



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:13 AM EDT

PDB ID : 4IQJ / pdb\_00004iqj  
Title : Structure of PolIIIalpha-Tauc-DNA complex suggests an atomic model of the replisome  
Authors : Liu, B.; Lin, J.; Steitz, T.  
Deposited on : 2013-01-11  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

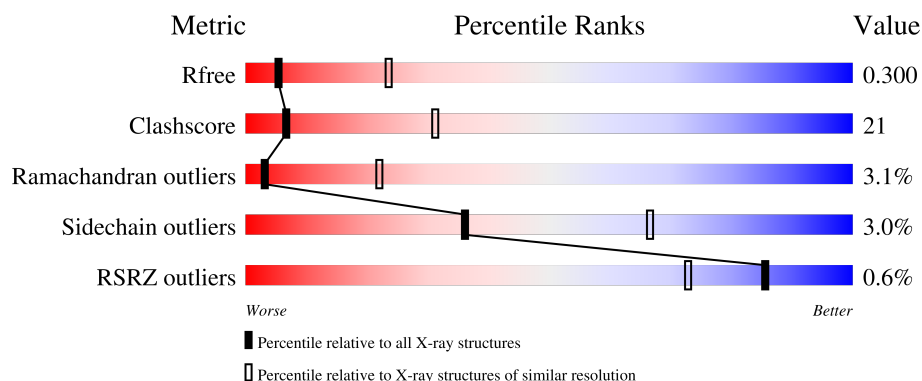
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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   | E     | 20     |                  |
| 1   | G     | 20     |                  |
| 1   | K     | 20     |                  |
| 2   | F     | 28     |                  |
| 2   | H     | 28     |                  |

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| Mol | Chain | Length | Quality of chain                                                                                         |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------|
| 2   | J     | 28     | <div><div></div><div>75%</div><div>7%</div><div>18%</div></div>                                          |
| 2   | L     | 28     | <div><div></div><div>79%</div><div>7%</div><div>14%</div></div>                                          |
| 3   | I     | 21     | <div><div>10%</div><div></div><div>71%</div><div>24%</div><div>5%</div></div>                            |
| 4   | A     | 1220   | <div><div></div><div>74%</div><div>20%</div><div>5%</div></div>                                          |
| 4   | B     | 1220   | <div><div>%</div><div></div><div>73%</div><div>21%</div><div>.</div><div>.</div></div>                   |
| 4   | C     | 1220   | <div><div></div><div>73%</div><div>20%</div><div>.</div><div>.</div></div>                               |
| 4   | D     | 1220   | <div><div>%</div><div></div><div>71%</div><div>23%</div><div>.</div><div>.</div><div>.</div></div>       |
| 5   | M     | 177    | <div><div>2%</div><div></div><div>27%</div><div>28%</div><div>17%</div><div>6%</div><div>22%</div></div> |
| 5   | N     | 177    | <div><div></div><div>35%</div><div>28%</div><div>11%</div><div>.</div><div>24%</div></div>               |
| 5   | O     | 177    | <div><div>%</div><div></div><div>28%</div><div>32%</div><div>13%</div><div>.</div><div>24%</div></div>   |
| 5   | P     | 177    | <div><div>2%</div><div></div><div>25%</div><div>29%</div><div>17%</div><div>7%</div><div>22%</div></div> |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 45265 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(P\*CP\*GP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*A)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1   | E     | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 411   | 193 | 83 | 115 | 20 |         |         |       |
| 1   | G     | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 411   | 193 | 83 | 115 | 20 |         |         |       |
| 1   | K     | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 411   | 193 | 83 | 115 | 20 |         |         |       |

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*GP\*TP\*GP\*GP\*CP\*AP\*CP\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*CP\*G)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | F     | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 409   | 194 | 70 | 125 | 20 |         |         |       |
| 2   | H     | 27       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 551   | 264 | 87 | 173 | 27 |         |         |       |
| 2   | J     | 23       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 471   | 224 | 79 | 145 | 23 |         |         |       |
| 2   | L     | 24       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 491   | 234 | 81 | 152 | 24 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 3   | I     | 21       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 429   | 202 | 86 | 120 | 21 |         |         |       |

- Molecule 4 is a protein called DNA polymerase III subunit alpha.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 4   | A     | 1164     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9280  | 5918 | 1620 | 1714 | 28 |         |         |       |
| 4   | B     | 1167     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9295  | 5926 | 1623 | 1716 | 30 |         |         |       |
| 4   | C     | 1166     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9293  | 5930 | 1621 | 1714 | 28 |         |         |       |
| 4   | D     | 1185     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9445  | 6026 | 1651 | 1738 | 30 |         |         |       |

- Molecule 5 is a protein called DNA polymerase III subunit gamma/tau.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | M     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1103  | 702 | 203 | 197 | 1 |         |         |       |
| 5   | N     | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1078  | 687 | 200 | 190 | 1 |         |         |       |
| 5   | O     | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1078  | 687 | 200 | 190 | 1 |         |         |       |
| 5   | P     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1093  | 695 | 203 | 194 | 1 |         |         |       |

There are 40 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| M     | 367     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| M     | 368     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| M     | 369     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| M     | 370     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| M     | 371     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| M     | 372     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| M     | 373     | LYS      | GLU    | conflict       | UNP A0A0M9ACL9 |
| M     | 541     | MET      | -      | expression tag | UNP A0A0M9ACL9 |
| M     | 542     | PRO      | -      | expression tag | UNP A0A0M9ACL9 |
| M     | 543     | PRO      | -      | expression tag | UNP A0A0M9ACL9 |
| N     | 367     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| N     | 368     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| N     | 369     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| N     | 370     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| N     | 371     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| N     | 372     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| N     | 373     | LYS      | GLU    | conflict       | UNP A0A0M9ACL9 |
| N     | 541     | MET      | -      | expression tag | UNP A0A0M9ACL9 |
| N     | 542     | PRO      | -      | expression tag | UNP A0A0M9ACL9 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| N     | 543     | PRO      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 367     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 368     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 369     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 370     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 371     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 372     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 373     | LYS      | GLU    | conflict       | UNP A0A0M9ACL9 |
| O     | 541     | MET      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 542     | PRO      | -      | expression tag | UNP A0A0M9ACL9 |
| O     | 543     | PRO      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 367     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 368     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 369     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 370     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 371     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 372     | HIS      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 373     | LYS      | GLU    | conflict       | UNP A0A0M9ACL9 |
| P     | 541     | MET      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 542     | PRO      | -      | expression tag | UNP A0A0M9ACL9 |
| P     | 543     | PRO      | -      | expression tag | UNP A0A0M9ACL9 |

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6   | A     | 3        | Total Zn<br>3 3 | 0       | 0       |
| 6   | B     | 3        | Total Zn<br>3 3 | 0       | 0       |
| 6   | C     | 3        | Total Zn<br>3 3 | 0       | 0       |
| 6   | D     | 3        | Total Zn<br>3 3 | 0       | 0       |

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 7   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 7   | C     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 7   | D     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

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

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

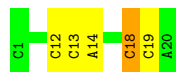
- Molecule 1: DNA (5'-D(P\*CP\*GP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*T P\*GP\*CP\*CP\*A)-3')

Chain E: 

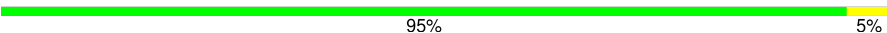


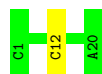
- Molecule 1: DNA (5'-D(P\*CP\*GP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*T P\*GP\*CP\*CP\*A)-3')

Chain G: 



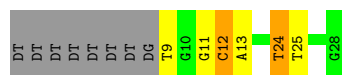
- Molecule 1: DNA (5'-D(P\*CP\*GP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*T P\*GP\*CP\*CP\*A)-3')

Chain K: 



- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*GP\*TP\*GP\*GP\*CP\*AP\*CP\*TP\*GP \*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*CP\*G)-3')

Chain F: 



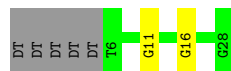
- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*GP\*TP\*GP\*GP\*CP\*AP\*CP\*TP\*GP \*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*CP\*G)-3')

Chain H: 

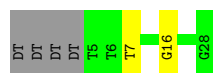
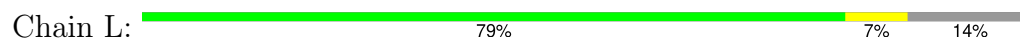




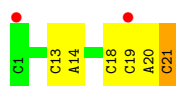
- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*GP\*TP\*GP\*GP\*CP\*AP\*CP\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*CP\*G)-3')



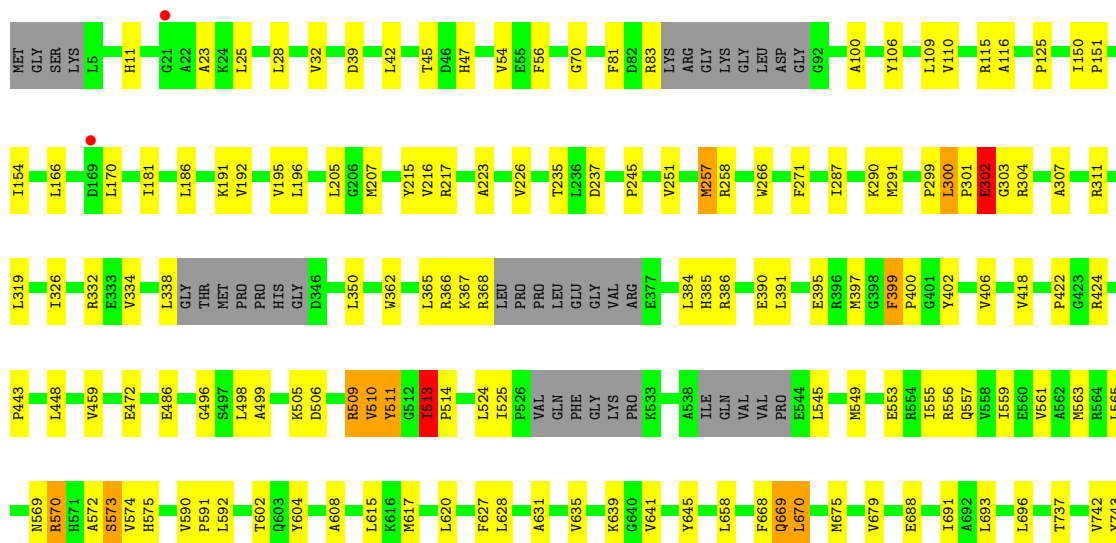
- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*GP\*TP\*GP\*GP\*CP\*AP\*CP\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*CP\*G)-3')

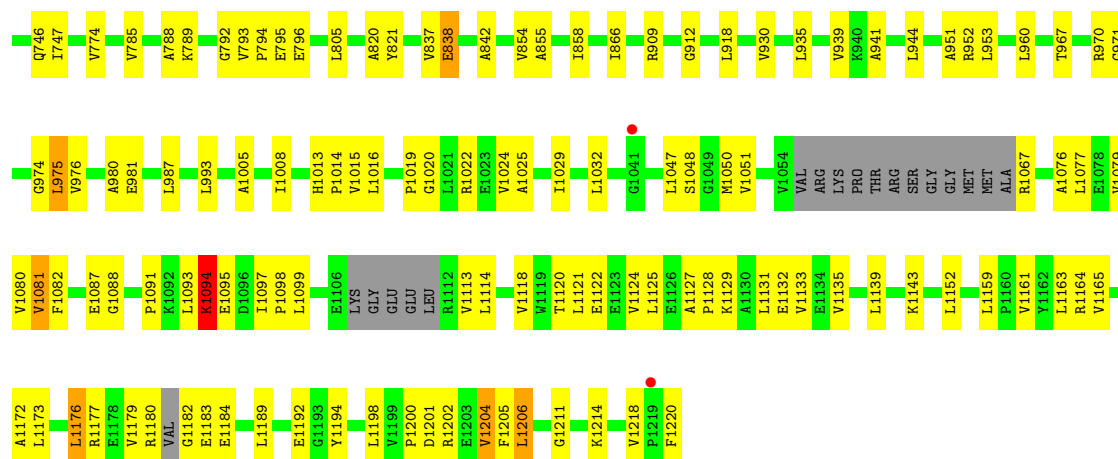


- Molecule 3: DNA (5'-D(P\*CP\*GP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*T\*P\*GP\*CP\*CP\*AP\*(DOC))-3')

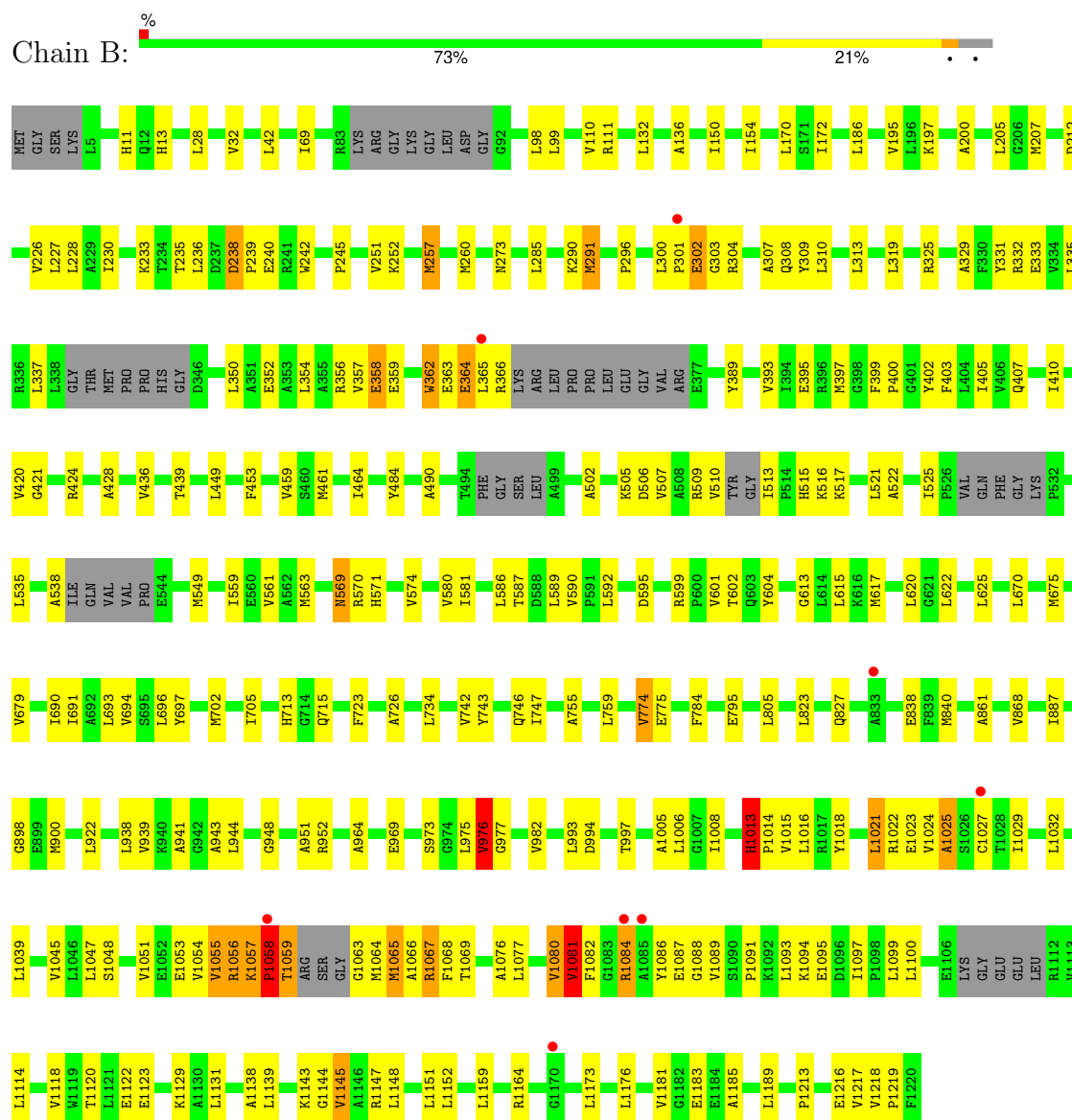


- Molecule 4: DNA polymerase III subunit alpha



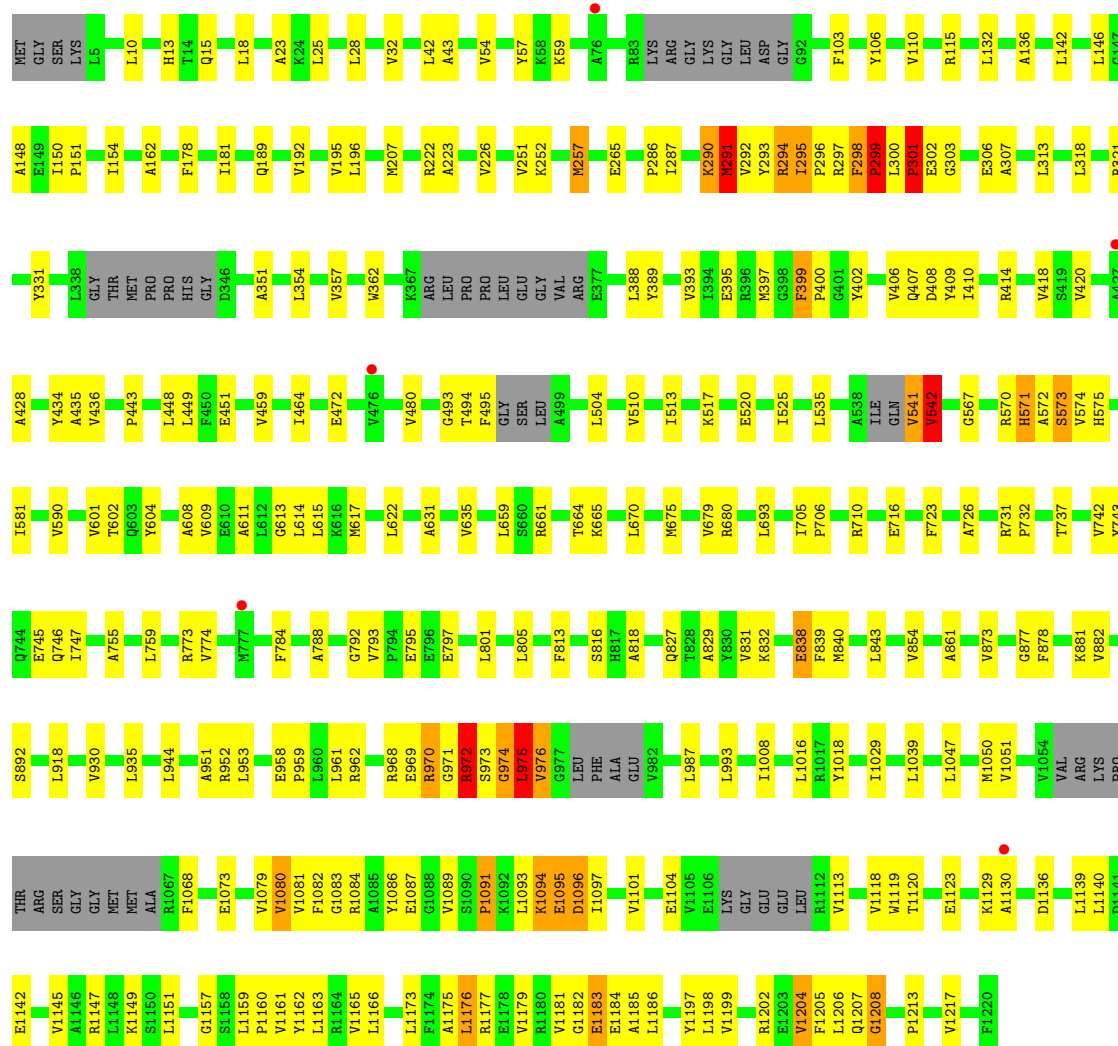


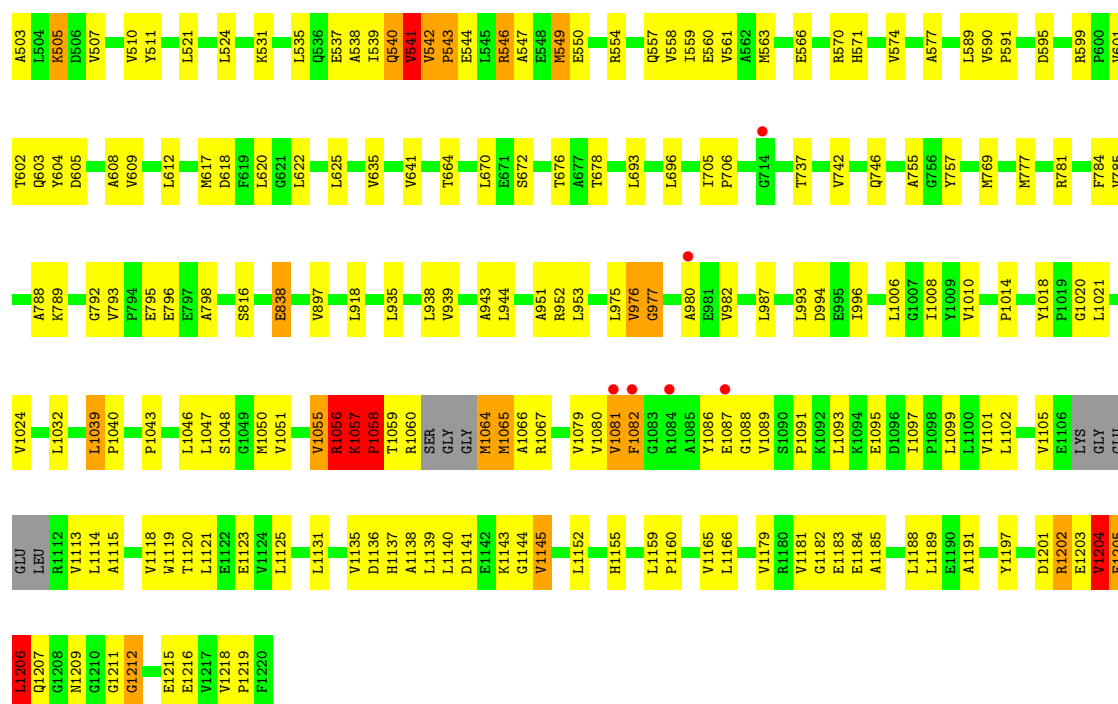
• Molecule 4: DNA polymerase III subunit alpha



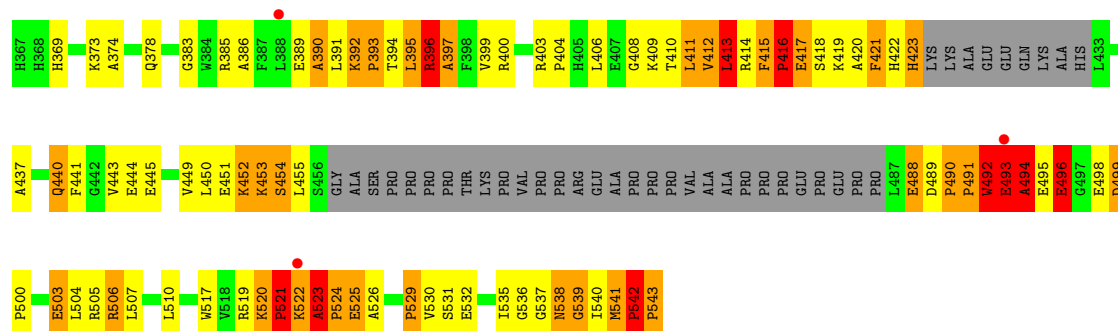
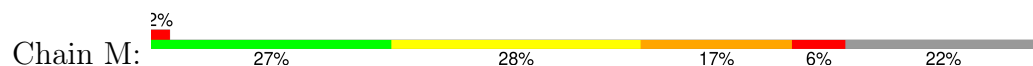
• Molecule 4: DNA polymerase III subunit alpha

Chain C:  73% 20%

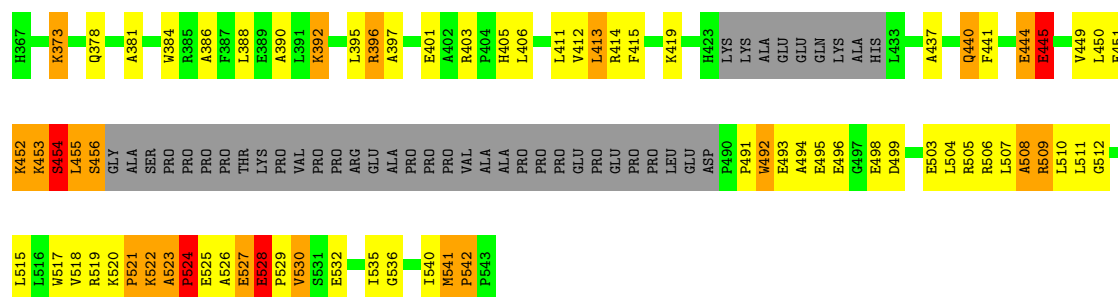




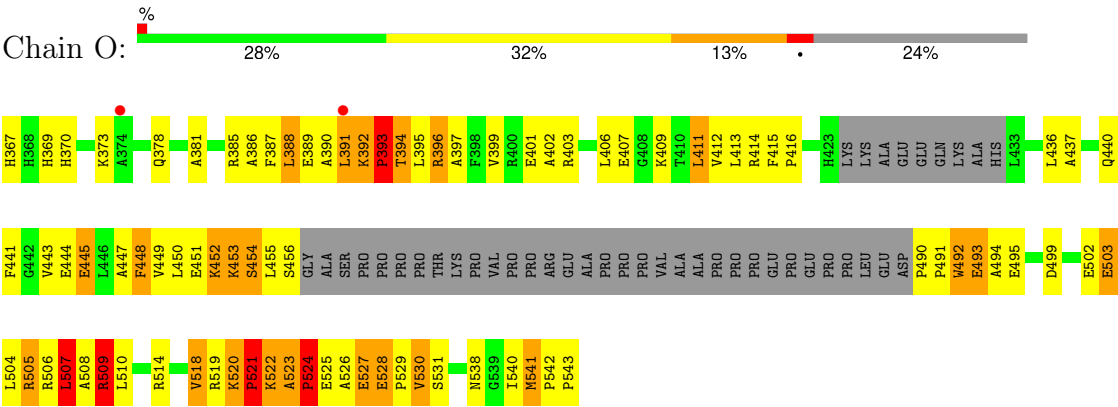
• Molecule 5: DNA polymerase III subunit gamma/tau



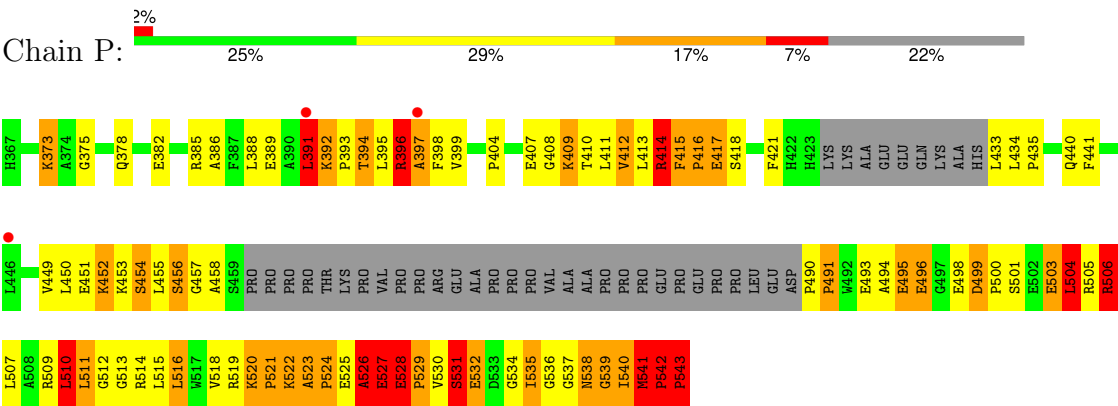
• Molecule 5: DNA polymerase III subunit gamma/tau



• Molecule 5: DNA polymerase III subunit gamma/tau



● Molecule 5: DNA polymerase III subunit gamma/tau



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 188.53Å 94.97Å 204.08Å<br>90.00° 89.97° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.20<br>20.00 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.0 (20.00-3.20)<br>95.5 (20.00-3.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.04                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 15.90 (at 3.22Å)                                            | Xtriage          |
| Refinement program                                                      | REFMAC 5.5.0109                                             | Depositor        |
| R, $R_{free}$                                                           | 0.264 , 0.305<br>0.258 , 0.300                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 11336 reflections (9.44%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 99.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.095                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 73.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction                                             | 0.018 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 45265                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 151.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DOC, 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   | E     | 0.33         | 0/462           | 0.66        | 0/710            |
| 1   | G     | 0.34         | 0/462           | 0.71        | 1/710 (0.1%)     |
| 1   | K     | 0.32         | 0/462           | 0.72        | 0/710            |
| 2   | F     | 0.32         | 0/456           | 0.82        | 2/702 (0.3%)     |
| 2   | H     | 0.35         | 0/613           | 0.82        | 1/945 (0.1%)     |
| 2   | J     | 0.32         | 0/525           | 0.77        | 0/809            |
| 2   | L     | 0.34         | 0/547           | 0.77        | 0/843            |
| 3   | I     | 0.34         | 0/462           | 0.71        | 0/710            |
| 4   | A     | 0.72         | 3/9466 (0.0%)   | 0.83        | 6/12781 (0.0%)   |
| 4   | B     | 0.71         | 2/9480 (0.0%)   | 0.83        | 6/12800 (0.0%)   |
| 4   | C     | 0.72         | 2/9481 (0.0%)   | 0.85        | 13/12805 (0.1%)  |
| 4   | D     | 0.75         | 2/9638 (0.0%)   | 0.86        | 18/13019 (0.1%)  |
| 5   | M     | 1.16         | 8/1133 (0.7%)   | 1.48        | 30/1528 (2.0%)   |
| 5   | N     | 0.92         | 0/1108          | 1.14        | 5/1493 (0.3%)    |
| 5   | O     | 0.95         | 0/1108          | 1.19        | 7/1493 (0.5%)    |
| 5   | P     | 1.14         | 7/1123 (0.6%)   | 1.43        | 30/1513 (2.0%)   |
| All | All   | 0.74         | 24/46526 (0.1%) | 0.89        | 119/63571 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 4   | A     | 0                   | 1                   |
| 4   | B     | 0                   | 1                   |
| 4   | C     | 0                   | 3                   |
| 4   | D     | 0                   | 4                   |
| 5   | M     | 0                   | 7                   |
| 5   | N     | 0                   | 1                   |
| 5   | O     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | P     | 0                   | 7                   |
| All | All   | 0                   | 26                  |

All (24) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | P     | 541  | MET  | C-N    | 6.64  | 1.41        | 1.33     |
| 5   | M     | 541  | MET  | C-N    | 6.39  | 1.41        | 1.33     |
| 5   | M     | 490  | PRO  | C-N    | 6.27  | 1.41        | 1.34     |
| 4   | C     | 295  | ILE  | C-N    | 6.12  | 1.40        | 1.33     |
| 5   | P     | 543  | PRO  | N-CD   | 6.00  | 1.56        | 1.47     |
| 4   | A     | 47   | HIS  | CG-CD2 | 5.94  | 1.42        | 1.35     |
| 5   | M     | 494  | ALA  | C-N    | 5.91  | 1.41        | 1.33     |
| 5   | M     | 416  | PRO  | N-CD   | 5.77  | 1.55        | 1.47     |
| 5   | P     | 539  | GLY  | C-O    | 5.76  | 1.30        | 1.23     |
| 5   | M     | 524  | PRO  | N-CD   | 5.75  | 1.55        | 1.47     |
| 5   | P     | 415  | PHE  | C-N    | 5.75  | 1.41        | 1.34     |
| 4   | D     | 1058 | PRO  | N-CD   | 5.57  | 1.55        | 1.47     |
| 5   | M     | 491  | PRO  | N-CD   | 5.51  | 1.55        | 1.47     |
| 5   | P     | 538  | ASN  | C-O    | -5.47 | 1.17        | 1.24     |
| 4   | A     | 39   | ASP  | N-CA   | 5.41  | 1.50        | 1.46     |
| 5   | M     | 543  | PRO  | N-CD   | 5.40  | 1.55        | 1.47     |
| 4   | B     | 1058 | PRO  | N-CD   | 5.22  | 1.55        | 1.47     |
| 5   | P     | 524  | PRO  | N-CD   | 5.20  | 1.55        | 1.47     |
| 5   | M     | 523  | ALA  | C-N    | 5.14  | 1.44        | 1.34     |
| 5   | P     | 412  | VAL  | N-CA   | -5.11 | 1.40        | 1.46     |
| 4   | A     | 11   | HIS  | CG-CD2 | 5.09  | 1.41        | 1.35     |
| 4   | C     | 13   | HIS  | CG-CD2 | 5.09  | 1.41        | 1.35     |
| 4   | D     | 214  | HIS  | CG-CD2 | 5.04  | 1.41        | 1.35     |
| 4   | B     | 13   | HIS  | CG-CD2 | 5.01  | 1.41        | 1.35     |

