



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:45 PM UTC

PDB ID : 1F1H / pdb\_00001f1h  
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM  
SALMONELLA TYPHIMURIUM WITH THALLIUM IONS  
Authors : Gill, H.S.; Eisenberg, D.  
Deposited on : 2000-05-19  
Resolution : 2.67 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                                                             |

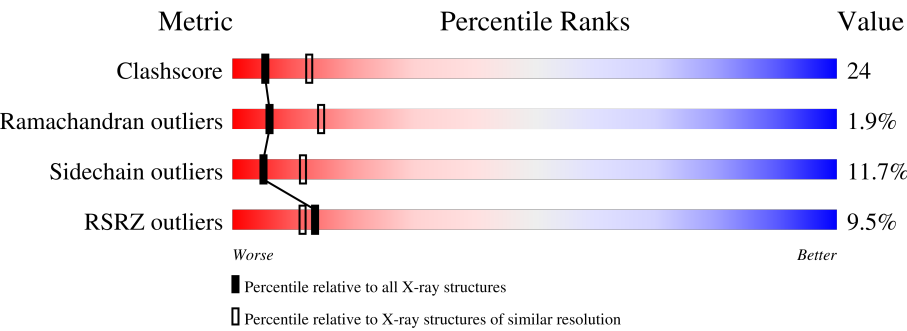
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 5409 (2.70-2.66)                                      |
| Ramachandran outliers | 187476                      | 5324 (2.70-2.66)                                      |
| Sidechain outliers    | 187428                      | 5324 (2.70-2.66)                                      |
| RSRZ outliers         | 180081                      | 5070 (2.70-2.66)                                      |

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     | 468    | <div><div>17%</div><div><div></div><div>66%</div><div>25%</div><div>7%</div><div>.</div></div></div> |
| 1   | B     | 468    | <div><div>8%</div><div><div></div><div>67%</div><div>24%</div><div>7%</div><div>.</div></div></div>  |
| 1   | C     | 468    | <div><div>9%</div><div><div></div><div>66%</div><div>25%</div><div>7%</div><div>.</div></div></div>  |
| 1   | D     | 468    | <div><div>6%</div><div><div></div><div>66%</div><div>24%</div><div>7%</div><div>.</div></div></div>  |
| 1   | E     | 468    | <div><div>7%</div><div><div></div><div>66%</div><div>24%</div><div>7%</div><div>.</div></div></div>  |
| 1   | F     | 468    | <div><div>7%</div><div><div></div><div>66%</div><div>25%</div><div>7%</div><div>.</div></div></div>  |
| 1   | G     | 468    | <div><div>7%</div><div><div></div><div>67%</div><div>24%</div><div>8%</div><div>.</div></div></div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | H     | 468    |                  |
| 1   | I     | 468    |                  |
| 1   | J     | 468    |                  |
| 1   | K     | 468    |                  |
| 1   | L     | 468    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 5   | MPD  | A     | 1483 | -         | -        | X       | -                |
| 5   | MPD  | B     | 1484 | -         | -        | X       | -                |
| 5   | MPD  | C     | 1485 | -         | -        | X       | -                |
| 5   | MPD  | D     | 1486 | -         | -        | X       | -                |
| 5   | MPD  | E     | 1487 | -         | -        | X       | -                |
| 5   | MPD  | F     | 1488 | -         | -        | X       | -                |
| 5   | MPD  | G     | 1489 | -         | -        | X       | -                |
| 5   | MPD  | H     | 1490 | -         | -        | X       | -                |
| 5   | MPD  | I     | 1491 | -         | -        | X       | -                |
| 5   | MPD  | J     | 1492 | -         | -        | X       | -                |
| 5   | MPD  | K     | 1493 | -         | -        | X       | -                |
| 5   | MPD  | L     | 1494 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 45564 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 PROTEIN (GLUTAMINE SYNTHETASE).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | B     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | C     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | D     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | E     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | F     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | G     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | H     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | I     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | J     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | K     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |
| 1   | L     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3637  | 2301 | 624 | 692 | 20 |         |         |       |

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

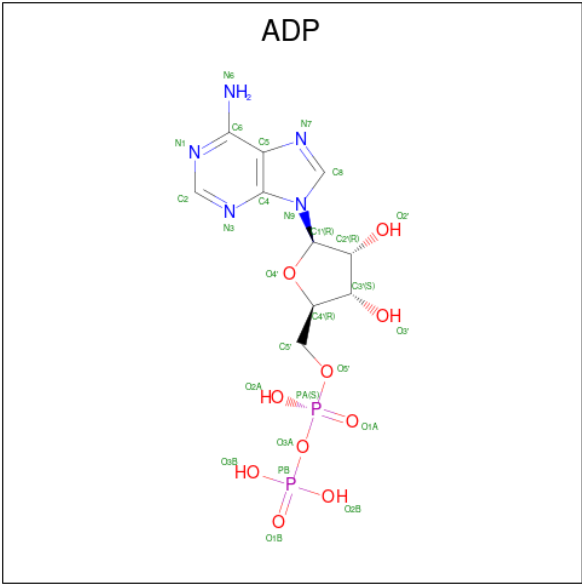
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | B     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | C     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | D     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | E     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | F     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | G     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | H     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | I     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | J     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | K     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | L     | 2        | Total | Mn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | I     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | J     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | K     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 3   | L     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

- Molecule 4 is THALLIUM (I) ION (CCD ID: TL) (formula: Tl).

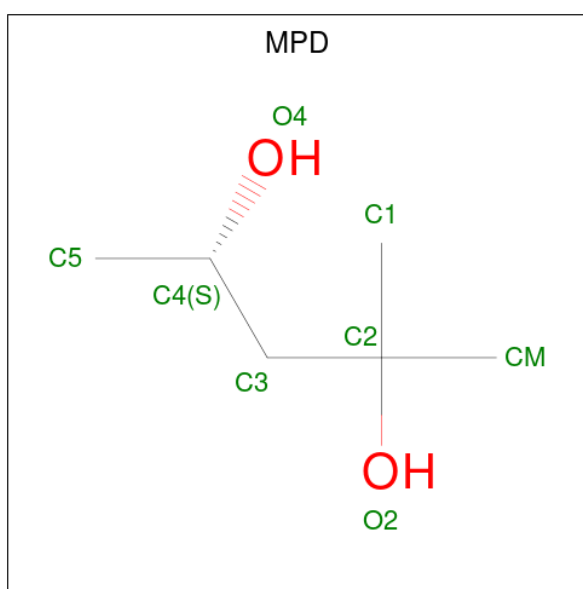
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | B     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | C     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | D     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | E     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | F     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | G     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | H     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | I     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | J     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | K     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | L     | 2        | Total | Tl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

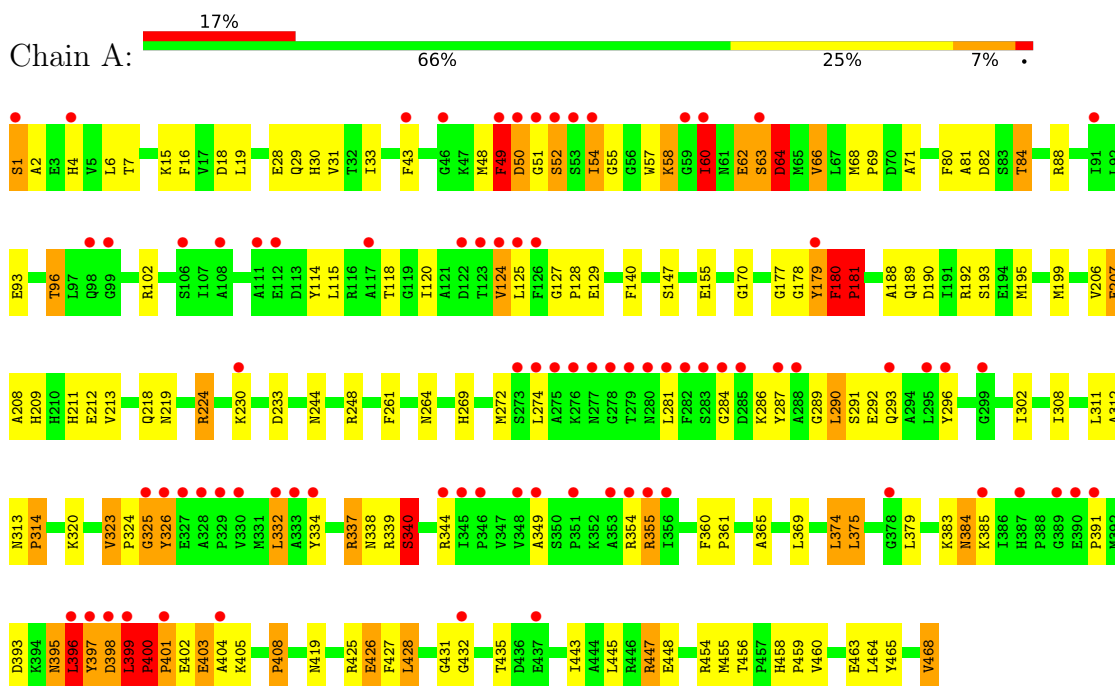
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 120      | Total | O   | 0       | 0       |
|     |       |          | 120   | 120 |         |         |
| 6   | B     | 121      | Total | O   | 0       | 0       |
|     |       |          | 121   | 121 |         |         |
| 6   | C     | 119      | Total | O   | 0       | 0       |
|     |       |          | 119   | 119 |         |         |
| 6   | D     | 122      | Total | O   | 0       | 0       |
|     |       |          | 122   | 122 |         |         |
| 6   | E     | 122      | Total | O   | 0       | 0       |
|     |       |          | 122   | 122 |         |         |
| 6   | F     | 121      | Total | O   | 0       | 0       |
|     |       |          | 121   | 121 |         |         |
| 6   | G     | 122      | Total | O   | 0       | 0       |
|     |       |          | 122   | 122 |         |         |
| 6   | H     | 121      | Total | O   | 0       | 0       |
|     |       |          | 121   | 121 |         |         |
| 6   | I     | 122      | Total | O   | 0       | 0       |
|     |       |          | 122   | 122 |         |         |
| 6   | J     | 120      | Total | O   | 0       | 0       |
|     |       |          | 120   | 120 |         |         |
| 6   | K     | 123      | Total | O   | 0       | 0       |
|     |       |          | 123   | 123 |         |         |
| 6   | L     | 119      | Total | O   | 0       | 0       |
|     |       |          | 119   | 119 |         |         |

