



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 11:25 AM UTC

PDB ID : 3OGL / pdb\_00003ogl  
Title : Structure of COI1-ASK1 in complex with JA-isoleucine and the JAZ1 degron  
Authors : Sheard, L.B.; Tan, X.; Mao, H.; Withers, J.; Ben-Nissan, G.; Hinds, T.R.;  
Hsu, F.; Sharon, M.; Browse, J.; He, S.Y.; Rizo, J.; Howe, G.A.; Zheng, N.  
Deposited on : 2010-08-17  
Resolution : 3.18 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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

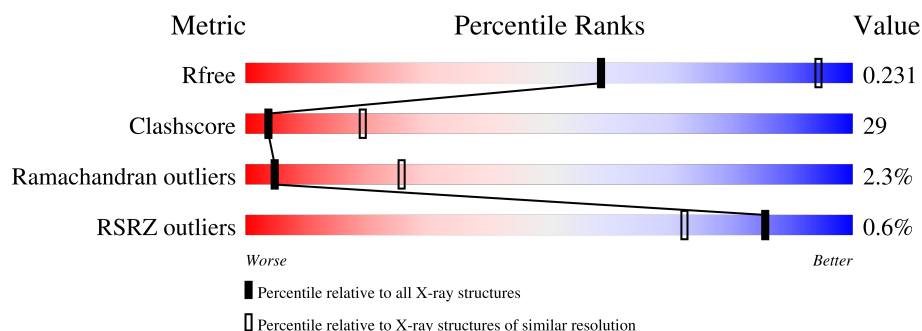
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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.



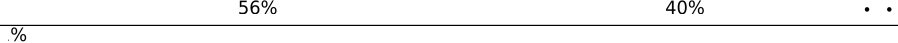
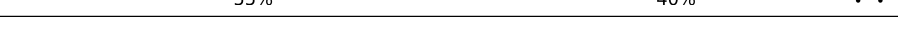
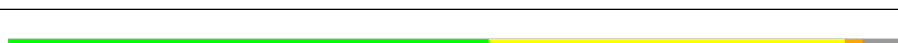
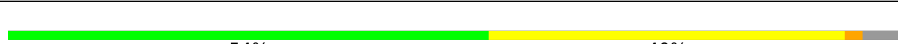
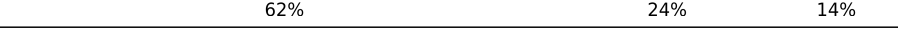
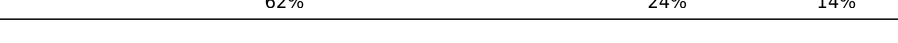
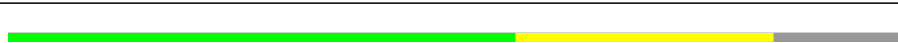
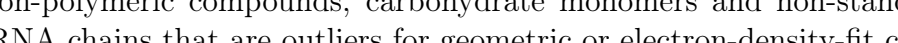
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2001 (3.20-3.16)                                      |
| Clashscore            | 190562                      | 2119 (3.20-3.16)                                      |
| Ramachandran outliers | 187476                      | 2070 (3.20-3.16)                                      |
| RSRZ outliers         | 180081                      | 2001 (3.20-3.16)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 1   | A     | 160    | <div> <div>%</div> <div> <div></div> <div>49%</div> <div>40%</div> <div>• 10%</div> </div> </div> |
| 1   | C     | 160    | <div> <div>%</div> <div> <div></div> <div>51%</div> <div>38%</div> <div>• 10%</div> </div> </div> |
| 1   | E     | 160    | <div> <div>%</div> <div> <div></div> <div>52%</div> <div>36%</div> <div>• 10%</div> </div> </div> |
| 1   | G     | 160    | <div> <div></div> <div> <div>48%</div> <div>39%</div> <div>• 10%</div> </div> </div>              |
| 1   | I     | 160    | <div> <div>%</div> <div> <div></div> <div>46%</div> <div>40%</div> <div>• 10%</div> </div> </div> |
| 1   | K     | 160    | <div> <div></div> <div> <div>50%</div> <div>38%</div> <div>• 10%</div> </div> </div>              |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | M     | 160    |    |
| 1   | O     | 160    |    |
| 2   | B     | 592    |    |
| 2   | D     | 592    |    |
| 2   | F     | 592    |    |
| 2   | H     | 592    |    |
| 2   | J     | 592    |    |
| 2   | L     | 592    |    |
| 2   | N     | 592    |    |
| 2   | P     | 592    |    |
| 3   | Q     | 21     |   |
| 3   | R     | 21     |  |
| 3   | S     | 21     |  |
| 3   | U     | 21     |  |
| 3   | V     | 21     |  |
| 3   | W     | 21     |  |
| 3   | X     | 21     |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | 7JA  | B     | 1100 | -         | -        | X       | -                |
| 4   | 7JA  | D     | 1100 | -         | -        | X       | -                |
| 4   | 7JA  | F     | 1100 | -         | -        | X       | -                |
| 4   | 7JA  | H     | 1100 | -         | -        | X       | -                |
| 4   | 7JA  | J     | 1100 | -         | -        | X       | -                |
| 4   | 7JA  | L     | 1100 | -         | -        | X       | -                |
| 4   | 7JA  | N     | 1100 | -         | -        | X       | -                |
| 4   | 7JA  | P     | 1100 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 5   | PO4  | B     | 1101 | -         | X        | -       | -                |
| 5   | PO4  | B     | 1102 | -         | X        | -       | -                |
| 5   | PO4  | B     | 1103 | -         | X        | X       | -                |
| 5   | PO4  | B     | 1104 | -         | X        | -       | -                |
| 5   | PO4  | D     | 1101 | -         | X        | -       | -                |
| 5   | PO4  | D     | 1102 | -         | X        | -       | -                |
| 5   | PO4  | D     | 1103 | -         | X        | X       | -                |
| 5   | PO4  | F     | 1101 | -         | X        | -       | -                |
| 5   | PO4  | F     | 1102 | -         | X        | -       | -                |
| 5   | PO4  | F     | 1103 | -         | X        | X       | -                |
| 5   | PO4  | F     | 1104 | -         | X        | -       | -                |
| 5   | PO4  | H     | 1101 | -         | X        | -       | -                |
| 5   | PO4  | H     | 1102 | -         | X        | -       | -                |
| 5   | PO4  | H     | 1103 | -         | X        | X       | -                |
| 5   | PO4  | H     | 1104 | -         | X        | -       | -                |
| 5   | PO4  | J     | 1101 | -         | X        | -       | -                |
| 5   | PO4  | J     | 1102 | -         | X        | -       | -                |
| 5   | PO4  | J     | 1103 | -         | X        | X       | -                |
| 5   | PO4  | J     | 1104 | -         | X        | -       | -                |
| 5   | PO4  | L     | 1101 | -         | X        | -       | -                |
| 5   | PO4  | L     | 1102 | -         | X        | -       | -                |
| 5   | PO4  | L     | 1103 | -         | X        | X       | -                |
| 5   | PO4  | L     | 1104 | -         | X        | -       | -                |
| 5   | PO4  | N     | 1101 | -         | X        | -       | -                |
| 5   | PO4  | N     | 1102 | -         | X        | -       | -                |
| 5   | PO4  | N     | 1103 | -         | X        | X       | -                |
| 5   | PO4  | N     | 1104 | -         | X        | -       | -                |
| 5   | PO4  | P     | 1101 | -         | X        | -       | -                |
| 5   | PO4  | P     | 1102 | -         | X        | -       | -                |
| 5   | PO4  | P     | 1103 | -         | X        | X       | -                |
| 5   | PO4  | P     | 1104 | -         | X        | -       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SKP1-like protein 1A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 720 | 185 | 235 | 6 |         |         |       |
| 1   | C     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 720 | 185 | 235 | 6 |         |         |       |
| 1   | E     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 720 | 185 | 235 | 6 |         |         |       |
| 1   | G     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 720 | 185 | 235 | 6 |         |         |       |
| 1   | I     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 720 | 185 | 235 | 6 |         |         |       |
| 1   | K     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 720 | 185 | 235 | 6 |         |         |       |
| 1   | M     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 720 | 185 | 235 | 6 |         |         |       |
| 1   | O     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 720 | 185 | 235 | 6 |         |         |       |

- Molecule 2 is a protein called Coronatine-insensitive protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 568      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4541  | 2873 | 790 | 842 | 36 |         |         |       |
| 2   | D     | 568      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4541  | 2873 | 790 | 842 | 36 |         |         |       |
| 2   | F     | 568      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4541  | 2873 | 790 | 842 | 36 |         |         |       |
| 2   | H     | 562      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4486  | 2840 | 779 | 831 | 36 |         |         |       |
| 2   | J     | 568      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4541  | 2873 | 790 | 842 | 36 |         |         |       |
| 2   | L     | 568      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4541  | 2873 | 790 | 842 | 36 |         |         |       |

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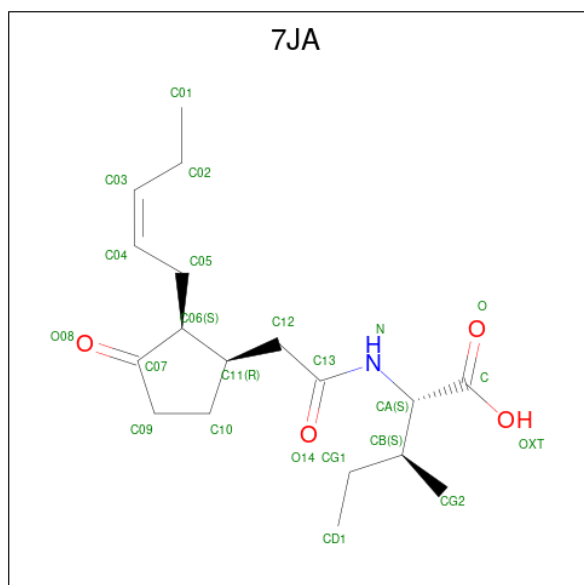
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| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | N     | 568      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4541  | 2873 | 790 | 842 | 36 |         |         |       |
| 2   | P     | 568      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4541  | 2873 | 790 | 842 | 36 |         |         |       |

- Molecule 3 is a protein called JAZ1 incomplete degron peptide.

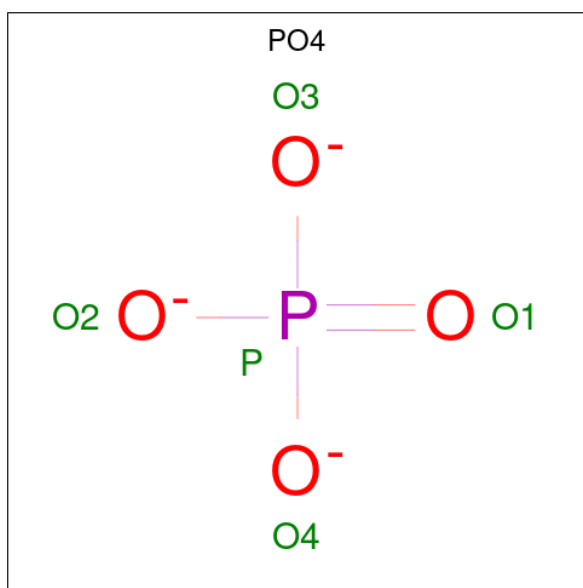
| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 3   | Q     | 18       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 156   | 99 | 34 | 23 |         |         |       |
| 3   | R     | 18       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 156   | 99 | 34 | 23 |         |         |       |
| 3   | S     | 18       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 156   | 99 | 34 | 23 |         |         |       |
| 3   | U     | 18       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 156   | 99 | 34 | 23 |         |         |       |
| 3   | V     | 18       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 156   | 99 | 34 | 23 |         |         |       |
| 3   | W     | 18       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 156   | 99 | 34 | 23 |         |         |       |
| 3   | X     | 18       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 156   | 99 | 34 | 23 |         |         |       |

- Molecule 4 is N-((1R,2S)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetyl)-L-isoleucine (CCD ID: 7JA) (formula: C<sub>18</sub>H<sub>29</sub>NO<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 18 | 1 | 4 |         |         |
| 4   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 18 | 1 | 4 |         |         |
| 4   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 18 | 1 | 4 |         |         |
| 4   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 18 | 1 | 4 |         |         |
| 4   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 18 | 1 | 4 |         |         |
| 4   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 18 | 1 | 4 |         |         |
| 4   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 18 | 1 | 4 |         |         |
| 4   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 23    | 18 | 1 | 4 |         |         |

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | H     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | H     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | H     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | H     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | J     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | J     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | J     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | J     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | L     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | L     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | L     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | L     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | N     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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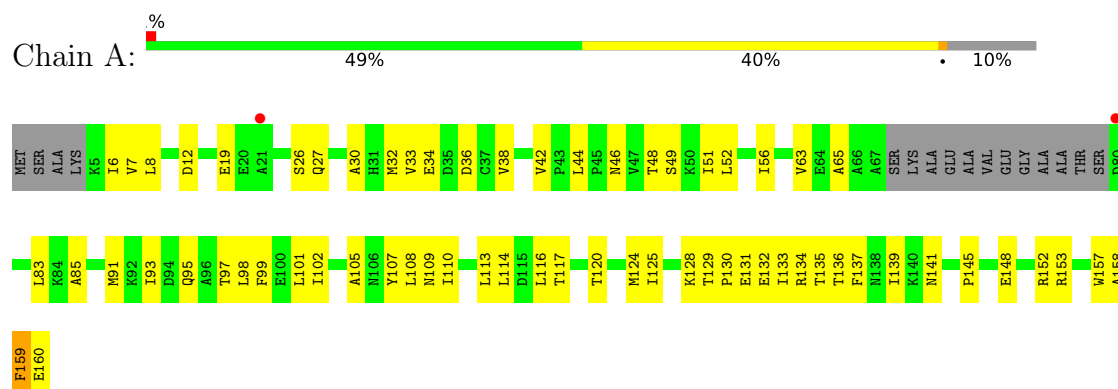
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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | N     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | N     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | N     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | P     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | P     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | P     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | P     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

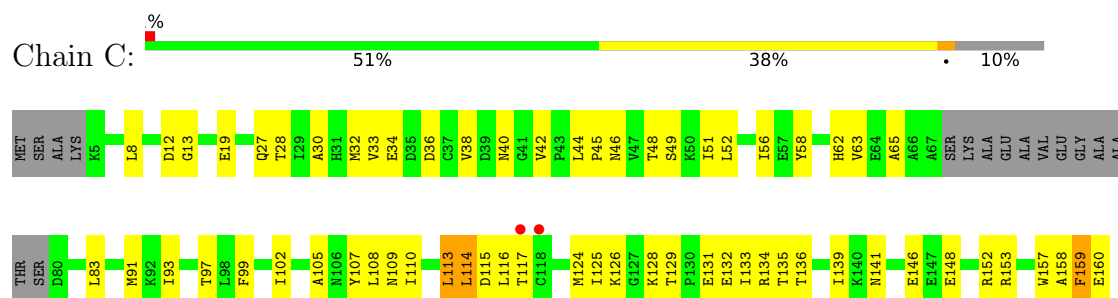
### 3 Residue-property plots [i](#)

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.

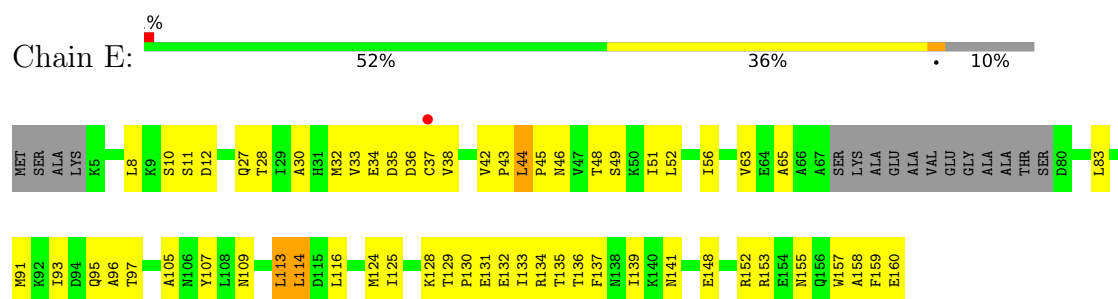
#### • Molecule 1: SKP1-like protein 1A



#### • Molecule 1: SKP1-like protein 1A

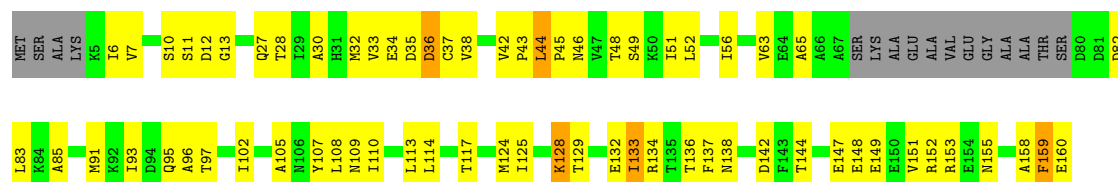


#### • Molecule 1: SKP1-like protein 1A

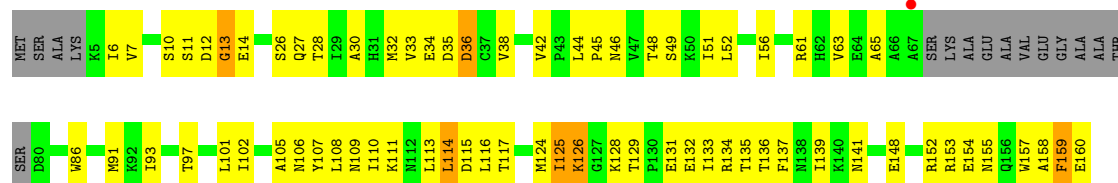


#### • Molecule 1: SKP1-like protein 1A

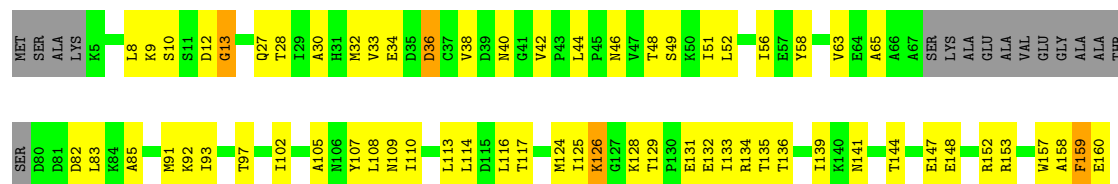




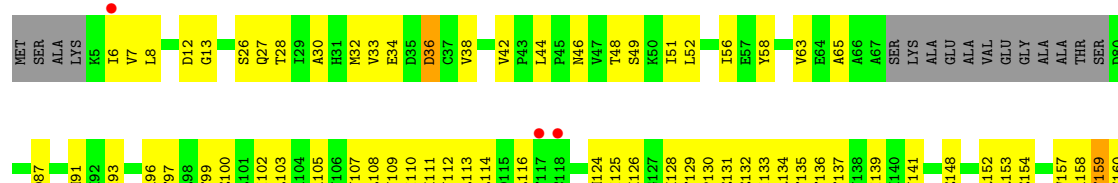
- Molecule 1: SKP1-like protein 1A



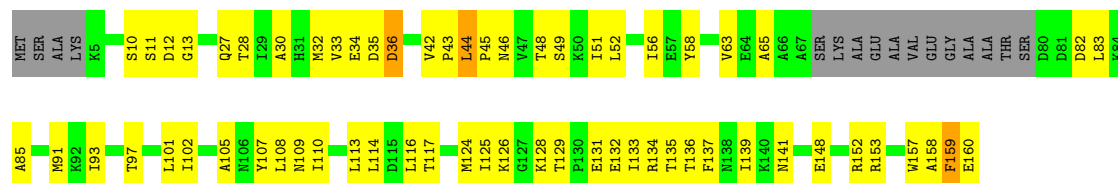
- Molecule 1: SKP1-like protein 1A



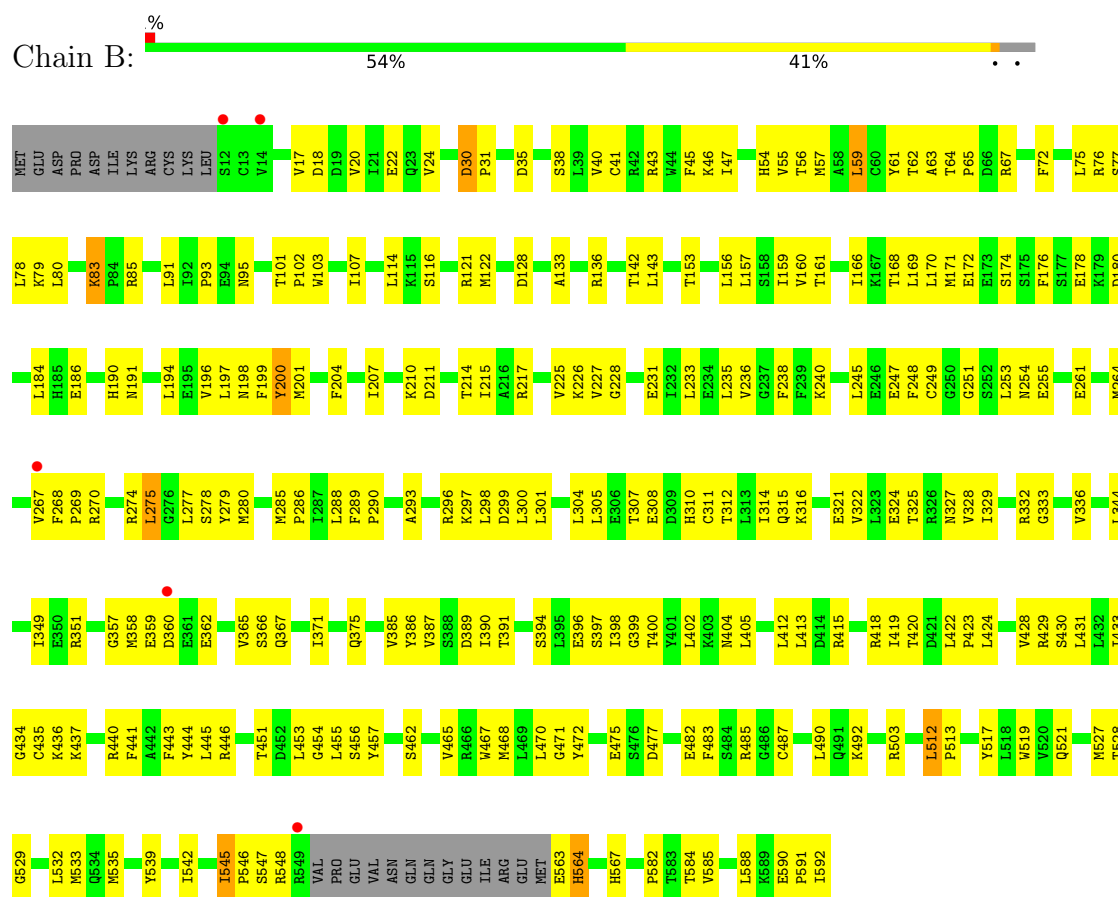
- Molecule 1: SKP1-like protein 1A



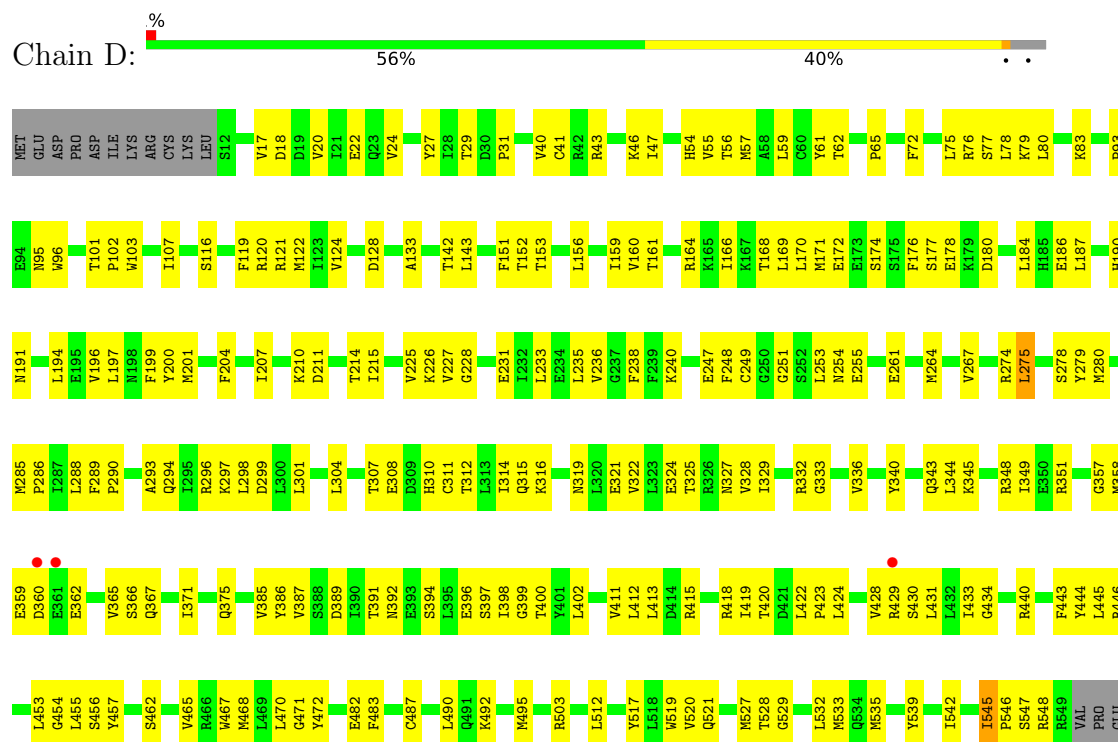
- Molecule 1: SKP1-like protein 1A



- Molecule 2: Coronatine-insensitive protein 1



• Molecule 2: Coronatine-insensitive protein 1



|     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| VAL | ASN | GLN | GLN | GLY | GLY | ILE | ARG | GLU | MET | E563 | H564 | P565 | A566 | H567 | R578 | T579 | D580 | C581 | P582 | T583 | T584 | L588 | K589 | E590 | P591 | I592 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

• Molecule 2: Coronatine-insensitive protein 1

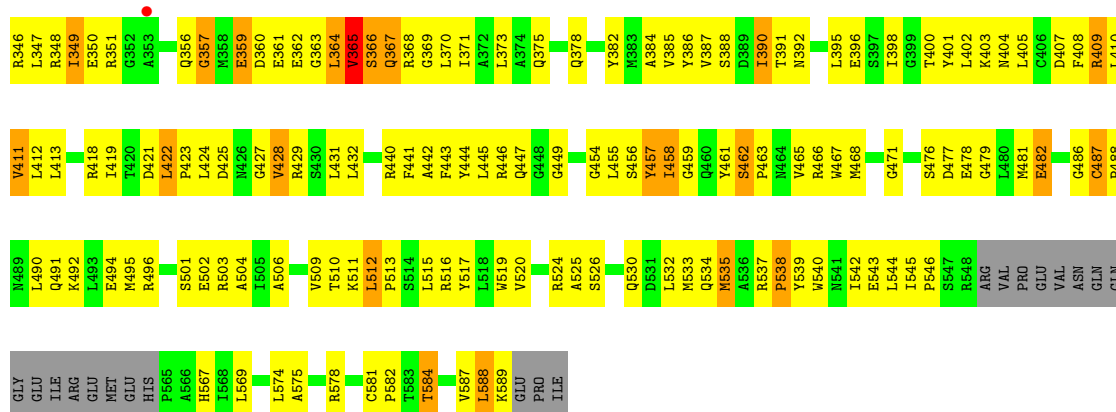


|     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| MET | GLU  | ASP  | PRO  | ASP  | ILE  | LYS  | ARG  | CYS  | LYS  | LEU  | S12  | C13  | V14  | V17  | V20  | T21  | E22  | Q23  | V24  | P31  | K32  | V40  | C41  | K46  | I47  | E50  | H54  | V55  | T56  | M57  | A58  | L59  | C60  | V61  | T62  | F72  | L75  | R76  | S77  | L80  | K83  | P84  | B85  | L91  | I92  | P93  | E94  |      |      |      |      |
|     | N95  | W96  | G97  | G98  | T101 | P102 | W103 | I107 | L111 | R112 | Q113 | L114 | K115 | S116 | R120 | R121 | M122 | I123 | V124 | D128 | A133 | R136 | D139 | T142 | L143 | F151 | T152 | T153 | L157 | S158 | I159 | V160 | T161 | I166 | K167 | T168 | L169 | M171 | L170 | E172 | S174 | E173 | S175 | F176 | S177 | E178 | K179 | D180 |      |      |      |
|     | L184 | H185 | L186 | L187 | A188 | N191 | L194 | P195 | V196 | L197 | N198 | F199 | Y200 | F204 | T207 | K210 | D211 | L212 | E213 | T214 | I215 | V225 | K226 | V227 | G228 | E231 | L232 | L233 | E234 | L235 | V236 | G237 | F238 | F239 | K240 | L245 | E246 | E247 | F248 | G251 | S252 | L253 | E255 | E256 | E261 | M264 | I267 | V267 |      |      |      |
|     | R274 | L275 | S278 | Y279 | M280 | M285 | P286 | L288 | F289 | P290 | K297 | L298 | D299 | L300 | L301 | L304 | T307 | E308 | D309 | H310 | C311 | T312 | L313 | I314 | Q315 | K316 | L320 | E321 | S322 | L323 | E324 | N327 | V328 | L329 | G330 | D331 | R332 | G333 | V336 | Y340 | Q343 | L344 | K345 | L347 | R348 | E349 | S350 |      |      |      |      |
|     | R351 | G357 | K358 | E359 | D360 | E362 | V365 | S366 | Q367 | I371 | Q375 | V385 | Y386 | V387 | S388 | D389 | L390 | T391 | E392 | E393 | S394 | L395 | E396 | S397 | L398 | Q399 | T400 | Y401 | L402 | L405 | R409 | L412 | L413 | D414 | R415 | R418 | T419 | T420 | D421 | L422 | P423 | L424 | V428 | R429 | S430 | L431 | L432 | I433 | G434 |      |      |
|     | C435 | R440 | F441 | A442 | F443 | Y444 | L445 | R446 | Q447 | G448 | G449 | L450 | T451 | D452 | L453 | G454 | L455 | S456 | Y457 | I458 | V465 | R466 | W467 | M468 | L469 | L470 | G471 | Y472 | E475 | E482 | F483 | S484 | R485 | T486 | C487 | L490 | Q491 | K492 | L493 | E494 | R503 | L512 | P513 | Y517 | L518 | W519 | V520 | Q521 | M527 | T528 | G529 |
|     | L532 | M533 | Q534 | M535 | Y539 | T542 | F545 | S547 | R548 | H549 | VAL  | PRO  | GLU  | VAL  | ASN  | GLN  | GLY  | GLU  | ILE  | ARG  | GLU  | MET  | E563 | H564 | P565 | A566 | H567 | R578 | P582 | T583 | T584 | L588 | K589 | E590 | P591 | I592 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |

• Molecule 2: Coronatine-insensitive protein 1

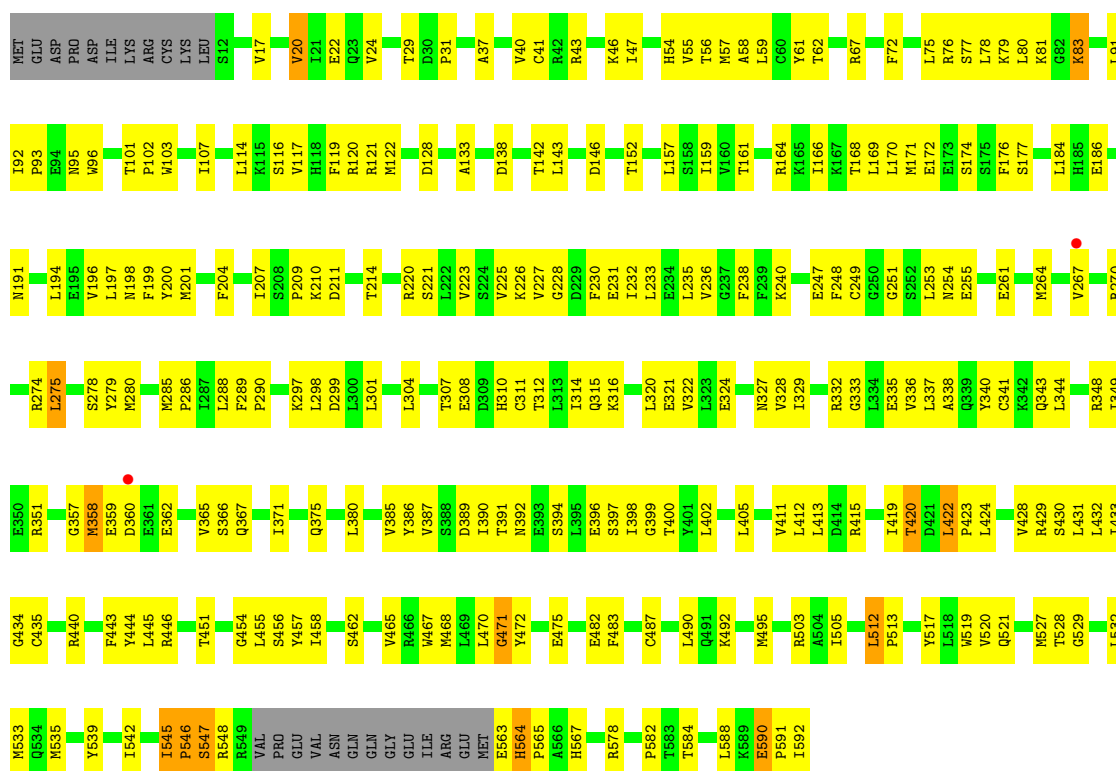


|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| MET  | GLU  | ASP  | PRO  | ASP  | ILE  | LYS  | ARG  | CYS  | LYS  | LEU  | S12  | T16  | V17  | D18  | D19  | V20  | T21  | E22  | Q23  | V24  | M25  | I28  | P31  | K32  | D33  | R34  | D35  | S36  | A37  | S38  | L39  | V40  | R43  | W44  | L47  | D48  | S49  | T51  | R52  | H53  | H54  | V55  | T56  | M57  | A58  | L59  | C60  | L61  | T62  | A63  | T64  | P65  | D66  |      |      |      |      |      |      |      |
| R67  |      | R71  | F72  | P73  | N74  | L75  | R76  | S77  | L78  | K79  | K83  | P84  | R85  | A86  | M87  | M88  | F89  | N90  | L91  | I92  | P93  | E94  | N95  | G96  | G97  | H98  | L99  | V100 | T101 | S102 | W103 |      | E106 | I107 | S108 | N109 | N110 | L111 | R112 | Q113 | L114 | K115 | S116 | V117 | H118 | F119 | R120 | M121 | M122 | I123 | V124 | S125 | D126 | L127 | D128 | A63  | T64  | P65  | D66  |      |
| R136 | A137 | D138 | D139 | L140 | E141 | L142 | L143 | K144 | L145 | D146 | K147 | F151 | T152 | T153 |      | L156 |      | I159 | V160 | T161 | H162 | C163 | R164 |      | T168 | L169 | G170 | H171 | E172 | E173 |      | F176 | S177 | E178 | K179 | D180 | G181 | K182 | L183 | L184 | H185 | L186 | L187 | A188 | Q189 | H190 | F191 | H192 | N191 | T192 | S193 |      | V196 | L197 | N198 | F199 | Y200 | M201 | T202 | E203 |
| F204 | A205 | K206 | I207 |      | D211 | L212 | E213 | T214 | L215 | A216 |      | R220 |      | S224 | V225 | K226 | V227 | G228 | D229 | E231 | L232 | L233 | E234 | L235 | V236 | G237 | F238 |      | E247 | F248 | C249 | G250 |      | L253 | M254 | E255 | D256 | T257 | G258 | M259 | P260 | E261 | K262 | Y263 |      | L266 | V267 | F268 | P269 | R270 | K271 | L272 | C273 | R274 |      | L277 | S278 | Y279 |      |      |
| M280 |      | N283 | E284 | M285 | P286 | L287 | L288 | F289 | P290 | F291 | A292 |      | T295 | R296 | K297 | L298 | D299 | L300 | L301 | Y302 | A303 | L304 | L305 | E306 | T307 | E308 | D309 | H310 | C311 | T312 | L313 | Q314 | Q315 | K316 | C317 | L320 | E321 | V322 | L323 | E324 | T325 | R326 | N327 | V328 |      | D331 | R332 | G333 |      | V336 | L337 |      | C341 | K342 | Q343 | L344 | K345 |      |      |      |



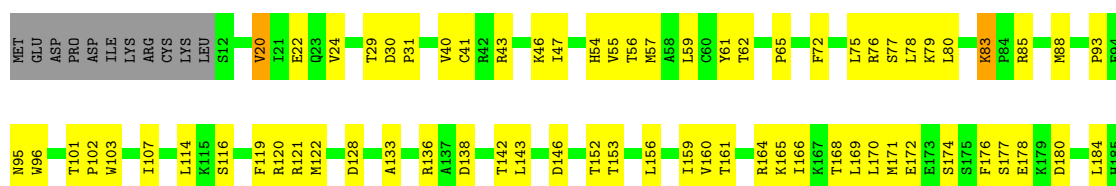
• Molecule 2: Coronatine-insensitive protein 1

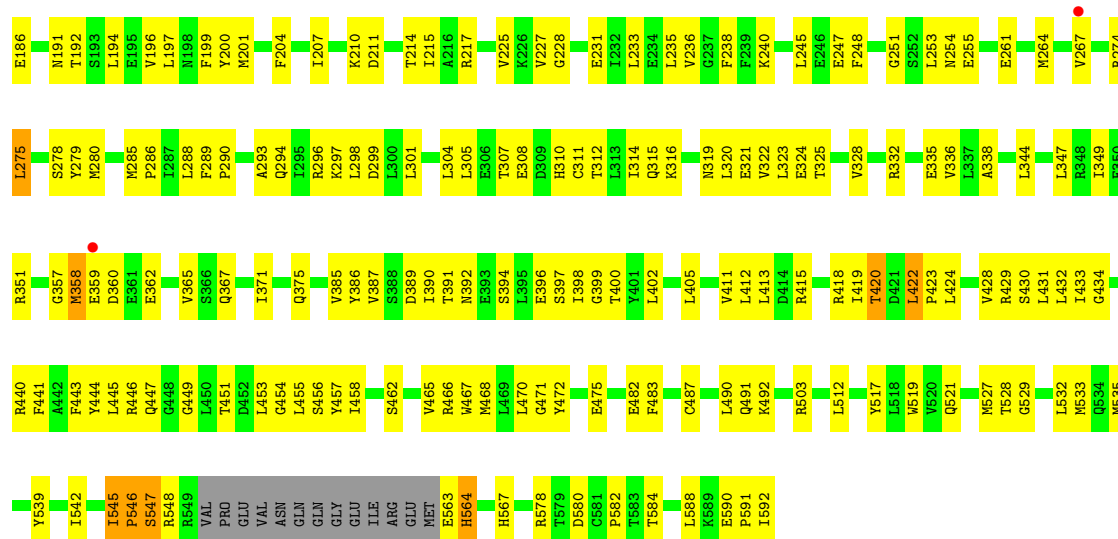
Chain J: 54% 40%



• Molecule 2: Coronatine-insensitive protein 1

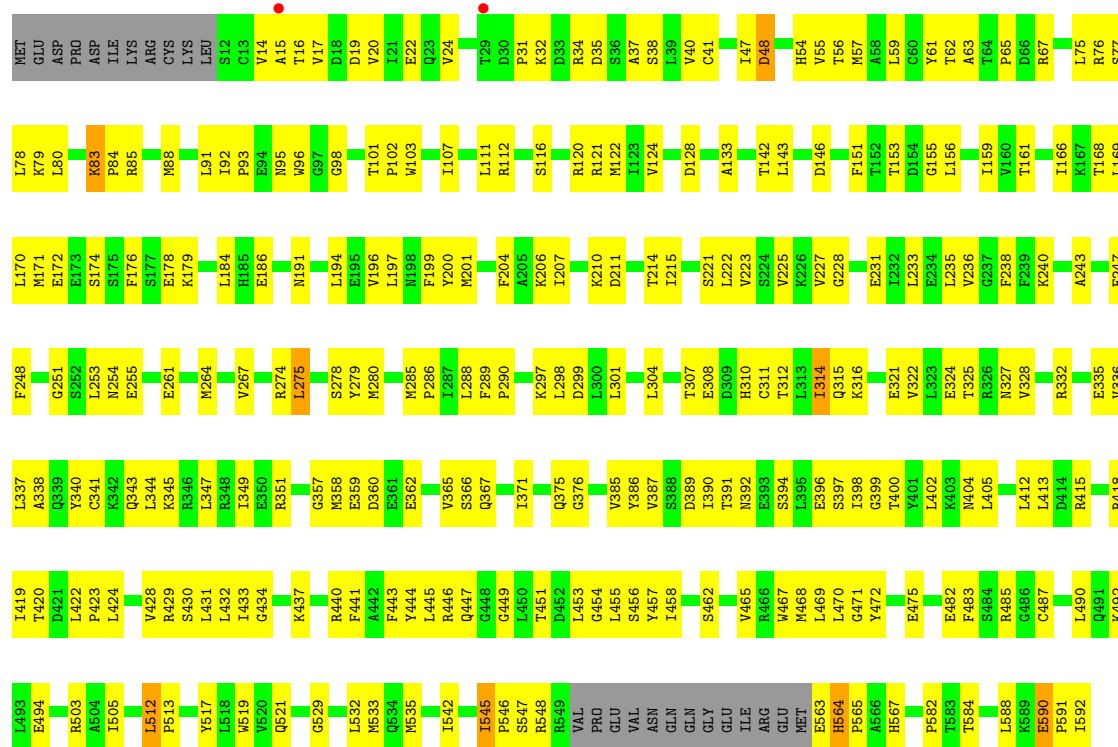
Chain L: 54% 40%





• Molecule 2: Coronatine-insensitive protein 1

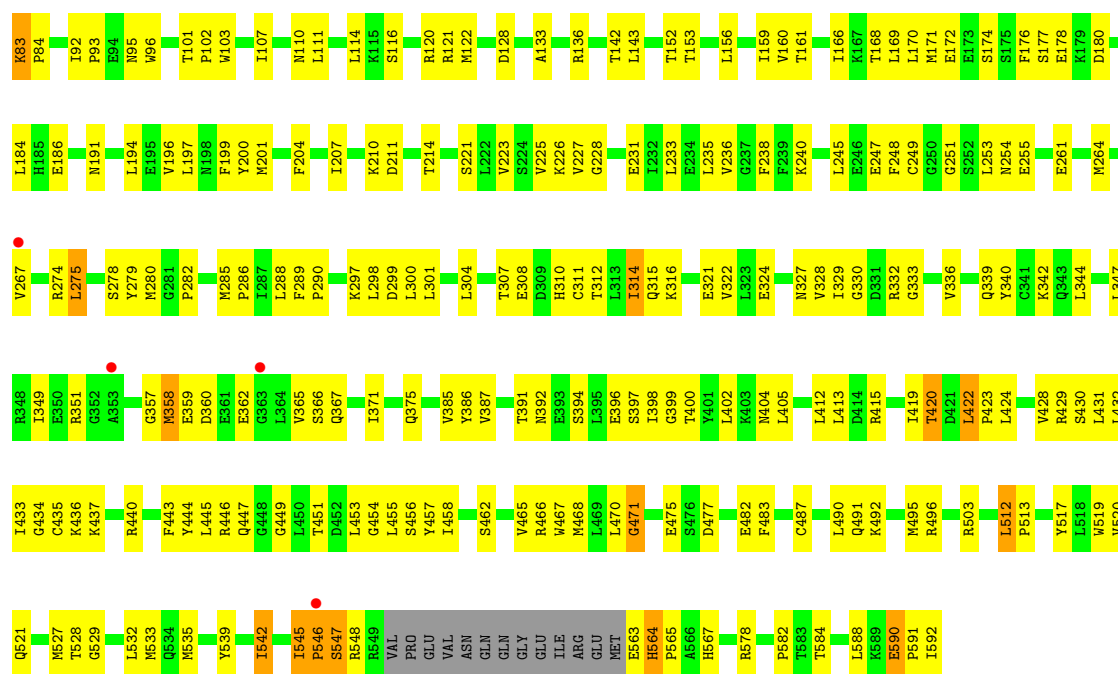
Chain N: 53% 42%



• Molecule 2: Coronatine-insensitive protein 1

Chain P: 53% 40%





- Molecule 3: JAZ1 incomplete degnon peptide

Chain Q: 62% 24% 14%



- Molecule 3: JAZ1 incomplete degnon peptide

Chain R: 62% 24% 14%



- Molecule 3: JAZ1 incomplete degnon peptide

Chain S: 62% 24% 14%



- Molecule 3: JAZ1 incomplete degnon peptide

Chain U: 62% 24% 14%



- Molecule 3: JAZ1 incomplete degnon peptide



Chain V:  62% 24% 14%



- Molecule 3: JAZ1 incomplete degron peptide

Chain W:  67% 19% 14%



- Molecule 3: JAZ1 incomplete degron peptide

Chain X:  57% 29% 14%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 122.35Å 220.82Å 148.67Å<br>90.00° 104.52° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 49.68 – 3.18<br>49.68 – 3.18                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.1 (49.68-3.18)<br>91.1 (49.68-3.18)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.38 (at 3.19Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine)                                      | Depositor        |
| R, $R_{free}$                                                           | 0.215 , 0.263<br>(Not available) , 0.231                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (1.62%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 61.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.248                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 46.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 46877                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 72.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7JA, PO4

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$      |
| 1   | A     | 0.63         | 0/1162         | 0.88        | 1/1571 (0.1%)    |
| 1   | C     | 0.71         | 2/1162 (0.2%)  | 0.91        | 4/1571 (0.3%)    |
| 1   | E     | 0.73         | 2/1162 (0.2%)  | 0.98        | 5/1571 (0.3%)    |
| 1   | G     | 0.71         | 0/1162         | 1.01        | 6/1571 (0.4%)    |
| 1   | I     | 0.61         | 0/1162         | 0.92        | 4/1571 (0.3%)    |
| 1   | K     | 0.62         | 0/1162         | 0.90        | 1/1571 (0.1%)    |
| 1   | M     | 0.62         | 0/1162         | 0.89        | 1/1571 (0.1%)    |
| 1   | O     | 0.62         | 0/1162         | 0.91        | 3/1571 (0.2%)    |
| 2   | B     | 0.78         | 1/4623 (0.0%)  | 1.07        | 25/6238 (0.4%)   |
| 2   | D     | 0.75         | 0/4623         | 1.07        | 15/6238 (0.2%)   |
| 2   | F     | 0.68         | 0/4623         | 1.05        | 19/6238 (0.3%)   |
| 2   | H     | 0.78         | 1/4566 (0.0%)  | 1.23        | 38/6161 (0.6%)   |
| 2   | J     | 0.69         | 0/4623         | 1.06        | 19/6238 (0.3%)   |
| 2   | L     | 0.67         | 0/4623         | 1.06        | 19/6238 (0.3%)   |
| 2   | N     | 0.71         | 0/4623         | 1.08        | 20/6238 (0.3%)   |
| 2   | P     | 0.65         | 1/4623 (0.0%)  | 1.07        | 20/6238 (0.3%)   |
| 3   | Q     | 0.66         | 0/158          | 0.83        | 0/208            |
| 3   | R     | 0.60         | 0/158          | 0.85        | 0/208            |
| 3   | S     | 0.53         | 0/158          | 0.79        | 0/208            |
| 3   | U     | 0.58         | 0/158          | 0.80        | 0/208            |
| 3   | V     | 0.49         | 0/158          | 0.83        | 0/208            |
| 3   | W     | 0.56         | 0/158          | 0.80        | 0/208            |
| 3   | X     | 0.57         | 0/158          | 0.77        | 0/208            |
| All | All   | 0.70         | 7/47329 (0.0%) | 1.05        | 200/63851 (0.3%) |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 114 | LEU  | N-CA  | 7.21  | 1.56        | 1.47     |
| 1   | C     | 113 | LEU  | C-N   | 6.70  | 1.44        | 1.33     |
| 1   | E     | 113 | LEU  | C-N   | -6.18 | 1.25        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | P     | 542 | ILE  | CA-CB | 5.45  | 1.61        | 1.54     |
| 2   | B     | 59  | LEU  | CA-C  | -5.22 | 1.47        | 1.52     |
| 2   | H     | 159 | ILE  | CA-CB | 5.19  | 1.61        | 1.54     |
| 1   | E     | 114 | LEU  | N-CA  | -5.15 | 1.39        | 1.46     |