All (119) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 5   | N     | 384  | TRP  | N-CA-C | 13.69  | 125.93      | 111.14   |
| 4   | D     | 1184 | GLU  | N-CA-C | -12.02 | 97.19       | 113.18   |
| 4   | C     | 291  | MET  | N-CA-C | 11.03  | 123.82      | 110.91   |
| 5   | M     | 494  | ALA  | N-CA-C | -10.42 | 93.59       | 109.94   |
| 4   | A     | 796  | GLU  | N-CA-C | -10.00 | 89.50       | 110.80   |
| 4   | D     | 542  | VAL  | N-CA-C | 9.76   | 129.97      | 108.88   |
| 5   | M     | 493  | GLU  | N-CA-C | 9.31   | 130.64      | 110.80   |
| 5   | M     | 541  | MET  | CA-C-N | -8.81  | 111.30      | 120.38   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5   | M     | 541  | MET  | C-N-CA    | -8.81 | 111.30      | 120.38   |
| 5   | P     | 541  | MET  | CA-C-N    | -8.77 | 111.35      | 120.38   |
| 5   | P     | 541  | MET  | C-N-CA    | -8.77 | 111.35      | 120.38   |
| 5   | P     | 531  | SER  | N-CA-C    | 8.71  | 120.54      | 111.14   |
| 4   | B     | 1057 | LYS  | C-N-CD    | 8.13  | 138.49      | 120.60   |
| 4   | D     | 542  | VAL  | N-CA-CB   | -8.08 | 99.90       | 111.21   |
| 4   | D     | 505  | LYS  | N-CA-C    | 8.05  | 119.68      | 111.07   |
| 5   | M     | 541  | MET  | N-CA-C    | 8.03  | 124.56      | 113.16   |
| 4   | C     | 971  | GLY  | N-CA-C    | -8.01 | 103.12      | 112.73   |
| 4   | A     | 669  | GLN  | N-CA-CB   | -7.93 | 106.17      | 114.10   |
| 5   | O     | 508  | ALA  | N-CA-C    | 7.89  | 125.51      | 113.51   |
| 5   | O     | 507  | LEU  | N-CA-C    | 7.54  | 121.79      | 111.54   |
| 2   | F     | 24   | DT   | P-O3'-C3' | 7.53  | 131.50      | 120.20   |
| 4   | D     | 1057 | LYS  | C-N-CD    | 7.53  | 137.16      | 120.60   |
| 5   | P     | 542  | PRO  | CA-N-CD   | -7.44 | 101.58      | 112.00   |
| 4   | C     | 975  | LEU  | CA-C-N    | -7.38 | 108.68      | 121.97   |
| 4   | C     | 975  | LEU  | C-N-CA    | -7.38 | 108.68      | 121.97   |
| 4   | A     | 670  | LEU  | N-CA-CB   | 7.34  | 121.98      | 111.19   |
| 5   | P     | 510  | LEU  | N-CA-C    | -7.31 | 103.45      | 113.18   |
| 5   | P     | 526  | ALA  | N-CA-C    | 7.22  | 126.17      | 110.80   |
| 5   | P     | 415  | PHE  | CA-C-N    | -7.16 | 111.04      | 118.85   |
| 5   | P     | 415  | PHE  | C-N-CA    | -7.16 | 111.04      | 118.85   |
| 5   | M     | 542  | PRO  | CA-N-CD   | -6.90 | 102.34      | 112.00   |
| 5   | P     | 540  | ILE  | CA-C-N    | 6.89  | 128.70      | 120.09   |
| 5   | P     | 540  | ILE  | C-N-CA    | 6.89  | 128.70      | 120.09   |
| 5   | P     | 541  | MET  | N-CA-C    | 6.86  | 122.91      | 113.16   |
| 4   | A     | 774  | VAL  | N-CA-C    | 6.85  | 117.36      | 110.23   |
| 5   | M     | 492  | TRP  | N-CA-C    | 6.84  | 120.98      | 111.74   |
| 5   | M     | 523  | ALA  | C-N-CD    | 6.75  | 135.46      | 120.60   |
| 5   | M     | 396  | ARG  | N-CA-C    | -6.70 | 101.69      | 110.53   |
| 5   | O     | 523  | ALA  | C-N-CD    | -6.59 | 106.11      | 120.60   |
| 5   | P     | 416  | PRO  | CA-N-CD   | -6.57 | 102.80      | 112.00   |
| 4   | D     | 796  | GLU  | N-CA-C    | -6.57 | 96.81       | 110.80   |
| 5   | P     | 524  | PRO  | CA-N-CD   | -6.53 | 102.36      | 111.50   |
| 4   | D     | 1056 | ARG  | O-C-N     | -6.51 | 113.92      | 122.59   |
| 4   | B     | 362  | TRP  | N-CA-C    | -6.47 | 104.15      | 111.07   |
| 5   | O     | 509  | ARG  | N-CA-C    | -6.42 | 103.97      | 113.61   |
| 4   | C     | 295  | ILE  | CA-C-N    | -6.36 | 114.08      | 120.31   |
| 4   | C     | 295  | ILE  | C-N-CA    | -6.36 | 114.08      | 120.31   |
| 4   | C     | 970  | ARG  | N-CA-C    | -6.28 | 104.36      | 111.07   |
| 5   | N     | 509  | ARG  | N-CA-C    | 6.22  | 119.97      | 112.38   |
| 5   | P     | 409  | LYS  | N-CA-C    | -6.16 | 98.95       | 108.31   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5   | O     | 524  | PRO  | CA-N-CD   | -6.15 | 102.89      | 111.50   |
| 4   | A     | 796  | GLU  | N-CA-CB   | 6.13  | 120.85      | 110.49   |
| 5   | M     | 521  | PRO  | CA-N-CD   | -6.11 | 103.45      | 112.00   |
| 5   | P     | 409  | LYS  | CB-CA-C   | -6.10 | 109.53      | 116.54   |
| 5   | N     | 528  | GLU  | CA-C-N    | -6.07 | 114.36      | 120.31   |
| 5   | N     | 528  | GLU  | C-N-CA    | -6.07 | 114.36      | 120.31   |
| 4   | D     | 1058 | PRO  | CA-N-CD   | -6.00 | 103.11      | 111.50   |
| 4   | C     | 742  | VAL  | CB-CA-C   | -5.91 | 104.50      | 111.94   |
| 5   | M     | 539  | GLY  | N-CA-C    | 5.88  | 120.30      | 112.77   |
| 4   | D     | 292  | VAL  | N-CA-C    | -5.88 | 99.59       | 108.17   |
| 1   | G     | 18   | DC   | P-O3'-C3' | 5.85  | 128.97      | 120.20   |
| 4   | B     | 150  | ILE  | CB-CA-C   | -5.84 | 108.15      | 113.70   |
| 2   | F     | 12   | DC   | P-O3'-C3' | 5.77  | 128.85      | 120.20   |
| 5   | P     | 539  | GLY  | N-CA-C    | 5.76  | 120.15      | 112.77   |
| 5   | M     | 390  | ALA  | N-CA-C    | -5.75 | 98.36       | 108.08   |
| 4   | A     | 1184 | GLU  | N-CA-C    | -5.71 | 98.63       | 110.80   |
| 4   | B     | 948  | GLY  | N-CA-C    | 5.69  | 117.85      | 110.45   |
| 5   | M     | 413  | LEU  | N-CA-C    | -5.68 | 106.05      | 112.87   |
| 5   | M     | 537  | GLY  | N-CA-C    | -5.66 | 105.94      | 112.73   |
| 4   | D     | 438  | ILE  | N-CA-C    | -5.59 | 105.65      | 110.74   |
| 5   | M     | 415  | PHE  | CA-C-N    | -5.58 | 112.86      | 119.05   |
| 5   | M     | 415  | PHE  | C-N-CA    | -5.58 | 112.86      | 119.05   |
| 5   | O     | 521  | PRO  | CA-N-CD   | -5.56 | 104.21      | 112.00   |
| 5   | N     | 524  | PRO  | CA-N-CD   | -5.55 | 103.73      | 111.50   |
| 5   | M     | 392  | LYS  | C-N-CD    | -5.52 | 108.45      | 120.60   |
| 4   | D     | 290  | LYS  | N-CA-C    | -5.50 | 101.71      | 109.96   |
| 4   | D     | 1056 | ARG  | CA-C-N    | -5.49 | 108.41      | 121.80   |
| 4   | D     | 1056 | ARG  | C-N-CA    | -5.49 | 108.41      | 121.80   |
| 4   | D     | 505  | LYS  | CA-C-N    | 5.48  | 127.63      | 120.28   |
| 4   | D     | 505  | LYS  | C-N-CA    | 5.48  | 127.63      | 120.28   |
| 5   | M     | 538  | ASN  | CA-C-N    | 5.47  | 126.01      | 120.00   |
| 5   | M     | 538  | ASN  | C-N-CA    | 5.47  | 126.01      | 120.00   |
| 5   | M     | 415  | PHE  | N-CA-C    | -5.44 | 105.36      | 112.75   |
| 4   | C     | 972  | ARG  | N-CA-C    | -5.43 | 105.26      | 111.07   |
| 4   | D     | 1212 | GLY  | CA-C-N    | -5.42 | 113.03      | 119.05   |
| 4   | D     | 1212 | GLY  | C-N-CA    | -5.42 | 113.03      | 119.05   |
| 5   | M     | 493  | GLU  | O-C-N     | 5.38  | 129.75      | 122.59   |
| 5   | M     | 415  | PHE  | O-C-N     | 5.36  | 125.25      | 120.48   |
| 4   | B     | 1055 | VAL  | O-C-N     | -5.36 | 116.98      | 122.82   |
| 2   | H     | 6    | DT   | P-O3'-C3' | 5.35  | 128.23      | 120.20   |
| 5   | P     | 543  | PRO  | CA-N-CD   | -5.34 | 104.52      | 112.00   |
| 5   | P     | 541  | MET  | C-N-CD    | 5.31  | 146.79      | 125.00   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | P     | 539  | GLY  | CA-C-O  | 5.29  | 126.27      | 120.66   |
| 5   | M     | 417  | GLU  | N-CA-C  | -5.25 | 105.56      | 111.28   |
| 4   | C     | 301  | PRO  | CA-C-N  | 5.23  | 131.12      | 121.70   |
| 4   | C     | 301  | PRO  | C-N-CA  | 5.23  | 131.12      | 121.70   |
| 5   | P     | 516  | LEU  | CA-C-N  | 5.21  | 127.71      | 120.63   |
| 5   | P     | 516  | LEU  | C-N-CA  | 5.21  | 127.71      | 120.63   |
| 5   | P     | 415  | PHE  | O-C-N   | 5.20  | 125.11      | 120.48   |
| 5   | M     | 494  | ALA  | O-C-N   | -5.17 | 115.53      | 122.14   |
| 4   | C     | 296  | PRO  | CA-N-CD | -5.16 | 104.78      | 112.00   |
| 5   | P     | 415  | PHE  | C-N-CD  | 5.16  | 146.15      | 125.00   |
| 5   | P     | 538  | ASN  | CA-C-O  | -5.16 | 115.08      | 120.55   |
| 4   | D     | 1165 | VAL  | CB-CA-C | -5.14 | 106.35      | 111.80   |
| 5   | O     | 508  | ALA  | N-CA-CB | -5.14 | 108.96      | 114.10   |
| 5   | M     | 493  | GLU  | CA-C-N  | 5.13  | 132.58      | 122.73   |
| 5   | M     | 493  | GLU  | C-N-CA  | 5.13  | 132.58      | 122.73   |
| 5   | M     | 541  | MET  | C-N-CD  | 5.13  | 146.02      | 125.00   |
| 4   | C     | 1184 | GLU  | N-CA-C  | -5.11 | 107.10      | 113.38   |
| 5   | M     | 520  | LYS  | CA-C-N  | -5.11 | 113.46      | 119.84   |
| 5   | M     | 520  | LYS  | C-N-CA  | -5.11 | 113.46      | 119.84   |
| 5   | P     | 414  | ARG  | N-CA-C  | -5.11 | 105.72      | 111.28   |
| 4   | B     | 1058 | PRO  | CA-N-CD | -5.08 | 104.38      | 111.50   |
| 5   | P     | 506  | ARG  | CA-C-N  | 5.08  | 131.25      | 121.54   |
| 5   | P     | 506  | ARG  | C-N-CA  | 5.08  | 131.25      | 121.54   |
| 5   | P     | 527  | GLU  | N-CA-C  | 5.06  | 121.58      | 110.80   |
| 5   | M     | 542  | PRO  | N-CA-C  | -5.05 | 104.54      | 110.70   |
| 5   | P     | 495  | GLU  | CA-C-N  | 5.05  | 130.78      | 121.70   |
| 5   | P     | 495  | GLU  | C-N-CA  | 5.05  | 130.78      | 121.70   |

There are no chirality outliers.

All (26) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 4   | A     | 570  | ARG  | Peptide   |
| 4   | B     | 1084 | ARG  | Sidechain |
| 4   | C     | 1080 | VAL  | Peptide   |
| 4   | C     | 972  | ARG  | Mainchain |
| 4   | C     | 974  | GLY  | Peptide   |
| 4   | D     | 1057 | LYS  | Peptide   |
| 4   | D     | 1206 | LEU  | Peptide   |
| 4   | D     | 541  | VAL  | Peptide   |
| 4   | D     | 546  | ARG  | Sidechain |
| 5   | M     | 396  | ARG  | Peptide   |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 5   | M     | 397 | ALA  | Peptide           |
| 5   | M     | 412 | VAL  | Peptide           |
| 5   | M     | 493 | GLU  | Mainchain,Peptide |
| 5   | M     | 494 | ALA  | Mainchain         |
| 5   | M     | 521 | PRO  | Peptide           |
| 5   | N     | 508 | ALA  | Peptide           |
| 5   | O     | 507 | LEU  | Peptide           |
| 5   | O     | 509 | ARG  | Sidechain         |
| 5   | P     | 391 | LEU  | Peptide           |
| 5   | P     | 394 | THR  | Peptide           |
| 5   | P     | 411 | LEU  | Mainchain,Peptide |
| 5   | P     | 504 | LEU  | Peptide           |
| 5   | P     | 506 | ARG  | Peptide           |
| 5   | P     | 531 | SER  | 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   | E     | 411   | 0        | 222      | 2       | 0            |
| 1   | G     | 411   | 0        | 222      | 6       | 0            |
| 1   | K     | 411   | 0        | 222      | 1       | 0            |
| 2   | F     | 409   | 0        | 227      | 5       | 0            |
| 2   | H     | 551   | 0        | 310      | 4       | 0            |
| 2   | J     | 471   | 0        | 262      | 2       | 0            |
| 2   | L     | 491   | 0        | 274      | 2       | 0            |
| 3   | I     | 429   | 0        | 233      | 5       | 0            |
| 4   | A     | 9280  | 0        | 9298     | 235     | 2            |
| 4   | B     | 9295  | 0        | 9323     | 312     | 3            |
| 4   | C     | 9293  | 0        | 9318     | 286     | 0            |
| 4   | D     | 9445  | 0        | 9488     | 392     | 2            |
| 5   | M     | 1103  | 0        | 1085     | 180     | 0            |
| 5   | N     | 1078  | 0        | 1065     | 140     | 1            |
| 5   | O     | 1078  | 0        | 1065     | 148     | 0            |
| 5   | P     | 1093  | 0        | 1078     | 211     | 2            |
| 6   | A     | 3     | 0        | 0        | 0       | 0            |
| 6   | B     | 3     | 0        | 0        | 0       | 0            |
| 6   | C     | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | D     | 3     | 0        | 0        | 0       | 0            |
| 7   | A     | 1     | 0        | 0        | 0       | 0            |
| 7   | B     | 1     | 0        | 0        | 0       | 0            |
| 7   | C     | 1     | 0        | 0        | 0       | 0            |
| 7   | D     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 45265 | 0        | 43692    | 1908    | 7            |

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 21.