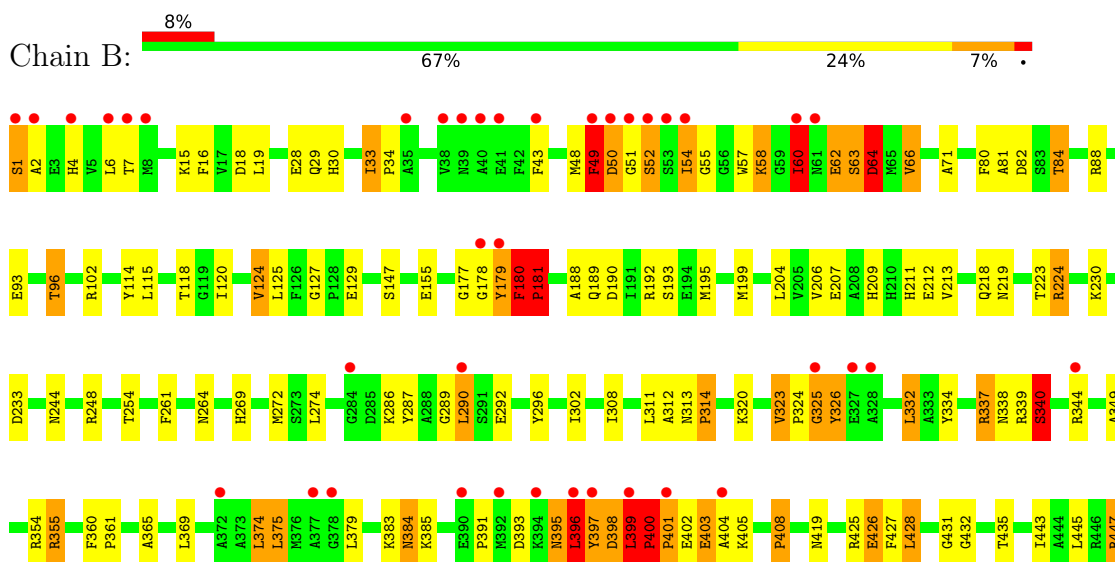
### 3 Residue-property plots

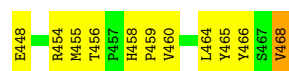
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