All (200) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 114 | LEU  | N-CA-C | -9.90 | 101.08      | 113.55   |
| 2   | F     | 545 | ILE  | CA-C-N | 9.84  | 132.14      | 119.84   |
| 2   | F     | 545 | ILE  | C-N-CA | 9.84  | 132.14      | 119.84   |
| 2   | P     | 545 | ILE  | CA-C-N | 9.67  | 131.92      | 119.84   |
| 2   | P     | 545 | ILE  | C-N-CA | 9.67  | 131.92      | 119.84   |
| 2   | L     | 545 | ILE  | CA-C-N | 9.40  | 131.59      | 119.84   |
| 2   | L     | 545 | ILE  | C-N-CA | 9.40  | 131.59      | 119.84   |
| 2   | D     | 545 | ILE  | CA-C-N | 9.36  | 131.54      | 119.84   |
| 2   | D     | 545 | ILE  | C-N-CA | 9.36  | 131.54      | 119.84   |
| 2   | H     | 366 | SER  | N-CA-C | -9.27 | 96.79       | 110.23   |
| 2   | N     | 545 | ILE  | CA-C-N | 9.02  | 131.11      | 119.84   |
| 2   | N     | 545 | ILE  | C-N-CA | 9.02  | 131.11      | 119.84   |
| 2   | B     | 545 | ILE  | CA-C-N | 8.98  | 131.06      | 119.84   |
| 2   | B     | 545 | ILE  | C-N-CA | 8.98  | 131.06      | 119.84   |
| 2   | J     | 545 | ILE  | CA-C-N | 8.05  | 129.91      | 119.84   |
| 2   | J     | 545 | ILE  | C-N-CA | 8.05  | 129.91      | 119.84   |
| 2   | H     | 462 | SER  | CA-C-N | 7.98  | 129.82      | 119.84   |
| 2   | H     | 462 | SER  | C-N-CA | 7.98  | 129.82      | 119.84   |
| 2   | H     | 101 | THR  | CA-C-N | 7.67  | 129.43      | 119.84   |
| 2   | H     | 101 | THR  | C-N-CA | 7.67  | 129.43      | 119.84   |
| 1   | G     | 114 | LEU  | N-CA-C | -7.33 | 103.22      | 111.07   |
| 2   | H     | 367 | GLN  | N-CA-C | -7.32 | 102.38      | 111.75   |
| 2   | J     | 76  | ARG  | N-CA-C | -7.19 | 105.04      | 113.88   |
| 2   | N     | 275 | LEU  | N-CA-C | 7.13  | 119.01      | 108.60   |
| 2   | D     | 275 | LEU  | N-CA-C | 7.05  | 118.90      | 108.60   |
| 2   | H     | 126 | ASP  | N-CA-C | -7.05 | 103.60      | 111.28   |
| 2   | N     | 76  | ARG  | N-CA-C | -7.04 | 105.22      | 113.88   |
| 2   | P     | 275 | LEU  | N-CA-C | 7.03  | 118.87      | 108.60   |
| 2   | H     | 422 | LEU  | N-CA-C | 6.99  | 118.16      | 110.13   |
| 2   | H     | 404 | ASN  | N-CA-C | 6.82  | 119.61      | 110.88   |
| 2   | L     | 275 | LEU  | N-CA-C | 6.76  | 118.47      | 108.60   |
| 2   | L     | 76  | ARG  | N-CA-C | -6.59 | 105.78      | 113.88   |
| 2   | B     | 72  | PHE  | CA-C-N | 6.57  | 126.26      | 119.56   |
| 2   | B     | 72  | PHE  | C-N-CA | 6.57  | 126.26      | 119.56   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 76  | ARG  | N-CA-C  | -6.54 | 105.84      | 113.88   |
| 2   | L     | 512 | LEU  | CA-C-N  | 6.53  | 125.97      | 118.85   |
| 2   | L     | 512 | LEU  | C-N-CA  | 6.53  | 125.97      | 118.85   |
| 2   | F     | 76  | ARG  | N-CA-C  | -6.50 | 105.89      | 113.88   |
| 2   | B     | 462 | SER  | CA-C-N  | 6.48  | 126.05      | 119.19   |
| 2   | B     | 462 | SER  | C-N-CA  | 6.48  | 126.05      | 119.19   |
| 2   | H     | 83  | LYS  | CA-C-N  | 6.45  | 126.63      | 120.31   |
| 2   | H     | 83  | LYS  | C-N-CA  | 6.45  | 126.63      | 120.31   |
| 2   | D     | 462 | SER  | CA-C-N  | 6.41  | 125.99      | 119.19   |
| 2   | D     | 462 | SER  | C-N-CA  | 6.41  | 125.99      | 119.19   |
| 2   | F     | 275 | LEU  | N-CA-C  | 6.39  | 117.94      | 108.60   |
| 1   | G     | 159 | PHE  | N-CA-C  | 6.37  | 119.87      | 109.24   |
| 2   | J     | 72  | PHE  | CA-C-N  | 6.36  | 126.05      | 119.56   |
| 2   | J     | 72  | PHE  | C-N-CA  | 6.36  | 126.05      | 119.56   |
| 2   | H     | 390 | ILE  | CB-CA-C | -6.34 | 102.50      | 111.38   |
| 2   | J     | 505 | ILE  | CB-CA-C | -6.33 | 103.90      | 111.81   |
| 2   | B     | 512 | LEU  | CA-C-N  | 6.29  | 126.03      | 119.05   |
| 2   | B     | 512 | LEU  | C-N-CA  | 6.29  | 126.03      | 119.05   |
| 2   | H     | 268 | PHE  | CA-C-N  | 6.28  | 127.68      | 119.84   |
| 2   | H     | 268 | PHE  | C-N-CA  | 6.28  | 127.68      | 119.84   |
| 2   | J     | 275 | LEU  | N-CA-C  | 6.27  | 117.75      | 108.60   |
| 2   | H     | 535 | MET  | N-CA-C  | -6.27 | 106.60      | 114.56   |
| 2   | J     | 462 | SER  | CA-C-N  | 6.23  | 125.80      | 119.19   |
| 2   | J     | 462 | SER  | C-N-CA  | 6.23  | 125.80      | 119.19   |
| 2   | H     | 349 | ILE  | CB-CA-C | -6.22 | 104.18      | 111.09   |
| 2   | P     | 76  | ARG  | N-CA-C  | -6.20 | 106.26      | 113.88   |
| 2   | D     | 512 | LEU  | CA-C-N  | 6.08  | 125.80      | 119.05   |
| 2   | D     | 512 | LEU  | C-N-CA  | 6.08  | 125.80      | 119.05   |
| 2   | J     | 512 | LEU  | CA-C-N  | 6.03  | 125.74      | 119.05   |
| 2   | J     | 512 | LEU  | C-N-CA  | 6.03  | 125.74      | 119.05   |
| 2   | P     | 83  | LYS  | CA-C-N  | 6.02  | 127.37      | 119.84   |
| 2   | P     | 83  | LYS  | C-N-CA  | 6.02  | 127.37      | 119.84   |
| 2   | B     | 180 | ASP  | N-CA-C  | 6.01  | 115.79      | 107.73   |
| 2   | H     | 226 | LYS  | N-CA-C  | -6.01 | 100.39      | 109.95   |
| 2   | D     | 580 | ASP  | N-CA-C  | 5.97  | 119.30      | 112.97   |
| 2   | N     | 83  | LYS  | CA-C-N  | 5.96  | 127.30      | 119.84   |
| 2   | N     | 83  | LYS  | C-N-CA  | 5.96  | 127.30      | 119.84   |
| 2   | L     | 72  | PHE  | CA-C-N  | 5.94  | 125.61      | 119.56   |
| 2   | L     | 72  | PHE  | C-N-CA  | 5.94  | 125.61      | 119.56   |
| 2   | D     | 72  | PHE  | CA-C-N  | 5.90  | 125.58      | 119.56   |
| 2   | D     | 72  | PHE  | C-N-CA  | 5.90  | 125.58      | 119.56   |
| 2   | D     | 529 | GLY  | N-CA-C  | -5.89 | 108.07      | 115.08   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 275 | LEU  | N-CA-C  | 5.88  | 117.18      | 108.60   |
| 2   | B     | 300 | LEU  | N-CA-C  | -5.87 | 106.75      | 112.97   |
| 1   | I     | 114 | LEU  | N-CA-C  | -5.86 | 104.80      | 111.07   |
| 2   | F     | 390 | ILE  | CB-CA-C | -5.85 | 103.18      | 111.19   |
| 2   | N     | 462 | SER  | CA-C-N  | 5.85  | 125.39      | 119.19   |
| 2   | N     | 462 | SER  | C-N-CA  | 5.85  | 125.39      | 119.19   |
| 2   | F     | 98  | GLY  | N-CA-C  | -5.80 | 106.49      | 116.01   |
| 2   | H     | 479 | GLY  | N-CA-C  | -5.78 | 105.80      | 112.50   |
| 2   | P     | 72  | PHE  | CA-C-N  | 5.75  | 125.42      | 119.56   |
| 2   | P     | 72  | PHE  | C-N-CA  | 5.75  | 125.42      | 119.56   |
| 2   | D     | 76  | ARG  | N-CA-C  | -5.73 | 106.83      | 113.88   |
| 1   | G     | 133 | ILE  | CB-CA-C | -5.73 | 104.65      | 111.81   |
| 2   | H     | 581 | CYS  | N-CA-C  | 5.70  | 116.58      | 109.57   |
| 2   | B     | 83  | LYS  | CA-C-N  | 5.69  | 126.95      | 119.84   |
| 2   | B     | 83  | LYS  | C-N-CA  | 5.69  | 126.95      | 119.84   |
| 2   | F     | 72  | PHE  | CA-C-N  | 5.68  | 125.35      | 119.56   |
| 2   | F     | 72  | PHE  | C-N-CA  | 5.68  | 125.35      | 119.56   |
| 1   | C     | 113 | LEU  | CA-C-N  | 5.64  | 129.55      | 121.71   |
| 1   | C     | 113 | LEU  | C-N-CA  | 5.64  | 129.55      | 121.71   |
| 2   | H     | 466 | ARG  | N-CA-C  | -5.64 | 106.56      | 113.50   |
| 2   | P     | 180 | ASP  | N-CA-C  | 5.60  | 115.23      | 107.73   |
| 2   | P     | 512 | LEU  | CA-C-N  | 5.57  | 125.24      | 119.05   |
| 2   | P     | 512 | LEU  | C-N-CA  | 5.57  | 125.24      | 119.05   |
| 2   | J     | 92  | ILE  | CA-C-N  | 5.56  | 125.57      | 119.90   |
| 2   | J     | 92  | ILE  | C-N-CA  | 5.56  | 125.57      | 119.90   |
| 1   | E     | 155 | ASN  | N-CA-C  | 5.56  | 117.34      | 111.28   |
| 2   | H     | 224 | SER  | N-CA-C  | 5.55  | 118.48      | 108.48   |
| 2   | L     | 180 | ASP  | N-CA-C  | 5.54  | 115.16      | 107.73   |
| 1   | K     | 159 | PHE  | N-CA-C  | 5.54  | 118.05      | 107.75   |
| 2   | H     | 409 | ARG  | N-CA-C  | 5.53  | 116.47      | 107.23   |
| 2   | P     | 92  | ILE  | CA-C-N  | 5.53  | 125.53      | 119.89   |
| 2   | P     | 92  | ILE  | C-N-CA  | 5.53  | 125.53      | 119.89   |
| 2   | H     | 172 | GLU  | N-CA-C  | 5.53  | 117.76      | 111.02   |
| 2   | P     | 529 | GLY  | N-CA-C  | -5.52 | 108.51      | 115.08   |
| 2   | B     | 529 | GLY  | N-CA-C  | -5.52 | 108.52      | 115.08   |
| 2   | N     | 529 | GLY  | N-CA-C  | -5.51 | 108.52      | 115.08   |
| 2   | L     | 580 | ASP  | N-CA-C  | 5.50  | 118.80      | 112.97   |
| 2   | N     | 48  | ASP  | N-CA-C  | -5.48 | 105.39      | 111.36   |
| 2   | H     | 458 | ILE  | CB-CA-C | -5.47 | 102.32      | 111.29   |
| 1   | M     | 159 | PHE  | N-CA-C  | 5.46  | 117.91      | 107.75   |
| 2   | N     | 512 | LEU  | CA-C-N  | 5.44  | 125.09      | 119.05   |
| 2   | N     | 512 | LEU  | C-N-CA  | 5.44  | 125.09      | 119.05   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | P     | 462 | SER  | CA-C-N  | 5.44  | 124.95      | 119.19   |
| 2   | P     | 462 | SER  | C-N-CA  | 5.44  | 124.95      | 119.19   |
| 2   | P     | 300 | LEU  | N-CA-C  | -5.42 | 107.22      | 112.97   |
| 1   | G     | 158 | ALA  | N-CA-C  | 5.41  | 120.54      | 113.88   |
| 1   | I     | 159 | PHE  | N-CA-C  | 5.40  | 117.43      | 108.20   |
| 1   | I     | 125 | ILE  | CB-CA-C | -5.39 | 104.97      | 112.04   |
| 1   | E     | 114 | LEU  | N-CA-CB | -5.38 | 102.60      | 110.40   |
| 2   | P     | 564 | HIS  | CA-C-N  | 5.36  | 126.11      | 120.11   |
| 2   | P     | 564 | HIS  | C-N-CA  | 5.36  | 126.11      | 120.11   |
| 2   | H     | 530 | GLN  | CB-CA-C | -5.36 | 104.63      | 111.22   |
| 2   | F     | 529 | GLY  | N-CA-C  | -5.35 | 108.71      | 115.08   |
| 2   | P     | 314 | ILE  | CB-CA-C | -5.35 | 105.03      | 112.04   |
| 2   | B     | 564 | HIS  | CA-C-N  | 5.34  | 126.52      | 119.84   |
| 2   | B     | 564 | HIS  | C-N-CA  | 5.34  | 126.52      | 119.84   |
| 2   | H     | 457 | TYR  | N-CA-C  | -5.34 | 104.89      | 111.40   |
| 2   | F     | 180 | ASP  | N-CA-C  | 5.33  | 114.88      | 107.73   |
| 2   | B     | 585 | VAL  | N-CA-C  | 5.33  | 115.57      | 108.11   |
| 1   | A     | 159 | PHE  | N-CA-C  | 5.32  | 117.30      | 108.20   |
| 2   | N     | 92  | ILE  | CA-C-N  | 5.32  | 125.32      | 119.89   |
| 2   | N     | 92  | ILE  | C-N-CA  | 5.32  | 125.32      | 119.89   |
| 2   | F     | 200 | TYR  | CA-C-N  | -5.31 | 115.87      | 123.20   |
| 2   | F     | 200 | TYR  | C-N-CA  | -5.31 | 115.87      | 123.20   |
| 2   | H     | 110 | ASN  | N-CA-C  | 5.30  | 120.75      | 113.97   |
| 2   | B     | 17  | VAL  | CB-CA-C | -5.29 | 105.00      | 112.14   |
| 2   | H     | 411 | VAL  | CB-CA-C | -5.28 | 103.29      | 110.42   |
| 2   | H     | 378 | GLN  | N-CA-C  | -5.28 | 106.79      | 114.12   |
| 2   | N     | 564 | HIS  | CA-C-N  | 5.25  | 126.40      | 119.84   |
| 2   | N     | 564 | HIS  | C-N-CA  | 5.25  | 126.40      | 119.84   |
| 2   | B     | 200 | TYR  | N-CA-C  | 5.22  | 117.06      | 111.36   |
| 1   | O     | 159 | PHE  | N-CA-C  | 5.21  | 117.44      | 107.75   |
| 2   | H     | 487 | CYS  | CA-C-N  | 5.20  | 125.50      | 119.47   |
| 2   | H     | 487 | CYS  | C-N-CA  | 5.20  | 125.50      | 119.47   |
| 2   | N     | 505 | ILE  | CB-CA-C | -5.19 | 105.33      | 111.81   |
| 2   | L     | 390 | ILE  | N-CA-C  | 5.18  | 116.32      | 108.96   |
| 2   | F     | 83  | LYS  | CA-C-N  | 5.18  | 126.31      | 119.84   |
| 2   | F     | 83  | LYS  | C-N-CA  | 5.18  | 126.31      | 119.84   |
| 2   | L     | 564 | HIS  | CA-C-N  | 5.17  | 126.30      | 119.84   |
| 2   | L     | 564 | HIS  | C-N-CA  | 5.17  | 126.30      | 119.84   |
| 2   | F     | 564 | HIS  | CA-C-N  | 5.17  | 126.30      | 119.84   |
| 2   | F     | 564 | HIS  | C-N-CA  | 5.17  | 126.30      | 119.84   |
| 2   | N     | 314 | ILE  | CB-CA-C | -5.17 | 105.27      | 112.04   |
| 2   | J     | 564 | HIS  | CA-C-N  | 5.17  | 126.30      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | J     | 564 | HIS  | C-N-CA  | 5.17  | 126.30      | 119.84   |
| 2   | L     | 529 | GLY  | N-CA-C  | -5.17 | 108.93      | 115.08   |
| 2   | F     | 512 | LEU  | CA-C-N  | 5.15  | 124.33      | 118.97   |
| 2   | F     | 512 | LEU  | C-N-CA  | 5.15  | 124.33      | 118.97   |
| 2   | J     | 529 | GLY  | N-CA-C  | -5.14 | 108.96      | 115.08   |
| 2   | H     | 584 | THR  | CB-CA-C | -5.12 | 99.76       | 109.95   |
| 1   | C     | 113 | LEU  | CA-C-O  | -5.11 | 113.10      | 119.18   |
| 2   | B     | 64  | THR  | CA-C-N  | -5.11 | 114.40      | 119.56   |
| 2   | B     | 64  | THR  | C-N-CA  | -5.11 | 114.40      | 119.56   |
| 2   | J     | 390 | ILE  | N-CA-C  | 5.11  | 116.21      | 108.96   |
| 2   | L     | 83  | LYS  | CA-C-N  | 5.11  | 126.22      | 119.84   |
| 2   | L     | 83  | LYS  | C-N-CA  | 5.11  | 126.22      | 119.84   |
| 2   | L     | 462 | SER  | CA-C-N  | 5.10  | 124.59      | 119.19   |
| 2   | L     | 462 | SER  | C-N-CA  | 5.10  | 124.59      | 119.19   |
| 2   | F     | 17  | VAL  | CB-CA-C | -5.10 | 105.26      | 112.14   |
| 1   | E     | 44  | LEU  | CA-C-N  | 5.08  | 126.20      | 119.84   |
| 1   | E     | 44  | LEU  | C-N-CA  | 5.08  | 126.20      | 119.84   |
| 2   | D     | 564 | HIS  | CA-C-N  | 5.08  | 126.20      | 119.84   |
| 2   | D     | 564 | HIS  | C-N-CA  | 5.08  | 126.20      | 119.84   |
| 2   | N     | 390 | ILE  | N-CA-C  | 5.08  | 116.18      | 108.96   |
| 2   | L     | 390 | ILE  | CB-CA-C | -5.08 | 104.23      | 111.19   |
| 2   | B     | 390 | ILE  | CB-CA-C | -5.07 | 104.24      | 111.19   |
| 1   | C     | 159 | PHE  | N-CA-C  | 5.07  | 117.18      | 107.75   |
| 2   | J     | 83  | LYS  | CA-C-N  | 5.06  | 126.17      | 119.84   |
| 2   | J     | 83  | LYS  | C-N-CA  | 5.06  | 126.17      | 119.84   |
| 2   | H     | 326 | ARG  | N-CA-C  | -5.06 | 103.04      | 110.52   |
| 2   | B     | 30  | ASP  | CA-C-N  | 5.05  | 124.71      | 119.56   |
| 2   | B     | 30  | ASP  | C-N-CA  | 5.05  | 124.71      | 119.56   |
| 2   | H     | 588 | LEU  | N-CA-C  | 5.05  | 117.48      | 109.96   |
| 2   | N     | 98  | GLY  | N-CA-C  | -5.05 | 107.73      | 116.01   |
| 1   | O     | 44  | LEU  | CA-C-N  | 5.04  | 126.15      | 119.84   |
| 1   | O     | 44  | LEU  | C-N-CA  | 5.04  | 126.15      | 119.84   |
| 2   | H     | 512 | LEU  | CA-C-N  | 5.04  | 125.86      | 120.47   |
| 2   | H     | 512 | LEU  | C-N-CA  | 5.04  | 125.86      | 120.47   |
| 2   | H     | 365 | VAL  | CB-CA-C | -5.01 | 103.07      | 111.29   |
| 1   | G     | 44  | LEU  | CA-C-N  | 5.01  | 126.10      | 119.84   |
| 1   | G     | 44  | LEU  | C-N-CA  | 5.01  | 126.10      | 119.84   |
| 1   | I     | 155 | ASN  | N-CA-C  | 5.01  | 117.39      | 111.33   |
| 2   | H     | 428 | VAL  | CB-CA-C | -5.01 | 105.47      | 111.88   |
| 2   | D     | 180 | ASP  | N-CA-C  | 5.00  | 114.44      | 107.73   |

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1146  | 0        | 1117     | 64      | 0            |
| 1   | C     | 1146  | 0        | 1117     | 69      | 0            |
| 1   | E     | 1146  | 0        | 1117     | 66      | 0            |
| 1   | G     | 1146  | 0        | 1117     | 64      | 0            |
| 1   | I     | 1146  | 0        | 1117     | 66      | 2            |
| 1   | K     | 1146  | 0        | 1117     | 62      | 0            |
| 1   | M     | 1146  | 0        | 1117     | 99      | 0            |
| 1   | O     | 1146  | 0        | 1117     | 60      | 0            |
| 2   | B     | 4541  | 0        | 4583     | 239     | 0            |
| 2   | D     | 4541  | 0        | 4583     | 250     | 2            |
| 2   | F     | 4541  | 0        | 4583     | 243     | 0            |
| 2   | H     | 4486  | 0        | 4534     | 456     | 0            |
| 2   | J     | 4541  | 0        | 4583     | 250     | 0            |
| 2   | L     | 4541  | 0        | 4583     | 256     | 0            |
| 2   | N     | 4541  | 0        | 4583     | 285     | 0            |
| 2   | P     | 4541  | 0        | 4583     | 244     | 0            |
| 3   | Q     | 156   | 0        | 171      | 5       | 0            |
| 3   | R     | 156   | 0        | 171      | 5       | 0            |
| 3   | S     | 156   | 0        | 171      | 5       | 0            |
| 3   | U     | 156   | 0        | 171      | 5       | 0            |
| 3   | V     | 156   | 0        | 171      | 5       | 0            |
| 3   | W     | 156   | 0        | 171      | 4       | 0            |
| 3   | X     | 156   | 0        | 171      | 5       | 0            |
| 4   | B     | 23    | 0        | 29       | 16      | 0            |
| 4   | D     | 23    | 0        | 28       | 15      | 0            |
| 4   | F     | 23    | 0        | 28       | 19      | 0            |
| 4   | H     | 23    | 0        | 29       | 21      | 0            |
| 4   | J     | 23    | 0        | 28       | 17      | 0            |
| 4   | L     | 23    | 0        | 28       | 16      | 0            |
| 4   | N     | 23    | 0        | 28       | 17      | 0            |
| 4   | P     | 23    | 0        | 28       | 15      | 0            |
| 5   | B     | 20    | 0        | 0        | 2       | 0            |
| 5   | D     | 20    | 0        | 0        | 3       | 0            |
| 5   | F     | 20    | 0        | 0        | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | H     | 20    | 0        | 0        | 3       | 0            |
| 5   | J     | 20    | 0        | 0        | 2       | 0            |
| 5   | L     | 20    | 0        | 0        | 3       | 0            |
| 5   | N     | 20    | 0        | 0        | 2       | 0            |
| 5   | P     | 20    | 0        | 0        | 3       | 0            |
| All | All   | 46877 | 0        | 46974    | 2702    | 2            |

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 29.