All (1908) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:528:GLU:CG    | 5:P:529:PRO:HD3   | 1.29                     | 1.53              |
| 5:O:387:PHE:CE2   | 5:O:441:PHE:CE2   | 2.03                     | 1.47              |
| 4:D:1080:VAL:HG11 | 4:D:1082:PHE:CE2  | 1.50                     | 1.45              |
| 5:P:523:ALA:CB    | 5:P:524:PRO:HA    | 1.38                     | 1.43              |
| 4:D:1080:VAL:HA   | 4:D:1081:VAL:CG2  | 1.47                     | 1.41              |
| 4:D:549:MET:CE    | 4:D:559:ILE:HD12  | 1.49                     | 1.40              |
| 4:D:1082:PHE:CE1  | 4:D:1114:LEU:HG   | 1.58                     | 1.39              |
| 5:O:519:ARG:HD3   | 5:O:520:LYS:NZ    | 1.35                     | 1.35              |
| 4:D:1066:ALA:O    | 4:D:1081:VAL:HG13 | 1.27                     | 1.30              |
| 5:N:523:ALA:CB    | 5:N:524:PRO:HA    | 1.63                     | 1.29              |
| 4:D:1080:VAL:HA   | 4:D:1081:VAL:CB   | 1.59                     | 1.27              |
| 5:P:524:PRO:HD2   | 5:P:525:GLU:O     | 1.30                     | 1.25              |
| 4:D:1082:PHE:HE1  | 4:D:1114:LEU:CD1  | 1.51                     | 1.24              |
| 4:B:1057:LYS:NZ   | 4:B:1064:MET:HE2  | 1.51                     | 1.23              |
| 4:D:1057:LYS:HG2  | 4:D:1064:MET:CA   | 1.67                     | 1.23              |
| 4:B:1066:ALA:O    | 4:B:1081:VAL:HB   | 1.32                     | 1.22              |
| 4:D:1057:LYS:CG   | 4:D:1064:MET:HA   | 1.69                     | 1.22              |
| 4:D:1082:PHE:HE1  | 4:D:1114:LEU:CG   | 1.52                     | 1.21              |
| 5:P:524:PRO:HD2   | 5:P:525:GLU:C     | 1.63                     | 1.21              |
| 4:D:549:MET:CE    | 4:D:559:ILE:CD1   | 2.19                     | 1.21              |
| 4:D:1082:PHE:CE1  | 4:D:1114:LEU:CG   | 2.23                     | 1.21              |
| 5:M:492:TRP:O     | 5:M:493:GLU:HG2   | 1.37                     | 1.20              |
| 4:B:357:VAL:HG12  | 4:B:358:GLU:HG3   | 1.21                     | 1.19              |
| 4:D:1080:VAL:CA   | 4:D:1081:VAL:HG23 | 1.72                     | 1.19              |
| 5:N:505:ARG:HD3   | 5:N:510:LEU:HD23  | 1.19                     | 1.18              |
| 4:A:971:GLY:HA2   | 4:A:975:LEU:CB    | 1.74                     | 1.17              |
| 5:O:519:ARG:CD    | 5:O:520:LYS:HZ2   | 1.56                     | 1.17              |
| 5:O:450:LEU:HB3   | 5:O:451:GLU:C     | 1.69                     | 1.17              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1056:ARG:HG3  | 4:B:1057:LYS:CG   | 1.75                     | 1.16              |
| 5:O:387:PHE:CZ    | 5:O:441:PHE:CE2   | 2.32                     | 1.16              |
| 5:O:519:ARG:CD    | 5:O:520:LYS:NZ    | 2.06                     | 1.16              |
| 4:B:1057:LYS:CE   | 4:B:1064:MET:HE2  | 1.77                     | 1.15              |
| 5:P:528:GLU:CG    | 5:P:529:PRO:CD    | 2.24                     | 1.15              |
| 5:P:523:ALA:HB3   | 5:P:524:PRO:HA    | 1.27                     | 1.15              |
| 4:B:1066:ALA:O    | 4:B:1081:VAL:CB   | 1.94                     | 1.13              |
| 4:C:1080:VAL:HG12 | 4:C:1082:PHE:CD2  | 1.81                     | 1.13              |
| 4:B:357:VAL:HB    | 4:B:358:GLU:HB2   | 1.20                     | 1.13              |
| 5:P:505:ARG:HB3   | 5:P:510:LEU:HD12  | 1.31                     | 1.13              |
| 5:P:523:ALA:CB    | 5:P:524:PRO:CA    | 2.25                     | 1.13              |
| 4:D:1080:VAL:HA   | 4:D:1081:VAL:HG23 | 1.23                     | 1.12              |
| 4:B:1159:LEU:HD11 | 4:B:1183:GLU:HG3  | 1.13                     | 1.12              |
| 4:A:1080:VAL:CG2  | 4:A:1114:LEU:HA   | 1.78                     | 1.11              |
| 5:O:388:LEU:HD21  | 5:O:399:VAL:HG23  | 1.33                     | 1.11              |
| 5:P:505:ARG:HD2   | 5:P:514:ARG:CZ    | 1.81                     | 1.10              |
| 4:C:1080:VAL:HG12 | 4:C:1082:PHE:HD2  | 1.02                     | 1.10              |
| 5:P:494:ALA:CB    | 5:P:495:GLU:HA    | 1.79                     | 1.10              |
| 5:P:528:GLU:HG3   | 5:P:529:PRO:HD3   | 1.14                     | 1.10              |
| 4:D:537:GLU:O     | 4:D:540:GLN:HG3   | 1.53                     | 1.09              |
| 5:M:421:PHE:CD2   | 5:M:422:HIS:ND1   | 2.20                     | 1.09              |
| 5:N:523:ALA:HB1   | 5:N:524:PRO:CA    | 1.83                     | 1.09              |
| 5:O:387:PHE:CZ    | 5:O:441:PHE:CD2   | 2.41                     | 1.08              |
| 4:B:1080:VAL:HA   | 4:B:1081:VAL:HG22 | 1.11                     | 1.08              |
| 4:D:1065:MET:SD   | 4:D:1082:PHE:HA   | 1.92                     | 1.08              |
| 5:N:506:ARG:HB2   | 5:N:510:LEU:HB2   | 1.16                     | 1.08              |
| 4:C:1093:LEU:HD11 | 4:C:1097:ILE:CG2  | 1.83                     | 1.08              |
| 4:D:1080:VAL:CG1  | 4:D:1082:PHE:CE2  | 2.35                     | 1.08              |
| 4:D:1082:PHE:CE1  | 4:D:1114:LEU:CD1  | 2.36                     | 1.08              |
| 5:N:494:ALA:CB    | 5:N:495:GLU:HA    | 1.82                     | 1.08              |
| 4:D:537:GLU:HA    | 4:D:540:GLN:CG    | 1.84                     | 1.07              |
| 5:P:505:ARG:HD2   | 5:P:514:ARG:NH2   | 1.69                     | 1.07              |
| 5:P:532:GLU:HA    | 5:P:535:ILE:HD13  | 1.36                     | 1.07              |
| 4:D:549:MET:HE2   | 4:D:559:ILE:HD12  | 1.11                     | 1.07              |
| 5:M:421:PHE:CE2   | 5:M:422:HIS:ND1   | 2.20                     | 1.07              |
| 5:N:523:ALA:HB1   | 5:N:524:PRO:HA    | 1.32                     | 1.07              |
| 5:P:505:ARG:CB    | 5:P:510:LEU:HD12  | 1.83                     | 1.07              |
| 4:A:1080:VAL:HA   | 4:A:1081:VAL:HB   | 1.33                     | 1.07              |
| 4:D:1080:VAL:CA   | 4:D:1081:VAL:CG2  | 2.32                     | 1.06              |
| 5:N:505:ARG:CD    | 5:N:510:LEU:HD23  | 1.83                     | 1.06              |
| 5:P:491:PRO:HB3   | 5:P:540:ILE:HG21  | 1.36                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:O:450:LEU:HB3   | 5:O:451:GLU:O     | 1.54                     | 1.06              |
| 4:A:572:ALA:HB1   | 4:A:573:SER:HB2   | 1.36                     | 1.06              |
| 4:B:1056:ARG:CG   | 4:B:1057:LYS:HG3  | 1.85                     | 1.06              |
| 5:P:524:PRO:CD    | 5:P:525:GLU:O     | 2.03                     | 1.06              |
| 4:A:572:ALA:HB1   | 4:A:573:SER:CB    | 1.84                     | 1.06              |
| 4:D:549:MET:HE3   | 4:D:559:ILE:CD1   | 1.85                     | 1.06              |
| 4:D:549:MET:HE3   | 4:D:559:ILE:HD12  | 1.38                     | 1.06              |
| 4:B:1057:LYS:HB3  | 4:B:1058:PRO:HA   | 1.37                     | 1.05              |
| 5:M:507:LEU:H     | 5:M:510:LEU:HD22  | 1.14                     | 1.05              |
| 5:N:523:ALA:HB3   | 5:N:524:PRO:HA    | 1.37                     | 1.05              |
| 4:C:292:VAL:O     | 4:C:294:ARG:NH2   | 1.88                     | 1.05              |
| 5:M:519:ARG:HB3   | 5:M:520:LYS:HB2   | 1.08                     | 1.05              |
| 5:N:524:PRO:HD2   | 5:N:525:GLU:HA    | 1.30                     | 1.05              |
| 4:C:972:ARG:O     | 4:C:974:GLY:N     | 1.89                     | 1.05              |
| 4:D:549:MET:HE1   | 4:D:559:ILE:HB    | 1.34                     | 1.05              |
| 5:N:508:ALA:HA    | 5:N:510:LEU:H     | 1.19                     | 1.05              |
| 4:A:1080:VAL:HG22 | 4:A:1114:LEU:HA   | 1.35                     | 1.04              |
| 4:D:498:LEU:HD21  | 4:D:503:ALA:HB2   | 1.38                     | 1.04              |
| 4:B:1057:LYS:HG2  | 4:B:1064:MET:CA   | 1.88                     | 1.04              |
| 5:P:412:VAL:HB    | 5:P:415:PHE:CD2   | 1.92                     | 1.04              |
| 4:B:1066:ALA:O    | 4:B:1081:VAL:CG1  | 2.06                     | 1.03              |
| 5:O:523:ALA:HB1   | 5:O:524:PRO:HB3   | 1.35                     | 1.03              |
| 4:D:549:MET:HE1   | 4:D:559:ILE:CB    | 1.87                     | 1.03              |
| 5:P:528:GLU:HG2   | 5:P:529:PRO:CD    | 1.84                     | 1.03              |
| 4:B:1057:LYS:CG   | 4:B:1064:MET:HA   | 1.89                     | 1.03              |
| 4:D:1080:VAL:HA   | 4:D:1081:VAL:HB   | 1.34                     | 1.03              |
| 4:B:1056:ARG:HD2  | 4:B:1057:LYS:HE3  | 1.42                     | 1.02              |
| 5:P:523:ALA:HB1   | 5:P:524:PRO:HA    | 1.05                     | 1.02              |
| 5:O:388:LEU:HD21  | 5:O:399:VAL:CG2   | 1.89                     | 1.02              |
| 4:A:1080:VAL:HG21 | 4:A:1114:LEU:CD2  | 1.90                     | 1.02              |
| 5:N:505:ARG:HB3   | 5:N:506:ARG:HB3   | 1.40                     | 1.01              |
| 5:O:494:ALA:CB    | 5:O:495:GLU:HA    | 1.90                     | 1.01              |
| 5:P:501:SER:HB3   | 5:P:514:ARG:HD2   | 1.42                     | 1.01              |
| 5:O:502:GLU:O     | 5:O:503:GLU:HB2   | 1.60                     | 1.01              |
| 4:A:971:GLY:HA2   | 4:A:975:LEU:HB3   | 1.03                     | 1.01              |
| 4:D:1057:LYS:HB3  | 4:D:1058:PRO:HA   | 1.43                     | 1.01              |
| 4:B:1093:LEU:HD11 | 4:B:1097:ILE:HG21 | 1.39                     | 1.00              |
| 4:D:1059:THR:HG22 | 4:D:1065:MET:HE3  | 1.43                     | 1.00              |
| 5:N:524:PRO:HB2   | 5:N:525:GLU:C     | 1.84                     | 1.00              |
| 4:D:500:SER:HB3   | 4:D:535:LEU:CD1   | 1.91                     | 1.00              |
| 5:N:505:ARG:HD2   | 5:N:510:LEU:HB3   | 1.42                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:501:SER:HB2   | 5:P:504:LEU:O     | 1.61                     | 1.00              |
| 4:B:1080:VAL:HA   | 4:B:1081:VAL:CG2  | 1.92                     | 1.00              |
| 4:B:1080:VAL:CA   | 4:B:1081:VAL:HG22 | 1.91                     | 1.00              |
| 4:C:287:ILE:HA    | 4:C:291:MET:HB3   | 1.41                     | 1.00              |
| 4:A:572:ALA:CB    | 4:A:573:SER:HB2   | 1.90                     | 0.99              |
| 4:D:501:LYS:HE3   | 4:D:505:LYS:NZ    | 1.77                     | 0.99              |
| 4:A:1080:VAL:HG21 | 4:A:1114:LEU:HD22 | 1.43                     | 0.99              |
| 5:P:505:ARG:CZ    | 5:P:532:GLU:OE1   | 2.11                     | 0.99              |
| 4:C:1093:LEU:HD11 | 4:C:1097:ILE:CB   | 1.93                     | 0.99              |
| 4:A:1029:ILE:HG23 | 4:A:1077:LEU:HD13 | 1.44                     | 0.99              |
| 4:D:1080:VAL:CA   | 4:D:1081:VAL:CB   | 2.37                     | 0.99              |
| 4:D:1080:VAL:HG11 | 4:D:1082:PHE:CD2  | 1.98                     | 0.99              |
| 5:N:520:LYS:N     | 5:N:521:PRO:HD3   | 1.77                     | 0.98              |
| 5:P:528:GLU:HG2   | 5:P:529:PRO:HD3   | 1.02                     | 0.98              |
| 5:O:387:PHE:CE2   | 5:O:441:PHE:CZ    | 2.50                     | 0.98              |
| 4:C:1129:LYS:HE2  | 4:C:1183:GLU:OE2  | 1.63                     | 0.98              |
| 5:P:506:ARG:HB2   | 5:P:506:ARG:HH11  | 1.28                     | 0.97              |
| 5:N:506:ARG:HB2   | 5:N:510:LEU:CB    | 1.94                     | 0.97              |
| 4:D:1202:ARG:HG2  | 4:D:1202:ARG:HH11 | 1.25                     | 0.97              |
| 5:M:519:ARG:CB    | 5:M:520:LYS:HB2   | 1.94                     | 0.97              |
| 5:M:396:ARG:HA    | 5:M:397:ALA:HB3   | 1.44                     | 0.97              |
| 5:M:519:ARG:HD3   | 5:M:520:LYS:HE2   | 1.45                     | 0.97              |
| 5:M:413:LEU:C     | 5:M:416:PRO:HD2   | 1.89                     | 0.96              |
| 5:N:494:ALA:HB3   | 5:N:495:GLU:HA    | 1.45                     | 0.96              |
| 4:B:357:VAL:CG1   | 4:B:358:GLU:HG3   | 1.94                     | 0.96              |
| 5:M:396:ARG:HB2   | 5:M:397:ALA:O     | 1.65                     | 0.96              |
| 5:M:421:PHE:HE2   | 5:M:422:HIS:HD1   | 0.98                     | 0.96              |
| 4:C:1080:VAL:HB   | 4:C:1082:PHE:N    | 1.79                     | 0.96              |
| 5:N:523:ALA:CB    | 5:N:524:PRO:CA    | 2.34                     | 0.96              |
| 4:D:181:ILE:HD12  | 4:D:207:MET:HE3   | 1.45                     | 0.96              |
| 5:P:494:ALA:HB3   | 5:P:495:GLU:HA    | 1.43                     | 0.95              |
| 4:D:284:ASP:HB3   | 4:D:290:LYS:CE    | 1.96                     | 0.95              |
| 4:B:1057:LYS:HE2  | 4:B:1064:MET:CE   | 1.96                     | 0.95              |
| 4:D:1080:VAL:CA   | 4:D:1081:VAL:HB   | 1.96                     | 0.95              |
| 4:D:1080:VAL:CG1  | 4:D:1082:PHE:HE2  | 1.76                     | 0.95              |
| 4:A:971:GLY:CA    | 4:A:975:LEU:HB3   | 1.94                     | 0.95              |
| 4:C:1093:LEU:HD11 | 4:C:1097:ILE:HG21 | 1.43                     | 0.95              |
| 4:D:1082:PHE:CE1  | 4:D:1114:LEU:HD12 | 1.99                     | 0.95              |
| 5:M:505:ARG:HB3   | 5:M:506:ARG:HB3   | 1.48                     | 0.95              |
| 4:A:1067:ARG:CA   | 4:A:1081:VAL:HG21 | 1.97                     | 0.94              |
| 4:B:357:VAL:HB    | 4:B:358:GLU:CB    | 1.96                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:494:ALA:HB1   | 5:M:495:GLU:HA    | 1.47                     | 0.94              |
| 4:D:1060:ARG:HG2  | 4:D:1060:ARG:HH11 | 1.33                     | 0.94              |
| 5:P:528:GLU:HG3   | 5:P:529:PRO:CD    | 1.94                     | 0.94              |
| 5:N:505:ARG:HB3   | 5:N:506:ARG:CB    | 1.96                     | 0.94              |
| 5:M:525:GLU:HG2   | 5:M:530:VAL:HG23  | 1.47                     | 0.94              |
| 4:D:1080:VAL:HG21 | 4:D:1082:PHE:CE2  | 2.03                     | 0.93              |
| 5:N:453:LYS:O     | 5:N:454:SER:HB2   | 1.64                     | 0.93              |
| 5:P:412:VAL:HB    | 5:P:415:PHE:HD2   | 1.28                     | 0.93              |
| 5:M:419:LYS:HA    | 5:M:422:HIS:CD2   | 2.04                     | 0.93              |
| 5:P:532:GLU:HA    | 5:P:535:ILE:CD1   | 1.98                     | 0.93              |
| 5:M:507:LEU:N     | 5:M:510:LEU:HD22  | 1.82                     | 0.93              |
| 5:M:418:SER:O     | 5:M:422:HIS:NE2   | 2.02                     | 0.93              |
| 5:P:499:ASP:HB2   | 5:P:515:LEU:HD22  | 1.48                     | 0.92              |
| 4:A:1014:PRO:HB2  | 4:A:1050:MET:HE3  | 1.51                     | 0.92              |
| 4:D:284:ASP:HB3   | 4:D:290:LYS:HE3   | 1.48                     | 0.92              |
| 5:P:523:ALA:HB3   | 5:P:524:PRO:CA    | 1.95                     | 0.92              |
| 4:D:994:ASP:HB2   | 5:P:528:GLU:OE1   | 1.69                     | 0.92              |
| 4:D:1205:PHE:CD1  | 4:D:1206:LEU:HD12 | 2.04                     | 0.92              |
| 5:N:505:ARG:NH2   | 5:N:532:GLU:OE1   | 2.02                     | 0.92              |
| 4:A:1067:ARG:HA   | 4:A:1081:VAL:HG21 | 1.50                     | 0.92              |
| 5:N:541:MET:N     | 5:N:542:PRO:HD2   | 1.85                     | 0.92              |
| 5:M:506:ARG:C     | 5:M:507:LEU:HD22  | 1.94                     | 0.92              |
| 5:O:390:ALA:HB3   | 5:O:393:PRO:CG    | 2.00                     | 0.92              |
| 4:D:1056:ARG:HA   | 4:D:1066:ALA:HB2  | 1.52                     | 0.92              |
| 5:N:524:PRO:CD    | 5:N:525:GLU:HA    | 1.98                     | 0.91              |
| 5:P:540:ILE:HD12  | 5:P:541:MET:N     | 1.85                     | 0.91              |
| 4:A:513:ILE:HG22  | 4:A:514:PRO:HD3   | 1.48                     | 0.91              |
| 5:M:505:ARG:HB3   | 5:M:506:ARG:CB    | 1.99                     | 0.91              |
| 4:B:615:LEU:HD21  | 4:B:617:MET:HE2   | 1.51                     | 0.91              |
| 4:B:1064:MET:HE3  | 4:B:1087:GLU:OE1  | 1.70                     | 0.91              |
| 5:N:523:ALA:HB1   | 5:N:524:PRO:C     | 1.95                     | 0.91              |
| 5:P:505:ARG:CZ    | 5:P:510:LEU:HD13  | 2.00                     | 0.91              |
| 5:P:522:LYS:HG3   | 5:P:523:ALA:H     | 1.34                     | 0.91              |
| 5:N:395:LEU:HA    | 5:N:396:ARG:HB2   | 1.51                     | 0.91              |
| 5:P:523:ALA:HB1   | 5:P:524:PRO:CA    | 1.93                     | 0.91              |
| 4:D:1102:LEU:HD12 | 4:D:1206:LEU:HG   | 1.52                     | 0.91              |
| 5:O:388:LEU:CD2   | 5:O:399:VAL:CG2   | 2.48                     | 0.91              |
| 5:N:508:ALA:HA    | 5:N:510:LEU:N     | 1.85                     | 0.91              |
| 4:B:1093:LEU:HD11 | 4:B:1097:ILE:CG2  | 2.01                     | 0.91              |
| 4:B:1057:LYS:HE2  | 4:B:1064:MET:HE2  | 1.47                     | 0.90              |
| 4:A:747:ILE:HG23  | 4:A:805:LEU:HD22  | 1.51                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:181:ILE:CD1   | 4:D:207:MET:HE3   | 2.01                     | 0.90              |
| 4:B:1056:ARG:CD   | 4:B:1057:LYS:HE3  | 2.02                     | 0.90              |
| 4:B:1159:LEU:CD1  | 4:B:1183:GLU:HG3  | 2.02                     | 0.90              |
| 4:D:501:LYS:HE3   | 4:D:505:LYS:HZ2   | 1.32                     | 0.90              |
| 4:D:1102:LEU:CD1  | 4:D:1206:LEU:HG   | 2.02                     | 0.90              |
| 5:O:450:LEU:CB    | 5:O:451:GLU:C     | 2.45                     | 0.89              |
| 4:A:1067:ARG:N    | 4:A:1081:VAL:HG21 | 1.88                     | 0.89              |
| 4:B:1067:ARG:HA   | 4:B:1081:VAL:HG21 | 1.54                     | 0.89              |
| 4:D:1082:PHE:CZ   | 4:D:1114:LEU:HA   | 2.07                     | 0.89              |
| 4:D:1057:LYS:HB3  | 4:D:1058:PRO:CA   | 2.02                     | 0.89              |
| 4:C:154:ILE:HD11  | 4:C:195:VAL:HB    | 1.54                     | 0.88              |
| 4:C:494:THR:N     | 4:C:573:SER:O     | 2.06                     | 0.88              |
| 5:O:494:ALA:HB1   | 5:O:495:GLU:HA    | 1.52                     | 0.88              |
| 4:A:1133:VAL:CG2  | 4:A:1189:LEU:HD11 | 2.03                     | 0.88              |
| 5:M:396:ARG:HB2   | 5:M:397:ALA:C     | 1.97                     | 0.88              |
| 4:D:1006:LEU:HD13 | 4:D:1010:VAL:HG21 | 1.53                     | 0.88              |
| 5:P:506:ARG:HB2   | 5:P:506:ARG:NH1   | 1.89                     | 0.88              |
| 4:B:1013:HIS:NE2  | 4:B:1016:LEU:HD11 | 1.89                     | 0.88              |
| 4:A:855:ALA:HB2   | 4:A:1008:ILE:HD11 | 1.56                     | 0.88              |
| 5:M:519:ARG:HD3   | 5:M:520:LYS:CE    | 2.03                     | 0.88              |
| 5:M:539:GLY:HA2   | 5:M:542:PRO:HD2   | 1.56                     | 0.88              |
| 5:M:492:TRP:O     | 5:M:493:GLU:CG    | 2.22                     | 0.87              |
| 4:D:1066:ALA:O    | 4:D:1081:VAL:CG1  | 2.19                     | 0.87              |
| 5:P:532:GLU:CD    | 5:P:535:ILE:HD11  | 1.98                     | 0.87              |
| 5:M:523:ALA:HB1   | 5:M:524:PRO:O     | 1.75                     | 0.87              |
| 4:A:1080:VAL:HA   | 4:A:1081:VAL:CB   | 2.05                     | 0.87              |
| 4:B:357:VAL:HG12  | 4:B:358:GLU:CG    | 2.05                     | 0.87              |
| 4:B:1057:LYS:HE2  | 4:B:1064:MET:CG   | 2.05                     | 0.87              |
| 5:M:523:ALA:HB1   | 5:M:524:PRO:C     | 2.00                     | 0.87              |
| 5:M:525:GLU:OE1   | 5:M:525:GLU:N     | 2.08                     | 0.87              |
| 4:C:1080:VAL:CG1  | 4:C:1082:PHE:HD2  | 1.88                     | 0.86              |
| 4:C:1080:VAL:CG1  | 4:C:1113:VAL:O    | 2.23                     | 0.86              |
| 5:O:387:PHE:HE2   | 5:O:441:PHE:CZ    | 1.92                     | 0.86              |
| 4:B:1057:LYS:CE   | 4:B:1064:MET:HG3  | 2.05                     | 0.86              |
| 4:B:1056:ARG:HG3  | 4:B:1057:LYS:HG3  | 0.89                     | 0.86              |
| 4:C:1129:LYS:CE   | 4:C:1183:GLU:OE2  | 2.23                     | 0.86              |
| 5:N:541:MET:N     | 5:N:542:PRO:CD    | 2.37                     | 0.86              |
| 4:D:537:GLU:HA    | 4:D:540:GLN:HG2   | 1.57                     | 0.86              |
| 5:P:505:ARG:HG3   | 5:P:514:ARG:HE    | 1.39                     | 0.86              |
| 4:C:968:ARG:O     | 4:C:972:ARG:HG3   | 1.75                     | 0.85              |
| 4:C:1093:LEU:HD11 | 4:C:1097:ILE:HB   | 1.57                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1032:LEU:HD11 | 4:A:1047:LEU:HD11 | 1.59                     | 0.85              |
| 4:D:1080:VAL:HG11 | 4:D:1082:PHE:HE2  | 0.90                     | 0.85              |
| 5:O:389:GLU:HB2   | 5:O:445:GLU:HB2   | 1.57                     | 0.85              |
| 5:O:390:ALA:HB3   | 5:O:393:PRO:HG2   | 1.57                     | 0.85              |
| 5:M:421:PHE:HD2   | 5:M:422:HIS:ND1   | 1.72                     | 0.85              |
| 5:M:524:PRO:HB2   | 5:M:525:GLU:C     | 2.02                     | 0.85              |
| 5:P:529:PRO:HB2   | 5:P:530:VAL:HA    | 1.59                     | 0.84              |
| 4:C:298:PHE:CD2   | 4:C:299:PRO:HD2   | 2.12                     | 0.84              |
| 5:M:519:ARG:CD    | 5:M:520:LYS:HE2   | 2.08                     | 0.84              |
| 5:M:418:SER:O     | 5:M:422:HIS:CD2   | 2.31                     | 0.84              |
| 4:A:572:ALA:CA    | 4:A:573:SER:HB2   | 2.07                     | 0.84              |
| 4:A:1127:ALA:HB1  | 4:A:1128:PRO:HD2  | 1.57                     | 0.84              |
| 4:C:970:ARG:HH21  | 4:C:975:LEU:CD2   | 1.90                     | 0.84              |
| 4:B:1013:HIS:HB3  | 4:B:1014:PRO:HA   | 1.60                     | 0.83              |
| 4:D:1064:MET:O    | 4:D:1065:MET:HE2  | 1.78                     | 0.83              |
| 5:O:387:PHE:HE2   | 5:O:441:PHE:CE2   | 1.91                     | 0.83              |
| 5:P:505:ARG:CG    | 5:P:514:ARG:HH21  | 1.91                     | 0.83              |
| 5:N:506:ARG:HG2   | 5:N:507:LEU:N     | 1.92                     | 0.83              |
| 4:A:1133:VAL:HG23 | 4:A:1189:LEU:HD11 | 1.60                     | 0.83              |
| 4:D:1079:VAL:HG23 | 4:D:1113:VAL:HG11 | 1.60                     | 0.83              |
| 5:M:392:LYS:HB3   | 5:M:395:LEU:O     | 1.78                     | 0.83              |
| 5:O:389:GLU:HB2   | 5:O:445:GLU:CB    | 2.09                     | 0.83              |
| 5:O:502:GLU:O     | 5:O:503:GLU:CB    | 2.26                     | 0.83              |
| 4:A:513:ILE:HG22  | 4:A:514:PRO:CD    | 2.07                     | 0.83              |
| 5:P:494:ALA:HB1   | 5:P:495:GLU:HA    | 1.61                     | 0.83              |
| 4:D:1080:VAL:C    | 4:D:1081:VAL:HG23 | 2.01                     | 0.82              |
| 4:B:570:ARG:HG2   | 4:B:571:HIS:H     | 1.44                     | 0.82              |
| 5:P:505:ARG:NE    | 5:P:510:LEU:CD1   | 2.43                     | 0.82              |
| 4:D:1119:TRP:CH2  | 4:D:1206:LEU:HA   | 2.14                     | 0.82              |
| 4:B:1089:VAL:HG22 | 4:B:1118:VAL:HG12 | 1.62                     | 0.82              |
| 5:M:396:ARG:CA    | 5:M:397:ALA:HB3   | 2.10                     | 0.82              |
| 5:P:532:GLU:OE2   | 5:P:535:ILE:HD11  | 1.79                     | 0.82              |
| 4:C:541:VAL:HG23  | 4:C:542:VAL:HA    | 1.61                     | 0.82              |
| 5:O:450:LEU:HB3   | 5:O:451:GLU:HB2   | 1.61                     | 0.82              |
| 5:P:396:ARG:O     | 5:P:397:ALA:O     | 1.96                     | 0.82              |
| 4:B:1143:LYS:N    | 4:B:1144:GLY:HA2  | 1.94                     | 0.81              |
| 4:D:539:ILE:O     | 4:D:541:VAL:HG23  | 1.78                     | 0.81              |
| 5:P:501:SER:CB    | 5:P:504:LEU:O     | 2.28                     | 0.81              |
| 4:B:1054:VAL:HG21 | 4:B:1094:LYS:NZ   | 1.96                     | 0.81              |
| 5:M:539:GLY:CA    | 5:M:542:PRO:HD2   | 2.10                     | 0.81              |
| 5:N:527:GLU:N     | 5:N:528:GLU:HA    | 1.95                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:539:GLY:O     | 5:P:542:PRO:HD2   | 1.80                     | 0.81              |
| 4:B:1057:LYS:HG2  | 4:B:1064:MET:HA   | 0.93                     | 0.81              |
| 4:D:1057:LYS:HE3  | 4:D:1064:MET:N    | 1.96                     | 0.81              |
| 5:O:387:PHE:HZ    | 5:O:441:PHE:CD2   | 1.98                     | 0.81              |
| 5:M:418:SER:O     | 5:M:422:HIS:CE1   | 2.34                     | 0.81              |
| 4:D:549:MET:CE    | 4:D:559:ILE:HB    | 2.11                     | 0.81              |
| 4:D:1080:VAL:CG1  | 4:D:1082:PHE:CD2  | 2.59                     | 0.81              |
| 4:D:537:GLU:CA    | 4:D:540:GLN:CG    | 2.58                     | 0.81              |
| 5:M:390:ALA:O     | 5:M:391:LEU:HD12  | 1.81                     | 0.81              |
| 5:M:539:GLY:C     | 5:M:542:PRO:HD2   | 2.04                     | 0.81              |
| 5:O:450:LEU:CB    | 5:O:451:GLU:HB2   | 2.11                     | 0.81              |
| 5:O:387:PHE:CE2   | 5:O:441:PHE:HE2   | 1.94                     | 0.81              |
| 5:N:453:LYS:O     | 5:N:454:SER:CB    | 2.21                     | 0.80              |
| 4:C:1080:VAL:CG1  | 4:C:1082:PHE:CD2  | 2.62                     | 0.80              |
| 5:O:505:ARG:HH11  | 5:O:505:ARG:HG2   | 1.47                     | 0.80              |
| 5:M:389:GLU:O     | 5:M:390:ALA:HB3   | 1.79                     | 0.80              |
| 5:M:408:GLY:HA3   | 5:M:415:PHE:HD1   | 1.46                     | 0.80              |
| 4:D:1056:ARG:CA   | 4:D:1066:ALA:HB2  | 2.12                     | 0.80              |
| 4:D:1079:VAL:O    | 4:D:1081:VAL:HG23 | 1.82                     | 0.80              |
| 5:P:505:ARG:CD    | 5:P:514:ARG:CZ    | 2.58                     | 0.80              |
| 5:N:520:LYS:N     | 5:N:521:PRO:CD    | 2.44                     | 0.80              |
| 5:N:525:GLU:CG    | 5:N:528:GLU:O     | 2.30                     | 0.80              |
| 5:O:396:ARG:HA    | 5:O:397:ALA:C     | 2.06                     | 0.80              |
| 4:D:284:ASP:HB3   | 4:D:290:LYS:NZ    | 1.95                     | 0.80              |
| 5:M:505:ARG:HB3   | 5:M:506:ARG:CA    | 2.11                     | 0.80              |
| 5:N:523:ALA:HB1   | 5:N:524:PRO:O     | 1.81                     | 0.80              |
| 4:A:569:ASN:HA    | 4:A:570:ARG:HB3   | 1.60                     | 0.80              |
| 5:P:505:ARG:CD    | 5:P:514:ARG:NH2   | 2.42                     | 0.80              |
| 4:C:301:PRO:HB2   | 4:C:302:GLU:HB2   | 1.64                     | 0.80              |
| 5:P:524:PRO:CD    | 5:P:525:GLU:C     | 2.52                     | 0.80              |
| 4:D:1059:THR:HG22 | 4:D:1065:MET:CE   | 2.11                     | 0.80              |
| 5:N:506:ARG:HA    | 5:N:510:LEU:HD22  | 1.63                     | 0.80              |
| 4:C:1080:VAL:HG13 | 4:C:1113:VAL:O    | 1.82                     | 0.79              |
| 4:C:737:THR:HG21  | 4:C:746:GLN:HE22  | 1.47                     | 0.79              |
| 4:D:537:GLU:HA    | 4:D:540:GLN:CD    | 2.06                     | 0.79              |
| 5:O:388:LEU:HD23  | 5:O:394:THR:HG21  | 1.65                     | 0.79              |
| 4:D:549:MET:HE1   | 4:D:559:ILE:CG2   | 2.11                     | 0.79              |
| 5:P:413:LEU:CA    | 5:P:416:PRO:HD2   | 2.13                     | 0.79              |
| 4:A:967:THR:HG23  | 4:A:981:GLU:HG2   | 1.64                     | 0.79              |
| 5:M:490:PRO:O     | 5:M:492:TRP:NE1   | 2.16                     | 0.79              |
| 4:A:975:LEU:HD12  | 4:A:975:LEU:O     | 1.82                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:1093:LEU:CD1  | 4:C:1097:ILE:HG21 | 2.13                     | 0.78              |
| 5:P:409:LYS:HG3   | 5:P:410:THR:N     | 1.98                     | 0.78              |
| 4:B:1054:VAL:CG2  | 4:B:1094:LYS:NZ   | 2.46                     | 0.78              |
| 4:D:500:SER:HB3   | 4:D:535:LEU:HD13  | 1.64                     | 0.78              |
| 4:C:407:GLN:OE1   | 4:C:436:VAL:HG11  | 1.84                     | 0.78              |
| 5:P:505:ARG:NE    | 5:P:510:LEU:HD13  | 1.98                     | 0.78              |
| 5:M:506:ARG:HA    | 5:M:510:LEU:HD23  | 1.64                     | 0.78              |
| 5:P:490:PRO:HD2   | 5:P:522:LYS:HE3   | 1.63                     | 0.78              |
| 4:D:1082:PHE:CZ   | 4:D:1114:LEU:CB   | 2.65                     | 0.78              |
| 4:D:696:LEU:HD21  | 4:D:742:VAL:HG22  | 1.66                     | 0.78              |
| 4:B:1057:LYS:HZ3  | 4:B:1064:MET:HE2  | 1.45                     | 0.77              |
| 4:A:980:ALA:C     | 4:A:981:GLU:HG3   | 2.09                     | 0.77              |
| 5:M:539:GLY:O     | 5:M:542:PRO:HD2   | 1.83                     | 0.77              |
| 4:B:1057:LYS:CB   | 4:B:1058:PRO:HA   | 2.08                     | 0.77              |
| 5:M:419:LYS:HA    | 5:M:422:HIS:HD2   | 1.49                     | 0.77              |
| 4:D:546:ARG:HD2   | 4:D:546:ARG:C     | 2.09                     | 0.77              |
| 5:N:494:ALA:CB    | 5:N:495:GLU:CA    | 2.62                     | 0.77              |
| 5:M:494:ALA:CB    | 5:M:495:GLU:HA    | 2.15                     | 0.77              |
| 3:I:19:DC:O2      | 2:J:11:DG:N2      | 2.18                     | 0.77              |
| 4:C:1051:VAL:HG21 | 4:C:1094:LYS:O    | 1.85                     | 0.77              |
| 4:D:302:GLU:HB3   | 4:D:303:GLY:CA    | 2.14                     | 0.77              |
| 4:D:549:MET:CE    | 4:D:559:ILE:CB    | 2.63                     | 0.77              |
| 5:M:413:LEU:O     | 5:M:417:GLU:HG3   | 1.85                     | 0.77              |
| 5:M:505:ARG:HD2   | 5:M:510:LEU:HD23  | 1.66                     | 0.77              |
| 5:N:505:ARG:HB3   | 5:N:506:ARG:CA    | 2.14                     | 0.77              |
| 4:B:1057:LYS:HZ1  | 4:B:1064:MET:HE2  | 1.48                     | 0.76              |
| 4:D:549:MET:HE2   | 4:D:559:ILE:CD1   | 1.99                     | 0.76              |
| 5:N:494:ALA:HB1   | 5:N:495:GLU:HA    | 1.64                     | 0.76              |
| 4:D:1082:PHE:HZ   | 4:D:1114:LEU:CB   | 1.98                     | 0.76              |
| 5:M:392:LYS:CG    | 5:M:397:ALA:HB2   | 2.16                     | 0.76              |
| 5:M:521:PRO:HG2   | 5:M:522:LYS:O     | 1.85                     | 0.76              |
| 5:M:394:THR:O     | 5:M:395:LEU:HB2   | 1.84                     | 0.76              |
| 5:P:511:LEU:O     | 5:P:515:LEU:HD23  | 1.85                     | 0.76              |
| 5:P:494:ALA:CB    | 5:P:495:GLU:CA    | 2.60                     | 0.76              |
| 5:O:507:LEU:HD23  | 5:O:507:LEU:H     | 1.50                     | 0.76              |
| 5:O:519:ARG:CD    | 5:O:520:LYS:HZ1   | 1.96                     | 0.76              |
| 4:C:407:GLN:CD    | 4:C:436:VAL:HG11  | 2.10                     | 0.76              |
| 4:C:970:ARG:O     | 4:C:973:SER:N     | 2.18                     | 0.76              |
| 5:P:412:VAL:O     | 5:P:415:PHE:N     | 2.17                     | 0.76              |
| 5:O:390:ALA:CB    | 5:O:393:PRO:HG2   | 2.14                     | 0.75              |
| 5:P:491:PRO:HB3   | 5:P:540:ILE:CG2   | 2.15                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1013:HIS:CD2  | 4:B:1016:LEU:HD11 | 2.21                     | 0.75              |
| 4:B:1056:ARG:HG2  | 4:B:1056:ARG:HH11 | 1.50                     | 0.75              |
| 4:B:1057:LYS:HE3  | 4:B:1064:MET:HG3  | 1.66                     | 0.75              |
| 4:A:971:GLY:CA    | 4:A:975:LEU:CB    | 2.61                     | 0.75              |
| 4:B:1084:ARG:HD2  | 4:B:1089:VAL:CG1  | 2.17                     | 0.75              |
| 4:B:1056:ARG:HA   | 4:B:1066:ALA:HB2  | 1.67                     | 0.75              |
| 4:B:1057:LYS:HD3  | 4:B:1063:GLY:O    | 1.86                     | 0.75              |
| 5:M:540:ILE:O     | 5:M:543:PRO:HD3   | 1.85                     | 0.75              |
| 4:C:1129:LYS:NZ   | 4:C:1183:GLU:OE2  | 2.18                     | 0.75              |
| 4:B:1054:VAL:HG23 | 4:B:1094:LYS:CE   | 2.16                     | 0.75              |
| 5:O:519:ARG:NE    | 5:O:520:LYS:NZ    | 2.35                     | 0.75              |
| 4:C:590:VAL:HG13  | 4:C:604:TYR:CD1   | 2.22                     | 0.74              |
| 5:O:541:MET:N     | 5:O:542:PRO:CD    | 2.50                     | 0.74              |
| 4:D:542:VAL:HG13  | 4:D:543:PRO:HD3   | 1.67                     | 0.74              |
| 4:D:939:VAL:HG22  | 4:D:944:LEU:HD12  | 1.67                     | 0.74              |
| 5:N:411:LEU:CB    | 5:N:412:VAL:HA    | 2.17                     | 0.74              |
| 5:P:409:LYS:HG3   | 5:P:410:THR:H     | 1.52                     | 0.74              |
| 4:B:154:ILE:HD13  | 4:B:195:VAL:HB    | 1.69                     | 0.74              |
| 4:D:1039:LEU:HD12 | 4:D:1040:PRO:CD   | 2.16                     | 0.74              |
| 5:M:524:PRO:HD2   | 5:M:525:GLU:HA    | 1.69                     | 0.74              |
| 5:O:390:ALA:HB3   | 5:O:393:PRO:HG3   | 1.67                     | 0.74              |
| 4:D:537:GLU:C     | 4:D:540:GLN:HG3   | 2.12                     | 0.74              |
| 4:B:679:VAL:HG22  | 4:B:693:LEU:HD21  | 1.69                     | 0.74              |
| 5:P:505:ARG:NH2   | 5:P:532:GLU:OE1   | 2.20                     | 0.74              |
| 4:A:1051:VAL:HG21 | 4:A:1099:LEU:HD12 | 1.69                     | 0.74              |
| 4:D:1080:VAL:CB   | 4:D:1081:VAL:HB   | 2.17                     | 0.74              |
| 5:N:403:ARG:NE    | 5:N:437:ALA:HB1   | 2.02                     | 0.74              |
| 5:P:522:LYS:HG3   | 5:P:523:ALA:N     | 2.02                     | 0.74              |
| 5:M:506:ARG:HB2   | 5:M:510:LEU:HB3   | 1.67                     | 0.74              |
| 5:P:499:ASP:CB    | 5:P:515:LEU:HD22  | 2.17                     | 0.73              |
| 4:D:498:LEU:CD2   | 4:D:503:ALA:HB2   | 2.17                     | 0.73              |
| 4:D:546:ARG:HD2   | 4:D:546:ARG:O     | 1.87                     | 0.73              |
| 5:O:411:LEU:CB    | 5:O:412:VAL:HA    | 2.19                     | 0.73              |
| 4:B:1056:ARG:HD2  | 4:B:1057:LYS:CE   | 2.17                     | 0.73              |
| 5:N:411:LEU:HB2   | 5:N:412:VAL:HA    | 1.71                     | 0.73              |
| 4:C:1080:VAL:HB   | 4:C:1082:PHE:H    | 1.52                     | 0.73              |
| 4:D:542:VAL:HG13  | 4:D:543:PRO:CD    | 2.19                     | 0.73              |
| 4:D:549:MET:HE3   | 4:D:559:ILE:HD13  | 1.66                     | 0.73              |
| 4:D:1080:VAL:CB   | 4:D:1082:PHE:CD2  | 2.71                     | 0.73              |
| 5:M:539:GLY:HA2   | 5:M:542:PRO:CD    | 2.17                     | 0.73              |
| 4:B:505:LYS:HE3   | 4:B:522:ALA:HB3   | 1.70                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1159:LEU:HD11 | 4:B:1183:GLU:CG   | 2.07                     | 0.73              |
| 4:D:541:VAL:HG13  | 4:D:544:GLU:HB2   | 1.69                     | 0.73              |
| 5:O:450:LEU:CA    | 5:O:451:GLU:HB2   | 2.18                     | 0.73              |
| 4:B:1023:GLU:O    | 4:B:1164:ARG:NH2  | 2.22                     | 0.73              |
| 5:O:494:ALA:CB    | 5:O:495:GLU:CA    | 2.67                     | 0.73              |
| 5:M:505:ARG:CB    | 5:M:506:ARG:HB3   | 2.17                     | 0.73              |
| 5:O:507:LEU:HD23  | 5:O:507:LEU:N     | 2.04                     | 0.73              |
| 5:P:504:LEU:N     | 5:P:504:LEU:HD12  | 2.04                     | 0.73              |
| 4:A:319:LEU:HD23  | 4:A:326:ILE:HG22  | 1.71                     | 0.72              |
| 4:D:289:ASP:N     | 4:D:289:ASP:OD1   | 2.22                     | 0.72              |
| 4:B:1013:HIS:CE1  | 4:B:1016:LEU:HD11 | 2.24                     | 0.72              |
| 4:B:1054:VAL:HG21 | 4:B:1094:LYS:HZ2  | 1.53                     | 0.72              |
| 4:B:1066:ALA:C    | 4:B:1081:VAL:HB   | 2.14                     | 0.72              |
| 4:D:1082:PHE:CZ   | 4:D:1114:LEU:CG   | 2.73                     | 0.72              |
| 5:P:505:ARG:HB2   | 5:P:510:LEU:HD12  | 1.72                     | 0.72              |
| 4:B:1066:ALA:O    | 4:B:1081:VAL:HG11 | 1.87                     | 0.72              |
| 5:O:388:LEU:CD2   | 5:O:399:VAL:HG21  | 2.18                     | 0.72              |
| 4:D:1135:VAL:HG11 | 4:D:1139:LEU:HD11 | 1.71                     | 0.72              |
| 4:B:615:LEU:HD21  | 4:B:617:MET:CE    | 2.19                     | 0.72              |
| 4:D:1080:VAL:HB   | 4:D:1082:PHE:CD2  | 2.24                     | 0.72              |
| 4:D:1080:VAL:CG2  | 4:D:1082:PHE:CE2  | 2.72                     | 0.72              |
| 5:M:421:PHE:CD2   | 5:M:422:HIS:CE1   | 2.78                     | 0.72              |
| 5:N:505:ARG:CB    | 5:N:506:ARG:HB3   | 2.18                     | 0.72              |
| 5:O:450:LEU:HA    | 5:O:451:GLU:HB2   | 1.71                     | 0.72              |
| 5:O:505:ARG:HG2   | 5:O:505:ARG:NH1   | 2.01                     | 0.72              |
| 4:C:1161:VAL:HG13 | 4:C:1176:LEU:HD23 | 1.71                     | 0.72              |
| 5:P:540:ILE:HD12  | 5:P:540:ILE:C     | 2.15                     | 0.71              |
| 4:A:572:ALA:HB1   | 4:A:573:SER:HB3   | 1.70                     | 0.71              |
| 4:B:352:GLU:OE1   | 4:B:356:ARG:NH2   | 2.23                     | 0.71              |
| 5:P:396:ARG:C     | 5:P:397:ALA:O     | 2.33                     | 0.71              |
| 5:P:413:LEU:C     | 5:P:416:PRO:HD2   | 2.16                     | 0.71              |
| 4:C:1161:VAL:CG1  | 4:C:1176:LEU:HD23 | 2.19                     | 0.71              |
| 4:D:1080:VAL:HG21 | 4:D:1114:LEU:HA   | 1.72                     | 0.71              |
| 5:O:519:ARG:HB3   | 5:O:520:LYS:HB2   | 1.71                     | 0.71              |
| 4:B:1066:ALA:HB3  | 4:B:1084:ARG:CZ   | 2.19                     | 0.71              |
| 4:C:1176:LEU:HD22 | 4:C:1179:VAL:HG23 | 1.72                     | 0.71              |
| 5:O:411:LEU:HB2   | 5:O:412:VAL:HA    | 1.72                     | 0.71              |
| 5:P:504:LEU:HB2   | 5:P:505:ARG:HG2   | 1.72                     | 0.71              |
| 5:P:504:LEU:HB3   | 5:P:505:ARG:HA    | 1.72                     | 0.71              |
| 4:B:363:GLU:O     | 4:B:366:ARG:HB2   | 1.90                     | 0.71              |
| 5:O:450:LEU:HB3   | 5:O:451:GLU:CB    | 2.20                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1054:VAL:HG23 | 4:B:1094:LYS:HD3  | 1.71                     | 0.71              |
| 4:D:498:LEU:HD21  | 4:D:503:ALA:CB    | 2.17                     | 0.71              |
| 5:P:538:ASN:O     | 5:P:541:MET:HB3   | 1.90                     | 0.71              |
| 5:N:506:ARG:CB    | 5:N:510:LEU:HB2   | 2.09                     | 0.71              |
| 5:O:455:LEU:HA    | 5:O:456:SER:C     | 2.16                     | 0.71              |
| 4:C:975:LEU:HD23  | 4:C:975:LEU:C     | 2.15                     | 0.71              |
| 4:D:507:VAL:HG12  | 4:D:558:VAL:HG13  | 1.72                     | 0.71              |
| 5:P:408:GLY:O     | 5:P:409:LYS:C     | 2.33                     | 0.71              |
| 4:A:1029:ILE:HG23 | 4:A:1077:LEU:CD1  | 2.20                     | 0.71              |
| 5:M:419:LYS:O     | 5:M:423:HIS:CE1   | 2.44                     | 0.71              |
| 4:A:975:LEU:HD12  | 4:A:975:LEU:C     | 2.16                     | 0.71              |
| 4:A:1159:LEU:O    | 4:A:1159:LEU:HD12 | 1.89                     | 0.70              |
| 4:B:525:ILE:HD11  | 4:B:538:ALA:CB    | 2.20                     | 0.70              |
| 4:D:537:GLU:O     | 4:D:540:GLN:CG    | 2.36                     | 0.70              |
| 4:D:1119:TRP:HH2  | 4:D:1206:LEU:HA   | 1.55                     | 0.70              |
| 5:O:495:GLU:HG3   | 5:O:503:GLU:HG3   | 1.73                     | 0.70              |
| 5:M:507:LEU:O     | 5:M:510:LEU:HD13  | 1.90                     | 0.70              |
| 4:C:1084:ARG:HG3  | 4:C:1089:VAL:HG22 | 1.73                     | 0.70              |
| 4:C:1159:LEU:CD1  | 4:C:1183:GLU:HG3  | 2.22                     | 0.70              |
| 5:M:532:GLU:O     | 5:M:535:ILE:HG22  | 1.91                     | 0.70              |
| 5:N:524:PRO:HB2   | 5:N:525:GLU:CA    | 2.20                     | 0.70              |
| 5:N:525:GLU:CD    | 5:N:525:GLU:H     | 1.99                     | 0.70              |
| 4:B:1057:LYS:CE   | 4:B:1064:MET:CE   | 2.56                     | 0.70              |
| 5:P:505:ARG:HB3   | 5:P:510:LEU:CD1   | 2.17                     | 0.70              |
| 4:C:918:LEU:HD22  | 4:C:953:LEU:CD2   | 2.21                     | 0.70              |
| 4:D:409:TYR:OH    | 4:D:617:MET:HE2   | 1.92                     | 0.70              |
| 5:O:540:ILE:C     | 5:O:542:PRO:HD2   | 2.16                     | 0.70              |
| 4:A:788:ALA:HB1   | 4:A:793:VAL:CG2   | 2.22                     | 0.70              |
| 4:A:1161:VAL:HG21 | 4:A:1179:VAL:CG2  | 2.22                     | 0.70              |
| 4:B:332:ARG:HG3   | 4:B:350:LEU:HD21  | 1.73                     | 0.70              |
| 5:O:450:LEU:HB3   | 5:O:451:GLU:CA    | 2.21                     | 0.70              |
| 4:C:1207:GLN:HB3  | 4:C:1208:GLY:HA2  | 1.73                     | 0.70              |
| 5:M:415:PHE:HB2   | 5:M:416:PRO:HD3   | 1.74                     | 0.70              |
| 5:P:538:ASN:O     | 5:P:542:PRO:HD3   | 1.91                     | 0.70              |
| 5:M:506:ARG:HB2   | 5:M:510:LEU:CB    | 2.21                     | 0.70              |
| 5:P:532:GLU:CA    | 5:P:535:ILE:HD13  | 2.18                     | 0.70              |
| 4:A:617:MET:HE2   | 4:A:617:MET:HA    | 1.74                     | 0.69              |
| 4:B:310:LEU:HD13  | 4:B:403:PHE:CD2   | 2.27                     | 0.69              |
| 4:C:854:VAL:HG23  | 4:C:1008:ILE:HD13 | 1.72                     | 0.69              |
| 5:N:519:ARG:HB3   | 5:N:520:LYS:HB2   | 1.73                     | 0.69              |
| 4:C:1176:LEU:HD22 | 4:C:1179:VAL:CG2  | 2.22                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:951:ALA:HB2   | 4:C:993:LEU:HG    | 1.72                     | 0.69              |
| 4:D:1082:PHE:CZ   | 4:D:1114:LEU:HG   | 2.23                     | 0.69              |
| 4:D:1082:PHE:CZ   | 4:D:1114:LEU:CA   | 2.75                     | 0.69              |
| 5:M:519:ARG:HB3   | 5:M:520:LYS:CB    | 2.04                     | 0.69              |
| 4:A:574:VAL:HG12  | 4:A:575:HIS:N     | 2.06                     | 0.69              |
| 4:A:1080:VAL:HG21 | 4:A:1114:LEU:HD23 | 1.73                     | 0.69              |
| 4:D:50:LEU:HD11   | 4:D:591:PRO:HG3   | 1.75                     | 0.69              |
| 4:D:1080:VAL:CB   | 4:D:1082:PHE:CE2  | 2.75                     | 0.69              |
| 4:B:1055:VAL:O    | 4:B:1066:ALA:CB   | 2.40                     | 0.69              |
| 5:M:506:ARG:O     | 5:M:507:LEU:HD22  | 1.93                     | 0.69              |
| 5:P:505:ARG:CG    | 5:P:514:ARG:NH2   | 2.55                     | 0.69              |
| 5:N:520:LYS:H     | 5:N:521:PRO:HD3   | 1.53                     | 0.69              |
| 4:B:357:VAL:CB    | 4:B:358:GLU:HB2   | 2.13                     | 0.69              |
| 4:C:970:ARG:HH21  | 4:C:975:LEU:HD21  | 1.58                     | 0.69              |
| 4:B:357:VAL:CB    | 4:B:358:GLU:HG3   | 2.22                     | 0.69              |
| 4:D:590:VAL:HG13  | 4:D:604:TYR:CD1   | 2.27                     | 0.69              |
| 5:P:391:LEU:C     | 5:P:393:PRO:HD3   | 2.17                     | 0.69              |
| 4:A:1165:VAL:HG13 | 4:A:1172:ALA:HB3  | 1.75                     | 0.68              |
| 4:B:515:HIS:HB2   | 4:B:516:LYS:HA    | 1.76                     | 0.68              |
| 4:D:492:ILE:HA    | 4:D:602:THR:HG22  | 1.75                     | 0.68              |
| 5:M:505:ARG:HB3   | 5:M:506:ARG:HA    | 1.73                     | 0.68              |
| 5:P:494:ALA:HB1   | 5:P:495:GLU:CA    | 2.23                     | 0.68              |
| 5:N:540:ILE:C     | 5:N:542:PRO:HD2   | 2.17                     | 0.68              |
| 5:P:504:LEU:HB2   | 5:P:505:ARG:CG    | 2.23                     | 0.68              |
| 4:D:635:VAL:HG12  | 4:D:641:VAL:HG13  | 1.75                     | 0.68              |
| 4:D:1039:LEU:HD12 | 4:D:1040:PRO:HD2  | 1.74                     | 0.68              |
| 4:C:291:MET:HE1   | 4:C:613:GLY:CA    | 2.24                     | 0.68              |
| 5:M:524:PRO:CD    | 5:M:525:GLU:HA    | 2.24                     | 0.68              |
| 4:C:154:ILE:CG2   | 4:C:192:VAL:HG22  | 2.23                     | 0.68              |
| 4:D:116:ALA:HB1   | 4:D:125:PRO:HB2   | 1.76                     | 0.68              |
| 4:D:302:GLU:HB3   | 4:D:303:GLY:C     | 2.19                     | 0.68              |
| 4:B:186:LEU:HD21  | 4:B:245:PRO:HB2   | 1.75                     | 0.68              |
| 4:D:1202:ARG:HG2  | 4:D:1202:ARG:NH1  | 1.98                     | 0.68              |
| 4:D:994:ASP:CB    | 5:P:528:GLU:OE1   | 2.42                     | 0.68              |
| 4:D:996:ILE:HD12  | 5:P:528:GLU:OE2   | 1.94                     | 0.68              |
| 4:A:572:ALA:HA    | 4:A:573:SER:HB2   | 1.75                     | 0.68              |
| 4:D:538:ALA:O     | 4:D:541:VAL:HG22  | 1.93                     | 0.68              |
| 4:D:1059:THR:CG2  | 4:D:1065:MET:CE   | 2.71                     | 0.68              |
| 5:P:412:VAL:O     | 5:P:416:PRO:HD2   | 1.94                     | 0.68              |
| 4:B:570:ARG:CG    | 4:B:571:HIS:H     | 2.03                     | 0.68              |
| 4:B:1055:VAL:O    | 4:B:1066:ALA:HB1  | 1.93                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:411:LEU:N     | 5:M:412:VAL:HG22  | 2.09                     | 0.67              |
| 5:O:541:MET:N     | 5:O:542:PRO:HD2   | 2.08                     | 0.67              |
| 5:P:412:VAL:HB    | 5:P:415:PHE:CE2   | 2.29                     | 0.67              |
| 4:B:357:VAL:O     | 4:B:362:TRP:CZ2   | 2.47                     | 0.67              |
| 4:D:1060:ARG:HG2  | 4:D:1060:ARG:NH1  | 2.06                     | 0.67              |
| 5:N:412:VAL:O     | 5:N:414:ARG:N     | 2.27                     | 0.67              |
| 5:P:395:LEU:O     | 5:P:397:ALA:N     | 2.26                     | 0.67              |
| 4:C:291:MET:HE2   | 4:C:291:MET:O     | 1.95                     | 0.67              |
| 5:M:506:ARG:O     | 5:M:507:LEU:HD13  | 1.93                     | 0.67              |
| 5:O:494:ALA:HB3   | 5:O:495:GLU:HA    | 1.71                     | 0.67              |
| 5:P:392:LYS:N     | 5:P:393:PRO:CD    | 2.58                     | 0.67              |
| 5:O:388:LEU:HD23  | 5:O:399:VAL:HG21  | 1.77                     | 0.67              |
| 5:P:525:GLU:H     | 5:P:525:GLU:CD    | 2.03                     | 0.67              |
| 4:C:151:PRO:O     | 4:C:154:ILE:HG22  | 1.94                     | 0.67              |
| 5:O:518:VAL:HG23  | 5:O:519:ARG:HB2   | 1.76                     | 0.67              |
| 5:P:512:GLY:O     | 5:P:516:LEU:HG    | 1.93                     | 0.67              |
| 4:A:498:LEU:HB3   | 4:A:499:ALA:HB2   | 1.77                     | 0.67              |
| 4:B:352:GLU:CG    | 4:B:356:ARG:NH2   | 2.58                     | 0.67              |
| 4:D:1080:VAL:HG21 | 4:D:1082:PHE:CZ   | 2.29                     | 0.67              |
| 5:M:396:ARG:HA    | 5:M:397:ALA:CB    | 2.22                     | 0.67              |
| 4:A:1080:VAL:CG2  | 4:A:1114:LEU:CD2  | 2.72                     | 0.66              |
| 4:C:788:ALA:HB1   | 4:C:793:VAL:CG2   | 2.25                     | 0.66              |
| 4:C:878:PHE:O     | 4:C:892:SER:OG    | 2.08                     | 0.66              |
| 4:B:670:LEU:HD11  | 4:B:679:VAL:HG21  | 1.75                     | 0.66              |
| 4:B:1095:GLU:O    | 4:B:1097:ILE:HD12 | 1.95                     | 0.66              |
| 4:C:154:ILE:HD13  | 4:C:192:VAL:HA    | 1.76                     | 0.66              |
| 5:M:505:ARG:CD    | 5:M:510:LEU:HD23  | 2.25                     | 0.66              |
| 4:A:301:PRO:HA    | 4:A:302:GLU:HG2   | 1.77                     | 0.66              |
| 4:A:1080:VAL:CG2  | 4:A:1114:LEU:HD23 | 2.25                     | 0.66              |
| 4:A:1131:LEU:HD23 | 4:A:1132:GLU:N    | 2.11                     | 0.66              |
| 4:B:359:GLU:HA    | 4:B:362:TRP:HD1   | 1.59                     | 0.66              |
| 4:B:1054:VAL:HG23 | 4:B:1094:LYS:CD   | 2.24                     | 0.66              |
| 4:C:659:LEU:HD11  | 4:C:829:ALA:HB1   | 1.78                     | 0.66              |
| 5:M:507:LEU:O     | 5:M:510:LEU:HB2   | 1.95                     | 0.66              |
| 5:N:494:ALA:HB1   | 5:N:495:GLU:CA    | 2.25                     | 0.66              |
| 5:N:526:ALA:C     | 5:N:528:GLU:HA    | 2.20                     | 0.66              |
| 5:P:389:GLU:O     | 5:P:393:PRO:CD    | 2.44                     | 0.66              |
| 4:B:352:GLU:HG2   | 4:B:356:ARG:NH2   | 2.11                     | 0.66              |
| 4:C:181:ILE:CD1   | 4:C:207:MET:HE3   | 2.26                     | 0.66              |
| 4:D:539:ILE:C     | 4:D:541:VAL:HG23  | 2.19                     | 0.66              |
| 4:D:1079:VAL:O    | 4:D:1081:VAL:CG2  | 2.43                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:1082:PHE:HZ   | 4:D:1114:LEU:HB2  | 1.58                     | 0.66              |
| 5:P:456:SER:H     | 5:P:457:GLY:HA2   | 1.61                     | 0.66              |
| 5:P:499:ASP:CB    | 5:P:515:LEU:CD2   | 2.74                     | 0.66              |
| 4:B:357:VAL:CB    | 4:B:358:GLU:CB    | 2.73                     | 0.66              |
| 4:D:737:THR:HG21  | 4:D:746:GLN:HE22  | 1.60                     | 0.66              |
| 4:C:1095:GLU:HG2  | 4:C:1096:ASP:N    | 2.09                     | 0.66              |
| 4:D:1093:LEU:HD22 | 4:D:1099:LEU:CD1  | 2.25                     | 0.66              |
| 5:N:518:VAL:HG13  | 5:N:519:ARG:HB2   | 1.78                     | 0.66              |
| 4:A:631:ALA:O     | 4:A:635:VAL:HG23  | 1.96                     | 0.66              |
| 4:B:226:VAL:HG21  | 4:B:561:VAL:HG13  | 1.78                     | 0.66              |
| 4:B:1057:LYS:CE   | 4:B:1064:MET:CG   | 2.68                     | 0.66              |
| 4:D:1159:LEU:HD21 | 4:D:1183:GLU:CG   | 2.26                     | 0.66              |
| 4:C:106:TYR:O     | 4:C:110:VAL:HG23  | 1.96                     | 0.65              |
| 4:C:747:ILE:HG23  | 4:C:805:LEU:HD22  | 1.78                     | 0.65              |
| 4:C:918:LEU:HD22  | 4:C:953:LEU:HD23  | 1.77                     | 0.65              |
| 4:C:1093:LEU:C    | 4:C:1094:LYS:HG2  | 2.21                     | 0.65              |
| 5:M:493:GLU:OE1   | 5:M:517:TRP:CD1   | 2.50                     | 0.65              |
| 5:M:523:ALA:CB    | 5:M:524:PRO:HA    | 2.26                     | 0.65              |
| 5:P:531:SER:O     | 5:P:534:GLY:N     | 2.29                     | 0.65              |
| 4:A:980:ALA:O     | 4:A:981:GLU:HG3   | 1.96                     | 0.65              |
| 4:B:226:VAL:HG21  | 4:B:561:VAL:CG1   | 2.26                     | 0.65              |
| 4:B:941:ALA:HB1   | 4:B:1006:LEU:HD11 | 1.78                     | 0.65              |
| 4:B:1057:LYS:HE2  | 4:B:1064:MET:CB   | 2.26                     | 0.65              |
| 4:C:1051:VAL:CG2  | 4:C:1094:LYS:O    | 2.43                     | 0.65              |
| 4:C:1093:LEU:O    | 4:C:1094:LYS:CB   | 2.44                     | 0.65              |
| 5:M:392:LYS:HG3   | 5:M:397:ALA:HB2   | 1.77                     | 0.65              |
| 4:A:668:PHE:O     | 4:A:669:GLN:CB    | 2.41                     | 0.65              |
| 4:C:1161:VAL:HG12 | 4:C:1176:LEU:CD2  | 2.26                     | 0.65              |
| 5:M:507:LEU:H     | 5:M:510:LEU:CD2   | 2.00                     | 0.65              |
| 5:N:530:VAL:HG22  | 5:N:530:VAL:O     | 1.96                     | 0.65              |
| 4:A:785:VAL:CG1   | 4:A:795:GLU:HG3   | 2.26                     | 0.65              |
| 4:C:1029:ILE:HD13 | 4:C:1047:LEU:HD13 | 1.76                     | 0.65              |
| 4:B:300:LEU:HD22  | 4:B:309:TYR:CD2   | 2.32                     | 0.65              |
| 4:B:549:MET:HG2   | 4:B:559:ILE:HD12  | 1.79                     | 0.65              |
| 5:P:539:GLY:C     | 5:P:542:PRO:HD2   | 2.22                     | 0.65              |
| 4:A:951:ALA:HB2   | 4:A:993:LEU:CD2   | 2.27                     | 0.65              |
| 4:A:980:ALA:O     | 4:A:981:GLU:CG    | 2.45                     | 0.65              |
| 4:A:1133:VAL:HG21 | 4:A:1189:LEU:HD11 | 1.76                     | 0.65              |
| 4:B:1008:ILE:O    | 4:B:1008:ILE:HD12 | 1.97                     | 0.65              |
| 4:D:537:GLU:CA    | 4:D:540:GLN:HG2   | 2.25                     | 0.65              |
| 5:M:390:ALA:C     | 5:M:391:LEU:HD12  | 2.21                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:181:ILE:HD12  | 4:C:207:MET:HE3   | 1.79                     | 0.65              |
| 5:M:538:ASN:O     | 5:M:542:PRO:HD3   | 1.96                     | 0.65              |
| 5:N:499:ASP:OD2   | 5:N:515:LEU:HD11  | 1.96                     | 0.65              |
| 4:D:1057:LYS:HG2  | 4:D:1064:MET:HA   | 0.79                     | 0.65              |
| 5:M:421:PHE:HE2   | 5:M:422:HIS:ND1   | 1.73                     | 0.65              |
| 4:D:769:MET:HG2   | 4:D:777:MET:HE1   | 1.78                     | 0.64              |
| 5:O:505:ARG:HE    | 5:O:507:LEU:HD21  | 1.61                     | 0.64              |
| 4:B:535:LEU:HD23  | 4:B:559:ILE:HG23  | 1.78                     | 0.64              |
| 4:B:570:ARG:HG2   | 4:B:571:HIS:N     | 2.12                     | 0.64              |
| 4:B:1054:VAL:CG2  | 4:B:1094:LYS:HD3  | 2.26                     | 0.64              |
| 4:C:410:ILE:HG23  | 4:C:420:VAL:HG11  | 1.79                     | 0.64              |
| 5:M:505:ARG:HD2   | 5:M:510:LEU:CD2   | 2.26                     | 0.64              |
| 4:C:154:ILE:HG21  | 4:C:192:VAL:HG22  | 1.79                     | 0.64              |
| 4:D:338:LEU:HD11  | 4:D:365:LEU:HD11  | 1.78                     | 0.64              |
| 4:D:1014:PRO:HB2  | 4:D:1050:MET:HE3  | 1.80                     | 0.64              |
| 5:O:519:ARG:HD3   | 5:O:520:LYS:HZ2   | 0.65                     | 0.64              |
| 4:A:785:VAL:HG11  | 4:A:795:GLU:HG3   | 1.79                     | 0.64              |
| 4:D:1064:MET:O    | 4:D:1065:MET:HB2  | 1.96                     | 0.64              |
| 5:P:521:PRO:O     | 5:P:522:LYS:HB3   | 1.96                     | 0.64              |
| 5:P:535:ILE:HG12  | 5:P:536:GLY:N     | 2.13                     | 0.64              |
| 4:B:1021:LEU:HD21 | 4:B:1100:LEU:HD13 | 1.79                     | 0.64              |
| 4:B:1080:VAL:HG22 | 4:B:1114:LEU:HA   | 1.79                     | 0.64              |
| 4:C:590:VAL:HG11  | 4:C:602:THR:HG23  | 1.80                     | 0.64              |
| 4:D:1101:VAL:HG22 | 4:D:1118:VAL:HG22 | 1.79                     | 0.64              |
| 5:P:412:VAL:C     | 5:P:416:PRO:HD2   | 2.22                     | 0.64              |
| 5:P:524:PRO:N     | 5:P:525:GLU:HA    | 2.13                     | 0.64              |
| 4:B:1054:VAL:CG2  | 4:B:1094:LYS:HZ3  | 2.11                     | 0.64              |
| 5:P:506:ARG:O     | 5:P:510:LEU:HG    | 1.98                     | 0.64              |
| 4:D:222:ARG:O     | 4:D:226:VAL:HG13  | 1.98                     | 0.63              |
| 4:D:542:VAL:HG22  | 4:D:543:PRO:HD3   | 1.80                     | 0.63              |
| 5:M:495:GLU:HB2   | 5:M:496:GLU:HG2   | 1.79                     | 0.63              |
| 4:B:509:ARG:HA    | 4:B:513:ILE:HG21  | 1.79                     | 0.63              |
| 5:M:413:LEU:O     | 5:M:416:PRO:HD2   | 1.97                     | 0.63              |
| 5:M:415:PHE:O     | 5:M:418:SER:HB3   | 1.98                     | 0.63              |
| 5:N:525:GLU:HG3   | 5:N:529:PRO:HA    | 1.79                     | 0.63              |
| 5:O:494:ALA:HB3   | 5:O:495:GLU:CD    | 2.22                     | 0.63              |
| 5:P:413:LEU:HA    | 5:P:416:PRO:HD2   | 1.79                     | 0.63              |
| 4:A:1025:ALA:HB2  | 4:A:1048:SER:OG   | 1.98                     | 0.63              |
| 4:B:319:LEU:HD23  | 4:B:319:LEU:C     | 2.22                     | 0.63              |
| 4:B:1057:LYS:HE2  | 4:B:1064:MET:HB2  | 1.81                     | 0.63              |
| 4:C:299:PRO:HG2   | 4:C:300:LEU:H     | 1.64                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:897:VAL:HG21  | 4:D:938:LEU:HD13  | 1.80                     | 0.63              |
| 4:D:1136:ASP:OD2  | 4:D:1166:LEU:HD11 | 1.99                     | 0.63              |
| 4:D:1205:PHE:HD1  | 4:D:1206:LEU:HD12 | 1.61                     | 0.63              |
| 4:A:1135:VAL:HG13 | 4:A:1194:TYR:CE1  | 2.34                     | 0.63              |
| 5:M:525:GLU:H     | 5:M:525:GLU:CD    | 2.03                     | 0.63              |
| 5:O:504:LEU:HD13  | 5:O:514:ARG:HH22  | 1.63                     | 0.63              |
| 5:O:505:ARG:HH11  | 5:O:505:ARG:CG    | 2.11                     | 0.63              |
| 5:O:523:ALA:HB1   | 5:O:524:PRO:CB    | 2.20                     | 0.63              |
| 5:P:505:ARG:HG3   | 5:P:514:ARG:NE    | 2.13                     | 0.63              |
| 4:B:449:LEU:HD22  | 4:B:759:LEU:HD21  | 1.80                     | 0.62              |
| 4:B:670:LEU:HD12  | 4:B:675:MET:HG3   | 1.79                     | 0.62              |
| 4:B:1151:LEU:HD13 | 4:B:1189:LEU:HD13 | 1.80                     | 0.62              |
| 4:D:547:ALA:O     | 4:D:550:GLU:N     | 2.29                     | 0.62              |
| 5:N:411:LEU:N     | 5:N:412:VAL:HG22  | 2.14                     | 0.62              |
| 5:P:532:GLU:O     | 5:P:535:ILE:HG12  | 1.98                     | 0.62              |
| 4:A:918:LEU:HD22  | 4:A:953:LEU:HD23  | 1.80                     | 0.62              |
| 4:A:1076:ALA:O    | 4:A:1077:LEU:HD12 | 1.99                     | 0.62              |
| 4:D:226:VAL:CG1   | 4:D:510:VAL:HG11  | 2.29                     | 0.62              |
| 4:D:50:LEU:HD12   | 4:D:50:LEU:O      | 1.99                     | 0.62              |
| 5:P:416:PRO:HG2   | 5:P:417:GLU:N     | 2.14                     | 0.62              |
| 4:D:635:VAL:CG1   | 4:D:641:VAL:HG13  | 2.30                     | 0.62              |
| 4:D:1039:LEU:HD12 | 4:D:1040:PRO:HD3  | 1.80                     | 0.62              |
| 5:P:513:GLY:HA2   | 5:P:516:LEU:HD12  | 1.79                     | 0.62              |
| 4:A:1161:VAL:HG21 | 4:A:1179:VAL:HG21 | 1.80                     | 0.62              |
| 5:M:523:ALA:HB1   | 5:M:524:PRO:CA    | 2.28                     | 0.62              |
| 5:P:505:ARG:CD    | 5:P:514:ARG:NE    | 2.62                     | 0.62              |
| 5:P:522:LYS:CG    | 5:P:523:ALA:N     | 2.62                     | 0.62              |
| 4:B:1018:TYR:OH   | 5:N:530:VAL:HG12  | 2.00                     | 0.62              |
| 4:B:1056:ARG:CG   | 4:B:1056:ARG:HH11 | 2.13                     | 0.62              |
| 4:C:968:ARG:O     | 4:C:972:ARG:CG    | 2.48                     | 0.62              |
| 5:N:499:ASP:OD1   | 5:N:515:LEU:HD21  | 1.99                     | 0.62              |
| 5:O:388:LEU:HD23  | 5:O:399:VAL:CG2   | 2.30                     | 0.62              |
| 5:P:537:GLY:O     | 5:P:540:ILE:HG13  | 1.99                     | 0.62              |
| 4:B:354:LEU:O     | 4:B:362:TRP:CZ2   | 2.52                     | 0.62              |
| 5:O:506:ARG:O     | 5:O:510:LEU:HD22  | 2.00                     | 0.62              |
| 4:B:1066:ALA:HB3  | 4:B:1084:ARG:NH1  | 2.15                     | 0.62              |
| 4:B:976:VAL:HG11  | 4:C:115:ARG:HD3   | 1.82                     | 0.62              |
| 4:C:1094:LYS:N    | 4:C:1094:LYS:HD2  | 2.14                     | 0.62              |
| 4:D:284:ASP:CB    | 4:D:290:LYS:HE3   | 2.25                     | 0.62              |
| 4:D:302:GLU:HB3   | 4:D:303:GLY:HA3   | 1.80                     | 0.62              |
| 4:D:1135:VAL:CG1  | 4:D:1139:LEU:HD11 | 2.29                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:974:GLY:O     | 4:A:975:LEU:HB3   | 1.98                     | 0.61              |
| 4:C:854:VAL:CG2   | 4:C:1008:ILE:HD13 | 2.30                     | 0.61              |
| 5:O:392:LYS:HA    | 5:O:393:PRO:C     | 2.25                     | 0.61              |
| 4:D:664:THR:OG1   | 4:D:676:THR:HG22  | 1.98                     | 0.61              |
| 4:D:1006:LEU:CD1  | 4:D:1010:VAL:HG21 | 2.27                     | 0.61              |
| 4:D:498:LEU:HD23  | 4:D:566:GLU:HA    | 1.81                     | 0.61              |
| 5:M:535:ILE:HG23  | 5:M:536:GLY:N     | 2.15                     | 0.61              |
| 5:P:413:LEU:HA    | 5:P:416:PRO:CD    | 2.31                     | 0.61              |
| 4:A:668:PHE:O     | 4:A:669:GLN:HB2   | 2.01                     | 0.61              |
| 4:A:1139:LEU:HD12 | 4:A:1143:LYS:HE3  | 1.81                     | 0.61              |
| 4:B:1080:VAL:CB   | 4:B:1081:VAL:HG22 | 2.29                     | 0.61              |
| 4:C:675:MET:O     | 4:C:679:VAL:HG23  | 2.00                     | 0.61              |
| 4:C:1093:LEU:O    | 4:C:1094:LYS:HG2  | 2.00                     | 0.61              |
| 4:D:560:GLU:HA    | 4:D:563:MET:HE3   | 1.81                     | 0.61              |
| 4:C:1162:TYR:C    | 4:C:1163:LEU:HD12 | 2.26                     | 0.61              |
| 5:M:408:GLY:CA    | 5:M:415:PHE:HD1   | 2.13                     | 0.61              |
| 4:B:670:LEU:HD11  | 4:B:679:VAL:CG2   | 2.30                     | 0.61              |
| 4:C:1093:LEU:C    | 4:C:1094:LYS:CG   | 2.67                     | 0.61              |
| 5:O:494:ALA:HB3   | 5:O:495:GLU:CA    | 2.29                     | 0.61              |
| 4:B:1089:VAL:HG22 | 4:B:1118:VAL:CG1  | 2.28                     | 0.61              |
| 5:N:505:ARG:HH22  | 5:N:532:GLU:CD    | 2.09                     | 0.61              |
| 4:B:1084:ARG:HD2  | 4:B:1089:VAL:HG12 | 1.82                     | 0.61              |
| 4:D:795:GLU:O     | 4:D:795:GLU:HG2   | 2.00                     | 0.61              |
| 5:M:418:SER:C     | 5:M:422:HIS:NE2   | 2.58                     | 0.61              |
| 5:N:411:LEU:H     | 5:N:412:VAL:HG22  | 1.66                     | 0.61              |
| 4:A:1161:VAL:CG2  | 4:A:1179:VAL:HG22 | 2.31                     | 0.60              |
| 4:D:1181:VAL:HG11 | 4:D:1185:ALA:HB3  | 1.84                     | 0.60              |
| 5:O:519:ARG:CB    | 5:O:520:LYS:HB2   | 2.31                     | 0.60              |
| 4:B:1032:LEU:HD22 | 4:B:1077:LEU:HD11 | 1.84                     | 0.60              |
| 4:B:1064:MET:HG2  | 4:B:1084:ARG:HH21 | 1.66                     | 0.60              |
| 4:B:1066:ALA:HB3  | 4:B:1084:ARG:NH2  | 2.15                     | 0.60              |
| 4:C:291:MET:CE    | 4:C:613:GLY:HA3   | 2.30                     | 0.60              |
| 4:D:549:MET:HE1   | 4:D:559:ILE:HG21  | 1.81                     | 0.60              |
| 4:C:299:PRO:HG2   | 4:C:300:LEU:N     | 2.16                     | 0.60              |
| 4:C:1081:VAL:HG13 | 4:C:1081:VAL:O    | 2.01                     | 0.60              |
| 5:O:450:LEU:CB    | 5:O:451:GLU:O     | 2.41                     | 0.60              |
| 5:O:450:LEU:HA    | 5:O:451:GLU:CB    | 2.30                     | 0.60              |
| 4:A:1080:VAL:HB   | 4:A:1082:PHE:N    | 2.15                     | 0.60              |
| 5:M:409:LYS:HB3   | 5:M:412:VAL:HG21  | 1.83                     | 0.60              |
| 5:P:409:LYS:CG    | 5:P:410:THR:H     | 2.10                     | 0.60              |
| 4:B:1054:VAL:CG2  | 4:B:1094:LYS:CD   | 2.79                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1032:LEU:HD11 | 4:A:1047:LEU:CD1  | 2.30                     | 0.60              |
| 4:D:507:VAL:CG1   | 4:D:558:VAL:HG13  | 2.31                     | 0.60              |
| 4:D:1204:VAL:HG22 | 4:D:1205:PHE:N    | 2.16                     | 0.60              |
| 5:M:421:PHE:HD2   | 5:M:422:HIS:CE1   | 2.18                     | 0.60              |
| 4:A:443:PRO:HA    | 4:A:448:LEU:HD12  | 1.83                     | 0.60              |
| 4:B:291:MET:HE3   | 4:B:613:GLY:HA2   | 1.84                     | 0.60              |
| 4:D:549:MET:CE    | 4:D:559:ILE:CG1   | 2.79                     | 0.60              |
| 5:M:499:ASP:HB3   | 5:M:500:PRO:HA    | 1.83                     | 0.60              |
| 4:A:1161:VAL:CG2  | 4:A:1179:VAL:CG2  | 2.80                     | 0.60              |
| 4:B:1054:VAL:CG2  | 4:B:1094:LYS:CE   | 2.80                     | 0.60              |
| 4:B:1056:ARG:CG   | 4:B:1057:LYS:CG   | 2.63                     | 0.60              |
| 4:D:537:GLU:C     | 4:D:540:GLN:CG    | 2.74                     | 0.60              |
| 4:D:1079:VAL:C    | 4:D:1081:VAL:HG23 | 2.26                     | 0.60              |
| 4:D:300:LEU:HD22  | 4:D:304:ARG:HB2   | 1.84                     | 0.59              |
| 4:D:1046:LEU:HD22 | 4:D:1205:PHE:CE2  | 2.36                     | 0.59              |
| 5:O:388:LEU:HD23  | 5:O:394:THR:CG2   | 2.32                     | 0.59              |
| 4:D:1209:ASN:O    | 4:D:1211:GLY:N    | 2.31                     | 0.59              |
| 4:B:774:VAL:HG12  | 4:B:775:GLU:HG3   | 1.83                     | 0.59              |
| 4:C:298:PHE:CG    | 4:C:299:PRO:CD    | 2.85                     | 0.59              |
| 4:D:537:GLU:CA    | 4:D:540:GLN:HG3   | 2.31                     | 0.59              |
| 4:C:970:ARG:HH21  | 4:C:975:LEU:CD1   | 2.15                     | 0.59              |
| 5:P:396:ARG:O     | 5:P:397:ALA:C     | 2.45                     | 0.59              |
| 5:P:397:ALA:HA    | 5:P:398:PHE:O     | 2.03                     | 0.59              |
| 4:A:1152:LEU:HD13 | 4:A:1179:VAL:HG21 | 1.83                     | 0.59              |
| 4:B:615:LEU:CD2   | 4:B:617:MET:HE2   | 2.28                     | 0.59              |
| 4:D:1067:ARG:HA   | 4:D:1081:VAL:HG22 | 1.84                     | 0.59              |
| 4:D:1204:VAL:O    | 4:D:1205:PHE:HD1  | 1.85                     | 0.59              |
| 5:N:525:GLU:HG3   | 5:N:528:GLU:O     | 2.01                     | 0.59              |
| 4:A:1165:VAL:CG1  | 4:A:1172:ALA:HB3  | 2.32                     | 0.59              |
| 4:B:747:ILE:HG23  | 4:B:805:LEU:HD22  | 1.84                     | 0.59              |
| 4:C:292:VAL:HG12  | 4:C:293:TYR:N     | 2.17                     | 0.59              |
| 5:P:413:LEU:HA    | 5:P:416:PRO:CG    | 2.32                     | 0.59              |
| 5:P:505:ARG:HG2   | 5:P:514:ARG:HH21  | 1.65                     | 0.59              |
| 2:F:9:DT:O4       | 4:A:511:TYR:HA    | 2.02                     | 0.59              |
| 4:C:839:PHE:CE2   | 4:C:843:LEU:HD11  | 2.38                     | 0.59              |
| 4:D:334:VAL:HG21  | 4:D:384:LEU:HD11  | 1.84                     | 0.59              |
| 5:O:450:LEU:CA    | 5:O:451:GLU:CB    | 2.77                     | 0.59              |
| 4:A:226:VAL:HG21  | 4:A:561:VAL:HG11  | 1.85                     | 0.59              |
| 4:B:389:TYR:O     | 4:B:393:VAL:HG23  | 2.02                     | 0.59              |
| 4:B:1013:HIS:CE1  | 4:B:1016:LEU:HD21 | 2.36                     | 0.59              |
| 4:C:57:TYR:CE2    | 4:C:287:ILE:HD11  | 2.38                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:450:LEU:HB3   | 5:M:451:GLU:C     | 2.28                     | 0.59              |
| 5:N:525:GLU:HG2   | 5:N:528:GLU:O     | 2.02                     | 0.59              |
| 5:N:529:PRO:CA    | 5:N:530:VAL:HB    | 2.33                     | 0.59              |
| 4:B:333:GLU:O     | 4:B:337:LEU:HD12  | 2.03                     | 0.59              |
| 4:D:300:LEU:HD22  | 4:D:304:ARG:CB    | 2.32                     | 0.59              |
| 4:D:501:LYS:HE3   | 4:D:505:LYS:HZ1   | 1.64                     | 0.59              |
| 5:O:519:ARG:CG    | 5:O:520:LYS:HB2   | 2.32                     | 0.59              |
| 4:A:1087:GLU:HG3  | 4:A:1088:GLY:HA3  | 1.83                     | 0.59              |
| 4:D:100:ALA:HB2   | 4:D:109:LEU:HD12  | 1.84                     | 0.59              |
| 5:O:389:GLU:HB2   | 5:O:445:GLU:HB3   | 1.85                     | 0.59              |
| 5:P:541:MET:C     | 5:P:541:MET:HE2   | 2.28                     | 0.59              |
| 4:A:555:ILE:C     | 4:A:555:ILE:HD12  | 2.28                     | 0.58              |
| 4:A:559:ILE:HG22  | 4:A:563:MET:HE3   | 1.83                     | 0.58              |
| 4:B:1084:ARG:HD2  | 4:B:1089:VAL:HG11 | 1.84                     | 0.58              |
| 4:C:975:LEU:HD23  | 4:C:976:VAL:N     | 2.18                     | 0.58              |
| 4:C:1207:GLN:HB3  | 4:C:1208:GLY:CA   | 2.32                     | 0.58              |
| 5:P:395:LEU:C     | 5:P:397:ALA:N     | 2.61                     | 0.58              |
| 4:A:1161:VAL:HG22 | 4:A:1179:VAL:HG22 | 1.84                     | 0.58              |
| 4:B:976:VAL:HG21  | 4:C:115:ARG:CZ    | 2.34                     | 0.58              |
| 4:C:298:PHE:CG    | 4:C:299:PRO:HD2   | 2.37                     | 0.58              |
| 4:D:1166:LEU:HD12 | 4:D:1166:LEU:O    | 2.02                     | 0.58              |
| 4:B:233:LYS:HG2   | 4:B:510:VAL:HG11  | 1.85                     | 0.58              |
| 4:C:291:MET:HE1   | 4:C:613:GLY:HA3   | 1.84                     | 0.58              |
| 4:C:428:ALA:HB3   | 4:C:816:SER:HB2   | 1.85                     | 0.58              |
| 4:D:1081:VAL:O    | 4:D:1081:VAL:HG12 | 2.02                     | 0.58              |
| 5:M:389:GLU:O     | 5:M:390:ALA:CB    | 2.49                     | 0.58              |
| 5:N:450:LEU:HB3   | 5:N:451:GLU:HB2   | 1.85                     | 0.58              |
| 5:O:395:LEU:CB    | 5:O:396:ARG:HB2   | 2.34                     | 0.58              |
| 5:M:524:PRO:N     | 5:M:525:GLU:HA    | 2.18                     | 0.58              |
| 5:P:456:SER:N     | 5:P:457:GLY:HA2   | 2.18                     | 0.58              |
| 4:A:639:LYS:O     | 4:A:641:VAL:HG23  | 2.03                     | 0.58              |
| 4:A:1093:LEU:HD13 | 4:A:1099:LEU:HG   | 1.85                     | 0.58              |
| 4:A:181:ILE:CD1   | 4:A:207:MET:HE3   | 2.34                     | 0.58              |
| 4:A:669:GLN:HE22  | 4:A:821:TYR:HB3   | 1.69                     | 0.58              |
| 4:C:1165:VAL:O    | 4:C:1165:VAL:HG13 | 2.04                     | 0.58              |
| 4:D:1119:TRP:CZ2  | 4:D:1206:LEU:HA   | 2.38                     | 0.58              |
| 5:M:412:VAL:O     | 5:M:414:ARG:N     | 2.37                     | 0.58              |
| 5:P:413:LEU:O     | 5:P:417:GLU:HB2   | 2.03                     | 0.58              |
| 4:C:290:LYS:O     | 4:C:291:MET:HG3   | 2.03                     | 0.58              |
| 4:D:1082:PHE:HZ   | 4:D:1114:LEU:CA   | 2.16                     | 0.58              |
| 5:M:421:PHE:CE2   | 5:M:422:HIS:CE1   | 2.91                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:N:395:LEU:HA    | 5:N:396:ARG:CB    | 2.29                     | 0.58              |
| 5:N:406:LEU:HD22  | 5:N:419:LYS:HG2   | 1.86                     | 0.58              |
| 5:P:493:GLU:O     | 5:P:504:LEU:HD13  | 2.04                     | 0.58              |
| 4:B:461:MET:HE1   | 4:B:615:LEU:HA    | 1.86                     | 0.58              |
| 4:C:659:LEU:HD11  | 4:C:829:ALA:CB    | 2.33                     | 0.58              |
| 5:P:524:PRO:HG2   | 5:P:526:ALA:HB2   | 1.86                     | 0.58              |
| 5:P:529:PRO:CB    | 5:P:530:VAL:HA    | 2.30                     | 0.58              |
| 4:C:1051:VAL:HG12 | 4:C:1068:PHE:CD1  | 2.39                     | 0.57              |
| 5:M:421:PHE:CD2   | 5:M:422:HIS:N     | 2.72                     | 0.57              |
| 5:P:456:SER:H     | 5:P:457:GLY:CA    | 2.17                     | 0.57              |
| 4:A:1093:LEU:HD23 | 4:A:1094:LYS:O    | 2.04                     | 0.57              |
| 4:A:1204:VAL:HG12 | 4:A:1205:PHE:H    | 1.69                     | 0.57              |
| 4:C:418:VAL:HG13  | 4:C:472:GLU:HB2   | 1.85                     | 0.57              |
| 4:C:1129:LYS:HE2  | 4:C:1198:LEU:HD21 | 1.86                     | 0.57              |
| 4:D:285:LEU:O     | 4:D:287:ILE:N     | 2.37                     | 0.57              |
| 5:M:408:GLY:HA3   | 5:M:415:PHE:CD1   | 2.35                     | 0.57              |
| 5:O:529:PRO:HA    | 5:O:530:VAL:HB    | 1.86                     | 0.57              |
| 4:A:32:VAL:HG21   | 4:A:42:LEU:HD22   | 1.86                     | 0.57              |
| 4:A:1080:VAL:CG2  | 4:A:1114:LEU:CA   | 2.70                     | 0.57              |
| 4:B:1067:ARG:CA   | 4:B:1081:VAL:HG21 | 2.32                     | 0.57              |
| 5:N:518:VAL:HG22  | 5:N:519:ARG:HG3   | 1.86                     | 0.57              |
| 4:D:1201:ASP:O    | 4:D:1204:VAL:HG12 | 2.03                     | 0.57              |
| 5:M:419:LYS:CA    | 5:M:422:HIS:CD2   | 2.84                     | 0.57              |
| 5:O:453:LYS:O     | 5:O:454:SER:HB3   | 2.04                     | 0.57              |
| 4:A:307:ALA:HB1   | 4:A:395:GLU:HG2   | 1.86                     | 0.57              |
| 4:B:1056:ARG:HG3  | 4:B:1057:LYS:CD   | 2.34                     | 0.57              |
| 4:C:541:VAL:N     | 4:C:542:VAL:HG13  | 2.19                     | 0.57              |
| 4:D:951:ALA:HB2   | 4:D:993:LEU:HG    | 1.86                     | 0.57              |
| 5:M:523:ALA:HB1   | 5:M:524:PRO:HA    | 1.87                     | 0.57              |
| 5:O:490:PRO:HD2   | 5:O:522:LYS:HD2   | 1.86                     | 0.57              |
| 4:A:1204:VAL:HG12 | 4:A:1205:PHE:N    | 2.20                     | 0.57              |
| 4:C:1161:VAL:CG1  | 4:C:1176:LEU:CD2  | 2.83                     | 0.57              |
| 4:B:354:LEU:O     | 4:B:362:TRP:CH2   | 2.58                     | 0.57              |
| 4:D:418:VAL:HG13  | 4:D:472:GLU:HB2   | 1.85                     | 0.57              |
| 4:D:1212:GLY:O    | 4:D:1216:GLU:HG2  | 2.04                     | 0.57              |
| 5:M:524:PRO:HG2   | 5:M:526:ALA:CB    | 2.35                     | 0.57              |
| 5:O:403:ARG:HE    | 5:O:437:ALA:HB3   | 1.70                     | 0.57              |
| 4:B:525:ILE:HD11  | 4:B:538:ALA:HB2   | 1.86                     | 0.57              |
| 4:D:159:LEU:HD22  | 4:D:195:VAL:HG11  | 1.86                     | 0.57              |
| 4:D:1119:TRP:CZ2  | 4:D:1206:LEU:CA   | 2.88                     | 0.57              |
| 4:D:1144:GLY:HA2  | 4:D:1145:VAL:HG13 | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:403:ARG:HE    | 5:M:437:ALA:HB3   | 1.70                     | 0.57              |
| 1:E:20:DA:N6      | 4:A:510:VAL:O     | 2.38                     | 0.57              |
| 4:B:28:LEU:HD11   | 4:B:251:VAL:HG21  | 1.86                     | 0.57              |
| 4:B:357:VAL:CG1   | 4:B:358:GLU:CG    | 2.75                     | 0.57              |
| 4:D:935:LEU:O     | 4:D:939:VAL:HG23  | 2.05                     | 0.57              |
| 5:M:406:LEU:HA    | 5:M:419:LYS:HG2   | 1.86                     | 0.57              |
| 5:M:523:ALA:CB    | 5:M:524:PRO:CA    | 2.83                     | 0.57              |
| 4:D:1055:VAL:HG21 | 4:D:1067:ARG:C    | 2.29                     | 0.57              |
| 5:M:392:LYS:HG2   | 5:M:397:ALA:HB2   | 1.87                     | 0.57              |
| 4:D:226:VAL:HG12  | 4:D:510:VAL:HG11  | 1.86                     | 0.56              |
| 5:P:493:GLU:HB2   | 5:P:494:ALA:HA    | 1.86                     | 0.56              |
| 5:P:539:GLY:HA2   | 5:P:542:PRO:HD2   | 1.86                     | 0.56              |
| 4:A:386:ARG:NH1   | 4:A:390:GLU:OE1   | 2.38                     | 0.56              |
| 4:A:590:VAL:HG11  | 4:A:602:THR:HG23  | 1.87                     | 0.56              |
| 4:B:490:ALA:O     | 4:B:580:VAL:HG12  | 2.05                     | 0.56              |
| 4:D:444:LEU:HD12  | 4:D:445:ARG:N     | 2.21                     | 0.56              |
| 5:M:413:LEU:CA    | 5:M:416:PRO:HD2   | 2.35                     | 0.56              |
| 5:O:395:LEU:N     | 5:O:396:ARG:O     | 2.37                     | 0.56              |
| 5:O:518:VAL:HA    | 5:O:519:ARG:HG3   | 1.88                     | 0.56              |
| 4:C:331:TYR:CD2   | 4:C:354:LEU:HD11  | 2.40                     | 0.56              |
| 4:C:1159:LEU:HD11 | 4:C:1183:GLU:HG3  | 1.88                     | 0.56              |
| 4:D:67:PRO:O      | 4:D:68:ILE:HD13   | 2.04                     | 0.56              |
| 4:D:106:TYR:O     | 4:D:110:VAL:HG23  | 2.04                     | 0.56              |
| 4:D:181:ILE:HD12  | 4:D:207:MET:CE    | 2.30                     | 0.56              |
| 4:D:975:LEU:CB    | 4:D:980:ALA:HB2   | 2.35                     | 0.56              |
| 4:D:1032:LEU:HD12 | 4:D:1047:LEU:HD11 | 1.87                     | 0.56              |
| 4:D:1055:VAL:HB   | 4:D:1066:ALA:HB1  | 1.88                     | 0.56              |
| 5:O:530:VAL:HG13  | 5:O:530:VAL:O     | 2.05                     | 0.56              |
| 5:P:392:LYS:N     | 5:P:393:PRO:HD3   | 2.20                     | 0.56              |
| 4:B:132:LEU:O     | 4:B:136:ALA:HB2   | 2.05                     | 0.56              |
| 4:B:235:THR:HG22  | 4:B:236:LEU:H     | 1.70                     | 0.56              |
| 4:C:1080:VAL:HB   | 4:C:1081:VAL:C    | 2.29                     | 0.56              |
| 5:O:402:ALA:O     | 5:O:406:LEU:HD13  | 2.05                     | 0.56              |
| 5:P:389:GLU:HG2   | 5:P:393:PRO:HG2   | 1.87                     | 0.56              |
| 5:P:450:LEU:HB3   | 5:P:451:GLU:C     | 2.30                     | 0.56              |
| 4:B:1056:ARG:C    | 4:B:1057:LYS:HG3  | 2.26                     | 0.56              |
| 5:N:505:ARG:HD2   | 5:N:510:LEU:CB    | 2.26                     | 0.56              |
| 5:P:540:ILE:O     | 5:P:543:PRO:HD3   | 2.04                     | 0.56              |
| 4:B:357:VAL:CB    | 4:B:358:GLU:CG    | 2.84                     | 0.56              |
| 5:M:506:ARG:HA    | 5:M:510:LEU:CD2   | 2.33                     | 0.56              |
| 5:N:455:LEU:HA    | 5:N:456:SER:C     | 2.30                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:54:VAL:HG11   | 4:D:608:ALA:HB1   | 1.87                     | 0.56              |
| 4:D:535:LEU:O     | 4:D:539:ILE:HG12  | 2.06                     | 0.56              |
| 5:N:494:ALA:HB1   | 5:N:495:GLU:C     | 2.30                     | 0.56              |
| 5:P:399:VAL:HG11  | 5:P:441:PHE:CZ    | 2.40                     | 0.56              |
| 4:A:737:THR:HG21  | 4:A:746:GLN:HE22  | 1.69                     | 0.56              |
| 4:D:192:VAL:HG12  | 4:D:196:LEU:CD1   | 2.35                     | 0.56              |
| 4:D:287:ILE:O     | 4:D:290:LYS:HG3   | 2.05                     | 0.56              |
| 4:A:1080:VAL:HG22 | 4:A:1113:VAL:O    | 2.05                     | 0.56              |
| 4:D:188:GLU:O     | 4:D:192:VAL:HG23  | 2.06                     | 0.56              |
| 4:D:1080:VAL:HG12 | 4:D:1081:VAL:HB   | 1.87                     | 0.56              |
| 4:D:1205:PHE:CE1  | 4:D:1206:LEU:CD1  | 2.89                     | 0.56              |
| 5:P:525:GLU:O     | 5:P:526:ALA:HB3   | 2.06                     | 0.56              |
| 4:D:397:MET:HE2   | 4:D:399:PHE:HE1   | 1.70                     | 0.56              |
| 5:O:392:LYS:HD2   | 5:O:397:ALA:HB3   | 1.88                     | 0.56              |
| 4:C:295:ILE:HG23  | 4:C:295:ILE:O     | 2.05                     | 0.55              |
| 4:D:1204:VAL:HG22 | 4:D:1205:PHE:H    | 1.71                     | 0.55              |
| 5:N:504:LEU:HD13  | 5:N:535:ILE:HD12  | 1.88                     | 0.55              |
| 5:O:506:ARG:O     | 5:O:510:LEU:HB2   | 2.06                     | 0.55              |
| 5:P:518:VAL:HA    | 5:P:519:ARG:HG3   | 1.87                     | 0.55              |
| 4:A:300:LEU:N     | 4:A:301:PRO:CD    | 2.70                     | 0.55              |
| 5:N:505:ARG:HD2   | 5:N:510:LEU:HD23  | 1.78                     | 0.55              |
| 5:N:529:PRO:HA    | 5:N:530:VAL:HB    | 1.88                     | 0.55              |
| 4:C:351:ALA:HA    | 4:C:354:LEU:HD12  | 1.87                     | 0.55              |
| 5:N:395:LEU:HD23  | 5:N:396:ARG:CB    | 2.36                     | 0.55              |
| 5:N:529:PRO:CB    | 5:N:530:VAL:HB    | 2.36                     | 0.55              |
| 4:A:399:PHE:N     | 4:A:400:PRO:CD    | 2.70                     | 0.55              |
| 4:A:1133:VAL:HG13 | 4:A:1163:LEU:HD12 | 1.88                     | 0.55              |
| 5:P:451:GLU:O     | 5:P:452:LYS:HB2   | 2.07                     | 0.55              |
| 5:P:504:LEU:CB    | 5:P:505:ARG:HG2   | 2.36                     | 0.55              |
| 4:B:1024:VAL:O    | 4:B:1025:ALA:C    | 2.49                     | 0.55              |
| 4:C:590:VAL:HG11  | 4:C:602:THR:CG2   | 2.37                     | 0.55              |
| 4:D:975:LEU:HB3   | 4:D:980:ALA:HB2   | 1.88                     | 0.55              |
| 4:D:1102:LEU:CD1  | 4:D:1206:LEU:CG   | 2.82                     | 0.55              |
| 5:N:510:LEU:O     | 5:N:511:LEU:C     | 2.49                     | 0.55              |
| 4:A:980:ALA:C     | 4:A:981:GLU:CG    | 2.79                     | 0.55              |
| 4:B:1123:GLU:HG2  | 4:B:1216:GLU:HB3  | 1.88                     | 0.55              |
| 4:D:286:PRO:HA    | 4:D:290:LYS:HB2   | 1.89                     | 0.55              |
| 4:D:500:SER:HB3   | 4:D:535:LEU:HD12  | 1.86                     | 0.55              |
| 4:D:1051:VAL:HG21 | 4:D:1093:LEU:CD2  | 2.37                     | 0.55              |
| 5:P:499:ASP:HB3   | 5:P:515:LEU:CD2   | 2.37                     | 0.55              |
| 4:B:569:ASN:O     | 4:B:570:ARG:HB3   | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1093:LEU:HD22 | 4:B:1099:LEU:HG   | 1.89                     | 0.55              |
| 4:C:1079:VAL:HG12 | 4:C:1080:VAL:N    | 2.22                     | 0.55              |
| 4:C:1093:LEU:CD1  | 4:C:1097:ILE:HB   | 2.34                     | 0.55              |
| 5:M:535:ILE:O     | 5:M:538:ASN:HB3   | 2.07                     | 0.55              |
| 4:B:1056:ARG:CG   | 4:B:1057:LYS:CD   | 2.84                     | 0.55              |
| 4:D:664:THR:HG21  | 4:D:670:LEU:HD13  | 1.89                     | 0.55              |
| 4:D:1080:VAL:C    | 4:D:1081:VAL:CG2  | 2.74                     | 0.55              |
| 5:O:505:ARG:HH12  | 5:O:506:ARG:NH1   | 2.05                     | 0.55              |
| 5:P:529:PRO:HB2   | 5:P:530:VAL:CA    | 2.32                     | 0.55              |
| 1:G:19:DC:N4      | 2:H:10:DG:C6      | 2.75                     | 0.54              |
| 4:C:307:ALA:HB1   | 4:C:395:GLU:CD    | 2.32                     | 0.54              |
| 4:C:788:ALA:HB1   | 4:C:793:VAL:HG21  | 1.89                     | 0.54              |
| 5:P:498:GLU:HB2   | 5:P:499:ASP:HA    | 1.90                     | 0.54              |
| 4:A:170:LEU:HD21  | 4:A:205:LEU:HD22  | 1.89                     | 0.54              |
| 4:D:982:VAL:HG13  | 4:D:982:VAL:O     | 2.07                     | 0.54              |
| 5:M:394:THR:O     | 5:M:394:THR:HG22  | 2.06                     | 0.54              |
| 5:P:493:GLU:O     | 5:P:504:LEU:CD1   | 2.55                     | 0.54              |
| 4:A:970:ARG:O     | 4:A:974:GLY:O     | 2.24                     | 0.54              |
| 4:A:1177:ARG:O    | 4:A:1179:VAL:HG13 | 2.07                     | 0.54              |
| 4:B:670:LEU:HD12  | 4:B:675:MET:CG    | 2.37                     | 0.54              |
| 4:B:696:LEU:HD21  | 4:B:742:VAL:HG22  | 1.89                     | 0.54              |
| 4:B:1099:LEU:HD22 | 4:B:1118:VAL:HG22 | 1.90                     | 0.54              |
| 4:B:1053:GLU:HB3  | 4:B:1068:PHE:HA   | 1.89                     | 0.54              |
| 4:C:154:ILE:CD1   | 4:C:195:VAL:HB    | 2.33                     | 0.54              |
| 5:M:419:LYS:O     | 5:M:423:HIS:CD2   | 2.60                     | 0.54              |
| 4:A:1013:HIS:CD2  | 4:A:1015:VAL:HG12 | 2.42                     | 0.54              |
| 4:B:951:ALA:HB2   | 4:B:993:LEU:HG    | 1.90                     | 0.54              |
| 5:M:541:MET:O     | 5:M:543:PRO:HD2   | 2.08                     | 0.54              |
| 4:A:918:LEU:HD22  | 4:A:953:LEU:CD2   | 2.38                     | 0.54              |
| 4:A:1080:VAL:HG23 | 4:A:1114:LEU:HA   | 1.81                     | 0.54              |
| 4:C:723:PHE:HB3   | 4:C:726:ALA:HB3   | 1.88                     | 0.54              |
| 4:D:287:ILE:HG22  | 4:D:288:GLY:N     | 2.22                     | 0.54              |
| 4:D:1218:VAL:HB   | 4:D:1219:PRO:HD3  | 1.88                     | 0.54              |
| 4:B:410:ILE:HG23  | 4:B:420:VAL:HG11  | 1.88                     | 0.54              |
| 4:C:146:LEU:HD11  | 4:C:189:GLN:HG2   | 1.90                     | 0.54              |
| 4:D:1087:GLU:HB3  | 4:D:1088:GLY:HA3  | 1.88                     | 0.54              |
| 4:C:1093:LEU:O    | 4:C:1094:LYS:HB2  | 2.08                     | 0.54              |
| 4:D:1057:LYS:CB   | 4:D:1058:PRO:CA   | 2.83                     | 0.54              |
| 4:B:1058:PRO:HG2  | 4:B:1059:THR:N    | 2.22                     | 0.54              |
| 4:C:854:VAL:HG23  | 4:C:1008:ILE:HG21 | 1.89                     | 0.54              |
| 5:M:519:ARG:HD3   | 5:M:520:LYS:HE3   | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:417:GLU:O     | 5:P:418:SER:C     | 2.51                     | 0.54              |
| 4:C:287:ILE:CA    | 4:C:291:MET:HB3   | 2.27                     | 0.54              |
| 4:C:854:VAL:CG2   | 4:C:1008:ILE:HG21 | 2.38                     | 0.54              |
| 4:C:1205:PHE:O    | 4:C:1206:LEU:HG   | 2.08                     | 0.54              |
| 4:D:154:ILE:C     | 4:D:154:ILE:HD12  | 2.33                     | 0.54              |
| 4:D:1080:VAL:CG2  | 4:D:1115:ALA:H    | 2.21                     | 0.54              |
| 5:P:541:MET:C     | 5:P:543:PRO:HD3   | 2.33                     | 0.54              |
| 3:I:20:DA:C2      | 3:I:21:DOC:C2     | 2.91                     | 0.53              |
| 4:A:1099:LEU:HD13 | 4:A:1118:VAL:HG11 | 1.90                     | 0.53              |
| 4:D:549:MET:CE    | 4:D:559:ILE:HG21  | 2.38                     | 0.53              |
| 4:D:589:LEU:HG    | 4:D:612:LEU:HD21  | 1.90                     | 0.53              |
| 4:D:672:SER:O     | 4:D:676:THR:HG23  | 2.08                     | 0.53              |
| 4:D:1095:GLU:O    | 4:D:1097:ILE:HD12 | 2.08                     | 0.53              |
| 5:O:390:ALA:C     | 5:O:393:PRO:HG2   | 2.33                     | 0.53              |
| 4:A:951:ALA:HB2   | 4:A:993:LEU:HD21  | 1.90                     | 0.53              |
| 4:B:1080:VAL:HA   | 4:B:1081:VAL:CB   | 2.37                     | 0.53              |
| 4:D:546:ARG:NH1   | 4:D:550:GLU:OE2   | 2.41                     | 0.53              |
| 4:D:1159:LEU:HD21 | 4:D:1183:GLU:HG2  | 1.90                     | 0.53              |
| 4:B:590:VAL:HG13  | 4:B:604:TYR:CD1   | 2.43                     | 0.53              |
| 4:B:1057:LYS:CB   | 4:B:1058:PRO:CA   | 2.84                     | 0.53              |
| 4:C:28:LEU:HD11   | 4:C:251:VAL:HG21  | 1.90                     | 0.53              |
| 4:C:631:ALA:O     | 4:C:635:VAL:HG23  | 2.08                     | 0.53              |
| 5:N:395:LEU:HD23  | 5:N:396:ARG:CD    | 2.38                     | 0.53              |
| 4:B:308:GLN:HE21  | 4:B:356:ARG:HA    | 1.74                     | 0.53              |
| 4:D:28:LEU:CD1    | 4:D:251:VAL:HG21  | 2.39                     | 0.53              |
| 4:D:535:LEU:O     | 4:D:538:ALA:HB3   | 2.08                     | 0.53              |
| 4:D:788:ALA:HB1   | 4:D:793:VAL:CG2   | 2.38                     | 0.53              |
| 4:A:170:LEU:HD21  | 4:A:205:LEU:CD2   | 2.38                     | 0.53              |
| 4:B:358:GLU:C     | 4:B:362:TRP:CD1   | 2.86                     | 0.53              |
| 4:C:1051:VAL:HG22 | 4:C:1097:ILE:O    | 2.07                     | 0.53              |
| 4:D:1089:VAL:HG12 | 4:D:1091:PRO:HD3  | 1.89                     | 0.53              |
| 4:D:1144:GLY:HA2  | 4:D:1145:VAL:CG1  | 2.38                     | 0.53              |
| 4:D:1205:PHE:CD1  | 4:D:1206:LEU:CD1  | 2.85                     | 0.53              |
| 5:P:494:ALA:HB1   | 5:P:495:GLU:C     | 2.34                     | 0.53              |
| 4:A:691:ILE:HG22  | 4:A:743:TYR:OH    | 2.09                     | 0.53              |
| 4:A:1067:ARG:N    | 4:A:1081:VAL:CG2  | 2.67                     | 0.53              |
| 4:D:115:ARG:NH1   | 4:D:131:ILE:HD12  | 2.23                     | 0.53              |
| 4:A:257:MET:HE2   | 4:A:257:MET:HA    | 1.90                     | 0.53              |
| 4:A:319:LEU:HD23  | 4:A:326:ILE:O     | 2.08                     | 0.53              |
| 4:A:459:VAL:HG13  | 4:A:459:VAL:O     | 2.09                     | 0.53              |
| 4:B:257:MET:HA    | 4:B:257:MET:HE2   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:252:LYS:HD2   | 4:B:257:MET:HE3   | 1.90                     | 0.53              |
| 4:C:513:ILE:HG23  | 4:C:517:LYS:NZ    | 2.24                     | 0.53              |
| 4:C:541:VAL:N     | 4:C:542:VAL:HG22  | 2.23                     | 0.53              |
| 4:B:319:LEU:HD23  | 4:B:319:LEU:O     | 2.08                     | 0.53              |
| 5:O:409:LYS:HD3   | 5:O:412:VAL:HG21  | 1.91                     | 0.53              |
| 4:C:318:LEU:HD12  | 4:C:435:ALA:HB1   | 1.91                     | 0.53              |
| 4:C:570:ARG:C     | 4:C:571:HIS:CG    | 2.87                     | 0.53              |
| 5:M:396:ARG:CB    | 5:M:397:ALA:HB3   | 2.39                     | 0.53              |
| 5:N:378:GLN:HA    | 5:N:381:ALA:HB3   | 1.91                     | 0.53              |
| 5:O:416:PRO:HB3   | 5:O:436:LEU:HD21  | 1.91                     | 0.53              |
| 5:O:453:LYS:O     | 5:O:454:SER:CB    | 2.56                     | 0.53              |
| 4:B:230:ILE:HG12  | 4:B:507:VAL:HG13  | 1.91                     | 0.52              |
| 4:B:1181:VAL:CG1  | 4:B:1185:ALA:HB3  | 2.38                     | 0.52              |
| 4:C:1129:LYS:O    | 4:C:1159:LEU:HD22 | 2.10                     | 0.52              |
| 4:D:952:ARG:HD3   | 4:D:987:LEU:HD23  | 1.91                     | 0.52              |
| 4:D:1205:PHE:O    | 4:D:1206:LEU:HD12 | 2.09                     | 0.52              |
| 4:A:1121:LEU:HD11 | 4:A:1125:LEU:HD11 | 1.90                     | 0.52              |
| 4:C:54:VAL:HG23   | 4:C:604:TYR:CE2   | 2.45                     | 0.52              |
| 4:C:1081:VAL:HG23 | 4:C:1084:ARG:HB3  | 1.91                     | 0.52              |
| 4:D:148:ALA:HB3   | 4:D:151:PRO:CG    | 2.38                     | 0.52              |
| 4:D:158:ARG:HG2   | 4:D:161:LEU:HD22  | 1.91                     | 0.52              |
| 5:N:505:ARG:CD    | 5:N:510:LEU:CD2   | 2.75                     | 0.52              |
| 4:A:952:ARG:HD3   | 4:A:987:LEU:HD23  | 1.90                     | 0.52              |
| 4:A:1080:VAL:CA   | 4:A:1081:VAL:HB   | 2.21                     | 0.52              |
| 4:C:970:ARG:HE    | 4:C:975:LEU:HD13  | 1.74                     | 0.52              |
| 4:C:1213:PRO:O    | 4:C:1217:VAL:HG23 | 2.09                     | 0.52              |
| 4:D:307:ALA:HB1   | 4:D:395:GLU:CD    | 2.34                     | 0.52              |
| 4:D:498:LEU:HD22  | 4:D:570:ARG:HH21  | 1.74                     | 0.52              |
| 4:D:1065:MET:HG3  | 4:D:1081:VAL:O    | 2.09                     | 0.52              |
| 5:N:512:GLY:HA2   | 5:N:515:LEU:HD13  | 1.91                     | 0.52              |
| 5:O:538:ASN:HA    | 5:O:541:MET:HE3   | 1.92                     | 0.52              |
| 5:P:542:PRO:C     | 5:P:543:PRO:OXT   | 2.51                     | 0.52              |
| 2:F:24:DT:H1'     | 2:F:25:DT:H5''    | 1.90                     | 0.52              |
| 4:A:1135:VAL:HG21 | 4:A:1163:LEU:HD11 | 1.91                     | 0.52              |
| 4:B:1013:HIS:HB3  | 4:B:1014:PRO:CA   | 2.37                     | 0.52              |
| 5:M:403:ARG:HG2   | 5:M:437:ALA:HB1   | 1.92                     | 0.52              |
| 4:A:332:ARG:HG3   | 4:A:350:LEU:HD21  | 1.90                     | 0.52              |
| 4:A:951:ALA:HB2   | 4:A:993:LEU:HG    | 1.92                     | 0.52              |
| 4:C:970:ARG:NH2   | 4:C:975:LEU:CD1   | 2.73                     | 0.52              |
| 4:C:1129:LYS:CE   | 4:C:1198:LEU:HD21 | 2.40                     | 0.52              |
| 4:D:788:ALA:HB1   | 4:D:793:VAL:HG21  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:N:455:LEU:N     | 5:N:456:SER:CB    | 2.72                     | 0.52              |
| 5:O:521:PRO:HD2   | 5:O:522:LYS:H     | 1.73                     | 0.52              |
| 4:A:154:ILE:HD13  | 4:A:195:VAL:HB    | 1.92                     | 0.52              |
| 4:A:569:ASN:HA    | 4:A:570:ARG:CB    | 2.34                     | 0.52              |
| 4:A:574:VAL:CG1   | 4:A:575:HIS:N     | 2.73                     | 0.52              |
| 4:C:1086:TYR:HB2  | 4:C:1087:GLU:C    | 2.35                     | 0.52              |
| 4:D:1051:VAL:HB   | 4:D:1093:LEU:HD23 | 1.92                     | 0.52              |
| 4:A:1016:LEU:HD23 | 4:A:1022:ARG:HD2  | 1.92                     | 0.52              |
| 4:B:1122:GLU:OE2  | 5:N:530:VAL:HG11  | 2.09                     | 0.52              |
| 4:C:1093:LEU:CD1  | 4:C:1097:ILE:CG2  | 2.71                     | 0.52              |
| 4:C:1166:LEU:O    | 4:C:1166:LEU:HD12 | 2.10                     | 0.52              |
| 4:D:112:LEU:CD2   | 4:D:131:ILE:HG22  | 2.38                     | 0.52              |
| 5:M:385:ARG:HB2   | 5:M:386:ALA:HA    | 1.91                     | 0.52              |
| 5:N:508:ALA:HB1   | 5:N:509:ARG:C     | 2.35                     | 0.52              |
| 5:P:499:ASP:HB3   | 5:P:515:LEU:HD21  | 1.92                     | 0.52              |
| 5:P:524:PRO:N     | 5:P:525:GLU:CA    | 2.73                     | 0.52              |
| 4:A:424:ARG:CZ    | 4:A:620:LEU:HD22  | 2.39                     | 0.52              |
| 4:B:1055:VAL:O    | 4:B:1066:ALA:HB2  | 2.08                     | 0.52              |
| 5:O:395:LEU:HB2   | 5:O:396:ARG:O     | 2.09                     | 0.52              |
| 4:A:1081:VAL:O    | 4:A:1081:VAL:HG12 | 2.09                     | 0.52              |
| 4:C:574:VAL:HG12  | 4:C:575:HIS:O     | 2.09                     | 0.52              |
| 4:C:1182:GLY:O    | 4:C:1183:GLU:HB2  | 2.10                     | 0.52              |
| 5:M:505:ARG:CB    | 5:M:506:ARG:CA    | 2.82                     | 0.52              |
| 5:M:524:PRO:HG2   | 5:M:526:ALA:HB3   | 1.92                     | 0.52              |
| 5:N:524:PRO:CB    | 5:N:525:GLU:CA    | 2.86                     | 0.52              |
| 4:A:561:VAL:O     | 4:A:565:LEU:HD13  | 2.10                     | 0.52              |
| 4:A:1051:VAL:HB   | 4:A:1093:LEU:HD22 | 1.92                     | 0.52              |
| 4:A:1159:LEU:HD11 | 4:A:1180:ARG:HD2  | 1.92                     | 0.52              |
| 4:B:260:MET:HE2   | 4:B:260:MET:HA    | 1.92                     | 0.52              |
| 4:D:1102:LEU:HD11 | 4:D:1206:LEU:HG   | 1.87                     | 0.52              |
| 5:N:395:LEU:CA    | 5:N:396:ARG:HB2   | 2.31                     | 0.52              |
| 5:P:504:LEU:CB    | 5:P:505:ARG:HA    | 2.36                     | 0.52              |
| 1:E:15:DG:O6      | 2:F:13:DA:N6      | 2.43                     | 0.51              |
| 4:D:537:GLU:HB3   | 4:D:540:GLN:NE2   | 2.26                     | 0.51              |
| 4:D:1152:LEU:HD22 | 4:D:1181:VAL:HG21 | 1.92                     | 0.51              |
| 5:O:519:ARG:HB3   | 5:O:520:LYS:CB    | 2.40                     | 0.51              |
| 4:B:1147:ARG:HG3  | 4:B:1148:LEU:HD12 | 1.92                     | 0.51              |
| 4:C:292:VAL:CG1   | 4:C:293:TYR:N     | 2.73                     | 0.51              |
| 5:M:415:PHE:HB2   | 5:M:416:PRO:CD    | 2.41                     | 0.51              |
| 4:A:291:MET:HG2   | 4:A:291:MET:O     | 2.10                     | 0.51              |
| 4:A:971:GLY:HA2   | 4:A:975:LEU:HB2   | 1.85                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1214:LYS:O    | 4:A:1218:VAL:HG23 | 2.09                     | 0.51              |
| 4:C:293:TYR:N     | 4:C:293:TYR:CD1   | 2.78                     | 0.51              |
| 5:M:535:ILE:CG2   | 5:M:536:GLY:N     | 2.72                     | 0.51              |
| 5:O:407:GLU:OE1   | 5:O:436:LEU:HD22  | 2.10                     | 0.51              |
| 4:B:1056:ARG:CZ   | 4:B:1056:ARG:HB2  | 2.38                     | 0.51              |
| 4:C:293:TYR:N     | 4:C:293:TYR:HD1   | 2.07                     | 0.51              |
| 4:C:399:PHE:N     | 4:C:400:PRO:CD    | 2.74                     | 0.51              |
| 4:C:813:PHE:CE2   | 4:C:818:ALA:HB2   | 2.45                     | 0.51              |
| 4:D:1120:THR:HG22 | 4:D:1121:LEU:H    | 1.76                     | 0.51              |
| 5:P:416:PRO:HG2   | 5:P:417:GLU:H     | 1.75                     | 0.51              |
| 4:A:795:GLU:O     | 4:A:795:GLU:HG2   | 2.10                     | 0.51              |
| 4:B:357:VAL:HB    | 4:B:358:GLU:CG    | 2.41                     | 0.51              |
| 4:B:1016:LEU:C    | 4:B:1016:LEU:HD12 | 2.36                     | 0.51              |
| 4:C:301:PRO:HB2   | 4:C:302:GLU:CB    | 2.38                     | 0.51              |
| 4:D:1057:LYS:CE   | 4:D:1064:MET:N    | 2.71                     | 0.51              |
| 4:D:1159:LEU:CD2  | 4:D:1183:GLU:CG   | 2.88                     | 0.51              |
| 4:B:690:ILE:O     | 4:B:694:VAL:HG23  | 2.10                     | 0.51              |
| 4:B:982:VAL:O     | 4:B:982:VAL:HG13  | 2.11                     | 0.51              |
| 4:D:1152:LEU:HB3  | 4:D:1179:VAL:HG11 | 1.93                     | 0.51              |
| 5:N:505:ARG:HB3   | 5:N:506:ARG:HA    | 1.89                     | 0.51              |
| 5:N:508:ALA:CA    | 5:N:510:LEU:N     | 2.67                     | 0.51              |
| 5:P:539:GLY:HA2   | 5:P:542:PRO:CD    | 2.41                     | 0.51              |
| 5:P:541:MET:O     | 5:P:541:MET:HE3   | 2.10                     | 0.51              |
| 4:B:407:GLN:HG3   | 4:B:436:VAL:HG12  | 1.92                     | 0.51              |
| 4:B:1027:CYS:O    | 4:B:1047:LEU:HD13 | 2.11                     | 0.51              |
| 4:B:1151:LEU:HD12 | 4:B:1152:LEU:CD1  | 2.41                     | 0.51              |
| 4:C:54:VAL:HG23   | 4:C:604:TYR:CZ    | 2.45                     | 0.51              |
| 4:C:504:LEU:HD12  | 4:C:525:ILE:HD11  | 1.92                     | 0.51              |
| 4:C:1181:VAL:CG1  | 4:C:1185:ALA:HB3  | 2.41                     | 0.51              |
| 4:D:146:LEU:HD11  | 4:D:189:GLN:HG3   | 1.92                     | 0.51              |
| 5:N:395:LEU:HD23  | 5:N:396:ARG:HD2   | 1.92                     | 0.51              |
| 4:D:1125:LEU:HD13 | 5:P:530:VAL:CG1   | 2.40                     | 0.51              |
| 5:N:495:GLU:HB2   | 5:N:496:GLU:HB2   | 1.91                     | 0.51              |
| 5:P:539:GLY:CA    | 5:P:542:PRO:HD2   | 2.41                     | 0.51              |
| 4:A:106:TYR:O     | 4:A:110:VAL:HG23  | 2.10                     | 0.51              |
| 4:B:1055:VAL:CG1  | 4:B:1066:ALA:HA   | 2.41                     | 0.51              |
| 4:C:951:ALA:HB2   | 4:C:993:LEU:CG    | 2.41                     | 0.51              |
| 4:C:952:ARG:HD3   | 4:C:987:LEU:HD23  | 1.93                     | 0.51              |
| 4:C:976:VAL:O     | 4:C:976:VAL:HG13  | 2.10                     | 0.51              |
| 4:C:1161:VAL:HG12 | 4:C:1176:LEU:HD21 | 1.93                     | 0.51              |
| 4:D:1080:VAL:CG1  | 4:D:1081:VAL:HB   | 2.39                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:406:LEU:HD22  | 5:M:419:LYS:HG2   | 1.92                     | 0.51              |
| 5:M:492:TRP:C     | 5:M:493:GLU:HG2   | 2.29                     | 0.51              |
| 5:N:524:PRO:HD2   | 5:N:525:GLU:CA    | 2.21                     | 0.51              |
| 5:O:447:ALA:O     | 5:O:448:PHE:CD1   | 2.64                     | 0.51              |
| 5:P:528:GLU:H     | 5:P:529:PRO:CD    | 2.23                     | 0.51              |
| 4:A:25:LEU:HD21   | 4:A:56:PHE:HA     | 1.93                     | 0.51              |
| 4:C:226:VAL:HG12  | 4:C:510:VAL:HG11  | 1.92                     | 0.51              |
| 5:M:543:PRO:HG2   | 5:M:543:PRO:O     | 2.11                     | 0.51              |
| 4:C:975:LEU:HD23  | 4:C:976:VAL:HA    | 1.93                     | 0.50              |
| 5:P:499:ASP:HB2   | 5:P:515:LEU:CD2   | 2.27                     | 0.50              |
| 4:B:1027:CYS:SG   | 4:B:1045:VAL:HG11 | 2.51                     | 0.50              |
| 4:B:1058:PRO:HG2  | 4:B:1059:THR:H    | 1.76                     | 0.50              |
| 4:B:1058:PRO:CG   | 4:B:1059:THR:N    | 2.73                     | 0.50              |
| 4:C:223:ALA:O     | 4:C:226:VAL:HG22  | 2.12                     | 0.50              |
| 4:C:918:LEU:HD22  | 4:C:953:LEU:HD22  | 1.92                     | 0.50              |
| 4:D:1080:VAL:N    | 4:D:1081:VAL:HG23 | 2.23                     | 0.50              |
| 5:O:505:ARG:NE    | 5:O:507:LEU:HD21  | 2.24                     | 0.50              |
| 3:I:14:DA:C2      | 2:J:16:DG:N2      | 2.80                     | 0.50              |
| 4:A:1093:LEU:HD11 | 4:A:1097:ILE:HG22 | 1.93                     | 0.50              |
| 4:C:154:ILE:HD11  | 4:C:195:VAL:CB    | 2.36                     | 0.50              |
| 4:D:1159:LEU:CD1  | 4:D:1183:GLU:HG3  | 2.41                     | 0.50              |
| 5:P:541:MET:C     | 5:P:543:PRO:CD    | 2.85                     | 0.50              |
| 4:A:362:TRP:CE3   | 4:A:365:LEU:HD12  | 2.47                     | 0.50              |
| 4:B:227:LEU:HA    | 4:B:230:ILE:HD12  | 1.92                     | 0.50              |
| 4:B:405:ILE:HG23  | 4:B:484:TYR:OH    | 2.11                     | 0.50              |
| 4:B:515:HIS:HB2   | 4:B:516:LYS:CA    | 2.40                     | 0.50              |
| 4:B:1151:LEU:HD12 | 4:B:1152:LEU:HD12 | 1.92                     | 0.50              |
| 4:C:1089:VAL:HG23 | 4:C:1091:PRO:HD3  | 1.94                     | 0.50              |
| 4:C:1093:LEU:O    | 4:C:1094:LYS:CG   | 2.59                     | 0.50              |
| 4:D:537:GLU:HB3   | 4:D:540:GLN:HE21  | 1.76                     | 0.50              |
| 5:N:440:GLN:CB    | 5:N:441:PHE:HA    | 2.41                     | 0.50              |
| 4:A:186:LEU:HD21  | 4:A:245:PRO:HB2   | 1.93                     | 0.50              |
| 4:D:1082:PHE:CZ   | 4:D:1114:LEU:HB2  | 2.39                     | 0.50              |
| 5:M:369:HIS:O     | 5:M:378:GLN:NE2   | 2.44                     | 0.50              |
| 5:O:494:ALA:HB3   | 5:O:495:GLU:CG    | 2.42                     | 0.50              |
| 4:A:658:LEU:HD23  | 4:A:658:LEU:C     | 2.37                     | 0.50              |
| 4:A:1093:LEU:HD13 | 4:A:1099:LEU:CG   | 2.41                     | 0.50              |
| 4:C:604:TYR:HB3   | 4:C:608:ALA:HB3   | 1.93                     | 0.50              |
| 4:C:1093:LEU:HD12 | 4:C:1097:ILE:HD12 | 1.92                     | 0.50              |
| 4:C:1136:ASP:O    | 4:C:1139:LEU:HD23 | 2.11                     | 0.50              |
| 4:D:397:MET:HE3   | 4:D:459:VAL:HA    | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:406:LEU:HD22  | 5:M:419:LYS:CG    | 2.42                     | 0.50              |
| 5:M:419:LYS:O     | 5:M:423:HIS:NE2   | 2.45                     | 0.50              |
| 5:N:440:GLN:HB2   | 5:N:441:PHE:HB2   | 1.92                     | 0.50              |
| 4:C:406:VAL:HG11  | 4:C:464:ILE:HG21  | 1.94                     | 0.50              |
| 4:C:970:ARG:NE    | 4:C:975:LEU:HD13  | 2.26                     | 0.50              |
| 4:D:1159:LEU:CD2  | 4:D:1183:GLU:HG3  | 2.42                     | 0.50              |
| 5:M:541:MET:C     | 5:M:543:PRO:CD    | 2.85                     | 0.50              |
| 5:O:385:ARG:HB2   | 5:O:386:ALA:HA    | 1.94                     | 0.50              |
| 5:P:505:ARG:CG    | 5:P:514:ARG:HE    | 2.17                     | 0.50              |
| 4:B:922:LEU:CD1   | 4:B:964:ALA:HB2   | 2.42                     | 0.50              |
| 4:D:542:VAL:CG1   | 4:D:543:PRO:HD3   | 2.40                     | 0.50              |
| 5:O:390:ALA:O     | 5:O:391:LEU:O     | 2.29                     | 0.50              |
| 4:B:1218:VAL:N    | 4:B:1219:PRO:HD2  | 2.27                     | 0.50              |
| 5:N:395:LEU:CA    | 5:N:396:ARG:CB    | 2.89                     | 0.50              |
| 5:P:501:SER:OG    | 5:P:504:LEU:O     | 2.29                     | 0.50              |
| 4:A:116:ALA:HB1   | 4:A:125:PRO:HB2   | 1.94                     | 0.49              |
| 4:A:366:ARG:HD3   | 4:A:385:HIS:NE2   | 2.27                     | 0.49              |
| 4:B:352:GLU:HG2   | 4:B:356:ARG:CZ    | 2.41                     | 0.49              |
| 5:M:538:ASN:O     | 5:M:541:MET:HB3   | 2.12                     | 0.49              |
| 2:L:7:DT:OP2      | 4:D:1067:ARG:NH1  | 2.45                     | 0.49              |
| 4:A:513:ILE:CG2   | 4:A:514:PRO:CD    | 2.85                     | 0.49              |
| 4:A:789:LYS:HE3   | 4:A:795:GLU:OE1   | 2.12                     | 0.49              |
| 4:A:1152:LEU:HD13 | 4:A:1179:VAL:CG2  | 2.41                     | 0.49              |
| 4:B:32:VAL:HG21   | 4:B:42:LEU:HD22   | 1.95                     | 0.49              |
| 4:B:1027:CYS:SG   | 4:B:1045:VAL:CG1  | 3.00                     | 0.49              |
| 4:C:1173:LEU:HD13 | 4:C:1202:ARG:HH22 | 1.78                     | 0.49              |
| 4:D:635:VAL:HG22  | 4:D:838:GLU:HG3   | 1.94                     | 0.49              |
| 4:A:590:VAL:CG1   | 4:A:602:THR:HG23  | 2.42                     | 0.49              |
| 4:A:628:LEU:HD22  | 4:A:645:TYR:CE2   | 2.47                     | 0.49              |
| 4:B:590:VAL:CG1   | 4:B:602:THR:HG23  | 2.42                     | 0.49              |
| 4:B:1099:LEU:HD23 | 4:B:1120:THR:HA   | 1.93                     | 0.49              |
| 4:C:961:LEU:HD12  | 4:C:962:ARG:N     | 2.27                     | 0.49              |
| 4:D:23:ALA:HB2    | 4:D:215:TYR:HA    | 1.94                     | 0.49              |
| 4:D:1067:ARG:HA   | 4:D:1081:VAL:CG2  | 2.42                     | 0.49              |
| 5:M:499:ASP:HB3   | 5:M:500:PRO:CA    | 2.42                     | 0.49              |
| 5:N:395:LEU:HD23  | 5:N:396:ARG:HB3   | 1.93                     | 0.49              |
| 5:O:452:LYS:HZ2   | 5:O:509:ARG:CZ    | 2.25                     | 0.49              |
| 5:O:527:GLU:N     | 5:O:528:GLU:HA    | 2.26                     | 0.49              |
| 5:P:541:MET:C     | 5:P:541:MET:CE    | 2.85                     | 0.49              |
| 4:B:1068:PHE:H    | 4:B:1081:VAL:HG11 | 1.75                     | 0.49              |
| 4:C:28:LEU:CD1    | 4:C:251:VAL:HG21  | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:32:VAL:HG21   | 4:C:42:LEU:HD22   | 1.94                     | 0.49              |
| 4:C:132:LEU:O     | 4:C:136:ALA:HB2   | 2.12                     | 0.49              |
| 4:C:661:ARG:O     | 4:C:680:ARG:NH1   | 2.46                     | 0.49              |
| 5:P:389:GLU:O     | 5:P:393:PRO:HD2   | 2.13                     | 0.49              |
| 4:B:1055:VAL:HG12 | 4:B:1056:ARG:N    | 2.26                     | 0.49              |
| 4:B:1057:LYS:HE2  | 4:B:1064:MET:SD   | 2.51                     | 0.49              |
| 4:C:148:ALA:HB3   | 4:C:151:PRO:CG    | 2.42                     | 0.49              |
| 5:M:390:ALA:C     | 5:M:391:LEU:CD1   | 2.85                     | 0.49              |
| 5:P:453:LYS:O     | 5:P:454:SER:HB3   | 2.13                     | 0.49              |
| 4:A:1098:PRO:CG   | 4:A:1121:LEU:HD22 | 2.42                     | 0.49              |
| 4:B:397:MET:HE3   | 4:B:459:VAL:HA    | 1.94                     | 0.49              |
| 4:D:319:LEU:HD11  | 4:D:328:GLU:OE2   | 2.13                     | 0.49              |
| 4:D:1205:PHE:CD1  | 4:D:1205:PHE:C    | 2.90                     | 0.49              |
| 5:O:412:VAL:O     | 5:O:414:ARG:N     | 2.45                     | 0.49              |
| 5:N:526:ALA:O     | 5:N:527:GLU:HB2   | 2.13                     | 0.49              |
| 5:O:403:ARG:HG2   | 5:O:437:ALA:HB1   | 1.95                     | 0.49              |
| 5:O:505:ARG:NH1   | 5:O:506:ARG:NH1   | 2.60                     | 0.49              |
| 4:A:54:VAL:HG13   | 4:A:287:ILE:HD11  | 1.94                     | 0.49              |
| 4:A:181:ILE:HD13  | 4:A:266:TRP:CZ3   | 2.48                     | 0.49              |
| 4:A:854:VAL:O     | 4:A:858:ILE:HG23  | 2.13                     | 0.49              |
| 4:A:1098:PRO:HG2  | 4:A:1121:LEU:HD22 | 1.95                     | 0.49              |
| 4:D:1202:ARG:NH1  | 4:D:1202:ARG:CG   | 2.73                     | 0.49              |
| 5:P:504:LEU:N     | 5:P:504:LEU:CD1   | 2.73                     | 0.49              |
| 4:A:1122:GLU:HB3  | 4:A:1220:PHE:CD1  | 2.48                     | 0.49              |
| 5:N:498:GLU:HB2   | 5:N:499:ASP:HA    | 1.95                     | 0.49              |
| 5:O:395:LEU:HB3   | 5:O:396:ARG:HB2   | 1.95                     | 0.49              |
| 5:P:522:LYS:CG    | 5:P:523:ALA:H     | 2.13                     | 0.49              |
| 4:C:362:TRP:CD1   | 4:C:388:LEU:HD13  | 2.48                     | 0.48              |
| 4:D:996:ILE:CD1   | 5:P:528:GLU:OE2   | 2.59                     | 0.48              |
| 4:D:1020:GLY:O    | 4:D:1024:VAL:HG23 | 2.13                     | 0.48              |
| 4:D:1065:MET:SD   | 4:D:1082:PHE:CA   | 2.83                     | 0.48              |
| 5:N:455:LEU:CA    | 5:N:456:SER:C     | 2.86                     | 0.48              |
| 4:C:397:MET:HE3   | 4:C:459:VAL:HA    | 1.96                     | 0.48              |
| 4:C:975:LEU:HD23  | 4:C:976:VAL:CA    | 2.42                     | 0.48              |
| 5:P:382:GLU:HG3   | 5:P:388:LEU:HD21  | 1.94                     | 0.48              |
| 5:P:518:VAL:HG13  | 5:P:519:ARG:HB2   | 1.93                     | 0.48              |
| 4:A:1189:LEU:O    | 4:A:1189:LEU:HD23 | 2.12                     | 0.48              |
| 4:A:970:ARG:HG3   | 4:A:980:ALA:HA    | 1.95                     | 0.48              |
| 4:A:1164:ARG:HG2  | 4:A:1173:LEU:HD21 | 1.94                     | 0.48              |
| 4:B:302:GLU:CD    | 4:B:304:ARG:NH1   | 2.71                     | 0.48              |
| 4:B:1181:VAL:HG13 | 4:B:1185:ALA:HB3  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:335:LEU:HD21  | 4:D:354:LEU:HG    | 1.94                     | 0.48              |
| 4:D:1046:LEU:HD13 | 4:D:1205:PHE:HD2  | 1.78                     | 0.48              |
| 5:M:505:ARG:HD2   | 5:M:510:LEU:CG    | 2.43                     | 0.48              |
| 4:D:1205:PHE:CE1  | 4:D:1206:LEU:HD12 | 2.45                     | 0.48              |
| 5:N:493:GLU:HB2   | 5:N:494:ALA:HA    | 1.95                     | 0.48              |
| 4:A:1124:VAL:HG13 | 4:A:1200:PRO:CG   | 2.42                     | 0.48              |
| 4:C:679:VAL:HG22  | 4:C:693:LEU:HD21  | 1.96                     | 0.48              |
| 4:C:1080:VAL:CB   | 4:C:1082:PHE:H    | 2.23                     | 0.48              |
| 4:D:755:ALA:HB2   | 4:D:784:PHE:CD1   | 2.49                     | 0.48              |
| 4:D:1119:TRP:CH2  | 4:D:1206:LEU:CA   | 2.93                     | 0.48              |
| 5:M:491:PRO:C     | 5:M:492:TRP:CG    | 2.91                     | 0.48              |
| 5:N:498:GLU:HB3   | 5:N:499:ASP:C     | 2.39                     | 0.48              |
| 4:A:574:VAL:HG12  | 4:A:575:HIS:H     | 1.76                     | 0.48              |
| 4:B:356:ARG:O     | 4:B:357:VAL:CG1   | 2.62                     | 0.48              |
| 4:D:589:LEU:HD21  | 4:D:612:LEU:HG    | 1.96                     | 0.48              |
| 4:A:28:LEU:HD11   | 4:A:251:VAL:HG21  | 1.96                     | 0.48              |
| 4:C:252:LYS:HD2   | 4:C:257:MET:HE3   | 1.94                     | 0.48              |
| 4:C:300:LEU:HB3   | 4:C:302:GLU:O     | 2.14                     | 0.48              |
| 4:C:1051:VAL:HG12 | 4:C:1068:PHE:CE1  | 2.48                     | 0.48              |
| 5:M:411:LEU:CB    | 5:M:412:VAL:HA    | 2.43                     | 0.48              |
| 5:N:527:GLU:N     | 5:N:528:GLU:CA    | 2.70                     | 0.48              |
| 5:P:535:ILE:HG12  | 5:P:536:GLY:H     | 1.79                     | 0.48              |
| 4:B:352:GLU:CD    | 4:B:356:ARG:NH2   | 2.72                     | 0.48              |
| 4:C:1101:VAL:HG22 | 4:C:1118:VAL:HG12 | 1.94                     | 0.48              |
| 5:M:524:PRO:HB2   | 5:M:525:GLU:O     | 2.14                     | 0.48              |
| 5:N:523:ALA:HB3   | 5:N:524:PRO:CA    | 2.24                     | 0.48              |
| 5:N:525:GLU:HG3   | 5:N:530:VAL:HA    | 1.95                     | 0.48              |
| 4:A:311:ARG:HG2   | 4:A:391:LEU:HD13  | 1.94                     | 0.48              |
| 4:A:620:LEU:N     | 4:A:620:LEU:HD12  | 2.29                     | 0.48              |
| 4:B:424:ARG:NE    | 4:B:620:LEU:HD22  | 2.28                     | 0.48              |
| 4:B:535:LEU:HB3   | 4:B:563:MET:HE2   | 1.95                     | 0.48              |
| 4:B:1056:ARG:CG   | 4:B:1056:ARG:NH1  | 2.73                     | 0.48              |
| 4:C:970:ARG:NH2   | 4:C:975:LEU:HD21  | 2.28                     | 0.48              |
| 4:D:13:HIS:NE2    | 4:D:72:GLU:OE1    | 2.47                     | 0.48              |
| 4:D:1099:LEU:HD23 | 4:D:1120:THR:HA   | 1.95                     | 0.48              |
| 5:N:522:LYS:HG2   | 5:N:523:ALA:H     | 1.78                     | 0.48              |
| 4:C:1096:ASP:O    | 4:C:1097:ILE:HG13 | 2.14                     | 0.47              |
| 5:M:419:LYS:O     | 5:M:423:HIS:CG    | 2.66                     | 0.47              |
| 4:B:356:ARG:O     | 4:B:357:VAL:HG13  | 2.13                     | 0.47              |
| 4:B:517:LYS:O     | 4:B:521:LEU:HD13  | 2.13                     | 0.47              |
| 4:B:941:ALA:CB    | 4:B:1006:LEU:HD11 | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:154:ILE:HD11  | 4:D:192:VAL:HG22  | 1.96                     | 0.47              |
| 5:M:492:TRP:CZ3   | 5:M:495:GLU:O     | 2.68                     | 0.47              |
| 2:F:11:DG:H2"     | 2:F:12:DC:C6      | 2.49                     | 0.47              |
| 4:A:498:LEU:HB3   | 4:A:499:ALA:CB    | 2.43                     | 0.47              |
| 4:A:525:ILE:H     | 4:A:525:ILE:HD12  | 1.79                     | 0.47              |
| 4:C:389:TYR:O     | 4:C:393:VAL:HG23  | 2.14                     | 0.47              |
| 4:C:570:ARG:C     | 4:C:571:HIS:ND1   | 2.72                     | 0.47              |
| 4:C:1157:GLY:HA3  | 4:C:1182:GLY:HA2  | 1.95                     | 0.47              |
| 4:D:15:GLN:N      | 4:D:23:ALA:O      | 2.47                     | 0.47              |
| 4:D:314:THR:HG21  | 4:D:391:LEU:HD11  | 1.96                     | 0.47              |
| 5:M:391:LEU:O     | 5:M:392:LYS:C     | 2.57                     | 0.47              |
| 5:O:523:ALA:CB    | 5:O:524:PRO:HB3   | 2.25                     | 0.47              |
| 4:A:1051:VAL:CG2  | 4:A:1099:LEU:HD12 | 2.43                     | 0.47              |
| 4:B:951:ALA:HB2   | 4:B:993:LEU:CD2   | 2.45                     | 0.47              |
| 4:C:287:ILE:HG22  | 4:C:611:ALA:O     | 2.14                     | 0.47              |
| 4:D:574:VAL:HG22  | 4:D:601:VAL:HG21  | 1.95                     | 0.47              |
| 4:D:918:LEU:HD22  | 4:D:953:LEU:CD2   | 2.44                     | 0.47              |
| 4:D:1140:LEU:HG   | 4:D:1144:GLY:HA3  | 1.97                     | 0.47              |
| 5:P:525:GLU:HB2   | 5:P:528:GLU:O     | 2.14                     | 0.47              |
| 4:B:354:LEU:O     | 4:B:362:TRP:HZ2   | 1.98                     | 0.47              |
| 4:B:590:VAL:HG11  | 4:B:602:THR:HG23  | 1.97                     | 0.47              |
| 4:C:969:GLU:O     | 4:C:973:SER:N     | 2.40                     | 0.47              |
| 4:C:1140:LEU:HD12 | 4:C:1142:GLU:H    | 1.80                     | 0.47              |
| 4:D:203:TYR:HB2   | 4:D:205:LEU:HD13  | 1.96                     | 0.47              |
| 4:D:622:LEU:HD23  | 4:D:625:LEU:HD13  | 1.97                     | 0.47              |
| 5:M:505:ARG:CB    | 5:M:506:ARG:HA    | 2.39                     | 0.47              |
| 5:P:505:ARG:CG    | 5:P:514:ARG:NE    | 2.76                     | 0.47              |
| 4:A:553:GLU:O     | 4:A:556:ARG:HG2   | 2.13                     | 0.47              |
| 4:B:197:LYS:HA    | 4:B:207:MET:HE2   | 1.96                     | 0.47              |
| 4:B:1029:ILE:HD13 | 4:B:1047:LEU:HD21 | 1.96                     | 0.47              |
| 4:C:480:VAL:HG11  | 4:C:581:ILE:HD11  | 1.95                     | 0.47              |
| 4:C:617:MET:HA    | 4:C:617:MET:HE2   | 1.97                     | 0.47              |
| 4:D:252:LYS:HD2   | 4:D:257:MET:HE3   | 1.96                     | 0.47              |
| 4:D:302:GLU:OE2   | 4:D:304:ARG:NH1   | 2.47                     | 0.47              |
| 4:D:557:GLN:O     | 4:D:561:VAL:HG23  | 2.14                     | 0.47              |
| 5:M:506:ARG:HB2   | 5:M:510:LEU:HB2   | 1.95                     | 0.47              |
| 5:O:396:ARG:CA    | 5:O:397:ALA:C     | 2.84                     | 0.47              |
| 5:P:417:GLU:HG2   | 5:P:421:PHE:CE2   | 2.50                     | 0.47              |
| 1:K:12:DC:N4      | 2:L:16:DG:O6      | 2.48                     | 0.47              |
| 4:A:939:VAL:HG22  | 4:A:944:LEU:HD12  | 1.97                     | 0.47              |
| 4:A:1173:LEU:HD12 | 4:A:1202:ARG:HD2  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:675:MET:HE1   | 4:B:697:TYR:HB3   | 1.96                     | 0.47              |
| 4:B:1080:VAL:HG21 | 4:B:1114:LEU:HD22 | 1.96                     | 0.47              |
| 4:C:257:MET:HE2   | 4:C:257:MET:HA    | 1.97                     | 0.47              |
| 4:C:291:MET:HB2   | 4:C:291:MET:HE3   | 1.65                     | 0.47              |
| 4:C:1094:LYS:N    | 4:C:1094:LYS:CD   | 2.72                     | 0.47              |
| 4:D:235:THR:HG22  | 4:D:236:LEU:H     | 1.80                     | 0.47              |
| 4:D:399:PHE:N     | 4:D:400:PRO:CD    | 2.77                     | 0.47              |
| 4:D:1086:TYR:HB2  | 4:D:1087:GLU:C    | 2.40                     | 0.47              |
| 4:D:1099:LEU:HD22 | 4:D:1118:VAL:CG1  | 2.44                     | 0.47              |
| 5:M:418:SER:O     | 5:M:422:HIS:CG    | 2.68                     | 0.47              |
| 5:P:528:GLU:HG3   | 5:P:529:PRO:CG    | 2.43                     | 0.47              |
| 2:F:12:DC:C4      | 2:F:13:DA:C6      | 3.02                     | 0.47              |
| 4:B:238:ASP:HB3   | 4:B:239:PRO:CA    | 2.44                     | 0.47              |
| 4:C:1176:LEU:HD12 | 4:C:1177:ARG:N    | 2.30                     | 0.47              |
| 4:D:1093:LEU:HD11 | 4:D:1097:ILE:HG22 | 1.97                     | 0.47              |
| 4:D:1119:TRP:HZ2  | 4:D:1206:LEU:C    | 2.22                     | 0.47              |
| 4:A:975:LEU:C     | 4:A:975:LEU:CD1   | 2.87                     | 0.47              |
| 4:C:495:PHE:CD1   | 4:C:572:ALA:HB2   | 2.50                     | 0.47              |
| 4:C:1197:TYR:CD2  | 4:C:1199:VAL:HG12 | 2.50                     | 0.47              |
| 4:D:511:TYR:O     | 4:D:554:ARG:NH2   | 2.47                     | 0.47              |
| 4:D:1211:GLY:N    | 4:D:1212:GLY:HA2  | 2.30                     | 0.47              |
| 5:M:453:LYS:O     | 5:M:454:SER:CB    | 2.63                     | 0.47              |
| 5:N:403:ARG:HE    | 5:N:437:ALA:HB1   | 1.80                     | 0.47              |
| 5:N:505:ARG:CB    | 5:N:506:ARG:CA    | 2.85                     | 0.47              |
| 5:O:390:ALA:CB    | 5:O:393:PRO:CG    | 2.78                     | 0.47              |
| 5:P:505:ARG:NE    | 5:P:510:LEU:HD12  | 2.29                     | 0.47              |
| 5:P:506:ARG:NH1   | 5:P:506:ARG:CB    | 2.72                     | 0.47              |
| 2:H:6:DT:H2"      | 2:H:7:DT:OP2      | 2.15                     | 0.47              |
| 4:B:331:TYR:O     | 4:B:335:LEU:HD13  | 2.15                     | 0.47              |
| 4:C:970:ARG:NH2   | 4:C:975:LEU:HD11  | 2.30                     | 0.47              |
| 4:C:1080:VAL:HG11 | 4:C:1113:VAL:O    | 2.10                     | 0.47              |
| 4:D:793:VAL:HG21  | 4:D:798:ALA:HB2   | 1.97                     | 0.47              |
| 4:D:1043:PRO:HD2  | 4:D:1105:VAL:HG23 | 1.96                     | 0.47              |
| 5:M:411:LEU:H     | 5:M:412:VAL:HG22  | 1.76                     | 0.47              |
| 5:M:495:GLU:N     | 5:M:496:GLU:C     | 2.73                     | 0.47              |
| 5:P:395:LEU:HG    | 5:P:396:ARG:N     | 2.29                     | 0.47              |
| 4:B:364:GLU:C     | 4:B:366:ARG:H     | 2.23                     | 0.46              |
| 4:B:675:MET:O     | 4:B:679:VAL:HG23  | 2.14                     | 0.46              |
| 4:B:734:LEU:HD23  | 4:B:746:GLN:NE2   | 2.29                     | 0.46              |
| 4:B:922:LEU:HD13  | 4:B:964:ALA:HB2   | 1.96                     | 0.46              |
| 4:C:710:ARG:NH1   | 4:C:716:GLU:OE1   | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:1186:LEU:HD23 | 4:C:1186:LEU:C    | 2.40                     | 0.46              |
| 5:O:395:LEU:H     | 5:O:396:ARG:C     | 2.23                     | 0.46              |
| 4:C:590:VAL:CG1   | 4:C:602:THR:HG23  | 2.45                     | 0.46              |
| 4:D:1079:VAL:HG23 | 4:D:1113:VAL:CG1  | 2.40                     | 0.46              |
| 5:M:373:LYS:O     | 5:M:374:ALA:HB3   | 2.15                     | 0.46              |
| 5:O:378:GLN:HA    | 5:O:381:ALA:HB2   | 1.97                     | 0.46              |
| 4:B:200:ALA:HB3   | 4:B:207:MET:HE3   | 1.97                     | 0.46              |
| 4:B:840:MET:HG2   | 4:B:861:ALA:HB2   | 1.96                     | 0.46              |
| 4:C:1016:LEU:HD21 | 4:C:1073:GLU:CD   | 2.40                     | 0.46              |
| 4:D:595:ASP:OD1   | 4:D:599:ARG:N     | 2.44                     | 0.46              |
| 4:D:1060:ARG:O    | 4:D:1060:ARG:HG3  | 2.16                     | 0.46              |
| 4:D:1082:PHE:CE2  | 4:D:1113:VAL:O    | 2.69                     | 0.46              |
| 5:M:525:GLU:HB3   | 5:M:529:PRO:CD    | 2.44                     | 0.46              |
| 5:O:395:LEU:HB2   | 5:O:396:ARG:HB2   | 1.97                     | 0.46              |
| 5:O:529:PRO:HB2   | 5:O:530:VAL:HG12  | 1.96                     | 0.46              |
| 5:P:455:LEU:HA    | 5:P:456:SER:HB2   | 1.96                     | 0.46              |
| 4:A:1099:LEU:HD23 | 4:A:1120:THR:HA   | 1.97                     | 0.46              |
| 4:A:1161:VAL:HG11 | 4:A:1179:VAL:HG23 | 1.98                     | 0.46              |
| 4:C:504:LEU:CD1   | 4:C:525:ILE:HD11  | 2.45                     | 0.46              |
| 5:N:452:LYS:O     | 5:N:453:LYS:C     | 2.58                     | 0.46              |
| 5:P:522:LYS:O     | 5:P:523:ALA:C     | 2.57                     | 0.46              |
| 4:B:399:PHE:N     | 4:B:400:PRO:CD    | 2.78                     | 0.46              |
| 4:B:994:ASP:OD1   | 4:B:997:THR:HG22  | 2.16                     | 0.46              |
| 4:D:215:TYR:CE1   | 4:D:250:TYR:HB3   | 2.50                     | 0.46              |
| 5:M:419:LYS:HA    | 5:M:419:LYS:HD2   | 1.61                     | 0.46              |
| 5:M:519:ARG:NE    | 5:M:520:LYS:HE2   | 2.30                     | 0.46              |
| 4:A:549:MET:HA    | 4:A:555:ILE:CD1   | 2.45                     | 0.46              |
| 4:A:837:VAL:HA    | 4:A:866:ILE:HD13  | 1.97                     | 0.46              |
| 4:B:622:LEU:HD23  | 4:B:625:LEU:HD13  | 1.97                     | 0.46              |
| 4:B:1008:ILE:HD12 | 4:B:1008:ILE:C    | 2.40                     | 0.46              |
| 4:B:1054:VAL:HG23 | 4:B:1094:LYS:HE2  | 1.95                     | 0.46              |
| 4:D:102:ASP:C     | 4:D:283:VAL:HG22  | 2.40                     | 0.46              |
| 4:D:406:VAL:HG12  | 4:D:410:ILE:HD12  | 1.97                     | 0.46              |
| 5:O:520:LYS:O     | 5:O:520:LYS:HG2   | 2.16                     | 0.46              |
| 5:P:540:ILE:C     | 5:P:540:ILE:CD1   | 2.85                     | 0.46              |
| 4:A:258:ARG:HG2   | 4:A:271:PHE:CZ    | 2.51                     | 0.46              |
| 4:B:28:LEU:CD1    | 4:B:251:VAL:HG21  | 2.45                     | 0.46              |
| 4:C:1147:ARG:O    | 4:C:1151:LEU:HD13 | 2.15                     | 0.46              |
| 4:C:1162:TYR:CD2  | 4:C:1175:ALA:HB2  | 2.50                     | 0.46              |
| 4:D:57:TYR:CD2    | 4:D:287:ILE:HD12  | 2.50                     | 0.46              |
| 4:D:1057:LYS:HB3  | 4:D:1058:PRO:CB   | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:1160:PRO:CG   | 4:D:1201:ASP:OD2  | 2.63                     | 0.46              |
| 4:B:98:LEU:O      | 4:B:99:LEU:HD23   | 2.16                     | 0.46              |
| 4:B:331:TYR:HB3   | 4:B:350:LEU:HD23  | 1.97                     | 0.46              |
| 4:B:702:MET:HG3   | 4:B:705:ILE:HD12  | 1.97                     | 0.46              |
| 4:D:938:LEU:HG    | 4:D:943:ALA:HB3   | 1.97                     | 0.46              |
| 4:D:1155:HIS:NE2  | 4:D:1188:LEU:HD21 | 2.31                     | 0.46              |
| 5:O:411:LEU:H     | 5:O:412:VAL:HG22  | 1.81                     | 0.46              |
| 5:P:412:VAL:O     | 5:P:415:PHE:HB2   | 2.16                     | 0.46              |
| 5:P:495:GLU:H     | 5:P:496:GLU:HG2   | 1.81                     | 0.46              |
| 2:H:10:DG:H2"     | 2:H:11:DG:C8      | 2.51                     | 0.46              |
| 4:B:233:LYS:CG    | 4:B:510:VAL:HG11  | 2.45                     | 0.46              |
| 4:C:28:LEU:O      | 4:C:32:VAL:HG23   | 2.16                     | 0.46              |
| 4:C:602:THR:HG22  | 4:C:604:TYR:H     | 1.79                     | 0.46              |
| 4:D:223:ALA:O     | 4:D:226:VAL:HG22  | 2.15                     | 0.46              |
| 4:D:789:LYS:HG3   | 4:D:795:GLU:HB2   | 1.98                     | 0.46              |
| 5:O:451:GLU:O     | 5:O:452:LYS:HB3   | 2.16                     | 0.46              |
| 1:G:14:DA:OP1     | 4:B:898:GLY:HA2   | 2.16                     | 0.46              |
| 4:A:402:TYR:O     | 4:A:406:VAL:HG23  | 2.16                     | 0.46              |
| 4:A:1164:ARG:NH1  | 4:A:1173:LEU:HD11 | 2.31                     | 0.46              |
| 4:B:357:VAL:HA    | 4:B:358:GLU:HG3   | 1.98                     | 0.46              |
| 4:C:443:PRO:HA    | 4:C:448:LEU:HD12  | 1.97                     | 0.46              |
| 4:C:525:ILE:HD11  | 4:C:535:LEU:HD21  | 1.98                     | 0.46              |
| 5:M:524:PRO:HD2   | 5:M:526:ALA:N     | 2.30                     | 0.46              |
| 5:N:536:GLY:O     | 5:N:540:ILE:HG12  | 2.16                     | 0.46              |
| 4:A:226:VAL:HG21  | 4:A:561:VAL:CG1   | 2.47                     | 0.45              |
| 4:A:555:ILE:C     | 4:A:555:ILE:CD1   | 2.89                     | 0.45              |
| 4:A:604:TYR:HB3   | 4:A:608:ALA:HB3   | 1.98                     | 0.45              |
| 4:A:1189:LEU:HD23 | 4:A:1194:TYR:O    | 2.16                     | 0.45              |
| 4:B:308:GLN:NE2   | 4:B:356:ARG:HA    | 2.30                     | 0.45              |
| 4:B:595:ASP:OD1   | 4:B:599:ARG:N     | 2.49                     | 0.45              |
| 4:C:298:PHE:CZ    | 4:C:408:ASP:HB2   | 2.51                     | 0.45              |
| 4:D:678:THR:HG22  | 4:D:693:LEU:HD11  | 1.98                     | 0.45              |
| 4:D:785:VAL:HG13  | 4:D:795:GLU:HG3   | 1.97                     | 0.45              |
| 5:O:521:PRO:O     | 5:O:522:LYS:CB    | 2.63                     | 0.45              |
| 4:A:524:LEU:HD22  | 4:A:545:LEU:HD22  | 1.97                     | 0.45              |
| 4:B:586:LEU:HD13  | 4:B:592:LEU:HD21  | 1.98                     | 0.45              |
| 4:B:723:PHE:HB3   | 4:B:726:ALA:HB3   | 1.99                     | 0.45              |
| 4:C:451:GLU:CD    | 4:C:759:LEU:HD23  | 2.41                     | 0.45              |
| 4:C:951:ALA:HB2   | 4:C:993:LEU:CD2   | 2.46                     | 0.45              |
| 4:D:1080:VAL:CG2  | 4:D:1114:LEU:HA   | 2.44                     | 0.45              |
| 5:M:408:GLY:C     | 5:M:415:PHE:HD1   | 2.25                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:450:LEU:HB3   | 5:M:451:GLU:HB2   | 1.97                     | 0.45              |
| 4:A:557:GLN:O     | 4:A:561:VAL:HG23  | 2.17                     | 0.45              |
| 4:B:939:VAL:HG22  | 4:B:944:LEU:HD12  | 1.99                     | 0.45              |
| 4:B:1051:VAL:HG21 | 4:B:1093:LEU:HD23 | 1.97                     | 0.45              |
| 4:B:1055:VAL:HG12 | 4:B:1066:ALA:HA   | 1.98                     | 0.45              |
| 4:C:297:ARG:HD3   | 4:C:306:GLU:OE2   | 2.16                     | 0.45              |
| 4:C:743:TYR:H     | 4:C:746:GLN:HE21  | 1.64                     | 0.45              |
| 5:M:489:ASP:O     | 5:M:490:PRO:C     | 2.57                     | 0.45              |
| 4:A:511:TYR:HB3   | 4:A:513:ILE:HD11  | 1.99                     | 0.45              |
| 4:B:1015:VAL:HG13 | 4:B:1016:LEU:N    | 2.30                     | 0.45              |
| 4:C:1082:PHE:C    | 4:C:1084:ARG:N    | 2.73                     | 0.45              |
| 4:D:1043:PRO:O    | 4:D:1105:VAL:HG22 | 2.16                     | 0.45              |
| 5:M:525:GLU:HB3   | 5:M:529:PRO:HD2   | 1.98                     | 0.45              |
| 5:O:389:GLU:CB    | 5:O:445:GLU:HB3   | 2.46                     | 0.45              |
| 5:O:529:PRO:CA    | 5:O:530:VAL:HB    | 2.46                     | 0.45              |
| 4:A:302:GLU:O     | 4:A:304:ARG:N     | 2.49                     | 0.45              |
| 4:A:591:PRO:C     | 4:A:592:LEU:HD12  | 2.41                     | 0.45              |
| 4:B:238:ASP:HB3   | 4:B:239:PRO:HA    | 1.99                     | 0.45              |
| 4:B:1086:TYR:N    | 4:B:1087:GLU:HA   | 2.31                     | 0.45              |
| 4:C:25:LEU:HD23   | 4:C:59:LYS:HD2    | 1.99                     | 0.45              |
| 4:C:797:GLU:O     | 4:C:801:LEU:N     | 2.45                     | 0.45              |
| 4:D:1137:HIS:O    | 4:D:1139:LEU:N    | 2.48                     | 0.45              |
| 5:N:450:LEU:HB3   | 5:N:451:GLU:C     | 2.42                     | 0.45              |
| 5:N:498:GLU:CB    | 5:N:499:ASP:CA    | 2.94                     | 0.45              |
| 5:N:528:GLU:H     | 5:N:529:PRO:CD    | 2.29                     | 0.45              |
| 5:P:494:ALA:HB1   | 5:P:495:GLU:O     | 2.15                     | 0.45              |
| 4:C:590:VAL:HG13  | 4:C:604:TYR:CE1   | 2.52                     | 0.45              |
| 5:M:488:GLU:HA    | 5:M:489:ASP:HA    | 1.71                     | 0.45              |
| 5:N:386:ALA:HB1   | 5:N:388:LEU:HG    | 1.98                     | 0.45              |
| 5:N:506:ARG:HD3   | 5:N:506:ARG:N     | 2.31                     | 0.45              |
| 5:O:450:LEU:CB    | 5:O:451:GLU:CA    | 2.90                     | 0.45              |
| 4:A:397:MET:HE3   | 4:A:459:VAL:HA    | 1.98                     | 0.45              |
| 4:A:418:VAL:HG22  | 4:A:472:GLU:HB3   | 1.99                     | 0.45              |
| 4:A:1127:ALA:HB1  | 4:A:1128:PRO:CD   | 2.37                     | 0.45              |
| 4:B:421:GLY:N     | 4:B:625:LEU:HD21  | 2.31                     | 0.45              |
| 4:B:755:ALA:HB2   | 4:B:784:PHE:CD1   | 2.51                     | 0.45              |
| 4:B:1131:LEU:CD2  | 4:B:1181:VAL:HG21 | 2.47                     | 0.45              |
| 4:C:1029:ILE:CD1  | 4:C:1047:LEU:HD13 | 2.44                     | 0.45              |
| 4:C:1145:VAL:HG13 | 4:C:1149:LYS:HD2  | 1.98                     | 0.45              |
| 5:M:451:GLU:O     | 5:M:452:LYS:HG2   | 2.16                     | 0.45              |
| 5:M:507:LEU:N     | 5:M:507:LEU:HD22  | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:N:506:ARG:CA    | 5:N:510:LEU:HD22  | 2.42                     | 0.45              |
| 4:A:1205:PHE:O    | 4:A:1206:LEU:HD12 | 2.16                     | 0.45              |
| 4:B:69:ILE:HD11   | 4:B:285:LEU:HD11  | 1.97                     | 0.45              |
| 4:B:358:GLU:O     | 4:B:362:TRP:CD1   | 2.70                     | 0.45              |
| 4:B:1143:LYS:N    | 4:B:1144:GLY:CA   | 2.74                     | 0.45              |
| 4:C:755:ALA:HB2   | 4:C:784:PHE:CD1   | 2.52                     | 0.45              |
| 4:C:840:MET:HG2   | 4:C:861:ALA:HB2   | 1.99                     | 0.45              |
| 5:M:414:ARG:HA    | 5:M:417:GLU:CD    | 2.41                     | 0.45              |
| 5:O:394:THR:HG21  | 5:O:399:VAL:CG2   | 2.47                     | 0.45              |
| 5:P:434:LEU:N     | 5:P:435:PRO:CD    | 2.80                     | 0.45              |
| 4:A:23:ALA:HB2    | 4:A:215:TYR:HA    | 1.99                     | 0.45              |
| 4:A:549:MET:HA    | 4:A:555:ILE:HD13  | 1.98                     | 0.45              |
| 4:C:570:ARG:O     | 4:C:571:HIS:CG    | 2.70                     | 0.45              |
| 4:C:1095:GLU:HG2  | 4:C:1096:ASP:HB2  | 1.99                     | 0.45              |
| 4:D:58:LYS:HA     | 4:D:61:THR:HG22   | 1.99                     | 0.45              |
| 4:D:591:PRO:HG2   | 4:D:603:GLN:HB2   | 1.98                     | 0.45              |
| 4:D:1080:VAL:CG1  | 4:D:1082:PHE:HD2  | 2.25                     | 0.45              |
| 5:N:499:ASP:CG    | 5:N:515:LEU:HD11  | 2.42                     | 0.45              |
| 5:O:387:PHE:CD2   | 5:O:387:PHE:O     | 2.70                     | 0.45              |
| 5:P:525:GLU:CD    | 5:P:525:GLU:N     | 2.72                     | 0.45              |
| 4:B:1056:ARG:O    | 4:B:1065:MET:C    | 2.61                     | 0.44              |
| 4:C:1207:GLN:CB   | 4:C:1208:GLY:CA   | 2.94                     | 0.44              |
| 4:D:260:MET:HE2   | 4:D:260:MET:N     | 2.31                     | 0.44              |
| 4:D:1140:LEU:CG   | 4:D:1144:GLY:HA3  | 2.46                     | 0.44              |
| 4:D:1160:PRO:HG3  | 4:D:1201:ASP:OD2  | 2.16                     | 0.44              |
| 5:M:490:PRO:O     | 5:M:492:TRP:CD1   | 2.70                     | 0.44              |
| 5:O:369:HIS:CE1   | 5:O:370:HIS:NE2   | 2.84                     | 0.44              |
| 5:P:412:VAL:O     | 5:P:415:PHE:HD2   | 1.99                     | 0.44              |
| 5:P:499:ASP:HB3   | 5:P:500:PRO:HA    | 1.99                     | 0.44              |
| 4:B:333:GLU:O     | 4:B:337:LEU:CD1   | 2.65                     | 0.44              |
| 4:B:1029:ILE:HG21 | 4:B:1076:ALA:N    | 2.33                     | 0.44              |
| 4:C:300:LEU:HD13  | 4:C:303:GLY:HA2   | 1.99                     | 0.44              |
| 4:D:696:LEU:HD21  | 4:D:742:VAL:CG2   | 2.40                     | 0.44              |
| 4:D:785:VAL:CG1   | 4:D:795:GLU:HG3   | 2.46                     | 0.44              |
| 4:D:1051:VAL:CB   | 4:D:1093:LEU:HD23 | 2.47                     | 0.44              |
| 5:N:454:SER:HA    | 5:N:456:SER:HB2   | 1.99                     | 0.44              |
| 5:N:494:ALA:HB1   | 5:N:495:GLU:O     | 2.17                     | 0.44              |
| 5:N:524:PRO:N     | 5:N:525:GLU:HA    | 2.28                     | 0.44              |
| 5:P:412:VAL:O     | 5:P:415:PHE:CD2   | 2.70                     | 0.44              |
| 5:P:507:LEU:HD23  | 5:P:507:LEU:C     | 2.42                     | 0.44              |
| 4:A:191:LYS:O     | 4:A:195:VAL:HG23  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:941:ALA:HB2   | 4:A:1005:ALA:HB1  | 2.00                     | 0.44              |
| 4:B:110:VAL:HG11  | 4:B:589:LEU:C     | 2.43                     | 0.44              |
| 4:B:170:LEU:HD21  | 4:B:205:LEU:CD2   | 2.47                     | 0.44              |
| 4:B:230:ILE:CG1   | 4:B:507:VAL:HG13  | 2.48                     | 0.44              |
| 4:B:235:THR:HG22  | 4:B:236:LEU:N     | 2.30                     | 0.44              |
| 4:B:402:TYR:CE1   | 4:B:617:MET:HE1   | 2.52                     | 0.44              |
| 4:C:449:LEU:HD13  | 4:C:745:GLU:HB3   | 2.00                     | 0.44              |
| 4:C:838:GLU:HB3   | 4:C:882:VAL:HG21  | 2.00                     | 0.44              |
| 4:D:238:ASP:HB3   | 4:D:239:PRO:CA    | 2.47                     | 0.44              |
| 5:N:412:VAL:O     | 5:N:413:LEU:C     | 2.60                     | 0.44              |
| 5:N:508:ALA:HB2   | 5:N:511:LEU:HG    | 1.99                     | 0.44              |
| 5:O:370:HIS:CE1   | 5:O:401:GLU:HG3   | 2.52                     | 0.44              |
| 4:C:1104:GLU:O    | 4:C:1113:VAL:HG13 | 2.17                     | 0.44              |
| 4:D:1205:PHE:CD1  | 4:D:1205:PHE:O    | 2.70                     | 0.44              |
| 5:M:490:PRO:O     | 5:M:492:TRP:CE2   | 2.70                     | 0.44              |
| 5:N:517:TRP:HH2   | 5:N:524:PRO:HD3   | 1.82                     | 0.44              |
| 4:A:688:GLU:OE1   | 4:A:688:GLU:N     | 2.50                     | 0.44              |
| 4:A:1024:VAL:HG11 | 4:A:1205:PHE:CE2  | 2.53                     | 0.44              |
| 4:B:679:VAL:HG22  | 4:B:693:LEU:CD2   | 2.43                     | 0.44              |
| 4:B:1087:GLU:HB3  | 4:B:1088:GLY:HA3  | 2.00                     | 0.44              |
| 4:D:150:ILE:N     | 4:D:151:PRO:HD2   | 2.32                     | 0.44              |
| 4:D:421:GLY:N     | 4:D:625:LEU:HD21  | 2.33                     | 0.44              |
| 4:D:781:ARG:O     | 4:D:785:VAL:HG23  | 2.18                     | 0.44              |
| 5:M:505:ARG:HD2   | 5:M:510:LEU:HG    | 2.00                     | 0.44              |
| 5:N:508:ALA:HB2   | 5:N:511:LEU:H     | 1.82                     | 0.44              |
| 5:P:512:GLY:O     | 5:P:516:LEU:CD1   | 2.65                     | 0.44              |
| 4:A:301:PRO:HA    | 4:A:302:GLU:O     | 2.18                     | 0.44              |
| 4:A:951:ALA:HB2   | 4:A:993:LEU:CG    | 2.48                     | 0.44              |
| 4:A:1095:GLU:O    | 4:A:1097:ILE:HD12 | 2.18                     | 0.44              |
| 4:B:111:ARG:HG2   | 4:B:587:THR:HG22  | 2.00                     | 0.44              |
| 4:C:54:VAL:HG11   | 4:C:608:ALA:HB1   | 1.98                     | 0.44              |
| 4:C:1130:ALA:HB1  | 4:C:1160:PRO:O    | 2.18                     | 0.44              |
| 4:D:1188:LEU:HD12 | 4:D:1189:LEU:N    | 2.33                     | 0.44              |
| 5:M:423:HIS:N     | 5:M:423:HIS:ND1   | 2.63                     | 0.44              |
| 5:O:394:THR:HG21  | 5:O:399:VAL:HG21  | 2.00                     | 0.44              |
| 5:O:493:GLU:HB2   | 5:O:494:ALA:HA    | 2.00                     | 0.44              |
| 4:A:365:LEU:O     | 4:A:368:ARG:HB2   | 2.18                     | 0.44              |
| 4:A:635:VAL:HG22  | 4:A:838:GLU:HG3   | 1.99                     | 0.44              |
| 4:B:402:TYR:CE1   | 4:B:461:MET:HE3   | 2.53                     | 0.44              |
| 4:B:823:LEU:CD2   | 4:B:827:GLN:NE2   | 2.80                     | 0.44              |
| 4:C:1081:VAL:O    | 4:C:1082:PHE:CD1  | 2.70                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:1205:PHE:O    | 4:C:1206:LEU:HD23 | 2.18                     | 0.44              |
| 4:D:1203:GLU:O    | 4:D:1205:PHE:CE1  | 2.70                     | 0.44              |
| 4:D:1204:VAL:O    | 4:D:1205:PHE:CD1  | 2.69                     | 0.44              |
| 5:O:392:LYS:CD    | 5:O:397:ALA:HB3   | 2.48                     | 0.44              |
| 5:P:382:GLU:CG    | 5:P:388:LEU:HD21  | 2.48                     | 0.44              |
| 4:C:15:GLN:NE2    | 4:C:567:GLY:O     | 2.50                     | 0.44              |
| 4:C:151:PRO:C     | 4:C:154:ILE:HG22  | 2.43                     | 0.44              |
| 4:C:705:ILE:N     | 4:C:706:PRO:CD    | 2.81                     | 0.44              |
| 4:C:1204:VAL:HG12 | 4:C:1205:PHE:H    | 1.83                     | 0.44              |
| 4:D:501:LYS:O     | 4:D:505:LYS:HG3   | 2.18                     | 0.44              |
| 5:N:511:LEU:O     | 5:N:515:LEU:HD12  | 2.18                     | 0.44              |
| 4:A:45:THR:HG22   | 4:A:70:GLY:HA3    | 2.00                     | 0.43              |
| 4:B:525:ILE:HD11  | 4:B:538:ALA:HB3   | 1.98                     | 0.43              |
| 4:B:1080:VAL:HG11 | 4:B:1082:PHE:CE2  | 2.53                     | 0.43              |
| 4:C:291:MET:CE    | 4:C:613:GLY:CA    | 2.92                     | 0.43              |
| 4:C:737:THR:HG21  | 4:C:746:GLN:NE2   | 2.26                     | 0.43              |
| 4:C:970:ARG:HH21  | 4:C:975:LEU:HD22  | 1.76                     | 0.43              |
| 4:C:1093:LEU:CD1  | 4:C:1097:ILE:HD12 | 2.47                     | 0.43              |
| 4:C:1182:GLY:O    | 4:C:1183:GLU:CB   | 2.66                     | 0.43              |
| 5:M:491:PRO:O     | 5:M:492:TRP:CD2   | 2.70                     | 0.43              |
| 5:P:450:LEU:HB3   | 5:P:451:GLU:HB2   | 1.99                     | 0.43              |
| 4:B:11:HIS:CD2    | 4:B:212:ASP:OD1   | 2.70                     | 0.43              |
| 4:B:502:ALA:HB1   | 4:B:506:ASP:CG    | 2.43                     | 0.43              |
| 4:C:146:LEU:HD11  | 4:C:189:GLN:CG    | 2.47                     | 0.43              |
| 4:C:418:VAL:HG22  | 4:C:472:GLU:HB3   | 2.00                     | 0.43              |
| 4:C:731:ARG:HB3   | 4:C:732:PRO:HD3   | 2.00                     | 0.43              |
| 4:D:18:LEU:HD13   | 4:D:571:HIS:HA    | 2.00                     | 0.43              |
| 4:D:976:VAL:C     | 4:D:980:ALA:HB3   | 2.43                     | 0.43              |
| 4:D:1131:LEU:HD12 | 4:D:1197:TYR:O    | 2.17                     | 0.43              |
| 5:M:406:LEU:HD11  | 5:M:440:GLN:NE2   | 2.33                     | 0.43              |
| 5:M:419:LYS:HD2   | 5:M:422:HIS:CD2   | 2.52                     | 0.43              |
| 5:P:505:ARG:HG3   | 5:P:514:ARG:HH21  | 1.79                     | 0.43              |
| 5:P:505:ARG:NH1   | 5:P:532:GLU:OE1   | 2.48                     | 0.43              |
| 4:D:307:ALA:HB1   | 4:D:395:GLU:HG2   | 1.99                     | 0.43              |
| 4:D:542:VAL:CG2   | 4:D:543:PRO:HD3   | 2.48                     | 0.43              |
| 5:M:529:PRO:CB    | 5:M:530:VAL:HA    | 2.48                     | 0.43              |
| 5:N:506:ARG:HG2   | 5:N:507:LEU:H     | 1.76                     | 0.43              |
| 4:A:696:LEU:HD21  | 4:A:742:VAL:HG22  | 2.01                     | 0.43              |
| 4:B:226:VAL:HG21  | 4:B:561:VAL:HG11  | 1.97                     | 0.43              |
| 4:B:1145:VAL:O    | 4:B:1145:VAL:HG22 | 2.17                     | 0.43              |
| 4:C:930:VAL:HG12  | 4:C:935:LEU:HG    | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:577:ALA:HB1   | 4:D:618:ASP:HB3   | 2.00                     | 0.43              |
| 4:D:1093:LEU:HD11 | 4:D:1097:ILE:CG2  | 2.48                     | 0.43              |
| 5:M:443:VAL:HG13  | 5:M:444:GLU:CD    | 2.44                     | 0.43              |
| 5:N:401:GLU:O     | 5:N:405:HIS:CD2   | 2.71                     | 0.43              |
| 4:A:555:ILE:HD12  | 4:A:556:ARG:N     | 2.34                     | 0.43              |
| 4:B:424:ARG:CD    | 4:B:620:LEU:HD22  | 2.48                     | 0.43              |
| 4:C:1050:MET:HE3  | 4:C:1097:ILE:N    | 2.33                     | 0.43              |
| 4:D:1093:LEU:HD22 | 4:D:1099:LEU:HD11 | 2.00                     | 0.43              |
| 5:N:440:GLN:HB2   | 5:N:441:PHE:CB    | 2.47                     | 0.43              |
| 5:O:542:PRO:N     | 5:O:543:PRO:CD    | 2.82                     | 0.43              |
| 5:P:504:LEU:HB2   | 5:P:505:ARG:HG3   | 1.96                     | 0.43              |
| 4:B:938:LEU:HG    | 4:B:943:ALA:HB3   | 2.01                     | 0.43              |
| 4:C:635:VAL:HG22  | 4:C:838:GLU:HG3   | 1.99                     | 0.43              |
| 4:D:35:THR:HG23   | 4:D:253:THR:HG22  | 2.00                     | 0.43              |
| 5:N:492:TRP:O     | 5:N:493:GLU:C     | 2.62                     | 0.43              |
| 5:P:413:LEU:O     | 5:P:414:ARG:C     | 2.60                     | 0.43              |
| 4:A:151:PRO:HB3   | 4:A:192:VAL:HG11  | 2.01                     | 0.43              |
| 4:A:192:VAL:HG12  | 4:A:196:LEU:HD12  | 2.00                     | 0.43              |
| 4:B:868:VAL:HG22  | 4:B:887:ILE:HB    | 2.01                     | 0.43              |
| 4:C:290:LYS:O     | 4:C:291:MET:CG    | 2.67                     | 0.43              |
| 4:C:297:ARG:CZ    | 4:C:306:GLU:HB2   | 2.49                     | 0.43              |
| 4:C:574:VAL:HG22  | 4:C:601:VAL:HG21  | 2.00                     | 0.43              |
| 4:C:665:LYS:HB2   | 4:C:832:LYS:HZ2   | 1.82                     | 0.43              |
| 4:D:155:LEU:HD13  | 4:D:192:VAL:HG22  | 2.01                     | 0.43              |
| 4:D:390:GLU:OE2   | 4:D:432:VAL:HG23  | 2.19                     | 0.43              |
| 5:N:518:VAL:HA    | 5:N:519:ARG:HG3   | 1.99                     | 0.43              |
| 5:O:502:GLU:O     | 5:O:503:GLU:CG    | 2.66                     | 0.43              |
| 4:A:788:ALA:HB1   | 4:A:793:VAL:HG22  | 2.00                     | 0.43              |
| 4:C:150:ILE:HG23  | 4:C:162:ALA:HB1   | 2.00                     | 0.43              |
| 4:C:357:VAL:HB    | 4:C:362:TRP:CH2   | 2.53                     | 0.43              |
| 4:C:1080:VAL:CB   | 4:C:1082:PHE:CD2  | 3.01                     | 0.43              |
| 5:M:524:PRO:HG2   | 5:M:526:ALA:HB2   | 2.01                     | 0.43              |
| 4:A:366:ARG:O     | 4:A:368:ARG:N     | 2.43                     | 0.43              |
| 4:A:930:VAL:HG12  | 4:A:935:LEU:HG    | 2.01                     | 0.43              |
| 4:B:300:LEU:O     | 4:B:302:GLU:N     | 2.52                     | 0.43              |
| 4:B:307:ALA:HB1   | 4:B:395:GLU:CD    | 2.44                     | 0.43              |
| 4:D:302:GLU:HB3   | 4:D:304:ARG:N     | 2.32                     | 0.43              |
| 4:D:473:ARG:NH1   | 4:D:477:ILE:HD11  | 2.34                     | 0.43              |
| 5:M:504:LEU:HD13  | 5:M:536:GLY:HA2   | 2.00                     | 0.43              |
| 5:N:454:SER:C     | 5:N:456:SER:HB2   | 2.44                     | 0.43              |
| 4:A:1099:LEU:HD22 | 4:A:1118:VAL:HG12 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1099:LEU:CD2  | 4:A:1120:THR:HG22 | 2.48                     | 0.43              |
| 4:C:1176:LEU:CD1  | 4:C:1177:ARG:N    | 2.81                     | 0.43              |
| 4:A:334:VAL:HG21  | 4:A:384:LEU:HD11  | 2.00                     | 0.42              |
| 4:A:338:LEU:HD11  | 4:A:365:LEU:HD11  | 2.02                     | 0.42              |
| 4:A:572:ALA:CB    | 4:A:573:SER:CB    | 2.63                     | 0.42              |
| 4:B:356:ARG:C     | 4:B:357:VAL:HG13  | 2.43                     | 0.42              |
| 4:C:493:GLY:HA2   | 4:C:573:SER:O     | 2.19                     | 0.42              |
| 4:C:1079:VAL:CG1  | 4:C:1080:VAL:N    | 2.82                     | 0.42              |
| 4:C:1205:PHE:C    | 4:C:1206:LEU:HG   | 2.44                     | 0.42              |
| 4:D:100:ALA:HB2   | 4:D:109:LEU:CD1   | 2.49                     | 0.42              |
| 5:O:492:TRP:O     | 5:O:493:GLU:C     | 2.62                     | 0.42              |
| 5:P:504:LEU:CB    | 5:P:505:ARG:CG    | 2.94                     | 0.42              |
| 4:A:150:ILE:HD11  | 4:A:166:LEU:HA    | 2.02                     | 0.42              |
| 4:A:971:GLY:HA3   | 4:A:975:LEU:HD22  | 1.69                     | 0.42              |
| 4:B:1129:LYS:O    | 4:B:1159:LEU:HD22 | 2.18                     | 0.42              |
| 4:D:1057:LYS:CD   | 4:D:1064:MET:N    | 2.82                     | 0.42              |
| 5:M:403:ARG:HE    | 5:M:437:ALA:CB    | 2.32                     | 0.42              |
| 4:B:574:VAL:HG22  | 4:B:601:VAL:HG21  | 2.00                     | 0.42              |
| 4:C:459:VAL:HG23  | 4:C:459:VAL:O     | 2.19                     | 0.42              |
| 5:O:493:GLU:O     | 5:O:504:LEU:HD12  | 2.19                     | 0.42              |
| 5:O:519:ARG:HG2   | 5:O:520:LYS:HB2   | 1.98                     | 0.42              |
| 5:P:385:ARG:HB3   | 5:P:386:ALA:HA    | 2.02                     | 0.42              |
| 5:P:503:GLU:HB3   | 5:P:504:LEU:HD12  | 2.00                     | 0.42              |
| 4:B:230:ILE:CD1   | 4:B:507:VAL:HG22  | 2.49                     | 0.42              |
| 4:C:1119:TRP:CD1  | 4:C:1123:GLU:HB2  | 2.54                     | 0.42              |
| 4:D:428:ALA:HB3   | 4:D:816:SER:HB2   | 2.01                     | 0.42              |
| 5:N:440:GLN:CB    | 5:N:441:PHE:CA    | 2.97                     | 0.42              |
| 5:O:447:ALA:C     | 5:O:448:PHE:CG    | 2.96                     | 0.42              |
| 4:A:28:LEU:CD1    | 4:A:251:VAL:HG21  | 2.50                     | 0.42              |
| 4:B:362:TRP:O     | 4:B:363:GLU:C     | 2.59                     | 0.42              |
| 4:B:1213:PRO:O    | 4:B:1217:VAL:HG23 | 2.19                     | 0.42              |
| 4:C:103:PHE:CE1   | 4:C:286:PRO:HD3   | 2.54                     | 0.42              |
| 4:C:827:GLN:O     | 4:C:831:VAL:HG23  | 2.19                     | 0.42              |
| 4:C:1096:ASP:O    | 4:C:1097:ILE:CG1  | 2.67                     | 0.42              |
| 4:D:1080:VAL:HG23 | 4:D:1115:ALA:H    | 1.83                     | 0.42              |
| 5:M:440:GLN:CB    | 5:M:441:PHE:HA    | 2.50                     | 0.42              |
| 5:M:490:PRO:HB2   | 5:M:492:TRP:CD1   | 2.55                     | 0.42              |
| 5:M:494:ALA:CB    | 5:M:503:GLU:OE2   | 2.68                     | 0.42              |
| 5:O:392:LYS:HA    | 5:O:394:THR:N     | 2.34                     | 0.42              |
| 5:O:450:LEU:HA    | 5:O:451:GLU:HG3   | 2.01                     | 0.42              |
| 5:P:455:LEU:N     | 5:P:456:SER:HA    | 2.33                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:498:GLU:HB2   | 5:P:499:ASP:CA    | 2.49                     | 0.42              |
| 4:A:675:MET:O     | 4:A:679:VAL:HG23  | 2.20                     | 0.42              |
| 4:B:260:MET:HE2   | 4:B:260:MET:CA    | 2.49                     | 0.42              |
| 4:B:357:VAL:CA    | 4:B:358:GLU:HG3   | 2.49                     | 0.42              |
| 4:B:952:ARG:NH1   | 5:N:373:LYS:HB3   | 2.34                     | 0.42              |
| 4:B:976:VAL:HG21  | 4:C:115:ARG:NH1   | 2.34                     | 0.42              |
| 4:B:1093:LEU:HG   | 4:B:1097:ILE:HB   | 2.01                     | 0.42              |
| 4:C:321:ARG:HD3   | 4:C:434:TYR:CE2   | 2.54                     | 0.42              |
| 4:C:609:VAL:HG13  | 4:C:614:LEU:HD12  | 2.01                     | 0.42              |
| 4:D:186:LEU:HD21  | 4:D:245:PRO:HB2   | 2.01                     | 0.42              |
| 4:D:259:ALA:C     | 4:D:260:MET:HE2   | 2.43                     | 0.42              |
| 5:O:452:LYS:HZ2   | 5:O:509:ARG:NH2   | 2.18                     | 0.42              |
| 5:P:505:ARG:CZ    | 5:P:510:LEU:CD1   | 2.80                     | 0.42              |
| 5:P:532:GLU:HA    | 5:P:535:ILE:HD11  | 1.93                     | 0.42              |
| 4:A:1182:GLY:O    | 4:A:1183:GLU:C    | 2.61                     | 0.42              |
| 4:D:238:ASP:HB3   | 4:D:239:PRO:C     | 2.45                     | 0.42              |
| 4:D:1102:LEU:HD11 | 4:D:1206:LEU:CG   | 2.46                     | 0.42              |
| 4:B:313:LEU:HB3   | 4:B:436:VAL:HG13  | 2.02                     | 0.42              |
| 4:C:321:ARG:HD3   | 4:C:434:TYR:CZ    | 2.55                     | 0.42              |
| 4:C:407:GLN:CD    | 4:C:436:VAL:CG1   | 2.89                     | 0.42              |
| 4:C:541:VAL:CG2   | 4:C:542:VAL:HA    | 2.40                     | 0.42              |
| 4:D:226:VAL:HB    | 4:D:510:VAL:HG21  | 2.01                     | 0.42              |
| 4:D:424:ARG:NH1   | 4:D:620:LEU:HD22  | 2.35                     | 0.42              |
| 4:D:554:ARG:O     | 4:D:558:VAL:HG23  | 2.20                     | 0.42              |
| 4:D:1082:PHE:CZ   | 4:D:1113:VAL:O    | 2.73                     | 0.42              |
| 4:D:1181:VAL:HG12 | 4:D:1182:GLY:N    | 2.34                     | 0.42              |
| 4:A:237:ASP:OD1   | 4:A:237:ASP:N     | 2.53                     | 0.42              |
| 4:C:406:VAL:HA    | 4:C:409:TYR:CE2   | 2.55                     | 0.42              |
| 4:D:897:VAL:CG2   | 4:D:938:LEU:HD13  | 2.49                     | 0.42              |
| 5:N:504:LEU:CD1   | 5:N:535:ILE:HD12  | 2.50                     | 0.42              |
| 5:O:455:LEU:N     | 5:O:456:SER:HB3   | 2.35                     | 0.42              |
| 3:I:18:DC:H2"     | 3:I:19:DC:C6      | 2.55                     | 0.42              |
| 4:A:1093:LEU:HD23 | 4:A:1093:LEU:C    | 2.45                     | 0.42              |
| 4:A:1161:VAL:HG23 | 4:A:1176:LEU:HD11 | 2.02                     | 0.42              |
| 4:B:602:THR:HG22  | 4:B:604:TYR:H     | 1.84                     | 0.42              |
| 4:B:1069:THR:HG23 | 4:B:1077:LEU:O    | 2.19                     | 0.42              |
| 4:D:1093:LEU:HD22 | 4:D:1099:LEU:HD12 | 2.01                     | 0.42              |
| 5:M:383:GLY:O     | 5:M:386:ALA:HB2   | 2.20                     | 0.42              |
| 5:M:498:GLU:HB2   | 5:M:499:ASP:HA    | 2.02                     | 0.42              |
| 5:N:524:PRO:CB    | 5:N:525:GLU:HA    | 2.49                     | 0.42              |
| 5:O:443:VAL:HG13  | 5:O:444:GLU:N     | 2.35                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:O:505:ARG:HH12  | 5:O:506:ARG:HH12 | 1.67                     | 0.42              |
| 5:P:524:PRO:HD2   | 5:P:526:ALA:CB   | 2.50                     | 0.42              |
| 5:P:527:GLU:N     | 5:P:528:GLU:HA   | 2.35                     | 0.42              |
| 4:B:200:ALA:HB3   | 4:B:207:MET:CE   | 2.50                     | 0.41              |
| 4:B:335:LEU:HD12  | 4:B:354:LEU:HD21 | 2.02                     | 0.41              |
| 4:C:958:GLU:HB3   | 4:C:959:PRO:HD3  | 2.02                     | 0.41              |
| 4:D:498:LEU:HD13  | 4:D:570:ARG:HE   | 1.85                     | 0.41              |
| 4:D:952:ARG:HD2   | 5:P:375:GLY:H    | 1.85                     | 0.41              |
| 4:D:1024:VAL:HG12 | 4:D:1046:LEU:CD1 | 2.50                     | 0.41              |
| 5:M:524:PRO:HD2   | 5:M:525:GLU:CA   | 2.46                     | 0.41              |
| 5:N:440:GLN:HB3   | 5:N:441:PHE:HA   | 2.02                     | 0.41              |
| 4:B:691:ILE:HG22  | 4:B:743:TYR:OH   | 2.20                     | 0.41              |
| 4:B:1021:LEU:HD22 | 4:B:1048:SER:CB  | 2.50                     | 0.41              |
| 4:C:18:LEU:HD13   | 4:C:571:HIS:HB3  | 2.01                     | 0.41              |
| 4:C:192:VAL:HG12  | 4:C:196:LEU:CD1  | 2.49                     | 0.41              |
| 4:D:25:LEU:HD23   | 4:D:59:LYS:HD2   | 2.02                     | 0.41              |
| 4:D:402:TYR:O     | 4:D:406:VAL:HG23 | 2.20                     | 0.41              |
| 4:D:705:ILE:HB    | 4:D:706:PRO:HD3  | 2.01                     | 0.41              |
| 4:D:939:VAL:CG2   | 4:D:944:LEU:HD12 | 2.44                     | 0.41              |
| 5:M:400:ARG:O     | 5:M:404:PRO:CD   | 2.68                     | 0.41              |
| 5:N:390:ALA:C     | 5:N:392:LYS:H    | 2.28                     | 0.41              |
| 5:O:525:GLU:O     | 5:O:526:ALA:C    | 2.61                     | 0.41              |
| 5:P:416:PRO:CG    | 5:P:417:GLU:N    | 2.80                     | 0.41              |
| 4:A:909:ARG:O     | 4:A:912:GLY:O    | 2.37                     | 0.41              |
| 4:C:142:LEU:HD23  | 4:C:178:PHE:HB2  | 2.02                     | 0.41              |
| 4:C:297:ARG:HD3   | 4:C:297:ARG:HA   | 1.97                     | 0.41              |
| 4:C:410:ILE:HG22  | 4:C:414:ARG:NH1  | 2.35                     | 0.41              |
| 4:D:413:ALA:HB1   | 4:D:418:VAL:HB   | 2.01                     | 0.41              |
| 4:D:1123:GLU:HG2  | 4:D:1216:GLU:HB3 | 2.02                     | 0.41              |
| 5:M:393:PRO:O     | 5:M:394:THR:CB   | 2.68                     | 0.41              |
| 5:O:521:PRO:HG2   | 5:O:523:ALA:H    | 1.83                     | 0.41              |
| 5:P:528:GLU:HG2   | 5:P:528:GLU:H    | 1.58                     | 0.41              |
| 4:A:216:VAL:HG12  | 4:A:217:ARG:HG3  | 2.02                     | 0.41              |
| 4:A:615:LEU:HD21  | 4:A:617:MET:HE3  | 2.02                     | 0.41              |
| 4:B:941:ALA:HB2   | 4:B:1005:ALA:HB1 | 2.02                     | 0.41              |
| 4:B:1021:LEU:HD22 | 4:B:1048:SER:OG  | 2.20                     | 0.41              |
| 4:C:313:LEU:CD1   | 4:C:407:GLN:NE2  | 2.83                     | 0.41              |
| 4:C:574:VAL:HG22  | 4:C:601:VAL:CG2  | 2.50                     | 0.41              |
| 4:D:605:ASP:O     | 4:D:609:VAL:HG23 | 2.20                     | 0.41              |
| 1:G:18:DC:H1'     | 1:G:19:DC:C5     | 2.56                     | 0.41              |
| 1:G:19:DC:C4      | 2:H:10:DG:C6     | 3.08                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1129:LYS:HB3  | 4:A:1198:LEU:HG   | 2.01                     | 0.41              |
| 4:B:453:PHE:CZ    | 4:B:464:ILE:HD11  | 2.54                     | 0.41              |
| 4:B:1089:VAL:CG2  | 4:B:1118:VAL:HG12 | 2.44                     | 0.41              |
| 4:D:110:VAL:HG13  | 4:D:591:PRO:N     | 2.35                     | 0.41              |
| 4:D:300:LEU:HD22  | 4:D:304:ARG:HB3   | 2.01                     | 0.41              |
| 4:D:407:GLN:HG3   | 4:D:436:VAL:CG1   | 2.51                     | 0.41              |
| 4:D:1008:ILE:O    | 4:D:1010:VAL:N    | 2.54                     | 0.41              |
| 5:M:494:ALA:HB2   | 5:M:503:GLU:CD    | 2.46                     | 0.41              |
| 5:N:505:ARG:HD2   | 5:N:510:LEU:CD2   | 2.46                     | 0.41              |
| 5:O:367:HIS:CE1   | 5:O:401:GLU:HG2   | 2.55                     | 0.41              |
| 5:P:404:PRO:HA    | 5:P:433:LEU:HD13  | 2.02                     | 0.41              |
| 5:P:412:VAL:CB    | 5:P:415:PHE:HD2   | 2.14                     | 0.41              |
| 4:A:794:PRO:O     | 4:A:795:GLU:C     | 2.64                     | 0.41              |
| 4:B:1032:LEU:CD2  | 4:B:1077:LEU:HD11 | 2.50                     | 0.41              |
| 5:M:419:LYS:O     | 5:M:423:HIS:ND1   | 2.53                     | 0.41              |
| 5:M:538:ASN:O     | 5:M:542:PRO:CD    | 2.66                     | 0.41              |
| 5:N:506:ARG:CG    | 5:N:507:LEU:N     | 2.73                     | 0.41              |
| 5:P:519:ARG:HB3   | 5:P:520:LYS:CB    | 2.50                     | 0.41              |
| 1:G:12:DC:H2"     | 1:G:13:DC:C6      | 2.55                     | 0.41              |
| 4:A:1099:LEU:HD22 | 4:A:1118:VAL:CG1  | 2.51                     | 0.41              |
| 4:A:1189:LEU:HD23 | 4:A:1189:LEU:C    | 2.46                     | 0.41              |
| 4:B:1047:LEU:HD12 | 4:B:1048:SER:H    | 1.85                     | 0.41              |
| 4:D:1099:LEU:HD22 | 4:D:1118:VAL:HG13 | 2.02                     | 0.41              |
| 5:N:504:LEU:HD11  | 5:N:536:GLY:HA2   | 2.02                     | 0.41              |
| 5:N:507:LEU:N     | 5:N:507:LEU:HD23  | 2.35                     | 0.41              |
| 5:P:407:GLU:O     | 5:P:415:PHE:HB3   | 2.20                     | 0.41              |
| 4:A:81:PHE:O      | 4:A:83:ARG:HG3    | 2.21                     | 0.41              |
| 4:A:223:ALA:O     | 4:A:226:VAL:HG22  | 2.21                     | 0.41              |
| 4:A:679:VAL:HG22  | 4:A:693:LEU:CD2   | 2.51                     | 0.41              |
| 4:B:296:PRO:HG2   | 4:B:581:ILE:HG22  | 2.03                     | 0.41              |
| 4:B:329:ALA:O     | 4:B:333:GLU:HG3   | 2.21                     | 0.41              |
| 4:B:357:VAL:CA    | 4:B:358:GLU:CB    | 2.99                     | 0.41              |
| 4:D:284:ASP:HB3   | 4:D:290:LYS:HZ1   | 1.82                     | 0.41              |
| 4:D:1008:ILE:O    | 4:D:1010:VAL:HG23 | 2.20                     | 0.41              |
| 4:D:1057:LYS:HG2  | 4:D:1064:MET:N    | 2.28                     | 0.41              |
| 4:D:1059:THR:HG23 | 4:D:1064:MET:O    | 2.21                     | 0.41              |
| 5:P:395:LEU:HG    | 5:P:396:ARG:H     | 1.85                     | 0.41              |
| 1:G:13:DC:OP1     | 4:B:900:MET:HE2   | 2.21                     | 0.41              |
| 4:A:627:PHE:CE1   | 4:A:842:ALA:HB3   | 2.55                     | 0.41              |
| 4:B:1054:VAL:HG13 | 4:B:1054:VAL:O    | 2.20                     | 0.41              |
| 4:B:1080:VAL:HG11 | 4:B:1082:PHE:CD2  | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:10:LEU:HA     | 4:C:43:ALA:HB3    | 2.03                     | 0.41              |
| 4:C:664:THR:HG21  | 4:C:670:LEU:HD13  | 2.02                     | 0.41              |
| 4:C:873:VAL:HG11  | 4:C:944:LEU:HD21  | 2.02                     | 0.41              |
| 4:D:410:ILE:CD1   | 4:D:438:ILE:HG23  | 2.50                     | 0.41              |
| 4:D:1021:LEU:HB3  | 4:D:1048:SER:HB2  | 2.02                     | 0.41              |
| 4:D:1093:LEU:HD21 | 4:D:1097:ILE:O    | 2.21                     | 0.41              |
| 4:D:1204:VAL:HG13 | 4:D:1205:PHE:H    | 1.86                     | 0.41              |
| 5:M:420:ALA:O     | 5:M:421:PHE:C     | 2.63                     | 0.41              |
| 5:N:444:GLU:O     | 5:N:445:GLU:C     | 2.64                     | 0.41              |
| 5:N:530:VAL:O     | 5:N:530:VAL:CG2   | 2.66                     | 0.41              |
| 5:P:373:LYS:HG2   | 5:P:378:GLN:HB2   | 2.03                     | 0.41              |
| 5:P:520:LYS:N     | 5:P:521:PRO:HD3   | 2.36                     | 0.41              |
| 5:P:526:ALA:O     | 5:P:527:GLU:CB    | 2.69                     | 0.41              |
| 5:P:526:ALA:O     | 5:P:527:GLU:HG3   | 2.21                     | 0.41              |
| 4:A:100:ALA:HB2   | 4:A:109:LEU:HD12  | 2.02                     | 0.41              |
| 4:A:1019:PRO:O    | 4:A:1020:GLY:C    | 2.62                     | 0.41              |
| 4:B:228:LEU:HD22  | 4:B:242:TRP:CE3   | 2.55                     | 0.41              |
| 4:C:222:ARG:O     | 4:C:226:VAL:HG13  | 2.21                     | 0.41              |
| 4:C:451:GLU:OE1   | 4:C:451:GLU:N     | 2.53                     | 0.41              |
| 4:D:521:LEU:HA    | 4:D:524:LEU:HD23  | 2.03                     | 0.41              |
| 5:M:392:LYS:NZ    | 5:M:399:VAL:HG21  | 2.36                     | 0.41              |
| 5:O:490:PRO:CD    | 5:O:522:LYS:HD2   | 2.51                     | 0.41              |
| 5:P:540:ILE:O     | 5:P:543:PRO:CD    | 2.69                     | 0.41              |
| 4:A:422:PRO:HG2   | 4:A:820:ALA:HB1   | 2.03                     | 0.40              |
| 4:A:918:LEU:HD23  | 4:A:960:LEU:CD1   | 2.50                     | 0.40              |
| 4:B:302:GLU:OE2   | 4:B:304:ARG:NH1   | 2.54                     | 0.40              |
| 4:B:428:ALA:HA    | 4:B:439:THR:HG21  | 2.03                     | 0.40              |
| 4:B:1081:VAL:O    | 4:B:1081:VAL:HG23 | 2.20                     | 0.40              |
| 4:D:1065:MET:HB3  | 4:D:1066:ALA:H    | 1.18                     | 0.40              |
| 5:O:519:ARG:CZ    | 5:O:520:LYS:HZ3   | 2.33                     | 0.40              |
| 5:O:542:PRO:N     | 5:O:543:PRO:HD3   | 2.36                     | 0.40              |
| 5:P:528:GLU:N     | 5:P:529:PRO:CD    | 2.82                     | 0.40              |
| 4:B:509:ARG:CA    | 4:B:513:ILE:HG21  | 2.49                     | 0.40              |
| 4:B:1056:ARG:CA   | 4:B:1066:ALA:HB2  | 2.46                     | 0.40              |
| 4:C:877:GLY:H     | 4:C:881:LYS:HZ1   | 1.69                     | 0.40              |
| 4:D:1140:LEU:HD11 | 4:D:1144:GLY:HA3  | 2.02                     | 0.40              |
| 4:D:1207:GLN:HG3  | 4:D:1207:GLN:O    | 2.20                     | 0.40              |
| 4:D:1207:GLN:O    | 4:D:1207:GLN:CG   | 2.70                     | 0.40              |
| 5:M:412:VAL:C     | 5:M:414:ARG:N     | 2.76                     | 0.40              |
| 5:N:450:LEU:CB    | 5:N:451:GLU:HB2   | 2.50                     | 0.40              |
| 5:N:495:GLU:HB2   | 5:N:496:GLU:CG    | 2.51                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:O:415:PHE:HB2   | 5:O:416:PRO:HD3  | 2.02                     | 0.40              |
| 5:O:519:ARG:NE    | 5:O:520:LYS:HZ3  | 2.18                     | 0.40              |
| 5:P:504:LEU:CB    | 5:P:505:ARG:CA   | 2.99                     | 0.40              |
| 4:A:498:LEU:HB3   | 4:A:499:ALA:CA   | 2.51                     | 0.40              |
| 4:A:505:LYS:HB3   | 4:A:509:ARG:HB2  | 2.04                     | 0.40              |
| 4:C:773:ARG:O     | 4:C:774:VAL:C    | 2.65                     | 0.40              |
| 4:C:1094:LYS:CE   | 4:C:1094:LYS:CA  | 2.98                     | 0.40              |
| 4:D:678:THR:CG2   | 4:D:693:LEU:HD11 | 2.52                     | 0.40              |
| 4:D:1205:PHE:O    | 4:D:1206:LEU:CG  | 2.70                     | 0.40              |
| 5:M:453:LYS:O     | 5:M:454:SER:HB3  | 2.22                     | 0.40              |
| 5:O:373:LYS:HG2   | 5:O:378:GLN:HB2  | 2.02                     | 0.40              |
| 5:P:498:GLU:CB    | 5:P:499:ASP:CA   | 3.00                     | 0.40              |
| 5:P:504:LEU:HD12  | 5:P:504:LEU:H    | 1.82                     | 0.40              |
| 5:P:512:GLY:O     | 5:P:516:LEU:CG   | 2.66                     | 0.40              |
| 3:I:13:DC:H1'     | 3:I:14:DA:C8     | 2.57                     | 0.40              |
| 4:A:1124:VAL:HG13 | 4:A:1200:PRO:HG2 | 2.04                     | 0.40              |
| 4:B:620:LEU:HD12  | 4:B:620:LEU:N    | 2.36                     | 0.40              |
| 4:B:1008:ILE:C    | 4:B:1008:ILE:CD1 | 2.94                     | 0.40              |
| 4:B:1093:LEU:HD22 | 4:B:1099:LEU:CG  | 2.52                     | 0.40              |
| 4:C:15:GLN:N      | 4:C:23:ALA:O     | 2.54                     | 0.40              |
| 4:D:918:LEU:HD22  | 4:D:953:LEU:HD23 | 2.04                     | 0.40              |
| 4:D:1058:PRO:O    | 4:D:1058:PRO:CD  | 2.70                     | 0.40              |
| 4:D:1120:THR:HG22 | 4:D:1121:LEU:N   | 2.36                     | 0.40              |
| 4:D:1188:LEU:O    | 4:D:1191:ALA:HB3 | 2.20                     | 0.40              |
| 4:D:1204:VAL:C    | 4:D:1205:PHE:CD1 | 2.99                     | 0.40              |
| 5:M:409:LYS:HB2   | 5:M:415:PHE:HE1  | 1.87                     | 0.40              |
| 5:O:455:LEU:CA    | 5:O:456:SER:C    | 2.92                     | 0.40              |
| 4:B:574:VAL:HG22  | 4:B:601:VAL:CG2  | 2.52                     | 0.40              |
| 4:C:402:TYR:HE1   | 4:C:615:LEU:HD11 | 1.87                     | 0.40              |
| 4:C:788:ALA:HB1   | 4:C:793:VAL:HG22 | 1.99                     | 0.40              |
| 4:C:1082:PHE:O    | 4:C:1083:GLY:C   | 2.65                     | 0.40              |
| 4:D:183:ASN:OD1   | 4:D:184:HIS:O    | 2.39                     | 0.40              |
| 4:D:976:VAL:HG23  | 4:D:977:GLY:H    | 1.87                     | 0.40              |
| 4:D:1057:LYS:CB   | 4:D:1058:PRO:HA  | 2.29                     | 0.40              |
| 5:O:518:VAL:CG2   | 5:O:519:ARG:HB2  | 2.46                     | 0.40              |