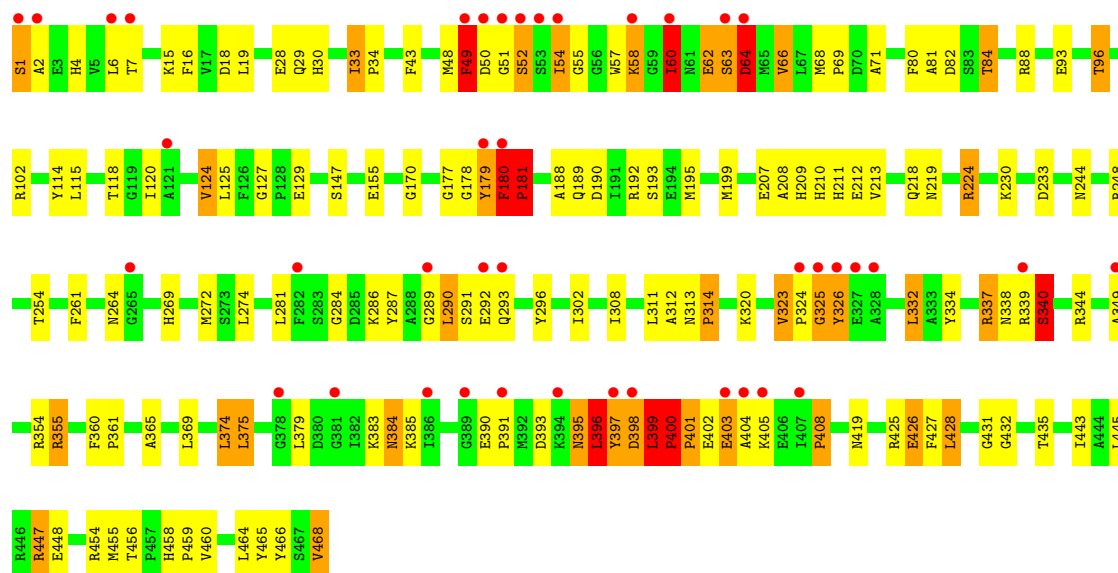


#### • Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

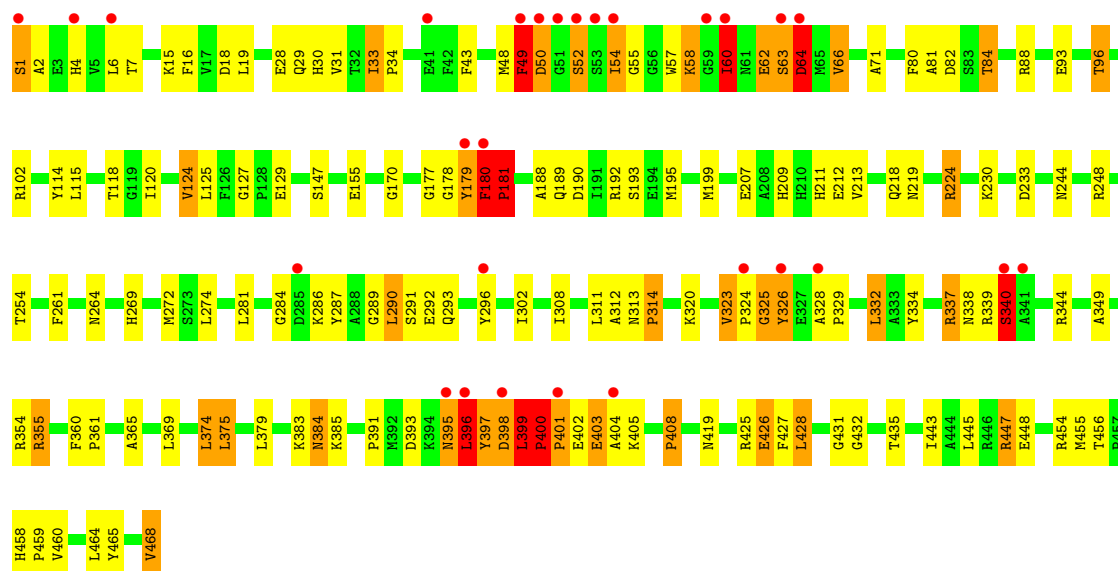




• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

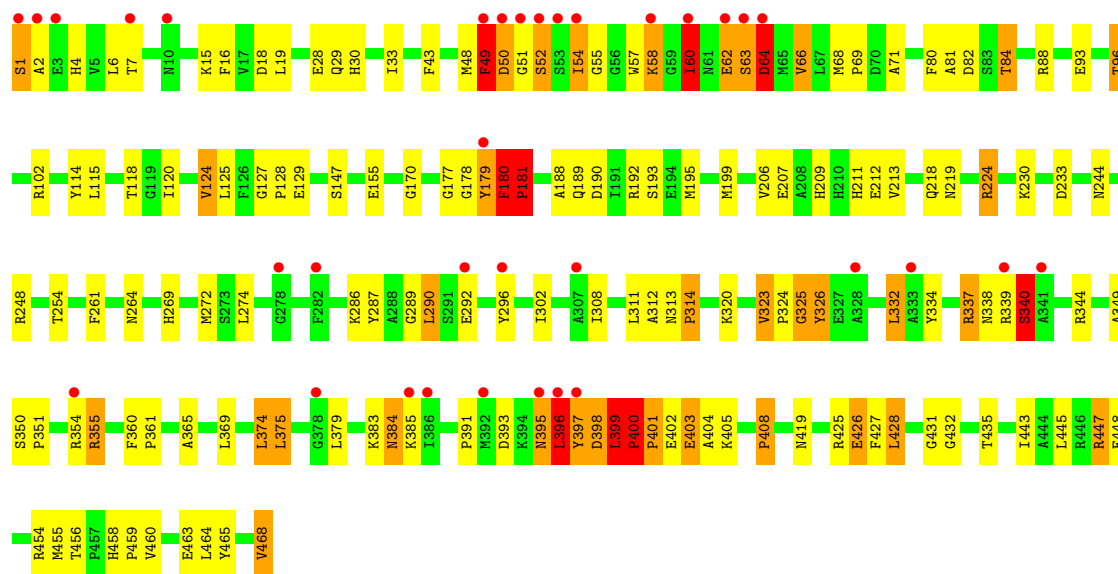


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

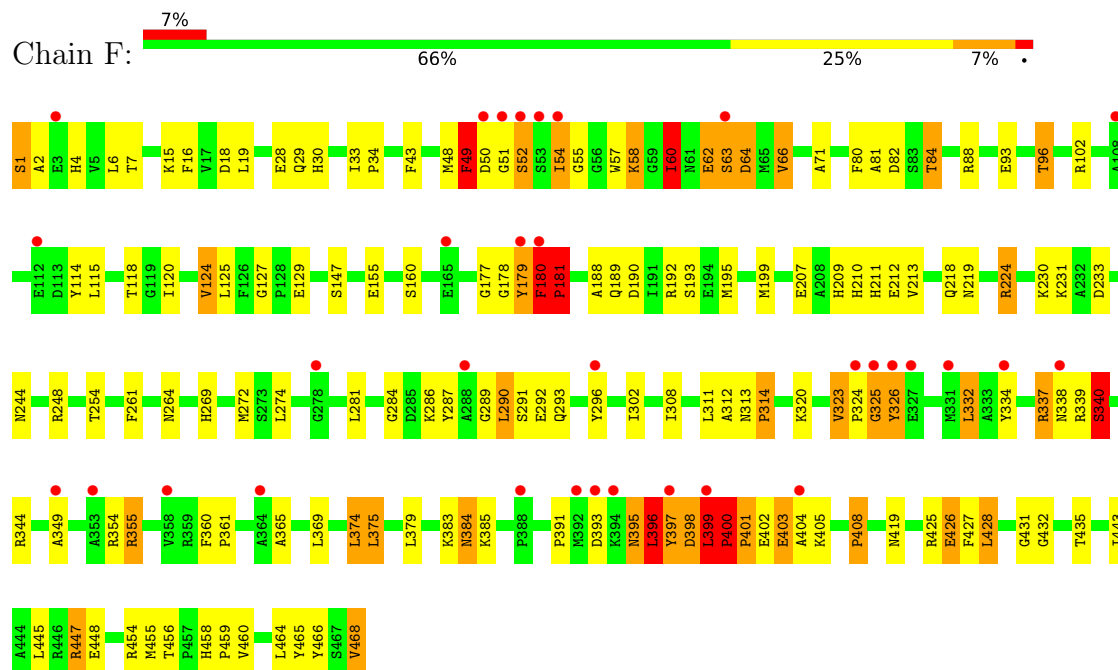


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

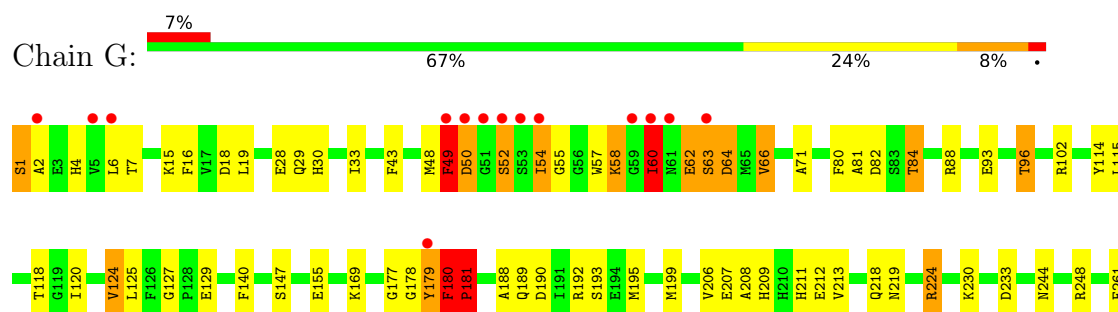


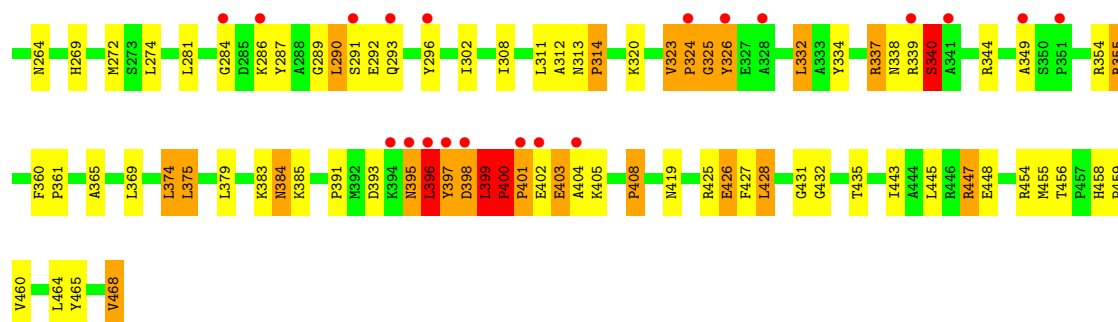


- Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

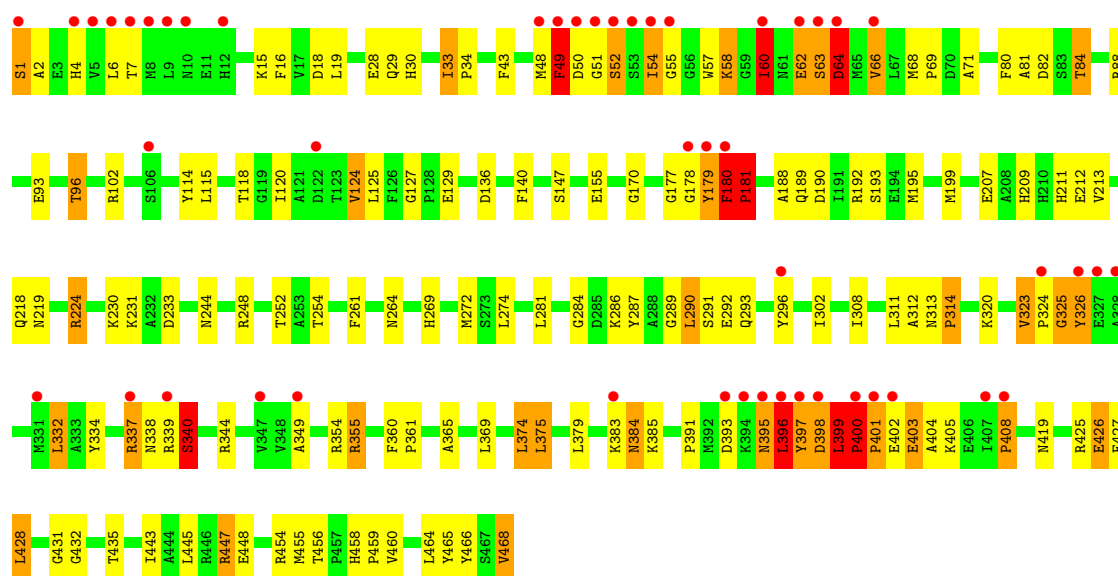


- Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

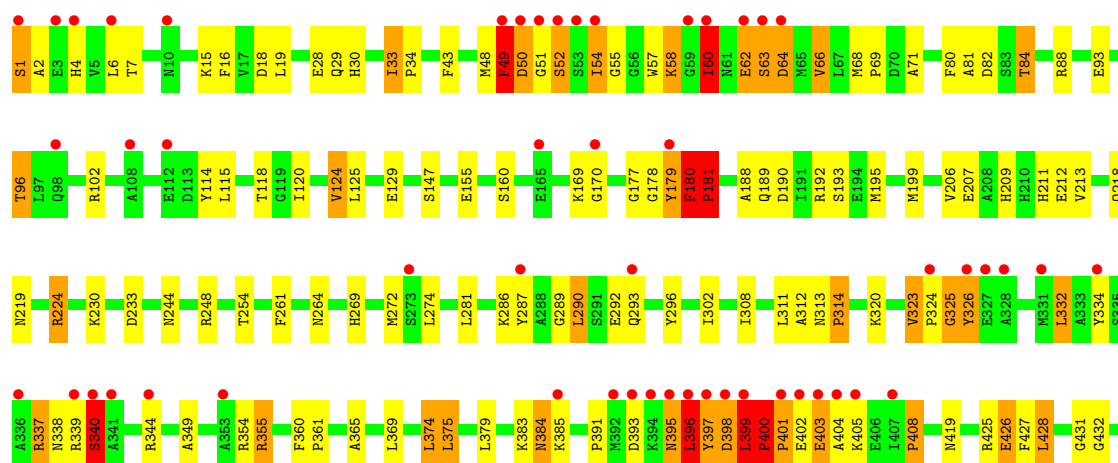




• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

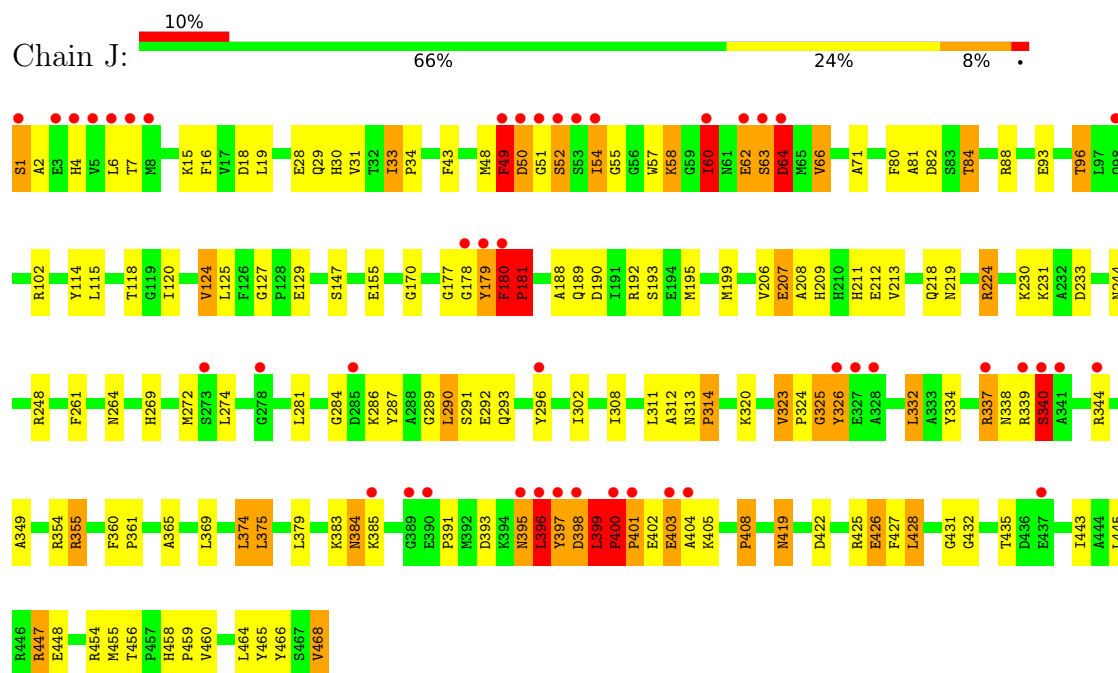


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

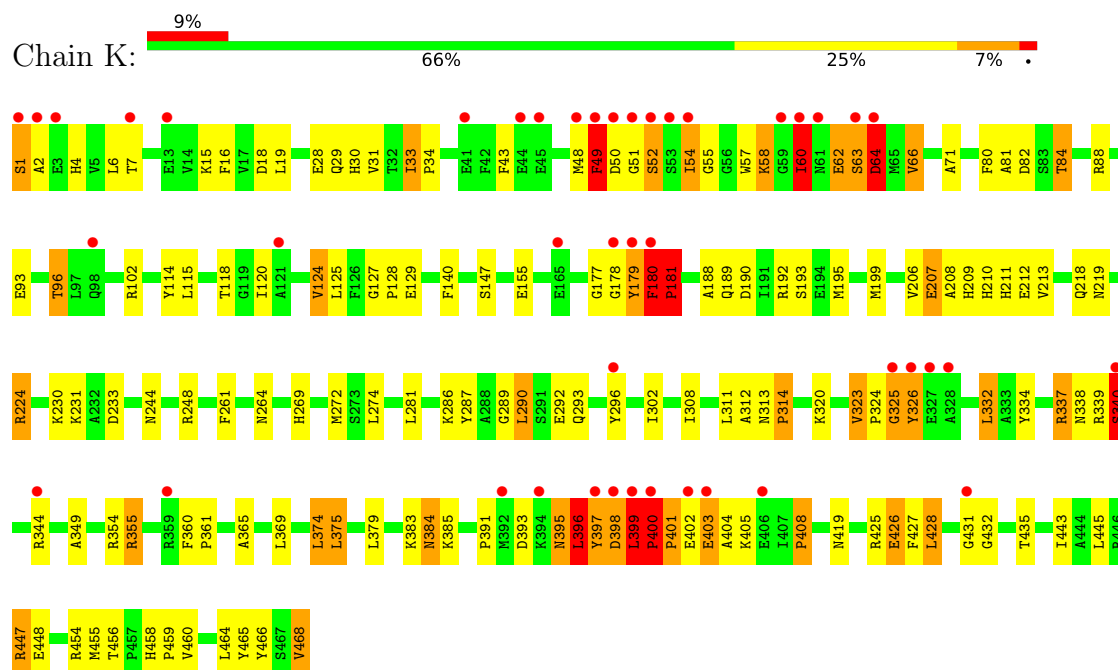




• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

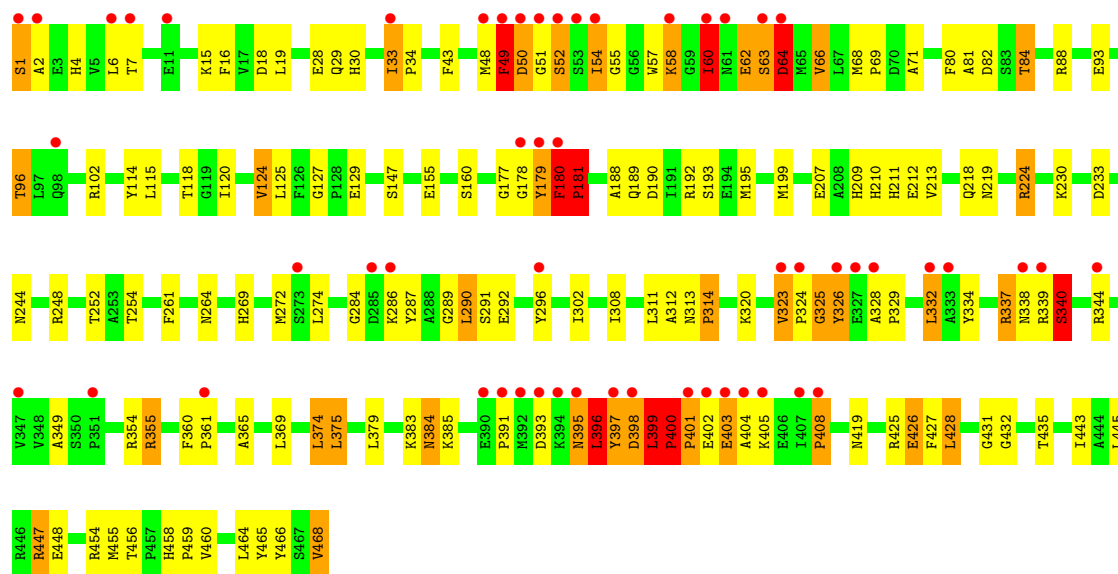


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 231.13Å 132.79Å 196.78Å<br>90.00° 102.44° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 32.00 – 2.67<br>32.00 – 2.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 82.0 (32.00-2.67)<br>81.9 (32.00-2.70)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.33 (at 2.68Å)                                             | Xtriage          |
| Refinement program                                                      | X-PLOR 3.843                                                | Depositor        |
| R, $R_{free}$                                                           | 0.232 , 0.263<br>0.231 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 45.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.135                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 60.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 45564                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 46.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: MN, ADP, TL, MPD