All (2702) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:168:THR:HB   | 2:B:196:VAL:HG13  | 1.28                     | 1.14              |
| 2:L:168:THR:HB   | 2:L:196:VAL:HG13  | 1.22                     | 1.14              |
| 2:F:168:THR:HB   | 2:F:196:VAL:HG13  | 1.27                     | 1.13              |
| 4:J:1100:7JA:H12 | 4:J:1100:7JA:H04  | 1.29                     | 1.13              |
| 1:G:151:VAL:HG11 | 2:H:39:LEU:HD21   | 1.28                     | 1.13              |
| 4:F:1100:7JA:H04 | 4:F:1100:7JA:H12  | 1.27                     | 1.13              |
| 4:D:1100:7JA:H12 | 4:D:1100:7JA:H04  | 1.29                     | 1.12              |
| 2:D:168:THR:HB   | 2:D:196:VAL:HG13  | 1.25                     | 1.11              |
| 2:H:390:ILE:HD11 | 2:H:412:LEU:HD21  | 1.28                     | 1.11              |
| 2:J:168:THR:HB   | 2:J:196:VAL:HG13  | 1.26                     | 1.11              |
| 4:P:1100:7JA:H04 | 4:P:1100:7JA:H12  | 1.30                     | 1.11              |
| 2:H:519:TRP:HE1  | 4:H:1100:7JA:H01A | 0.97                     | 1.10              |
| 4:L:1100:7JA:H12 | 4:L:1100:7JA:H04  | 1.29                     | 1.10              |
| 4:N:1100:7JA:H04 | 4:N:1100:7JA:H12  | 1.33                     | 1.10              |
| 4:B:1100:7JA:H12 | 4:B:1100:7JA:H04  | 1.29                     | 1.09              |
| 2:N:168:THR:HB   | 2:N:196:VAL:HG13  | 1.27                     | 1.08              |
| 4:F:1100:7JA:H04 | 4:F:1100:7JA:C12  | 1.83                     | 1.07              |
| 2:P:168:THR:HB   | 2:P:196:VAL:HG13  | 1.24                     | 1.07              |
| 4:B:1100:7JA:H04 | 4:B:1100:7JA:C12  | 1.84                     | 1.07              |
| 4:D:1100:7JA:H04 | 4:D:1100:7JA:C12  | 1.84                     | 1.06              |
| 1:M:102:ILE:HD12 | 2:N:20:VAL:HG21   | 1.38                     | 1.06              |
| 4:L:1100:7JA:H04 | 4:L:1100:7JA:C12  | 1.86                     | 1.05              |
| 2:H:442:ALA:HB3  | 4:H:1100:7JA:HD1  | 1.36                     | 1.04              |
| 2:H:398:ILE:HG23 | 2:H:402:LEU:HD11  | 1.39                     | 1.03              |
| 4:J:1100:7JA:H04 | 4:J:1100:7JA:C12  | 1.87                     | 1.03              |
| 4:P:1100:7JA:H04 | 4:P:1100:7JA:C12  | 1.87                     | 1.02              |
| 2:H:366:SER:HB3  | 2:H:368:ARG:HG2   | 1.36                     | 1.02              |
| 4:N:1100:7JA:H04 | 4:N:1100:7JA:C12  | 1.89                     | 1.01              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:P:93:PRO:HA    | 2:P:548:ARG:HB2   | 1.42                     | 1.01              |
| 1:G:151:VAL:CG1  | 2:H:39:LEU:HD21   | 1.91                     | 1.01              |
| 2:H:274:ARG:HG2  | 2:H:297:LYS:HB3   | 1.43                     | 1.00              |
| 2:L:93:PRO:HA    | 2:L:548:ARG:HB2   | 1.43                     | 0.99              |
| 2:H:364:LEU:HB3  | 2:H:365:VAL:HG22  | 1.44                     | 0.99              |
| 2:F:93:PRO:HA    | 2:F:548:ARG:HB2   | 1.45                     | 0.99              |
| 2:D:386:TYR:CE1  | 4:D:1100:7JA:HG2  | 1.98                     | 0.98              |
| 2:N:93:PRO:HA    | 2:N:548:ARG:HB2   | 1.42                     | 0.98              |
| 2:H:519:TRP:NE1  | 4:H:1100:7JA:H01A | 1.78                     | 0.98              |
| 2:N:519:TRP:HE1  | 4:N:1100:7JA:H01A | 1.28                     | 0.98              |
| 1:M:102:ILE:CD1  | 2:N:20:VAL:HG21   | 1.93                     | 0.98              |
| 2:H:347:LEU:HD12 | 2:H:348:ARG:N     | 1.78                     | 0.97              |
| 2:D:93:PRO:HA    | 2:D:548:ARG:HB2   | 1.46                     | 0.97              |
| 2:N:386:TYR:CE1  | 4:N:1100:7JA:HG2  | 1.98                     | 0.97              |
| 2:H:323:LEU:HD11 | 2:H:325:THR:HG22  | 1.46                     | 0.97              |
| 2:N:444:TYR:HA   | 2:N:471:GLY:HA3   | 1.46                     | 0.97              |
| 2:H:283:ASN:O    | 2:H:286:PRO:HD2   | 1.64                     | 0.97              |
| 2:L:542:ILE:HD11 | 2:L:588:LEU:HD12  | 1.45                     | 0.96              |
| 4:B:1100:7JA:C12 | 4:B:1100:7JA:C04  | 2.42                     | 0.96              |
| 2:B:444:TYR:HA   | 2:B:471:GLY:HA3   | 1.47                     | 0.96              |
| 2:L:386:TYR:CE1  | 4:L:1100:7JA:HG2  | 2.00                     | 0.96              |
| 2:D:444:TYR:HA   | 2:D:471:GLY:HA3   | 1.47                     | 0.95              |
| 2:D:80:LEU:HB2   | 2:D:122:MET:HE1   | 1.47                     | 0.95              |
| 2:F:386:TYR:CE1  | 4:F:1100:7JA:HG2  | 2.00                     | 0.95              |
| 2:F:444:TYR:HA   | 2:F:471:GLY:HA3   | 1.49                     | 0.95              |
| 2:N:116:SER:HB2  | 2:N:142:THR:HG23  | 1.48                     | 0.95              |
| 2:J:164:ARG:HE   | 2:N:112:ARG:HG3   | 1.32                     | 0.95              |
| 2:B:93:PRO:HA    | 2:B:548:ARG:HB2   | 1.46                     | 0.95              |
| 2:P:519:TRP:HE1  | 4:P:1100:7JA:H01A | 1.30                     | 0.94              |
| 2:H:409:ARG:HB3  | 4:H:1100:7JA:H29  | 1.49                     | 0.94              |
| 2:N:80:LEU:HB2   | 2:N:122:MET:HE1   | 1.50                     | 0.94              |
| 4:N:1100:7JA:C12 | 4:N:1100:7JA:C04  | 2.46                     | 0.93              |
| 2:F:519:TRP:HE1  | 4:F:1100:7JA:H01A | 1.32                     | 0.93              |
| 2:N:546:PRO:HG2  | 2:N:584:THR:HB    | 1.50                     | 0.93              |
| 2:J:386:TYR:CE1  | 4:J:1100:7JA:HG2  | 2.03                     | 0.93              |
| 1:M:102:ILE:HG21 | 2:N:20:VAL:CG2    | 1.98                     | 0.93              |
| 4:L:1100:7JA:C12 | 4:L:1100:7JA:C04  | 2.45                     | 0.93              |
| 2:P:429:ARG:O    | 2:P:433:ILE:HG13  | 1.67                     | 0.93              |
| 2:H:366:SER:CB   | 2:H:368:ARG:HG2   | 1.98                     | 0.92              |
| 2:D:101:THR:HG22 | 2:D:128:ASP:OD1   | 1.69                     | 0.92              |
| 2:J:93:PRO:HA    | 2:J:548:ARG:HB2   | 1.49                     | 0.92              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:101:THR:HG22 | 2:B:128:ASP:OD1   | 1.69                     | 0.91              |
| 2:F:101:THR:HG22 | 2:F:128:ASP:OD1   | 1.70                     | 0.91              |
| 2:H:332:ARG:HG2  | 2:H:332:ARG:HH11  | 1.34                     | 0.91              |
| 4:F:1100:7JA:C12 | 4:F:1100:7JA:C04  | 2.46                     | 0.91              |
| 4:J:1100:7JA:C12 | 4:J:1100:7JA:C04  | 2.47                     | 0.91              |
| 2:B:386:TYR:CE1  | 4:B:1100:7JA:HG2  | 2.04                     | 0.91              |
| 2:B:542:ILE:HD11 | 2:B:588:LEU:HD12  | 1.51                     | 0.91              |
| 2:P:101:THR:HG22 | 2:P:128:ASP:OD1   | 1.70                     | 0.91              |
| 4:D:1100:7JA:C12 | 4:D:1100:7JA:C04  | 2.46                     | 0.90              |
| 2:P:386:TYR:CE1  | 4:P:1100:7JA:HG2  | 2.06                     | 0.90              |
| 2:J:519:TRP:NE1  | 4:J:1100:7JA:H01A | 1.86                     | 0.90              |
| 2:J:542:ILE:HD11 | 2:J:588:LEU:HD12  | 1.52                     | 0.90              |
| 2:B:519:TRP:HE1  | 4:B:1100:7JA:H01A | 1.34                     | 0.90              |
| 2:F:542:ILE:HD11 | 2:F:588:LEU:HD12  | 1.52                     | 0.90              |
| 2:F:546:PRO:HG2  | 2:F:584:THR:HB    | 1.53                     | 0.90              |
| 4:P:1100:7JA:C12 | 4:P:1100:7JA:C04  | 2.47                     | 0.90              |
| 2:H:97:GLY:HA3   | 2:H:123:ILE:HD11  | 1.52                     | 0.90              |
| 4:B:1100:7JA:H12 | 4:B:1100:7JA:C04  | 2.01                     | 0.89              |
| 2:N:142:THR:HB   | 2:N:168:THR:HG23  | 1.54                     | 0.89              |
| 2:J:164:ARG:HE   | 2:N:112:ARG:CG    | 1.85                     | 0.89              |
| 2:L:101:THR:HG22 | 2:L:128:ASP:OD1   | 1.72                     | 0.89              |
| 2:P:444:TYR:HA   | 2:P:471:GLY:HA3   | 1.54                     | 0.89              |
| 2:J:519:TRP:HE1  | 4:J:1100:7JA:H01A | 1.35                     | 0.89              |
| 2:L:519:TRP:HE1  | 4:L:1100:7JA:H01A | 1.36                     | 0.89              |
| 2:B:590:GLU:HB3  | 2:B:591:PRO:HD2   | 1.55                     | 0.89              |
| 2:H:305:LEU:HD23 | 2:H:305:LEU:H     | 1.37                     | 0.89              |
| 2:P:519:TRP:NE1  | 4:P:1100:7JA:H01A | 1.88                     | 0.89              |
| 2:N:590:GLU:HB3  | 2:N:591:PRO:HD2   | 1.55                     | 0.88              |
| 2:P:590:GLU:HB3  | 2:P:591:PRO:HD2   | 1.55                     | 0.88              |
| 2:N:519:TRP:NE1  | 4:N:1100:7JA:H01A | 1.87                     | 0.88              |
| 2:J:444:TYR:HA   | 2:J:471:GLY:HA3   | 1.53                     | 0.88              |
| 2:N:429:ARG:O    | 2:N:433:ILE:HG13  | 1.72                     | 0.88              |
| 2:L:444:TYR:HA   | 2:L:471:GLY:HA3   | 1.54                     | 0.88              |
| 1:M:96:ALA:HB1   | 2:N:14:VAL:HG12   | 1.55                     | 0.88              |
| 2:P:542:ILE:HD11 | 2:P:588:LEU:HD12  | 1.54                     | 0.88              |
| 4:L:1100:7JA:H12 | 4:L:1100:7JA:C04  | 2.04                     | 0.88              |
| 2:B:519:TRP:NE1  | 4:B:1100:7JA:H01A | 1.88                     | 0.88              |
| 2:N:542:ILE:HD11 | 2:N:588:LEU:HD12  | 1.56                     | 0.88              |
| 1:C:48:THR:HG22  | 1:C:51:ILE:H      | 1.39                     | 0.87              |
| 2:D:590:GLU:HB3  | 2:D:591:PRO:HD2   | 1.55                     | 0.87              |
| 2:J:80:LEU:HB2   | 2:J:122:MET:HE1   | 1.54                     | 0.87              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:199:PHE:CZ   | 2:H:227:VAL:HG23  | 2.10                     | 0.87              |
| 2:P:80:LEU:HB2   | 2:P:122:MET:HE1   | 1.55                     | 0.87              |
| 2:D:80:LEU:HB2   | 2:D:122:MET:CE    | 2.03                     | 0.87              |
| 4:P:1100:7JA:H12 | 4:P:1100:7JA:C04  | 2.04                     | 0.87              |
| 2:H:142:THR:HB   | 2:H:168:THR:OG1   | 1.74                     | 0.86              |
| 2:F:519:TRP:NE1  | 4:F:1100:7JA:H01A | 1.88                     | 0.86              |
| 2:H:542:ILE:HD12 | 2:H:542:ILE:C     | 1.99                     | 0.86              |
| 2:D:116:SER:HB2  | 2:D:142:THR:HG23  | 1.57                     | 0.86              |
| 2:H:428:VAL:HG12 | 2:H:443:PHE:CZ    | 2.11                     | 0.86              |
| 2:H:201:MET:HG3  | 2:H:302:TYR:CE1   | 2.09                     | 0.86              |
| 4:J:1100:7JA:H12 | 4:J:1100:7JA:C04  | 2.04                     | 0.86              |
| 2:L:546:PRO:HG2  | 2:L:584:THR:HB    | 1.57                     | 0.86              |
| 2:H:311:CYS:HB3  | 2:H:336:VAL:HG21  | 1.55                     | 0.86              |
| 2:P:286:PRO:HA   | 2:P:289:PHE:CE2   | 2.11                     | 0.86              |
| 2:H:444:TYR:HA   | 2:H:471:GLY:HA3   | 1.58                     | 0.86              |
| 2:H:371:ILE:HG22 | 2:H:375:GLN:HE21  | 1.40                     | 0.86              |
| 2:D:519:TRP:NE1  | 4:D:1100:7JA:H01A | 1.91                     | 0.85              |
| 2:H:519:TRP:HH2  | 2:H:567:HIS:HD1   | 1.21                     | 0.85              |
| 2:B:116:SER:HB2  | 2:B:142:THR:HG23  | 1.56                     | 0.85              |
| 2:H:442:ALA:HB3  | 4:H:1100:7JA:CD1  | 2.04                     | 0.85              |
| 2:J:590:GLU:HB3  | 2:J:591:PRO:HD2   | 1.56                     | 0.85              |
| 2:L:590:GLU:HB3  | 2:L:591:PRO:HD2   | 1.55                     | 0.85              |
| 2:P:142:THR:HB   | 2:P:168:THR:HG23  | 1.57                     | 0.85              |
| 2:B:590:GLU:HB3  | 2:B:591:PRO:CD    | 2.07                     | 0.85              |
| 1:K:102:ILE:HG12 | 1:K:117:THR:HB    | 1.58                     | 0.85              |
| 2:P:546:PRO:HG2  | 2:P:584:THR:HB    | 1.58                     | 0.85              |
| 2:L:429:ARG:O    | 2:L:433:ILE:HG13  | 1.77                     | 0.85              |
| 2:L:519:TRP:NE1  | 4:L:1100:7JA:H01A | 1.91                     | 0.85              |
| 2:D:542:ILE:HD11 | 2:D:588:LEU:HD12  | 1.58                     | 0.84              |
| 2:D:590:GLU:HB3  | 2:D:591:PRO:CD    | 2.07                     | 0.84              |
| 2:F:116:SER:HB2  | 2:F:142:THR:HG23  | 1.59                     | 0.84              |
| 1:M:99:PHE:CD2   | 2:N:16:THR:C      | 2.56                     | 0.84              |
| 2:P:590:GLU:HB3  | 2:P:591:PRO:CD    | 2.07                     | 0.84              |
| 2:F:590:GLU:HB3  | 2:F:591:PRO:HD2   | 1.58                     | 0.84              |
| 4:F:1100:7JA:H12 | 4:F:1100:7JA:C04  | 2.05                     | 0.84              |
| 2:H:54:HIS:HE1   | 2:H:56:THR:OG1    | 1.61                     | 0.84              |
| 2:D:519:TRP:HE1  | 4:D:1100:7JA:H01A | 1.39                     | 0.84              |
| 2:N:101:THR:HG22 | 2:N:128:ASP:OD1   | 1.77                     | 0.84              |
| 2:H:409:ARG:HB3  | 4:H:1100:7JA:CG1  | 2.08                     | 0.84              |
| 1:I:48:THR:HG22  | 1:I:51:ILE:H      | 1.42                     | 0.84              |
| 2:J:101:THR:HG22 | 2:J:128:ASP:OD1   | 1.77                     | 0.84              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:80:LEU:HB2   | 2:F:122:MET:HE1   | 1.58                     | 0.83              |
| 2:H:286:PRO:HA   | 2:H:289:PHE:CE2   | 2.12                     | 0.83              |
| 2:N:590:GLU:HB3  | 2:N:591:PRO:CD    | 2.07                     | 0.83              |
| 2:P:116:SER:HB2  | 2:P:142:THR:HG23  | 1.59                     | 0.83              |
| 4:D:1100:7JA:H12 | 4:D:1100:7JA:C04  | 2.05                     | 0.83              |
| 1:E:48:THR:HG22  | 1:E:51:ILE:H      | 1.43                     | 0.83              |
| 2:J:429:ARG:O    | 2:J:433:ILE:HG13  | 1.78                     | 0.83              |
| 2:J:590:GLU:HB3  | 2:J:591:PRO:CD    | 2.08                     | 0.83              |
| 2:N:80:LEU:HB2   | 2:N:122:MET:CE    | 2.07                     | 0.83              |
| 2:B:429:ARG:O    | 2:B:433:ILE:HG13  | 1.78                     | 0.83              |
| 4:B:1100:7JA:C04 | 4:B:1100:7JA:H12A | 2.08                     | 0.83              |
| 2:J:546:PRO:HG2  | 2:J:584:THR:HB    | 1.60                     | 0.83              |
| 2:L:590:GLU:HB3  | 2:L:591:PRO:CD    | 2.09                     | 0.83              |
| 1:M:125:ILE:HG23 | 1:M:133:ILE:HD12  | 1.61                     | 0.83              |
| 1:G:48:THR:HG22  | 1:G:51:ILE:H      | 1.43                     | 0.82              |
| 1:C:125:ILE:HG23 | 1:C:133:ILE:HD12  | 1.59                     | 0.82              |
| 2:N:519:TRP:HE1  | 4:N:1100:7JA:C01  | 1.92                     | 0.82              |
| 2:L:80:LEU:HB2   | 2:L:122:MET:HE1   | 1.62                     | 0.82              |
| 2:H:390:ILE:HD12 | 2:H:410:LEU:HD21  | 1.62                     | 0.82              |
| 2:J:80:LEU:HB2   | 2:J:122:MET:CE    | 2.08                     | 0.82              |
| 2:F:429:ARG:O    | 2:F:433:ILE:HG13  | 1.79                     | 0.82              |
| 1:M:102:ILE:CD1  | 2:N:20:VAL:CG2    | 2.58                     | 0.82              |
| 2:H:492:LYS:NZ   | 2:H:516:ARG:HH11  | 1.77                     | 0.81              |
| 1:K:125:ILE:HG23 | 1:K:133:ILE:HD12  | 1.63                     | 0.81              |
| 2:F:142:THR:HB   | 2:F:168:THR:HG23  | 1.60                     | 0.81              |
| 2:J:116:SER:HB2  | 2:J:142:THR:HG23  | 1.61                     | 0.81              |
| 4:L:1100:7JA:C04 | 4:L:1100:7JA:H12A | 2.11                     | 0.81              |
| 2:F:590:GLU:HB3  | 2:F:591:PRO:CD    | 2.10                     | 0.81              |
| 1:G:151:VAL:HG11 | 2:H:39:LEU:CD2    | 2.09                     | 0.81              |
| 2:D:546:PRO:HG2  | 2:D:584:THR:HB    | 1.63                     | 0.81              |
| 2:J:142:THR:HB   | 2:J:168:THR:HG23  | 1.62                     | 0.81              |
| 1:K:93:ILE:HD12  | 1:K:97:THR:HG22   | 1.62                     | 0.81              |
| 2:H:409:ARG:HB3  | 4:H:1100:7JA:CD1  | 2.11                     | 0.81              |
| 2:J:519:TRP:HE1  | 4:J:1100:7JA:C01  | 1.94                     | 0.80              |
| 2:H:201:MET:HG3  | 2:H:302:TYR:HE1   | 1.46                     | 0.80              |
| 2:H:328:VAL:HG13 | 2:H:359:GLU:HG2   | 1.62                     | 0.80              |
| 1:M:96:ALA:HB1   | 2:N:14:VAL:CG1    | 2.10                     | 0.80              |
| 1:M:99:PHE:HD2   | 2:N:15:ALA:O      | 1.63                     | 0.80              |
| 1:A:93:ILE:HD12  | 1:A:97:THR:HG22   | 1.61                     | 0.80              |
| 1:C:93:ILE:HD12  | 1:C:97:THR:HG22   | 1.63                     | 0.80              |
| 2:F:112:ARG:HG2  | 2:L:164:ARG:HD2   | 1.64                     | 0.80              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:L:519:TRP:HE1  | 4:L:1100:7JA:C01  | 1.95                     | 0.80              |
| 1:M:93:ILE:HD12  | 1:M:97:THR:HG22   | 1.63                     | 0.80              |
| 2:L:116:SER:HB2  | 2:L:142:THR:HG23  | 1.62                     | 0.80              |
| 1:M:102:ILE:HG21 | 2:N:20:VAL:HG22   | 1.62                     | 0.80              |
| 4:N:1100:7JA:C04 | 4:N:1100:7JA:H12A | 2.10                     | 0.80              |
| 4:D:1100:7JA:C04 | 4:D:1100:7JA:H12A | 2.12                     | 0.80              |
| 1:A:48:THR:HG22  | 1:A:51:ILE:H      | 1.46                     | 0.80              |
| 2:B:142:THR:HB   | 2:B:168:THR:HG23  | 1.64                     | 0.80              |
| 2:J:164:ARG:HD2  | 2:N:112:ARG:HG2   | 1.63                     | 0.80              |
| 1:M:112:ASN:C    | 1:M:114:LEU:H     | 1.89                     | 0.80              |
| 2:B:519:TRP:HE1  | 4:B:1100:7JA:C01  | 1.95                     | 0.80              |
| 2:P:419:ILE:HD11 | 2:P:446:ARG:HH22  | 1.47                     | 0.79              |
| 1:O:48:THR:HG22  | 1:O:51:ILE:H      | 1.46                     | 0.79              |
| 2:L:80:LEU:HB2   | 2:L:122:MET:CE    | 2.12                     | 0.79              |
| 2:L:286:PRO:HA   | 2:L:289:PHE:CE2   | 2.18                     | 0.79              |
| 2:H:542:ILE:CG1  | 2:H:588:LEU:HB2   | 2.12                     | 0.79              |
| 2:L:142:THR:HB   | 2:L:168:THR:HG23  | 1.64                     | 0.79              |
| 2:H:266:LEU:HD13 | 2:H:267:VAL:H     | 1.48                     | 0.78              |
| 4:F:1100:7JA:C04 | 4:F:1100:7JA:H12A | 2.13                     | 0.78              |
| 1:M:48:THR:HG22  | 1:M:51:ILE:H      | 1.48                     | 0.78              |
| 2:P:519:TRP:HE1  | 4:P:1100:7JA:C01  | 1.96                     | 0.78              |
| 1:E:93:ILE:HD12  | 1:E:97:THR:HG22   | 1.66                     | 0.78              |
| 2:H:160:VAL:HG11 | 2:H:187:LEU:HG    | 1.65                     | 0.78              |
| 2:N:286:PRO:HA   | 2:N:289:PHE:CE2   | 2.18                     | 0.78              |
| 2:F:519:TRP:HE1  | 4:F:1100:7JA:C01  | 1.97                     | 0.78              |
| 1:K:48:THR:HG22  | 1:K:51:ILE:H      | 1.47                     | 0.78              |
| 2:H:125:SER:HB2  | 2:H:128:ASP:H     | 1.48                     | 0.78              |
| 2:H:230:PHE:HD1  | 2:H:235:LEU:HD21  | 1.49                     | 0.78              |
| 1:I:125:ILE:HG23 | 1:I:133:ILE:HD12  | 1.66                     | 0.77              |
| 2:F:80:LEU:HB2   | 2:F:122:MET:CE    | 2.14                     | 0.77              |
| 2:J:357:GLY:HA2  | 2:J:415:ARG:HH22  | 1.49                     | 0.77              |
| 2:L:308:GLU:HG3  | 2:L:332:ARG:HH22  | 1.50                     | 0.77              |
| 2:F:419:ILE:HD11 | 2:F:446:ARG:HH22  | 1.49                     | 0.77              |
| 1:G:155:ASN:HB3  | 2:H:35:ASP:OD2    | 1.85                     | 0.77              |
| 2:N:455:LEU:HD22 | 2:N:483:PHE:HB2   | 1.67                     | 0.77              |
| 2:D:308:GLU:HG3  | 2:D:332:ARG:HH22  | 1.50                     | 0.77              |
| 2:H:178:GLU:OE1  | 2:H:206:LYS:HB3   | 1.84                     | 0.77              |
| 2:D:429:ARG:O    | 2:D:433:ILE:HG13  | 1.84                     | 0.77              |
| 2:B:440:ARG:HB3  | 2:B:467:TRP:HE3   | 1.50                     | 0.76              |
| 1:O:159:PHE:O    | 1:O:160:GLU:HB2   | 1.84                     | 0.76              |
| 2:D:519:TRP:HE1  | 4:D:1100:7JA:C01  | 1.98                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:J:419:ILE:HD11 | 2:J:446:ARG:HH22  | 1.48                     | 0.76              |
| 2:F:455:LEU:HD22 | 2:F:483:PHE:HB2   | 1.67                     | 0.76              |
| 2:H:92:ILE:HD13  | 2:H:93:PRO:HD2    | 1.67                     | 0.76              |
| 2:P:80:LEU:HB2   | 2:P:122:MET:CE    | 2.15                     | 0.76              |
| 2:L:349:ILE:HG13 | 2:L:385:VAL:HG22  | 1.67                     | 0.76              |
| 1:O:113:LEU:O    | 1:O:113:LEU:HG    | 1.83                     | 0.76              |
| 2:J:398:ILE:HG23 | 2:J:402:LEU:HD11  | 1.68                     | 0.76              |
| 2:B:546:PRO:HG2  | 2:B:584:THR:HB    | 1.65                     | 0.76              |
| 2:D:419:ILE:HD11 | 2:D:446:ARG:HH22  | 1.49                     | 0.76              |
| 2:H:213:GLU:CD   | 2:H:237:GLY:HA3   | 2.10                     | 0.76              |
| 2:L:357:GLY:HA2  | 2:L:415:ARG:HH22  | 1.50                     | 0.76              |
| 2:H:331:ASP:OD2  | 2:H:366:SER:HB2   | 1.84                     | 0.76              |
| 1:O:125:ILE:HG23 | 1:O:133:ILE:HD12  | 1.67                     | 0.76              |
| 2:F:443:PHE:CE2  | 2:F:445:LEU:HD11  | 2.21                     | 0.75              |
| 2:H:373:LEU:O    | 2:H:373:LEU:HD12  | 1.85                     | 0.75              |
| 2:J:240:LYS:HG3  | 2:J:267:VAL:HG21  | 1.67                     | 0.75              |
| 2:F:59:LEU:HD22  | 2:F:61:TYR:H      | 1.49                     | 0.75              |
| 2:F:286:PRO:HA   | 2:F:289:PHE:CE2   | 2.21                     | 0.75              |
| 2:H:323:LEU:CD1  | 2:H:325:THR:HG22  | 2.16                     | 0.75              |
| 1:M:159:PHE:O    | 1:M:160:GLU:HB2   | 1.84                     | 0.75              |
| 2:D:431:LEU:C    | 2:D:431:LEU:HD12  | 2.11                     | 0.75              |
| 2:N:349:ILE:HG13 | 2:N:385:VAL:HG22  | 1.68                     | 0.75              |
| 2:H:519:TRP:HE1  | 4:H:1100:7JA:C01  | 1.90                     | 0.75              |
| 2:H:519:TRP:CH2  | 2:H:567:HIS:ND1   | 2.53                     | 0.75              |
| 4:P:1100:7JA:C04 | 4:P:1100:7JA:H12A | 2.16                     | 0.75              |
| 2:L:455:LEU:HD22 | 2:L:483:PHE:HB2   | 1.68                     | 0.75              |
| 2:P:310:HIS:O    | 2:P:314:ILE:HG12  | 1.87                     | 0.75              |
| 2:H:400:THR:O    | 2:H:403:LYS:HE2   | 1.87                     | 0.75              |
| 4:D:1100:7JA:H04 | 4:D:1100:7JA:H12A | 1.69                     | 0.75              |
| 2:P:357:GLY:HA2  | 2:P:415:ARG:HH22  | 1.52                     | 0.75              |
| 4:J:1100:7JA:C04 | 4:J:1100:7JA:H12A | 2.14                     | 0.75              |
| 2:P:55:VAL:HG23  | 2:P:75:LEU:HD21   | 1.68                     | 0.75              |
| 4:F:1100:7JA:H04 | 4:F:1100:7JA:H12A | 1.69                     | 0.74              |
| 2:H:286:PRO:HA   | 2:H:289:PHE:CD2   | 2.22                     | 0.74              |
| 1:K:159:PHE:O    | 1:K:160:GLU:HB2   | 1.85                     | 0.74              |
| 2:N:299:ASP:OD2  | 2:N:301:LEU:HB2   | 1.86                     | 0.74              |
| 2:B:286:PRO:HA   | 2:B:289:PHE:CE2   | 2.22                     | 0.74              |
| 2:H:396:GLU:O    | 2:H:400:THR:HG23  | 1.86                     | 0.74              |
| 1:C:159:PHE:O    | 1:C:160:GLU:HB2   | 1.87                     | 0.74              |
| 1:I:93:ILE:HD12  | 1:I:97:THR:HG22   | 1.69                     | 0.74              |
| 2:D:164:ARG:HD2  | 2:H:112:ARG:HD3   | 1.70                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:454:GLY:O    | 2:N:457:TYR:HB2  | 1.88                     | 0.74              |
| 2:P:308:GLU:HG3  | 2:P:332:ARG:HH22 | 1.52                     | 0.74              |
| 1:E:160:GLU:OE2  | 1:E:160:GLU:HA   | 1.86                     | 0.74              |
| 2:L:431:LEU:C    | 2:L:431:LEU:HD12 | 2.13                     | 0.74              |
| 2:N:419:ILE:HD11 | 2:N:446:ARG:HH22 | 1.51                     | 0.74              |
| 2:P:440:ARG:HB3  | 2:P:467:TRP:HE3  | 1.53                     | 0.74              |
| 2:B:308:GLU:HG3  | 2:B:332:ARG:HH22 | 1.53                     | 0.74              |
| 2:B:419:ILE:HD11 | 2:B:446:ARG:HH22 | 1.51                     | 0.74              |
| 2:N:55:VAL:HG23  | 2:N:75:LEU:HD21  | 1.67                     | 0.73              |
| 2:F:240:LYS:HG3  | 2:F:267:VAL:HG21 | 1.70                     | 0.73              |
| 1:G:160:GLU:HA   | 1:G:160:GLU:OE1  | 1.87                     | 0.73              |
| 1:I:160:GLU:HA   | 1:I:160:GLU:OE2  | 1.86                     | 0.73              |
| 2:P:455:LEU:HD22 | 2:P:483:PHE:HB2  | 1.69                     | 0.73              |
| 1:A:160:GLU:HA   | 1:A:160:GLU:OE2  | 1.86                     | 0.73              |
| 2:B:80:LEU:HB2   | 2:B:122:MET:CE   | 2.17                     | 0.73              |
| 2:H:285:MET:HE1  | 2:H:309:ASP:HB3  | 1.69                     | 0.73              |
| 2:J:440:ARG:HB3  | 2:J:467:TRP:HE3  | 1.53                     | 0.73              |
| 2:N:357:GLY:HA2  | 2:N:415:ARG:HH22 | 1.53                     | 0.73              |
| 2:B:191:ASN:HD21 | 2:B:194:LEU:H    | 1.34                     | 0.73              |
| 2:F:308:GLU:HG3  | 2:F:332:ARG:HH22 | 1.51                     | 0.73              |
| 2:H:280:MET:HE1  | 2:H:288:LEU:CD1  | 2.18                     | 0.73              |
| 2:N:240:LYS:HG3  | 2:N:267:VAL:HG21 | 1.71                     | 0.73              |
| 2:H:428:VAL:CG1  | 2:H:443:PHE:CZ   | 2.71                     | 0.73              |
| 2:L:443:PHE:CE2  | 2:L:445:LEU:HD11 | 2.24                     | 0.73              |
| 2:B:80:LEU:HB2   | 2:B:122:MET:HE1  | 1.68                     | 0.73              |
| 2:J:311:CYS:HB3  | 2:J:336:VAL:HG21 | 1.69                     | 0.73              |
| 1:O:93:ILE:HD12  | 1:O:97:THR:HG22  | 1.71                     | 0.73              |
| 1:A:159:PHE:O    | 1:A:160:GLU:HB2  | 1.89                     | 0.73              |
| 1:A:125:ILE:HG23 | 1:A:133:ILE:HD12 | 1.71                     | 0.72              |
| 2:D:440:ARG:HB3  | 2:D:467:TRP:HE3  | 1.53                     | 0.72              |
| 1:G:93:ILE:HD12  | 1:G:97:THR:HG22  | 1.71                     | 0.72              |
| 1:O:160:GLU:HA   | 1:O:160:GLU:OE2  | 1.89                     | 0.72              |
| 2:N:398:ILE:HG23 | 2:N:402:LEU:HD11 | 1.70                     | 0.72              |
| 2:B:357:GLY:HA2  | 2:B:415:ARG:HH22 | 1.53                     | 0.72              |
| 2:F:328:VAL:HG22 | 2:F:359:GLU:HB2  | 1.71                     | 0.72              |
| 1:M:48:THR:HG22  | 1:M:51:ILE:HB    | 1.71                     | 0.72              |
| 2:P:367:GLN:O    | 2:P:371:ILE:HG22 | 1.89                     | 0.72              |
| 2:D:357:GLY:HA2  | 2:D:415:ARG:HH22 | 1.55                     | 0.72              |
| 2:H:199:PHE:CE1  | 2:H:227:VAL:HG23 | 2.24                     | 0.72              |
| 2:J:286:PRO:HA   | 2:J:289:PHE:CE2  | 2.24                     | 0.72              |
| 2:J:308:GLU:HG3  | 2:J:332:ARG:HH22 | 1.53                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:L:398:ILE:HG23 | 2:L:402:LEU:HD11  | 1.71                     | 0.72              |
| 2:D:142:THR:HB   | 2:D:168:THR:HG23  | 1.71                     | 0.72              |
| 2:H:20:VAL:O     | 2:H:24:VAL:HG23   | 1.89                     | 0.72              |
| 2:L:240:LYS:HG3  | 2:L:267:VAL:HG21  | 1.70                     | 0.72              |
| 2:L:289:PHE:CD1  | 2:L:316:LYS:HD2   | 2.25                     | 0.72              |
| 1:M:96:ALA:CB    | 2:N:14:VAL:HG12   | 2.19                     | 0.72              |
| 2:P:240:LYS:HG3  | 2:P:267:VAL:HG21  | 1.72                     | 0.72              |
| 2:H:371:ILE:O    | 2:H:375:GLN:HG3   | 1.90                     | 0.72              |
| 2:J:349:ILE:HG13 | 2:J:385:VAL:HG22  | 1.70                     | 0.72              |
| 2:P:328:VAL:HG22 | 2:P:359:GLU:HB2   | 1.71                     | 0.72              |
| 2:F:545:ILE:HB   | 2:F:567:HIS:HB2   | 1.72                     | 0.72              |
| 1:E:159:PHE:O    | 1:E:160:GLU:HB2   | 1.90                     | 0.72              |
| 2:P:184:LEU:HD12 | 2:P:207:ILE:HB    | 1.71                     | 0.72              |
| 2:P:532:LEU:HD22 | 2:P:535:MET:HE2   | 1.71                     | 0.72              |
| 2:D:398:ILE:HG23 | 2:D:402:LEU:HD11  | 1.71                     | 0.71              |
| 2:D:328:VAL:HG22 | 2:D:359:GLU:HB2   | 1.72                     | 0.71              |
| 2:D:519:TRP:HH2  | 2:D:567:HIS:CE1   | 2.08                     | 0.71              |
| 3:S:203:ILE:H    | 3:S:203:ILE:HD12  | 1.55                     | 0.71              |
| 2:N:443:PHE:CE2  | 2:N:445:LEU:HD11  | 2.25                     | 0.71              |
| 2:D:191:ASN:HD21 | 2:D:194:LEU:H     | 1.39                     | 0.71              |
| 2:D:286:PRO:HA   | 2:D:289:PHE:CE2   | 2.26                     | 0.71              |
| 2:H:277:LEU:O    | 2:H:278:SER:O     | 2.08                     | 0.71              |
| 2:J:419:ILE:HD13 | 2:J:446:ARG:HH12  | 1.54                     | 0.71              |
| 2:F:357:GLY:HA2  | 2:F:415:ARG:HH22  | 1.55                     | 0.71              |
| 2:H:322:VAL:HG22 | 2:H:346:ARG:HB2   | 1.72                     | 0.71              |
| 2:L:184:LEU:HD12 | 2:L:207:ILE:HB    | 1.73                     | 0.71              |
| 2:N:308:GLU:HG3  | 2:N:332:ARG:HH22  | 1.54                     | 0.71              |
| 2:B:349:ILE:HG13 | 2:B:385:VAL:HG22  | 1.71                     | 0.71              |
| 2:D:240:LYS:HG3  | 2:D:267:VAL:HG21  | 1.71                     | 0.71              |
| 2:D:443:PHE:CE2  | 2:D:445:LEU:HD11  | 2.26                     | 0.70              |
| 2:H:364:LEU:HD22 | 2:H:387:VAL:HA    | 1.73                     | 0.70              |
| 2:P:59:LEU:HD22  | 2:P:61:TYR:H      | 1.54                     | 0.70              |
| 1:E:48:THR:HG22  | 1:E:51:ILE:HB     | 1.73                     | 0.70              |
| 2:L:419:ILE:HD11 | 2:L:446:ARG:HH22  | 1.54                     | 0.70              |
| 2:P:286:PRO:HA   | 2:P:289:PHE:CD2   | 2.26                     | 0.70              |
| 2:L:59:LEU:HD22  | 2:L:61:TYR:H      | 1.55                     | 0.70              |
| 4:P:1100:7JA:H04 | 4:P:1100:7JA:H12A | 1.73                     | 0.70              |
| 2:H:77:SER:HB3   | 2:H:116:SER:HB3   | 1.73                     | 0.70              |
| 2:F:310:HIS:O    | 2:F:314:ILE:HG12  | 1.91                     | 0.70              |
| 2:J:55:VAL:HG23  | 2:J:75:LEU:HD21   | 1.74                     | 0.70              |
| 2:B:59:LEU:HD22  | 2:B:61:TYR:H      | 1.57                     | 0.70              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:468:MET:HG3  | 2:H:490:LEU:HD21  | 1.73                     | 0.70              |
| 2:J:210:LYS:O    | 2:J:214:THR:HG22  | 1.92                     | 0.70              |
| 2:P:311:CYS:HB3  | 2:P:336:VAL:HG21  | 1.73                     | 0.70              |
| 2:H:160:VAL:CG1  | 2:H:187:LEU:HG    | 2.21                     | 0.70              |
| 1:C:160:GLU:HA   | 1:C:160:GLU:OE2   | 1.91                     | 0.69              |
| 2:F:398:ILE:HG23 | 2:F:402:LEU:HD11  | 1.73                     | 0.69              |
| 2:F:419:ILE:HD13 | 2:F:446:ARG:HH12  | 1.55                     | 0.69              |
| 2:F:454:GLY:O    | 2:F:457:TYR:HB2   | 1.92                     | 0.69              |
| 2:N:328:VAL:HG22 | 2:N:359:GLU:HB2   | 1.73                     | 0.69              |
| 2:J:328:VAL:HG22 | 2:J:359:GLU:HB2   | 1.74                     | 0.69              |
| 2:L:328:VAL:HG22 | 2:L:359:GLU:HB2   | 1.73                     | 0.69              |
| 2:P:545:ILE:HB   | 2:P:567:HIS:HB2   | 1.73                     | 0.69              |
| 2:D:59:LEU:HD22  | 2:D:61:TYR:H      | 1.58                     | 0.69              |
| 2:B:455:LEU:HD22 | 2:B:483:PHE:HB2   | 1.74                     | 0.69              |
| 1:M:102:ILE:CG2  | 2:N:20:VAL:CG2    | 2.69                     | 0.69              |
| 1:M:160:GLU:OE2  | 1:M:160:GLU:HA    | 1.91                     | 0.69              |
| 2:H:325:THR:OG1  | 2:H:326:ARG:O     | 2.11                     | 0.69              |
| 1:K:160:GLU:HA   | 1:K:160:GLU:OE2   | 1.90                     | 0.69              |
| 1:M:129:THR:O    | 1:M:133:ILE:HG12  | 1.92                     | 0.69              |
| 4:N:1100:7JA:H04 | 4:N:1100:7JA:H12A | 1.72                     | 0.69              |
| 2:P:398:ILE:HG23 | 2:P:402:LEU:HD11  | 1.74                     | 0.69              |
| 2:B:143:LEU:HD23 | 2:B:159:ILE:HD13  | 1.74                     | 0.69              |
| 2:D:251:GLY:O    | 2:D:278:SER:HB2   | 1.93                     | 0.69              |
| 2:J:59:LEU:HD22  | 2:J:61:TYR:H      | 1.57                     | 0.69              |
| 2:J:164:ARG:NE   | 2:N:112:ARG:CG    | 2.55                     | 0.69              |
| 3:U:203:ILE:H    | 3:U:203:ILE:HD12  | 1.57                     | 0.69              |
| 2:P:431:LEU:C    | 2:P:431:LEU:HD12  | 2.18                     | 0.69              |
| 2:F:431:LEU:HD12 | 2:F:431:LEU:C     | 2.18                     | 0.69              |
| 2:L:251:GLY:O    | 2:L:278:SER:HB2   | 1.93                     | 0.69              |
| 3:V:203:ILE:HD12 | 3:V:203:ILE:H     | 1.57                     | 0.69              |
| 2:D:563:GLU:HG3  | 2:D:563:GLU:O     | 1.93                     | 0.69              |
| 2:F:191:ASN:HD21 | 2:F:194:LEU:H     | 1.39                     | 0.69              |
| 2:H:327:ASN:CG   | 2:H:351:ARG:HB2   | 2.18                     | 0.69              |
| 2:N:431:LEU:HD12 | 2:N:431:LEU:C     | 2.17                     | 0.69              |
| 2:J:299:ASP:OD2  | 2:J:301:LEU:HB2   | 1.94                     | 0.68              |
| 2:F:349:ILE:HG13 | 2:F:385:VAL:HG22  | 1.75                     | 0.68              |
| 2:H:492:LYS:HZ3  | 2:H:516:ARG:HH11  | 1.39                     | 0.68              |
| 1:I:159:PHE:O    | 1:I:160:GLU:HB2   | 1.92                     | 0.68              |
| 2:N:59:LEU:HD22  | 2:N:61:TYR:H      | 1.56                     | 0.68              |
| 2:N:391:THR:HG23 | 2:N:394:SER:H     | 1.58                     | 0.68              |
| 2:P:143:LEU:HD23 | 2:P:159:ILE:HD13  | 1.74                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:251:GLY:O    | 2:P:278:SER:HB2  | 1.93                     | 0.68              |
| 2:J:563:GLU:O    | 2:J:563:GLU:HG3  | 1.93                     | 0.68              |
| 2:N:440:ARG:HB3  | 2:N:467:TRP:HE3  | 1.58                     | 0.68              |
| 2:B:210:LYS:O    | 2:B:214:THR:HG22 | 1.93                     | 0.68              |
| 2:B:240:LYS:HG3  | 2:B:267:VAL:HG21 | 1.76                     | 0.68              |
| 2:B:328:VAL:HG22 | 2:B:359:GLU:HB2  | 1.74                     | 0.68              |
| 2:B:351:ARG:HD3  | 2:B:413:LEU:HD11 | 1.75                     | 0.68              |
| 2:D:419:ILE:HD13 | 2:D:446:ARG:HH12 | 1.59                     | 0.68              |
| 2:D:545:ILE:HB   | 2:D:567:HIS:HB2  | 1.73                     | 0.68              |
| 2:H:367:GLN:O    | 2:H:371:ILE:HG13 | 1.93                     | 0.68              |
| 2:J:164:ARG:CD   | 2:N:112:ARG:HG2  | 2.23                     | 0.68              |
| 2:J:357:GLY:CA   | 2:J:415:ARG:HH22 | 2.07                     | 0.68              |
| 2:L:468:MET:HE3  | 2:L:470:LEU:HD21 | 1.74                     | 0.68              |
| 1:M:102:ILE:HD13 | 2:N:20:VAL:HG22  | 1.75                     | 0.68              |
| 2:H:428:VAL:HG23 | 2:H:429:ARG:N    | 2.08                     | 0.68              |
| 2:F:55:VAL:HG23  | 2:F:75:LEU:HD21  | 1.75                     | 0.68              |
| 2:H:278:SER:O    | 2:H:280:MET:N    | 2.26                     | 0.68              |
| 4:N:1100:7JA:H12 | 4:N:1100:7JA:C04 | 2.05                     | 0.68              |
| 1:O:48:THR:HG22  | 1:O:51:ILE:HB    | 1.76                     | 0.68              |
| 2:D:455:LEU:HD22 | 2:D:483:PHE:HB2  | 1.74                     | 0.68              |
| 2:P:349:ILE:HG13 | 2:P:385:VAL:HG22 | 1.75                     | 0.68              |
| 2:L:210:LYS:O    | 2:L:214:THR:HG22 | 1.92                     | 0.68              |
| 2:P:443:PHE:CE2  | 2:P:445:LEU:HD11 | 2.29                     | 0.68              |
| 2:B:487:CYS:HB3  | 2:B:490:LEU:HB2  | 1.75                     | 0.68              |
| 2:F:251:GLY:O    | 2:F:278:SER:HB2  | 1.93                     | 0.68              |
| 2:H:280:MET:HE1  | 2:H:288:LEU:HD11 | 1.76                     | 0.68              |
| 2:P:191:ASN:HD21 | 2:P:194:LEU:H    | 1.40                     | 0.68              |
| 2:D:289:PHE:CD1  | 2:D:316:LYS:HD2  | 2.29                     | 0.67              |
| 2:L:563:GLU:HG3  | 2:L:563:GLU:O    | 1.94                     | 0.67              |
| 2:N:307:THR:HG21 | 2:N:362:GLU:HB2  | 1.76                     | 0.67              |
| 3:W:203:ILE:H    | 3:W:203:ILE:HD12 | 1.59                     | 0.67              |
| 2:J:424:LEU:O    | 2:J:428:VAL:HG23 | 1.94                     | 0.67              |
| 2:L:391:THR:HG23 | 2:L:394:SER:H    | 1.59                     | 0.67              |
| 1:G:132:GLU:O    | 1:G:136:THR:HG23 | 1.93                     | 0.67              |
| 2:H:168:THR:HB   | 2:H:196:VAL:HG13 | 1.76                     | 0.67              |
| 2:N:367:GLN:O    | 2:N:371:ILE:HG22 | 1.95                     | 0.67              |
| 2:N:487:CYS:HB3  | 2:N:490:LEU:HB2  | 1.76                     | 0.67              |
| 2:H:443:PHE:CE2  | 2:H:445:LEU:HD11 | 2.29                     | 0.67              |
| 2:L:311:CYS:HB3  | 2:L:336:VAL:HG21 | 1.77                     | 0.67              |
| 2:N:545:ILE:HB   | 2:N:567:HIS:HB2  | 1.75                     | 0.67              |
| 2:H:232:ILE:HG13 | 2:H:253:LEU:CD2  | 2.25                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:477:ASP:OD2  | 2:H:501:SER:OG   | 2.09                     | 0.67              |
| 2:J:365:VAL:HG23 | 2:J:387:VAL:HA   | 1.77                     | 0.67              |
| 2:J:455:LEU:HD22 | 2:J:483:PHE:HB2  | 1.76                     | 0.67              |
| 2:P:357:GLY:CA   | 2:P:415:ARG:HH22 | 2.07                     | 0.67              |
| 1:E:125:ILE:HG23 | 1:E:133:ILE:HD12 | 1.77                     | 0.67              |
| 1:G:30:ALA:O     | 1:G:33:VAL:HG22  | 1.94                     | 0.67              |
| 2:H:347:LEU:HD12 | 2:H:348:ARG:H    | 1.59                     | 0.67              |
| 2:J:191:ASN:HD21 | 2:J:194:LEU:H    | 1.42                     | 0.67              |
| 1:M:102:ILE:HD13 | 2:N:20:VAL:CG2   | 2.23                     | 0.67              |
| 2:B:365:VAL:HG23 | 2:B:387:VAL:HA   | 1.75                     | 0.67              |
| 1:E:45:PRO:HG3   | 2:L:293:ALA:HB3  | 1.75                     | 0.67              |
| 2:F:286:PRO:HA   | 2:F:289:PHE:CD2  | 2.30                     | 0.67              |
| 2:H:431:LEU:HD23 | 2:H:431:LEU:C    | 2.20                     | 0.67              |
| 2:H:441:PHE:CZ   | 2:H:443:PHE:CD1  | 2.83                     | 0.67              |
| 1:A:48:THR:HG22  | 1:A:51:ILE:HB    | 1.77                     | 0.67              |
| 2:D:307:THR:HG21 | 2:D:362:GLU:HB2  | 1.77                     | 0.67              |
| 1:I:158:ALA:HA   | 2:J:62:THR:HG21  | 1.77                     | 0.67              |
| 2:J:184:LEU:HD12 | 2:J:207:ILE:HB   | 1.74                     | 0.67              |
| 2:J:545:ILE:HB   | 2:J:567:HIS:HB2  | 1.75                     | 0.67              |
| 2:L:431:LEU:HD12 | 2:L:431:LEU:O    | 1.95                     | 0.67              |
| 2:P:289:PHE:CD1  | 2:P:316:LYS:HD2  | 2.29                     | 0.67              |
| 2:B:431:LEU:C    | 2:B:431:LEU:HD12 | 2.19                     | 0.67              |
| 2:D:95:ASN:O     | 2:D:582:PRO:HG3  | 1.95                     | 0.67              |
| 1:G:48:THR:CG2   | 1:G:51:ILE:H     | 2.07                     | 0.67              |
| 2:H:542:ILE:HD11 | 2:H:588:LEU:HB2  | 1.76                     | 0.67              |
| 2:B:519:TRP:HH2  | 2:B:567:HIS:CE1  | 2.13                     | 0.66              |
| 2:L:357:GLY:CA   | 2:L:415:ARG:HH22 | 2.07                     | 0.66              |
| 2:B:468:MET:HE3  | 2:B:470:LEU:HD21 | 1.76                     | 0.66              |
| 2:D:349:ILE:HG13 | 2:D:385:VAL:HG22 | 1.77                     | 0.66              |
| 2:F:311:CYS:HB3  | 2:F:336:VAL:HG21 | 1.77                     | 0.66              |
| 2:J:431:LEU:C    | 2:J:431:LEU:HD12 | 2.20                     | 0.66              |
| 2:P:93:PRO:HA    | 2:P:548:ARG:CB   | 2.22                     | 0.66              |
| 2:B:55:VAL:HG23  | 2:B:75:LEU:HD21  | 1.77                     | 0.66              |
| 2:B:357:GLY:CA   | 2:B:415:ARG:HH22 | 2.08                     | 0.66              |
| 2:D:468:MET:HE3  | 2:D:470:LEU:HD21 | 1.76                     | 0.66              |
| 2:F:289:PHE:CD1  | 2:F:316:LYS:HD2  | 2.31                     | 0.66              |
| 2:J:251:GLY:O    | 2:J:278:SER:HB2  | 1.96                     | 0.66              |
| 2:P:468:MET:HE3  | 2:P:470:LEU:HD21 | 1.76                     | 0.66              |
| 1:G:48:THR:HG22  | 1:G:51:ILE:HB    | 1.77                     | 0.66              |
| 2:H:545:ILE:HB   | 2:H:567:HIS:HB2  | 1.77                     | 0.66              |
| 2:P:454:GLY:O    | 2:P:457:TYR:HB2  | 1.94                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:184:LEU:HD12 | 2:F:207:ILE:HB   | 1.78                     | 0.66              |
| 2:F:211:ASP:HA   | 2:F:214:THR:HG23 | 1.78                     | 0.66              |
| 2:H:258:GLY:C    | 2:H:260:PRO:HD3  | 2.20                     | 0.66              |
| 2:D:54:HIS:HD2   | 2:D:77:SER:OG    | 1.78                     | 0.66              |
| 2:J:454:GLY:O    | 2:J:457:TYR:HB2  | 1.96                     | 0.66              |
| 2:P:519:TRP:HH2  | 2:P:567:HIS:CE1  | 2.13                     | 0.66              |
| 2:D:365:VAL:HG23 | 2:D:387:VAL:HA   | 1.77                     | 0.66              |
| 3:R:203:ILE:H    | 3:R:203:ILE:HD12 | 1.61                     | 0.66              |
| 2:H:332:ARG:HH11 | 2:H:332:ARG:CG   | 2.07                     | 0.66              |
| 1:I:153:ARG:HG2  | 1:I:157:TRP:CZ3  | 2.30                     | 0.66              |
| 2:N:211:ASP:HA   | 2:N:214:THR:HG23 | 1.78                     | 0.66              |
| 2:B:311:CYS:HB3  | 2:B:336:VAL:HG21 | 1.76                     | 0.66              |
| 1:G:128:LYS:HE3  | 1:G:136:THR:HG21 | 1.78                     | 0.66              |
| 2:H:392:ASN:O    | 2:H:396:GLU:HG3  | 1.95                     | 0.66              |
| 2:N:286:PRO:HA   | 2:N:289:PHE:CD2  | 2.31                     | 0.66              |
| 1:A:102:ILE:CG1  | 1:A:117:THR:HB   | 2.25                     | 0.66              |
| 2:J:289:PHE:CD1  | 2:J:316:LYS:HD2  | 2.30                     | 0.66              |
| 2:L:55:VAL:HG23  | 2:L:75:LEU:HD21  | 1.76                     | 0.66              |
| 1:G:144:THR:HG23 | 1:G:147:GLU:OE2  | 1.96                     | 0.65              |
| 2:H:533:MET:C    | 2:H:535:MET:H    | 2.05                     | 0.65              |
| 2:H:584:THR:O    | 2:H:584:THR:HG22 | 1.95                     | 0.65              |
| 2:J:443:PHE:CE2  | 2:J:445:LEU:HD11 | 2.31                     | 0.65              |
| 2:D:351:ARG:HD3  | 2:D:413:LEU:HD11 | 1.77                     | 0.65              |
| 2:F:487:CYS:HB3  | 2:F:490:LEU:HB2  | 1.77                     | 0.65              |
| 2:H:211:ASP:O    | 2:H:215:ILE:HG13 | 1.97                     | 0.65              |
| 2:H:351:ARG:HD2  | 2:H:359:GLU:O    | 1.96                     | 0.65              |
| 2:J:519:TRP:HH2  | 2:J:567:HIS:CE1  | 2.14                     | 0.65              |
| 2:L:227:VAL:HG13 | 2:L:228:GLY:N    | 2.10                     | 0.65              |
| 2:L:440:ARG:HB3  | 2:L:467:TRP:HE3  | 1.59                     | 0.65              |
| 2:P:563:GLU:HG3  | 2:P:563:GLU:O    | 1.94                     | 0.65              |
| 2:B:419:ILE:HD13 | 2:B:446:ARG:HH12 | 1.61                     | 0.65              |
| 2:L:231:GLU:HG2  | 2:L:254:ASN:HD22 | 1.60                     | 0.65              |
| 2:N:184:LEU:HD12 | 2:N:207:ILE:HB   | 1.78                     | 0.65              |
| 3:X:203:ILE:H    | 3:X:203:ILE:HD12 | 1.60                     | 0.65              |
| 2:D:386:TYR:HE1  | 4:D:1100:7JA:HG2 | 1.61                     | 0.65              |
| 1:M:99:PHE:CD2   | 2:N:15:ALA:O     | 2.48                     | 0.65              |
| 2:N:93:PRO:HA    | 2:N:548:ARG:CB   | 2.24                     | 0.65              |
| 2:N:456:SER:HB3  | 2:N:482:GLU:HB3  | 1.79                     | 0.65              |
| 2:H:54:HIS:CE1   | 2:H:56:THR:OG1   | 2.47                     | 0.65              |
| 2:J:211:ASP:HA   | 2:J:214:THR:HG23 | 1.78                     | 0.65              |
| 2:L:307:THR:HG21 | 2:L:362:GLU:HB2  | 1.79                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:P:211:ASP:HA   | 2:P:214:THR:HG23  | 1.78                     | 0.65              |
| 2:B:563:GLU:O    | 2:B:563:GLU:HG3   | 1.94                     | 0.65              |
| 2:F:563:GLU:HG3  | 2:F:563:GLU:O     | 1.95                     | 0.65              |
| 2:H:441:PHE:O    | 2:H:468:MET:HA    | 1.95                     | 0.65              |
| 2:L:419:ILE:HD13 | 2:L:446:ARG:HH12  | 1.61                     | 0.65              |
| 2:N:468:MET:HE1  | 2:N:483:PHE:CE1   | 2.32                     | 0.65              |
| 2:N:251:GLY:O    | 2:N:278:SER:HB2   | 1.96                     | 0.65              |
| 2:N:419:ILE:HD13 | 2:N:446:ARG:HH12  | 1.62                     | 0.65              |
| 1:A:98:LEU:HD21  | 1:A:120:THR:HG22  | 1.78                     | 0.65              |
| 2:H:390:ILE:HD11 | 2:H:412:LEU:CD2   | 2.15                     | 0.65              |
| 4:L:1100:7JA:H04 | 4:L:1100:7JA:H12A | 1.71                     | 0.65              |
| 2:N:191:ASN:HD21 | 2:N:194:LEU:H     | 1.44                     | 0.65              |
| 2:N:289:PHE:CD1  | 2:N:316:LYS:HD2   | 2.31                     | 0.65              |
| 2:F:365:VAL:HG23 | 2:F:387:VAL:HA    | 1.79                     | 0.65              |
| 2:H:56:THR:HG23  | 2:H:79:LYS:HB3    | 1.77                     | 0.65              |
| 2:H:56:THR:HG23  | 2:H:79:LYS:HD2    | 1.79                     | 0.65              |
| 2:H:99:TYR:CD2   | 2:H:123:ILE:HD12  | 2.32                     | 0.65              |
| 2:L:454:GLY:O    | 2:L:457:TYR:HB2   | 1.96                     | 0.65              |
| 2:P:365:VAL:HG23 | 2:P:387:VAL:HA    | 1.79                     | 0.65              |
| 1:E:30:ALA:O     | 1:E:33:VAL:HG22   | 1.97                     | 0.64              |
| 2:F:231:GLU:HG2  | 2:F:254:ASN:HD22  | 1.61                     | 0.64              |
| 2:H:34:ARG:NH1   | 2:H:48:ASP:OD1    | 2.27                     | 0.64              |
| 2:H:305:LEU:HD23 | 2:H:305:LEU:N     | 2.10                     | 0.64              |
| 2:D:319:ASN:ND2  | 1:G:43:PRO:HG3    | 2.12                     | 0.64              |
| 2:H:259:MET:C    | 2:H:261:GLU:H     | 2.06                     | 0.64              |
| 2:N:357:GLY:CA   | 2:N:415:ARG:HH22  | 2.09                     | 0.64              |
| 2:P:419:ILE:HD13 | 2:P:446:ARG:HH12  | 1.61                     | 0.64              |
| 2:B:307:THR:HG21 | 2:B:362:GLU:HB2   | 1.78                     | 0.64              |
| 2:H:343:GLN:CD   | 2:H:343:GLN:H     | 2.05                     | 0.64              |
| 2:B:443:PHE:CE2  | 2:B:445:LEU:HD11  | 2.31                     | 0.64              |
| 2:D:299:ASP:OD2  | 2:D:301:LEU:HB2   | 1.98                     | 0.64              |
| 1:E:48:THR:CG2   | 1:E:51:ILE:H      | 2.09                     | 0.64              |
| 2:F:468:MET:HE3  | 2:F:470:LEU:HD21  | 1.80                     | 0.64              |
| 1:O:30:ALA:O     | 1:O:33:VAL:HG22   | 1.98                     | 0.64              |
| 2:B:398:ILE:HG23 | 2:B:402:LEU:HD11  | 1.79                     | 0.64              |
| 2:D:210:LYS:O    | 2:D:214:THR:HG22  | 1.97                     | 0.64              |
| 2:D:487:CYS:HB3  | 2:D:490:LEU:HB2   | 1.80                     | 0.64              |
| 2:F:299:ASP:OD2  | 2:F:301:LEU:HB2   | 1.98                     | 0.64              |
| 2:H:532:LEU:O    | 2:H:535:MET:HB3   | 1.98                     | 0.64              |
| 2:J:54:HIS:HE1   | 2:J:56:THR:OG1    | 1.81                     | 0.64              |
| 2:N:563:GLU:HG3  | 2:N:563:GLU:O     | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:431:LEU:HD12 | 2:P:431:LEU:O    | 1.97                     | 0.64              |
| 2:D:412:LEU:O    | 2:D:412:LEU:HD12 | 1.98                     | 0.64              |
| 2:F:424:LEU:O    | 2:F:428:VAL:HG23 | 1.97                     | 0.64              |
| 2:H:143:LEU:HD12 | 2:H:144:LYS:H    | 1.62                     | 0.64              |
| 1:I:30:ALA:O     | 1:I:33:VAL:HG22  | 1.97                     | 0.64              |
| 2:L:121:ARG:NH2  | 5:L:1103:PO4:O4  | 2.31                     | 0.64              |
| 1:M:102:ILE:HG21 | 2:N:20:VAL:HG23  | 1.78                     | 0.64              |
| 2:N:519:TRP:HH2  | 2:N:567:HIS:CE1  | 2.16                     | 0.64              |
| 2:B:54:HIS:HE1   | 2:B:56:THR:OG1   | 1.80                     | 0.64              |
| 2:B:299:ASP:OD2  | 2:B:301:LEU:HB2  | 1.98                     | 0.64              |
| 2:D:55:VAL:HG23  | 2:D:75:LEU:HD21  | 1.79                     | 0.64              |
| 1:E:113:LEU:HG   | 1:E:113:LEU:O    | 1.98                     | 0.64              |
| 2:L:487:CYS:HB3  | 2:L:490:LEU:HB2  | 1.80                     | 0.64              |
| 1:M:112:ASN:C    | 1:M:114:LEU:N    | 2.55                     | 0.64              |
| 2:B:310:HIS:O    | 2:B:314:ILE:HG12 | 1.98                     | 0.64              |
| 1:C:91:MET:HE2   | 1:C:91:MET:HA    | 1.78                     | 0.64              |
| 2:H:291:PHE:N    | 2:H:291:PHE:CD2  | 2.65                     | 0.64              |
| 2:N:170:LEU:C    | 2:N:170:LEU:HD23 | 2.23                     | 0.64              |
| 2:H:85:ARG:NH2   | 4:H:1100:7JA:O14 | 2.31                     | 0.63              |
| 2:L:191:ASN:HD21 | 2:L:194:LEU:H    | 1.46                     | 0.63              |
| 2:L:286:PRO:HA   | 2:L:289:PHE:CD2  | 2.33                     | 0.63              |
| 1:M:131:GLU:HA   | 1:M:131:GLU:OE2  | 1.97                     | 0.63              |
| 1:K:48:THR:HG22  | 1:K:51:ILE:HB    | 1.78                     | 0.63              |
| 2:J:231:GLU:HG2  | 2:J:254:ASN:HD22 | 1.62                     | 0.63              |
| 2:F:93:PRO:HA    | 2:F:548:ARG:CB   | 2.26                     | 0.63              |
| 2:L:365:VAL:HG23 | 2:L:387:VAL:HA   | 1.78                     | 0.63              |
| 2:B:286:PRO:HA   | 2:B:289:PHE:CD2  | 2.34                     | 0.63              |
| 2:D:159:ILE:HD12 | 2:D:166:ILE:HD11 | 1.81                     | 0.63              |
| 2:D:294:GLN:NE2  | 1:G:107:TYR:OH   | 2.31                     | 0.63              |
| 2:J:487:CYS:HB3  | 2:J:490:LEU:HB2  | 1.80                     | 0.63              |
| 2:P:227:VAL:HG13 | 2:P:228:GLY:N    | 2.13                     | 0.63              |
| 2:B:412:LEU:HD12 | 2:B:412:LEU:O    | 1.99                     | 0.63              |
| 2:F:519:TRP:HH2  | 2:F:567:HIS:CE1  | 2.17                     | 0.63              |
| 1:K:102:ILE:CG1  | 1:K:117:THR:HB   | 2.27                     | 0.63              |
| 1:M:102:ILE:CG2  | 2:N:20:VAL:HG23  | 2.28                     | 0.63              |
| 2:H:143:LEU:HD12 | 2:H:144:LYS:N    | 2.14                     | 0.63              |
| 2:H:307:THR:HB   | 2:H:328:VAL:O    | 1.99                     | 0.63              |
| 2:B:440:ARG:HB3  | 2:B:467:TRP:CE3  | 2.34                     | 0.63              |
| 3:Q:203:ILE:HD12 | 3:Q:203:ILE:H    | 1.63                     | 0.63              |
| 2:D:424:LEU:O    | 2:D:428:VAL:HG23 | 1.99                     | 0.63              |
| 2:F:357:GLY:CA   | 2:F:415:ARG:HH22 | 2.10                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:391:THR:HG23 | 2:F:394:SER:H    | 1.64                     | 0.63              |
| 2:H:542:ILE:CD1  | 2:H:588:LEU:HB2  | 2.29                     | 0.63              |
| 2:L:519:TRP:HH2  | 2:L:567:HIS:CE1  | 2.16                     | 0.63              |
| 1:M:100:GLU:HG2  | 2:N:15:ALA:CB    | 2.29                     | 0.63              |
| 2:N:365:VAL:HG23 | 2:N:387:VAL:HA   | 1.81                     | 0.63              |
| 1:O:48:THR:CG2   | 1:O:51:ILE:H     | 2.12                     | 0.63              |
| 2:H:95:ASN:O     | 2:H:582:PRO:HG3  | 1.98                     | 0.63              |
| 2:J:307:THR:HG21 | 2:J:362:GLU:HB2  | 1.79                     | 0.63              |
| 2:L:310:HIS:O    | 2:L:314:ILE:HG12 | 1.99                     | 0.63              |
| 2:P:199:PHE:CE1  | 2:P:227:VAL:HG22 | 2.33                     | 0.63              |
| 2:F:307:THR:HG21 | 2:F:362:GLU:HB2  | 1.80                     | 0.62              |
| 2:N:301:LEU:HD23 | 2:N:324:GLU:HB3  | 1.81                     | 0.62              |
| 2:N:310:HIS:O    | 2:N:314:ILE:HG12 | 1.98                     | 0.62              |
| 2:P:299:ASP:OD2  | 2:P:301:LEU:HB2  | 1.98                     | 0.62              |
| 2:B:184:LEU:HD12 | 2:B:207:ILE:HB   | 1.79                     | 0.62              |
| 2:B:289:PHE:CD1  | 2:B:316:LYS:HD2  | 2.33                     | 0.62              |
| 2:H:382:TYR:C    | 2:H:382:TYR:CD1  | 2.77                     | 0.62              |
| 2:B:454:GLY:O    | 2:B:457:TYR:HB2  | 1.97                     | 0.62              |
| 2:D:231:GLU:HG2  | 2:D:254:ASN:HD22 | 1.64                     | 0.62              |
| 2:F:468:MET:HE1  | 2:F:483:PHE:CE1  | 2.35                     | 0.62              |
| 2:N:396:GLU:O    | 2:N:400:THR:HB   | 1.98                     | 0.62              |
| 2:B:545:ILE:HB   | 2:B:567:HIS:HB2  | 1.80                     | 0.62              |
| 2:D:357:GLY:CA   | 2:D:415:ARG:HH22 | 2.11                     | 0.62              |
| 2:J:286:PRO:HA   | 2:J:289:PHE:CD2  | 2.35                     | 0.62              |
| 1:M:96:ALA:CB    | 2:N:14:VAL:CG1   | 2.76                     | 0.62              |
| 2:B:251:GLY:O    | 2:B:278:SER:HB2  | 1.99                     | 0.62              |
| 2:H:284:GLU:O    | 2:H:287:ILE:HD13 | 1.99                     | 0.62              |
| 2:H:442:ALA:CB   | 4:H:1100:7JA:CD1 | 2.75                     | 0.62              |
| 2:L:542:ILE:CD1  | 2:L:588:LEU:HD12 | 2.27                     | 0.62              |
| 2:H:125:SER:O    | 2:H:129:LEU:HB2  | 2.00                     | 0.62              |
| 2:H:365:VAL:HG21 | 2:H:387:VAL:HG13 | 1.81                     | 0.62              |
| 2:H:409:ARG:HB3  | 4:H:1100:7JA:HD1 | 1.80                     | 0.62              |
| 2:L:121:ARG:HH22 | 5:L:1103:PO4:P   | 2.23                     | 0.62              |
| 2:L:424:LEU:O    | 2:L:428:VAL:HG23 | 1.99                     | 0.62              |
| 1:M:100:GLU:HG2  | 2:N:15:ALA:HB2   | 1.81                     | 0.62              |
| 1:K:48:THR:CG2   | 1:K:51:ILE:H     | 2.13                     | 0.62              |
| 2:N:532:LEU:HD22 | 2:N:535:MET:HE2  | 1.81                     | 0.62              |
| 2:H:322:VAL:CG1  | 2:H:323:LEU:N    | 2.62                     | 0.62              |
| 2:H:542:ILE:C    | 2:H:542:ILE:CD1  | 2.69                     | 0.62              |
| 2:J:310:HIS:O    | 2:J:314:ILE:HG12 | 1.98                     | 0.62              |
| 2:N:231:GLU:HG2  | 2:N:254:ASN:HD22 | 1.64                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:371:ILE:O    | 2:B:375:GLN:HG3  | 2.00                     | 0.62              |
| 2:D:310:HIS:O    | 2:D:314:ILE:HG12 | 1.99                     | 0.62              |
| 2:F:50:GLU:OE1   | 2:L:217:ARG:NH1  | 2.33                     | 0.62              |
| 2:H:144:LYS:HG2  | 2:H:170:LEU:HD13 | 1.82                     | 0.62              |
| 1:M:99:PHE:CE2   | 2:N:17:VAL:N     | 2.68                     | 0.62              |
| 2:P:351:ARG:HD3  | 2:P:413:LEU:HD11 | 1.82                     | 0.62              |
| 2:B:93:PRO:HA    | 2:B:548:ARG:CB   | 2.27                     | 0.62              |
| 1:C:113:LEU:O    | 1:C:117:THR:HG23 | 1.99                     | 0.62              |
| 2:F:297:LYS:HE2  | 2:F:322:VAL:HG21 | 1.82                     | 0.62              |
| 2:H:78:LEU:HD12  | 2:H:79:LYS:H     | 1.63                     | 0.62              |
| 2:J:412:LEU:HD12 | 2:J:412:LEU:O    | 1.99                     | 0.62              |
| 1:M:87:ASP:OD2   | 1:M:116:LEU:HD22 | 2.00                     | 0.62              |
| 1:A:48:THR:CG2   | 1:A:51:ILE:H     | 2.13                     | 0.61              |
| 2:B:533:MET:CE   | 2:B:588:LEU:HD13 | 2.29                     | 0.61              |
| 2:B:533:MET:HE3  | 2:B:588:LEU:HD13 | 1.80                     | 0.61              |
| 2:H:25:MET:HA    | 2:H:28:ILE:HD12  | 1.82                     | 0.61              |
| 2:H:443:PHE:HE2  | 2:H:445:LEU:HD11 | 1.65                     | 0.61              |
| 2:L:211:ASP:HA   | 2:L:214:THR:HG23 | 1.82                     | 0.61              |
| 2:L:412:LEU:HD12 | 2:L:412:LEU:O    | 1.98                     | 0.61              |
| 2:L:532:LEU:HD22 | 2:L:535:MET:HE2  | 1.82                     | 0.61              |
| 2:D:519:TRP:CH2  | 2:D:567:HIS:ND1  | 2.68                     | 0.61              |
| 2:L:93:PRO:HA    | 2:L:548:ARG:CB   | 2.25                     | 0.61              |
| 2:B:391:THR:HG23 | 2:B:394:SER:H    | 1.65                     | 0.61              |
| 2:D:171:MET:O    | 2:D:174:SER:HB2  | 1.99                     | 0.61              |
| 1:E:107:TYR:OH   | 2:L:294:GLN:NE2  | 2.33                     | 0.61              |
| 2:H:225:VAL:O    | 2:H:248:PHE:HA   | 2.00                     | 0.61              |
| 2:H:286:PRO:C    | 2:H:288:LEU:H    | 2.09                     | 0.61              |
| 2:N:468:MET:HE3  | 2:N:470:LEU:HD21 | 1.81                     | 0.61              |
| 2:D:367:GLN:O    | 2:D:371:ILE:HG22 | 1.99                     | 0.61              |
| 2:J:419:ILE:HD13 | 2:J:446:ARG:NH1  | 2.15                     | 0.61              |
| 2:D:211:ASP:HA   | 2:D:214:THR:HG23 | 1.81                     | 0.61              |
| 2:D:227:VAL:HG13 | 2:D:228:GLY:N    | 2.15                     | 0.61              |
| 2:F:440:ARG:HB3  | 2:F:467:TRP:HE3  | 1.65                     | 0.61              |
| 2:J:233:LEU:O    | 2:J:236:VAL:HG23 | 2.00                     | 0.61              |
| 1:K:158:ALA:HA   | 2:L:62:THR:HG21  | 1.81                     | 0.61              |
| 2:N:444:TYR:HA   | 2:N:471:GLY:CA   | 2.28                     | 0.61              |
| 2:D:431:LEU:HD12 | 2:D:431:LEU:O    | 1.99                     | 0.61              |
| 2:L:299:ASP:OD2  | 2:L:301:LEU:HB2  | 2.00                     | 0.61              |
| 1:M:99:PHE:HB2   | 2:N:15:ALA:CB    | 2.31                     | 0.61              |
| 2:N:311:CYS:HB3  | 2:N:336:VAL:HG21 | 1.82                     | 0.61              |
| 1:M:48:THR:CG2   | 1:M:51:ILE:H     | 2.14                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:N:412:LEU:HD12 | 2:N:412:LEU:O     | 2.01                     | 0.61              |
| 2:B:397:SER:O    | 2:B:400:THR:HG22  | 2.00                     | 0.61              |
| 2:J:532:LEU:HD22 | 2:J:535:MET:HE2   | 1.82                     | 0.61              |
| 1:O:158:ALA:HA   | 2:P:62:THR:HG21   | 1.82                     | 0.61              |
| 1:C:48:THR:CG2   | 1:C:51:ILE:H      | 2.11                     | 0.60              |
| 2:D:143:LEU:HD23 | 2:D:159:ILE:HD13  | 1.83                     | 0.60              |
| 2:F:419:ILE:HD13 | 2:F:446:ARG:NH1   | 2.16                     | 0.60              |
| 2:H:395:LEU:CD2  | 2:H:395:LEU:H     | 2.13                     | 0.60              |
| 2:J:391:THR:HG23 | 2:J:394:SER:H     | 1.65                     | 0.60              |
| 2:J:468:MET:HE3  | 2:J:470:LEU:HD21  | 1.83                     | 0.60              |
| 2:L:472:TYR:OH   | 3:V:201:LEU:HB2   | 2.00                     | 0.60              |
| 2:P:54:HIS:HE1   | 2:P:56:THR:OG1    | 1.83                     | 0.60              |
| 2:P:371:ILE:O    | 2:P:375:GLN:HG3   | 2.01                     | 0.60              |
| 2:P:456:SER:CB   | 2:P:482:GLU:HB3   | 2.31                     | 0.60              |
| 2:H:386:TYR:CE1  | 4:H:1100:7JA:HG2B | 2.36                     | 0.60              |
| 4:J:1100:7JA:H04 | 4:J:1100:7JA:H12A | 1.73                     | 0.60              |
| 2:N:386:TYR:CE1  | 4:N:1100:7JA:CG2  | 2.81                     | 0.60              |
| 2:B:227:VAL:HG13 | 2:B:228:GLY:N     | 2.16                     | 0.60              |
| 2:H:57:MET:HE3   | 2:H:62:THR:HG22   | 1.83                     | 0.60              |
| 2:H:361:GLU:HA   | 2:H:364:LEU:HD12  | 1.81                     | 0.60              |
| 2:L:351:ARG:HD3  | 2:L:413:LEU:HD11  | 1.83                     | 0.60              |
| 2:D:293:ALA:HB3  | 1:G:45:PRO:HG3    | 1.84                     | 0.60              |
| 2:D:412:LEU:HD12 | 2:D:412:LEU:C     | 2.25                     | 0.60              |
| 2:H:477:ASP:OD2  | 2:H:504:ALA:HB2   | 2.01                     | 0.60              |
| 1:I:131:GLU:HA   | 1:I:131:GLU:OE2   | 2.01                     | 0.60              |
| 2:J:93:PRO:HA    | 2:J:548:ARG:CB    | 2.30                     | 0.60              |
| 2:J:95:ASN:O     | 2:J:582:PRO:HG3   | 2.01                     | 0.60              |
| 2:N:143:LEU:HD23 | 2:N:159:ILE:HD13  | 1.82                     | 0.60              |
| 1:A:30:ALA:O     | 1:A:33:VAL:HG22   | 2.01                     | 0.60              |
| 2:F:170:LEU:C    | 2:F:170:LEU:HD23  | 2.26                     | 0.60              |
| 1:G:153:ARG:NH2  | 2:H:539:TYR:HE1   | 1.99                     | 0.60              |
| 2:H:386:TYR:CZ   | 4:H:1100:7JA:HG2B | 2.37                     | 0.60              |
| 2:N:211:ASP:O    | 2:N:215:ILE:HG13  | 2.02                     | 0.60              |
| 2:P:456:SER:HB3  | 2:P:482:GLU:HB3   | 1.83                     | 0.60              |
| 2:B:412:LEU:HD12 | 2:B:412:LEU:C     | 2.27                     | 0.60              |
| 1:C:30:ALA:O     | 1:C:33:VAL:HG22   | 2.00                     | 0.60              |
| 2:L:170:LEU:HD23 | 2:L:170:LEU:C     | 2.26                     | 0.60              |
| 1:M:30:ALA:O     | 1:M:33:VAL:HG22   | 2.01                     | 0.60              |
| 2:N:133:ALA:HB2  | 2:N:159:ILE:HG22  | 1.84                     | 0.60              |
| 2:N:521:GLN:HG3  | 2:N:567:HIS:HD2   | 1.66                     | 0.60              |
| 2:P:159:ILE:HD12 | 2:P:166:ILE:HD11  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:472:TYR:OH   | 3:R:201:LEU:HB2  | 2.02                     | 0.60              |
| 2:H:285:MET:HG2  | 2:H:286:PRO:HD3  | 1.83                     | 0.60              |
| 2:J:412:LEU:HD12 | 2:J:412:LEU:C    | 2.27                     | 0.60              |
| 2:L:54:HIS:HD2   | 2:L:77:SER:OG    | 1.84                     | 0.60              |
| 1:M:99:PHE:CZ    | 2:N:17:VAL:HG22  | 2.37                     | 0.60              |
| 2:P:546:PRO:O    | 2:P:547:SER:HB2  | 2.01                     | 0.60              |
| 2:D:184:LEU:HD12 | 2:D:207:ILE:HB   | 1.83                     | 0.60              |
| 2:H:407:ASP:OD1  | 2:H:440:ARG:HD2  | 2.01                     | 0.60              |
| 2:J:367:GLN:O    | 2:J:371:ILE:HG22 | 2.01                     | 0.60              |
| 2:J:533:MET:HE3  | 2:J:588:LEU:HD13 | 1.82                     | 0.60              |
| 2:N:397:SER:O    | 2:N:400:THR:HG22 | 2.02                     | 0.60              |
| 2:P:170:LEU:HD23 | 2:P:170:LEU:C    | 2.27                     | 0.60              |
| 2:B:231:GLU:HG2  | 2:B:254:ASN:HD22 | 1.66                     | 0.60              |
| 1:K:30:ALA:O     | 1:K:33:VAL:HG22  | 2.00                     | 0.60              |
| 2:B:211:ASP:HA   | 2:B:214:THR:HG23 | 1.84                     | 0.60              |
| 2:L:231:GLU:HG2  | 2:L:254:ASN:ND2  | 2.17                     | 0.60              |
| 1:O:131:GLU:HA   | 1:O:131:GLU:OE2  | 2.02                     | 0.60              |
| 2:D:419:ILE:HD13 | 2:D:446:ARG:NH1  | 2.17                     | 0.59              |
| 2:H:92:ILE:HG22  | 2:H:93:PRO:O     | 2.02                     | 0.59              |
| 2:H:262:LYS:HD2  | 2:H:263:TYR:CE1  | 2.36                     | 0.59              |
| 2:N:54:HIS:HE1   | 2:N:56:THR:OG1   | 1.85                     | 0.59              |
| 2:N:121:ARG:NH2  | 5:N:1103:PO4:O4  | 2.35                     | 0.59              |
| 2:F:386:TYR:CE1  | 4:F:1100:7JA:CG2 | 2.83                     | 0.59              |
| 2:P:231:GLU:HG2  | 2:P:254:ASN:HD22 | 1.67                     | 0.59              |
| 2:P:391:THR:HG23 | 2:P:394:SER:H    | 1.65                     | 0.59              |
| 2:P:412:LEU:HD12 | 2:P:412:LEU:O    | 2.01                     | 0.59              |
| 2:B:279:TYR:HA   | 2:B:304:LEU:HD22 | 1.83                     | 0.59              |
| 2:D:440:ARG:HB3  | 2:D:467:TRP:CE3  | 2.35                     | 0.59              |
| 2:H:347:LEU:HD11 | 2:H:349:ILE:HG13 | 1.83                     | 0.59              |
| 1:M:27:GLN:HB2   | 1:M:109:ASN:HB3  | 1.83                     | 0.59              |
| 2:B:121:ARG:NH2  | 5:B:1103:PO4:O4  | 2.36                     | 0.59              |
| 2:B:217:ARG:NH1  | 2:P:50:GLU:OE1   | 2.36                     | 0.59              |
| 1:C:131:GLU:OE2  | 1:C:131:GLU:HA   | 2.00                     | 0.59              |
| 2:F:261:GLU:HG2  | 2:F:264:MET:HG3  | 1.84                     | 0.59              |
| 2:F:431:LEU:HD12 | 2:F:431:LEU:O    | 2.01                     | 0.59              |
| 2:N:456:SER:CB   | 2:N:482:GLU:HB3  | 2.32                     | 0.59              |
| 2:H:284:GLU:CD   | 2:H:284:GLU:H    | 2.10                     | 0.59              |
| 2:P:351:ARG:O    | 2:P:351:ARG:HG3  | 2.03                     | 0.59              |
| 2:P:487:CYS:HB3  | 2:P:490:LEU:HB2  | 1.83                     | 0.59              |
| 2:F:112:ARG:HG3  | 2:L:164:ARG:HE   | 1.68                     | 0.59              |
| 2:F:472:TYR:OH   | 3:S:201:LEU:HB2  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:532:LEU:HD22 | 2:F:535:MET:HE2  | 1.84                     | 0.59              |
| 2:H:125:SER:HB3  | 2:H:127:LEU:H    | 1.66                     | 0.59              |
| 2:H:402:LEU:HD13 | 2:H:405:LEU:HG   | 1.85                     | 0.59              |
| 2:L:297:LYS:HE2  | 2:L:322:VAL:HG21 | 1.83                     | 0.59              |
| 2:L:367:GLN:O    | 2:L:371:ILE:HG22 | 2.01                     | 0.59              |
| 1:K:105:ALA:HB2  | 1:K:113:LEU:HD23 | 1.85                     | 0.59              |
| 2:N:546:PRO:O    | 2:N:547:SER:HB2  | 2.03                     | 0.59              |
| 1:O:91:MET:HE2   | 1:O:91:MET:HA    | 1.85                     | 0.59              |
| 1:I:48:THR:CG2   | 1:I:51:ILE:H     | 2.15                     | 0.59              |
| 1:C:158:ALA:HA   | 2:D:62:THR:HG21  | 1.84                     | 0.59              |
| 2:F:227:VAL:HG13 | 2:F:228:GLY:N    | 2.17                     | 0.59              |
| 2:H:191:ASN:ND2  | 2:H:193:SER:H    | 2.01                     | 0.59              |
| 2:H:375:GLN:HG2  | 2:H:401:TYR:CD1  | 2.38                     | 0.59              |
| 2:P:412:LEU:HD12 | 2:P:412:LEU:C    | 2.28                     | 0.59              |
| 2:J:164:ARG:NE   | 2:N:112:ARG:HG2  | 2.18                     | 0.59              |
| 1:M:153:ARG:HG2  | 1:M:157:TRP:CZ3  | 2.37                     | 0.59              |
| 1:M:158:ALA:HA   | 2:N:62:THR:HG21  | 1.83                     | 0.59              |
| 2:N:275:LEU:HD11 | 2:N:288:LEU:HD21 | 1.84                     | 0.59              |
| 2:P:103:TRP:O    | 2:P:107:ILE:HG13 | 2.03                     | 0.59              |
| 2:P:279:TYR:HA   | 2:P:304:LEU:HD22 | 1.84                     | 0.59              |
| 2:B:424:LEU:O    | 2:B:428:VAL:HG23 | 2.02                     | 0.58              |
| 1:C:12:ASP:O     | 1:K:40:ASN:CB    | 2.50                     | 0.58              |
| 2:D:311:CYS:HB3  | 2:D:336:VAL:HG21 | 1.83                     | 0.58              |
| 2:F:456:SER:HB3  | 2:F:482:GLU:HB3  | 1.85                     | 0.58              |
| 2:P:468:MET:HE1  | 2:P:483:PHE:CE1  | 2.38                     | 0.58              |
| 2:D:546:PRO:O    | 2:D:547:SER:HB2  | 2.02                     | 0.58              |
| 2:F:533:MET:CE   | 2:F:588:LEU:HD13 | 2.33                     | 0.58              |
| 2:H:233:LEU:O    | 2:H:236:VAL:HG23 | 2.03                     | 0.58              |
| 2:J:143:LEU:HD23 | 2:J:159:ILE:HD13 | 1.85                     | 0.58              |
| 2:J:546:PRO:O    | 2:J:547:SER:HB2  | 2.03                     | 0.58              |
| 2:L:54:HIS:HE1   | 2:L:56:THR:OG1   | 1.84                     | 0.58              |
| 2:L:159:ILE:HD12 | 2:L:166:ILE:HD11 | 1.84                     | 0.58              |
| 2:N:261:GLU:HG2  | 2:N:264:MET:HG3  | 1.85                     | 0.58              |
| 1:A:102:ILE:HG13 | 1:A:117:THR:HB   | 1.84                     | 0.58              |
| 2:B:367:GLN:O    | 2:B:371:ILE:HG22 | 2.04                     | 0.58              |
| 2:H:371:ILE:CG2  | 2:H:375:GLN:HE21 | 2.14                     | 0.58              |
| 2:H:392:ASN:HD21 | 2:H:422:LEU:HD13 | 1.68                     | 0.58              |
| 2:J:422:LEU:HB3  | 2:J:423:PRO:HD3  | 1.85                     | 0.58              |
| 2:J:440:ARG:HB3  | 2:J:467:TRP:CE3  | 2.36                     | 0.58              |
| 2:P:301:LEU:HD23 | 2:P:324:GLU:HB3  | 1.85                     | 0.58              |
| 1:C:27:GLN:HB2   | 1:C:109:ASN:HB3  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:159:ILE:HD12 | 2:N:166:ILE:HD11 | 1.86                     | 0.58              |
| 2:N:199:PHE:CE1  | 2:N:227:VAL:HG22 | 2.38                     | 0.58              |
| 2:N:424:LEU:O    | 2:N:428:VAL:HG23 | 2.02                     | 0.58              |
| 1:C:132:GLU:O    | 1:C:136:THR:HG23 | 2.03                     | 0.58              |
| 2:H:509:VAL:HG21 | 2:H:535:MET:SD   | 2.43                     | 0.58              |
| 1:M:148:GLU:HG2  | 1:M:152:ARG:HH12 | 1.68                     | 0.58              |
| 1:O:91:MET:SD    | 1:O:117:THR:HG22 | 2.44                     | 0.58              |
| 1:A:158:ALA:HA   | 2:B:62:THR:HG21  | 1.85                     | 0.58              |
| 2:B:161:THR:HG22 | 2:B:186:GLU:HG2  | 1.86                     | 0.58              |
| 1:C:48:THR:HG22  | 1:C:51:ILE:N     | 2.14                     | 0.58              |
| 1:C:102:ILE:HG21 | 2:D:20:VAL:CG2   | 2.34                     | 0.58              |
| 2:F:546:PRO:HG2  | 2:F:584:THR:CB   | 2.32                     | 0.58              |
| 2:H:310:HIS:O    | 2:H:314:ILE:HG12 | 2.03                     | 0.58              |
| 2:P:172:GLU:HG3  | 2:P:200:TYR:HB3  | 1.85                     | 0.58              |
| 2:F:40:VAL:O     | 2:F:41:CYS:HB3   | 2.02                     | 0.58              |
| 1:I:35:ASP:HB3   | 2:N:243:ALA:HB1  | 1.85                     | 0.58              |
| 2:L:95:ASN:O     | 2:L:582:PRO:HG3  | 2.02                     | 0.58              |
| 2:L:412:LEU:HD12 | 2:L:412:LEU:C    | 2.29                     | 0.58              |
| 2:L:419:ILE:HD13 | 2:L:446:ARG:NH1  | 2.19                     | 0.58              |
| 1:C:48:THR:HG22  | 1:C:51:ILE:HB    | 1.85                     | 0.58              |
| 1:C:114:LEU:C    | 1:C:116:LEU:H    | 2.12                     | 0.58              |
| 2:D:286:PRO:HA   | 2:D:289:PHE:CD2  | 2.38                     | 0.58              |
| 1:E:153:ARG:HG2  | 1:E:157:TRP:CZ3  | 2.39                     | 0.58              |
| 2:F:159:ILE:HD12 | 2:F:166:ILE:HD11 | 1.85                     | 0.58              |
| 2:H:37:ALA:O     | 2:H:40:VAL:HG13  | 2.03                     | 0.58              |
| 2:H:487:CYS:N    | 2:H:488:PRO:HD3  | 2.18                     | 0.58              |
| 2:N:546:PRO:HG2  | 2:N:584:THR:CB   | 2.30                     | 0.58              |
| 2:P:419:ILE:HD13 | 2:P:446:ARG:NH1  | 2.19                     | 0.58              |
| 2:F:275:LEU:HD11 | 2:F:288:LEU:HD21 | 1.86                     | 0.58              |
| 2:H:125:SER:HB3  | 2:H:127:LEU:N    | 2.18                     | 0.58              |
| 2:N:440:ARG:HB3  | 2:N:467:TRP:CE3  | 2.39                     | 0.58              |
| 2:B:159:ILE:HD11 | 2:B:169:LEU:HD13 | 1.86                     | 0.58              |
| 2:F:133:ALA:HB2  | 2:F:159:ILE:HG22 | 1.86                     | 0.58              |
| 2:H:99:TYR:CE2   | 2:H:123:ILE:HD12 | 2.39                     | 0.58              |
| 2:J:431:LEU:HD12 | 2:J:431:LEU:O    | 2.04                     | 0.58              |
| 2:L:307:THR:HG22 | 2:L:360:ASP:OD2  | 2.04                     | 0.58              |
| 1:M:128:LYS:HB2  | 1:M:133:ILE:CD1  | 2.34                     | 0.58              |
| 2:P:440:ARG:HB3  | 2:P:467:TRP:CE3  | 2.36                     | 0.58              |
| 2:B:159:ILE:HD12 | 2:B:166:ILE:HD11 | 1.86                     | 0.57              |
| 2:B:253:LEU:HD12 | 2:B:280:MET:HB2  | 1.86                     | 0.57              |
| 2:D:386:TYR:CE1  | 4:D:1100:7JA:CG2 | 2.83                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:227:VAL:CG1  | 2:L:228:GLY:N    | 2.66                     | 0.57              |
| 2:L:545:ILE:HB   | 2:L:567:HIS:HB2  | 1.85                     | 0.57              |
| 2:N:431:LEU:HD12 | 2:N:431:LEU:O    | 2.04                     | 0.57              |
| 2:D:454:GLY:O    | 2:D:457:TYR:HB2  | 2.04                     | 0.57              |
| 2:J:227:VAL:HG13 | 2:J:228:GLY:N    | 2.19                     | 0.57              |
| 2:P:133:ALA:HB2  | 2:P:159:ILE:HG22 | 1.85                     | 0.57              |
| 2:P:397:SER:O    | 2:P:400:THR:HG22 | 2.04                     | 0.57              |
| 2:F:143:LEU:HD23 | 2:F:159:ILE:HD13 | 1.86                     | 0.57              |
| 2:F:210:LYS:O    | 2:F:214:THR:HG22 | 2.04                     | 0.57              |
| 2:H:96:TRP:HA    | 2:H:582:PRO:HG2  | 1.85                     | 0.57              |
| 2:L:456:SER:HB3  | 2:L:482:GLU:HB3  | 1.86                     | 0.57              |
| 2:N:297:LYS:HG3  | 2:N:322:VAL:HB   | 1.86                     | 0.57              |
| 2:N:521:GLN:HG3  | 2:N:567:HIS:CD2  | 2.39                     | 0.57              |
| 1:O:159:PHE:O    | 1:O:160:GLU:CB   | 2.52                     | 0.57              |
| 1:A:134:ARG:HH11 | 2:B:40:VAL:HA    | 1.70                     | 0.57              |
| 1:C:102:ILE:HG12 | 1:C:117:THR:HB   | 1.85                     | 0.57              |
| 1:E:105:ALA:HB3  | 1:E:114:LEU:HD13 | 1.87                     | 0.57              |
| 2:J:422:LEU:O    | 2:J:423:PRO:C    | 2.45                     | 0.57              |
| 1:K:102:ILE:HG12 | 1:K:117:THR:CB   | 2.32                     | 0.57              |
| 2:B:419:ILE:HD13 | 2:B:446:ARG:NH1  | 2.20                     | 0.57              |
| 1:E:141:ASN:C    | 1:E:141:ASN:OD1  | 2.47                     | 0.57              |
| 2:J:307:THR:HG22 | 2:J:360:ASP:OD2  | 2.03                     | 0.57              |
| 1:O:153:ARG:HG2  | 1:O:157:TRP:CZ3  | 2.39                     | 0.57              |
| 2:L:456:SER:CB   | 2:L:482:GLU:HB3  | 2.35                     | 0.57              |
| 1:M:132:GLU:O    | 1:M:136:THR:HG23 | 2.05                     | 0.57              |
| 2:N:351:ARG:HG3  | 2:N:351:ARG:O    | 2.04                     | 0.57              |
| 2:N:396:GLU:HG2  | 2:N:430:SER:OG   | 2.05                     | 0.57              |
| 1:E:43:PRO:HG3   | 2:L:319:ASN:ND2  | 2.20                     | 0.57              |
| 1:G:48:THR:HG22  | 1:G:51:ILE:N     | 2.18                     | 0.57              |
| 2:H:180:ASP:OD1  | 2:H:182:LYS:HB2  | 2.04                     | 0.57              |
| 2:N:297:LYS:HE2  | 2:N:322:VAL:HG21 | 1.86                     | 0.57              |
| 2:B:546:PRO:O    | 2:B:547:SER:HB2  | 2.03                     | 0.57              |
| 2:D:547:SER:HB3  | 2:D:564:HIS:HB2  | 1.86                     | 0.57              |
| 2:F:231:GLU:HG2  | 2:F:254:ASN:ND2  | 2.18                     | 0.57              |
| 2:J:121:ARG:HH22 | 5:J:1103:PO4:P   | 2.28                     | 0.57              |
| 2:J:170:LEU:HD23 | 2:J:170:LEU:C    | 2.30                     | 0.57              |
| 2:J:279:TYR:HA   | 2:J:304:LEU:HD22 | 1.86                     | 0.57              |
| 2:J:533:MET:CE   | 2:J:588:LEU:HD13 | 2.35                     | 0.57              |
| 2:B:592:ILE:H    | 2:B:592:ILE:HD12 | 1.69                     | 0.57              |
| 2:D:233:LEU:O    | 2:D:236:VAL:HG23 | 2.05                     | 0.57              |
| 2:D:580:ASP:HA   | 2:N:206:LYS:HE3  | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:147:LYS:HE2  | 2:H:173:GLU:OE1  | 2.04                     | 0.57              |
| 2:L:397:SER:O    | 2:L:400:THR:HG22 | 2.04                     | 0.57              |
| 2:H:289:PHE:CE1  | 2:H:316:LYS:HD3  | 2.40                     | 0.57              |
| 2:J:275:LEU:HD11 | 2:J:288:LEU:HD21 | 1.87                     | 0.57              |
| 1:A:131:GLU:HA   | 1:A:131:GLU:OE2  | 2.04                     | 0.56              |
| 2:D:170:LEU:HD23 | 2:D:170:LEU:C    | 2.30                     | 0.56              |
| 2:D:307:THR:HG22 | 2:D:360:ASP:OD2  | 2.04                     | 0.56              |
| 2:D:391:THR:HG23 | 2:D:394:SER:H    | 1.70                     | 0.56              |
| 2:J:351:ARG:HG3  | 2:J:351:ARG:O    | 2.04                     | 0.56              |
| 1:C:40:ASN:HB3   | 1:K:13:GLY:O     | 2.04                     | 0.56              |
| 2:H:386:TYR:HD2  | 2:H:413:LEU:HD21 | 1.70                     | 0.56              |
| 2:J:519:TRP:CH2  | 2:J:567:HIS:ND1  | 2.73                     | 0.56              |
| 2:L:592:ILE:H    | 2:L:592:ILE:HD12 | 1.70                     | 0.56              |
| 1:C:52:LEU:O     | 1:C:56:ILE:HG13  | 2.06                     | 0.56              |
| 2:D:121:ARG:HH22 | 5:D:1103:PO4:P   | 2.28                     | 0.56              |
| 1:G:102:ILE:HG12 | 1:G:117:THR:OG1  | 2.06                     | 0.56              |
| 2:H:100:VAL:HG23 | 2:H:122:MET:HE2  | 1.88                     | 0.56              |
| 2:H:136:ARG:HA   | 2:H:136:ARG:NE   | 2.19                     | 0.56              |
| 2:H:216:ALA:HB2  | 2:H:238:PHE:CD1  | 2.40                     | 0.56              |
| 2:H:331:ASP:CG   | 2:H:366:SER:H    | 2.13                     | 0.56              |
| 2:H:362:GLU:O    | 2:H:363:GLY:C    | 2.48                     | 0.56              |
| 2:J:54:HIS:HD2   | 2:J:77:SER:OG    | 1.88                     | 0.56              |
| 2:L:386:TYR:CE1  | 4:L:1100:7JA:CG2 | 2.83                     | 0.56              |
| 2:L:440:ARG:HB3  | 2:L:467:TRP:CE3  | 2.40                     | 0.56              |
| 1:M:105:ALA:HB2  | 1:M:113:LEU:HD23 | 1.86                     | 0.56              |
| 2:N:95:ASN:O     | 2:N:582:PRO:HG3  | 2.05                     | 0.56              |
| 2:N:210:LYS:O    | 2:N:214:THR:HG22 | 2.05                     | 0.56              |
| 1:O:153:ARG:NH2  | 2:P:539:TYR:CE1  | 2.73                     | 0.56              |
| 2:P:533:MET:HE3  | 2:P:588:LEU:HD13 | 1.87                     | 0.56              |
| 2:B:532:LEU:HD22 | 2:B:535:MET:HE2  | 1.87                     | 0.56              |
| 2:F:199:PHE:CE1  | 2:F:227:VAL:HG22 | 2.40                     | 0.56              |
| 2:H:87:ALA:HB2   | 2:H:92:ILE:HB    | 1.87                     | 0.56              |
| 2:H:431:LEU:HD22 | 2:H:432:LEU:HD23 | 1.88                     | 0.56              |
| 2:J:159:ILE:HD12 | 2:J:166:ILE:HD11 | 1.86                     | 0.56              |
| 2:J:231:GLU:HG2  | 2:J:254:ASN:ND2  | 2.20                     | 0.56              |
| 2:J:547:SER:HB3  | 2:J:564:HIS:HB2  | 1.86                     | 0.56              |
| 2:N:533:MET:HE3  | 2:N:588:LEU:HD13 | 1.87                     | 0.56              |
| 2:P:275:LEU:HD11 | 2:P:288:LEU:HD21 | 1.87                     | 0.56              |
| 2:B:170:LEU:HD23 | 2:B:170:LEU:C    | 2.31                     | 0.56              |
| 2:D:519:TRP:CZ3  | 2:D:567:HIS:ND1  | 2.73                     | 0.56              |
| 2:D:533:MET:CE   | 2:D:588:LEU:HD13 | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:444:TYR:HA   | 2:H:471:GLY:CA   | 2.31                     | 0.56              |
| 1:I:91:MET:HA    | 1:I:91:MET:HE2   | 1.88                     | 0.56              |
| 2:J:396:GLU:HG2  | 2:J:430:SER:OG   | 2.06                     | 0.56              |
| 2:N:171:MET:O    | 2:N:174:SER:HB2  | 2.06                     | 0.56              |
| 2:B:444:TYR:HA   | 2:B:471:GLY:CA   | 2.30                     | 0.56              |
| 1:G:124:MET:O    | 1:G:128:LYS:HE2  | 2.05                     | 0.56              |
| 2:H:178:GLU:CD   | 2:H:206:LYS:HB3  | 2.30                     | 0.56              |
| 2:J:351:ARG:HD3  | 2:J:413:LEU:HD11 | 1.86                     | 0.56              |
| 1:K:131:GLU:HA   | 1:K:131:GLU:OE2  | 2.05                     | 0.56              |
| 2:B:547:SER:HB3  | 2:B:564:HIS:HB2  | 1.88                     | 0.56              |
| 2:J:308:GLU:O    | 2:J:312:THR:HG23 | 2.06                     | 0.56              |
| 2:J:456:SER:CB   | 2:J:482:GLU:HB3  | 2.36                     | 0.56              |
| 2:L:199:PHE:CE1  | 2:L:227:VAL:HG22 | 2.41                     | 0.56              |
| 2:L:547:SER:HB3  | 2:L:564:HIS:HB2  | 1.88                     | 0.56              |
| 2:P:248:PHE:C    | 2:P:248:PHE:CD2  | 2.83                     | 0.56              |
| 1:A:132:GLU:O    | 1:A:136:THR:HG23 | 2.05                     | 0.56              |
| 2:D:371:ILE:O    | 2:D:375:GLN:HG3  | 2.06                     | 0.56              |
| 2:F:521:GLN:HG3  | 2:F:567:HIS:HD2  | 1.71                     | 0.56              |
| 2:F:533:MET:HE3  | 2:F:588:LEU:HD13 | 1.88                     | 0.56              |
| 2:H:101:THR:HB   | 2:H:102:PRO:CD   | 2.36                     | 0.56              |
| 2:H:170:LEU:HB2  | 2:H:198:ASN:HB3  | 1.88                     | 0.56              |
| 2:J:261:GLU:HG2  | 2:J:264:MET:HG3  | 1.87                     | 0.56              |
| 2:J:592:ILE:H    | 2:J:592:ILE:HD12 | 1.70                     | 0.56              |
| 2:L:143:LEU:HD23 | 2:L:159:ILE:HD13 | 1.88                     | 0.56              |
| 2:N:351:ARG:HD3  | 2:N:413:LEU:HD11 | 1.87                     | 0.56              |
| 1:O:148:GLU:HG2  | 1:O:152:ARG:HH12 | 1.70                     | 0.56              |
| 2:F:412:LEU:C    | 2:F:412:LEU:HD12 | 2.30                     | 0.56              |
| 2:F:546:PRO:HD3  | 2:F:584:THR:O    | 2.06                     | 0.56              |
| 1:G:91:MET:HE2   | 1:G:91:MET:HA    | 1.87                     | 0.56              |
| 2:H:156:LEU:O    | 2:H:160:VAL:HG22 | 2.05                     | 0.56              |
| 2:H:542:ILE:HD12 | 2:H:543:GLU:N    | 2.21                     | 0.56              |
| 2:L:386:TYR:HE1  | 4:L:1100:7JA:HG2 | 1.63                     | 0.56              |
| 1:M:99:PHE:HB2   | 2:N:15:ALA:HB3   | 1.88                     | 0.56              |
| 1:M:124:MET:O    | 1:M:128:LYS:HE2  | 2.04                     | 0.56              |
| 1:O:27:GLN:HB2   | 1:O:109:ASN:HB3  | 1.86                     | 0.56              |
| 2:P:307:THR:HG21 | 2:P:362:GLU:HB2  | 1.86                     | 0.56              |
| 2:P:307:THR:HG22 | 2:P:360:ASP:OD2  | 2.06                     | 0.56              |
| 2:D:456:SER:HB3  | 2:D:482:GLU:HB3  | 1.88                     | 0.56              |
| 1:E:129:THR:O    | 1:E:133:ILE:HG12 | 2.06                     | 0.56              |
| 2:F:412:LEU:HD12 | 2:F:412:LEU:O    | 2.05                     | 0.56              |
| 2:H:259:MET:O    | 2:H:261:GLU:N    | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:27:GLN:HB2   | 1:I:109:ASN:HB3  | 1.88                     | 0.56              |
| 2:J:456:SER:HB3  | 2:J:482:GLU:HB3  | 1.88                     | 0.56              |
| 2:D:422:LEU:O    | 2:D:423:PRO:C    | 2.48                     | 0.55              |
| 1:E:30:ALA:C     | 1:E:32:MET:H     | 2.15                     | 0.55              |
| 2:H:47:ILE:O     | 2:H:51:THR:HG23  | 2.05                     | 0.55              |
| 2:H:304:LEU:HD13 | 2:H:304:LEU:O    | 2.05                     | 0.55              |
| 2:H:428:VAL:CG2  | 2:H:429:ARG:N    | 2.68                     | 0.55              |
| 2:N:546:PRO:HD3  | 2:N:584:THR:O    | 2.05                     | 0.55              |
| 2:P:121:ARG:NH2  | 5:P:1103:PO4:O4  | 2.38                     | 0.55              |
| 2:B:227:VAL:CG1  | 2:B:228:GLY:N    | 2.70                     | 0.55              |
| 2:D:261:GLU:HG2  | 2:D:264:MET:HG3  | 1.87                     | 0.55              |
| 2:D:296:ARG:HH22 | 1:G:35:ASP:HB2   | 1.71                     | 0.55              |
| 2:D:532:LEU:HD22 | 2:D:535:MET:HE2  | 1.87                     | 0.55              |
| 2:H:136:ARG:HH11 | 2:H:136:ARG:HG3  | 1.71                     | 0.55              |
| 2:H:366:SER:C    | 2:H:368:ARG:N    | 2.60                     | 0.55              |
| 1:I:108:LEU:HD12 | 1:I:110:ILE:HD11 | 1.87                     | 0.55              |
| 2:J:521:GLN:HG3  | 2:J:567:HIS:HD2  | 1.71                     | 0.55              |
| 2:J:521:GLN:HG3  | 2:J:567:HIS:CD2  | 2.42                     | 0.55              |
| 2:N:472:TYR:OH   | 3:W:201:LEU:HB2  | 2.06                     | 0.55              |
| 1:O:129:THR:O    | 1:O:133:ILE:HG12 | 2.06                     | 0.55              |
| 2:D:301:LEU:HD23 | 2:D:324:GLU:HB3  | 1.88                     | 0.55              |
| 2:H:322:VAL:HG12 | 2:H:323:LEU:N    | 2.19                     | 0.55              |
| 2:J:121:ARG:NH2  | 5:J:1103:PO4:O4  | 2.39                     | 0.55              |
| 2:N:327:ASN:HD22 | 2:N:328:VAL:N    | 2.04                     | 0.55              |
| 2:B:307:THR:HG22 | 2:B:360:ASP:OD2  | 2.05                     | 0.55              |
| 1:E:105:ALA:HB2  | 1:E:113:LEU:HD23 | 1.88                     | 0.55              |
| 2:L:533:MET:CE   | 2:L:588:LEU:HD13 | 2.36                     | 0.55              |
| 2:L:546:PRO:O    | 2:L:547:SER:HB2  | 2.05                     | 0.55              |
| 2:B:519:TRP:CH2  | 2:B:567:HIS:ND1  | 2.75                     | 0.55              |
| 1:E:148:GLU:HG2  | 1:E:152:ARG:HH12 | 1.70                     | 0.55              |
| 2:F:592:ILE:H    | 2:F:592:ILE:HD12 | 1.71                     | 0.55              |
| 1:G:27:GLN:HB2   | 1:G:109:ASN:HB3  | 1.88                     | 0.55              |
| 2:J:297:LYS:HE2  | 2:J:322:VAL:HG21 | 1.89                     | 0.55              |
| 1:M:99:PHE:CE2   | 2:N:16:THR:C     | 2.84                     | 0.55              |
| 1:M:159:PHE:O    | 1:M:160:GLU:CB   | 2.52                     | 0.55              |
| 2:N:172:GLU:HG3  | 2:N:200:TYR:HB3  | 1.89                     | 0.55              |
| 1:A:153:ARG:HG2  | 1:A:157:TRP:CZ3  | 2.41                     | 0.55              |
| 2:B:396:GLU:O    | 2:B:400:THR:HB   | 2.06                     | 0.55              |
| 2:F:211:ASP:O    | 2:F:215:ILE:HG13 | 2.07                     | 0.55              |
| 2:H:291:PHE:N    | 2:H:291:PHE:HD2  | 2.02                     | 0.55              |
| 1:K:108:LEU:HD12 | 1:K:110:ILE:HD11 | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:134:ARG:HH11 | 2:L:40:VAL:HA    | 1.72                     | 0.55              |
| 2:N:57:MET:HE3   | 2:N:62:THR:HG22  | 1.89                     | 0.55              |
| 2:N:519:TRP:NE1  | 4:N:1100:7JA:C01 | 2.61                     | 0.55              |
| 1:E:91:MET:HE2   | 1:E:91:MET:HA    | 1.89                     | 0.55              |
| 2:H:84:PRO:HB3   | 2:H:517:TYR:OH   | 2.07                     | 0.55              |
| 2:H:286:PRO:O    | 2:H:288:LEU:N    | 2.40                     | 0.55              |
| 2:H:305:LEU:H    | 2:H:305:LEU:CD2  | 2.14                     | 0.55              |
| 2:H:419:ILE:O    | 2:H:419:ILE:HG13 | 2.06                     | 0.55              |
| 2:H:533:MET:CE   | 2:H:588:LEU:HD13 | 2.37                     | 0.55              |
| 2:H:533:MET:HE3  | 2:H:588:LEU:HD13 | 1.88                     | 0.55              |
| 2:H:543:GLU:C    | 2:H:544:LEU:HD23 | 2.32                     | 0.55              |
| 1:I:128:LYS:HB2  | 1:I:133:ILE:CD1  | 2.37                     | 0.55              |
| 2:J:172:GLU:HG3  | 2:J:200:TYR:HB3  | 1.88                     | 0.55              |
| 1:K:132:GLU:O    | 1:K:136:THR:HG23 | 2.06                     | 0.55              |
| 1:M:102:ILE:HD12 | 2:N:20:VAL:CG2   | 2.24                     | 0.55              |
| 1:O:113:LEU:O    | 1:O:113:LEU:CG   | 2.54                     | 0.55              |
| 2:P:297:LYS:HE2  | 2:P:322:VAL:HG21 | 1.89                     | 0.55              |
| 1:A:135:THR:HG22 | 1:A:136:THR:N    | 2.22                     | 0.55              |
| 2:B:431:LEU:HD12 | 2:B:431:LEU:O    | 2.07                     | 0.55              |
| 2:H:456:SER:OG   | 2:H:482:GLU:HB3  | 2.06                     | 0.55              |
| 2:N:347:LEU:HD21 | 2:N:349:ILE:HD11 | 1.89                     | 0.55              |
| 2:B:101:THR:CG2  | 2:B:128:ASP:OD1  | 2.51                     | 0.55              |
| 2:D:296:ARG:NH2  | 1:G:37:CYS:SG    | 2.80                     | 0.55              |
| 2:F:521:GLN:HG3  | 2:F:567:HIS:CD2  | 2.42                     | 0.55              |
| 1:G:159:PHE:O    | 1:G:160:GLU:HB2  | 2.05                     | 0.55              |
| 2:H:153:THR:HG23 | 2:H:178:GLU:HA   | 1.89                     | 0.55              |
| 2:H:502:GLU:OE1  | 2:H:526:SER:HB2  | 2.07                     | 0.55              |
| 2:J:419:ILE:CD1  | 2:J:446:ARG:HH12 | 2.20                     | 0.55              |
| 2:L:533:MET:HE3  | 2:L:588:LEU:HD13 | 1.87                     | 0.55              |
| 2:N:412:LEU:HD12 | 2:N:412:LEU:C    | 2.32                     | 0.55              |
| 2:P:191:ASN:ND2  | 2:P:194:LEU:H    | 2.04                     | 0.55              |
| 1:A:102:ILE:HG12 | 1:A:117:THR:HB   | 1.87                     | 0.55              |
| 2:B:275:LEU:HD11 | 2:B:288:LEU:HD21 | 1.89                     | 0.55              |
| 2:D:93:PRO:HA    | 2:D:548:ARG:CB   | 2.28                     | 0.55              |
| 1:E:132:GLU:O    | 1:E:136:THR:HG23 | 2.07                     | 0.55              |
| 2:F:542:ILE:CD1  | 2:F:588:LEU:HD12 | 2.34                     | 0.55              |
| 2:H:78:LEU:HD12  | 2:H:79:LYS:N     | 2.22                     | 0.55              |
| 2:H:176:PHE:CZ   | 2:H:204:PHE:CZ   | 2.95                     | 0.55              |
| 2:N:311:CYS:O    | 2:N:315:GLN:HB2  | 2.06                     | 0.55              |
| 2:P:592:ILE:H    | 2:P:592:ILE:HD12 | 1.72                     | 0.55              |
| 2:D:54:HIS:CD2   | 2:D:77:SER:OG    | 2.58                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:396:GLU:O    | 2:F:400:THR:HB   | 2.07                     | 0.54              |
| 2:F:546:PRO:O    | 2:F:547:SER:HB2  | 2.06                     | 0.54              |
| 2:H:138:ASP:OD2  | 2:H:164:ARG:HG3  | 2.07                     | 0.54              |
| 1:I:148:GLU:HG2  | 1:I:152:ARG:HH12 | 1.72                     | 0.54              |
| 2:J:235:LEU:O    | 2:J:238:PHE:HB3  | 2.07                     | 0.54              |
| 2:L:519:TRP:CH2  | 2:L:567:HIS:ND1  | 2.75                     | 0.54              |
| 1:M:91:MET:HE2   | 1:M:91:MET:HA    | 1.89                     | 0.54              |
| 1:A:102:ILE:HG12 | 1:A:117:THR:CB   | 2.37                     | 0.54              |
| 2:B:521:GLN:HG3  | 2:B:567:HIS:HD2  | 1.72                     | 0.54              |
| 1:E:128:LYS:HB2  | 1:E:133:ILE:CD1  | 2.37                     | 0.54              |
| 1:I:26:SER:HG    | 1:I:108:LEU:HB3  | 1.72                     | 0.54              |
| 1:I:129:THR:O    | 1:I:133:ILE:HG12 | 2.06                     | 0.54              |
| 1:M:125:ILE:HG23 | 1:M:133:ILE:CD1  | 2.36                     | 0.54              |
| 2:N:419:ILE:HD13 | 2:N:446:ARG:NH1  | 2.21                     | 0.54              |
| 1:A:99:PHE:HZ    | 1:A:137:PHE:HE1  | 1.55                     | 0.54              |
| 1:C:134:ARG:HH11 | 2:D:40:VAL:HA    | 1.73                     | 0.54              |
| 2:F:279:TYR:HA   | 2:F:304:LEU:HD22 | 1.89                     | 0.54              |
| 2:H:49:SER:HB2   | 2:H:71:ARG:O     | 2.07                     | 0.54              |
| 2:H:232:ILE:HG13 | 2:H:253:LEU:HD23 | 1.89                     | 0.54              |
| 2:L:519:TRP:NE1  | 4:L:1100:7JA:C01 | 2.62                     | 0.54              |
| 2:P:396:GLU:O    | 2:P:400:THR:HB   | 2.07                     | 0.54              |
| 2:F:456:SER:CB   | 2:F:482:GLU:HB3  | 2.37                     | 0.54              |
| 2:H:83:LYS:HA    | 2:H:96:TRP:CZ3   | 2.43                     | 0.54              |
| 2:H:274:ARG:CG   | 2:H:297:LYS:HB3  | 2.27                     | 0.54              |
| 1:A:141:ASN:C    | 1:A:141:ASN:OD1  | 2.50                     | 0.54              |
| 1:C:12:ASP:OD2   | 1:C:49:SER:HB2   | 2.08                     | 0.54              |
| 1:C:114:LEU:C    | 1:C:116:LEU:N    | 2.63                     | 0.54              |
| 1:E:44:LEU:HD12  | 1:E:44:LEU:O     | 2.07                     | 0.54              |
| 2:H:106:GLU:OE1  | 2:H:106:GLU:HA   | 2.08                     | 0.54              |
| 2:H:277:LEU:O    | 2:H:278:SER:C    | 2.51                     | 0.54              |
| 1:K:114:LEU:C    | 1:K:116:LEU:H    | 2.16                     | 0.54              |
| 1:M:48:THR:HG22  | 1:M:51:ILE:CB    | 2.38                     | 0.54              |
| 1:O:128:LYS:HB2  | 1:O:133:ILE:CD1  | 2.38                     | 0.54              |
| 4:D:1100:7JA:CG2 | 4:D:1100:7JA:OXT | 2.53                     | 0.54              |
| 1:E:135:THR:HG22 | 1:E:136:THR:N    | 2.21                     | 0.54              |
| 2:F:253:LEU:HD12 | 2:F:280:MET:HB2  | 1.89                     | 0.54              |
| 2:F:367:GLN:O    | 2:F:371:ILE:HG22 | 2.07                     | 0.54              |
| 2:H:64:THR:O     | 2:H:65:PRO:C     | 2.47                     | 0.54              |
| 2:J:103:TRP:O    | 2:J:107:ILE:HG13 | 2.08                     | 0.54              |
| 2:P:519:TRP:CH2  | 2:P:567:HIS:ND1  | 2.76                     | 0.54              |
| 2:P:547:SER:HB3  | 2:P:564:HIS:HB2  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:255:GLU:HG3  | 2:B:255:GLU:O    | 2.08                     | 0.54              |
| 2:H:492:LYS:NZ   | 2:H:516:ARG:NH1  | 2.54                     | 0.54              |
| 2:J:357:GLY:HA2  | 2:J:415:ARG:NH2  | 2.20                     | 0.54              |
| 2:L:396:GLU:O    | 2:L:400:THR:HB   | 2.07                     | 0.54              |
| 2:B:297:LYS:HE2  | 2:B:322:VAL:HG21 | 1.90                     | 0.54              |
| 2:H:391:THR:O    | 2:H:395:LEU:HD23 | 2.07                     | 0.54              |
| 2:J:397:SER:O    | 2:J:400:THR:HG22 | 2.08                     | 0.54              |
| 2:P:533:MET:CE   | 2:P:588:LEU:HD13 | 2.38                     | 0.54              |
| 1:A:27:GLN:HB2   | 1:A:109:ASN:HB3  | 1.90                     | 0.54              |
| 2:B:233:LEU:O    | 2:B:236:VAL:HG23 | 2.06                     | 0.54              |
| 2:D:227:VAL:CG1  | 2:D:228:GLY:N    | 2.70                     | 0.54              |
| 2:H:328:VAL:HG13 | 2:H:359:GLU:CG   | 2.37                     | 0.54              |
| 2:H:373:LEU:HD12 | 2:H:373:LEU:C    | 2.32                     | 0.54              |
| 1:I:48:THR:HG22  | 1:I:51:ILE:HB    | 1.90                     | 0.54              |
| 1:I:105:ALA:HB2  | 1:I:113:LEU:HD23 | 1.89                     | 0.54              |
| 2:J:101:THR:OG1  | 2:J:102:PRO:HD3  | 2.08                     | 0.54              |
| 2:J:519:TRP:NE1  | 4:J:1100:7JA:C01 | 2.60                     | 0.54              |
| 1:M:148:GLU:HG2  | 1:M:152:ARG:NH1  | 2.23                     | 0.54              |
| 2:P:176:PHE:CZ   | 2:P:204:PHE:CZ   | 2.96                     | 0.54              |
| 2:P:227:VAL:CG1  | 2:P:228:GLY:N    | 2.69                     | 0.54              |
| 2:P:308:GLU:O    | 2:P:312:THR:HG23 | 2.08                     | 0.54              |
| 2:P:424:LEU:O    | 2:P:428:VAL:HG23 | 2.07                     | 0.54              |
| 2:D:54:HIS:HE1   | 2:D:56:THR:OG1   | 1.91                     | 0.54              |
| 2:D:121:ARG:NH2  | 5:D:1103:PO4:O4  | 2.41                     | 0.54              |
| 2:D:456:SER:CB   | 2:D:482:GLU:HB3  | 2.38                     | 0.54              |
| 2:D:492:LYS:HE3  | 2:D:517:TYR:CE2  | 2.43                     | 0.54              |
| 1:E:37:CYS:SG    | 2:L:296:ARG:NH2  | 2.81                     | 0.54              |
| 2:F:542:ILE:HG13 | 2:F:588:LEU:HB2  | 1.90                     | 0.54              |
| 2:H:533:MET:CE   | 2:H:588:LEU:HB3  | 2.37                     | 0.54              |
| 2:L:279:TYR:HA   | 2:L:304:LEU:HD22 | 1.90                     | 0.54              |
| 2:N:307:THR:HG22 | 2:N:360:ASP:OD2  | 2.07                     | 0.54              |
| 2:B:171:MET:O    | 2:B:174:SER:HB2  | 2.08                     | 0.53              |
| 2:B:261:GLU:HG2  | 2:B:264:MET:HG3  | 1.90                     | 0.53              |
| 2:B:357:GLY:HA2  | 2:B:415:ARG:NH2  | 2.23                     | 0.53              |
| 2:D:159:ILE:HD11 | 2:D:169:LEU:HD13 | 1.90                     | 0.53              |
| 2:D:422:LEU:HB3  | 2:D:423:PRO:HD3  | 1.89                     | 0.53              |
| 1:E:107:TYR:HE1  | 2:L:294:GLN:HE22 | 1.56                     | 0.53              |
| 2:F:227:VAL:CG1  | 2:F:228:GLY:N    | 2.72                     | 0.53              |
| 2:H:118:HIS:HE1  | 2:H:146:ASP:OD2  | 1.90                     | 0.53              |
| 2:H:170:LEU:HD23 | 2:H:170:LEU:C    | 2.33                     | 0.53              |
| 1:I:132:GLU:O    | 1:I:136:THR:HG23 | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:54:HIS:HD2   | 2:P:77:SER:OG    | 1.90                     | 0.53              |
| 2:P:422:LEU:HB3  | 2:P:423:PRO:HD3  | 1.90                     | 0.53              |
| 4:B:1100:7JA:O   | 4:B:1100:7JA:CG2 | 2.52                     | 0.53              |
| 2:D:231:GLU:HG2  | 2:D:254:ASN:ND2  | 2.22                     | 0.53              |
| 1:E:158:ALA:HA   | 2:F:62:THR:HG21  | 1.89                     | 0.53              |
| 2:H:268:PHE:O    | 2:H:270:ARG:N    | 2.41                     | 0.53              |
| 1:I:105:ALA:HB3  | 1:I:114:LEU:CD1  | 2.38                     | 0.53              |
| 2:J:386:TYR:CE1  | 4:J:1100:7JA:CG2 | 2.86                     | 0.53              |
| 2:N:468:MET:HE1  | 2:N:483:PHE:HE1  | 1.71                     | 0.53              |
| 1:A:48:THR:HG22  | 1:A:51:ILE:N     | 2.20                     | 0.53              |
| 2:B:121:ARG:HH22 | 5:B:1103:PO4:P   | 2.32                     | 0.53              |
| 1:C:30:ALA:C     | 1:C:32:MET:H     | 2.16                     | 0.53              |
| 2:H:390:ILE:HB   | 2:H:395:LEU:HD21 | 1.90                     | 0.53              |
| 2:L:227:VAL:HG13 | 2:L:228:GLY:H    | 1.73                     | 0.53              |
| 2:N:465:VAL:HG11 | 2:N:468:MET:HG3  | 1.90                     | 0.53              |
| 2:N:547:SER:HB3  | 2:N:564:HIS:HB2  | 1.90                     | 0.53              |
| 2:F:351:ARG:HG3  | 2:F:351:ARG:O    | 2.09                     | 0.53              |
| 2:F:422:LEU:HB3  | 2:F:423:PRO:HD3  | 1.91                     | 0.53              |
| 2:J:289:PHE:N    | 2:J:290:PRO:HD2  | 2.23                     | 0.53              |
| 2:J:371:ILE:O    | 2:J:375:GLN:HG3  | 2.08                     | 0.53              |
| 1:C:153:ARG:HG2  | 1:C:157:TRP:CZ3  | 2.44                     | 0.53              |
| 1:C:159:PHE:O    | 1:C:160:GLU:CB   | 2.55                     | 0.53              |
| 1:E:27:GLN:HB2   | 1:E:109:ASN:HB3  | 1.90                     | 0.53              |
| 1:E:134:ARG:HH11 | 2:F:40:VAL:HA    | 1.74                     | 0.53              |
| 2:H:18:ASP:OD2   | 2:H:43:ARG:NH1   | 2.34                     | 0.53              |
| 2:H:533:MET:HE1  | 2:H:588:LEU:HB3  | 1.91                     | 0.53              |
| 1:I:102:ILE:CG1  | 1:I:117:THR:HB   | 2.38                     | 0.53              |
| 2:L:542:ILE:CG1  | 2:L:588:LEU:HB2  | 2.38                     | 0.53              |
| 2:N:545:ILE:HG22 | 2:N:546:PRO:N    | 2.24                     | 0.53              |
| 2:B:103:TRP:O    | 2:B:107:ILE:HG13 | 2.08                     | 0.53              |
| 2:B:191:ASN:ND2  | 2:B:194:LEU:H    | 2.06                     | 0.53              |
| 2:B:456:SER:CB   | 2:B:482:GLU:HB3  | 2.38                     | 0.53              |
| 2:F:113:GLN:HE22 | 2:L:192:THR:CB   | 2.21                     | 0.53              |
| 1:I:52:LEU:O     | 1:I:56:ILE:HG13  | 2.09                     | 0.53              |
| 2:J:468:MET:HE1  | 2:J:483:PHE:CE1  | 2.43                     | 0.53              |
| 2:L:465:VAL:HG11 | 2:L:468:MET:HG3  | 1.91                     | 0.53              |
| 1:O:52:LEU:O     | 1:O:56:ILE:HG13  | 2.09                     | 0.53              |
| 2:P:367:GLN:HB3  | 2:P:391:THR:HG22 | 1.91                     | 0.53              |
| 2:P:521:GLN:HG3  | 2:P:567:HIS:HD2  | 1.73                     | 0.53              |
| 1:A:101:LEU:HB3  | 1:A:117:THR:HG21 | 1.91                     | 0.53              |
| 2:D:235:LEU:O    | 2:D:238:PHE:HB3  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:396:GLU:HG2  | 2:D:430:SER:OG   | 2.08                     | 0.53              |
| 1:E:159:PHE:O    | 1:E:160:GLU:CB   | 2.57                     | 0.53              |
| 2:F:307:THR:HG22 | 2:F:360:ASP:OD2  | 2.09                     | 0.53              |
| 2:F:547:SER:HB3  | 2:F:564:HIS:HB2  | 1.90                     | 0.53              |
| 2:H:262:LYS:HD2  | 2:H:263:TYR:CZ   | 2.44                     | 0.53              |
| 2:H:365:VAL:HG12 | 2:H:370:LEU:HG   | 1.89                     | 0.53              |
| 2:H:503:ARG:HE   | 2:H:503:ARG:H    | 1.57                     | 0.53              |
| 1:K:141:ASN:C    | 1:K:141:ASN:OD1  | 2.52                     | 0.53              |
| 2:L:255:GLU:HG3  | 2:L:255:GLU:O    | 2.08                     | 0.53              |
| 2:L:289:PHE:N    | 2:L:290:PRO:HD2  | 2.24                     | 0.53              |
| 2:L:547:SER:HB3  | 2:L:564:HIS:CB   | 2.39                     | 0.53              |
| 1:A:159:PHE:O    | 1:A:160:GLU:CB   | 2.57                     | 0.53              |
| 2:D:101:THR:OG1  | 2:N:179:LYS:NZ   | 2.42                     | 0.53              |
| 2:D:397:SER:O    | 2:D:400:THR:HG22 | 2.09                     | 0.53              |
| 1:E:48:THR:HG22  | 1:E:51:ILE:N     | 2.19                     | 0.53              |
| 1:G:30:ALA:C     | 1:G:32:MET:H     | 2.17                     | 0.53              |
| 1:G:48:THR:HG22  | 1:G:51:ILE:CB    | 2.38                     | 0.53              |
| 2:J:78:LEU:HD12  | 2:J:79:LYS:H     | 1.74                     | 0.53              |
| 2:N:197:LEU:O    | 2:N:225:VAL:HA   | 2.09                     | 0.53              |
| 2:P:78:LEU:HD12  | 2:P:79:LYS:H     | 1.73                     | 0.53              |
| 2:B:95:ASN:O     | 2:B:582:PRO:HG3  | 2.08                     | 0.53              |
| 2:B:231:GLU:HG2  | 2:B:254:ASN:ND2  | 2.24                     | 0.53              |
| 2:D:161:THR:HG22 | 2:D:186:GLU:HG2  | 1.90                     | 0.53              |
| 2:F:397:SER:O    | 2:F:400:THR:HG22 | 2.09                     | 0.53              |
| 2:H:327:ASN:HD22 | 2:H:364:LEU:HD21 | 1.73                     | 0.53              |
| 2:H:343:GLN:CD   | 2:H:343:GLN:N    | 2.67                     | 0.53              |
| 2:N:422:LEU:O    | 2:N:423:PRO:C    | 2.50                     | 0.53              |
| 2:P:253:LEU:HD12 | 2:P:280:MET:HB2  | 1.91                     | 0.53              |
| 2:B:422:LEU:HB3  | 2:B:423:PRO:HD3  | 1.91                     | 0.53              |
| 2:B:456:SER:HB3  | 2:B:482:GLU:HB3  | 1.90                     | 0.53              |
| 2:B:472:TYR:OH   | 3:Q:201:LEU:HB2  | 2.08                     | 0.53              |
| 1:E:148:GLU:HG2  | 1:E:152:ARG:NH1  | 2.24                     | 0.53              |
| 2:F:542:ILE:CG1  | 2:F:588:LEU:HB2  | 2.39                     | 0.53              |
| 1:G:153:ARG:NH2  | 2:H:539:TYR:CE1  | 2.76                     | 0.53              |
| 2:H:418:ARG:HB3  | 2:H:421:ASP:HB2  | 1.91                     | 0.53              |
| 1:K:27:GLN:HB2   | 1:K:109:ASN:HB3  | 1.89                     | 0.53              |
| 2:L:542:ILE:HG13 | 2:L:588:LEU:HB2  | 1.91                     | 0.53              |
| 2:D:248:PHE:C    | 2:D:248:PHE:CD2  | 2.86                     | 0.52              |
| 2:H:91:LEU:HD21  | 2:H:496:ARG:NH2  | 2.23                     | 0.52              |
| 2:H:269:PRO:O    | 2:H:271:LYS:N    | 2.42                     | 0.52              |
| 2:H:363:GLY:O    | 2:H:365:VAL:N    | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:428:VAL:HG12 | 2:H:443:PHE:CE1  | 2.44                     | 0.52              |
| 2:J:311:CYS:CB   | 2:J:336:VAL:HG21 | 2.38                     | 0.52              |
| 2:J:547:SER:HB3  | 2:J:564:HIS:CB   | 2.38                     | 0.52              |
| 2:L:371:ILE:O    | 2:L:375:GLN:HG3  | 2.08                     | 0.52              |
| 2:N:121:ARG:HH22 | 5:N:1103:PO4:P   | 2.32                     | 0.52              |
| 2:P:422:LEU:O    | 2:P:423:PRO:C    | 2.51                     | 0.52              |
| 2:P:519:TRP:CZ3  | 2:P:567:HIS:ND1  | 2.77                     | 0.52              |
| 1:A:12:ASP:OD2   | 1:A:49:SER:HB2   | 2.10                     | 0.52              |
| 2:B:386:TYR:CE1  | 4:B:1100:7JA:CG2 | 2.87                     | 0.52              |
| 1:C:148:GLU:HG2  | 1:C:152:ARG:HH12 | 1.74                     | 0.52              |
| 2:D:80:LEU:CB    | 2:D:122:MET:HE1  | 2.32                     | 0.52              |
| 2:J:545:ILE:HG22 | 2:J:546:PRO:N    | 2.25                     | 0.52              |
| 1:K:46:ASN:HB2   | 1:K:107:TYR:CZ   | 2.44                     | 0.52              |
| 1:A:30:ALA:C     | 1:A:32:MET:H     | 2.17                     | 0.52              |
| 2:F:161:THR:HG22 | 2:F:186:GLU:HG2  | 1.90                     | 0.52              |
| 2:J:138:ASP:OD2  | 2:J:164:ARG:HG3  | 2.08                     | 0.52              |
| 2:J:248:PHE:C    | 2:J:248:PHE:CD2  | 2.87                     | 0.52              |
| 1:M:141:ASN:C    | 1:M:141:ASN:OD1  | 2.51                     | 0.52              |
| 2:P:357:GLY:HA2  | 2:P:415:ARG:NH2  | 2.22                     | 0.52              |
| 2:D:279:TYR:HA   | 2:D:304:LEU:HD22 | 1.89                     | 0.52              |
| 2:F:54:HIS:HD2   | 2:F:77:SER:OG    | 1.93                     | 0.52              |
| 2:F:396:GLU:HG2  | 2:F:430:SER:OG   | 2.09                     | 0.52              |
| 2:H:391:THR:O    | 2:H:392:ASN:C    | 2.52                     | 0.52              |
| 2:J:171:MET:O    | 2:J:174:SER:HB2  | 2.09                     | 0.52              |
| 4:L:1100:7JA:CG2 | 4:L:1100:7JA:OXT | 2.55                     | 0.52              |
| 1:M:87:ASP:HB3   | 1:M:116:LEU:HD21 | 1.92                     | 0.52              |
| 1:O:148:GLU:HG2  | 1:O:152:ARG:NH1  | 2.24                     | 0.52              |
| 2:P:386:TYR:CE1  | 4:P:1100:7JA:CG2 | 2.88                     | 0.52              |
| 2:B:545:ILE:HG22 | 2:B:546:PRO:N    | 2.23                     | 0.52              |
| 1:E:105:ALA:HB3  | 1:E:114:LEU:CD1  | 2.40                     | 0.52              |
| 2:F:357:GLY:HA2  | 2:F:415:ARG:NH2  | 2.24                     | 0.52              |
| 2:F:519:TRP:CH2  | 2:F:567:HIS:ND1  | 2.77                     | 0.52              |
| 1:I:46:ASN:HB2   | 1:I:107:TYR:CZ   | 2.44                     | 0.52              |
| 2:N:371:ILE:O    | 2:N:375:GLN:HG3  | 2.09                     | 0.52              |
| 2:N:399:GLY:O    | 2:N:434:GLY:HA3  | 2.10                     | 0.52              |
| 2:P:121:ARG:HH22 | 5:P:1103:PO4:P   | 2.31                     | 0.52              |
| 1:A:98:LEU:CD2   | 1:A:120:THR:HG22 | 2.39                     | 0.52              |
| 2:D:519:TRP:CH2  | 2:D:567:HIS:CE1  | 2.94                     | 0.52              |
| 2:H:107:ILE:HG12 | 2:H:114:LEU:CD2  | 2.40                     | 0.52              |
| 1:K:48:THR:HG22  | 1:K:51:ILE:N     | 2.21                     | 0.52              |
| 1:K:159:PHE:O    | 1:K:160:GLU:CB   | 2.56                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:367:GLN:HB3  | 2:N:391:THR:HG22 | 1.92                     | 0.52              |
| 2:P:444:TYR:HA   | 2:P:471:GLY:CA   | 2.35                     | 0.52              |
| 2:P:542:ILE:CG1  | 2:P:588:LEU:HB2  | 2.40                     | 0.52              |
| 2:B:422:LEU:O    | 2:B:423:PRO:C    | 2.51                     | 0.52              |
| 2:D:411:VAL:HG22 | 2:D:444:TYR:HB3  | 1.91                     | 0.52              |
| 2:H:542:ILE:HD12 | 2:H:542:ILE:O    | 2.09                     | 0.52              |
| 2:J:159:ILE:HD11 | 2:J:169:LEU:HD13 | 1.91                     | 0.52              |
| 2:L:197:LEU:O    | 2:L:225:VAL:HA   | 2.09                     | 0.52              |
| 2:N:308:GLU:O    | 2:N:312:THR:HG23 | 2.10                     | 0.52              |
| 2:B:542:ILE:CD1  | 2:B:588:LEU:HD12 | 2.33                     | 0.52              |
| 2:F:95:ASN:O     | 2:F:582:PRO:HG3  | 2.10                     | 0.52              |
| 2:J:199:PHE:CE1  | 2:J:227:VAL:HG22 | 2.44                     | 0.52              |
| 2:J:255:GLU:HG3  | 2:J:255:GLU:O    | 2.10                     | 0.52              |
| 2:L:253:LEU:HD12 | 2:L:280:MET:HB2  | 1.92                     | 0.52              |
| 2:N:176:PHE:CZ   | 2:N:204:PHE:CZ   | 2.98                     | 0.52              |
| 2:N:492:LYS:HE3  | 2:N:517:TYR:CE2  | 2.45                     | 0.52              |
| 2:P:197:LEU:O    | 2:P:225:VAL:HA   | 2.09                     | 0.52              |
| 1:C:105:ALA:HB2  | 1:C:113:LEU:HD23 | 1.91                     | 0.52              |
| 2:D:519:TRP:NE1  | 4:D:1100:7JA:C01 | 2.64                     | 0.52              |
| 2:F:371:ILE:O    | 2:F:375:GLN:HG3  | 2.09                     | 0.52              |
| 2:F:386:TYR:HE1  | 4:F:1100:7JA:HG2 | 1.66                     | 0.52              |
| 2:H:395:LEU:CD2  | 2:H:395:LEU:N    | 2.73                     | 0.52              |
| 1:K:129:THR:O    | 1:K:133:ILE:HG12 | 2.09                     | 0.52              |
| 2:L:351:ARG:HG3  | 2:L:351:ARG:O    | 2.10                     | 0.52              |
| 2:N:519:TRP:CH2  | 2:N:567:HIS:ND1  | 2.77                     | 0.52              |
| 2:P:210:LYS:O    | 2:P:214:THR:HG22 | 2.10                     | 0.52              |
| 2:H:321:GLU:HA   | 2:H:344:LEU:HA   | 1.92                     | 0.52              |
| 2:H:447:GLN:O    | 2:H:447:GLN:HG3  | 2.09                     | 0.52              |
| 2:N:386:TYR:HE1  | 4:N:1100:7JA:HG2 | 1.68                     | 0.52              |
| 2:B:54:HIS:HD2   | 2:B:77:SER:OG    | 1.93                     | 0.51              |
| 2:B:519:TRP:CZ3  | 2:B:567:HIS:ND1  | 2.78                     | 0.51              |
| 1:C:125:ILE:HG23 | 1:C:133:ILE:CD1  | 2.34                     | 0.51              |
| 2:F:468:MET:HE1  | 2:F:483:PHE:HE1  | 1.76                     | 0.51              |
| 1:I:124:MET:O    | 1:I:128:LYS:HE2  | 2.09                     | 0.51              |
| 1:I:141:ASN:C    | 1:I:141:ASN:OD1  | 2.52                     | 0.51              |
| 2:J:367:GLN:HB3  | 2:J:391:THR:HG22 | 1.92                     | 0.51              |
| 1:M:44:LEU:HD12  | 1:M:44:LEU:O     | 2.11                     | 0.51              |
| 1:M:102:ILE:CB   | 2:N:20:VAL:CG2   | 2.87                     | 0.51              |
| 1:O:132:GLU:O    | 1:O:136:THR:HG23 | 2.09                     | 0.51              |
| 1:O:134:ARG:HH11 | 2:P:40:VAL:HA    | 1.75                     | 0.51              |
| 2:P:399:GLY:O    | 2:P:434:GLY:HA3  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:542:ILE:HG13 | 2:P:588:LEU:HB2  | 1.92                     | 0.51              |
| 2:B:296:ARG:HH22 | 1:O:35:ASP:HB2   | 1.74                     | 0.51              |
| 2:D:365:VAL:CG2  | 2:D:387:VAL:HA   | 2.40                     | 0.51              |
| 2:H:91:LEU:HD21  | 2:H:496:ARG:HH22 | 1.75                     | 0.51              |
| 1:I:148:GLU:HG2  | 1:I:152:ARG:NH1  | 2.25                     | 0.51              |
| 2:J:301:LEU:HD23 | 2:J:324:GLU:HB3  | 1.91                     | 0.51              |
| 2:J:542:ILE:HG13 | 2:J:588:LEU:HB2  | 1.92                     | 0.51              |
| 2:L:54:HIS:CD2   | 2:L:77:SER:OG    | 2.63                     | 0.51              |
| 2:L:233:LEU:O    | 2:L:236:VAL:HG23 | 2.09                     | 0.51              |
| 2:L:248:PHE:C    | 2:L:248:PHE:CD2  | 2.88                     | 0.51              |
| 2:N:85:ARG:HG2   | 2:N:88:MET:HE2   | 1.92                     | 0.51              |
| 2:N:289:PHE:N    | 2:N:290:PRO:HD2  | 2.25                     | 0.51              |
| 2:N:592:ILE:HD12 | 2:N:592:ILE:H    | 1.75                     | 0.51              |
| 2:B:521:GLN:HG3  | 2:B:567:HIS:CD2  | 2.45                     | 0.51              |
| 1:C:135:THR:HG22 | 1:C:136:THR:N    | 2.25                     | 0.51              |
| 2:D:547:SER:HB3  | 2:D:564:HIS:CB   | 2.40                     | 0.51              |
| 2:H:199:PHE:CE1  | 2:H:227:VAL:CG2  | 2.92                     | 0.51              |
| 2:J:197:LEU:O    | 2:J:225:VAL:HA   | 2.11                     | 0.51              |
| 2:L:133:ALA:HB2  | 2:L:159:ILE:HG22 | 1.92                     | 0.51              |
| 2:P:311:CYS:CB   | 2:P:336:VAL:HG21 | 2.41                     | 0.51              |
| 2:P:396:GLU:HG2  | 2:P:430:SER:OG   | 2.10                     | 0.51              |
| 2:B:176:PHE:CZ   | 2:B:204:PHE:CZ   | 2.99                     | 0.51              |
| 2:D:592:ILE:H    | 2:D:592:ILE:HD12 | 1.76                     | 0.51              |
| 2:F:301:LEU:HD23 | 2:F:324:GLU:HB3  | 1.93                     | 0.51              |
| 2:F:419:ILE:CD1  | 2:F:446:ARG:HH12 | 2.23                     | 0.51              |
| 1:G:108:LEU:HD12 | 1:G:110:ILE:HD11 | 1.93                     | 0.51              |
| 1:G:160:GLU:HG2  | 2:H:52:ARG:HH21  | 1.76                     | 0.51              |
| 2:H:256:ASP:OD2  | 2:H:259:MET:HG2  | 2.10                     | 0.51              |
| 2:J:389:ASP:OD2  | 2:J:419:ILE:HG23 | 2.10                     | 0.51              |
| 2:N:231:GLU:HG2  | 2:N:254:ASN:ND2  | 2.25                     | 0.51              |
| 2:P:547:SER:HB3  | 2:P:564:HIS:CB   | 2.41                     | 0.51              |
| 2:B:289:PHE:N    | 2:B:290:PRO:CD   | 2.73                     | 0.51              |
| 1:C:108:LEU:HD12 | 1:C:110:ILE:HD11 | 1.92                     | 0.51              |
| 1:E:124:MET:O    | 1:E:128:LYS:HE2  | 2.10                     | 0.51              |
| 2:H:101:THR:HB   | 2:H:102:PRO:HD2  | 1.91                     | 0.51              |
| 2:H:405:LEU:HD13 | 2:H:408:PHE:HB2  | 1.91                     | 0.51              |
| 2:J:392:ASN:HD21 | 2:J:424:LEU:HA   | 1.75                     | 0.51              |
| 1:K:114:LEU:C    | 1:K:116:LEU:N    | 2.66                     | 0.51              |
| 2:L:65:PRO:HG3   | 2:L:103:TRP:CE2  | 2.46                     | 0.51              |
| 2:N:248:PHE:C    | 2:N:248:PHE:CD2  | 2.88                     | 0.51              |
| 2:N:357:GLY:HA2  | 2:N:415:ARG:NH2  | 2.24                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:519:TRP:NE1  | 4:P:1100:7JA:C01 | 2.65                     | 0.51              |
| 2:B:157:LEU:O    | 2:B:161:THR:HG23 | 2.11                     | 0.51              |
| 2:D:297:LYS:HE2  | 2:D:322:VAL:HG21 | 1.92                     | 0.51              |
| 2:H:247:GLU:HA   | 2:H:274:ARG:O    | 2.10                     | 0.51              |
| 2:H:459:GLY:O    | 2:H:486:GLY:HA3  | 2.10                     | 0.51              |
| 1:I:105:ALA:HB3  | 1:I:114:LEU:HD12 | 1.92                     | 0.51              |
| 2:J:57:MET:HE3   | 2:J:62:THR:HG22  | 1.92                     | 0.51              |
| 2:L:357:GLY:HA2  | 2:L:415:ARG:NH2  | 2.21                     | 0.51              |
| 2:L:521:GLN:HG3  | 2:L:567:HIS:HD2  | 1.75                     | 0.51              |