All (7) 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) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:D:175:ASP:OD1 | 5:P:414:ARG:NH1[2_655] | 1.84                     | 0.36              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:A:115:ARG:NE  | 4:A:976:VAL:CG1[2_555] | 1.90                     | 0.30              |
| 4:A:115:ARG:NH2 | 4:A:976:VAL:CG2[2_555] | 1.95                     | 0.25              |
| 4:B:363:GLU:OE2 | 4:B:969:GLU:OE2[1_545] | 2.01                     | 0.19              |
| 4:D:160:ASP:N   | 5:N:454:SER:OG[1_545]  | 2.01                     | 0.19              |
| 4:B:715:GLN:OE1 | 5:P:413:LEU:CD2[2_655] | 2.05                     | 0.15              |
| 4:B:273:ASN:OD1 | 4:B:1057:LYS:O[2_646]  | 2.16                     | 0.04              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 4   | A     | 1146/1220 (94%) | 1036 (90%) | 87 (8%)  | 23 (2%)  | 6           | 31 |
| 4   | B     | 1147/1220 (94%) | 1051 (92%) | 76 (7%)  | 20 (2%)  | 7           | 35 |
| 4   | C     | 1148/1220 (94%) | 1056 (92%) | 79 (7%)  | 13 (1%)  | 11          | 43 |
| 4   | D     | 1173/1220 (96%) | 1062 (90%) | 94 (8%)  | 17 (1%)  | 9           | 39 |
| 5   | M     | 132/177 (75%)   | 84 (64%)   | 31 (24%) | 17 (13%) | 0           | 1  |
| 5   | N     | 129/177 (73%)   | 76 (59%)   | 28 (22%) | 25 (19%) | 0           | 0  |
| 5   | O     | 129/177 (73%)   | 77 (60%)   | 28 (22%) | 24 (19%) | 0           | 0  |
| 5   | P     | 132/177 (75%)   | 80 (61%)   | 33 (25%) | 19 (14%) | 0           | 1  |
| All | All   | 5136/5588 (92%) | 4522 (88%) | 456 (9%) | 158 (3%) | 3           | 22 |