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     | 0.64         | 1/3724 (0.0%)   | 1.25        | 35/5043 (0.7%)   |
| 1   | B     | 0.64         | 1/3724 (0.0%)   | 1.25        | 33/5043 (0.7%)   |
| 1   | C     | 0.64         | 1/3724 (0.0%)   | 1.25        | 35/5043 (0.7%)   |
| 1   | D     | 0.64         | 1/3724 (0.0%)   | 1.25        | 35/5043 (0.7%)   |
| 1   | E     | 0.64         | 1/3724 (0.0%)   | 1.25        | 37/5043 (0.7%)   |
| 1   | F     | 0.64         | 1/3724 (0.0%)   | 1.25        | 33/5043 (0.7%)   |
| 1   | G     | 0.64         | 1/3724 (0.0%)   | 1.25        | 33/5043 (0.7%)   |
| 1   | H     | 0.64         | 1/3724 (0.0%)   | 1.25        | 37/5043 (0.7%)   |
| 1   | I     | 0.64         | 1/3724 (0.0%)   | 1.25        | 35/5043 (0.7%)   |
| 1   | J     | 0.64         | 1/3724 (0.0%)   | 1.25        | 35/5043 (0.7%)   |
| 1   | K     | 0.64         | 1/3724 (0.0%)   | 1.25        | 33/5043 (0.7%)   |
| 1   | L     | 0.64         | 1/3724 (0.0%)   | 1.25        | 33/5043 (0.7%)   |
| All | All   | 0.64         | 12/44688 (0.0%) | 1.25        | 414/60516 (0.7%) |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | I     | 54  | ILE  | CA-C  | 5.20 | 1.57        | 1.52     |
| 1   | D     | 54  | ILE  | CA-C  | 5.19 | 1.57        | 1.52     |
| 1   | G     | 54  | ILE  | CA-C  | 5.17 | 1.57        | 1.52     |
| 1   | H     | 54  | ILE  | CA-C  | 5.17 | 1.57        | 1.52     |
| 1   | K     | 54  | ILE  | CA-C  | 5.16 | 1.57        | 1.52     |
| 1   | C     | 54  | ILE  | CA-C  | 5.15 | 1.57        | 1.52     |
| 1   | A     | 54  | ILE  | CA-C  | 5.14 | 1.57        | 1.52     |
| 1   | J     | 54  | ILE  | CA-C  | 5.11 | 1.57        | 1.52     |
| 1   | F     | 54  | ILE  | CA-C  | 5.09 | 1.57        | 1.52     |
| 1   | B     | 54  | ILE  | CA-C  | 5.07 | 1.57        | 1.52     |
| 1   | L     | 54  | ILE  | CA-C  | 5.06 | 1.57        | 1.52     |
| 1   | E     | 54  | ILE  | CA-C  | 5.05 | 1.57        | 1.52     |