| 1:M:135:THR:HG22 | 1:M:136:THR:N    | 2.25                     | 0.51              |
| 1:A:48:THR:HG22  | 1:A:51:ILE:CB    | 2.40                     | 0.51              |
| 1:C:129:THR:O    | 1:C:133:ILE:HG12 | 2.11                     | 0.51              |
| 1:E:131:GLU:HA   | 1:E:131:GLU:OE2  | 2.11                     | 0.51              |
| 2:F:172:GLU:HG3  | 2:F:200:TYR:HB3  | 1.91                     | 0.51              |
| 1:I:28:THR:O     | 1:I:32:MET:HE2   | 2.11                     | 0.51              |
| 2:J:519:TRP:CZ3  | 2:J:567:HIS:ND1  | 2.78                     | 0.51              |
| 1:K:135:THR:HG22 | 1:K:136:THR:N    | 2.25                     | 0.51              |
| 1:M:58:TYR:CD2   | 1:M:113:LEU:HD13 | 2.46                     | 0.51              |
| 2:D:542:ILE:HG13 | 2:D:588:LEU:HB2  | 1.93                     | 0.51              |
| 2:F:171:MET:O    | 2:F:174:SER:HB2  | 2.10                     | 0.51              |
| 1:G:153:ARG:HB3  | 2:H:574:LEU:HD21 | 1.93                     | 0.51              |
| 2:H:124:VAL:O    | 2:H:151:PHE:HB3  | 2.11                     | 0.51              |
| 2:H:476:SER:C    | 2:H:478:GLU:N    | 2.67                     | 0.51              |
| 2:J:227:VAL:CG1  | 2:J:228:GLY:N    | 2.73                     | 0.51              |
| 2:L:289:PHE:N    | 2:L:290:PRO:CD   | 2.74                     | 0.51              |
| 2:B:293:ALA:HB3  | 1:O:45:PRO:HG3   | 1.93                     | 0.51              |
| 2:B:547:SER:HB3  | 2:B:564:HIS:CB   | 2.40                     | 0.51              |
| 1:C:128:LYS:HB2  | 1:C:133:ILE:CD1  | 2.41                     | 0.51              |
| 1:E:48:THR:HG22  | 1:E:51:ILE:CB    | 2.39                     | 0.51              |
| 2:F:440:ARG:HB3  | 2:F:467:TRP:CE3  | 2.46                     | 0.51              |
| 2:H:107:ILE:HG12 | 2:H:114:LEU:HD22 | 1.92                     | 0.51              |
| 2:H:347:LEU:HD12 | 2:H:347:LEU:C    | 2.33                     | 0.51              |
| 2:J:327:ASN:HD22 | 2:J:328:VAL:N    | 2.09                     | 0.51              |
| 2:L:176:PHE:CZ   | 2:L:204:PHE:CZ   | 2.98                     | 0.51              |
| 1:M:48:THR:HG22  | 1:M:51:ILE:N     | 2.21                     | 0.51              |
| 2:N:279:TYR:HA   | 2:N:304:LEU:HD22 | 1.93                     | 0.51              |
| 2:P:521:GLN:HG3  | 2:P:567:HIS:CD2  | 2.45                     | 0.51              |
| 2:B:539:TYR:OH   | 1:C:146:GLU:HA   | 2.10                     | 0.51              |
| 2:F:328:VAL:CG2  | 2:F:359:GLU:HB2  | 2.41                     | 0.51              |
| 2:F:482:GLU:O    | 2:F:485:ARG:HG2  | 2.11                     | 0.51              |
| 2:H:278:SER:C    | 2:H:280:MET:H    | 2.19                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:337:LEU:HD11 | 2:H:344:LEU:HD22 | 1.93                     | 0.51              |
| 2:H:542:ILE:HD11 | 2:H:588:LEU:CB   | 2.41                     | 0.51              |
| 2:L:57:MET:HE3   | 2:L:62:THR:HG22  | 1.93                     | 0.51              |
| 2:L:301:LEU:HD23 | 2:L:324:GLU:HB3  | 1.92                     | 0.51              |
| 2:N:83:LYS:HA    | 2:N:96:TRP:CZ3   | 2.46                     | 0.51              |
| 2:P:327:ASN:HD22 | 2:P:328:VAL:N    | 2.08                     | 0.51              |
| 2:P:365:VAL:CG2  | 2:P:387:VAL:HA   | 2.41                     | 0.51              |
| 1:G:151:VAL:HG12 | 2:H:39:LEU:HD21  | 1.86                     | 0.50              |
| 2:L:422:LEU:HB3  | 2:L:423:PRO:HD3  | 1.93                     | 0.50              |
| 2:N:227:VAL:HG13 | 2:N:228:GLY:N    | 2.26                     | 0.50              |
| 1:O:102:ILE:HD12 | 2:P:20:VAL:HG21  | 1.91                     | 0.50              |
| 2:B:351:ARG:O    | 2:B:351:ARG:HG3  | 2.11                     | 0.50              |
| 2:F:22:GLU:HG2   | 2:F:47:ILE:CD1   | 2.41                     | 0.50              |
| 2:F:547:SER:HB3  | 2:F:564:HIS:CB   | 2.42                     | 0.50              |
| 2:H:232:ILE:HG13 | 2:H:253:LEU:HD21 | 1.93                     | 0.50              |
| 2:H:332:ARG:O    | 2:H:336:VAL:HG23 | 2.11                     | 0.50              |
| 1:I:102:ILE:HG13 | 1:I:117:THR:HB   | 1.94                     | 0.50              |
| 1:I:106:ASN:N    | 1:I:114:LEU:HD13 | 2.26                     | 0.50              |
| 2:J:40:VAL:O     | 2:J:41:CYS:HB3   | 2.11                     | 0.50              |
| 2:J:191:ASN:ND2  | 2:J:194:LEU:HB2  | 2.27                     | 0.50              |
| 1:K:30:ALA:C     | 1:K:32:MET:H     | 2.19                     | 0.50              |
| 1:K:91:MET:HE2   | 1:K:91:MET:HA    | 1.93                     | 0.50              |
| 1:K:125:ILE:HG23 | 1:K:133:ILE:CD1  | 2.38                     | 0.50              |
| 2:N:159:ILE:HD11 | 2:N:169:LEU:HD13 | 1.92                     | 0.50              |
| 2:N:255:GLU:HG3  | 2:N:255:GLU:O    | 2.11                     | 0.50              |
| 1:A:52:LEU:O     | 1:A:56:ILE:HG13  | 2.11                     | 0.50              |
| 2:B:40:VAL:O     | 2:B:41:CYS:HB3   | 2.10                     | 0.50              |
| 2:D:253:LEU:HD12 | 2:D:280:MET:HB2  | 1.93                     | 0.50              |
| 2:F:121:ARG:NH2  | 5:F:1103:PO4:O4  | 2.43                     | 0.50              |
| 2:H:314:ILE:C    | 2:H:316:LYS:H    | 2.18                     | 0.50              |
| 2:H:366:SER:HB3  | 2:H:368:ARG:CG   | 2.25                     | 0.50              |
| 1:K:48:THR:HG22  | 1:K:51:ILE:CB    | 2.42                     | 0.50              |
| 2:D:396:GLU:O    | 2:D:400:THR:HB   | 2.12                     | 0.50              |
| 2:F:191:ASN:ND2  | 2:F:194:LEU:H    | 2.08                     | 0.50              |
| 2:H:303:ALA:HB1  | 2:H:305:LEU:CD2  | 2.42                     | 0.50              |
| 2:L:519:TRP:CZ3  | 2:L:567:HIS:ND1  | 2.79                     | 0.50              |
| 2:N:253:LEU:HD12 | 2:N:280:MET:HB2  | 1.92                     | 0.50              |
| 1:O:30:ALA:C     | 1:O:32:MET:H     | 2.20                     | 0.50              |
| 2:P:311:CYS:O    | 2:P:315:GLN:HB2  | 2.12                     | 0.50              |
| 1:A:91:MET:HA    | 1:A:91:MET:HE2   | 1.94                     | 0.50              |
| 2:F:54:HIS:HE1   | 2:F:56:THR:OG1   | 1.95                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:28:THR:O     | 1:G:32:MET:HE2   | 2.11                     | 0.50              |
| 2:H:76:ARG:HG2   | 2:H:76:ARG:HH11  | 1.76                     | 0.50              |
| 2:J:191:ASN:ND2  | 2:J:194:LEU:H    | 2.08                     | 0.50              |
| 1:M:12:ASP:OD2   | 1:M:49:SER:HB2   | 2.12                     | 0.50              |
| 2:P:83:LYS:HA    | 2:P:96:TRP:CZ3   | 2.47                     | 0.50              |
| 2:B:78:LEU:HD12  | 2:B:79:LYS:H     | 1.77                     | 0.50              |
| 2:B:270:ARG:HB3  | 1:O:107:TYR:CD1  | 2.47                     | 0.50              |
| 2:H:587:VAL:O    | 2:H:587:VAL:HG12 | 2.10                     | 0.50              |
| 1:I:48:THR:HG22  | 1:I:51:ILE:N     | 2.18                     | 0.50              |
| 2:L:431:LEU:C    | 2:L:431:LEU:CD1  | 2.84                     | 0.50              |
| 2:N:54:HIS:HD2   | 2:N:77:SER:OG    | 1.94                     | 0.50              |
| 2:N:321:GLU:HA   | 2:N:344:LEU:HA   | 1.92                     | 0.50              |
| 2:N:519:TRP:CZ3  | 2:N:567:HIS:ND1  | 2.80                     | 0.50              |
| 2:B:399:GLY:O    | 2:B:434:GLY:HA3  | 2.12                     | 0.50              |
| 1:G:52:LEU:O     | 1:G:56:ILE:HG13  | 2.11                     | 0.50              |
| 2:H:16:THR:O     | 2:H:17:VAL:C     | 2.54                     | 0.50              |
| 1:I:101:LEU:HB3  | 1:I:117:THR:HG21 | 1.93                     | 0.50              |
| 2:J:220:ARG:HH21 | 2:N:22:GLU:HB3   | 1.76                     | 0.50              |
| 2:L:40:VAL:O     | 2:L:41:CYS:HB3   | 2.10                     | 0.50              |
| 2:L:159:ILE:HD11 | 2:L:169:LEU:HD13 | 1.94                     | 0.50              |
| 2:N:35:ASP:O     | 2:N:38:SER:OG    | 2.29                     | 0.50              |
| 2:N:101:THR:OG1  | 2:N:102:PRO:HD3  | 2.12                     | 0.50              |
| 2:D:197:LEU:O    | 2:D:225:VAL:HA   | 2.11                     | 0.50              |
| 1:E:52:LEU:O     | 1:E:56:ILE:HG13  | 2.11                     | 0.50              |
| 2:H:462:SER:HB2  | 2:H:465:VAL:HB   | 1.92                     | 0.50              |
| 2:J:546:PRO:HG2  | 2:J:584:THR:CB   | 2.38                     | 0.50              |
| 1:K:52:LEU:O     | 1:K:56:ILE:HG13  | 2.12                     | 0.50              |
| 2:L:261:GLU:HG2  | 2:L:264:MET:HG3  | 1.94                     | 0.50              |
| 2:L:311:CYS:CB   | 2:L:336:VAL:HG21 | 2.42                     | 0.50              |
| 1:M:99:PHE:CD2   | 2:N:16:THR:O     | 2.65                     | 0.50              |
| 1:M:108:LEU:HD12 | 1:M:110:ILE:HD11 | 1.93                     | 0.50              |
| 2:P:261:GLU:HG2  | 2:P:264:MET:HG3  | 1.93                     | 0.50              |
| 1:A:148:GLU:HG2  | 1:A:152:ARG:HH12 | 1.76                     | 0.50              |
| 2:B:492:LYS:HE3  | 2:B:517:TYR:CE2  | 2.47                     | 0.50              |
| 2:B:519:TRP:NE1  | 4:B:1100:7JA:C01 | 2.62                     | 0.50              |
| 2:B:542:ILE:CG1  | 2:B:588:LEU:HB2  | 2.42                     | 0.50              |
| 1:C:28:THR:O     | 1:C:32:MET:HE2   | 2.12                     | 0.50              |
| 2:D:542:ILE:CG1  | 2:D:588:LEU:HB2  | 2.42                     | 0.50              |
| 2:H:40:VAL:HG11  | 2:H:44:TRP:CE3   | 2.46                     | 0.50              |
| 1:I:158:ALA:HA   | 2:J:62:THR:CG2   | 2.42                     | 0.50              |
| 2:J:226:LYS:HA   | 2:J:249:CYS:O    | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:503:ARG:NH1  | 2:L:503:ARG:HB3  | 2.27                     | 0.50              |
| 2:N:533:MET:HE1  | 2:N:588:LEU:HB3  | 1.93                     | 0.50              |
| 2:P:156:LEU:O    | 2:P:160:VAL:HG22 | 2.12                     | 0.50              |
| 2:B:386:TYR:HE1  | 4:B:1100:7JA:HG2 | 1.70                     | 0.49              |
| 2:B:542:ILE:HG13 | 2:B:588:LEU:HB2  | 1.94                     | 0.49              |
| 2:F:22:GLU:HG2   | 2:F:47:ILE:HD13  | 1.94                     | 0.49              |
| 2:F:297:LYS:HG3  | 2:F:322:VAL:HB   | 1.92                     | 0.49              |
| 2:H:100:VAL:CG2  | 2:H:119:PHE:CE1  | 2.95                     | 0.49              |
| 2:H:331:ASP:OD1  | 2:H:366:SER:N    | 2.44                     | 0.49              |
| 1:I:26:SER:OG    | 1:I:108:LEU:HB3  | 2.12                     | 0.49              |
| 2:J:419:ILE:O    | 2:J:420:THR:C    | 2.55                     | 0.49              |
| 1:M:111:LYS:O    | 1:M:114:LEU:HB2  | 2.11                     | 0.49              |
| 1:O:105:ALA:HB2  | 1:O:113:LEU:HD23 | 1.93                     | 0.49              |
| 2:P:546:PRO:HD3  | 2:P:584:THR:O    | 2.11                     | 0.49              |
| 2:B:22:GLU:HG2   | 2:B:47:ILE:CD1   | 2.42                     | 0.49              |
| 2:B:289:PHE:N    | 2:B:290:PRO:HD2  | 2.27                     | 0.49              |
| 1:C:44:LEU:O     | 1:C:44:LEU:HD12  | 2.12                     | 0.49              |
| 2:D:296:ARG:NE   | 1:G:37:CYS:SG    | 2.85                     | 0.49              |
| 2:F:176:PHE:CZ   | 2:F:204:PHE:CZ   | 3.01                     | 0.49              |
| 2:H:85:ARG:HB3   | 2:H:85:ARG:CZ    | 2.41                     | 0.49              |
| 1:I:44:LEU:HD12  | 1:I:44:LEU:O     | 2.12                     | 0.49              |
| 2:J:22:GLU:OE1   | 2:J:43:ARG:NH2   | 2.45                     | 0.49              |
| 2:J:365:VAL:CG2  | 2:J:387:VAL:HA   | 2.41                     | 0.49              |
| 2:L:85:ARG:NH2   | 4:L:1100:7JA:O14 | 2.40                     | 0.49              |
| 2:L:545:ILE:HG22 | 2:L:546:PRO:N    | 2.27                     | 0.49              |
| 2:N:78:LEU:HD12  | 2:N:79:LYS:H     | 1.77                     | 0.49              |
| 2:N:233:LEU:O    | 2:N:236:VAL:HG23 | 2.12                     | 0.49              |
| 2:N:547:SER:HB3  | 2:N:564:HIS:CB   | 2.42                     | 0.49              |
| 1:O:48:THR:HG22  | 1:O:51:ILE:CB    | 2.40                     | 0.49              |
| 1:A:108:LEU:HD12 | 1:A:110:ILE:HD11 | 1.95                     | 0.49              |
| 1:A:153:ARG:NH2  | 2:B:539:TYR:CE1  | 2.81                     | 0.49              |
| 2:D:357:GLY:HA2  | 2:D:415:ARG:NH2  | 2.25                     | 0.49              |
| 2:H:385:VAL:HG13 | 2:H:387:VAL:HG23 | 1.94                     | 0.49              |
| 2:L:80:LEU:HB2   | 2:L:122:MET:HE2  | 1.94                     | 0.49              |
| 2:N:22:GLU:HG2   | 2:N:47:ILE:HD13  | 1.93                     | 0.49              |
| 2:N:519:TRP:CH2  | 2:N:567:HIS:CG   | 3.00                     | 0.49              |
| 2:P:57:MET:HE3   | 2:P:62:THR:HG22  | 1.94                     | 0.49              |
| 2:D:176:PHE:CZ   | 2:D:204:PHE:CZ   | 3.00                     | 0.49              |
| 2:F:85:ARG:NH2   | 4:F:1100:7JA:O14 | 2.38                     | 0.49              |
| 2:F:365:VAL:CG2  | 2:F:387:VAL:HA   | 2.41                     | 0.49              |
| 1:G:137:PHE:CD1  | 2:H:17:VAL:HG13  | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:100:VAL:HG11 | 2:H:124:VAL:HG22 | 1.94                     | 0.49              |
| 2:H:298:LEU:HD22 | 2:H:300:LEU:HG   | 1.94                     | 0.49              |
| 1:K:12:ASP:OD2   | 1:K:49:SER:HB2   | 2.11                     | 0.49              |
| 2:P:199:PHE:CZ   | 2:P:227:VAL:HG22 | 2.47                     | 0.49              |
| 1:A:44:LEU:HD12  | 1:A:44:LEU:O     | 2.13                     | 0.49              |
| 2:H:176:PHE:HZ   | 2:H:204:PHE:CZ   | 2.30                     | 0.49              |
| 2:P:168:THR:HB   | 2:P:196:VAL:CG1  | 2.17                     | 0.49              |
| 2:B:57:MET:HE3   | 2:B:62:THR:HG22  | 1.94                     | 0.49              |
| 2:B:301:LEU:HD23 | 2:B:324:GLU:HB3  | 1.94                     | 0.49              |
| 2:B:327:ASN:HD22 | 2:B:328:VAL:N    | 2.11                     | 0.49              |
| 2:H:153:THR:CG2  | 2:H:178:GLU:HA   | 2.41                     | 0.49              |
| 2:H:390:ILE:HD11 | 2:H:410:LEU:HD11 | 1.94                     | 0.49              |
| 2:H:428:VAL:O    | 2:H:432:LEU:HG   | 2.13                     | 0.49              |
| 2:J:133:ALA:HB2  | 2:J:159:ILE:HG22 | 1.94                     | 0.49              |
| 2:L:161:THR:HG22 | 2:L:186:GLU:HG2  | 1.93                     | 0.49              |
| 2:L:311:CYS:O    | 2:L:315:GLN:HB2  | 2.13                     | 0.49              |
| 2:N:22:GLU:HG2   | 2:N:47:ILE:CD1   | 2.43                     | 0.49              |
| 2:N:275:LEU:HD11 | 2:N:288:LEU:CD2  | 2.43                     | 0.49              |
| 2:N:533:MET:CE   | 2:N:588:LEU:HD13 | 2.42                     | 0.49              |
| 2:D:419:ILE:CD1  | 2:D:446:ARG:HH12 | 2.24                     | 0.49              |
| 2:F:121:ARG:HH22 | 5:F:1103:PO4:P   | 2.36                     | 0.49              |
| 2:H:395:LEU:N    | 2:H:395:LEU:HD22 | 2.28                     | 0.49              |
| 1:I:159:PHE:O    | 1:I:160:GLU:CB   | 2.59                     | 0.49              |
| 2:J:253:LEU:HD12 | 2:J:280:MET:HB2  | 1.93                     | 0.49              |
| 2:J:337:LEU:HD12 | 2:J:341:CYS:SG   | 2.53                     | 0.49              |
| 2:P:280:MET:HE1  | 2:P:288:LEU:HD11 | 1.93                     | 0.49              |
| 2:D:275:LEU:HD11 | 2:D:288:LEU:HD21 | 1.94                     | 0.49              |
| 2:H:478:GLU:O    | 2:H:482:GLU:HG2  | 2.13                     | 0.49              |
| 2:L:542:ILE:HD11 | 2:L:588:LEU:CD1  | 2.31                     | 0.49              |
| 1:M:52:LEU:O     | 1:M:56:ILE:HG13  | 2.12                     | 0.49              |
| 2:N:116:SER:CB   | 2:N:142:THR:HG23 | 2.32                     | 0.49              |
| 2:N:124:VAL:O    | 2:N:151:PHE:HB3  | 2.12                     | 0.49              |
| 1:O:141:ASN:C    | 1:O:141:ASN:OD1  | 2.55                     | 0.49              |
| 1:A:46:ASN:HB2   | 1:A:107:TYR:CZ   | 2.47                     | 0.49              |
| 2:D:199:PHE:CE1  | 2:D:227:VAL:HG22 | 2.48                     | 0.49              |
| 2:D:444:TYR:HA   | 2:D:471:GLY:CA   | 2.31                     | 0.49              |
| 1:G:102:ILE:HG21 | 2:H:20:VAL:HG22  | 1.95                     | 0.49              |
| 2:H:65:PRO:HA    | 2:H:103:TRP:CZ3  | 2.48                     | 0.49              |
| 2:H:386:TYR:CD2  | 2:H:413:LEU:HD21 | 2.48                     | 0.49              |
| 1:M:99:PHE:HD2   | 2:N:15:ALA:C     | 2.20                     | 0.49              |
| 2:D:311:CYS:O    | 2:D:315:GLN:HB2  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:233:LEU:O    | 2:F:236:VAL:HG23 | 2.13                     | 0.49              |
| 2:F:367:GLN:HB3  | 2:F:391:THR:HG22 | 1.95                     | 0.49              |
| 2:F:399:GLY:O    | 2:F:434:GLY:HA3  | 2.13                     | 0.49              |
| 1:I:160:GLU:CG   | 2:J:31:PRO:HB3   | 2.43                     | 0.49              |
| 2:L:156:LEU:O    | 2:L:160:VAL:HG22 | 2.13                     | 0.49              |
| 1:M:28:THR:O     | 1:M:32:MET:HE2   | 2.13                     | 0.49              |
| 1:O:28:THR:O     | 1:O:32:MET:HE2   | 2.13                     | 0.49              |
| 2:B:275:LEU:HD11 | 2:B:288:LEU:CD2  | 2.42                     | 0.48              |
| 2:F:519:TRP:CZ3  | 2:F:567:HIS:ND1  | 2.81                     | 0.48              |
| 2:H:119:PHE:O    | 2:H:146:ASP:HB3  | 2.13                     | 0.48              |
| 2:H:331:ASP:OD2  | 2:H:366:SER:CB   | 2.59                     | 0.48              |
| 2:H:465:VAL:HG11 | 2:H:468:MET:HG2  | 1.95                     | 0.48              |
| 2:J:542:ILE:CG1  | 2:J:588:LEU:HB2  | 2.43                     | 0.48              |
| 2:N:65:PRO:HG3   | 2:N:103:TRP:CE2  | 2.48                     | 0.48              |
| 1:O:137:PHE:CD1  | 2:P:17:VAL:HG21  | 2.47                     | 0.48              |
| 2:P:22:GLU:HG2   | 2:P:47:ILE:HD13  | 1.94                     | 0.48              |
| 2:P:152:THR:HG22 | 2:P:177:SER:HB2  | 1.95                     | 0.48              |
| 2:P:171:MET:O    | 2:P:174:SER:HB2  | 2.12                     | 0.48              |
| 2:D:533:MET:HE3  | 2:D:588:LEU:HD13 | 1.94                     | 0.48              |
| 2:F:519:TRP:NE1  | 4:F:1100:7JA:C01 | 2.65                     | 0.48              |
| 1:G:147:GLU:O    | 1:G:148:GLU:C    | 2.54                     | 0.48              |
| 2:H:292:ALA:HA   | 2:H:295:ILE:HG12 | 1.95                     | 0.48              |
| 2:H:542:ILE:HG12 | 2:H:588:LEU:HB2  | 1.92                     | 0.48              |
| 1:K:158:ALA:HA   | 2:L:62:THR:CG2   | 2.43                     | 0.48              |
| 2:L:80:LEU:O     | 2:L:122:MET:HE2  | 2.13                     | 0.48              |
| 2:L:347:LEU:HD21 | 2:L:349:ILE:HD11 | 1.94                     | 0.48              |
| 2:L:422:LEU:O    | 2:L:423:PRO:C    | 2.53                     | 0.48              |
| 2:N:40:VAL:O     | 2:N:41:CYS:HB3   | 2.13                     | 0.48              |
| 2:B:297:LYS:HG3  | 2:B:322:VAL:HB   | 1.95                     | 0.48              |
| 2:D:542:ILE:CD1  | 2:D:588:LEU:HD12 | 2.38                     | 0.48              |
| 2:F:327:ASN:HD22 | 2:F:328:VAL:N    | 2.11                     | 0.48              |
| 1:G:152:ARG:O    | 1:G:153:ARG:C    | 2.56                     | 0.48              |
| 2:L:468:MET:HE1  | 2:L:483:PHE:CE1  | 2.48                     | 0.48              |
| 2:N:103:TRP:O    | 2:N:107:ILE:HG13 | 2.13                     | 0.48              |
| 2:N:392:ASN:HD21 | 2:N:424:LEU:HA   | 1.78                     | 0.48              |
| 2:N:432:LEU:CD1  | 2:N:458:ILE:HA   | 2.44                     | 0.48              |
| 2:B:20:VAL:O     | 2:B:24:VAL:HG23  | 2.13                     | 0.48              |
| 2:B:365:VAL:CG2  | 2:B:387:VAL:HA   | 2.41                     | 0.48              |
| 1:C:134:ARG:HB2  | 1:C:139:ILE:O    | 2.14                     | 0.48              |
| 2:D:211:ASP:O    | 2:D:215:ILE:HG13 | 2.13                     | 0.48              |
| 2:D:247:GLU:HA   | 2:D:274:ARG:O    | 2.14                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:280:MET:O    | 2:D:280:MET:HG2   | 2.13                     | 0.48              |
| 1:E:35:ASP:HB2   | 2:L:296:ARG:HH22  | 1.79                     | 0.48              |
| 2:J:465:VAL:HG11 | 2:J:468:MET:HG3   | 1.95                     | 0.48              |
| 1:K:128:LYS:HB2  | 1:K:133:ILE:CD1   | 2.44                     | 0.48              |
| 2:L:365:VAL:CG2  | 2:L:387:VAL:HA    | 2.43                     | 0.48              |
| 1:M:160:GLU:CG   | 2:N:31:PRO:HB3    | 2.43                     | 0.48              |
| 2:N:422:LEU:HB3  | 2:N:423:PRO:HD3   | 1.94                     | 0.48              |
| 1:O:12:ASP:OD2   | 1:O:49:SER:HB2    | 2.13                     | 0.48              |
| 2:P:492:LYS:HE3  | 2:P:517:TYR:CE2   | 2.48                     | 0.48              |
| 1:A:148:GLU:HG2  | 1:A:152:ARG:NH1   | 2.27                     | 0.48              |
| 2:B:101:THR:HG22 | 2:B:128:ASP:CG    | 2.37                     | 0.48              |
| 2:D:255:GLU:HG3  | 2:D:255:GLU:O     | 2.12                     | 0.48              |
| 2:D:296:ARG:CZ   | 1:G:37:CYS:SG     | 3.01                     | 0.48              |
| 2:D:519:TRP:CH2  | 2:D:567:HIS:CG    | 3.01                     | 0.48              |
| 2:F:315:GLN:HG2  | 2:F:340:TYR:CE1   | 2.49                     | 0.48              |
| 1:I:134:ARG:HH11 | 2:J:40:VAL:HA     | 1.78                     | 0.48              |
| 2:J:396:GLU:O    | 2:J:400:THR:HB    | 2.12                     | 0.48              |
| 2:L:308:GLU:O    | 2:L:312:THR:HG23  | 2.13                     | 0.48              |
| 2:L:396:GLU:HG2  | 2:L:430:SER:OG    | 2.13                     | 0.48              |
| 2:L:521:GLN:HG3  | 2:L:567:HIS:CD2   | 2.48                     | 0.48              |
| 1:M:46:ASN:HB2   | 1:M:107:TYR:CZ    | 2.48                     | 0.48              |
| 2:P:231:GLU:HG2  | 2:P:254:ASN:ND2   | 2.28                     | 0.48              |
| 2:B:197:LEU:O    | 2:B:225:VAL:HA    | 2.14                     | 0.48              |
| 4:B:1100:7JA:H04 | 4:B:1100:7JA:H12A | 1.69                     | 0.48              |
| 2:H:392:ASN:ND2  | 2:H:422:LEU:HD13  | 2.28                     | 0.48              |
| 2:L:297:LYS:HE3  | 2:L:297:LYS:HB2   | 1.66                     | 0.48              |
| 2:N:503:ARG:HB3  | 2:N:503:ARG:NH1   | 2.29                     | 0.48              |
| 2:F:235:LEU:O    | 2:F:238:PHE:HB3   | 2.13                     | 0.48              |
| 1:G:129:THR:OG1  | 1:G:132:GLU:HG3   | 2.14                     | 0.48              |
| 2:H:412:LEU:HD13 | 2:H:446:ARG:NH2   | 2.28                     | 0.48              |
| 2:H:442:ALA:CB   | 4:H:1100:7JA:HD1  | 2.25                     | 0.48              |
| 2:N:419:ILE:O    | 2:N:420:THR:C     | 2.57                     | 0.48              |
| 2:N:542:ILE:CG1  | 2:N:588:LEU:HB2   | 2.44                     | 0.48              |
| 2:P:233:LEU:O    | 2:P:236:VAL:HG23  | 2.13                     | 0.48              |
| 2:B:133:ALA:HB2  | 2:B:159:ILE:HG22  | 1.96                     | 0.48              |
| 2:B:396:GLU:HG2  | 2:B:430:SER:OG    | 2.14                     | 0.48              |
| 2:D:40:VAL:O     | 2:D:41:CYS:HB3    | 2.14                     | 0.48              |
| 2:F:311:CYS:O    | 2:F:315:GLN:HB2   | 2.14                     | 0.48              |
| 2:F:465:VAL:HG11 | 2:F:468:MET:HG3   | 1.96                     | 0.48              |
| 2:H:356:GLN:O    | 2:H:357:GLY:O     | 2.32                     | 0.48              |
| 2:J:176:PHE:CZ   | 2:J:204:PHE:CZ    | 3.01                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:519:TRP:CZ3  | 2:N:567:HIS:CG   | 3.01                     | 0.48              |
| 1:O:124:MET:O    | 1:O:128:LYS:HE2  | 2.14                     | 0.48              |
| 2:P:465:VAL:HG11 | 2:P:468:MET:HG3  | 1.96                     | 0.48              |
| 1:A:95:GLN:HG2   | 1:A:124:MET:HE1  | 1.95                     | 0.48              |
| 2:D:20:VAL:O     | 2:D:24:VAL:HG23  | 2.13                     | 0.48              |
| 2:D:190:HIS:HB3  | 2:H:112:ARG:HD2  | 1.94                     | 0.48              |
| 2:D:492:LYS:HG3  | 2:D:517:TYR:CD2  | 2.49                     | 0.48              |
| 1:E:134:ARG:HB2  | 1:E:139:ILE:O    | 2.12                     | 0.48              |
| 2:F:247:GLU:HA   | 2:F:274:ARG:O    | 2.14                     | 0.48              |
| 2:L:519:TRP:CH2  | 2:L:567:HIS:CG   | 3.02                     | 0.48              |
| 2:N:492:LYS:HG3  | 2:N:517:TYR:CD2  | 2.49                     | 0.48              |
| 2:P:46:LYS:HE3   | 2:P:46:LYS:HB2   | 1.49                     | 0.48              |
| 2:P:321:GLU:HA   | 2:P:344:LEU:HA   | 1.94                     | 0.48              |
| 2:B:156:LEU:O    | 2:B:160:VAL:HG22 | 2.14                     | 0.48              |
| 1:I:30:ALA:C     | 1:I:32:MET:H     | 2.22                     | 0.48              |
| 1:M:30:ALA:C     | 1:M:32:MET:H     | 2.21                     | 0.48              |
| 2:P:328:VAL:CG2  | 2:P:359:GLU:HB2  | 2.43                     | 0.48              |
| 2:P:546:PRO:HG2  | 2:P:584:THR:CB   | 2.37                     | 0.48              |
| 2:B:519:TRP:CH2  | 2:B:567:HIS:CG   | 3.02                     | 0.47              |
| 2:F:351:ARG:HD3  | 2:F:413:LEU:HD11 | 1.95                     | 0.47              |
| 1:G:10:SER:OG    | 1:G:11:SER:N     | 2.47                     | 0.47              |
| 2:H:71:ARG:HG2   | 2:H:72:PHE:CD1   | 2.49                     | 0.47              |
| 2:H:200:TYR:CD1  | 2:H:200:TYR:C    | 2.90                     | 0.47              |
| 2:H:395:LEU:H    | 2:H:395:LEU:HD23 | 1.79                     | 0.47              |
| 2:J:22:GLU:HG2   | 2:J:47:ILE:HD13  | 1.96                     | 0.47              |
| 2:J:285:MET:N    | 2:J:286:PRO:CD   | 2.77                     | 0.47              |
| 2:L:171:MET:O    | 2:L:174:SER:HB2  | 2.13                     | 0.47              |
| 2:L:419:ILE:CD1  | 2:L:446:ARG:HH12 | 2.27                     | 0.47              |
| 2:N:542:ILE:HG13 | 2:N:588:LEU:HB2  | 1.95                     | 0.47              |
| 2:P:289:PHE:N    | 2:P:290:PRO:CD   | 2.77                     | 0.47              |
| 2:P:468:MET:HE1  | 2:P:483:PHE:HE1  | 1.79                     | 0.47              |
| 2:P:503:ARG:HB3  | 2:P:503:ARG:NH1  | 2.28                     | 0.47              |
| 2:D:80:LEU:HB2   | 2:D:122:MET:HE2  | 1.88                     | 0.47              |
| 2:F:275:LEU:HD11 | 2:F:288:LEU:CD2  | 2.44                     | 0.47              |
| 4:F:1100:7JA:CG2 | 4:F:1100:7JA:OXT | 2.54                     | 0.47              |
| 2:H:101:THR:CB   | 2:H:102:PRO:CD   | 2.91                     | 0.47              |
| 2:H:121:ARG:HA   | 2:H:147:LYS:O    | 2.13                     | 0.47              |
| 2:J:143:LEU:CD2  | 2:J:159:ILE:HD13 | 2.44                     | 0.47              |
| 2:J:152:THR:HG22 | 2:J:177:SER:HB2  | 1.96                     | 0.47              |
| 4:J:1100:7JA:CG2 | 4:J:1100:7JA:OXT | 2.56                     | 0.47              |
| 1:K:148:GLU:HG2  | 1:K:152:ARG:HH12 | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:80:LEU:HB2   | 2:N:122:MET:HE2  | 1.95                     | 0.47              |
| 2:P:419:ILE:O    | 2:P:420:THR:C    | 2.57                     | 0.47              |
| 2:F:197:LEU:O    | 2:F:225:VAL:HA   | 2.14                     | 0.47              |
| 2:F:289:PHE:N    | 2:F:290:PRO:HD2  | 2.30                     | 0.47              |
| 2:J:533:MET:HE1  | 2:J:588:LEU:HB3  | 1.96                     | 0.47              |
| 2:N:389:ASP:OD2  | 2:N:419:ILE:HG23 | 2.14                     | 0.47              |
| 3:Q:212:PHE:CD2  | 3:Q:213:LEU:HD23 | 2.48                     | 0.47              |
| 2:D:124:VAL:O    | 2:D:151:PHE:HB3  | 2.15                     | 0.47              |
| 2:D:431:LEU:C    | 2:D:431:LEU:CD1  | 2.82                     | 0.47              |
| 2:F:157:LEU:O    | 2:F:161:THR:HG23 | 2.14                     | 0.47              |
| 1:G:82:ASP:O     | 1:G:85:ALA:HB3   | 2.14                     | 0.47              |
| 2:H:386:TYR:HB3  | 2:H:413:LEU:HD21 | 1.97                     | 0.47              |
| 1:M:134:ARG:NE   | 1:M:141:ASN:HB2  | 2.30                     | 0.47              |
| 2:N:153:THR:HG23 | 2:N:178:GLU:HA   | 1.95                     | 0.47              |
| 2:B:297:LYS:HB2  | 2:B:297:LYS:HE3  | 1.57                     | 0.47              |
| 2:B:468:MET:HE1  | 2:B:483:PHE:CE1  | 2.49                     | 0.47              |
| 1:C:124:MET:O    | 1:C:128:LYS:HE2  | 2.14                     | 0.47              |
| 2:H:59:LEU:HD22  | 2:H:61:TYR:HB2   | 1.96                     | 0.47              |
| 2:H:153:THR:HG23 | 2:H:177:SER:O    | 2.14                     | 0.47              |
| 2:H:201:MET:HG3  | 2:H:302:TYR:CD1  | 2.49                     | 0.47              |
| 2:J:289:PHE:N    | 2:J:290:PRO:CD   | 2.76                     | 0.47              |
| 2:N:297:LYS:HE3  | 2:N:297:LYS:HB2  | 1.68                     | 0.47              |
| 2:N:328:VAL:CG2  | 2:N:359:GLU:HB2  | 2.44                     | 0.47              |
| 1:A:129:THR:O    | 1:A:133:ILE:HG12 | 2.14                     | 0.47              |
| 2:B:248:PHE:C    | 2:B:248:PHE:CD2  | 2.92                     | 0.47              |
| 1:C:153:ARG:NH2  | 2:D:539:TYR:CE1  | 2.83                     | 0.47              |
| 2:D:289:PHE:N    | 2:D:290:PRO:HD2  | 2.29                     | 0.47              |
| 2:F:443:PHE:HE2  | 2:F:445:LEU:HD11 | 1.75                     | 0.47              |
| 2:H:122:MET:HE3  | 2:H:122:MET:HB3  | 1.71                     | 0.47              |
| 2:H:512:LEU:HA   | 2:H:513:PRO:HD3  | 1.64                     | 0.47              |
| 2:J:221:SER:O    | 2:J:223:VAL:HG23 | 2.15                     | 0.47              |
| 1:K:153:ARG:NH2  | 2:L:539:TYR:CE1  | 2.83                     | 0.47              |
| 2:L:46:LYS:HB2   | 2:L:46:LYS:HE3   | 1.53                     | 0.47              |
| 2:N:55:VAL:CG2   | 2:N:75:LEU:HD21  | 2.41                     | 0.47              |
| 2:N:468:MET:CE   | 2:N:470:LEU:HD11 | 2.43                     | 0.47              |
| 2:P:289:PHE:N    | 2:P:290:PRO:HD2  | 2.28                     | 0.47              |
| 2:P:366:SER:HB2  | 2:P:367:GLN:OE1  | 2.15                     | 0.47              |
| 2:B:46:LYS:HB2   | 2:B:46:LYS:HE3   | 1.47                     | 0.47              |
| 2:B:419:ILE:O    | 2:B:420:THR:C    | 2.57                     | 0.47              |
| 1:C:48:THR:HG22  | 1:C:51:ILE:CB    | 2.44                     | 0.47              |
| 1:C:148:GLU:HG2  | 1:C:152:ARG:NH1  | 2.29                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:275:LEU:HD11 | 2:D:288:LEU:CD2   | 2.44                     | 0.47              |
| 2:D:285:MET:N    | 2:D:286:PRO:CD    | 2.78                     | 0.47              |
| 2:F:112:ARG:CG   | 2:L:164:ARG:HD2   | 2.42                     | 0.47              |
| 2:F:308:GLU:O    | 2:F:312:THR:HG23  | 2.14                     | 0.47              |
| 2:F:422:LEU:O    | 2:F:423:PRO:C     | 2.57                     | 0.47              |
| 2:F:533:MET:HE1  | 2:F:588:LEU:HB3   | 1.97                     | 0.47              |
| 2:H:392:ASN:HD22 | 2:H:392:ASN:H     | 1.62                     | 0.47              |
| 2:H:492:LYS:HZ1  | 2:H:516:ARG:HH11  | 1.59                     | 0.47              |
| 2:H:502:GLU:CD   | 2:H:526:SER:HB2   | 2.40                     | 0.47              |
| 2:J:83:LYS:HA    | 2:J:96:TRP:CZ3    | 2.49                     | 0.47              |
| 2:J:444:TYR:HA   | 2:J:471:GLY:CA    | 2.36                     | 0.47              |
| 2:N:191:ASN:ND2  | 2:N:194:LEU:HB2   | 2.30                     | 0.47              |
| 2:N:512:LEU:HA   | 2:N:513:PRO:HD2   | 1.77                     | 0.47              |
| 1:O:46:ASN:HB2   | 1:O:107:TYR:CZ    | 2.50                     | 0.47              |
| 2:P:161:THR:HG22 | 2:P:186:GLU:HG2   | 1.96                     | 0.47              |
| 2:P:227:VAL:HG13 | 2:P:228:GLY:H     | 1.79                     | 0.47              |
| 2:P:329:ILE:O    | 2:P:333:GLY:HA3   | 2.14                     | 0.47              |
| 1:A:63:VAL:C     | 1:A:65:ALA:H      | 2.22                     | 0.47              |
| 4:B:1100:7JA:O   | 4:B:1100:7JA:HG2A | 2.10                     | 0.47              |
| 2:D:96:TRP:O     | 2:D:578:ARG:NH2   | 2.39                     | 0.47              |
| 2:H:85:ARG:O     | 2:H:88:MET:HG2    | 2.15                     | 0.47              |
| 2:H:87:ALA:C     | 2:H:89:PHE:H      | 2.23                     | 0.47              |
| 2:H:390:ILE:CD1  | 2:H:410:LEU:HD11  | 2.45                     | 0.47              |
| 2:H:442:ALA:CB   | 4:H:1100:7JA:H28  | 2.44                     | 0.47              |
| 2:L:78:LEU:HD21  | 2:L:80:LEU:HD21   | 1.96                     | 0.47              |
| 1:M:153:ARG:CG   | 1:M:157:TRP:CZ3   | 2.98                     | 0.47              |
| 2:P:22:GLU:HG2   | 2:P:47:ILE:CD1    | 2.45                     | 0.47              |
| 2:P:101:THR:OG1  | 2:P:102:PRO:HD3   | 2.15                     | 0.47              |
| 2:P:286:PRO:CA   | 2:P:289:PHE:CE2   | 2.92                     | 0.47              |
| 1:C:141:ASN:OD1  | 1:C:141:ASN:C     | 2.58                     | 0.47              |
| 2:D:468:MET:HE1  | 2:D:483:PHE:CE1   | 2.50                     | 0.47              |
| 2:F:503:ARG:HB3  | 2:F:503:ARG:NH1   | 2.29                     | 0.47              |
| 2:H:423:PRO:HA   | 2:H:449:GLY:O     | 2.15                     | 0.47              |
| 2:J:270:ARG:O    | 1:M:46:ASN:OD1    | 2.33                     | 0.47              |
| 2:L:492:LYS:HE3  | 2:L:517:TYR:CE2   | 2.50                     | 0.47              |
| 2:B:101:THR:OG1  | 2:B:102:PRO:HD3   | 2.15                     | 0.47              |
| 2:B:199:PHE:CE1  | 2:B:227:VAL:HG22  | 2.49                     | 0.47              |
| 2:B:465:VAL:HG11 | 2:B:468:MET:HG3   | 1.97                     | 0.47              |
| 1:C:113:LEU:O    | 1:C:117:THR:CG2   | 2.63                     | 0.47              |
| 2:F:103:TRP:O    | 2:F:107:ILE:HG13  | 2.15                     | 0.47              |
| 1:G:134:ARG:HD3  | 2:H:40:VAL:O      | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:95:ASN:HD22  | 2:H:95:ASN:N     | 2.12                     | 0.47              |
| 2:H:136:ARG:HG3  | 2:H:136:ARG:NH1  | 2.30                     | 0.47              |
| 2:H:185:HIS:O    | 2:H:188:ALA:HB3  | 2.15                     | 0.47              |
| 2:L:546:PRO:HG2  | 2:L:584:THR:CB   | 2.36                     | 0.47              |
| 2:N:337:LEU:HD12 | 2:N:341:CYS:SG   | 2.55                     | 0.47              |
| 2:P:419:ILE:CD1  | 2:P:446:ARG:HH12 | 2.26                     | 0.47              |
| 2:P:519:TRP:CH2  | 2:P:567:HIS:CE1  | 2.99                     | 0.47              |
| 2:B:492:LYS:HG3  | 2:B:517:TYR:CD2  | 2.50                     | 0.46              |
| 2:B:519:TRP:CH2  | 2:B:567:HIS:CE1  | 2.99                     | 0.46              |
| 1:C:58:TYR:CD2   | 1:C:113:LEU:HD13 | 2.50                     | 0.46              |
| 1:E:113:LEU:O    | 1:E:113:LEU:CG   | 2.63                     | 0.46              |
| 2:P:545:ILE:HG22 | 2:P:546:PRO:N    | 2.30                     | 0.46              |
| 2:D:190:HIS:HE1  | 2:H:110:ASN:HA   | 1.81                     | 0.46              |
| 2:D:289:PHE:N    | 2:D:290:PRO:CD   | 2.78                     | 0.46              |
| 2:F:101:THR:OG1  | 2:F:102:PRO:HD3  | 2.15                     | 0.46              |
| 1:G:12:ASP:OD2   | 1:G:49:SER:HB2   | 2.14                     | 0.46              |
| 1:G:83:LEU:HD23  | 1:G:83:LEU:HA    | 1.77                     | 0.46              |
| 1:G:105:ALA:HB2  | 1:G:113:LEU:HD23 | 1.97                     | 0.46              |
| 1:I:44:LEU:HA    | 1:I:45:PRO:HD3   | 1.71                     | 0.46              |
| 2:L:533:MET:HE1  | 2:L:588:LEU:HB3  | 1.97                     | 0.46              |
| 2:N:367:GLN:HG2  | 2:N:391:THR:HB   | 1.96                     | 0.46              |
| 2:P:285:MET:N    | 2:P:286:PRO:CD   | 2.78                     | 0.46              |
| 2:P:347:LEU:HD21 | 2:P:349:ILE:HD11 | 1.95                     | 0.46              |
| 2:B:533:MET:HE1  | 2:B:588:LEU:HB3  | 1.96                     | 0.46              |
| 2:H:59:LEU:CD2   | 2:H:61:TYR:HB2   | 2.45                     | 0.46              |
| 2:H:519:TRP:HH2  | 2:H:567:HIS:ND1  | 2.00                     | 0.46              |
| 2:L:546:PRO:HD3  | 2:L:584:THR:O    | 2.14                     | 0.46              |
| 1:M:114:LEU:C    | 1:M:116:LEU:N    | 2.72                     | 0.46              |
| 1:M:128:LYS:HB2  | 1:M:133:ILE:HD11 | 1.97                     | 0.46              |
| 1:M:134:ARG:HH11 | 2:N:40:VAL:HA    | 1.80                     | 0.46              |
| 2:P:477:ASP:OD1  | 2:P:477:ASP:N    | 2.48                     | 0.46              |
| 2:P:492:LYS:HG3  | 2:P:517:TYR:CD2  | 2.50                     | 0.46              |
| 1:A:128:LYS:HB2  | 1:A:133:ILE:CD1  | 2.46                     | 0.46              |
| 1:I:12:ASP:OD2   | 1:I:49:SER:HB2   | 2.16                     | 0.46              |
| 1:M:63:VAL:C     | 1:M:65:ALA:H     | 2.24                     | 0.46              |
| 1:M:102:ILE:HB   | 2:N:20:VAL:CG2   | 2.46                     | 0.46              |
| 1:A:160:GLU:CG   | 2:B:31:PRO:HB3   | 2.45                     | 0.46              |
| 2:B:321:GLU:HA   | 2:B:344:LEU:HA   | 1.96                     | 0.46              |
| 2:D:156:LEU:O    | 2:D:160:VAL:HG22 | 2.15                     | 0.46              |
| 2:H:266:LEU:CD1  | 2:H:267:VAL:H    | 2.26                     | 0.46              |
| 1:I:135:THR:HG22 | 1:I:136:THR:N    | 2.31                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:54:HIS:CE1   | 2:J:56:THR:OG1   | 2.66                     | 0.46              |
| 2:J:321:GLU:HA   | 2:J:344:LEU:HA   | 1.97                     | 0.46              |
| 1:K:28:THR:O     | 1:K:32:MET:HE2   | 2.16                     | 0.46              |
| 2:L:80:LEU:HD12  | 2:L:122:MET:HE1  | 1.98                     | 0.46              |
| 2:L:321:GLU:HA   | 2:L:344:LEU:HA   | 1.97                     | 0.46              |
| 1:M:158:ALA:HA   | 2:N:62:THR:CG2   | 2.46                     | 0.46              |
| 2:B:308:GLU:O    | 2:B:312:THR:HG23 | 2.16                     | 0.46              |
| 1:C:93:ILE:CD1   | 1:C:97:THR:HG22  | 2.42                     | 0.46              |
| 1:C:158:ALA:HA   | 2:D:62:THR:CG2   | 2.45                     | 0.46              |
| 2:D:367:GLN:HB3  | 2:D:391:THR:HG22 | 1.98                     | 0.46              |
| 2:F:55:VAL:CG2   | 2:F:75:LEU:HD21  | 2.45                     | 0.46              |
| 2:F:124:VAL:O    | 2:F:151:PHE:HB3  | 2.16                     | 0.46              |
| 2:F:444:TYR:HA   | 2:F:471:GLY:CA   | 2.33                     | 0.46              |
| 2:H:39:LEU:HA    | 2:H:39:LEU:HD23  | 1.56                     | 0.46              |
| 2:L:387:VAL:HG22 | 2:L:389:ASP:H    | 1.79                     | 0.46              |
| 1:M:114:LEU:C    | 1:M:116:LEU:H    | 2.24                     | 0.46              |
| 2:N:419:ILE:CD1  | 2:N:446:ARG:HH12 | 2.29                     | 0.46              |
| 4:N:1100:7JA:H27 | 4:N:1100:7JA:H05 | 1.74                     | 0.46              |
| 4:P:1100:7JA:CG2 | 4:P:1100:7JA:OXT | 2.58                     | 0.46              |
| 1:A:158:ALA:HA   | 2:B:62:THR:CG2   | 2.46                     | 0.46              |
| 2:B:235:LEU:O    | 2:B:238:PHE:HB3  | 2.16                     | 0.46              |
| 2:F:57:MET:HE3   | 2:F:62:THR:HG22  | 1.96                     | 0.46              |
| 2:F:80:LEU:O     | 2:F:122:MET:HE2  | 2.15                     | 0.46              |
| 2:F:419:ILE:O    | 2:F:420:THR:C    | 2.58                     | 0.46              |
| 2:J:472:TYR:OH   | 3:U:201:LEU:HB2  | 2.16                     | 0.46              |
| 2:L:399:GLY:O    | 2:L:434:GLY:HA3  | 2.16                     | 0.46              |
| 2:L:419:ILE:O    | 2:L:420:THR:C    | 2.58                     | 0.46              |
| 2:P:431:LEU:C    | 2:P:431:LEU:CD1  | 2.88                     | 0.46              |
| 2:D:103:TRP:O    | 2:D:107:ILE:HG13 | 2.14                     | 0.46              |
| 2:D:296:ARG:NH1  | 1:G:35:ASP:OD1   | 2.41                     | 0.46              |
| 2:D:465:VAL:HG11 | 2:D:468:MET:HG3  | 1.98                     | 0.46              |
| 2:F:83:LYS:HA    | 2:F:96:TRP:CZ3   | 2.51                     | 0.46              |
| 2:F:519:TRP:CH2  | 2:F:567:HIS:CE1  | 3.03                     | 0.46              |
| 2:H:168:THR:HB   | 2:H:196:VAL:CG1  | 2.45                     | 0.46              |
| 2:H:458:ILE:CG2  | 2:H:468:MET:HE1  | 2.45                     | 0.46              |
| 2:H:494:GLU:HA   | 2:H:519:TRP:O    | 2.15                     | 0.46              |
| 2:H:533:MET:O    | 2:H:535:MET:N    | 2.46                     | 0.46              |
| 1:I:134:ARG:NE   | 1:I:141:ASN:HB2  | 2.31                     | 0.46              |
| 1:K:148:GLU:HG2  | 1:K:152:ARG:NH1  | 2.31                     | 0.46              |
| 2:L:22:GLU:HG2   | 2:L:47:ILE:CD1   | 2.45                     | 0.46              |
| 3:V:201:LEU:HD23 | 3:V:201:LEU:HA   | 1.72                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:153:THR:HG23 | 2:P:178:GLU:HA   | 1.97                     | 0.46              |
| 2:P:226:LYS:HA   | 2:P:249:CYS:O    | 2.15                     | 0.46              |
| 2:P:533:MET:HE1  | 2:P:588:LEU:HB3  | 1.97                     | 0.46              |
| 2:D:191:ASN:ND2  | 2:D:194:LEU:HB2  | 2.30                     | 0.46              |
| 3:S:201:LEU:HA   | 3:S:201:LEU:HD23 | 1.61                     | 0.46              |
| 2:H:59:LEU:CD2   | 2:H:61:TYR:H     | 2.29                     | 0.46              |
| 2:H:108:SER:OG   | 2:H:135:ALA:HB2  | 2.16                     | 0.46              |
| 2:H:366:SER:OG   | 2:H:368:ARG:HG2  | 2.16                     | 0.46              |
| 1:M:134:ARG:HB2  | 1:M:139:ILE:O    | 2.15                     | 0.46              |
| 2:P:40:VAL:O     | 2:P:41:CYS:HB3   | 2.16                     | 0.46              |
| 2:P:194:LEU:HA   | 2:P:194:LEU:HD12 | 1.81                     | 0.46              |
| 2:P:297:LYS:HB2  | 2:P:297:LYS:HE3  | 1.68                     | 0.46              |
| 2:P:332:ARG:O    | 2:P:336:VAL:HG23 | 2.15                     | 0.46              |
| 2:P:542:ILE:CD1  | 2:P:588:LEU:HD12 | 2.36                     | 0.46              |
| 1:E:160:GLU:CG   | 2:F:31:PRO:HB3   | 2.45                     | 0.46              |
| 2:F:564:HIS:HA   | 2:F:565:PRO:HD2  | 1.76                     | 0.46              |
| 2:H:94:GLU:CG    | 2:H:95:ASN:H     | 2.29                     | 0.46              |
| 2:H:289:PHE:O    | 2:H:290:PRO:C    | 2.58                     | 0.46              |
| 2:J:329:ILE:O    | 2:J:333:GLY:HA3  | 2.16                     | 0.46              |
| 2:J:527:MET:O    | 2:J:528:THR:C    | 2.59                     | 0.46              |
| 2:J:542:ILE:CD1  | 2:J:588:LEU:HD12 | 2.36                     | 0.46              |
| 1:K:134:ARG:HB2  | 1:K:139:ILE:O    | 2.16                     | 0.46              |
| 1:K:160:GLU:CG   | 2:L:31:PRO:HB3   | 2.46                     | 0.46              |
| 2:N:443:PHE:HE2  | 2:N:445:LEU:HD11 | 1.80                     | 0.46              |
| 2:N:519:TRP:CH2  | 2:N:567:HIS:CE1  | 3.02                     | 0.46              |
| 2:N:519:TRP:CZ3  | 2:N:567:HIS:HB3  | 2.51                     | 0.46              |
| 1:O:42:VAL:HA    | 1:O:43:PRO:HD3   | 1.82                     | 0.46              |
| 2:P:432:LEU:CD1  | 2:P:458:ILE:HA   | 2.46                     | 0.46              |
| 2:B:419:ILE:HD11 | 2:B:446:ARG:NH2  | 2.27                     | 0.45              |
| 2:D:419:ILE:O    | 2:D:420:THR:C    | 2.59                     | 0.45              |
| 2:H:317:CYS:O    | 2:H:320:LEU:HB2  | 2.16                     | 0.45              |
| 2:H:327:ASN:HA   | 2:H:349:ILE:CG2  | 2.46                     | 0.45              |
| 1:I:34:GLU:C     | 1:I:36:ASP:H     | 2.24                     | 0.45              |
| 2:J:20:VAL:O     | 2:J:24:VAL:HG23  | 2.16                     | 0.45              |
| 2:L:285:MET:N    | 2:L:286:PRO:CD   | 2.79                     | 0.45              |
| 2:N:338:ALA:O    | 2:N:376:GLY:HA3  | 2.16                     | 0.45              |
| 1:O:63:VAL:C     | 1:O:65:ALA:H     | 2.23                     | 0.45              |
| 2:P:211:ASP:HA   | 2:P:214:THR:CG2  | 2.43                     | 0.45              |
| 2:P:275:LEU:HD11 | 2:P:288:LEU:CD2  | 2.46                     | 0.45              |
| 2:H:71:ARG:C     | 2:H:73:PRO:HD3   | 2.41                     | 0.45              |
| 2:L:172:GLU:HG3  | 2:L:200:TYR:HB3  | 1.96                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:527:MET:O    | 2:L:528:THR:C    | 2.58                     | 0.45              |
| 1:A:102:ILE:HG12 | 1:A:117:THR:OG1  | 2.16                     | 0.45              |
| 2:B:310:HIS:HE1  | 2:B:325:THR:OG1  | 1.98                     | 0.45              |
| 2:B:431:LEU:CD1  | 2:B:435:CYS:SG   | 3.04                     | 0.45              |
| 2:D:133:ALA:HB2  | 2:D:159:ILE:HG22 | 1.98                     | 0.45              |
| 1:E:130:PRO:O    | 1:E:134:ARG:HG2  | 2.16                     | 0.45              |
| 2:F:255:GLU:HG3  | 2:F:255:GLU:O    | 2.16                     | 0.45              |
| 2:H:286:PRO:C    | 2:H:288:LEU:N    | 2.69                     | 0.45              |
| 2:H:351:ARG:HG3  | 2:H:359:GLU:HB3  | 1.97                     | 0.45              |
| 2:H:375:GLN:HG2  | 2:H:401:TYR:CE1  | 2.51                     | 0.45              |
| 2:J:164:ARG:HE   | 2:N:112:ARG:HG2  | 1.69                     | 0.45              |
| 2:J:495:MET:O    | 2:J:520:VAL:HA   | 2.16                     | 0.45              |
| 2:L:194:LEU:HA   | 2:L:194:LEU:HD12 | 1.74                     | 0.45              |
| 1:M:103:LEU:HD11 | 2:N:19:ASP:HB3   | 1.98                     | 0.45              |
| 2:N:20:VAL:O     | 2:N:24:VAL:HG23  | 2.17                     | 0.45              |
| 2:P:159:ILE:HD11 | 2:P:169:LEU:HD13 | 1.99                     | 0.45              |
| 3:X:201:LEU:HD23 | 3:X:201:LEU:HA   | 1.69                     | 0.45              |
| 2:D:80:LEU:HD12  | 2:D:122:MET:HE1  | 1.97                     | 0.45              |
| 2:D:191:ASN:ND2  | 2:D:194:LEU:H    | 2.10                     | 0.45              |
| 2:D:321:GLU:HA   | 2:D:344:LEU:HA   | 1.98                     | 0.45              |
| 3:R:201:LEU:HD23 | 3:R:201:LEU:HA   | 1.74                     | 0.45              |
| 2:F:168:THR:HB   | 2:F:196:VAL:CG1  | 2.20                     | 0.45              |
| 2:F:321:GLU:HA   | 2:F:344:LEU:HA   | 1.99                     | 0.45              |
| 1:G:137:PHE:CD1  | 2:H:17:VAL:CG1   | 3.00                     | 0.45              |
| 2:H:314:ILE:HG22 | 2:H:341:CYS:SG   | 2.56                     | 0.45              |
| 2:H:327:ASN:HD22 | 2:H:364:LEU:CD2  | 2.30                     | 0.45              |
| 2:J:298:LEU:HD12 | 2:J:298:LEU:HA   | 1.67                     | 0.45              |
| 2:J:311:CYS:O    | 2:J:315:GLN:HB2  | 2.16                     | 0.45              |
| 1:K:134:ARG:NE   | 1:K:141:ASN:HB2  | 2.31                     | 0.45              |
| 1:K:158:ALA:CB   | 2:L:62:THR:HG23  | 2.47                     | 0.45              |
| 2:L:22:GLU:OE1   | 2:L:43:ARG:NH2   | 2.49                     | 0.45              |
| 2:L:275:LEU:HD11 | 2:L:288:LEU:HD21 | 1.97                     | 0.45              |
| 2:L:367:GLN:HG2  | 2:L:391:THR:HB   | 1.98                     | 0.45              |
| 2:N:201:MET:HE2  | 2:N:201:MET:HB2  | 1.86                     | 0.45              |
| 2:N:310:HIS:HE1  | 2:N:325:THR:OG1  | 2.00                     | 0.45              |
| 2:N:451:THR:HA   | 2:N:475:GLU:HG3  | 1.98                     | 0.45              |
| 2:B:503:ARG:NH1  | 2:B:503:ARG:HB3  | 2.31                     | 0.45              |
| 2:D:57:MET:HE3   | 2:D:62:THR:HG22  | 1.98                     | 0.45              |
| 2:D:101:THR:OG1  | 2:D:102:PRO:HD3  | 2.17                     | 0.45              |
| 2:D:194:LEU:HD12 | 2:D:194:LEU:HA   | 1.80                     | 0.45              |
| 2:D:297:LYS:HG3  | 2:D:322:VAL:HB   | 1.98                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:351:ARG:HG3  | 2:D:351:ARG:O     | 2.16                     | 0.45              |
| 2:F:20:VAL:O     | 2:F:24:VAL:HG23   | 2.17                     | 0.45              |
| 2:F:329:ILE:O    | 2:F:333:GLY:HA3   | 2.17                     | 0.45              |
| 2:H:230:PHE:CD1  | 2:H:235:LEU:HD21  | 2.39                     | 0.45              |
| 2:P:54:HIS:CE1   | 2:P:56:THR:OG1    | 2.66                     | 0.45              |
| 1:A:83:LEU:HD23  | 1:A:83:LEU:HA     | 1.84                     | 0.45              |
| 2:B:114:LEU:O    | 2:B:136:ARG:NH1   | 2.48                     | 0.45              |
| 2:B:545:ILE:HA   | 2:B:546:PRO:HD3   | 1.76                     | 0.45              |
| 2:B:546:PRO:HG2  | 2:B:584:THR:CB    | 2.42                     | 0.45              |
| 2:D:22:GLU:OE1   | 2:D:43:ARG:NH2    | 2.49                     | 0.45              |
| 2:D:329:ILE:O    | 2:D:333:GLY:HA3   | 2.17                     | 0.45              |
| 2:F:240:LYS:CG   | 2:F:267:VAL:HG21  | 2.44                     | 0.45              |
| 2:F:387:VAL:HG22 | 2:F:389:ASP:H     | 1.80                     | 0.45              |
| 2:H:32:LYS:HD3   | 2:H:32:LYS:HA     | 1.49                     | 0.45              |
| 2:J:54:HIS:CD2   | 2:J:77:SER:OG     | 2.69                     | 0.45              |
| 2:J:399:GLY:O    | 2:J:434:GLY:HA3   | 2.17                     | 0.45              |
| 2:J:519:TRP:CH2  | 2:J:567:HIS:CG    | 3.04                     | 0.45              |
| 1:K:44:LEU:O     | 1:K:44:LEU:HD12   | 2.17                     | 0.45              |
| 2:L:54:HIS:CE1   | 2:L:56:THR:OG1    | 2.69                     | 0.45              |
| 2:N:65:PRO:HA    | 2:N:103:TRP:CZ3   | 2.52                     | 0.45              |
| 2:N:404:ASN:HA   | 2:N:437:LYS:HD2   | 1.99                     | 0.45              |
| 2:N:418:ARG:C    | 2:N:419:ILE:HD12  | 2.42                     | 0.45              |
| 1:O:105:ALA:HB3  | 1:O:114:LEU:HD13  | 1.98                     | 0.45              |
| 2:P:63:ALA:HB1   | 2:P:67:ARG:HD2    | 1.99                     | 0.45              |
| 2:P:95:ASN:O     | 2:P:582:PRO:HG3   | 2.17                     | 0.45              |
| 2:D:546:PRO:HG2  | 2:D:584:THR:CB    | 2.40                     | 0.45              |
| 3:R:212:PHE:CD2  | 3:R:213:LEU:HD23  | 2.52                     | 0.45              |
| 4:F:1100:7JA:OXT | 4:F:1100:7JA:HG2A | 2.13                     | 0.45              |
| 1:I:153:ARG:NH2  | 2:J:539:TYR:CE1   | 2.85                     | 0.45              |
| 2:J:199:PHE:CZ   | 2:J:227:VAL:HG22  | 2.52                     | 0.45              |
| 2:J:201:MET:HE2  | 2:J:201:MET:HB2   | 1.93                     | 0.45              |
| 2:L:305:LEU:HD22 | 2:L:305:LEU:H     | 1.80                     | 0.45              |
| 1:M:112:ASN:O    | 1:M:114:LEU:N     | 2.46                     | 0.45              |
| 2:N:343:GLN:O    | 2:N:345:LYS:HG2   | 2.17                     | 0.45              |
| 2:P:255:GLU:HG3  | 2:P:255:GLU:O     | 2.16                     | 0.45              |
| 2:P:512:LEU:HA   | 2:P:513:PRO:HD2   | 1.76                     | 0.45              |
| 1:E:128:LYS:HB2  | 1:E:133:ILE:HD11  | 1.99                     | 0.45              |
| 1:E:137:PHE:CD1  | 2:F:17:VAL:HG21   | 2.52                     | 0.45              |
| 2:F:431:LEU:C    | 2:F:431:LEU:CD1   | 2.89                     | 0.45              |
| 4:F:1100:7JA:H05 | 4:F:1100:7JA:H27  | 1.65                     | 0.45              |
| 2:H:100:VAL:HG21 | 2:H:119:PHE:CZ    | 2.51                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:455:LEU:HD23 | 2:H:455:LEU:HA    | 1.66                     | 0.45              |
| 2:H:481:MET:O    | 2:H:482:GLU:C     | 2.57                     | 0.45              |
| 4:J:1100:7JA:OXT | 4:J:1100:7JA:HG2A | 2.12                     | 0.45              |
| 1:K:124:MET:O    | 1:K:128:LYS:HE2   | 2.16                     | 0.45              |
| 2:N:199:PHE:CZ   | 2:N:227:VAL:HG22  | 2.52                     | 0.45              |
| 2:N:247:GLU:HA   | 2:N:274:ARG:O     | 2.16                     | 0.45              |
| 2:N:398:ILE:CG2  | 2:N:402:LEU:HD11  | 2.45                     | 0.45              |
| 1:A:134:ARG:NH1  | 2:B:40:VAL:HA     | 2.31                     | 0.45              |
| 2:B:35:ASP:O     | 2:B:38:SER:OG     | 2.32                     | 0.45              |
| 2:B:245:LEU:HD12 | 2:B:245:LEU:HA    | 1.80                     | 0.45              |
| 2:D:419:ILE:HD11 | 2:D:446:ARG:NH2   | 2.25                     | 0.45              |
| 1:E:91:MET:HG3   | 1:E:116:LEU:HD11  | 1.98                     | 0.45              |
| 2:F:153:THR:HG23 | 2:F:178:GLU:HA    | 1.99                     | 0.45              |
| 2:F:392:ASN:HD21 | 2:F:424:LEU:HA    | 1.82                     | 0.45              |
| 2:F:545:ILE:HG22 | 2:F:546:PRO:N     | 2.32                     | 0.45              |
| 2:H:371:ILE:HG22 | 2:H:375:GLN:NE2   | 2.20                     | 0.45              |
| 1:I:128:LYS:HB2  | 1:I:133:ILE:HD11  | 1.99                     | 0.45              |
| 2:J:80:LEU:HB2   | 2:J:122:MET:HE2   | 1.94                     | 0.45              |
| 1:K:153:ARG:HG2  | 1:K:157:TRP:CZ3   | 2.52                     | 0.45              |
| 2:N:91:LEU:O     | 2:N:567:HIS:HE1   | 2.00                     | 0.45              |
| 2:N:301:LEU:CD2  | 2:N:324:GLU:HB3   | 2.46                     | 0.45              |
| 1:A:8:LEU:HD23   | 1:A:42:VAL:HG13   | 1.98                     | 0.45              |
| 2:F:46:LYS:HE3   | 2:F:46:LYS:HB2    | 1.56                     | 0.45              |
| 2:H:477:ASP:HB3  | 2:H:504:ALA:CB    | 2.47                     | 0.45              |
| 2:J:37:ALA:O     | 2:J:40:VAL:HG13   | 2.17                     | 0.45              |
| 2:J:275:LEU:HD11 | 2:J:288:LEU:CD2   | 2.46                     | 0.45              |
| 1:O:134:ARG:HB2  | 1:O:139:ILE:O     | 2.17                     | 0.45              |
| 1:O:160:GLU:CG   | 2:P:31:PRO:HB3    | 2.47                     | 0.45              |
| 2:P:431:LEU:CD1  | 2:P:435:CYS:SG    | 3.05                     | 0.45              |
| 2:D:172:GLU:HG3  | 2:D:200:TYR:HB3   | 1.99                     | 0.44              |
| 2:D:429:ARG:HG2  | 2:D:433:ILE:HD11  | 1.99                     | 0.44              |
| 1:G:34:GLU:C     | 1:G:36:ASP:H      | 2.25                     | 0.44              |
| 2:H:34:ARG:O     | 2:H:35:ASP:C      | 2.59                     | 0.44              |
| 2:H:248:PHE:C    | 2:H:248:PHE:CD2   | 2.95                     | 0.44              |
| 2:H:310:HIS:NE2  | 2:H:328:VAL:HG23  | 2.31                     | 0.44              |
| 2:H:410:LEU:HD13 | 2:H:411:VAL:N     | 2.32                     | 0.44              |
| 1:I:134:ARG:HB2  | 1:I:139:ILE:O     | 2.17                     | 0.44              |
| 1:I:158:ALA:CB   | 2:J:62:THR:HG23   | 2.47                     | 0.44              |
| 1:M:99:PHE:HZ    | 2:N:17:VAL:HG22   | 1.82                     | 0.44              |
| 2:P:301:LEU:CD2  | 2:P:324:GLU:HB3   | 2.47                     | 0.44              |
| 2:P:405:LEU:HD23 | 2:P:405:LEU:HA    | 1.80                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:419:ILE:CD1  | 2:B:446:ARG:HH12 | 2.27                     | 0.44              |
| 1:E:63:VAL:C     | 1:E:65:ALA:H     | 2.26                     | 0.44              |
| 2:H:142:THR:HA   | 2:H:168:THR:O    | 2.17                     | 0.44              |
| 2:H:161:THR:HG22 | 2:H:186:GLU:HG2  | 1.99                     | 0.44              |
| 2:H:313:LEU:O    | 2:H:314:ILE:C    | 2.60                     | 0.44              |
| 2:H:332:ARG:O    | 2:H:333:GLY:C    | 2.59                     | 0.44              |
| 1:K:34:GLU:C     | 1:K:36:ASP:H     | 2.25                     | 0.44              |
| 1:M:111:LYS:O    | 1:M:114:LEU:CB   | 2.65                     | 0.44              |
| 2:N:469:LEU:HA   | 2:N:494:GLU:O    | 2.17                     | 0.44              |
| 2:P:101:THR:CG2  | 2:P:128:ASP:OD1  | 2.55                     | 0.44              |
| 2:B:389:ASP:OD2  | 2:B:419:ILE:HG23 | 2.17                     | 0.44              |
| 2:F:301:LEU:CD2  | 2:F:324:GLU:HB3  | 2.48                     | 0.44              |
| 2:H:161:THR:HG22 | 2:H:186:GLU:CD   | 2.42                     | 0.44              |
| 2:H:366:SER:O    | 2:H:369:GLY:N    | 2.49                     | 0.44              |
| 2:H:461:TYR:C    | 2:H:463:PRO:HD3  | 2.41                     | 0.44              |
| 2:J:22:GLU:HG2   | 2:J:47:ILE:CD1   | 2.46                     | 0.44              |
| 2:J:164:ARG:NE   | 2:N:112:ARG:HG3  | 2.14                     | 0.44              |
| 2:J:432:LEU:CD1  | 2:J:458:ILE:HA   | 2.48                     | 0.44              |
| 2:J:468:MET:HE1  | 2:J:483:PHE:HE1  | 1.82                     | 0.44              |
| 2:J:519:TRP:CH2  | 2:J:567:HIS:CE1  | 3.00                     | 0.44              |
| 2:L:101:THR:OG1  | 2:L:102:PRO:HD3  | 2.17                     | 0.44              |
| 2:L:532:LEU:HA   | 2:L:532:LEU:HD23 | 1.75                     | 0.44              |
| 2:N:227:VAL:CG1  | 2:N:228:GLY:N    | 2.81                     | 0.44              |
| 1:O:34:GLU:C     | 1:O:36:ASP:H     | 2.26                     | 0.44              |
| 1:O:48:THR:HG22  | 1:O:51:ILE:N     | 2.22                     | 0.44              |
| 2:P:245:LEU:HD12 | 2:P:245:LEU:HA   | 1.85                     | 0.44              |
| 2:P:519:TRP:CH2  | 2:P:567:HIS:CG   | 3.05                     | 0.44              |
| 2:P:532:LEU:HA   | 2:P:532:LEU:HD23 | 1.70                     | 0.44              |
| 2:B:328:VAL:CG2  | 2:B:359:GLU:HB2  | 2.45                     | 0.44              |
| 2:D:46:LYS:HB2   | 2:D:46:LYS:HE3   | 1.51                     | 0.44              |
| 2:D:521:GLN:HG3  | 2:D:567:HIS:HD2  | 1.82                     | 0.44              |
| 1:E:44:LEU:HA    | 1:E:45:PRO:HD3   | 1.71                     | 0.44              |
| 2:H:56:THR:CG2   | 2:H:79:LYS:HD2   | 2.46                     | 0.44              |
| 2:H:64:THR:O     | 2:H:67:ARG:N     | 2.47                     | 0.44              |
| 2:H:117:VAL:HG11 | 2:H:119:PHE:CZ   | 2.52                     | 0.44              |
| 2:J:519:TRP:CD1  | 2:J:519:TRP:C    | 2.95                     | 0.44              |
| 2:L:199:PHE:CZ   | 2:L:227:VAL:HG22 | 2.52                     | 0.44              |
| 1:M:154:GLU:OE1  | 2:N:67:ARG:NH1   | 2.51                     | 0.44              |
| 2:N:34:ARG:NH1   | 2:N:48:ASP:OD1   | 2.50                     | 0.44              |
| 1:E:153:ARG:NH2  | 2:F:539:TYR:CE1  | 2.85                     | 0.44              |
| 2:F:366:SER:HB2  | 2:F:367:GLN:OE1  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:71:ARG:HG2   | 2:H:72:PHE:CE1   | 2.52                     | 0.44              |
| 2:H:121:ARG:NH2  | 5:H:1103:PO4:O4  | 2.49                     | 0.44              |
| 2:H:320:LEU:HD12 | 2:H:320:LEU:HA   | 1.71                     | 0.44              |
| 2:H:363:GLY:O    | 2:H:364:LEU:C    | 2.60                     | 0.44              |
| 2:H:409:ARG:CB   | 4:H:1100:7JA:HD1 | 2.48                     | 0.44              |
| 2:H:495:MET:HB2  | 2:H:520:VAL:HG22 | 1.99                     | 0.44              |
| 2:H:506:ALA:HB1  | 2:H:535:MET:HB2  | 1.99                     | 0.44              |
| 2:J:431:LEU:CD1  | 2:J:435:CYS:SG   | 3.05                     | 0.44              |
| 2:L:441:PHE:O    | 2:L:468:MET:HA   | 2.18                     | 0.44              |
| 1:M:130:PRO:O    | 1:M:134:ARG:HG2  | 2.17                     | 0.44              |
| 2:N:101:THR:N    | 2:N:102:PRO:CD   | 2.81                     | 0.44              |
| 2:N:351:ARG:HB3  | 2:N:386:TYR:CG   | 2.52                     | 0.44              |
| 2:P:443:PHE:HE2  | 2:P:445:LEU:HD11 | 1.82                     | 0.44              |
| 1:A:105:ALA:HB2  | 1:A:113:LEU:HD23 | 1.99                     | 0.44              |
| 2:B:172:GLU:HG3  | 2:B:200:TYR:HB3  | 1.98                     | 0.44              |
| 2:B:247:GLU:HA   | 2:B:274:ARG:O    | 2.17                     | 0.44              |
| 2:B:519:TRP:CZ3  | 2:B:567:HIS:CG   | 3.06                     | 0.44              |
| 1:C:46:ASN:HB2   | 1:C:107:TYR:CZ   | 2.53                     | 0.44              |
| 2:D:308:GLU:O    | 2:D:312:THR:HG23 | 2.18                     | 0.44              |
| 1:G:125:ILE:HG23 | 1:G:133:ILE:CD1  | 2.48                     | 0.44              |
| 2:H:75:LEU:HD23  | 2:H:75:LEU:HA    | 1.60                     | 0.44              |
| 2:H:211:ASP:HA   | 2:H:214:THR:HG23 | 1.99                     | 0.44              |
| 2:H:390:ILE:HD13 | 2:H:390:ILE:N    | 2.32                     | 0.44              |
| 2:H:392:ASN:ND2  | 2:H:392:ASN:H    | 2.15                     | 0.44              |
| 2:H:424:LEU:O    | 2:H:427:GLY:N    | 2.50                     | 0.44              |
| 2:J:117:VAL:HG11 | 2:J:119:PHE:CZ   | 2.52                     | 0.44              |
| 2:L:444:TYR:HA   | 2:L:471:GLY:CA   | 2.37                     | 0.44              |
| 2:L:519:TRP:CZ3  | 2:L:567:HIS:CG   | 3.06                     | 0.44              |
| 2:L:578:ARG:H    | 2:L:578:ARG:HG3  | 1.46                     | 0.44              |
| 2:N:315:GLN:HG2  | 2:N:340:TYR:CE1  | 2.53                     | 0.44              |
| 1:O:125:ILE:HG23 | 1:O:133:ILE:CD1  | 2.42                     | 0.44              |
| 2:P:83:LYS:HA    | 2:P:84:PRO:HD3   | 1.88                     | 0.44              |
| 2:P:495:MET:O    | 2:P:520:VAL:HA   | 2.16                     | 0.44              |
| 2:P:519:TRP:CZ3  | 2:P:567:HIS:CG   | 3.05                     | 0.44              |
| 4:P:1100:7JA:H27 | 4:P:1100:7JA:H05 | 1.67                     | 0.44              |
| 3:R:201:LEU:HA   | 3:R:202:PRO:HD3  | 1.83                     | 0.44              |
| 1:E:158:ALA:HA   | 2:F:62:THR:CG2   | 2.48                     | 0.44              |
| 2:F:492:LYS:HG3  | 2:F:517:TYR:CD2  | 2.53                     | 0.44              |
| 2:H:96:TRP:O     | 2:H:578:ARG:NH2  | 2.51                     | 0.44              |
| 2:H:121:ARG:NH2  | 5:H:1103:PO4:P   | 2.91                     | 0.44              |
| 2:H:189:GLN:C    | 2:H:190:HIS:ND1  | 2.75                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:367:GLN:CD   | 2:H:367:GLN:N    | 2.75                     | 0.44              |
| 2:H:424:LEU:N    | 2:H:449:GLY:O    | 2.47                     | 0.44              |
| 2:J:546:PRO:HD3  | 2:J:584:THR:O    | 2.18                     | 0.44              |
| 2:N:155:GLY:O    | 2:N:156:LEU:C    | 2.61                     | 0.44              |
| 3:W:201:LEU:HD23 | 3:W:201:LEU:HA   | 1.68                     | 0.44              |
| 2:P:191:ASN:HD21 | 2:P:194:LEU:N    | 2.09                     | 0.44              |
| 2:P:456:SER:HB2  | 2:P:482:GLU:HB3  | 1.97                     | 0.44              |
| 2:B:22:GLU:OE1   | 2:B:43:ARG:NH2   | 2.51                     | 0.44              |
| 1:C:34:GLU:C     | 1:C:36:ASP:H     | 2.26                     | 0.44              |
| 1:C:134:ARG:NE   | 1:C:141:ASN:HB2  | 2.33                     | 0.44              |
| 1:E:34:GLU:C     | 1:E:36:ASP:H     | 2.26                     | 0.44              |
| 2:F:311:CYS:CB   | 2:F:336:VAL:HG21 | 2.45                     | 0.44              |
| 2:F:429:ARG:HG2  | 2:F:433:ILE:HD11 | 2.00                     | 0.44              |
| 2:J:46:LYS:HE3   | 2:J:46:LYS:HB2   | 1.50                     | 0.44              |
| 2:J:80:LEU:O     | 2:J:122:MET:HE2  | 2.17                     | 0.44              |
| 1:K:63:VAL:C     | 1:K:65:ALA:H     | 2.26                     | 0.44              |
| 2:L:545:ILE:HA   | 2:L:546:PRO:HD3  | 1.74                     | 0.44              |
| 1:M:99:PHE:CD2   | 2:N:16:THR:CA    | 3.00                     | 0.44              |
| 2:N:431:LEU:C    | 2:N:431:LEU:CD1  | 2.88                     | 0.44              |
| 2:N:441:PHE:O    | 2:N:468:MET:HA   | 2.17                     | 0.44              |
| 2:B:80:LEU:HB2   | 2:B:122:MET:HE2  | 1.94                     | 0.44              |
| 1:E:12:ASP:OD2   | 1:E:49:SER:HB2   | 2.17                     | 0.44              |
| 2:F:343:GLN:O    | 2:F:345:LYS:HG2  | 2.18                     | 0.44              |
| 2:F:405:LEU:HA   | 2:F:405:LEU:HD23 | 1.77                     | 0.44              |
| 2:H:255:GLU:HB3  | 2:H:263:TYR:HE1  | 1.83                     | 0.44              |
| 2:L:320:LEU:HD21 | 2:L:323:LEU:HB2  | 1.99                     | 0.44              |
| 1:A:34:GLU:C     | 1:A:36:ASP:H     | 2.26                     | 0.43              |
| 1:A:125:ILE:HG23 | 1:A:133:ILE:CD1  | 2.45                     | 0.43              |
| 2:B:285:MET:N    | 2:B:286:PRO:CD   | 2.81                     | 0.43              |
| 2:B:542:ILE:HD11 | 2:B:588:LEU:CD1  | 2.37                     | 0.43              |
| 1:C:8:LEU:HD23   | 1:C:42:VAL:HG13  | 1.99                     | 0.43              |
| 2:H:124:VAL:CG1  | 2:H:129:LEU:HD13 | 2.48                     | 0.43              |
| 2:H:140:LEU:HD23 | 2:H:163:CYS:SG   | 2.58                     | 0.43              |
| 2:H:206:LYS:HE3  | 2:H:206:LYS:HB2  | 1.81                     | 0.43              |
| 2:H:314:ILE:O    | 2:H:316:LYS:N    | 2.51                     | 0.43              |
| 2:H:431:LEU:C    | 2:H:431:LEU:CD2  | 2.88                     | 0.43              |
| 2:L:103:TRP:O    | 2:L:107:ILE:HG13 | 2.18                     | 0.43              |
| 2:L:138:ASP:OD2  | 2:L:164:ARG:HG3  | 2.18                     | 0.43              |
| 2:L:310:HIS:HE1  | 2:L:325:THR:OG1  | 2.00                     | 0.43              |
| 2:L:328:VAL:CG2  | 2:L:359:GLU:HB2  | 2.43                     | 0.43              |
| 2:L:519:TRP:CH2  | 2:L:567:HIS:CE1  | 3.02                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:37:ALA:O     | 2:N:40:VAL:HG13  | 2.18                     | 0.43              |
| 2:P:451:THR:HB   | 2:P:475:GLU:OE2  | 2.18                     | 0.43              |
| 2:B:83:LYS:O     | 2:B:121:ARG:HD2  | 2.19                     | 0.43              |
| 2:B:546:PRO:HD3  | 2:B:584:THR:O    | 2.18                     | 0.43              |
| 2:D:22:GLU:HG2   | 2:D:47:ILE:HD13  | 2.01                     | 0.43              |
| 2:D:297:LYS:HB2  | 2:D:297:LYS:HE3  | 1.67                     | 0.43              |
| 2:D:348:ARG:HH22 | 4:D:1100:7JA:C   | 2.32                     | 0.43              |
| 2:F:199:PHE:CZ   | 2:F:227:VAL:HG22 | 2.53                     | 0.43              |
| 2:F:432:LEU:CD1  | 2:F:458:ILE:HA   | 2.48                     | 0.43              |
| 2:F:519:TRP:CH2  | 2:F:567:HIS:CG   | 3.06                     | 0.43              |
| 2:H:225:VAL:O    | 2:H:225:VAL:HG23 | 2.17                     | 0.43              |
| 2:H:328:VAL:CG1  | 2:H:359:GLU:HG2  | 2.40                     | 0.43              |
| 1:I:6:ILE:HG22   | 1:I:7:VAL:N      | 2.33                     | 0.43              |
| 1:M:34:GLU:C     | 1:M:36:ASP:H     | 2.26                     | 0.43              |
| 1:M:137:PHE:CD1  | 2:N:17:VAL:HG21  | 2.52                     | 0.43              |
| 1:O:128:LYS:HB2  | 1:O:133:ILE:HD11 | 1.99                     | 0.43              |
| 2:P:235:LEU:O    | 2:P:238:PHE:HB3  | 2.17                     | 0.43              |
| 2:B:477:ASP:OD1  | 2:B:477:ASP:N    | 2.50                     | 0.43              |
| 1:C:13:GLY:HA3   | 1:K:9:LYS:NZ     | 2.32                     | 0.43              |
| 2:D:519:TRP:CZ3  | 2:D:567:HIS:CG   | 3.06                     | 0.43              |
| 2:D:546:PRO:HD3  | 2:D:584:THR:O    | 2.17                     | 0.43              |
| 2:H:351:ARG:HH11 | 2:H:360:ASP:HA   | 1.83                     | 0.43              |
| 2:H:542:ILE:HD13 | 2:H:544:LEU:HD21 | 2.00                     | 0.43              |
| 2:J:490:LEU:HD23 | 2:J:490:LEU:HA   | 1.86                     | 0.43              |
| 2:L:211:ASP:HA   | 2:L:214:THR:CG2  | 2.47                     | 0.43              |
| 1:M:6:ILE:HG22   | 1:M:7:VAL:N      | 2.33                     | 0.43              |
| 1:M:36:ASP:C     | 1:M:38:VAL:H     | 2.26                     | 0.43              |
| 2:N:482:GLU:O    | 2:N:485:ARG:HG2  | 2.18                     | 0.43              |
| 2:N:545:ILE:HG23 | 2:N:546:PRO:HD2  | 2.01                     | 0.43              |
| 2:B:546:PRO:HB2  | 2:B:547:SER:H    | 1.60                     | 0.43              |
| 2:D:398:ILE:CG2  | 2:D:402:LEU:HD11 | 2.43                     | 0.43              |
| 2:F:297:LYS:HE2  | 2:F:322:VAL:CG2  | 2.48                     | 0.43              |
| 2:F:422:LEU:O    | 2:F:424:LEU:HG   | 2.18                     | 0.43              |
| 1:G:142:ASP:OD2  | 1:G:142:ASP:N    | 2.51                     | 0.43              |
| 1:G:151:VAL:O    | 1:G:152:ARG:C    | 2.61                     | 0.43              |
| 2:H:491:GLN:HA   | 2:H:515:LEU:HA   | 1.99                     | 0.43              |
| 2:J:357:GLY:C    | 2:J:358:MET:O    | 2.61                     | 0.43              |
| 3:U:212:PHE:CD2  | 3:U:213:LEU:HD23 | 2.53                     | 0.43              |
| 2:L:114:LEU:HD12 | 2:L:114:LEU:HA   | 1.80                     | 0.43              |
| 2:L:297:LYS:HE2  | 2:L:322:VAL:CG2  | 2.48                     | 0.43              |
| 1:M:8:LEU:HD23   | 1:M:42:VAL:HG13  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:O:108:LEU:HD12 | 1:O:110:ILE:HD11  | 2.00                     | 0.43              |
| 2:P:114:LEU:O    | 2:P:136:ARG:NH1   | 2.49                     | 0.43              |
| 2:P:285:MET:HB3  | 2:P:286:PRO:HD3   | 2.00                     | 0.43              |
| 2:D:78:LEU:HD12  | 2:D:79:LYS:H      | 1.83                     | 0.43              |
| 2:D:503:ARG:NH1  | 2:D:503:ARG:HB3   | 2.34                     | 0.43              |
| 2:F:101:THR:N    | 2:F:102:PRO:CD    | 2.82                     | 0.43              |
| 2:H:328:VAL:CG1  | 2:H:359:GLU:CG    | 2.96                     | 0.43              |
| 2:H:364:LEU:HD13 | 2:H:388:SER:CB    | 2.49                     | 0.43              |
| 4:H:1100:7JA:H12 | 4:H:1100:7JA:H05A | 1.84                     | 0.43              |
| 1:I:42:VAL:O     | 1:I:42:VAL:HG22   | 2.18                     | 0.43              |
| 2:J:503:ARG:NH1  | 2:J:503:ARG:HB3   | 2.34                     | 0.43              |
| 2:L:247:GLU:HA   | 2:L:274:ARG:O     | 2.18                     | 0.43              |
| 2:N:194:LEU:HA   | 2:N:194:LEU:HD12  | 1.73                     | 0.43              |
| 2:N:298:LEU:HA   | 2:N:298:LEU:HD12  | 1.70                     | 0.43              |
| 2:P:80:LEU:O     | 2:P:122:MET:HE2   | 2.18                     | 0.43              |
| 2:B:198:ASN:OD1  | 2:B:198:ASN:C     | 2.61                     | 0.43              |
| 1:C:63:VAL:C     | 1:C:65:ALA:H      | 2.26                     | 0.43              |
| 2:D:521:GLN:HG3  | 2:D:567:HIS:CD2   | 2.53                     | 0.43              |
| 1:E:46:ASN:HB2   | 1:E:107:TYR:CZ    | 2.54                     | 0.43              |
| 1:G:46:ASN:HB2   | 1:G:107:TYR:CZ    | 2.53                     | 0.43              |
| 1:G:63:VAL:C     | 1:G:65:ALA:H      | 2.26                     | 0.43              |
| 1:G:148:GLU:HG2  | 1:G:152:ARG:NH1   | 2.33                     | 0.43              |
| 2:J:398:ILE:CG2  | 2:J:402:LEU:HD11  | 2.43                     | 0.43              |
| 2:J:512:LEU:HA   | 2:J:513:PRO:HD2   | 1.73                     | 0.43              |
| 2:L:85:ARG:NH1   | 5:L:1101:PO4:O3   | 2.51                     | 0.43              |
| 2:L:405:LEU:HD23 | 2:L:405:LEU:HA    | 1.84                     | 0.43              |
| 1:O:158:ALA:HA   | 2:P:62:THR:CG2    | 2.46                     | 0.43              |
| 2:P:315:GLN:HG2  | 2:P:340:TYR:CE1   | 2.54                     | 0.43              |
| 2:P:453:LEU:HD11 | 2:P:457:TYR:OH    | 2.18                     | 0.43              |
| 2:B:404:ASN:HA   | 2:B:437:LYS:HD2   | 2.01                     | 0.43              |
| 2:B:451:THR:HA   | 2:B:475:GLU:HG3   | 2.00                     | 0.43              |
| 2:D:187:LEU:HA   | 2:D:187:LEU:HD23  | 1.85                     | 0.43              |
| 2:D:578:ARG:H    | 2:D:578:ARG:HG3   | 1.48                     | 0.43              |
| 1:E:91:MET:HG2   | 1:E:116:LEU:HD21  | 2.00                     | 0.43              |
| 2:F:409:ARG:HB3  | 4:F:1100:7JA:HG1  | 2.01                     | 0.43              |
| 2:H:96:TRP:HA    | 2:H:582:PRO:CG    | 2.47                     | 0.43              |
| 2:H:207:ILE:HD12 | 2:H:230:PHE:HZ    | 1.84                     | 0.43              |
| 2:H:213:GLU:OE2  | 2:H:237:GLY:HA3   | 2.18                     | 0.43              |
| 2:H:233:LEU:HD11 | 2:H:262:LYS:HD3   | 2.01                     | 0.43              |
| 2:H:385:VAL:HG13 | 2:H:387:VAL:CG2   | 2.48                     | 0.43              |
| 1:I:126:LYS:HZ3  | 2:J:29:THR:H      | 1.67                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:120:ARG:HD2  | 2:J:146:ASP:OD2  | 2.18                     | 0.43              |
| 2:J:280:MET:HE1  | 2:J:288:LEU:HD11 | 2.00                     | 0.43              |
| 2:J:315:GLN:HG2  | 2:J:340:TYR:CE1  | 2.54                     | 0.43              |
| 2:J:411:VAL:HG22 | 2:J:444:TYR:HB3  | 1.99                     | 0.43              |
| 2:J:547:SER:CB   | 2:J:564:HIS:CB   | 2.96                     | 0.43              |
| 2:L:114:LEU:O    | 2:L:136:ARG:NH1  | 2.50                     | 0.43              |
| 2:L:297:LYS:HG3  | 2:L:322:VAL:HB   | 2.01                     | 0.43              |
| 2:L:429:ARG:HG2  | 2:L:433:ILE:HD11 | 2.01                     | 0.43              |
| 2:N:83:LYS:HA    | 2:N:84:PRO:HD3   | 1.88                     | 0.43              |
| 2:P:357:GLY:C    | 2:P:358:MET:O    | 2.61                     | 0.43              |
| 2:P:563:GLU:O    | 2:P:563:GLU:CG   | 2.66                     | 0.43              |
| 1:A:124:MET:O    | 1:A:128:LYS:HE2  | 2.18                     | 0.43              |
| 2:B:85:ARG:NH2   | 4:B:1100:7JA:O14 | 2.45                     | 0.43              |
| 2:D:547:SER:CB   | 2:D:564:HIS:CB   | 2.97                     | 0.43              |
| 2:F:107:ILE:HG12 | 2:F:111:LEU:HD12 | 2.00                     | 0.43              |
| 2:F:112:ARG:HG2  | 2:L:164:ARG:CD   | 2.43                     | 0.43              |
| 2:H:227:VAL:O    | 2:H:250:GLY:HA3  | 2.19                     | 0.43              |
| 2:H:307:THR:O    | 2:H:311:CYS:SG   | 2.77                     | 0.43              |
| 2:J:191:ASN:HD21 | 2:J:194:LEU:N    | 2.12                     | 0.43              |
| 2:J:344:LEU:HD23 | 2:J:380:LEU:HD21 | 2.00                     | 0.43              |
| 2:L:20:VAL:O     | 2:L:24:VAL:HG23  | 2.19                     | 0.43              |
| 2:L:78:LEU:HD12  | 2:L:79:LYS:H     | 1.84                     | 0.43              |
| 2:L:389:ASP:OD2  | 2:L:419:ILE:HG23 | 2.18                     | 0.43              |
| 2:L:419:ILE:HD11 | 2:L:446:ARG:NH2  | 2.29                     | 0.43              |
| 2:N:311:CYS:CB   | 2:N:336:VAL:HG21 | 2.48                     | 0.43              |
| 1:O:114:LEU:C    | 1:O:116:LEU:N    | 2.76                     | 0.43              |
| 1:O:153:ARG:CG   | 1:O:157:TRP:CZ3  | 3.02                     | 0.43              |
| 2:P:52:ARG:HH11  | 2:P:52:ARG:HD3   | 1.70                     | 0.43              |
| 2:P:339:GLN:HA   | 2:P:342:LYS:HE2  | 2.00                     | 0.43              |
| 2:B:65:PRO:HG3   | 2:B:103:TRP:CE2  | 2.54                     | 0.43              |
| 2:F:114:LEU:HD12 | 2:F:114:LEU:HA   | 1.79                     | 0.43              |
| 2:F:211:ASP:HA   | 2:F:214:THR:CG2  | 2.48                     | 0.43              |
| 2:H:100:VAL:HG21 | 2:H:119:PHE:CE1  | 2.53                     | 0.43              |
| 2:H:121:ARG:HH22 | 5:H:1103:PO4:P   | 2.41                     | 0.43              |
| 2:H:137:ALA:C    | 2:H:139:ASP:H    | 2.26                     | 0.43              |
| 2:J:80:LEU:HD12  | 2:J:122:MET:HE1  | 2.00                     | 0.43              |
| 2:J:297:LYS:HG3  | 2:J:322:VAL:HB   | 2.00                     | 0.43              |
| 2:J:492:LYS:HG3  | 2:J:517:TYR:CD2  | 2.54                     | 0.43              |
| 1:K:126:LYS:HZ3  | 2:L:29:THR:H     | 1.67                     | 0.43              |
| 2:N:365:VAL:CG2  | 2:N:387:VAL:HA   | 2.46                     | 0.43              |
| 1:O:135:THR:HG22 | 1:O:136:THR:N    | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:304:LEU:HD11 | 3:X:216:ARG:HG3  | 2.00                     | 0.43              |
| 2:B:143:LEU:CD2  | 2:B:159:ILE:HD13 | 2.47                     | 0.43              |
| 2:B:357:GLY:C    | 2:B:358:MET:O    | 2.61                     | 0.43              |
| 2:B:367:GLN:HG2  | 2:B:391:THR:HB   | 2.01                     | 0.43              |
| 1:C:126:LYS:HZ3  | 2:D:29:THR:H     | 1.65                     | 0.43              |
| 1:C:160:GLU:CG   | 2:D:31:PRO:HB3   | 2.49                     | 0.43              |
| 2:D:328:VAL:CG2  | 2:D:359:GLU:HB2  | 2.44                     | 0.43              |
| 2:D:357:GLY:C    | 2:D:358:MET:O    | 2.61                     | 0.43              |
| 2:H:467:TRP:CZ3  | 2:H:494:GLU:OE1  | 2.72                     | 0.43              |
| 2:H:542:ILE:HG13 | 2:H:588:LEU:HB2  | 1.97                     | 0.43              |
| 1:I:102:ILE:HG12 | 1:I:117:THR:HB   | 2.01                     | 0.43              |
| 2:L:280:MET:HE1  | 2:L:288:LEU:HD11 | 2.01                     | 0.43              |
| 2:L:451:THR:HA   | 2:L:475:GLU:HG3  | 2.00                     | 0.43              |
| 1:M:26:SER:OG    | 1:M:108:LEU:HB3  | 2.19                     | 0.43              |
| 2:N:542:ILE:CD1  | 2:N:588:LEU:HD12 | 2.39                     | 0.43              |
| 2:B:441:PHE:O    | 2:B:468:MET:HA   | 2.19                     | 0.42              |
| 1:C:19:GLU:OE1   | 1:C:19:GLU:N     | 2.49                     | 0.42              |
| 2:D:495:MET:O    | 2:D:520:VAL:HA   | 2.19                     | 0.42              |
| 2:F:245:LEU:HD12 | 2:F:245:LEU:HA   | 1.79                     | 0.42              |
| 1:G:149:GLU:OE1  | 1:G:153:ARG:NE   | 2.52                     | 0.42              |
| 2:H:43:ARG:NH2   | 2:H:47:ILE:HD11  | 2.34                     | 0.42              |
| 2:H:487:CYS:N    | 2:H:488:PRO:CD   | 2.82                     | 0.42              |
| 2:L:418:ARG:C    | 2:L:419:ILE:HD12 | 2.44                     | 0.42              |
| 2:L:432:LEU:CD1  | 2:L:458:ILE:HA   | 2.49                     | 0.42              |
| 2:L:443:PHE:HE2  | 2:L:445:LEU:HD11 | 1.80                     | 0.42              |
| 2:L:468:MET:CE   | 2:L:470:LEU:HD11 | 2.49                     | 0.42              |
| 2:N:161:THR:HG22 | 2:N:186:GLU:HG2  | 2.00                     | 0.42              |
| 2:N:447:GLN:C    | 2:N:449:GLY:H    | 2.27                     | 0.42              |
| 2:P:17:VAL:O     | 2:P:20:VAL:HG12  | 2.19                     | 0.42              |
| 2:P:282:PRO:HA   | 2:P:285:MET:HE2  | 2.00                     | 0.42              |
| 2:P:447:GLN:C    | 2:P:449:GLY:H    | 2.27                     | 0.42              |
| 2:P:545:ILE:HA   | 2:P:546:PRO:HD3  | 1.76                     | 0.42              |
| 1:A:134:ARG:HB2  | 1:A:139:ILE:O    | 2.19                     | 0.42              |
| 2:B:418:ARG:C    | 2:B:419:ILE:HD12 | 2.43                     | 0.42              |
| 3:Q:201:LEU:HA   | 3:Q:202:PRO:HD3  | 1.81                     | 0.42              |
| 1:C:12:ASP:O     | 1:K:40:ASN:HB2   | 2.19                     | 0.42              |
| 2:D:527:MET:O    | 2:D:528:THR:C    | 2.62                     | 0.42              |
| 2:F:139:ASP:CG   | 2:L:165:LYS:HZ1  | 2.27                     | 0.42              |
| 2:F:289:PHE:N    | 2:F:290:PRO:CD   | 2.81                     | 0.42              |
| 2:F:563:GLU:O    | 2:F:563:GLU:CG   | 2.67                     | 0.42              |
| 2:H:94:GLU:CG    | 2:H:95:ASN:N     | 2.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:198:ASN:O    | 2:H:198:ASN:OD1  | 2.38                     | 0.42              |
| 2:H:289:PHE:N    | 2:H:290:PRO:HD2  | 2.34                     | 0.42              |
| 2:H:440:ARG:HB3  | 2:H:467:TRP:CD1  | 2.54                     | 0.42              |
| 2:J:58:ALA:O     | 2:J:81:LYS:HB2   | 2.19                     | 0.42              |
| 2:L:168:THR:HB   | 2:L:196:VAL:CG1  | 2.16                     | 0.42              |
| 2:L:233:LEU:HD23 | 2:L:233:LEU:HA   | 1.88                     | 0.42              |
| 2:N:453:LEU:HD11 | 2:N:457:TYR:OH   | 2.19                     | 0.42              |
| 2:N:564:HIS:HA   | 2:N:565:PRO:HD2  | 1.76                     | 0.42              |
| 2:P:297:LYS:HG3  | 2:P:322:VAL:HB   | 1.99                     | 0.42              |
| 2:B:527:MET:O    | 2:B:528:THR:C    | 2.61                     | 0.42              |
| 2:D:453:LEU:HD11 | 2:D:457:TYR:OH   | 2.19                     | 0.42              |
| 1:E:134:ARG:NH1  | 2:F:40:VAL:HA    | 2.34                     | 0.42              |
| 2:F:32:LYS:HD2   | 2:F:32:LYS:HA    | 1.91                     | 0.42              |
| 2:F:248:PHE:C    | 2:F:248:PHE:CD2  | 2.97                     | 0.42              |
| 2:F:298:LEU:HB2  | 2:F:320:LEU:HD11 | 2.02                     | 0.42              |
| 2:F:527:MET:O    | 2:F:528:THR:C    | 2.63                     | 0.42              |
| 2:H:92:ILE:CG2   | 2:H:93:PRO:O     | 2.68                     | 0.42              |
| 2:H:309:ASP:O    | 2:H:310:HIS:C    | 2.62                     | 0.42              |
| 2:H:537:ARG:HB3  | 2:H:538:PRO:CD   | 2.49                     | 0.42              |
| 2:H:542:ILE:HD12 | 2:H:543:GLU:CA   | 2.49                     | 0.42              |
| 2:J:96:TRP:O     | 2:J:578:ARG:NH2  | 2.45                     | 0.42              |
| 2:J:247:GLU:HA   | 2:J:274:ARG:O    | 2.20                     | 0.42              |
| 2:L:191:ASN:ND2  | 2:L:194:LEU:HB2  | 2.35                     | 0.42              |
| 2:P:37:ALA:O     | 2:P:40:VAL:HG13  | 2.20                     | 0.42              |
| 2:B:298:LEU:HD12 | 2:B:298:LEU:HA   | 1.77                     | 0.42              |
| 1:C:12:ASP:O     | 1:K:40:ASN:HB3   | 2.19                     | 0.42              |
| 1:C:99:PHE:CZ    | 2:D:17:VAL:HG22  | 2.55                     | 0.42              |
| 2:D:101:THR:CG2  | 2:D:128:ASP:OD1  | 2.55                     | 0.42              |
| 2:F:191:ASN:ND2  | 2:F:194:LEU:HB2  | 2.34                     | 0.42              |
| 2:F:578:ARG:H    | 2:F:578:ARG:HG3  | 1.48                     | 0.42              |
| 2:H:21:ILE:C     | 2:H:23:GLN:N     | 2.75                     | 0.42              |
| 2:H:21:ILE:HG23  | 2:H:47:ILE:HD13  | 2.02                     | 0.42              |
| 2:H:476:SER:C    | 2:H:478:GLU:H    | 2.27                     | 0.42              |
| 2:J:194:LEU:HA   | 2:J:194:LEU:HD12 | 1.74                     | 0.42              |
| 2:J:431:LEU:C    | 2:J:431:LEU:CD1  | 2.90                     | 0.42              |
| 1:K:8:LEU:HD23   | 1:K:42:VAL:HG13  | 2.00                     | 0.42              |
| 2:N:335:GLU:O    | 2:N:338:ALA:HB3  | 2.20                     | 0.42              |
| 1:O:82:ASP:O     | 1:O:85:ALA:HB3   | 2.19                     | 0.42              |
| 2:P:386:TYR:HE1  | 4:P:1100:7JA:HG2 | 1.72                     | 0.42              |
| 2:P:451:THR:HA   | 2:P:475:GLU:HG3  | 2.02                     | 0.42              |
| 1:A:160:GLU:HG3  | 2:B:31:PRO:HB3   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:10:SER:OG    | 1:E:11:SER:N     | 2.50                     | 0.42              |
| 2:F:96:TRP:O     | 2:F:578:ARG:NH2  | 2.45                     | 0.42              |
| 2:F:187:LEU:HD23 | 2:F:187:LEU:HA   | 1.83                     | 0.42              |
| 2:F:188:ALA:HA   | 2:F:215:ILE:HG12 | 2.02                     | 0.42              |
| 2:F:431:LEU:CD1  | 2:F:435:CYS:SG   | 3.08                     | 0.42              |
| 2:F:490:LEU:HD23 | 2:F:490:LEU:HA   | 1.89                     | 0.42              |
| 2:H:409:ARG:CB   | 4:H:1100:7JA:H29 | 2.35                     | 0.42              |
| 2:J:101:THR:CG2  | 2:J:128:ASP:OD1  | 2.59                     | 0.42              |
| 2:J:387:VAL:HG22 | 2:J:389:ASP:H    | 1.84                     | 0.42              |
| 2:J:419:ILE:HD11 | 2:J:446:ARG:NH2  | 2.25                     | 0.42              |
| 2:L:447:GLN:C    | 2:L:449:GLY:H    | 2.27                     | 0.42              |
| 1:M:87:ASP:CG    | 1:M:116:LEU:HD22 | 2.44                     | 0.42              |
| 1:M:100:GLU:CG   | 2:N:15:ALA:HB2   | 2.48                     | 0.42              |
| 2:N:297:LYS:HE2  | 2:N:322:VAL:CG2  | 2.49                     | 0.42              |
| 2:P:527:MET:O    | 2:P:528:THR:C    | 2.61                     | 0.42              |
| 3:X:201:LEU:HA   | 3:X:202:PRO:HD3  | 1.83                     | 0.42              |
| 1:A:36:ASP:C     | 1:A:38:VAL:H     | 2.28                     | 0.42              |
| 2:D:343:GLN:O    | 2:D:345:LYS:HG2  | 2.20                     | 0.42              |
| 2:H:345:LYS:NZ   | 2:H:345:LYS:HB3  | 2.35                     | 0.42              |
| 2:J:366:SER:HB2  | 2:J:367:GLN:OE1  | 2.19                     | 0.42              |
| 2:L:85:ARG:HG2   | 2:L:88:MET:HE2   | 2.01                     | 0.42              |
| 2:L:357:GLY:C    | 2:L:358:MET:O    | 2.60                     | 0.42              |
| 2:N:289:PHE:HB2  | 2:N:290:PRO:HD3  | 2.02                     | 0.42              |
| 1:O:44:LEU:HA    | 1:O:45:PRO:HD3   | 1.77                     | 0.42              |
| 2:P:466:ARG:HG2  | 2:P:491:GLN:OE1  | 2.19                     | 0.42              |
| 2:B:22:GLU:HG2   | 2:B:47:ILE:HD13  | 2.00                     | 0.42              |
| 2:B:226:LYS:HA   | 2:B:249:CYS:O    | 2.20                     | 0.42              |
| 2:F:532:LEU:HD23 | 2:F:532:LEU:HA   | 1.70                     | 0.42              |
| 1:G:160:GLU:HB3  | 2:H:31:PRO:HB3   | 2.02                     | 0.42              |
| 2:H:107:ILE:HA   | 2:H:111:LEU:HB2  | 2.02                     | 0.42              |
| 2:H:302:TYR:CD2  | 2:H:302:TYR:N    | 2.83                     | 0.42              |
| 2:H:343:GLN:N    | 2:H:343:GLN:NE2  | 2.67                     | 0.42              |
| 2:H:476:SER:O    | 2:H:477:ASP:C    | 2.57                     | 0.42              |
| 2:J:101:THR:N    | 2:J:102:PRO:CD   | 2.82                     | 0.42              |
| 2:J:231:GLU:O    | 2:J:232:ILE:C    | 2.63                     | 0.42              |
| 2:J:335:GLU:O    | 2:J:338:ALA:HB3  | 2.20                     | 0.42              |
| 2:L:22:GLU:HG2   | 2:L:47:ILE:HD13  | 2.01                     | 0.42              |
| 2:L:201:MET:HE2  | 2:L:201:MET:HB2  | 1.91                     | 0.42              |
| 2:L:235:LEU:O    | 2:L:238:PHE:HB3  | 2.19                     | 0.42              |
| 2:N:235:LEU:O    | 2:N:238:PHE:HB3  | 2.19                     | 0.42              |
| 2:N:285:MET:N    | 2:N:286:PRO:CD   | 2.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:N:1100:7JA:HN  | 4:N:1100:7JA:H10 | 1.85                     | 0.42              |
| 2:P:298:LEU:HD12 | 2:P:298:LEU:HA   | 1.87                     | 0.42              |
| 2:B:280:MET:HE1  | 2:B:288:LEU:HD11 | 2.02                     | 0.42              |
| 2:B:329:ILE:O    | 2:B:333:GLY:HA3  | 2.19                     | 0.42              |
| 2:B:419:ILE:HD12 | 2:B:419:ILE:N    | 2.35                     | 0.42              |
| 2:D:152:THR:HG22 | 2:D:177:SER:HB2  | 2.02                     | 0.42              |
| 2:D:411:VAL:HG22 | 2:D:444:TYR:CB   | 2.49                     | 0.42              |
| 1:E:36:ASP:C     | 1:E:38:VAL:H     | 2.27                     | 0.42              |
| 2:F:114:LEU:O    | 2:F:136:ARG:NH1  | 2.52                     | 0.42              |
| 2:F:285:MET:N    | 2:F:286:PRO:CD   | 2.81                     | 0.42              |
| 1:G:42:VAL:O     | 1:G:42:VAL:HG22  | 2.20                     | 0.42              |
| 2:H:64:THR:C     | 2:H:66:ASP:N     | 2.78                     | 0.42              |
| 2:H:96:TRP:NE1   | 2:H:578:ARG:HH12 | 2.16                     | 0.42              |
| 2:H:172:GLU:O    | 2:H:202:THR:CG2  | 2.68                     | 0.42              |
| 2:H:364:LEU:O    | 2:H:365:VAL:HG13 | 2.20                     | 0.42              |
| 2:H:510:THR:HG22 | 2:H:511:LYS:N    | 2.35                     | 0.42              |
| 1:I:63:VAL:C     | 1:I:65:ALA:H     | 2.27                     | 0.42              |
| 2:J:327:ASN:HD22 | 2:J:327:ASN:C    | 2.27                     | 0.42              |
| 2:J:328:VAL:CG2  | 2:J:359:GLU:HB2  | 2.44                     | 0.42              |
| 1:M:102:ILE:CB   | 2:N:20:VAL:HG21  | 2.50                     | 0.42              |
| 2:N:54:HIS:CD2   | 2:N:77:SER:OG    | 2.71                     | 0.42              |
| 3:X:212:PHE:CD2  | 3:X:213:LEU:HD23 | 2.55                     | 0.42              |
| 1:A:6:ILE:HG22   | 1:A:7:VAL:N      | 2.35                     | 0.42              |
| 2:B:277:LEU:HB2  | 2:B:280:MET:HE3  | 2.01                     | 0.42              |
| 2:B:305:LEU:H    | 2:B:305:LEU:HD22 | 1.85                     | 0.42              |
| 2:B:366:SER:HB2  | 2:B:367:GLN:OE1  | 2.19                     | 0.42              |
| 2:B:431:LEU:C    | 2:B:431:LEU:CD1  | 2.89                     | 0.42              |
| 2:B:545:ILE:HG23 | 2:B:546:PRO:HD2  | 2.01                     | 0.42              |
| 2:D:422:LEU:O    | 2:D:424:LEU:HG   | 2.20                     | 0.42              |
| 2:F:542:ILE:HD11 | 2:F:588:LEU:CD1  | 2.36                     | 0.42              |
| 1:G:95:GLN:O     | 1:G:96:ALA:C     | 2.63                     | 0.42              |
| 2:H:351:ARG:HD2  | 2:H:359:GLU:C    | 2.45                     | 0.42              |
| 1:I:10:SER:OG    | 1:I:11:SER:N     | 2.52                     | 0.42              |
| 1:I:111:LYS:O    | 1:I:115:ASP:HB2  | 2.19                     | 0.42              |
| 2:J:161:THR:HG22 | 2:J:186:GLU:HG2  | 2.02                     | 0.42              |
| 1:K:83:LEU:HD23  | 1:K:83:LEU:HA    | 1.81                     | 0.42              |
| 2:L:367:GLN:HB3  | 2:L:391:THR:HG22 | 2.01                     | 0.42              |
| 2:L:492:LYS:HG3  | 2:L:517:TYR:CD2  | 2.55                     | 0.42              |
| 1:A:93:ILE:CD1   | 1:A:97:THR:HG22  | 2.42                     | 0.42              |
| 2:B:30:ASP:HA    | 2:B:31:PRO:HD3   | 1.90                     | 0.42              |
| 2:B:387:VAL:HG22 | 2:B:389:ASP:H    | 1.84                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:547:SER:CB   | 2:B:564:HIS:CB    | 2.97                     | 0.42              |
| 2:D:226:LYS:HA   | 2:D:249:CYS:O     | 2.19                     | 0.42              |
| 2:F:159:ILE:HD11 | 2:F:169:LEU:HD13  | 2.02                     | 0.42              |
| 2:F:418:ARG:C    | 2:F:419:ILE:HD12  | 2.45                     | 0.42              |
| 2:F:419:ILE:HD11 | 2:F:446:ARG:NH2   | 2.27                     | 0.42              |
| 3:S:212:PHE:CD2  | 3:S:213:LEU:HD23  | 2.55                     | 0.42              |
| 1:I:48:THR:HG22  | 1:I:51:ILE:CB     | 2.50                     | 0.42              |
| 1:I:153:ARG:CG   | 1:I:157:TRP:CZ3   | 3.01                     | 0.42              |
| 2:J:405:LEU:HA   | 2:J:405:LEU:HD23  | 1.74                     | 0.42              |
| 1:M:102:ILE:HB   | 2:N:20:VAL:HG21   | 2.02                     | 0.42              |
| 2:N:63:ALA:HB1   | 2:N:67:ARG:HD2    | 2.02                     | 0.42              |
| 2:N:357:GLY:C    | 2:N:358:MET:O     | 2.63                     | 0.42              |
| 3:W:212:PHE:CD2  | 3:W:213:LEU:HD23  | 2.55                     | 0.42              |
| 2:B:482:GLU:O    | 2:B:485:ARG:HG2   | 2.20                     | 0.41              |
| 2:B:490:LEU:HD23 | 2:B:490:LEU:HA    | 1.85                     | 0.41              |
| 2:D:83:LYS:HA    | 2:D:96:TRP:CZ3    | 2.55                     | 0.41              |
| 2:D:315:GLN:HG2  | 2:D:340:TYR:CE1   | 2.55                     | 0.41              |
| 1:E:8:LEU:HD23   | 1:E:42:VAL:HG13   | 2.02                     | 0.41              |
| 2:H:114:LEU:O    | 2:H:136:ARG:NH1   | 2.53                     | 0.41              |
| 2:H:123:ILE:HD13 | 2:H:123:ILE:HG21  | 1.88                     | 0.41              |
| 2:H:227:VAL:HG22 | 2:H:228:GLY:H     | 1.85                     | 0.41              |
| 2:J:91:LEU:O     | 2:J:567:HIS:HE1   | 2.03                     | 0.41              |
| 2:J:532:LEU:HD23 | 2:J:532:LEU:HA    | 1.75                     | 0.41              |
| 1:K:160:GLU:HG3  | 2:L:31:PRO:HB3    | 2.02                     | 0.41              |
| 2:L:30:ASP:HA    | 2:L:31:PRO:HD3    | 1.93                     | 0.41              |
| 4:L:1100:7JA:OXT | 4:L:1100:7JA:HG2A | 2.11                     | 0.41              |
| 3:V:201:LEU:HA   | 3:V:202:PRO:HD3   | 1.83                     | 0.41              |
| 2:N:80:LEU:O     | 2:N:122:MET:HE2   | 2.20                     | 0.41              |
| 2:N:221:SER:O    | 2:N:223:VAL:HG23  | 2.19                     | 0.41              |
| 2:N:405:LEU:HA   | 2:N:405:LEU:HD23  | 1.80                     | 0.41              |
| 2:P:20:VAL:O     | 2:P:24:VAL:HG23   | 2.20                     | 0.41              |
| 2:P:392:ASN:HD21 | 2:P:424:LEU:HA    | 1.85                     | 0.41              |
| 2:B:18:ASP:CG    | 2:B:43:ARG:HH11   | 2.28                     | 0.41              |
| 2:D:392:ASN:HD21 | 2:D:424:LEU:HA    | 1.85                     | 0.41              |
| 2:D:545:ILE:HG22 | 2:D:546:PRO:N     | 2.35                     | 0.41              |
| 2:F:194:LEU:HD12 | 2:F:194:LEU:HA    | 1.79                     | 0.41              |
| 2:F:348:ARG:HH22 | 4:F:1100:7JA:C    | 2.33                     | 0.41              |
| 2:F:453:LEU:HD11 | 2:F:457:TYR:OH    | 2.20                     | 0.41              |
| 2:H:216:ALA:HB2  | 2:H:238:PHE:HD1   | 1.83                     | 0.41              |
| 2:H:350:GLU:O    | 2:H:350:GLU:HG3   | 2.20                     | 0.41              |
| 2:H:429:ARG:HB2  | 2:H:457:TYR:CD1   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:392:ASN:ND2  | 2:J:424:LEU:HA   | 2.34                     | 0.41              |
| 1:K:82:ASP:O     | 1:K:85:ALA:HB3   | 2.20                     | 0.41              |
| 2:L:75:LEU:HD23  | 2:L:75:LEU:HA    | 1.83                     | 0.41              |
| 1:A:145:PRO:HB2  | 2:D:539:TYR:CE2  | 2.54                     | 0.41              |
| 2:B:153:THR:HG23 | 2:B:178:GLU:HA   | 2.02                     | 0.41              |
| 1:C:128:LYS:HB2  | 1:C:133:ILE:HD11 | 2.03                     | 0.41              |
| 2:D:101:THR:HG22 | 2:D:128:ASP:CG   | 2.41                     | 0.41              |
| 2:D:343:GLN:CD   | 2:D:343:GLN:N    | 2.79                     | 0.41              |
| 1:I:36:ASP:C     | 1:I:38:VAL:H     | 2.28                     | 0.41              |
| 2:J:198:ASN:OD1  | 2:J:198:ASN:C    | 2.63                     | 0.41              |
| 2:J:297:LYS:HE3  | 2:J:297:LYS:HB2  | 1.69                     | 0.41              |
| 2:J:367:GLN:CG   | 2:J:391:THR:HG22 | 2.50                     | 0.41              |
| 2:J:451:THR:HA   | 2:J:475:GLU:HG3  | 2.02                     | 0.41              |
| 1:K:10:SER:HB2   | 1:K:52:LEU:HD23  | 2.02                     | 0.41              |
| 2:L:83:LYS:HA    | 2:L:96:TRP:CZ3   | 2.55                     | 0.41              |
| 2:L:392:ASN:HD21 | 2:L:424:LEU:HA   | 1.85                     | 0.41              |
| 2:N:304:LEU:HD12 | 2:N:304:LEU:HA   | 1.93                     | 0.41              |
| 1:O:10:SER:OG    | 1:O:11:SER:N     | 2.51                     | 0.41              |
| 2:P:201:MET:HE2  | 2:P:201:MET:HB2  | 1.86                     | 0.41              |
| 2:P:221:SER:O    | 2:P:223:VAL:HG23 | 2.20                     | 0.41              |
| 2:P:496:ARG:HA   | 2:P:521:GLN:O    | 2.21                     | 0.41              |
| 2:B:54:HIS:CE1   | 2:B:56:THR:OG1   | 2.65                     | 0.41              |
| 2:B:191:ASN:ND2  | 2:B:194:LEU:HB2  | 2.36                     | 0.41              |
| 1:C:134:ARG:NH1  | 2:D:40:VAL:HA    | 2.35                     | 0.41              |
| 2:D:18:ASP:CG    | 2:D:43:ARG:HH11  | 2.29                     | 0.41              |
| 2:D:22:GLU:HG2   | 2:D:47:ILE:CD1   | 2.50                     | 0.41              |
| 2:D:310:HIS:HE1  | 2:D:325:THR:OG1  | 2.03                     | 0.41              |
| 3:S:201:LEU:HA   | 3:S:202:PRO:HD3  | 1.82                     | 0.41              |
| 1:G:36:ASP:C     | 1:G:38:VAL:H     | 2.27                     | 0.41              |
| 2:H:301:LEU:HA   | 2:H:301:LEU:HD13 | 1.68                     | 0.41              |
| 2:L:422:LEU:O    | 2:L:424:LEU:HG   | 2.21                     | 0.41              |
| 2:L:453:LEU:HD11 | 2:L:457:TYR:OH   | 2.20                     | 0.41              |
| 2:N:32:LYS:HD2   | 2:N:32:LYS:HA    | 1.93                     | 0.41              |
| 1:O:58:TYR:CD2   | 1:O:113:LEU:HD13 | 2.55                     | 0.41              |
| 2:P:398:ILE:CG2  | 2:P:402:LEU:HD11 | 2.48                     | 0.41              |
| 2:P:399:GLY:HA3  | 2:P:431:LEU:HA   | 2.03                     | 0.41              |
| 1:A:83:LEU:C     | 1:A:85:ALA:N     | 2.76                     | 0.41              |
| 1:A:130:PRO:O    | 1:A:134:ARG:HG2  | 2.21                     | 0.41              |
| 2:B:63:ALA:HB1   | 2:B:67:ARG:HD2   | 2.02                     | 0.41              |
| 2:D:542:ILE:C    | 2:D:542:ILE:HD12 | 2.46                     | 0.41              |
| 2:H:152:THR:HB   | 2:H:177:SER:HB2  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:255:GLU:HB3  | 2:H:263:TYR:CE1  | 2.55                     | 0.41              |
| 2:H:314:ILE:HG12 | 2:H:314:ILE:H    | 1.51                     | 0.41              |
| 2:H:314:ILE:C    | 2:H:316:LYS:N    | 2.78                     | 0.41              |
| 2:H:409:ARG:HD2  | 4:H:1100:7JA:H29 | 2.02                     | 0.41              |
| 1:I:154:GLU:OE1  | 2:J:67:ARG:NH1   | 2.53                     | 0.41              |
| 2:J:456:SER:HB2  | 2:J:482:GLU:HB3  | 2.01                     | 0.41              |
| 2:L:305:LEU:H    | 2:L:305:LEU:CD2  | 2.33                     | 0.41              |
| 2:L:411:VAL:HG22 | 2:L:444:TYR:HB3  | 2.02                     | 0.41              |
| 2:N:222:LEU:HA   | 2:N:222:LEU:HD12 | 1.85                     | 0.41              |
| 2:B:80:LEU:HD12  | 2:B:122:MET:HE1  | 2.02                     | 0.41              |
| 2:B:299:ASP:C    | 2:B:301:LEU:H    | 2.27                     | 0.41              |
| 2:D:579:THR:O    | 2:N:206:LYS:NZ   | 2.52                     | 0.41              |
| 1:E:42:VAL:HA    | 1:E:43:PRO:HD3   | 1.84                     | 0.41              |
| 1:E:95:GLN:O     | 1:E:96:ALA:C     | 2.63                     | 0.41              |
| 2:F:198:ASN:OD1  | 2:F:198:ASN:C    | 2.64                     | 0.41              |
| 2:F:280:MET:HE1  | 2:F:288:LEU:HD11 | 2.01                     | 0.41              |
| 2:H:83:LYS:HA    | 2:H:84:PRO:HD3   | 1.88                     | 0.41              |
| 2:H:347:LEU:HD11 | 2:H:349:ILE:CG1  | 2.48                     | 0.41              |
| 2:H:492:LYS:HZ1  | 2:H:516:ARG:NH1  | 2.18                     | 0.41              |
| 2:H:495:MET:HE2  | 2:H:520:VAL:HG22 | 2.03                     | 0.41              |
| 1:K:58:TYR:CD2   | 1:K:113:LEU:HD13 | 2.55                     | 0.41              |
| 1:M:134:ARG:NH2  | 1:M:141:ASN:HD22 | 2.18                     | 0.41              |
| 1:O:44:LEU:HD12  | 1:O:44:LEU:O     | 2.20                     | 0.41              |
| 2:P:107:ILE:HG12 | 2:P:111:LEU:HD12 | 2.02                     | 0.41              |
| 2:P:436:LYS:HE2  | 2:P:436:LYS:HB3  | 1.89                     | 0.41              |
| 2:P:546:PRO:HB2  | 2:P:547:SER:H    | 1.63                     | 0.41              |
| 1:C:58:TYR:CE1   | 1:C:62:HIS:CE1   | 3.09                     | 0.41              |
| 1:C:115:ASP:HA   | 2:D:27:TYR:HE2   | 1.85                     | 0.41              |
| 2:D:304:LEU:HD12 | 2:D:304:LEU:HA   | 1.91                     | 0.41              |
| 2:D:443:PHE:HE2  | 2:D:445:LEU:HD11 | 1.80                     | 0.41              |
| 1:E:51:ILE:HD13  | 1:E:51:ILE:HA    | 1.91                     | 0.41              |
| 1:E:134:ARG:NE   | 1:E:141:ASN:HB2  | 2.34                     | 0.41              |
| 1:E:158:ALA:CB   | 2:F:62:THR:HG23  | 2.51                     | 0.41              |
| 2:F:91:LEU:O     | 2:F:567:HIS:HE1  | 2.03                     | 0.41              |
| 2:F:120:ARG:NH2  | 5:F:1103:PO4:O4  | 2.53                     | 0.41              |
| 1:G:83:LEU:C     | 1:G:85:ALA:N     | 2.75                     | 0.41              |
| 2:H:182:LYS:O    | 2:H:183:TRP:C    | 2.64                     | 0.41              |
| 2:H:442:ALA:HB1  | 4:H:1100:7JA:H28 | 2.02                     | 0.41              |
| 2:H:538:PRO:C    | 2:H:540:TRP:H    | 2.28                     | 0.41              |
| 2:H:587:VAL:HG12 | 2:H:589:LYS:HD3  | 2.02                     | 0.41              |
| 2:J:209:PRO:HD3  | 2:J:230:PHE:CE2  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:386:TYR:HE1  | 4:J:1100:7JA:HG2 | 1.73                     | 0.41              |
| 4:J:1100:7JA:H05 | 4:J:1100:7JA:H27 | 1.65                     | 0.41              |
| 2:N:280:MET:HE1  | 2:N:288:LEU:HD11 | 2.03                     | 0.41              |
| 2:N:289:PHE:N    | 2:N:290:PRO:CD   | 2.82                     | 0.41              |
| 2:B:45:PHE:CD2   | 2:B:45:PHE:C     | 2.98                     | 0.41              |
| 2:B:91:LEU:O     | 2:B:567:HIS:HE1  | 2.04                     | 0.41              |
| 2:B:405:LEU:HD23 | 2:B:405:LEU:HA   | 1.80                     | 0.41              |
| 2:D:120:ARG:NH2  | 5:D:1103:PO4:O4  | 2.54                     | 0.41              |
| 2:D:314:ILE:HG12 | 2:D:314:ILE:H    | 1.65                     | 0.41              |
| 2:D:327:ASN:HD22 | 2:D:328:VAL:N    | 2.19                     | 0.41              |
| 2:D:418:ARG:C    | 2:D:419:ILE:HD12 | 2.46                     | 0.41              |
| 2:F:447:GLN:C    | 2:F:449:GLY:H    | 2.28                     | 0.41              |
| 2:H:277:LEU:HB2  | 2:H:280:MET:HE3  | 2.02                     | 0.41              |
| 1:I:13:GLY:O     | 1:I:14:GLU:HG2   | 2.20                     | 0.41              |
| 2:J:564:HIS:HA   | 2:J:565:PRO:HD2  | 1.80                     | 0.41              |
| 2:L:120:ARG:HD2  | 2:L:146:ASP:OD2  | 2.20                     | 0.41              |
| 2:L:456:SER:HB2  | 2:L:482:GLU:HB3  | 2.01                     | 0.41              |
| 2:L:466:ARG:HG2  | 2:L:491:GLN:OE1  | 2.21                     | 0.41              |
| 3:V:212:PHE:CD2  | 3:V:213:LEU:HD23 | 2.56                     | 0.41              |
| 2:N:120:ARG:HD2  | 2:N:146:ASP:OD2  | 2.20                     | 0.41              |
| 1:O:134:ARG:NE   | 1:O:141:ASN:HB2  | 2.36                     | 0.41              |
| 1:A:19:GLU:OE1   | 1:A:19:GLU:N     | 2.52                     | 0.41              |
| 1:A:98:LEU:HD21  | 1:A:120:THR:CG2  | 2.48                     | 0.41              |
| 1:A:114:LEU:C    | 1:A:116:LEU:N    | 2.78                     | 0.41              |
| 2:B:55:VAL:CG2   | 2:B:75:LEU:HD21  | 2.46                     | 0.41              |
| 2:B:453:LEU:HD11 | 2:B:457:TYR:OH   | 2.21                     | 0.41              |
| 3:Q:201:LEU:HA   | 3:Q:201:LEU:HD23 | 1.74                     | 0.41              |
| 1:C:44:LEU:HA    | 1:C:45:PRO:HD3   | 1.76                     | 0.41              |
| 2:D:83:LYS:O     | 2:D:121:ARG:HD2  | 2.21                     | 0.41              |
| 2:D:389:ASP:OD2  | 2:D:419:ILE:HG23 | 2.21                     | 0.41              |
| 2:D:519:TRP:CD1  | 2:D:519:TRP:C    | 2.95                     | 0.41              |
| 2:D:532:LEU:HD23 | 2:D:532:LEU:HA   | 1.74                     | 0.41              |
| 2:D:533:MET:HE1  | 2:D:588:LEU:HB3  | 2.02                     | 0.41              |
| 1:E:28:THR:O     | 1:E:32:MET:HE2   | 2.21                     | 0.41              |
| 2:F:298:LEU:HA   | 2:F:298:LEU:HD12 | 1.73                     | 0.41              |
| 2:F:347:LEU:HD21 | 2:F:349:ILE:HD11 | 2.02                     | 0.41              |
| 2:F:451:THR:HA   | 2:F:475:GLU:HG3  | 2.03                     | 0.41              |
| 2:H:123:ILE:C    | 2:H:124:VAL:HG23 | 2.45                     | 0.41              |
| 2:H:300:LEU:HD23 | 2:H:300:LEU:HA   | 1.89                     | 0.41              |
| 2:H:431:LEU:CD2  | 2:H:432:LEU:HD23 | 2.48                     | 0.41              |
| 2:H:543:GLU:O    | 2:H:544:LEU:HD23 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:137:PHE:CD1  | 2:J:17:VAL:HG21   | 2.55                     | 0.41              |
| 2:J:55:VAL:HG12  | 2:J:56:THR:N      | 2.36                     | 0.41              |
| 2:J:57:MET:CE    | 2:J:62:THR:HG22   | 2.50                     | 0.41              |
| 2:J:157:LEU:O    | 2:J:161:THR:HG23  | 2.20                     | 0.41              |
| 2:J:211:ASP:HA   | 2:J:214:THR:CG2   | 2.47                     | 0.41              |
| 2:J:298:LEU:HB2  | 2:J:320:LEU:HD11  | 2.01                     | 0.41              |
| 2:J:367:GLN:HG2  | 2:J:391:THR:HB    | 2.03                     | 0.41              |
| 2:L:335:GLU:O    | 2:L:338:ALA:HB3   | 2.21                     | 0.41              |
| 2:L:419:ILE:HD12 | 2:L:419:ILE:N     | 2.36                     | 0.41              |
| 1:M:128:LYS:HB2  | 1:M:133:ILE:HD13  | 2.02                     | 0.41              |
| 2:N:386:TYR:OH   | 4:N:1100:7JA:HG2B | 2.21                     | 0.41              |
| 1:O:101:LEU:HD23 | 1:O:101:LEU:HA    | 1.92                     | 0.41              |
| 2:P:327:ASN:HD22 | 2:P:327:ASN:C     | 2.29                     | 0.41              |
| 2:P:367:GLN:HG2  | 2:P:391:THR:HB    | 2.03                     | 0.41              |
| 1:A:26:SER:OG    | 1:A:108:LEU:HB3   | 2.20                     | 0.41              |
| 2:D:366:SER:HB2  | 2:D:367:GLN:OE1   | 2.21                     | 0.41              |
| 1:E:105:ALA:CB   | 1:E:114:LEU:HD13  | 2.50                     | 0.41              |
| 2:F:297:LYS:HB2  | 2:F:297:LYS:HE3   | 1.67                     | 0.41              |
| 2:F:519:TRP:CZ3  | 2:F:567:HIS:CG    | 3.09                     | 0.41              |
| 2:F:545:ILE:HA   | 2:F:546:PRO:HD3   | 1.79                     | 0.41              |
| 1:G:44:LEU:O     | 1:G:44:LEU:HD12   | 2.20                     | 0.41              |
| 2:H:266:LEU:HD22 | 2:H:266:LEU:HA    | 1.89                     | 0.41              |
| 2:H:425:ASP:OD1  | 2:H:454:GLY:HA3   | 2.21                     | 0.41              |
| 2:H:511:LYS:HB2  | 2:H:511:LYS:HE2   | 1.91                     | 0.41              |
| 2:L:152:THR:HG22 | 2:L:177:SER:HB2   | 2.04                     | 0.41              |
| 2:L:211:ASP:O    | 2:L:215:ILE:HG13  | 2.21                     | 0.41              |
| 1:M:99:PHE:CB    | 2:N:15:ALA:HB1    | 2.51                     | 0.41              |
| 2:N:422:LEU:O    | 2:N:424:LEU:HG    | 2.21                     | 0.41              |
| 2:N:465:VAL:CG1  | 2:N:468:MET:HG3   | 2.50                     | 0.41              |
| 4:N:1100:7JA:CG2 | 4:N:1100:7JA:OXT  | 2.66                     | 0.41              |
| 2:P:55:VAL:CG2   | 2:P:75:LEU:HD21   | 2.42                     | 0.41              |
| 2:B:190:HIS:HE1  | 2:P:110:ASN:HA    | 1.86                     | 0.40              |
| 2:B:191:ASN:HD21 | 2:B:194:LEU:N     | 2.11                     | 0.40              |
| 2:B:546:PRO:O    | 2:B:547:SER:CB    | 2.70                     | 0.40              |
| 2:D:119:PHE:CD1  | 2:D:122:MET:HE3   | 2.55                     | 0.40              |
| 2:D:311:CYS:CB   | 2:D:336:VAL:HG21  | 2.47                     | 0.40              |
| 2:D:367:GLN:HG2  | 2:D:391:THR:HB    | 2.03                     | 0.40              |
| 2:D:495:MET:HB2  | 2:D:495:MET:HE3   | 1.72                     | 0.40              |
| 2:D:564:HIS:HA   | 2:D:565:PRO:HD2   | 1.77                     | 0.40              |
| 2:F:289:PHE:HB2  | 2:F:290:PRO:HD3   | 2.03                     | 0.40              |
| 2:H:220:ARG:NE   | 2:H:220:ARG:HA    | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:424:LEU:O    | 2:H:425:ASP:C    | 2.64                     | 0.40              |
| 2:H:490:LEU:HD23 | 2:H:490:LEU:HA   | 1.85                     | 0.40              |
| 2:H:533:MET:C    | 2:H:535:MET:N    | 2.76                     | 0.40              |
| 2:H:544:LEU:HD23 | 2:H:544:LEU:N    | 2.36                     | 0.40              |
| 1:I:114:LEU:C    | 1:I:116:LEU:H    | 2.29                     | 0.40              |
| 1:I:114:LEU:C    | 1:I:116:LEU:N    | 2.77                     | 0.40              |
| 3:U:201:LEU:HD23 | 3:U:201:LEU:HA   | 1.69                     | 0.40              |
| 1:K:144:THR:OG1  | 1:K:147:GLU:HG3  | 2.22                     | 0.40              |
| 2:L:55:VAL:CG2   | 2:L:75:LEU:HD21  | 2.49                     | 0.40              |
| 2:L:153:THR:HG23 | 2:L:178:GLU:HA   | 2.02                     | 0.40              |
| 2:N:545:ILE:HA   | 2:N:546:PRO:HD3  | 1.78                     | 0.40              |
| 1:O:83:LEU:HD23  | 1:O:83:LEU:HA    | 1.80                     | 0.40              |
| 2:P:247:GLU:HA   | 2:P:274:ARG:O    | 2.20                     | 0.40              |
| 2:B:532:LEU:HA   | 2:B:532:LEU:HD23 | 1.76                     | 0.40              |
| 1:C:36:ASP:C     | 1:C:38:VAL:H     | 2.30                     | 0.40              |
| 2:D:153:THR:HG23 | 2:D:178:GLU:HA   | 2.03                     | 0.40              |
| 2:F:80:LEU:HB2   | 2:F:122:MET:HE2  | 2.00                     | 0.40              |
| 2:H:279:TYR:O    | 2:H:304:LEU:HB2  | 2.22                     | 0.40              |
| 2:H:432:LEU:HD11 | 2:H:458:ILE:CD1  | 2.52                     | 0.40              |
| 2:J:75:LEU:HA    | 2:J:75:LEU:HD23  | 1.87                     | 0.40              |
| 2:J:348:ARG:HH22 | 4:J:1100:7JA:C   | 2.35                     | 0.40              |
| 2:L:191:ASN:ND2  | 2:L:194:LEU:H    | 2.16                     | 0.40              |
| 2:L:301:LEU:CD2  | 2:L:324:GLU:HB3  | 2.52                     | 0.40              |
| 2:N:107:ILE:HA   | 2:N:111:LEU:HB2  | 2.03                     | 0.40              |
| 2:P:58:ALA:O     | 2:P:81:LYS:HB2   | 2.22                     | 0.40              |
| 2:P:65:PRO:HG3   | 2:P:103:TRP:CE2  | 2.56                     | 0.40              |
| 1:A:101:LEU:HD23 | 1:A:101:LEU:HA   | 1.92                     | 0.40              |
| 2:B:512:LEU:HA   | 2:B:513:PRO:HD2  | 1.78                     | 0.40              |
| 1:C:158:ALA:CB   | 2:D:62:THR:HG23  | 2.51                     | 0.40              |
| 2:D:75:LEU:HD23  | 2:D:75:LEU:HA    | 1.85                     | 0.40              |
| 2:D:227:VAL:HG13 | 2:D:228:GLY:H    | 1.83                     | 0.40              |
| 2:D:267:VAL:HG23 | 2:D:267:VAL:O    | 2.22                     | 0.40              |
| 2:D:298:LEU:HA   | 2:D:298:LEU:HD12 | 1.72                     | 0.40              |
| 2:D:563:GLU:O    | 2:D:563:GLU:CG   | 2.65                     | 0.40              |
| 1:E:83:LEU:HA    | 1:E:83:LEU:HD23  | 1.82                     | 0.40              |
| 2:H:59:LEU:O     | 2:H:62:THR:HB    | 2.21                     | 0.40              |
| 2:H:348:ARG:HG3  | 2:H:384:ALA:HB3  | 2.03                     | 0.40              |
| 2:H:454:GLY:O    | 2:H:457:TYR:HB2  | 2.20                     | 0.40              |
| 2:H:487:CYS:HB3  | 2:H:490:LEU:HB2  | 2.03                     | 0.40              |
| 1:I:125:ILE:HG23 | 1:I:133:ILE:CD1  | 2.42                     | 0.40              |
| 2:J:233:LEU:HA   | 2:J:233:LEU:HD23 | 1.82                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:J:343:GLN:CD   | 2:J:343:GLN:N     | 2.79                     | 0.40              |
| 1:K:36:ASP:C     | 1:K:38:VAL:H      | 2.28                     | 0.40              |
| 2:P:429:ARG:HG2  | 2:P:433:ILE:HD11  | 2.04                     | 0.40              |
| 2:P:564:HIS:HA   | 2:P:565:PRO:HD2   | 1.78                     | 0.40              |
| 2:B:268:PHE:O    | 2:B:269:PRO:C     | 2.62                     | 0.40              |
| 2:B:311:CYS:O    | 2:B:315:GLN:HB2   | 2.21                     | 0.40              |
| 2:B:327:ASN:HD22 | 2:B:327:ASN:C     | 2.29                     | 0.40              |
| 1:C:102:ILE:HG21 | 2:D:20:VAL:HG22   | 2.02                     | 0.40              |
| 1:C:134:ARG:NH2  | 1:C:141:ASN:HD22  | 2.19                     | 0.40              |
| 2:D:65:PRO:HA    | 2:D:103:TRP:CZ3   | 2.57                     | 0.40              |
| 2:D:399:GLY:O    | 2:D:434:GLY:HA3   | 2.22                     | 0.40              |
| 2:F:285:MET:HB3  | 2:F:286:PRO:HD3   | 2.03                     | 0.40              |
| 2:H:21:ILE:C     | 2:H:23:GLN:H      | 2.28                     | 0.40              |
| 2:H:37:ALA:C     | 2:H:39:LEU:H      | 2.29                     | 0.40              |
| 2:H:482:GLU:HG2  | 2:H:482:GLU:H     | 1.60                     | 0.40              |
| 2:H:492:LYS:NZ   | 2:H:516:ARG:HD2   | 2.35                     | 0.40              |
| 2:H:501:SER:HB2  | 2:H:503:ARG:CZ    | 2.51                     | 0.40              |
| 2:H:517:TYR:CE1  | 2:H:569:LEU:HD11  | 2.57                     | 0.40              |
| 3:U:201:LEU:HA   | 3:U:202:PRO:HD3   | 1.80                     | 0.40              |
| 2:L:275:LEU:HD11 | 2:L:288:LEU:CD2   | 2.51                     | 0.40              |
| 2:L:547:SER:CB   | 2:L:564:HIS:CB    | 2.99                     | 0.40              |
| 2:B:201:MET:HE2  | 2:B:201:MET:HB2   | 1.91                     | 0.40              |
| 2:B:211:ASP:O    | 2:B:215:ILE:HG13  | 2.21                     | 0.40              |
| 2:B:436:LYS:HE2  | 2:B:436:LYS:HB3   | 1.96                     | 0.40              |
| 2:B:456:SER:HB2  | 2:B:482:GLU:HB3   | 2.03                     | 0.40              |
| 2:B:468:MET:HE1  | 2:B:483:PHE:HE1   | 1.86                     | 0.40              |
| 1:C:83:LEU:HA    | 1:C:83:LEU:HD23   | 1.84                     | 0.40              |
| 2:D:201:MET:HB2  | 2:D:201:MET:HE2   | 1.86                     | 0.40              |
| 1:E:30:ALA:C     | 1:E:32:MET:N      | 2.79                     | 0.40              |
| 2:F:85:ARG:NH1   | 5:F:1101:PO4:O3   | 2.54                     | 0.40              |
| 2:F:329:ILE:HG23 | 2:F:330:GLY:N     | 2.36                     | 0.40              |
| 2:F:441:PHE:O    | 2:F:468:MET:HA    | 2.22                     | 0.40              |
| 2:F:469:LEU:HA   | 2:F:494:GLU:O     | 2.22                     | 0.40              |
| 1:G:6:ILE:HG22   | 1:G:7:VAL:N       | 2.36                     | 0.40              |
| 2:H:306:GLU:OE2  | 2:H:307:THR:HG22  | 2.21                     | 0.40              |
| 4:H:1100:7JA:C04 | 4:H:1100:7JA:H12A | 2.50                     | 0.40              |
| 2:J:114:LEU:HD12 | 2:J:114:LEU:HA    | 1.72                     | 0.40              |
| 1:K:134:ARG:NH1  | 2:L:40:VAL:HA     | 2.35                     | 0.40              |
| 2:L:96:TRP:O     | 2:L:578:ARG:NH2   | 2.44                     | 0.40              |
| 2:L:119:PHE:CD1  | 2:L:122:MET:HE3   | 2.56                     | 0.40              |
| 2:L:245:LEU:HD12 | 2:L:245:LEU:HA    | 1.80                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:L:298:LEU:HD12 | 2:L:298:LEU:HA  | 1.82                     | 0.40              |
| 2:L:367:GLN:NE2  | 2:L:389:ASP:OD1 | 2.53                     | 0.40              |
| 2:L:588:LEU:HD23 | 2:L:588:LEU:HA  | 1.97                     | 0.40              |
| 2:N:366:SER:HB2  | 2:N:367:GLN:OE1 | 2.21                     | 0.40              |
| 2:P:120:ARG:NH2  | 5:P:1103:PO4:O4 | 2.52                     | 0.40              |
| 2:P:329:ILE:HG23 | 2:P:330:GLY:N   | 2.35                     | 0.40              |
| 2:P:404:ASN:HA   | 2:P:437:LYS:HD2 | 2.02                     | 0.40              |
| 2:P:422:LEU:O    | 2:P:424:LEU:HG  | 2.21                     | 0.40              |
| 2:P:578:ARG:H    | 2:P:578:ARG:HG3 | 1.41                     | 0.40              |