All (158) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | A     | 506  | ASP  |
| 4   | A     | 1081 | VAL  |
| 4   | A     | 1201 | ASP  |
| 4   | A     | 1204 | VAL  |
| 4   | B     | 301  | PRO  |
| 4   | B     | 1058 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | C     | 299  | PRO  |
| 4   | C     | 1204 | VAL  |
| 4   | D     | 301  | PRO  |
| 4   | D     | 543  | PRO  |
| 4   | D     | 1057 | LYS  |
| 4   | D     | 1065 | MET  |
| 4   | D     | 1081 | VAL  |
| 5   | M     | 393  | PRO  |
| 5   | M     | 452  | LYS  |
| 5   | M     | 454  | SER  |
| 5   | M     | 455  | LEU  |
| 5   | M     | 493  | GLU  |
| 5   | M     | 521  | PRO  |
| 5   | M     | 523  | ALA  |
| 5   | N     | 396  | ARG  |
| 5   | N     | 413  | LEU  |
| 5   | N     | 444  | GLU  |
| 5   | N     | 445  | GLU  |
| 5   | N     | 452  | LYS  |
| 5   | N     | 453  | LYS  |
| 5   | N     | 454  | SER  |
| 5   | N     | 492  | TRP  |
| 5   | N     | 523  | ALA  |
| 5   | N     | 530  | VAL  |
| 5   | N     | 542  | PRO  |
| 5   | O     | 391  | LEU  |
| 5   | O     | 393  | PRO  |
| 5   | O     | 413  | LEU  |
| 5   | O     | 454  | SER  |
| 5   | O     | 492  | TRP  |
| 5   | O     | 524  | PRO  |
| 5   | O     | 530  | VAL  |
| 5   | P     | 392  | LYS  |
| 5   | P     | 397  | ALA  |
| 5   | P     | 452  | LYS  |
| 5   | P     | 521  | PRO  |
| 5   | P     | 523  | ALA  |
| 5   | P     | 527  | GLU  |
| 4   | A     | 303  | GLY  |
| 4   | A     | 511  | TYR  |
| 4   | A     | 1192 | GLU  |
| 4   | B     | 302  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 1013 | HIS  |
| 4   | B     | 1025 | ALA  |
| 4   | B     | 1081 | VAL  |
| 4   | B     | 1091 | PRO  |
| 4   | B     | 1176 | LEU  |
| 4   | C     | 976  | VAL  |
| 4   | D     | 286  | PRO  |
| 4   | D     | 977  | GLY  |
| 4   | D     | 1082 | PHE  |
| 4   | D     | 1138 | ALA  |
| 4   | D     | 1204 | VAL  |
| 5   | M     | 449  | VAL  |
| 5   | M     | 453  | LYS  |
| 5   | M     | 488  | GLU  |
| 5   | N     | 373  | LYS  |
| 5   | N     | 397  | ALA  |
| 5   | N     | 440  | GLN  |
| 5   | N     | 491  | PRO  |
| 5   | N     | 527  | GLU  |
| 5   | O     | 394  | THR  |
| 5   | O     | 491  | PRO  |
| 5   | O     | 518  | VAL  |
| 5   | O     | 521  | PRO  |
| 5   | P     | 440  | GLN  |
| 5   | P     | 449  | VAL  |
| 5   | P     | 454  | SER  |
| 4   | A     | 290  | LYS  |
| 4   | A     | 302  | GLU  |
| 4   | A     | 367  | LYS  |
| 4   | A     | 573  | SER  |
| 4   | A     | 975  | LEU  |
| 4   | B     | 290  | LYS  |
| 4   | B     | 291  | MET  |
| 4   | B     | 365  | LEU  |
| 4   | B     | 977  | GLY  |
| 4   | C     | 265  | GLU  |
| 4   | C     | 298  | PHE  |
| 4   | C     | 542  | VAL  |
| 4   | D     | 238  | ASP  |
| 4   | D     | 1058 | PRO  |
| 5   | M     | 440  | GLN  |
| 5   | M     | 445  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | M     | 503  | GLU  |
| 5   | M     | 531  | SER  |
| 5   | N     | 415  | PHE  |
| 5   | N     | 503  | GLU  |
| 5   | O     | 396  | ARG  |
| 5   | O     | 411  | LEU  |
| 5   | O     | 440  | GLN  |
| 5   | O     | 445  | GLU  |
| 5   | O     | 448  | PHE  |
| 5   | O     | 493  | GLU  |
| 5   | O     | 503  | GLU  |
| 5   | O     | 527  | GLU  |
| 5   | P     | 491  | PRO  |
| 5   | P     | 526  | ALA  |
| 4   | A     | 513  | ILE  |
| 4   | A     | 1094 | LYS  |
| 4   | B     | 238  | ASP  |
| 4   | B     | 1138 | ALA  |
| 4   | C     | 290  | LYS  |
| 4   | C     | 792  | GLY  |
| 4   | C     | 1176 | LEU  |
| 4   | D     | 541  | VAL  |
| 4   | D     | 1141 | ASP  |
| 5   | M     | 496  | GLU  |
| 5   | M     | 529  | PRO  |
| 5   | N     | 392  | LYS  |
| 5   | N     | 521  | PRO  |
| 5   | N     | 528  | GLU  |
| 5   | N     | 541  | MET  |
| 5   | O     | 452  | LYS  |
| 5   | O     | 528  | GLU  |
| 5   | O     | 531  | SER  |
| 5   | P     | 373  | LYS  |
| 5   | P     | 391  | LEU  |
| 5   | P     | 503  | GLU  |
| 4   | A     | 509  | ARG  |
| 4   | A     | 510  | VAL  |
| 4   | B     | 973  | SER  |
| 4   | D     | 792  | GLY  |
| 4   | D     | 1056 | ARG  |
| 5   | M     | 410  | THR  |
| 5   | N     | 522  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | O     | 541  | MET  |
| 5   | P     | 396  | ARG  |
| 5   | P     | 529  | PRO  |
| 4   | A     | 299  | PRO  |
| 4   | A     | 300  | LEU  |
| 4   | A     | 1091 | PRO  |
| 4   | B     | 975  | LEU  |
| 4   | C     | 1091 | PRO  |
| 4   | C     | 1208 | GLY  |
| 5   | P     | 456  | SER  |
| 5   | P     | 458  | ALA  |
| 4   | B     | 774  | VAL  |
| 4   | B     | 976  | VAL  |
| 5   | N     | 449  | VAL  |
| 4   | A     | 792  | GLY  |
| 4   | A     | 1211 | GLY  |
| 4   | C     | 301  | PRO  |
| 4   | D     | 39   | ASP  |
| 4   | A     | 399  | PHE  |
| 4   | B     | 303  | GLY  |
| 4   | B     | 1145 | VAL  |
| 4   | C     | 399  | PHE  |
| 4   | A     | 496  | GLY  |
| 5   | O     | 449  | VAL  |
| 5   | P     | 528  | GLU  |
| 5   | N     | 524  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4   | A     | 965/1009 (96%) | 954 (99%) | 11 (1%)  | 65          | 79 |
| 4   | B     | 968/1009 (96%) | 944 (98%) | 24 (2%)  | 42          | 69 |
| 4   | C     | 968/1009 (96%) | 948 (98%) | 20 (2%)  | 47          | 71 |
| 4   | D     | 984/1009 (98%) | 959 (98%) | 25 (2%)  | 42          | 69 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 5   | M     | 112/144 (78%)   | 98 (88%)   | 14 (12%) | 4           | 21 |
| 5   | N     | 109/144 (76%)   | 105 (96%)  | 4 (4%)   | 30          | 63 |
| 5   | O     | 109/144 (76%)   | 99 (91%)   | 10 (9%)  | 8           | 33 |
| 5   | P     | 110/144 (76%)   | 89 (81%)   | 21 (19%) | 1           | 9  |
| All | All   | 4325/4612 (94%) | 4196 (97%) | 129 (3%) | 36          | 66 |