All (414) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 213 | VAL  | N-CA-C     | 9.11  | 119.91      | 110.62   |
| 1   | H     | 213 | VAL  | N-CA-C     | 9.08  | 119.88      | 110.62   |
| 1   | E     | 213 | VAL  | N-CA-C     | 9.07  | 119.87      | 110.62   |
| 1   | A     | 213 | VAL  | N-CA-C     | 9.07  | 119.87      | 110.62   |
| 1   | D     | 213 | VAL  | N-CA-C     | 9.07  | 119.87      | 110.62   |
| 1   | L     | 213 | VAL  | N-CA-C     | 9.06  | 119.87      | 110.62   |
| 1   | B     | 213 | VAL  | N-CA-C     | 9.06  | 119.86      | 110.62   |
| 1   | J     | 213 | VAL  | N-CA-C     | 9.06  | 119.86      | 110.62   |
| 1   | G     | 213 | VAL  | N-CA-C     | 9.05  | 119.85      | 110.62   |
| 1   | F     | 213 | VAL  | N-CA-C     | 9.05  | 119.85      | 110.62   |
| 1   | K     | 213 | VAL  | N-CA-C     | 9.04  | 119.84      | 110.62   |
| 1   | I     | 213 | VAL  | N-CA-C     | 9.03  | 119.83      | 110.62   |
| 1   | C     | 218 | GLN  | OE1-CD-NE2 | -8.83 | 113.77      | 122.60   |
| 1   | L     | 218 | GLN  | OE1-CD-NE2 | -8.80 | 113.80      | 122.60   |
| 1   | I     | 218 | GLN  | OE1-CD-NE2 | -8.80 | 113.80      | 122.60   |
| 1   | F     | 399 | LEU  | O-C-N      | 8.80  | 131.44      | 121.32   |
| 1   | E     | 218 | GLN  | OE1-CD-NE2 | -8.79 | 113.81      | 122.60   |
| 1   | A     | 218 | GLN  | OE1-CD-NE2 | -8.78 | 113.82      | 122.60   |
| 1   | J     | 218 | GLN  | OE1-CD-NE2 | -8.79 | 113.81      | 122.60   |
| 1   | K     | 399 | LEU  | O-C-N      | 8.78  | 131.41      | 121.32   |
| 1   | H     | 218 | GLN  | OE1-CD-NE2 | -8.77 | 113.83      | 122.60   |
| 1   | G     | 218 | GLN  | OE1-CD-NE2 | -8.77 | 113.83      | 122.60   |
| 1   | B     | 218 | GLN  | OE1-CD-NE2 | -8.76 | 113.84      | 122.60   |
| 1   | K     | 218 | GLN  | OE1-CD-NE2 | -8.76 | 113.84      | 122.60   |
| 1   | E     | 399 | LEU  | O-C-N      | 8.76  | 131.39      | 121.32   |
| 1   | J     | 399 | LEU  | O-C-N      | 8.76  | 131.39      | 121.32   |
| 1   | A     | 399 | LEU  | O-C-N      | 8.76  | 131.39      | 121.32   |
| 1   | B     | 399 | LEU  | O-C-N      | 8.76  | 131.39      | 121.32   |
| 1   | L     | 399 | LEU  | O-C-N      | 8.76  | 131.39      | 121.32   |
| 1   | H     | 399 | LEU  | O-C-N      | 8.75  | 131.38      | 121.32   |
| 1   | F     | 218 | GLN  | OE1-CD-NE2 | -8.75 | 113.85      | 122.60   |
| 1   | D     | 399 | LEU  | O-C-N      | 8.74  | 131.37      | 121.32   |
| 1   | C     | 399 | LEU  | O-C-N      | 8.73  | 131.37      | 121.32   |
| 1   | D     | 218 | GLN  | OE1-CD-NE2 | -8.72 | 113.88      | 122.60   |
| 1   | I     | 399 | LEU  | O-C-N      | 8.72  | 131.35      | 121.32   |
| 1   | G     | 399 | LEU  | O-C-N      | 8.72  | 131.35      | 121.32   |
| 1   | I     | 49  | PHE  | CA-CB-CG   | 8.37  | 122.17      | 113.80   |
| 1   | L     | 49  | PHE  | CA-CB-CG   | 8.35  | 122.15      | 113.80   |
| 1   | F     | 49  | PHE  | CA-CB-CG   | 8.33  | 122.13      | 113.80   |
| 1   | J     | 49  | PHE  | CA-CB-CG   | 8.32  | 122.12      | 113.80   |
| 1   | D     | 49  | PHE  | CA-CB-CG   | 8.32  | 122.12      | 113.80   |
| 1   | H     | 49  | PHE  | CA-CB-CG   | 8.32  | 122.12      | 113.80   |
| 1   | E     | 49  | PHE  | CA-CB-CG   | 8.31  | 122.11      | 113.80   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | K     | 49  | PHE  | CA-CB-CG | 8.31  | 122.11      | 113.80   |
| 1   | A     | 49  | PHE  | CA-CB-CG | 8.30  | 122.10      | 113.80   |
| 1   | G     | 49  | PHE  | CA-CB-CG | 8.29  | 122.09      | 113.80   |
| 1   | E     | 54  | ILE  | CA-C-N   | 8.28  | 129.57      | 121.62   |
| 1   | E     | 54  | ILE  | C-N-CA   | 8.28  | 129.57      | 121.62   |
| 1   | L     | 54  | ILE  | CA-C-N   | 8.28  | 129.57      | 121.62   |
| 1   | L     | 54  | ILE  | C-N-CA   | 8.28  | 129.57      | 121.62   |
| 1   | B     | 54  | ILE  | CA-C-N   | 8.28  | 129.57      | 121.62   |
| 1   | B     | 54  | ILE  | C-N-CA   | 8.28  | 129.57      | 121.62   |
| 1   | C     | 49  | PHE  | CA-CB-CG | 8.27  | 122.07      | 113.80   |
| 1   | B     | 49  | PHE  | CA-CB-CG | 8.27  | 122.07      | 113.80   |
| 1   | G     | 54  | ILE  | CA-C-N   | 8.27  | 129.56      | 121.62   |
| 1   | G     | 54  | ILE  | C-N-CA   | 8.27  | 129.56      | 121.62   |
| 1   | K     | 54  | ILE  | CA-C-N   | 8.27  | 129.56      | 121.62   |
| 1   | K     | 54  | ILE  | C-N-CA   | 8.27  | 129.56      | 121.62   |
| 1   | A     | 54  | ILE  | CA-C-N   | 8.26  | 129.55      | 121.62   |
| 1   | A     | 54  | ILE  | C-N-CA   | 8.26  | 129.55      | 121.62   |
| 1   | F     | 54  | ILE  | CA-C-N   | 8.26  | 129.55      | 121.62   |
| 1   | F     | 54  | ILE  | C-N-CA   | 8.26  | 129.55      | 121.62   |
| 1   | J     | 54  | ILE  | CA-C-N   | 8.25  | 129.54      | 121.62   |
| 1   | J     | 54  | ILE  | C-N-CA   | 8.25  | 129.54      | 121.62   |
| 1   | D     | 54  | ILE  | CA-C-N   | 8.24  | 129.53      | 121.62   |
| 1   | D     | 54  | ILE  | C-N-CA   | 8.24  | 129.53      | 121.62   |
| 1   | I     | 54  | ILE  | CA-C-N   | 8.24  | 129.53      | 121.62   |
| 1   | I     | 54  | ILE  | C-N-CA   | 8.24  | 129.53      | 121.62   |
| 1   | H     | 54  | ILE  | CA-C-N   | 8.23  | 129.53      | 121.62   |
| 1   | H     | 54  | ILE  | C-N-CA   | 8.23  | 129.53      | 121.62   |
| 1   | C     | 54  | ILE  | CA-C-N   | 8.20  | 129.50      | 121.62   |
| 1   | C     | 54  | ILE  | C-N-CA   | 8.20  | 129.50      | 121.62   |
| 1   | F     | 398 | ASP  | N-CA-C   | -7.70 | 103.77      | 113.01   |
| 1   | B     | 398 | ASP  | N-CA-C   | -7.69 | 103.78      | 113.01   |
| 1   | I     | 398 | ASP  | N-CA-C   | -7.67 | 103.80      | 113.01   |
| 1   | C     | 398 | ASP  | N-CA-C   | -7.67 | 103.81      | 113.01   |
| 1   | H     | 398 | ASP  | N-CA-C   | -7.67 | 103.81      | 113.01   |
| 1   | A     | 398 | ASP  | N-CA-C   | -7.67 | 103.81      | 113.01   |
| 1   | J     | 398 | ASP  | N-CA-C   | -7.66 | 103.81      | 113.01   |
| 1   | L     | 398 | ASP  | N-CA-C   | -7.66 | 103.81      | 113.01   |
| 1   | G     | 398 | ASP  | N-CA-C   | -7.66 | 103.82      | 113.01   |
| 1   | E     | 398 | ASP  | N-CA-C   | -7.66 | 103.82      | 113.01   |
| 1   | K     | 398 | ASP  | N-CA-C   | -7.64 | 103.84      | 113.01   |
| 1   | D     | 398 | ASP  | N-CA-C   | -7.64 | 103.84      | 113.01   |