All (2) 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) |
|-----------------|-----------------------|--------------------------|-------------------|
| 2:D:429:ARG:NH2 | 1:I:61:ARG:NH1[2_555] | 2.06                     | 0.14              |
| 2:D:429:ARG:NH1 | 1:I:86:TRP:CE3[2_555] | 2.14                     | 0.06              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | G     | 140/160 (88%) | 114 (81%) | 22 (16%) | 4 (3%)   | 3           | 21  |
| 1   | I     | 140/160 (88%) | 117 (84%) | 20 (14%) | 3 (2%)   | 5           | 27  |
| 1   | K     | 140/160 (88%) | 117 (84%) | 19 (14%) | 4 (3%)   | 3           | 21  |
| 1   | M     | 109/160 (68%) | 88 (81%)  | 18 (16%) | 3 (3%)   | 4           | 22  |
| 1   | O     | 140/160 (88%) | 112 (80%) | 25 (18%) | 3 (2%)   | 5           | 27  |
| 2   | B     | 36/592 (6%)   | 30 (83%)  | 6 (17%)  | 0        | 100         | 100 |
| 2   | D     | 24/592 (4%)   | 21 (88%)  | 3 (12%)  | 0        | 100         | 100 |
| 2   | H     | 558/592 (94%) | 430 (77%) | 98 (18%) | 30 (5%)  | 1           | 10  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 2   | J     | 564/592 (95%)   | 504 (89%)  | 52 (9%)   | 8 (1%)   | 9           | 36  |
| 2   | L     | 536/592 (90%)   | 480 (90%)  | 50 (9%)   | 6 (1%)   | 11          | 41  |
| 2   | N     | 65/592 (11%)    | 57 (88%)   | 7 (11%)   | 1 (2%)   | 8           | 35  |
| 2   | P     | 564/592 (95%)   | 500 (89%)  | 56 (10%)  | 8 (1%)   | 9           | 36  |
| 3   | S     | 4/21 (19%)      | 4 (100%)   | 0         | 0        | 100         | 100 |
| 3   | U     | 16/21 (76%)     | 15 (94%)   | 1 (6%)    | 0        | 100         | 100 |
| 3   | V     | 14/21 (67%)     | 13 (93%)   | 1 (7%)    | 0        | 100         | 100 |
| 3   | W     | 16/21 (76%)     | 15 (94%)   | 1 (6%)    | 0        | 100         | 100 |
| 3   | X     | 16/21 (76%)     | 15 (94%)   | 1 (6%)    | 0        | 100         | 100 |
| All | All   | 3082/5049 (61%) | 2632 (85%) | 380 (12%) | 70 (2%)  | 5           | 26  |