All (129) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | A     | 235  | THR  |
| 4   | A     | 257  | MET  |
| 4   | A     | 302  | GLU  |
| 4   | A     | 486  | GLU  |
| 4   | A     | 513  | ILE  |
| 4   | A     | 670  | LEU  |
| 4   | A     | 838  | GLU  |
| 4   | A     | 1079 | VAL  |
| 4   | A     | 1094 | LYS  |
| 4   | A     | 1176 | LEU  |
| 4   | A     | 1206 | LEU  |
| 4   | B     | 172  | ILE  |
| 4   | B     | 240  | GLU  |
| 4   | B     | 257  | MET  |
| 4   | B     | 325  | ARG  |
| 4   | B     | 358  | GLU  |
| 4   | B     | 364  | GLU  |
| 4   | B     | 569  | ASN  |
| 4   | B     | 713  | HIS  |
| 4   | B     | 795  | GLU  |
| 4   | B     | 838  | GLU  |
| 4   | B     | 976  | VAL  |
| 4   | B     | 1013 | HIS  |
| 4   | B     | 1021 | LEU  |
| 4   | B     | 1022 | ARG  |
| 4   | B     | 1039 | LEU  |
| 4   | B     | 1056 | ARG  |
| 4   | B     | 1058 | PRO  |
| 4   | B     | 1059 | THR  |
| 4   | B     | 1065 | MET  |
| 4   | B     | 1067 | ARG  |
| 4   | B     | 1080 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 1081 | VAL  |
| 4   | B     | 1139 | LEU  |
| 4   | B     | 1173 | LEU  |
| 4   | C     | 257  | MET  |
| 4   | C     | 291  | MET  |
| 4   | C     | 294  | ARG  |
| 4   | C     | 299  | PRO  |
| 4   | C     | 520  | GLU  |
| 4   | C     | 541  | VAL  |
| 4   | C     | 542  | VAL  |
| 4   | C     | 571  | HIS  |
| 4   | C     | 573  | SER  |
| 4   | C     | 622  | LEU  |
| 4   | C     | 795  | GLU  |
| 4   | C     | 838  | GLU  |
| 4   | C     | 975  | LEU  |
| 4   | C     | 1018 | TYR  |
| 4   | C     | 1039 | LEU  |
| 4   | C     | 1094 | LYS  |
| 4   | C     | 1095 | GLU  |
| 4   | C     | 1096 | ASP  |
| 4   | C     | 1120 | THR  |
| 4   | C     | 1183 | GLU  |
| 4   | D     | 154  | ILE  |
| 4   | D     | 257  | MET  |
| 4   | D     | 289  | ASP  |
| 4   | D     | 290  | LYS  |
| 4   | D     | 291  | MET  |
| 4   | D     | 366  | ARG  |
| 4   | D     | 531  | LYS  |
| 4   | D     | 540  | GLN  |
| 4   | D     | 549  | MET  |
| 4   | D     | 757  | TYR  |
| 4   | D     | 838  | GLU  |
| 4   | D     | 976  | VAL  |
| 4   | D     | 1018 | TYR  |
| 4   | D     | 1039 | LEU  |
| 4   | D     | 1055 | VAL  |
| 4   | D     | 1056 | ARG  |
| 4   | D     | 1058 | PRO  |
| 4   | D     | 1064 | MET  |
| 4   | D     | 1143 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | D     | 1145 | VAL  |
| 4   | D     | 1202 | ARG  |
| 4   | D     | 1204 | VAL  |
| 4   | D     | 1205 | PHE  |
| 4   | D     | 1206 | LEU  |
| 4   | D     | 1215 | GLU  |
| 5   | M     | 395  | LEU  |
| 5   | M     | 396  | ARG  |
| 5   | M     | 411  | LEU  |
| 5   | M     | 413  | LEU  |
| 5   | M     | 416  | PRO  |
| 5   | M     | 421  | PHE  |
| 5   | M     | 423  | HIS  |
| 5   | M     | 492  | TRP  |
| 5   | M     | 496  | GLU  |
| 5   | M     | 499  | ASP  |
| 5   | M     | 506  | ARG  |
| 5   | M     | 522  | LYS  |
| 5   | M     | 525  | GLU  |
| 5   | M     | 542  | PRO  |
| 5   | N     | 445  | GLU  |
| 5   | N     | 454  | SER  |
| 5   | N     | 455  | LEU  |
| 5   | N     | 456  | SER  |
| 5   | O     | 388  | LEU  |
| 5   | O     | 392  | LYS  |
| 5   | O     | 393  | PRO  |
| 5   | O     | 453  | LYS  |
| 5   | O     | 499  | ASP  |
| 5   | O     | 505  | ARG  |
| 5   | O     | 507  | LEU  |
| 5   | O     | 520  | LYS  |
| 5   | O     | 521  | PRO  |
| 5   | O     | 522  | LYS  |
| 5   | P     | 394  | THR  |
| 5   | P     | 396  | ARG  |
| 5   | P     | 414  | ARG  |
| 5   | P     | 417  | GLU  |
| 5   | P     | 496  | GLU  |
| 5   | P     | 499  | ASP  |
| 5   | P     | 504  | LEU  |
| 5   | P     | 506  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P     | 509 | ARG  |
| 5   | P     | 510 | LEU  |
| 5   | P     | 511 | LEU  |
| 5   | P     | 520 | LYS  |
| 5   | P     | 522 | LYS  |
| 5   | P     | 527 | GLU  |
| 5   | P     | 528 | GLU  |
| 5   | P     | 531 | SER  |
| 5   | P     | 532 | GLU  |
| 5   | P     | 535 | ILE  |
| 5   | P     | 541 | MET  |
| 5   | P     | 542 | PRO  |
| 5   | P     | 543 | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | A     | 49   | ASN  |
| 4   | A     | 167  | ASN  |
| 4   | A     | 231  | GLN  |
| 4   | A     | 273  | ASN  |
| 4   | A     | 411  | ASN  |
| 4   | A     | 669  | GLN  |
| 4   | A     | 746  | GLN  |
| 4   | A     | 849  | HIS  |
| 4   | A     | 896  | ASN  |
| 4   | A     | 1209 | ASN  |
| 4   | B     | 9    | HIS  |
| 4   | B     | 167  | ASN  |
| 4   | B     | 308  | GLN  |
| 4   | B     | 814  | ASN  |
| 4   | B     | 817  | HIS  |
| 4   | B     | 827  | GLN  |
| 4   | B     | 896  | ASN  |
| 4   | B     | 1116 | GLN  |
| 4   | C     | 26   | GLN  |
| 4   | C     | 49   | ASN  |
| 4   | C     | 135  | HIS  |
| 4   | C     | 407  | GLN  |
| 4   | C     | 746  | GLN  |
| 4   | C     | 778  | GLN  |
| 4   | C     | 817  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | C     | 896 | ASN  |
| 4   | D     | 13  | HIS  |
| 4   | D     | 167 | ASN  |
| 4   | D     | 231 | GLN  |
| 4   | D     | 407 | GLN  |
| 4   | D     | 440 | ASN  |
| 4   | D     | 540 | GLN  |
| 4   | D     | 715 | GLN  |
| 4   | D     | 749 | GLN  |
| 4   | D     | 814 | ASN  |
| 4   | D     | 827 | GLN  |
| 4   | D     | 849 | HIS  |
| 4   | D     | 896 | ASN  |
| 5   | M     | 440 | GLN  |
| 5   | N     | 367 | HIS  |
| 5   | N     | 405 | HIS  |
| 5   | N     | 423 | HIS  |
| 5   | N     | 440 | GLN  |
| 5   | O     | 369 | HIS  |
| 5   | O     | 371 | HIS  |
| 5   | O     | 440 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | DOC  | I     | 21  | 3,2  | 16,19,20     | 1.01 | 1 (6%)      | 20,26,29    | 1.38 | 4 (20%)     |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | DOC  | I     | 21  | 3,2  | -       | 1/7/18/19 | 0/2/2/2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | I     | 21  | DOC  | C6-C5 | 2.14 | 1.40        | 1.35     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | I     | 21  | DOC  | C3'-C2'-C1' | 2.89  | 106.20      | 102.87   |
| 3   | I     | 21  | DOC  | O4'-C1'-N1  | 2.45  | 112.22      | 107.86   |
| 3   | I     | 21  | DOC  | O4'-C4'-C3' | 2.37  | 108.71      | 104.81   |
| 3   | I     | 21  | DOC  | O2-C2-N3    | -2.36 | 118.62      | 122.33   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | I     | 21  | DOC  | C3'-C4'-C5'-O5' |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | I     | 21  | DOC  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | E     | 20/20 (100%)    | 0.11   | 0 100 100     | 159, 177, 203, 209    | 0     |
| 1   | G     | 20/20 (100%)    | 0.04   | 0 100 100     | 160, 175, 204, 216    | 0     |
| 1   | K     | 20/20 (100%)    | 0.24   | 0 100 100     | 157, 168, 206, 213    | 0     |
| 2   | F     | 20/28 (71%)     | 0.34   | 0 100 100     | 165, 187, 208, 217    | 0     |
| 2   | H     | 27/28 (96%)     | 0.07   | 0 100 100     | 145, 168, 184, 186    | 0     |
| 2   | J     | 23/28 (82%)     | 0.12   | 0 100 100     | 148, 171, 192, 201    | 0     |
| 2   | L     | 24/28 (85%)     | 0.11   | 0 100 100     | 150, 176, 197, 204    | 0     |
| 3   | I     | 20/21 (95%)     | 1.31   | 2 (10%) 12 8  | 198, 224, 252, 255    | 0     |
| 4   | A     | 1164/1220 (95%) | -0.06  | 4 (0%) 90 81  | 109, 140, 177, 212    | 0     |
| 4   | B     | 1167/1220 (95%) | -0.05  | 8 (0%) 84 69  | 107, 140, 174, 218    | 0     |
| 4   | C     | 1166/1220 (95%) | -0.06  | 5 (0%) 88 79  | 108, 148, 176, 203    | 0     |
| 4   | D     | 1185/1220 (97%) | -0.04  | 8 (0%) 84 69  | 111, 145, 175, 230    | 0     |
| 5   | M     | 138/177 (77%)   | 0.29   | 3 (2%) 62 42  | 159, 176, 196, 209    | 0     |
| 5   | N     | 135/177 (76%)   | 0.01   | 0 100 100     | 143, 169, 187, 203    | 0     |
| 5   | O     | 135/177 (76%)   | 0.13   | 2 (1%) 72 52  | 155, 181, 206, 227    | 0     |
| 5   | P     | 138/177 (77%)   | 0.23   | 3 (2%) 62 42  | 139, 177, 202, 226    | 0     |
| All | All   | 5402/5781 (93%) | -0.02  | 35 (0%) 85 73 | 107, 147, 186, 255    | 0     |