| 1   | C     | 49  | PHE  | N-CA-C   | 7.64  | 118.35      | 108.34   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | J     | 49  | PHE  | N-CA-C   | 7.62  | 118.33      | 108.34   |
| 1   | A     | 49  | PHE  | N-CA-C   | 7.62  | 118.32      | 108.34   |
| 1   | D     | 49  | PHE  | N-CA-C   | 7.61  | 118.31      | 108.34   |
| 1   | F     | 49  | PHE  | N-CA-C   | 7.61  | 118.31      | 108.34   |
| 1   | K     | 49  | PHE  | N-CA-C   | 7.61  | 118.31      | 108.34   |
| 1   | G     | 49  | PHE  | N-CA-C   | 7.60  | 118.30      | 108.34   |
| 1   | B     | 49  | PHE  | N-CA-C   | 7.60  | 118.30      | 108.34   |
| 1   | H     | 49  | PHE  | N-CA-C   | 7.60  | 118.30      | 108.34   |
| 1   | E     | 49  | PHE  | N-CA-C   | 7.60  | 118.29      | 108.34   |
| 1   | L     | 49  | PHE  | N-CA-C   | 7.60  | 118.30      | 108.34   |
| 1   | I     | 49  | PHE  | N-CA-C   | 7.58  | 118.27      | 108.34   |
| 1   | B     | 64  | ASP  | N-CA-C   | 7.16  | 120.91      | 109.24   |
| 1   | F     | 64  | ASP  | N-CA-C   | 7.15  | 120.90      | 109.24   |
| 1   | K     | 64  | ASP  | N-CA-C   | 7.15  | 120.89      | 109.24   |
| 1   | C     | 64  | ASP  | N-CA-C   | 7.14  | 120.89      | 109.24   |
| 1   | A     | 64  | ASP  | N-CA-C   | 7.14  | 120.88      | 109.24   |
| 1   | E     | 64  | ASP  | N-CA-C   | 7.14  | 120.87      | 109.24   |
| 1   | J     | 64  | ASP  | N-CA-C   | 7.14  | 120.87      | 109.24   |
| 1   | D     | 64  | ASP  | N-CA-C   | 7.13  | 120.86      | 109.24   |
| 1   | I     | 64  | ASP  | N-CA-C   | 7.13  | 120.86      | 109.24   |
| 1   | H     | 64  | ASP  | N-CA-C   | 7.12  | 120.85      | 109.24   |
| 1   | G     | 64  | ASP  | N-CA-C   | 7.12  | 120.85      | 109.24   |
| 1   | L     | 64  | ASP  | N-CA-C   | 7.12  | 120.84      | 109.24   |
| 1   | G     | 178 | GLY  | CA-C-N   | -7.07 | 113.02      | 122.42   |
| 1   | G     | 178 | GLY  | C-N-CA   | -7.07 | 113.02      | 122.42   |
| 1   | C     | 178 | GLY  | CA-C-N   | -7.07 | 113.02      | 122.42   |
| 1   | C     | 178 | GLY  | C-N-CA   | -7.07 | 113.02      | 122.42   |
| 1   | I     | 178 | GLY  | CA-C-N   | -7.06 | 113.03      | 122.42   |
| 1   | I     | 178 | GLY  | C-N-CA   | -7.06 | 113.03      | 122.42   |
| 1   | J     | 178 | GLY  | CA-C-N   | -7.05 | 113.04      | 122.42   |
| 1   | J     | 178 | GLY  | C-N-CA   | -7.05 | 113.04      | 122.42   |
| 1   | D     | 178 | GLY  | CA-C-N   | -7.05 | 113.05      | 122.42   |
| 1   | D     | 178 | GLY  | C-N-CA   | -7.05 | 113.05      | 122.42   |
| 1   | A     | 178 | GLY  | CA-C-N   | -7.04 | 113.05      | 122.42   |
| 1   | A     | 178 | GLY  | C-N-CA   | -7.04 | 113.05      | 122.42   |
| 1   | K     | 178 | GLY  | CA-C-N   | -7.04 | 113.06      | 122.42   |
| 1   | K     | 178 | GLY  | C-N-CA   | -7.04 | 113.06      | 122.42   |
| 1   | L     | 398 | ASP  | CA-CB-CG | -7.03 | 105.57      | 112.60   |
| 1   | B     | 178 | GLY  | CA-C-N   | -7.03 | 113.08      | 122.42   |
| 1   | B     | 178 | GLY  | C-N-CA   | -7.03 | 113.08      | 122.42   |
| 1   | E     | 188 | ALA  | N-CA-C   | 7.02  | 121.16      | 112.59   |
| 1   | F     | 398 | ASP  | CA-CB-CG | -7.02 | 105.58      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | F     | 178 | GLY  | CA-C-N   | -7.02 | 113.08      | 122.42   |
| 1   | F     | 178 | GLY  | C-N-CA   | -7.02 | 113.08      | 122.42   |
| 1   | K     | 398 | ASP  | CA-CB-CG | -7.02 | 105.58      | 112.60   |
| 1   | L     | 178 | GLY  | CA-C-N   | -7.02 | 113.08      | 122.42   |
| 1   | L     | 178 | GLY  | C-N-CA   | -7.02 | 113.08      | 122.42   |
| 1   | H     | 178 | GLY  | CA-C-N   | -7.02 | 113.09      | 122.42   |
| 1   | H     | 178 | GLY  | C-N-CA   | -7.02 | 113.09      | 122.42   |
| 1   | D     | 188 | ALA  | N-CA-C   | 7.01  | 121.14      | 112.59   |
| 1   | E     | 178 | GLY  | CA-C-N   | -7.01 | 113.10      | 122.42   |
| 1   | E     | 178 | GLY  | C-N-CA   | -7.01 | 113.10      | 122.42   |
| 1   | H     | 188 | ALA  | N-CA-C   | 7.01  | 121.14      | 112.59   |
| 1   | J     | 398 | ASP  | CA-CB-CG | -7.00 | 105.60      | 112.60   |
| 1   | K     | 188 | ALA  | N-CA-C   | 7.00  | 121.13      | 112.59   |
| 1   | A     | 398 | ASP  | CA-CB-CG | -7.00 | 105.60      | 112.60   |
| 1   | J     | 188 | ALA  | N-CA-C   | 7.00  | 121.13      | 112.59   |
| 1   | H     | 398 | ASP  | CA-CB-CG | -7.00 | 105.60      | 112.60   |
| 1   | I     | 398 | ASP  | CA-CB-CG | -7.00 | 105.60      | 112.60   |
| 1   | B     | 188 | ALA  | N-CA-C   | 6.99  | 121.11      | 112.59   |
| 1   | A     | 188 | ALA  | N-CA-C   | 6.98  | 121.11      | 112.59   |
| 1   | B     | 398 | ASP  | CA-CB-CG | -6.98 | 105.62      | 112.60   |
| 1   | G     | 398 | ASP  | CA-CB-CG | -6.98 | 105.62      | 112.60   |
| 1   | G     | 188 | ALA  | N-CA-C   | 6.98  | 121.10      | 112.59   |
| 1   | C     | 188 | ALA  | N-CA-C   | 6.97  | 121.10      | 112.59   |
| 1   | L     | 188 | ALA  | N-CA-C   | 6.97  | 121.10      | 112.59   |
| 1   | I     | 188 | ALA  | N-CA-C   | 6.97  | 121.09      | 112.59   |
| 1   | F     | 188 | ALA  | N-CA-C   | 6.96  | 121.08      | 112.59   |
| 1   | C     | 398 | ASP  | CA-CB-CG | -6.96 | 105.64      | 112.60   |
| 1   | E     | 398 | ASP  | CA-CB-CG | -6.95 | 105.65      | 112.60   |
| 1   | D     | 398 | ASP  | CA-CB-CG | -6.95 | 105.65      | 112.60   |
| 1   | K     | 180 | PHE  | CA-C-N   | -6.92 | 112.84      | 119.90   |
| 1   | K     | 180 | PHE  | C-N-CA   | -6.92 | 112.84      | 119.90   |
| 1   | L     | 180 | PHE  | CA-C-N   | -6.92 | 112.84      | 119.90   |
| 1   | L     | 180 | PHE  | C-N-CA   | -6.92 | 112.84      | 119.90   |
| 1   | E     | 180 | PHE  | CA-C-N   | -6.91 | 112.86      | 119.90   |
| 1   | E     | 180 | PHE  | C-N-CA   | -6.91 | 112.86      | 119.90   |
| 1   | C     | 180 | PHE  | CA-C-N   | -6.90 | 112.86      | 119.90   |
| 1   | C     | 180 | PHE  | C-N-CA   | -6.90 | 112.86      | 119.90   |
| 1   | I     | 180 | PHE  | CA-C-N   | -6.90 | 112.86      | 119.90   |
| 1   | I     | 180 | PHE  | C-N-CA   | -6.90 | 112.86      | 119.90   |
| 1   | J     | 180 | PHE  | CA-C-N   | -6.90 | 112.87      | 119.90   |
| 1   | J     | 180 | PHE  | C-N-CA   | -6.90 | 112.87      | 119.90   |