All (70) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 36  | ASP  |
| 2   | H     | 97  | GLY  |
| 2   | H     | 200 | TYR  |
| 2   | H     | 269 | PRO  |
| 2   | H     | 270 | ARG  |
| 2   | H     | 278 | SER  |
| 2   | H     | 364 | LEU  |
| 2   | H     | 365 | VAL  |
| 1   | I     | 36  | ASP  |
| 2   | J     | 420 | THR  |
| 2   | J     | 546 | PRO  |
| 1   | K     | 36  | ASP  |
| 2   | L     | 420 | THR  |
| 2   | L     | 546 | PRO  |
| 1   | M     | 36  | ASP  |
| 1   | O     | 36  | ASP  |
| 2   | P     | 420 | THR  |
| 2   | P     | 546 | PRO  |
| 1   | G     | 13  | GLY  |
| 1   | G     | 128 | LYS  |
| 2   | H     | 20  | VAL  |
| 2   | H     | 228 | GLY  |
| 2   | H     | 254 | ASN  |
| 2   | H     | 279 | TYR  |
| 2   | H     | 287 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 357 | GLY  |
| 1   | I     | 13  | GLY  |
| 2   | J     | 358 | MET  |
| 2   | J     | 590 | GLU  |
| 1   | K     | 13  | GLY  |
| 2   | L     | 20  | VAL  |
| 1   | M     | 13  | GLY  |
| 1   | M     | 126 | LYS  |
| 2   | N     | 590 | GLU  |
| 1   | O     | 13  | GLY  |
| 2   | P     | 20  | VAL  |
| 2   | P     | 590 | GLU  |
| 2   | H     | 102 | PRO  |
| 2   | H     | 524 | ARG  |
| 2   | H     | 525 | ALA  |
| 2   | H     | 534 | GLN  |
| 2   | H     | 538 | PRO  |
| 1   | I     | 126 | LYS  |
| 2   | J     | 20  | VAL  |
| 2   | J     | 547 | SER  |
| 1   | K     | 126 | LYS  |
| 2   | L     | 358 | MET  |
| 2   | L     | 547 | SER  |
| 2   | P     | 358 | MET  |
| 2   | P     | 547 | SER  |
| 2   | H     | 206 | LYS  |
| 2   | H     | 273 | CYS  |
| 2   | H     | 315 | GLN  |
| 2   | H     | 330 | GLY  |
| 2   | H     | 359 | GLU  |
| 2   | H     | 575 | ALA  |
| 2   | J     | 422 | LEU  |
| 1   | K     | 92  | LYS  |
| 1   | O     | 126 | LYS  |
| 1   | G     | 138 | ASN  |
| 2   | H     | 188 | ALA  |
| 2   | H     | 260 | PRO  |
| 2   | H     | 482 | GLU  |
| 2   | H     | 546 | PRO  |
| 2   | L     | 422 | LEU  |
| 2   | P     | 422 | LEU  |
| 2   | H     | 290 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 471 | GLY  |
| 2   | P     | 471 | GLY  |
| 2   | H     | 314 | ILE  |