All (35) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | I     | 19   | DC   | 3.3  |
| 4   | B     | 365  | LEU  | 3.2  |
| 4   | D     | 714  | GLY  | 3.0  |
| 4   | D     | 1082 | PHE  | 3.0  |
| 4   | A     | 1219 | PRO  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | B     | 833  | ALA  | 2.9  |
| 4   | D     | 1081 | VAL  | 2.8  |
| 5   | P     | 397  | ALA  | 2.7  |
| 5   | P     | 446  | LEU  | 2.7  |
| 4   | C     | 427  | ALA  | 2.7  |
| 4   | B     | 1085 | ALA  | 2.6  |
| 5   | O     | 374  | ALA  | 2.6  |
| 5   | O     | 391  | LEU  | 2.5  |
| 4   | D     | 22   | ALA  | 2.5  |
| 4   | C     | 777  | MET  | 2.4  |
| 4   | B     | 301  | PRO  | 2.4  |
| 4   | C     | 1130 | ALA  | 2.4  |
| 5   | M     | 522  | LYS  | 2.4  |
| 5   | M     | 388  | LEU  | 2.4  |
| 4   | B     | 1084 | ARG  | 2.3  |
| 4   | D     | 1087 | GLU  | 2.3  |
| 4   | C     | 76   | ALA  | 2.3  |
| 5   | M     | 493  | GLU  | 2.3  |
| 4   | D     | 980  | ALA  | 2.3  |
| 4   | D     | 1084 | ARG  | 2.2  |
| 4   | A     | 1041 | GLY  | 2.2  |
| 4   | B     | 1027 | CYS  | 2.2  |
| 4   | D     | 140  | ILE  | 2.1  |
| 3   | I     | 1    | DC   | 2.1  |
| 4   | B     | 1058 | PRO  | 2.1  |
| 4   | A     | 169  | ASP  | 2.1  |
| 4   | A     | 21   | GLY  | 2.0  |
| 4   | C     | 476  | VAL  | 2.0  |
| 5   | P     | 391  | LEU  | 2.0  |
| 4   | B     | 1170 | GLY  | 2.0  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | DOC  | I     | 21  | 18/19 | 0.57 | 0.17 | 173,185,229,232            | 0     |