| 1   | H     | 180 | PHE  | CA-C-N   | -6.89 | 112.87      | 119.90   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | H     | 180 | PHE  | C-N-CA    | -6.89 | 112.87      | 119.90   |
| 1   | A     | 180 | PHE  | CA-C-N    | -6.89 | 112.88      | 119.90   |
| 1   | A     | 180 | PHE  | C-N-CA    | -6.89 | 112.88      | 119.90   |
| 1   | D     | 180 | PHE  | CA-C-N    | -6.88 | 112.88      | 119.90   |
| 1   | D     | 180 | PHE  | C-N-CA    | -6.88 | 112.88      | 119.90   |
| 1   | G     | 180 | PHE  | CA-C-N    | -6.88 | 112.88      | 119.90   |
| 1   | G     | 180 | PHE  | C-N-CA    | -6.88 | 112.88      | 119.90   |
| 1   | B     | 180 | PHE  | CA-C-N    | -6.88 | 112.89      | 119.90   |
| 1   | B     | 180 | PHE  | C-N-CA    | -6.88 | 112.89      | 119.90   |
| 1   | F     | 180 | PHE  | CA-C-N    | -6.85 | 112.91      | 119.90   |
| 1   | F     | 180 | PHE  | C-N-CA    | -6.85 | 112.91      | 119.90   |
| 1   | J     | 218 | GLN  | CG-CD-NE2 | 6.72  | 126.47      | 116.40   |
| 1   | E     | 218 | GLN  | CG-CD-NE2 | 6.71  | 126.46      | 116.40   |
| 1   | C     | 218 | GLN  | CG-CD-NE2 | 6.70  | 126.45      | 116.40   |
| 1   | B     | 218 | GLN  | CG-CD-NE2 | 6.70  | 126.45      | 116.40   |
| 1   | I     | 218 | GLN  | CG-CD-NE2 | 6.70  | 126.45      | 116.40   |
| 1   | L     | 218 | GLN  | CG-CD-NE2 | 6.70  | 126.45      | 116.40   |
| 1   | K     | 218 | GLN  | CG-CD-NE2 | 6.70  | 126.44      | 116.40   |
| 1   | A     | 218 | GLN  | CG-CD-NE2 | 6.69  | 126.44      | 116.40   |
| 1   | G     | 218 | GLN  | CG-CD-NE2 | 6.69  | 126.43      | 116.40   |
| 1   | H     | 218 | GLN  | CG-CD-NE2 | 6.68  | 126.43      | 116.40   |
| 1   | D     | 218 | GLN  | CG-CD-NE2 | 6.67  | 126.40      | 116.40   |
| 1   | F     | 218 | GLN  | CG-CD-NE2 | 6.66  | 126.39      | 116.40   |
| 1   | I     | 66  | VAL  | N-CA-C    | 6.42  | 117.16      | 108.17   |
| 1   | D     | 66  | VAL  | N-CA-C    | 6.42  | 117.16      | 108.17   |
| 1   | J     | 66  | VAL  | N-CA-C    | 6.41  | 117.14      | 108.17   |
| 1   | K     | 66  | VAL  | N-CA-C    | 6.41  | 117.14      | 108.17   |
| 1   | L     | 66  | VAL  | N-CA-C    | 6.41  | 117.14      | 108.17   |
| 1   | C     | 66  | VAL  | N-CA-C    | 6.41  | 117.14      | 108.17   |
| 1   | A     | 66  | VAL  | N-CA-C    | 6.40  | 117.14      | 108.17   |
| 1   | E     | 66  | VAL  | N-CA-C    | 6.40  | 117.13      | 108.17   |
| 1   | G     | 66  | VAL  | N-CA-C    | 6.40  | 117.13      | 108.17   |
| 1   | B     | 66  | VAL  | N-CA-C    | 6.40  | 117.13      | 108.17   |
| 1   | F     | 66  | VAL  | N-CA-C    | 6.39  | 117.11      | 108.17   |
| 1   | H     | 66  | VAL  | N-CA-C    | 6.37  | 117.09      | 108.17   |
| 1   | E     | 425 | ARG  | N-CA-C    | 6.23  | 120.62      | 112.89   |
| 1   | I     | 425 | ARG  | N-CA-C    | 6.22  | 120.61      | 112.89   |
| 1   | D     | 425 | ARG  | N-CA-C    | 6.22  | 120.60      | 112.89   |
| 1   | G     | 425 | ARG  | N-CA-C    | 6.21  | 120.59      | 112.89   |
| 1   | F     | 425 | ARG  | N-CA-C    | 6.21  | 120.59      | 112.89   |
| 1   | C     | 425 | ARG  | N-CA-C    | 6.21  | 120.59      | 112.89   |
| 1   | A     | 425 | ARG  | N-CA-C    | 6.21  | 120.59      | 112.89   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | L     | 425 | ARG  | N-CA-C | 6.20  | 120.58      | 112.89   |
| 1   | J     | 425 | ARG  | N-CA-C | 6.20  | 120.58      | 112.89   |
| 1   | K     | 425 | ARG  | N-CA-C | 6.20  | 120.57      | 112.89   |
| 1   | B     | 425 | ARG  | N-CA-C | 6.19  | 120.57      | 112.89   |
| 1   | H     | 425 | ARG  | N-CA-C | 6.17  | 120.54      | 112.89   |
| 1   | D     | 325 | GLY  | N-CA-C | -5.95 | 104.41      | 112.57   |
| 1   | F     | 325 | GLY  | N-CA-C | -5.95 | 104.42      | 112.57   |
| 1   | G     | 325 | GLY  | N-CA-C | -5.95 | 104.42      | 112.57   |
| 1   | C     | 325 | GLY  | N-CA-C | -5.95 | 104.42      | 112.57   |
| 1   | J     | 325 | GLY  | N-CA-C | -5.94 | 104.43      | 112.57   |
| 1   | B     | 325 | GLY  | N-CA-C | -5.93 | 104.44      | 112.57   |
| 1   | A     | 325 | GLY  | N-CA-C | -5.93 | 104.44      | 112.57   |
| 1   | K     | 325 | GLY  | N-CA-C | -5.93 | 104.45      | 112.57   |
| 1   | L     | 325 | GLY  | N-CA-C | -5.92 | 104.46      | 112.57   |
| 1   | E     | 325 | GLY  | N-CA-C | -5.91 | 104.47      | 112.57   |
| 1   | H     | 325 | GLY  | N-CA-C | -5.90 | 104.49      | 112.57   |
| 1   | I     | 325 | GLY  | N-CA-C | -5.90 | 104.49      | 112.57   |
| 1   | H     | 58  | LYS  | N-CA-C | 5.79  | 117.90      | 108.63   |
| 1   | B     | 58  | LYS  | N-CA-C | 5.78  | 117.87      | 108.63   |
| 1   | E     | 58  | LYS  | N-CA-C | 5.77  | 117.86      | 108.63   |
| 1   | I     | 58  | LYS  | N-CA-C | 5.77  | 117.86      | 108.63   |
| 1   | A     | 58  | LYS  | N-CA-C | 5.76  | 117.85      | 108.63   |
| 1   | C     | 58  | LYS  | N-CA-C | 5.76  | 117.85      | 108.63   |
| 1   | D     | 58  | LYS  | N-CA-C | 5.75  | 117.82      | 108.63   |
| 1   | K     | 58  | LYS  | N-CA-C | 5.75  | 117.82      | 108.63   |
| 1   | L     | 58  | LYS  | N-CA-C | 5.75  | 117.82      | 108.63   |
| 1   | F     | 58  | LYS  | N-CA-C | 5.74  | 117.82      | 108.63   |
| 1   | G     | 58  | LYS  | N-CA-C | 5.73  | 117.80      | 108.63   |
| 1   | J     | 58  | LYS  | N-CA-C | 5.73  | 117.80      | 108.63   |
| 1   | C     | 244 | ASN  | N-CA-C | 5.70  | 119.41      | 112.23   |
| 1   | F     | 244 | ASN  | N-CA-C | 5.70  | 119.41      | 112.23   |
| 1   | K     | 244 | ASN  | N-CA-C | 5.69  | 119.40      | 112.23   |
| 1   | D     | 244 | ASN  | N-CA-C | 5.69  | 119.40      | 112.23   |
| 1   | B     | 244 | ASN  | N-CA-C | 5.68  | 119.39      | 112.23   |
| 1   | J     | 244 | ASN  | N-CA-C | 5.68  | 119.39      | 112.23   |
| 1   | A     | 244 | ASN  | N-CA-C | 5.67  | 119.37      | 112.23   |
| 1   | E     | 244 | ASN  | N-CA-C | 5.65  | 119.35      | 112.23   |
| 1   | H     | 244 | ASN  | N-CA-C | 5.65  | 119.35      | 112.23   |
| 1   | I     | 244 | ASN  | N-CA-C | 5.65  | 119.35      | 112.23   |
| 1   | L     | 60  | ILE  | N-CA-C | 5.65  | 116.29      | 110.36   |
| 1   | L     | 244 | ASN  | N-CA-C | 5.65  | 119.34      | 112.23   |
| 1   | G     | 244 | ASN  | N-CA-C | 5.64  | 119.34      | 112.23   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 60  | ILE  | N-CA-C | 5.63  | 116.27      | 110.36   |