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

40 ligands are 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 |
| 5   | PO4  | F     | 1101 | -    | 4,4,4        | 4.38 | 4 (100%) | 6,6,6       | 1.69 | 2 (33%)  |
| 5   | PO4  | B     | 1104 | -    | 4,4,4        | 4.43 | 4 (100%) | 6,6,6       | 1.03 | 0        |
| 4   | 7JA  | L     | 1100 | -    | 23,23,23     | 2.04 | 5 (21%)  | 25,30,30    | 1.88 | 5 (20%)  |
| 5   | PO4  | J     | 1104 | -    | 4,4,4        | 4.34 | 4 (100%) | 6,6,6       | 0.80 | 0        |
| 4   | 7JA  | P     | 1100 | -    | 23,23,23     | 2.03 | 5 (21%)  | 25,30,30    | 2.06 | 6 (24%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | 7JA  | N     | 1100 | -    | 23,23,23     | 2.18 | 6 (26%)  | 25,30,30    | 2.04 | 6 (24%)  |
| 5   | PO4  | J     | 1101 | -    | 4,4,4        | 4.27 | 4 (100%) | 6,6,6       | 0.95 | 0        |
| 5   | PO4  | L     | 1104 | -    | 4,4,4        | 4.33 | 4 (100%) | 6,6,6       | 0.81 | 0        |
| 4   | 7JA  | H     | 1100 | -    | 23,23,23     | 1.62 | 5 (21%)  | 25,30,30    | 2.02 | 8 (32%)  |
| 5   | PO4  | P     | 1102 | -    | 4,4,4        | 4.47 | 4 (100%) | 6,6,6       | 0.49 | 0        |
| 5   | PO4  | B     | 1101 | -    | 4,4,4        | 4.42 | 4 (100%) | 6,6,6       | 0.70 | 0        |
| 5   | PO4  | D     | 1104 | -    | 4,4,4        | 4.33 | 3 (75%)  | 6,6,6       | 1.13 | 0        |
| 5   | PO4  | B     | 1102 | -    | 4,4,4        | 4.33 | 4 (100%) | 6,6,6       | 0.69 | 0        |
| 4   | 7JA  | F     | 1100 | -    | 23,23,23     | 2.10 | 5 (21%)  | 25,30,30    | 2.12 | 5 (20%)  |
| 5   | PO4  | P     | 1104 | -    | 4,4,4        | 4.40 | 4 (100%) | 6,6,6       | 1.05 | 0        |
| 5   | PO4  | N     | 1102 | -    | 4,4,4        | 4.55 | 4 (100%) | 6,6,6       | 0.75 | 0        |
| 5   | PO4  | H     | 1101 | -    | 4,4,4        | 4.54 | 4 (100%) | 6,6,6       | 1.05 | 1 (16%)  |
| 5   | PO4  | F     | 1102 | -    | 4,4,4        | 4.58 | 4 (100%) | 6,6,6       | 0.38 | 0        |
| 5   | PO4  | N     | 1103 | -    | 4,4,4        | 4.31 | 4 (100%) | 6,6,6       | 1.16 | 0        |
| 5   | PO4  | F     | 1103 | -    | 4,4,4        | 4.20 | 4 (100%) | 6,6,6       | 0.73 | 0        |
| 5   | PO4  | H     | 1104 | -    | 4,4,4        | 4.41 | 4 (100%) | 6,6,6       | 1.91 | 1 (16%)  |
| 4   | 7JA  | B     | 1100 | -    | 23,23,23     | 1.66 | 4 (17%)  | 25,30,30    | 2.11 | 6 (24%)  |
| 5   | PO4  | F     | 1104 | -    | 4,4,4        | 4.31 | 4 (100%) | 6,6,6       | 1.32 | 0        |
| 5   | PO4  | P     | 1103 | -    | 4,4,4        | 4.44 | 4 (100%) | 6,6,6       | 0.96 | 0        |
| 5   | PO4  | B     | 1103 | -    | 4,4,4        | 4.12 | 4 (100%) | 6,6,6       | 0.74 | 0        |
| 4   | 7JA  | D     | 1100 | -    | 23,23,23     | 2.11 | 5 (21%)  | 25,30,30    | 2.02 | 5 (20%)  |
| 5   | PO4  | D     | 1102 | -    | 4,4,4        | 4.32 | 4 (100%) | 6,6,6       | 0.28 | 0        |
| 5   | PO4  | D     | 1103 | -    | 4,4,4        | 4.23 | 4 (100%) | 6,6,6       | 0.91 | 0        |
| 5   | PO4  | J     | 1103 | -    | 4,4,4        | 4.37 | 4 (100%) | 6,6,6       | 0.78 | 0        |
| 5   | PO4  | L     | 1101 | -    | 4,4,4        | 4.18 | 4 (100%) | 6,6,6       | 0.81 | 0        |
| 5   | PO4  | L     | 1103 | -    | 4,4,4        | 4.44 | 4 (100%) | 6,6,6       | 0.64 | 0        |
| 5   | PO4  | L     | 1102 | -    | 4,4,4        | 4.45 | 4 (100%) | 6,6,6       | 0.32 | 0        |
| 5   | PO4  | D     | 1101 | -    | 4,4,4        | 4.22 | 4 (100%) | 6,6,6       | 0.89 | 0        |
| 5   | PO4  | H     | 1103 | -    | 4,4,4        | 4.37 | 4 (100%) | 6,6,6       | 0.68 | 0        |
| 5   | PO4  | J     | 1102 | -    | 4,4,4        | 4.55 | 4 (100%) | 6,6,6       | 0.43 | 0        |
| 5   | PO4  | H     | 1102 | -    | 4,4,4        | 4.55 | 4 (100%) | 6,6,6       | 0.65 | 0        |
| 5   | PO4  | P     | 1101 | -    | 4,4,4        | 4.44 | 4 (100%) | 6,6,6       | 0.72 | 0        |
| 5   | PO4  | N     | 1104 | -    | 4,4,4        | 4.53 | 4 (100%) | 6,6,6       | 1.00 | 0        |
| 5   | PO4  | N     | 1101 | -    | 4,4,4        | 4.27 | 4 (100%) | 6,6,6       | 1.17 | 0        |
| 4   | 7JA  | J     | 1100 | -    | 23,23,23     | 2.11 | 6 (26%)  | 25,30,30    | 2.08 | 6 (24%)  |



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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 4   | 7JA  | B     | 1100 | -    | -       | 6/23/36/36  | 0/1/1/1 |
| 4   | 7JA  | F     | 1100 | -    | -       | 7/23/36/36  | 0/1/1/1 |
| 4   | 7JA  | L     | 1100 | -    | -       | 7/23/36/36  | 0/1/1/1 |
| 4   | 7JA  | D     | 1100 | -    | -       | 8/23/36/36  | 0/1/1/1 |
| 4   | 7JA  | P     | 1100 | -    | -       | 7/23/36/36  | 0/1/1/1 |
| 4   | 7JA  | J     | 1100 | -    | -       | 5/23/36/36  | 0/1/1/1 |
| 4   | 7JA  | N     | 1100 | -    | -       | 7/23/36/36  | 0/1/1/1 |
| 4   | 7JA  | H     | 1100 | -    | -       | 12/23/36/36 | 0/1/1/1 |

All (168) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 5   | F     | 1102 | PO4  | P-O1  | 7.07 | 1.67        | 1.50     |
| 5   | P     | 1103 | PO4  | P-O1  | 7.00 | 1.66        | 1.50     |
| 5   | J     | 1104 | PO4  | P-O1  | 6.97 | 1.66        | 1.50     |
| 4   | N     | 1100 | 7JA  | O-C   | 6.96 | 1.42        | 1.22     |
| 5   | P     | 1104 | PO4  | P-O1  | 6.92 | 1.66        | 1.50     |
| 5   | H     | 1102 | PO4  | P-O1  | 6.85 | 1.66        | 1.50     |
| 5   | N     | 1102 | PO4  | P-O1  | 6.79 | 1.66        | 1.50     |
| 5   | J     | 1102 | PO4  | P-O1  | 6.78 | 1.66        | 1.50     |
| 5   | N     | 1104 | PO4  | P-O1  | 6.72 | 1.66        | 1.50     |
| 5   | L     | 1103 | PO4  | P-O1  | 6.70 | 1.66        | 1.50     |
| 5   | D     | 1104 | PO4  | P-O1  | 6.62 | 1.65        | 1.50     |
| 5   | J     | 1103 | PO4  | P-O1  | 6.60 | 1.65        | 1.50     |
| 5   | P     | 1101 | PO4  | P-O1  | 6.60 | 1.65        | 1.50     |
| 5   | B     | 1104 | PO4  | P-O1  | 6.54 | 1.65        | 1.50     |
| 5   | D     | 1102 | PO4  | P-O1  | 6.49 | 1.65        | 1.50     |
| 5   | L     | 1102 | PO4  | P-O1  | 6.49 | 1.65        | 1.50     |
| 5   | P     | 1102 | PO4  | P-O1  | 6.47 | 1.65        | 1.50     |
| 4   | J     | 1100 | 7JA  | O-C   | 6.46 | 1.41        | 1.22     |
| 5   | B     | 1102 | PO4  | P-O1  | 6.46 | 1.65        | 1.50     |
| 5   | B     | 1101 | PO4  | P-O1  | 6.46 | 1.65        | 1.50     |
| 5   | N     | 1103 | PO4  | P-O1  | 6.45 | 1.65        | 1.50     |
| 4   | D     | 1100 | 7JA  | O-C   | 6.42 | 1.41        | 1.22     |
| 5   | L     | 1104 | PO4  | P-O1  | 6.39 | 1.65        | 1.50     |
| 5   | F     | 1103 | PO4  | P-O1  | 6.37 | 1.65        | 1.50     |
| 5   | F     | 1104 | PO4  | P-O1  | 6.33 | 1.65        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 5   | H     | 1104 | PO4  | P-O1  | 6.31 | 1.65        | 1.50     |
| 5   | F     | 1101 | PO4  | P-O1  | 6.31 | 1.65        | 1.50     |
| 5   | H     | 1103 | PO4  | P-O1  | 6.29 | 1.65        | 1.50     |
| 5   | H     | 1101 | PO4  | P-O1  | 6.24 | 1.65        | 1.50     |
| 5   | D     | 1103 | PO4  | P-O1  | 6.22 | 1.65        | 1.50     |
| 4   | F     | 1100 | 7JA  | O-C   | 6.22 | 1.40        | 1.22     |
| 5   | J     | 1101 | PO4  | P-O1  | 6.19 | 1.65        | 1.50     |
| 4   | L     | 1100 | 7JA  | O-C   | 6.19 | 1.40        | 1.22     |
| 5   | L     | 1101 | PO4  | P-O1  | 6.12 | 1.64        | 1.50     |
| 5   | N     | 1101 | PO4  | P-O1  | 6.05 | 1.64        | 1.50     |
| 5   | B     | 1103 | PO4  | P-O1  | 6.05 | 1.64        | 1.50     |
| 5   | D     | 1101 | PO4  | P-O1  | 5.97 | 1.64        | 1.50     |
| 4   | P     | 1100 | 7JA  | O-C   | 5.95 | 1.39        | 1.22     |
| 4   | B     | 1100 | 7JA  | C13-N | 5.35 | 1.45        | 1.34     |
| 4   | J     | 1100 | 7JA  | C13-N | 5.16 | 1.45        | 1.34     |
| 4   | F     | 1100 | 7JA  | C13-N | 5.16 | 1.45        | 1.34     |
| 4   | P     | 1100 | 7JA  | C13-N | 5.13 | 1.44        | 1.34     |
| 4   | L     | 1100 | 7JA  | C13-N | 4.89 | 1.44        | 1.34     |
| 4   | D     | 1100 | 7JA  | C13-N | 4.65 | 1.43        | 1.34     |
| 4   | N     | 1100 | 7JA  | C13-N | 4.59 | 1.43        | 1.34     |
| 4   | H     | 1100 | 7JA  | C13-N | 4.58 | 1.43        | 1.34     |
| 5   | H     | 1101 | PO4  | P-O4  | 4.39 | 1.67        | 1.54     |
| 5   | N     | 1101 | PO4  | P-O3  | 4.35 | 1.67        | 1.54     |
| 5   | H     | 1104 | PO4  | P-O3  | 4.28 | 1.67        | 1.54     |
| 5   | L     | 1103 | PO4  | P-O3  | 4.25 | 1.67        | 1.54     |
| 5   | N     | 1102 | PO4  | P-O4  | 4.17 | 1.66        | 1.54     |
| 5   | N     | 1104 | PO4  | P-O4  | 4.13 | 1.66        | 1.54     |
| 5   | F     | 1104 | PO4  | P-O3  | 4.08 | 1.66        | 1.54     |
| 5   | B     | 1101 | PO4  | P-O3  | 4.04 | 1.66        | 1.54     |
| 5   | H     | 1102 | PO4  | P-O4  | 4.01 | 1.66        | 1.54     |
| 5   | J     | 1102 | PO4  | P-O3  | 4.00 | 1.66        | 1.54     |
| 5   | P     | 1102 | PO4  | P-O3  | 4.00 | 1.66        | 1.54     |
| 5   | N     | 1104 | PO4  | P-O3  | 3.99 | 1.66        | 1.54     |
| 5   | P     | 1101 | PO4  | P-O4  | 3.96 | 1.66        | 1.54     |
| 5   | D     | 1102 | PO4  | P-O4  | 3.95 | 1.66        | 1.54     |
| 5   | P     | 1102 | PO4  | P-O4  | 3.94 | 1.66        | 1.54     |
| 5   | H     | 1101 | PO4  | P-O3  | 3.92 | 1.66        | 1.54     |
| 5   | L     | 1102 | PO4  | P-O3  | 3.91 | 1.66        | 1.54     |
| 5   | B     | 1104 | PO4  | P-O4  | 3.91 | 1.66        | 1.54     |
| 5   | J     | 1101 | PO4  | P-O3  | 3.90 | 1.66        | 1.54     |
| 5   | B     | 1104 | PO4  | P-O3  | 3.88 | 1.65        | 1.54     |
| 5   | L     | 1104 | PO4  | P-O4  | 3.87 | 1.65        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5   | H     | 1103 | PO4  | P-O4  | 3.86  | 1.65        | 1.54     |
| 5   | N     | 1102 | PO4  | P-O3  | 3.85  | 1.65        | 1.54     |
| 5   | N     | 1103 | PO4  | P-O4  | 3.83  | 1.65        | 1.54     |
| 5   | B     | 1102 | PO4  | P-O4  | 3.83  | 1.65        | 1.54     |
| 5   | H     | 1103 | PO4  | P-O3  | 3.79  | 1.65        | 1.54     |
| 5   | J     | 1101 | PO4  | P-O4  | 3.78  | 1.65        | 1.54     |
| 5   | H     | 1102 | PO4  | P-O3  | 3.78  | 1.65        | 1.54     |
| 5   | H     | 1104 | PO4  | P-O4  | 3.78  | 1.65        | 1.54     |
| 5   | F     | 1102 | PO4  | P-O4  | 3.77  | 1.65        | 1.54     |
| 5   | D     | 1104 | PO4  | P-O3  | 3.77  | 1.65        | 1.54     |
| 5   | F     | 1101 | PO4  | P-O3  | 3.76  | 1.65        | 1.54     |
| 5   | L     | 1104 | PO4  | P-O3  | 3.76  | 1.65        | 1.54     |
| 5   | J     | 1103 | PO4  | P-O4  | 3.75  | 1.65        | 1.54     |
| 5   | L     | 1102 | PO4  | P-O4  | 3.74  | 1.65        | 1.54     |
| 5   | D     | 1103 | PO4  | P-O3  | 3.72  | 1.65        | 1.54     |
| 5   | J     | 1102 | PO4  | P-O4  | 3.71  | 1.65        | 1.54     |
| 5   | L     | 1101 | PO4  | P-O3  | 3.71  | 1.65        | 1.54     |
| 5   | P     | 1101 | PO4  | P-O3  | 3.71  | 1.65        | 1.54     |
| 5   | D     | 1101 | PO4  | P-O4  | 3.70  | 1.65        | 1.54     |
| 5   | D     | 1101 | PO4  | P-O3  | 3.69  | 1.65        | 1.54     |
| 5   | P     | 1104 | PO4  | P-O4  | 3.66  | 1.65        | 1.54     |
| 5   | D     | 1104 | PO4  | P-O4  | 3.64  | 1.65        | 1.54     |
| 5   | P     | 1103 | PO4  | P-O4  | 3.61  | 1.65        | 1.54     |
| 5   | N     | 1101 | PO4  | P-O4  | 3.60  | 1.65        | 1.54     |
| 4   | D     | 1100 | 7JA  | OXT-C | -3.56 | 1.19        | 1.30     |
| 5   | P     | 1103 | PO4  | P-O3  | 3.55  | 1.65        | 1.54     |
| 4   | L     | 1100 | 7JA  | OXT-C | -3.49 | 1.19        | 1.30     |
| 5   | F     | 1103 | PO4  | P-O3  | 3.47  | 1.64        | 1.54     |
| 5   | B     | 1103 | PO4  | P-O3  | 3.46  | 1.64        | 1.54     |
| 4   | H     | 1100 | 7JA  | OXT-C | 3.45  | 1.41        | 1.30     |
| 5   | P     | 1104 | PO4  | P-O3  | 3.43  | 1.64        | 1.54     |
| 5   | N     | 1103 | PO4  | P-O3  | 3.42  | 1.64        | 1.54     |
| 5   | F     | 1101 | PO4  | P-O2  | -3.41 | 1.44        | 1.54     |
| 5   | J     | 1103 | PO4  | P-O3  | 3.38  | 1.64        | 1.54     |
| 4   | J     | 1100 | 7JA  | OXT-C | -3.34 | 1.20        | 1.30     |
| 5   | F     | 1101 | PO4  | P-O4  | 3.33  | 1.64        | 1.54     |
| 5   | F     | 1102 | PO4  | P-O3  | 3.32  | 1.64        | 1.54     |
| 5   | F     | 1104 | PO4  | P-O4  | 3.31  | 1.64        | 1.54     |
| 5   | J     | 1104 | PO4  | P-O4  | 3.30  | 1.64        | 1.54     |
| 4   | F     | 1100 | 7JA  | OXT-C | -3.30 | 1.20        | 1.30     |
| 5   | B     | 1101 | PO4  | P-O2  | -3.29 | 1.45        | 1.54     |
| 5   | B     | 1103 | PO4  | P-O4  | 3.29  | 1.64        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | L     | 1101 | PO4  | P-O4    | 3.25  | 1.64        | 1.54     |
| 4   | P     | 1100 | 7JA  | OXT-C   | -3.25 | 1.20        | 1.30     |
| 5   | F     | 1103 | PO4  | P-O4    | 3.20  | 1.64        | 1.54     |
| 5   | D     | 1102 | PO4  | P-O3    | 3.19  | 1.63        | 1.54     |
| 5   | J     | 1104 | PO4  | P-O3    | 3.18  | 1.63        | 1.54     |
| 5   | B     | 1102 | PO4  | P-O3    | 3.17  | 1.63        | 1.54     |
| 5   | D     | 1103 | PO4  | P-O4    | 3.09  | 1.63        | 1.54     |
| 5   | D     | 1103 | PO4  | P-O2    | -3.09 | 1.45        | 1.54     |
| 5   | B     | 1101 | PO4  | P-O4    | 3.05  | 1.63        | 1.54     |
| 4   | N     | 1100 | 7JA  | OXT-C   | -3.05 | 1.20        | 1.30     |
| 5   | L     | 1103 | PO4  | P-O4    | 3.04  | 1.63        | 1.54     |
| 4   | B     | 1100 | 7JA  | OXT-C   | 3.00  | 1.40        | 1.30     |
| 5   | F     | 1102 | PO4  | P-O2    | -2.97 | 1.46        | 1.54     |
| 5   | H     | 1101 | PO4  | P-O2    | -2.96 | 1.46        | 1.54     |
| 4   | F     | 1100 | 7JA  | O14-C13 | -2.95 | 1.17        | 1.23     |
| 5   | B     | 1103 | PO4  | P-O2    | -2.92 | 1.46        | 1.54     |
| 5   | B     | 1102 | PO4  | P-O2    | -2.91 | 1.46        | 1.54     |
| 5   | D     | 1101 | PO4  | P-O2    | -2.91 | 1.46        | 1.54     |
| 4   | N     | 1100 | 7JA  | CA-C    | 2.89  | 1.57        | 1.52     |
| 4   | D     | 1100 | 7JA  | O14-C13 | -2.88 | 1.17        | 1.23     |
| 4   | B     | 1100 | 7JA  | O08-C07 | -2.88 | 1.17        | 1.21     |
| 5   | L     | 1101 | PO4  | P-O2    | -2.84 | 1.46        | 1.54     |
| 5   | L     | 1102 | PO4  | P-O2    | -2.84 | 1.46        | 1.54     |
| 5   | F     | 1103 | PO4  | P-O2    | -2.78 | 1.46        | 1.54     |
| 4   | N     | 1100 | 7JA  | C09-C07 | 2.76  | 1.55        | 1.51     |
| 5   | H     | 1103 | PO4  | P-O2    | -2.73 | 1.46        | 1.54     |
| 5   | J     | 1103 | PO4  | P-O2    | -2.69 | 1.46        | 1.54     |
| 4   | H     | 1100 | 7JA  | C09-C07 | 2.66  | 1.55        | 1.51     |
| 4   | B     | 1100 | 7JA  | O14-C13 | -2.64 | 1.18        | 1.23     |
| 4   | H     | 1100 | 7JA  | O14-C13 | -2.62 | 1.18        | 1.23     |
| 5   | J     | 1102 | PO4  | P-O2    | -2.61 | 1.47        | 1.54     |
| 5   | F     | 1104 | PO4  | P-O2    | -2.59 | 1.47        | 1.54     |
| 5   | P     | 1102 | PO4  | P-O2    | -2.58 | 1.47        | 1.54     |
| 5   | L     | 1103 | PO4  | P-O2    | -2.56 | 1.47        | 1.54     |
| 5   | D     | 1102 | PO4  | P-O2    | -2.56 | 1.47        | 1.54     |
| 4   | F     | 1100 | 7JA  | O08-C07 | -2.56 | 1.17        | 1.21     |
| 4   | N     | 1100 | 7JA  | O14-C13 | -2.55 | 1.18        | 1.23     |
| 4   | P     | 1100 | 7JA  | C09-C07 | 2.52  | 1.55        | 1.51     |
| 5   | N     | 1103 | PO4  | P-O2    | -2.51 | 1.47        | 1.54     |
| 5   | J     | 1104 | PO4  | P-O2    | -2.43 | 1.47        | 1.54     |
| 4   | L     | 1100 | 7JA  | O14-C13 | -2.42 | 1.18        | 1.23     |
| 5   | P     | 1101 | PO4  | P-O2    | -2.41 | 1.47        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | J     | 1100 | 7JA  | O14-C13 | -2.39 | 1.18        | 1.23     |
| 5   | H     | 1102 | PO4  | P-O2    | -2.36 | 1.47        | 1.54     |
| 4   | J     | 1100 | 7JA  | O08-C07 | -2.35 | 1.17        | 1.21     |
| 5   | B     | 1104 | PO4  | P-O2    | -2.33 | 1.47        | 1.54     |
| 5   | H     | 1104 | PO4  | P-O2    | -2.33 | 1.47        | 1.54     |
| 5   | L     | 1104 | PO4  | P-O2    | -2.26 | 1.48        | 1.54     |
| 4   | D     | 1100 | 7JA  | O08-C07 | -2.25 | 1.18        | 1.21     |
| 4   | P     | 1100 | 7JA  | O14-C13 | -2.23 | 1.18        | 1.23     |
| 5   | J     | 1101 | PO4  | P-O2    | -2.23 | 1.48        | 1.54     |
| 4   | J     | 1100 | 7JA  | CA-C    | 2.11  | 1.55        | 1.52     |
| 5   | N     | 1101 | PO4  | P-O2    | -2.11 | 1.48        | 1.54     |
| 4   | L     | 1100 | 7JA  | C09-C07 | 2.10  | 1.54        | 1.51     |
| 5   | N     | 1102 | PO4  | P-O2    | -2.08 | 1.48        | 1.54     |
| 5   | P     | 1104 | PO4  | P-O2    | -2.08 | 1.48        | 1.54     |
| 5   | P     | 1103 | PO4  | P-O2    | -2.07 | 1.48        | 1.54     |
| 4   | H     | 1100 | 7JA  | O08-C07 | -2.05 | 1.18        | 1.21     |
| 5   | N     | 1104 | PO4  | P-O2    | -2.01 | 1.48        | 1.54     |

All (51) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | N     | 1100 | 7JA  | CB-CA-N     | -6.37 | 98.25       | 111.35   |
| 4   | J     | 1100 | 7JA  | CB-CA-N     | -5.79 | 99.44       | 111.35   |
| 4   | D     | 1100 | 7JA  | CB-CA-N     | -5.78 | 99.46       | 111.35   |
| 4   | B     | 1100 | 7JA  | CB-CA-N     | -5.76 | 99.51       | 111.35   |
| 4   | F     | 1100 | 7JA  | CB-CA-N     | -5.59 | 99.86       | 111.35   |
| 4   | P     | 1100 | 7JA  | C11-C12-C13 | 5.45  | 121.07      | 112.99   |
| 4   | J     | 1100 | 7JA  | C11-C12-C13 | 5.44  | 121.05      | 112.99   |
| 4   | F     | 1100 | 7JA  | C11-C12-C13 | 5.33  | 120.88      | 112.99   |
| 4   | P     | 1100 | 7JA  | CB-CA-N     | -5.28 | 100.48      | 111.35   |
| 4   | B     | 1100 | 7JA  | C11-C12-C13 | 5.14  | 120.61      | 112.99   |
| 4   | D     | 1100 | 7JA  | C11-C12-C13 | 5.13  | 120.59      | 112.99   |
| 4   | L     | 1100 | 7JA  | CB-CA-N     | -5.12 | 100.81      | 111.35   |
| 4   | H     | 1100 | 7JA  | C11-C12-C13 | 5.11  | 120.56      | 112.99   |
| 4   | L     | 1100 | 7JA  | C11-C12-C13 | 5.07  | 120.50      | 112.99   |
| 4   | N     | 1100 | 7JA  | C11-C12-C13 | 5.04  | 120.46      | 112.99   |
| 4   | F     | 1100 | 7JA  | O14-C13-C12 | -3.93 | 115.80      | 121.54   |
| 4   | H     | 1100 | 7JA  | CB-CA-N     | -3.89 | 103.36      | 111.35   |
| 5   | H     | 1104 | PO4  | O3-P-O2     | 3.75  | 119.59      | 107.91   |
| 4   | B     | 1100 | 7JA  | O14-C13-C12 | -3.57 | 116.31      | 121.54   |
| 4   | H     | 1100 | 7JA  | O14-C13-N   | -3.13 | 117.66      | 122.95   |
| 4   | H     | 1100 | 7JA  | C10-C11-C06 | 3.00  | 107.58      | 103.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | N     | 1100 | 7JA  | C10-C11-C12 | -2.92 | 107.98      | 113.41   |
| 4   | B     | 1100 | 7JA  | C10-C09-C07 | -2.92 | 102.50      | 105.39   |
| 4   | H     | 1100 | 7JA  | CG1-CB-CA   | -2.90 | 103.89      | 111.17   |
| 4   | H     | 1100 | 7JA  | C-CA-N      | 2.80  | 116.33      | 110.17   |
| 4   | P     | 1100 | 7JA  | OXT-C-CA    | 2.73  | 123.64      | 114.15   |
| 4   | P     | 1100 | 7JA  | C10-C11-C12 | -2.69 | 108.40      | 113.41   |
| 4   | D     | 1100 | 7JA  | CG2-CB-CA   | -2.68 | 104.60      | 110.98   |
| 4   | D     | 1100 | 7JA  | O14-C13-C12 | -2.61 | 117.72      | 121.54   |
| 4   | P     | 1100 | 7JA  | O14-C13-C12 | -2.59 | 117.75      | 121.54   |
| 4   | J     | 1100 | 7JA  | OXT-C-O     | -2.56 | 118.26      | 124.08   |
| 5   | F     | 1101 | PO4  | O3-P-O2     | 2.40  | 115.39      | 107.91   |
| 4   | B     | 1100 | 7JA  | C10-C11-C12 | -2.40 | 108.94      | 113.41   |
| 4   | J     | 1100 | 7JA  | O14-C13-C12 | -2.39 | 118.04      | 121.54   |
| 4   | P     | 1100 | 7JA  | OXT-C-O     | -2.39 | 118.66      | 124.08   |
| 4   | D     | 1100 | 7JA  | OXT-C-O     | -2.31 | 118.83      | 124.08   |
| 5   | H     | 1101 | PO4  | O4-P-O3     | 2.29  | 115.05      | 107.91   |
| 4   | F     | 1100 | 7JA  | OXT-C-O     | -2.28 | 118.92      | 124.08   |
| 4   | B     | 1100 | 7JA  | OXT-C-O     | -2.28 | 118.92      | 124.08   |
| 4   | F     | 1100 | 7JA  | OXT-C-CA    | 2.27  | 122.02      | 114.15   |
| 4   | L     | 1100 | 7JA  | OXT-C-O     | -2.25 | 118.97      | 124.08   |
| 4   | J     | 1100 | 7JA  | C10-C11-C12 | -2.23 | 109.25      | 113.41   |
| 4   | J     | 1100 | 7JA  | CG2-CB-CA   | -2.16 | 105.84      | 110.98   |
| 4   | N     | 1100 | 7JA  | O14-C13-C12 | -2.15 | 118.39      | 121.54   |
| 5   | F     | 1101 | PO4  | O4-P-O3     | 2.15  | 114.60      | 107.91   |
| 4   | L     | 1100 | 7JA  | CB-CA-C     | -2.13 | 105.84      | 111.64   |
| 4   | N     | 1100 | 7JA  | OXT-C-O     | -2.07 | 119.39      | 124.08   |
| 4   | N     | 1100 | 7JA  | CG2-CB-CA   | -2.04 | 106.12      | 110.98   |
| 4   | L     | 1100 | 7JA  | OXT-C-CA    | 2.03  | 121.19      | 114.15   |
| 4   | H     | 1100 | 7JA  | O08-C07-C09 | 2.03  | 128.43      | 125.52   |
| 4   | H     | 1100 | 7JA  | O08-C07-C06 | -2.03 | 123.00      | 125.60   |

There are no chirality outliers.