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 7   | MG   | A     | 1304 | 1/1   | 0.72 | 0.09 | 156,156,156,156             | 0     |
| 7   | MG   | B     | 1304 | 1/1   | 0.86 | 0.07 | 132,132,132,132             | 0     |
| 7   | MG   | D     | 1304 | 1/1   | 0.88 | 0.07 | 139,139,139,139             | 0     |
| 6   | ZN   | C     | 1301 | 1/1   | 0.93 | 0.08 | 197,197,197,197             | 0     |
| 6   | ZN   | C     | 1302 | 1/1   | 0.93 | 0.07 | 158,158,158,158             | 0     |
| 7   | MG   | C     | 1304 | 1/1   | 0.93 | 0.05 | 177,177,177,177             | 0     |
| 6   | ZN   | D     | 1302 | 1/1   | 0.93 | 0.08 | 159,159,159,159             | 0     |
| 6   | ZN   | C     | 1303 | 1/1   | 0.95 | 0.09 | 179,179,179,179             | 0     |
| 6   | ZN   | D     | 1301 | 1/1   | 0.96 | 0.09 | 233,233,233,233             | 0     |
| 6   | ZN   | B     | 1303 | 1/1   | 0.96 | 0.11 | 166,166,166,166             | 0     |
| 6   | ZN   | A     | 1302 | 1/1   | 0.97 | 0.11 | 168,168,168,168             | 0     |
| 6   | ZN   | B     | 1301 | 1/1   | 0.97 | 0.06 | 163,163,163,163             | 0     |
| 6   | ZN   | A     | 1301 | 1/1   | 0.97 | 0.08 | 187,187,187,187             | 0     |
| 6   | ZN   | B     | 1302 | 1/1   | 0.98 | 0.07 | 141,141,141,141             | 0     |
| 6   | ZN   | D     | 1303 | 1/1   | 0.98 | 0.07 | 176,176,176,176             | 0     |
| 6   | ZN   | A     | 1303 | 1/1   | 0.99 | 0.04 | 141,141,141,141             | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.