All (59) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | B     | 1100 | 7JA  | C11-C12-C13-N   |
| 4   | B     | 1100 | 7JA  | C11-C12-C13-O14 |
| 4   | D     | 1100 | 7JA  | C11-C12-C13-N   |
| 4   | D     | 1100 | 7JA  | C11-C12-C13-O14 |
| 4   | F     | 1100 | 7JA  | C11-C12-C13-N   |
| 4   | F     | 1100 | 7JA  | C11-C12-C13-O14 |
| 4   | H     | 1100 | 7JA  | C-CA-CB-CG1     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | H     | 1100 | 7JA  | N-CA-CB-CG2     |
| 4   | H     | 1100 | 7JA  | C11-C12-C13-O14 |
| 4   | J     | 1100 | 7JA  | C11-C12-C13-N   |
| 4   | J     | 1100 | 7JA  | C11-C12-C13-O14 |
| 4   | L     | 1100 | 7JA  | C11-C12-C13-N   |
| 4   | L     | 1100 | 7JA  | C11-C12-C13-O14 |
| 4   | N     | 1100 | 7JA  | C11-C12-C13-N   |
| 4   | N     | 1100 | 7JA  | C11-C12-C13-O14 |
| 4   | P     | 1100 | 7JA  | C-CA-N-C13      |
| 4   | P     | 1100 | 7JA  | C11-C12-C13-N   |
| 4   | P     | 1100 | 7JA  | C11-C12-C13-O14 |
| 4   | B     | 1100 | 7JA  | C-CA-N-C13      |
| 4   | D     | 1100 | 7JA  | C-CA-N-C13      |
| 4   | F     | 1100 | 7JA  | C-CA-N-C13      |
| 4   | J     | 1100 | 7JA  | C-CA-N-C13      |
| 4   | L     | 1100 | 7JA  | C-CA-N-C13      |
| 4   | N     | 1100 | 7JA  | C-CA-N-C13      |
| 4   | H     | 1100 | 7JA  | CA-CB-CG1-CD1   |
| 4   | H     | 1100 | 7JA  | C11-C12-C13-N   |
| 4   | H     | 1100 | 7JA  | N-CA-CB-CG1     |
| 4   | H     | 1100 | 7JA  | CG2-CB-CG1-CD1  |
| 4   | H     | 1100 | 7JA  | C01-C02-C03-C04 |
| 4   | L     | 1100 | 7JA  | C04-C05-C06-C11 |
| 4   | H     | 1100 | 7JA  | C04-C05-C06-C07 |
| 4   | H     | 1100 | 7JA  | C-CA-CB-CG2     |
| 4   | P     | 1100 | 7JA  | N-CA-CB-CG2     |
| 4   | F     | 1100 | 7JA  | C-CA-CB-CG2     |
| 4   | P     | 1100 | 7JA  | C-CA-CB-CG2     |
| 4   | D     | 1100 | 7JA  | C04-C05-C06-C11 |
| 4   | F     | 1100 | 7JA  | C04-C05-C06-C11 |
| 4   | H     | 1100 | 7JA  | C04-C05-C06-C11 |
| 4   | J     | 1100 | 7JA  | C04-C05-C06-C11 |
| 4   | P     | 1100 | 7JA  | C04-C05-C06-C11 |
| 4   | B     | 1100 | 7JA  | C01-C02-C03-C04 |
| 4   | N     | 1100 | 7JA  | C01-C02-C03-C04 |
| 4   | P     | 1100 | 7JA  | C01-C02-C03-C04 |
| 4   | B     | 1100 | 7JA  | C-CA-CB-CG1     |
| 4   | B     | 1100 | 7JA  | C-CA-CB-CG2     |
| 4   | D     | 1100 | 7JA  | C-CA-CB-CG1     |
| 4   | D     | 1100 | 7JA  | C-CA-CB-CG2     |
| 4   | J     | 1100 | 7JA  | C-CA-CB-CG2     |
| 4   | L     | 1100 | 7JA  | C-CA-CB-CG2     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | H     | 1100 | 7JA  | C12-C13-N-CA    |
| 4   | F     | 1100 | 7JA  | N-CA-CB-CG2     |
| 4   | D     | 1100 | 7JA  | N-CA-CB-CG2     |
| 4   | D     | 1100 | 7JA  | C01-C02-C03-C04 |
| 4   | F     | 1100 | 7JA  | C01-C02-C03-C04 |
| 4   | L     | 1100 | 7JA  | C01-C02-C03-C04 |
| 4   | N     | 1100 | 7JA  | C-CA-CB-CG2     |
| 4   | N     | 1100 | 7JA  | C02-C03-C04-C05 |
| 4   | N     | 1100 | 7JA  | N-CA-CB-CG2     |
| 4   | L     | 1100 | 7JA  | C02-C03-C04-C05 |

There are no ring outliers.

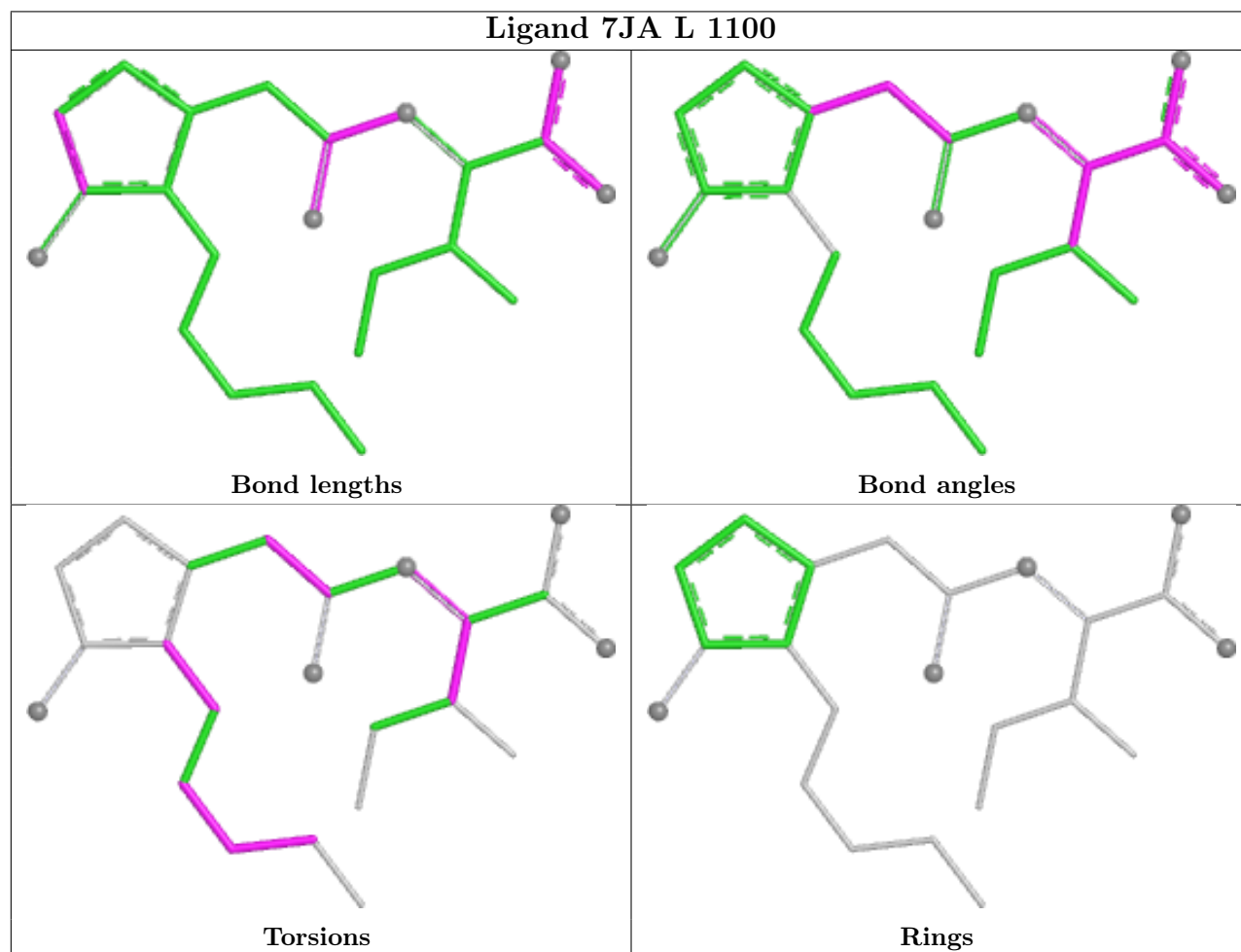
18 monomers are involved in 158 short contacts:

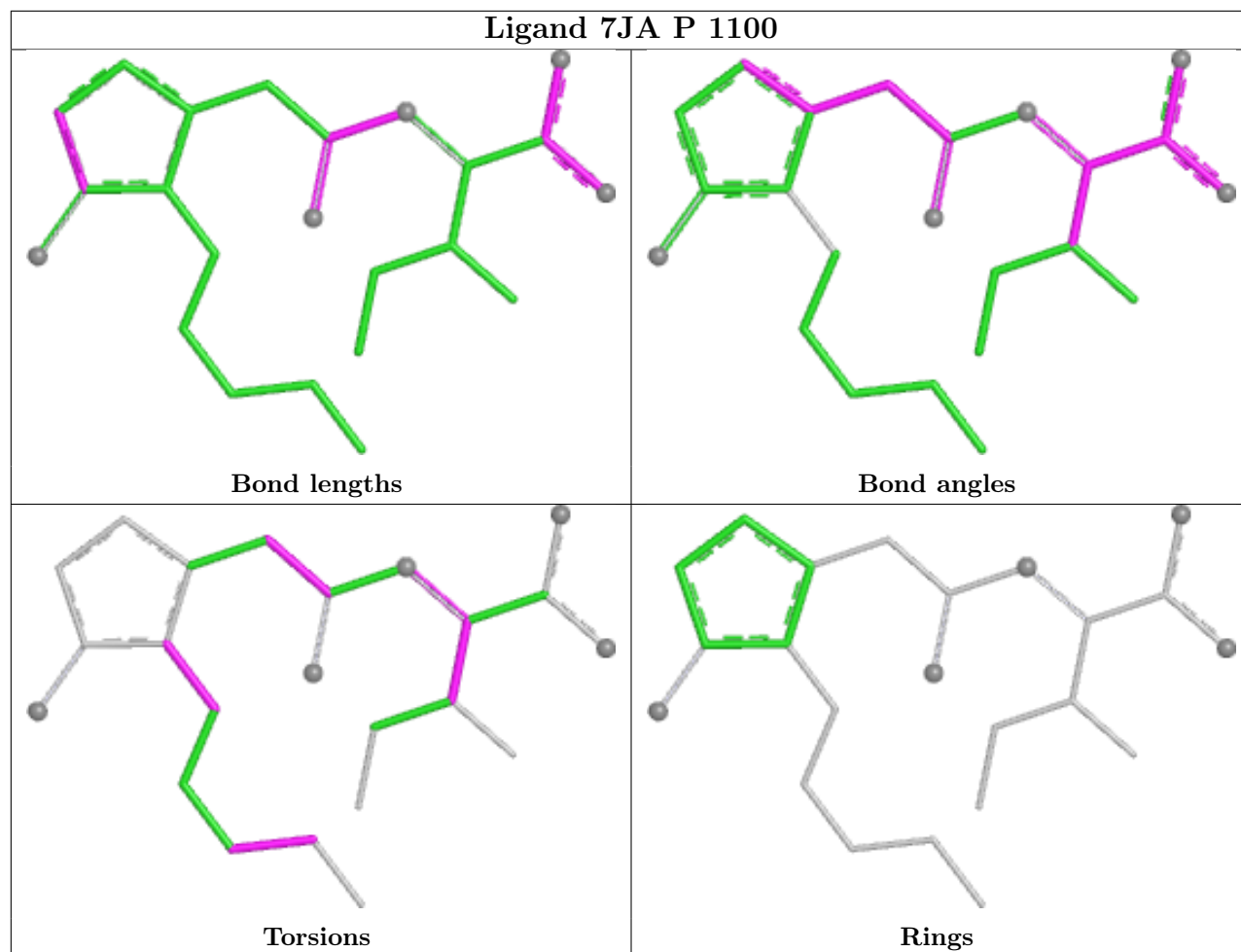
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | F     | 1101 | PO4  | 1       | 0            |
| 4   | L     | 1100 | 7JA  | 16      | 0            |
| 4   | P     | 1100 | 7JA  | 15      | 0            |
| 4   | N     | 1100 | 7JA  | 17      | 0            |
| 4   | H     | 1100 | 7JA  | 21      | 0            |
| 4   | F     | 1100 | 7JA  | 19      | 0            |
| 5   | N     | 1103 | PO4  | 2       | 0            |
| 5   | F     | 1103 | PO4  | 3       | 0            |
| 4   | B     | 1100 | 7JA  | 16      | 0            |
| 5   | P     | 1103 | PO4  | 3       | 0            |
| 5   | B     | 1103 | PO4  | 2       | 0            |
| 4   | D     | 1100 | 7JA  | 15      | 0            |
| 5   | D     | 1103 | PO4  | 3       | 0            |
| 5   | J     | 1103 | PO4  | 2       | 0            |
| 5   | L     | 1101 | PO4  | 1       | 0            |
| 5   | L     | 1103 | PO4  | 2       | 0            |
| 5   | H     | 1103 | PO4  | 3       | 0            |
| 4   | J     | 1100 | 7JA  | 17      | 0            |

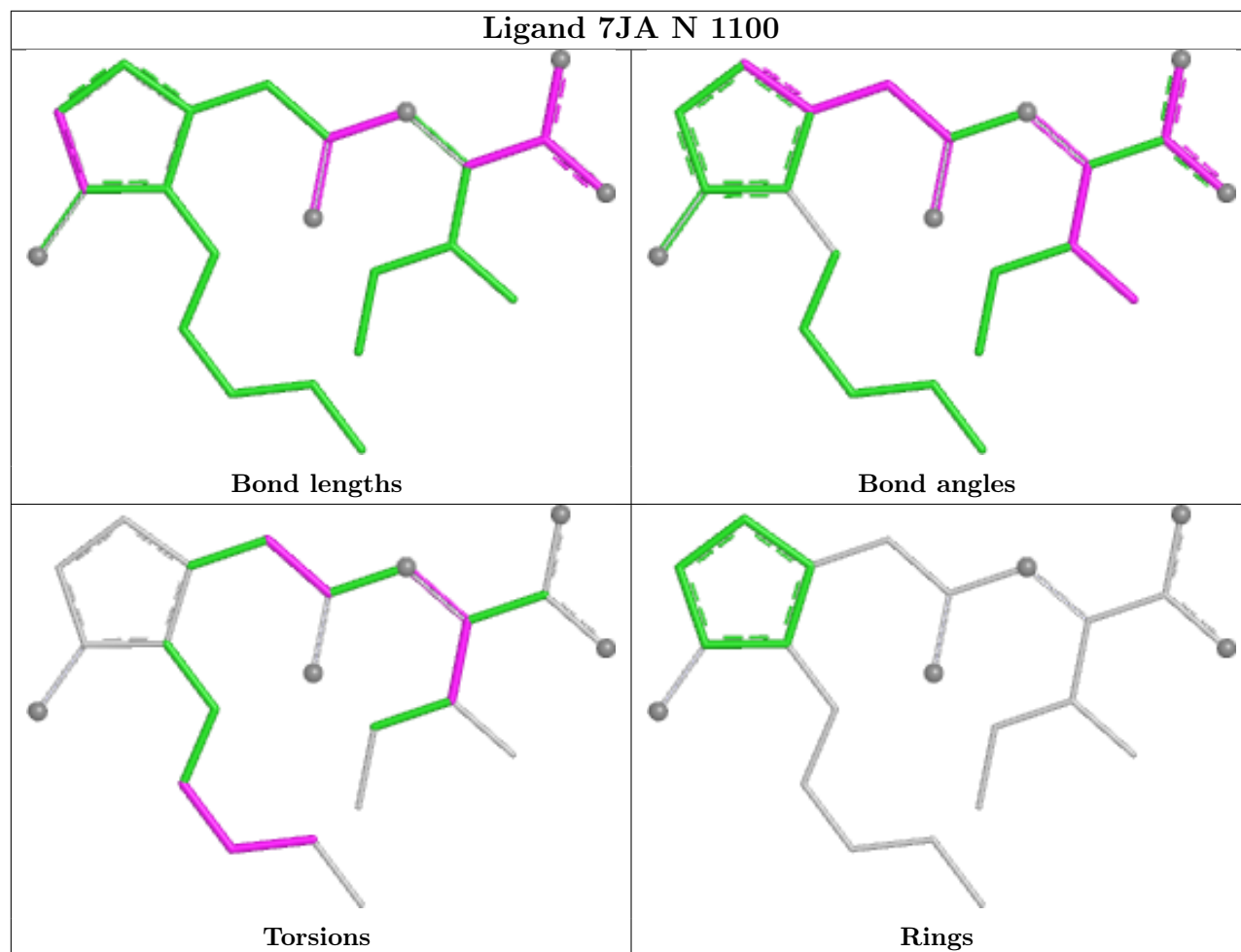
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

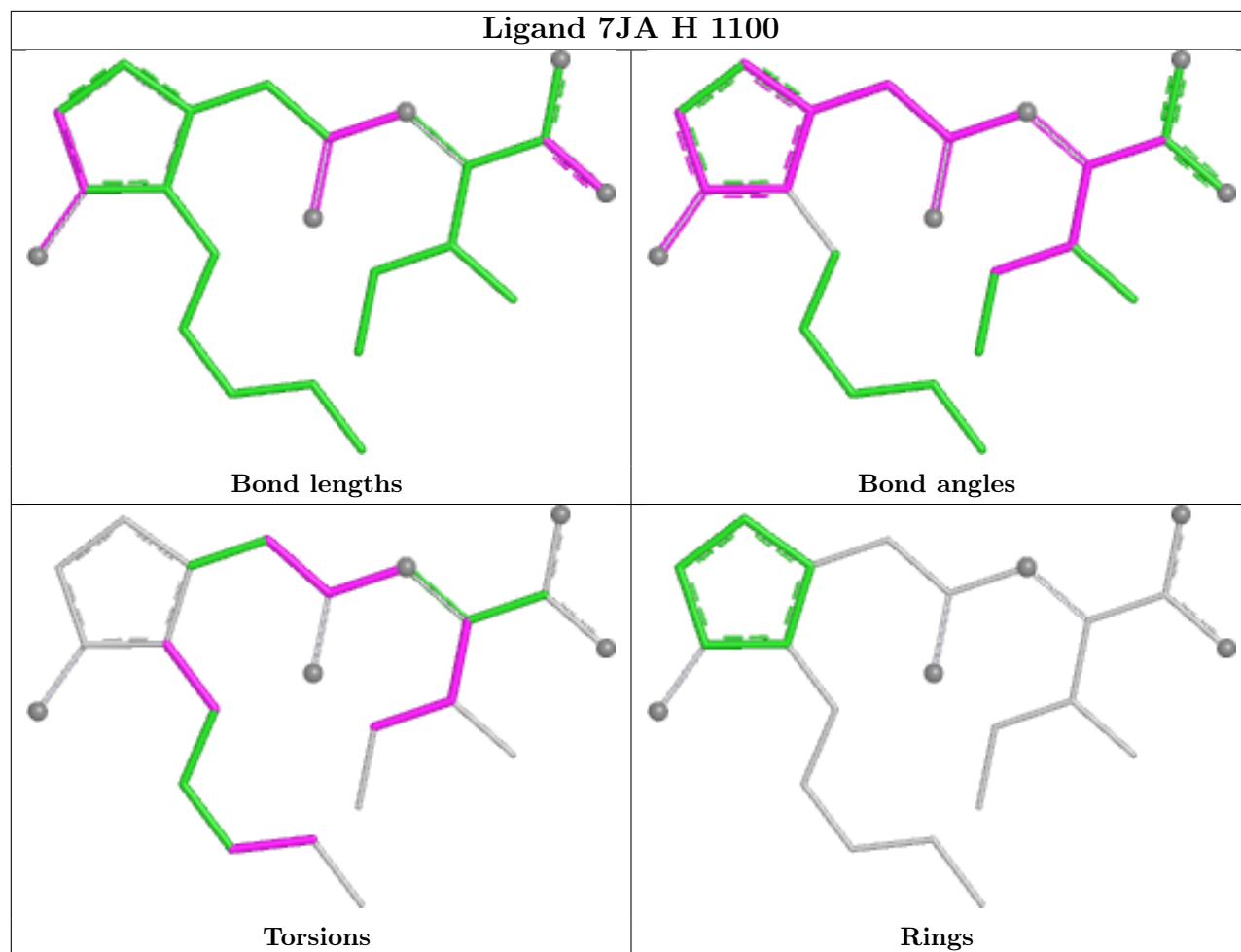


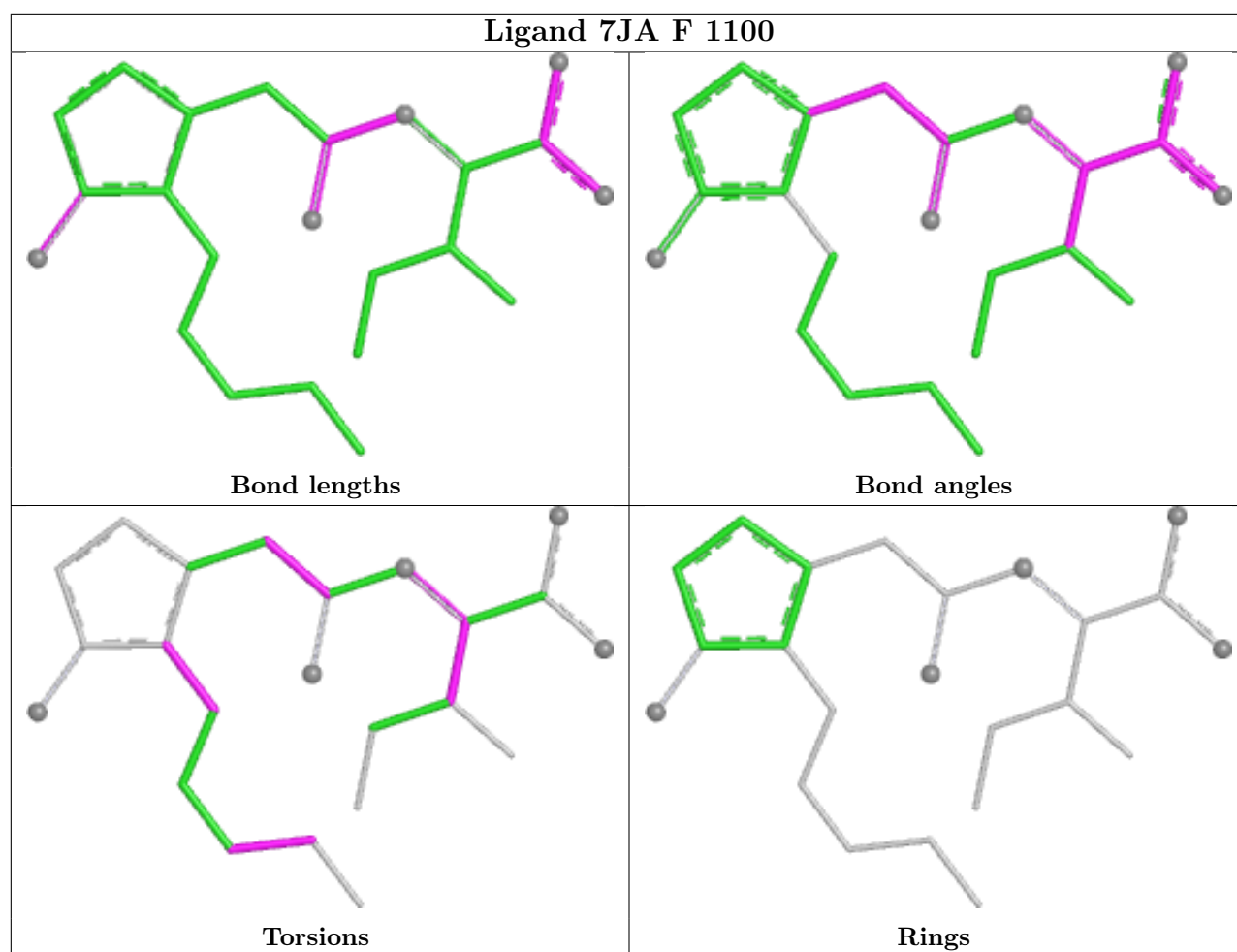
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

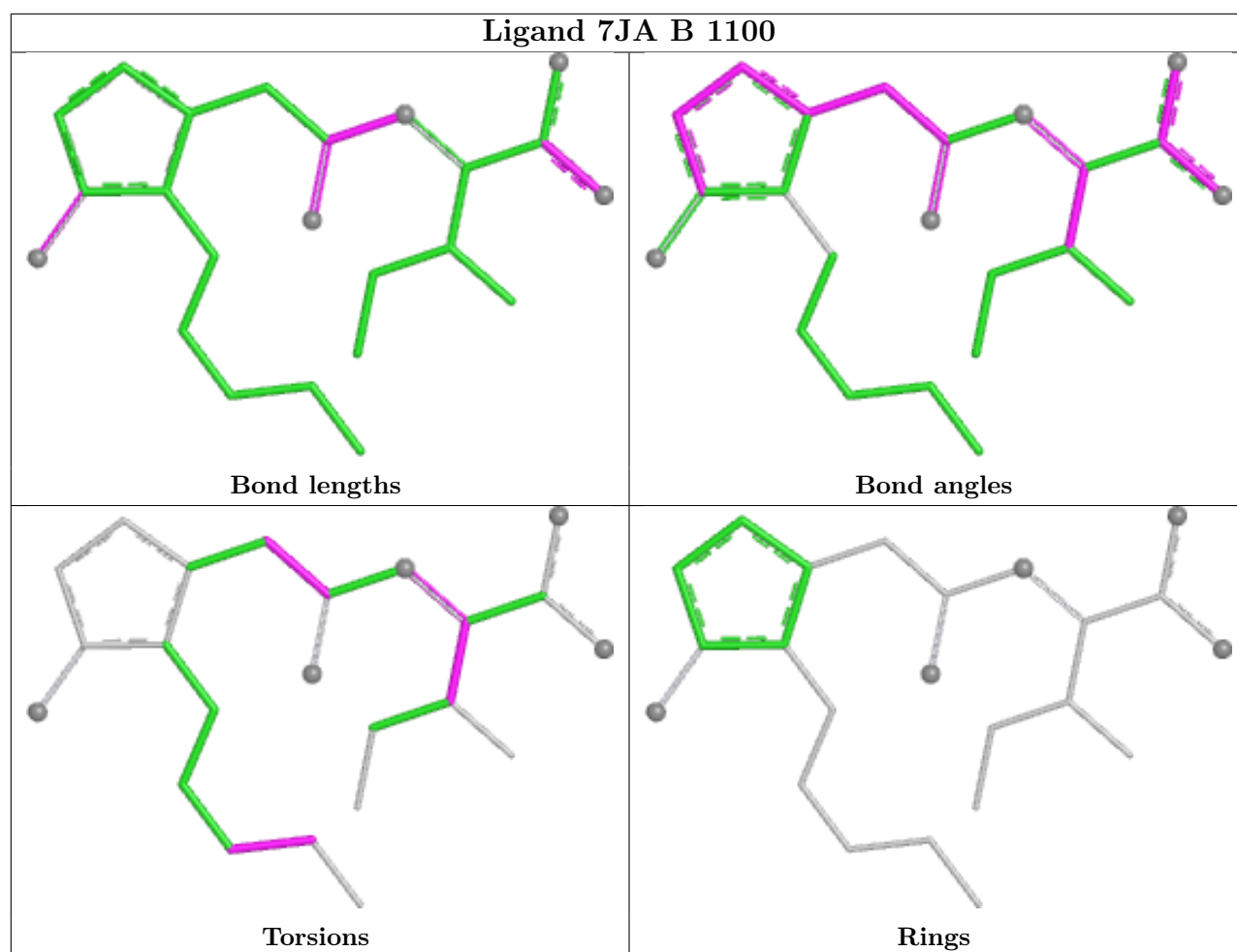


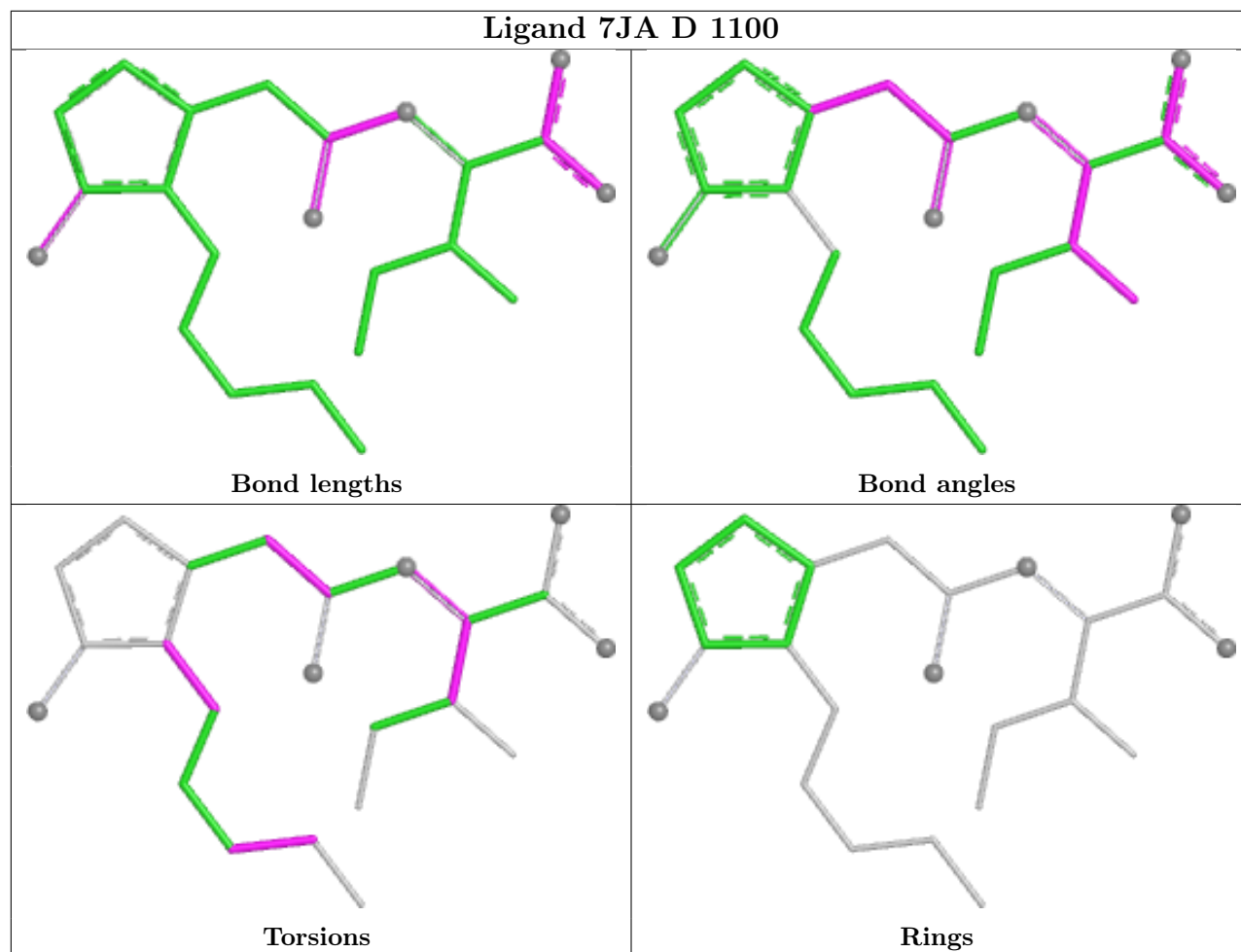


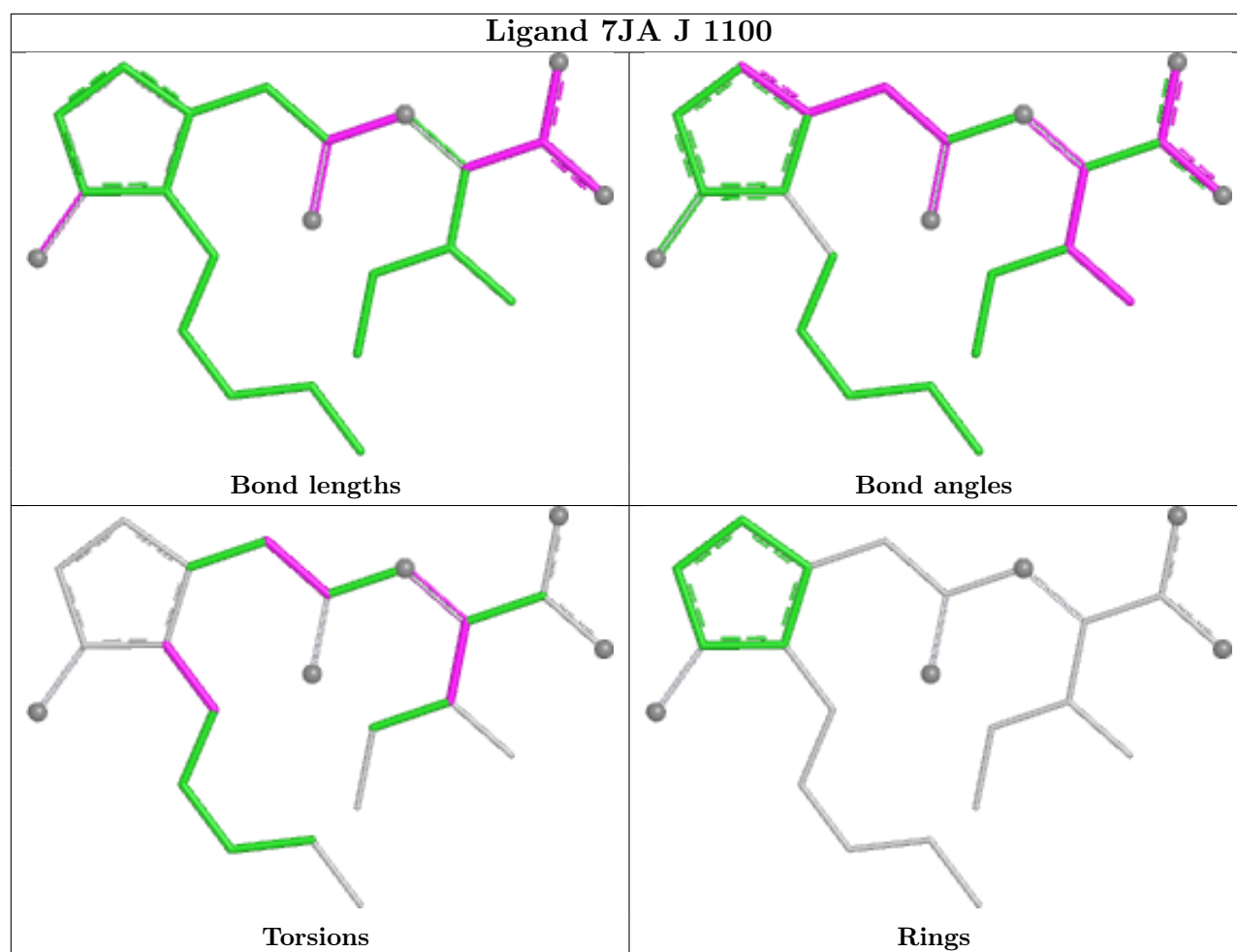












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 144/160 (90%)   | 0.10   | 2 (1%) 73 53  | 38, 87, 141, 157      | 0     |
| 1   | C     | 144/160 (90%)   | 0.12   | 2 (1%) 73 53  | 40, 90, 140, 159      | 0     |
| 1   | E     | 144/160 (90%)   | 0.16   | 1 (0%) 84 69  | 41, 85, 136, 157      | 0     |
| 1   | G     | 144/160 (90%)   | -0.20  | 0 100 100     | 37, 81, 136, 156      | 0     |
| 1   | I     | 144/160 (90%)   | 0.12   | 1 (0%) 84 69  | 43, 88, 138, 160      | 0     |
| 1   | K     | 144/160 (90%)   | -0.05  | 0 100 100     | 43, 89, 140, 158      | 0     |
| 1   | M     | 144/160 (90%)   | 0.22   | 3 (2%) 63 42  | 45, 89, 139, 163      | 0     |
| 1   | O     | 144/160 (90%)   | 0.01   | 0 100 100     | 43, 88, 138, 159      | 0     |
| 2   | B     | 568/592 (95%)   | -0.17  | 5 (0%) 81 64  | 31, 60, 122, 191      | 0     |
| 2   | D     | 568/592 (95%)   | -0.19  | 3 (0%) 87 75  | 33, 61, 124, 190      | 0     |
| 2   | F     | 568/592 (95%)   | -0.25  | 7 (1%) 76 57  | 32, 63, 125, 191      | 0     |
| 2   | H     | 562/592 (94%)   | -0.66  | 1 (0%) 91 85  | 29, 57, 106, 169      | 0     |
| 2   | J     | 568/592 (95%)   | -0.30  | 2 (0%) 88 78  | 33, 64, 124, 194      | 0     |
| 2   | L     | 568/592 (95%)   | -0.32  | 2 (0%) 88 78  | 33, 64, 125, 192      | 0     |
| 2   | N     | 568/592 (95%)   | 0.10   | 2 (0%) 88 78  | 33, 69, 126, 194      | 0     |
| 2   | P     | 568/592 (95%)   | -0.13  | 4 (0%) 84 69  | 34, 68, 126, 192      | 0     |
| 3   | Q     | 18/21 (85%)     | -0.05  | 0 100 100     | 61, 77, 108, 128      | 0     |
| 3   | R     | 18/21 (85%)     | -0.02  | 0 100 100     | 63, 78, 108, 131      | 0     |
| 3   | S     | 18/21 (85%)     | -0.35  | 0 100 100     | 64, 78, 109, 129      | 0     |
| 3   | U     | 18/21 (85%)     | 0.15   | 0 100 100     | 60, 80, 109, 130      | 0     |
| 3   | V     | 18/21 (85%)     | -0.21  | 0 100 100     | 61, 81, 108, 132      | 0     |
| 3   | W     | 18/21 (85%)     | 0.13   | 0 100 100     | 66, 83, 110, 132      | 0     |
| 3   | X     | 18/21 (85%)     | -0.18  | 0 100 100     | 65, 81, 109, 131      | 0     |
| All | All   | 5816/6163 (94%) | -0.18  | 35 (0%) 85 72 | 29, 68, 128, 194      | 0     |

All (35) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 360 | ASP  | 3.3  |
| 1   | C     | 118 | CYS  | 3.2  |
| 1   | C     | 117 | THR  | 3.1  |
| 2   | N     | 15  | ALA  | 2.9  |
| 2   | D     | 429 | ARG  | 2.7  |
| 2   | J     | 267 | VAL  | 2.6  |
| 2   | D     | 361 | GLU  | 2.6  |
| 2   | B     | 267 | VAL  | 2.6  |
| 2   | P     | 267 | VAL  | 2.5  |
| 1   | I     | 67  | ALA  | 2.5  |
| 2   | F     | 14  | VAL  | 2.4  |
| 1   | E     | 37  | CYS  | 2.4  |
| 2   | F     | 267 | VAL  | 2.4  |
| 2   | P     | 546 | PRO  | 2.4  |
| 2   | P     | 363 | GLY  | 2.4  |
| 2   | L     | 359 | GLU  | 2.4  |
| 2   | H     | 353 | ALA  | 2.3  |
| 2   | F     | 547 | SER  | 2.3  |
| 1   | M     | 6   | ILE  | 2.3  |
| 2   | B     | 12  | SER  | 2.3  |
| 2   | B     | 14  | VAL  | 2.3  |
| 2   | J     | 360 | ASP  | 2.2  |
| 1   | A     | 21  | ALA  | 2.2  |
| 2   | F     | 212 | LEU  | 2.2  |
| 2   | B     | 360 | ASP  | 2.2  |
| 1   | M     | 117 | THR  | 2.1  |
| 2   | L     | 267 | VAL  | 2.1  |
| 2   | P     | 353 | ALA  | 2.1  |
| 1   | A     | 80  | ASP  | 2.1  |
| 1   | M     | 118 | CYS  | 2.1  |
| 2   | B     | 549 | ARG  | 2.1  |
| 2   | N     | 29  | THR  | 2.0  |
| 2   | F     | 513 | PRO  | 2.0  |
| 2   | F     | 546 | PRO  | 2.0  |
| 2   | F     | 592 | ILE  | 2.0  |

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

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

## 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 5   | PO4  | H     | 1102 | 5/5   | 0.78 | 0.13 | 72,73,108,121               | 0     |
| 5   | PO4  | N     | 1102 | 5/5   | 0.80 | 0.12 | 64,78,83,116                | 0     |
| 5   | PO4  | P     | 1102 | 5/5   | 0.85 | 0.14 | 63,72,83,106                | 0     |
| 5   | PO4  | N     | 1104 | 5/5   | 0.86 | 0.10 | 56,57,89,100                | 0     |
| 5   | PO4  | F     | 1102 | 5/5   | 0.86 | 0.11 | 56,74,78,96                 | 0     |
| 5   | PO4  | B     | 1102 | 5/5   | 0.87 | 0.09 | 49,75,81,91                 | 0     |
| 5   | PO4  | D     | 1102 | 5/5   | 0.88 | 0.10 | 55,73,86,95                 | 0     |
| 5   | PO4  | H     | 1101 | 5/5   | 0.89 | 0.07 | 65,80,94,96                 | 0     |
| 5   | PO4  | H     | 1104 | 5/5   | 0.90 | 0.09 | 57,64,69,95                 | 0     |
| 5   | PO4  | D     | 1104 | 5/5   | 0.91 | 0.11 | 49,60,85,91                 | 0     |
| 5   | PO4  | P     | 1104 | 5/5   | 0.91 | 0.08 | 50,58,89,93                 | 0     |
| 5   | PO4  | J     | 1102 | 5/5   | 0.92 | 0.08 | 53,74,83,101                | 0     |
| 5   | PO4  | L     | 1104 | 5/5   | 0.92 | 0.08 | 52,60,91,94                 | 0     |
| 4   | 7JA  | N     | 1100 | 23/23 | 0.92 | 0.13 | 49,61,73,86                 | 0     |
| 4   | 7JA  | B     | 1100 | 23/23 | 0.93 | 0.16 | 34,55,70,87                 | 0     |
| 5   | PO4  | J     | 1104 | 5/5   | 0.93 | 0.11 | 57,60,82,86                 | 0     |
| 5   | PO4  | L     | 1102 | 5/5   | 0.93 | 0.05 | 64,67,83,96                 | 0     |
| 5   | PO4  | P     | 1103 | 5/5   | 0.93 | 0.08 | 47,55,70,76                 | 0     |
| 4   | 7JA  | H     | 1100 | 23/23 | 0.93 | 0.12 | 38,62,77,81                 | 0     |
| 5   | PO4  | N     | 1103 | 5/5   | 0.94 | 0.07 | 48,51,62,80                 | 0     |
| 5   | PO4  | F     | 1104 | 5/5   | 0.94 | 0.08 | 48,54,80,83                 | 0     |
| 4   | 7JA  | J     | 1100 | 23/23 | 0.94 | 0.13 | 39,55,72,83                 | 0     |
| 5   | PO4  | N     | 1101 | 5/5   | 0.94 | 0.08 | 42,48,74,75                 | 0     |
| 4   | 7JA  | P     | 1100 | 23/23 | 0.94 | 0.12 | 47,59,73,85                 | 0     |
| 4   | 7JA  | L     | 1100 | 23/23 | 0.95 | 0.10 | 42,58,72,86                 | 0     |
| 4   | 7JA  | F     | 1100 | 23/23 | 0.95 | 0.12 | 42,56,70,88                 | 0     |
| 5   | PO4  | B     | 1104 | 5/5   | 0.95 | 0.07 | 47,63,91,96                 | 0     |
| 5   | PO4  | P     | 1101 | 5/5   | 0.96 | 0.05 | 40,51,70,73                 | 0     |
| 5   | PO4  | B     | 1101 | 5/5   | 0.96 | 0.06 | 35,48,61,72                 | 0     |
| 5   | PO4  | F     | 1101 | 5/5   | 0.96 | 0.07 | 40,41,55,77                 | 0     |
| 4   | 7JA  | D     | 1100 | 23/23 | 0.96 | 0.10 | 37,55,68,85                 | 0     |
| 5   | PO4  | L     | 1103 | 5/5   | 0.97 | 0.06 | 45,48,58,71                 | 0     |

*Continued on next page...*

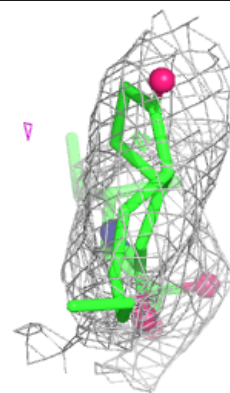
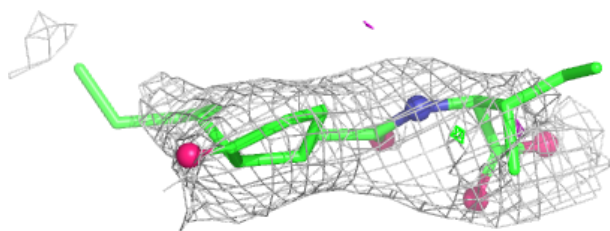
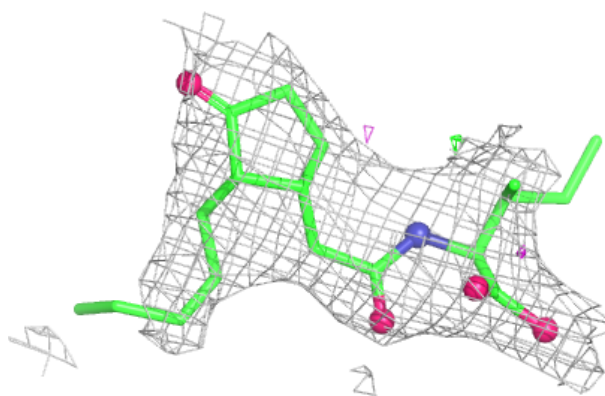
*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 5   | PO4  | D     | 1101 | 5/5   | 0.97 | 0.05 | 42,45,58,71                 | 0     |
| 5   | PO4  | F     | 1103 | 5/5   | 0.97 | 0.05 | 44,47,48,69                 | 0     |
| 5   | PO4  | L     | 1101 | 5/5   | 0.97 | 0.05 | 36,48,65,73                 | 0     |
| 5   | PO4  | D     | 1103 | 5/5   | 0.97 | 0.07 | 38,46,52,75                 | 0     |
| 5   | PO4  | H     | 1103 | 5/5   | 0.98 | 0.04 | 35,56,67,68                 | 0     |
| 5   | PO4  | J     | 1103 | 5/5   | 0.98 | 0.04 | 42,45,52,68                 | 0     |
| 5   | PO4  | J     | 1101 | 5/5   | 0.98 | 0.06 | 37,45,66,73                 | 0     |
| 5   | PO4  | B     | 1103 | 5/5   | 0.99 | 0.06 | 41,45,51,66                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

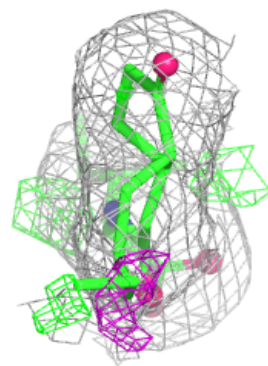
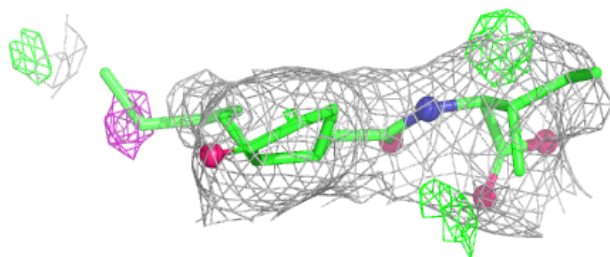
**Electron density around 7JA N 1100:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

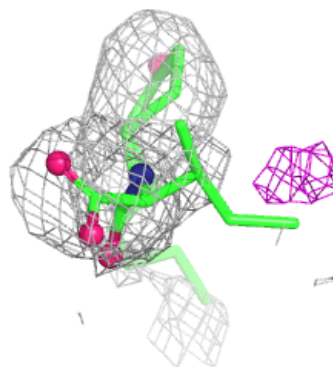
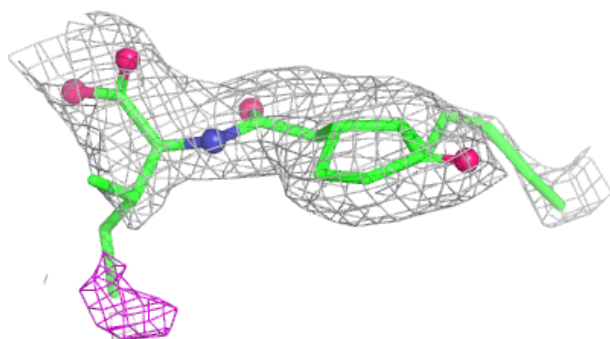
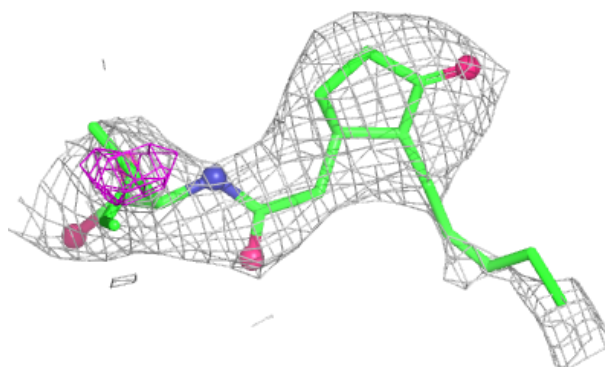


**Electron density around 7JA B 1100:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

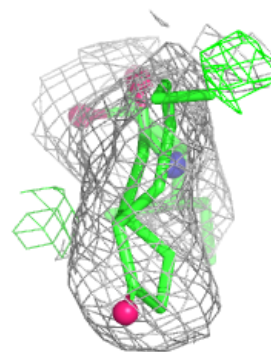
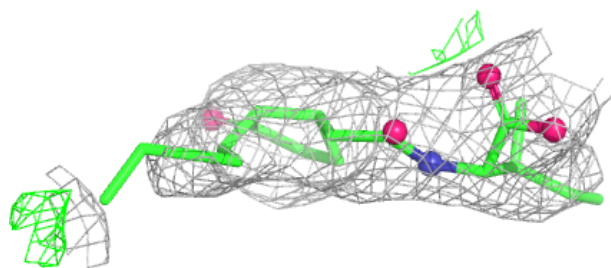
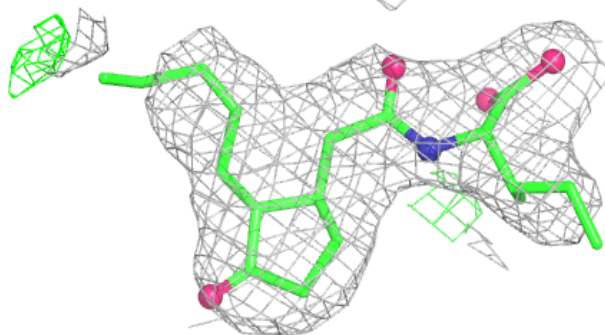
**Electron density around 7JA H 1100:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

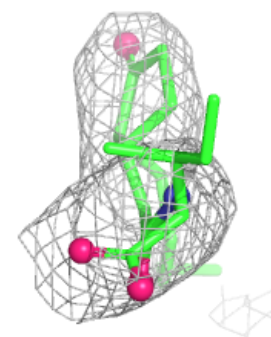
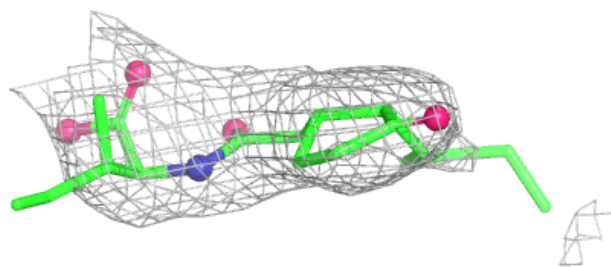
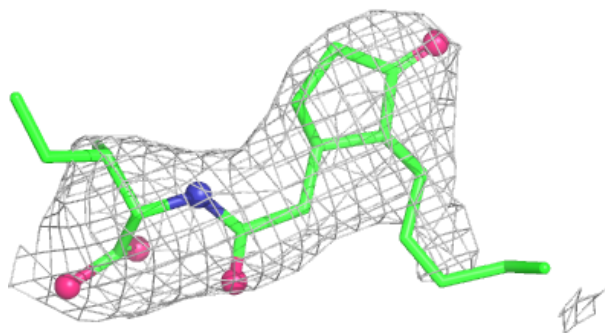


**Electron density around 7JA J 1100:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 7JA P 1100:**

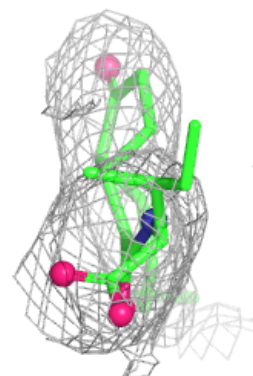
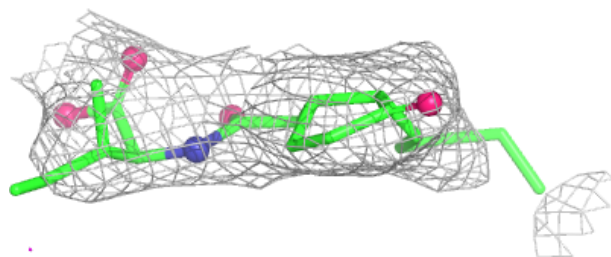
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



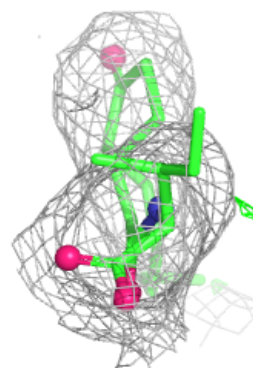
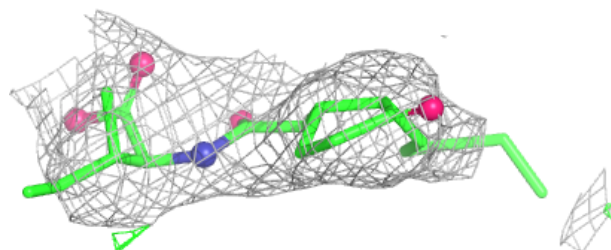
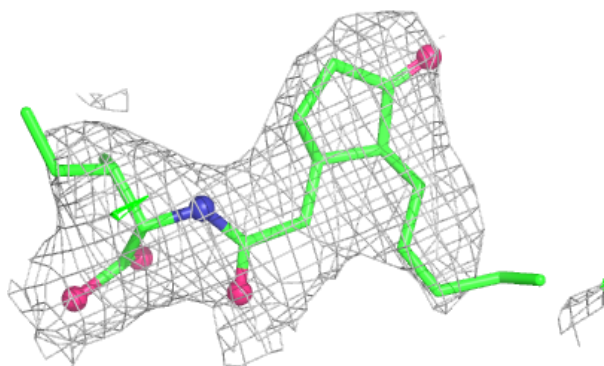


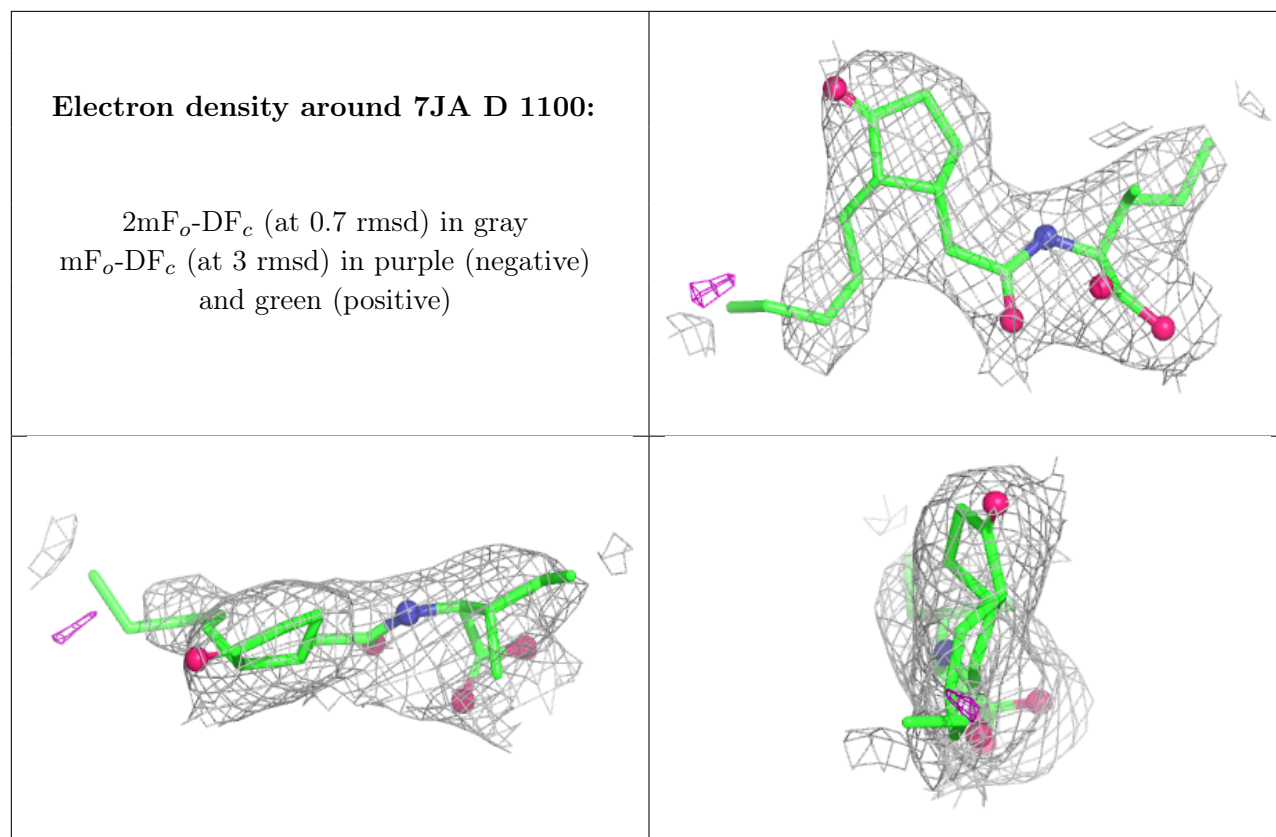
**Electron density around 7JA L 1100:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 7JA F 1100:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.