| 1   | F     | 60  | ILE  | N-CA-C | 5.63  | 116.27      | 110.36   |
| 1   | E     | 60  | ILE  | N-CA-C | 5.63  | 116.27      | 110.36   |
| 1   | G     | 60  | ILE  | N-CA-C | 5.62  | 116.27      | 110.36   |
| 1   | C     | 60  | ILE  | N-CA-C | 5.62  | 116.26      | 110.36   |
| 1   | J     | 60  | ILE  | N-CA-C | 5.62  | 116.26      | 110.36   |
| 1   | A     | 60  | ILE  | N-CA-C | 5.61  | 116.25      | 110.36   |
| 1   | I     | 60  | ILE  | N-CA-C | 5.61  | 116.25      | 110.36   |
| 1   | K     | 60  | ILE  | N-CA-C | 5.60  | 116.24      | 110.36   |
| 1   | H     | 60  | ILE  | N-CA-C | 5.59  | 116.23      | 110.36   |
| 1   | J     | 340 | SER  | N-CA-C | -5.59 | 105.96      | 112.89   |
| 1   | L     | 314 | PRO  | N-CA-C | 5.59  | 120.49      | 114.68   |
| 1   | D     | 60  | ILE  | N-CA-C | 5.58  | 116.22      | 110.36   |
| 1   | K     | 340 | SER  | N-CA-C | -5.58 | 105.97      | 112.89   |
| 1   | G     | 340 | SER  | N-CA-C | -5.58 | 105.97      | 112.89   |
| 1   | F     | 340 | SER  | N-CA-C | -5.57 | 105.98      | 112.89   |
| 1   | H     | 314 | PRO  | N-CA-C | 5.57  | 120.47      | 114.68   |
| 1   | E     | 340 | SER  | N-CA-C | -5.57 | 105.98      | 112.89   |
| 1   | A     | 340 | SER  | N-CA-C | -5.57 | 105.99      | 112.89   |
| 1   | H     | 340 | SER  | N-CA-C | -5.57 | 105.99      | 112.89   |
| 1   | D     | 340 | SER  | N-CA-C | -5.56 | 105.99      | 112.89   |
| 1   | G     | 314 | PRO  | N-CA-C | 5.56  | 120.47      | 114.68   |
| 1   | L     | 340 | SER  | N-CA-C | -5.56 | 105.99      | 112.89   |
| 1   | B     | 340 | SER  | N-CA-C | -5.55 | 106.01      | 112.89   |
| 1   | C     | 340 | SER  | N-CA-C | -5.55 | 106.01      | 112.89   |
| 1   | I     | 340 | SER  | N-CA-C | -5.55 | 106.01      | 112.89   |
| 1   | F     | 314 | PRO  | N-CA-C | 5.54  | 120.44      | 114.68   |
| 1   | A     | 314 | PRO  | N-CA-C | 5.54  | 120.44      | 114.68   |
| 1   | C     | 43  | PHE  | N-CA-C | 5.53  | 118.24      | 111.82   |
| 1   | F     | 43  | PHE  | N-CA-C | 5.53  | 118.24      | 111.82   |
| 1   | I     | 314 | PRO  | N-CA-C | 5.53  | 120.43      | 114.68   |
| 1   | D     | 314 | PRO  | N-CA-C | 5.53  | 120.43      | 114.68   |
| 1   | H     | 43  | PHE  | N-CA-C | 5.53  | 118.23      | 111.82   |
| 1   | J     | 43  | PHE  | N-CA-C | 5.52  | 118.23      | 111.82   |
| 1   | K     | 314 | PRO  | N-CA-C | 5.52  | 120.42      | 114.68   |
| 1   | A     | 43  | PHE  | N-CA-C | 5.52  | 118.22      | 111.82   |
| 1   | B     | 314 | PRO  | N-CA-C | 5.51  | 120.41      | 114.68   |
| 1   | K     | 43  | PHE  | N-CA-C | 5.51  | 118.21      | 111.82   |
| 1   | E     | 314 | PRO  | N-CA-C | 5.51  | 120.41      | 114.68   |
| 1   | I     | 43  | PHE  | N-CA-C | 5.51  | 118.21      | 111.82   |
| 1   | G     | 43  | PHE  | N-CA-C | 5.50  | 118.20      | 111.82   |
| 1   | L     | 43  | PHE  | N-CA-C | 5.50  | 118.20      | 111.82   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | D     | 426 | GLU  | N-CA-C | 5.50 | 117.98      | 111.33   |
| 1   | J     | 314 | PRO  | N-CA-C | 5.50 | 120.40      | 114.68   |
| 1   | B     | 43  | PHE  | N-CA-C | 5.50 | 118.20      | 111.82   |
| 1   | C     | 314 | PRO  | N-CA-C | 5.50 | 120.40      | 114.68   |
| 1   | D     | 43  | PHE  | N-CA-C | 5.49 | 118.19      | 111.82   |
| 1   | E     | 43  | PHE  | N-CA-C | 5.47 | 118.17      | 111.82   |
| 1   | J     | 426 | GLU  | N-CA-C | 5.47 | 117.95      | 111.33   |
| 1   | F     | 426 | GLU  | N-CA-C | 5.47 | 117.95      | 111.33   |
| 1   | L     | 426 | GLU  | N-CA-C | 5.47 | 117.95      | 111.33   |
| 1   | E     | 426 | GLU  | N-CA-C | 5.47 | 117.95      | 111.33   |
| 1   | I     | 426 | GLU  | N-CA-C | 5.45 | 117.93      | 111.33   |
| 1   | A     | 426 | GLU  | N-CA-C | 5.45 | 117.92      | 111.33   |
| 1   | C     | 426 | GLU  | N-CA-C | 5.45 | 117.92      | 111.33   |
| 1   | G     | 426 | GLU  | N-CA-C | 5.43 | 117.91      | 111.33   |
| 1   | H     | 426 | GLU  | N-CA-C | 5.43 | 117.90      | 111.33   |
| 1   | K     | 426 | GLU  | N-CA-C | 5.42 | 117.89      | 111.33   |
| 1   | B     | 426 | GLU  | N-CA-C | 5.41 | 117.88      | 111.33   |
| 1   | J     | 313 | ASN  | CA-C-N | 5.39 | 126.33      | 120.83   |
| 1   | J     | 313 | ASN  | C-N-CA | 5.39 | 126.33      | 120.83   |
| 1   | I     | 313 | ASN  | CA-C-N | 5.39 | 126.33      | 120.83   |
| 1   | I     | 313 | ASN  | C-N-CA | 5.39 | 126.33      | 120.83   |
| 1   | B     | 313 | ASN  | CA-C-N | 5.38 | 126.31      | 120.83   |
| 1   | B     | 313 | ASN  | C-N-CA | 5.38 | 126.31      | 120.83   |
| 1   | F     | 400 | PRO  | N-CA-C | 5.37 | 117.25      | 110.70   |
| 1   | D     | 313 | ASN  | CA-C-N | 5.37 | 126.31      | 120.83   |
| 1   | D     | 313 | ASN  | C-N-CA | 5.37 | 126.31      | 120.83   |
| 1   | F     | 313 | ASN  | CA-C-N | 5.37 | 126.30      | 120.83   |
| 1   | F     | 313 | ASN  | C-N-CA | 5.37 | 126.30      | 120.83   |
| 1   | L     | 400 | PRO  | N-CA-C | 5.37 | 117.25      | 110.70   |
| 1   | J     | 400 | PRO  | N-CA-C | 5.36 | 117.24      | 110.70   |
| 1   | B     | 400 | PRO  | N-CA-C | 5.36 | 117.24      | 110.70   |
| 1   | C     | 400 | PRO  | N-CA-C | 5.35 | 117.23      | 110.70   |
| 1   | E     | 400 | PRO  | N-CA-C | 5.35 | 117.23      | 110.70   |
| 1   | K     | 313 | ASN  | CA-C-N | 5.35 | 126.29      | 120.83   |
| 1   | K     | 313 | ASN  | C-N-CA | 5.35 | 126.29      | 120.83   |
| 1   | A     | 313 | ASN  | CA-C-N | 5.35 | 126.29      | 120.83   |
| 1   | A     | 313 | ASN  | C-N-CA | 5.35 | 126.29      | 120.83   |
| 1   | C     | 313 | ASN  | CA-C-N | 5.35 | 126.29      | 120.83   |
| 1   | C     | 313 | ASN  | C-N-CA | 5.35 | 126.29      | 120.83   |
| 1   | D     | 400 | PRO  | N-CA-C | 5.35 | 117.23      | 110.70   |
| 1   | G     | 400 | PRO  | N-CA-C | 5.35 | 117.22      | 110.70   |
| 1   | K     | 400 | PRO  | N-CA-C | 5.35 | 117.23      | 110.70   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | H     | 400 | PRO  | N-CA-C   | 5.35  | 117.22      | 110.70   |
| 1   | E     | 313 | ASN  | CA-C-N   | 5.35  | 126.28      | 120.83   |
| 1   | E     | 313 | ASN  | C-N-CA   | 5.35  | 126.28      | 120.83   |
| 1   | A     | 400 | PRO  | N-CA-C   | 5.34  | 117.22      | 110.70   |
| 1   | G     | 313 | ASN  | CA-C-N   | 5.34  | 126.28      | 120.83   |
| 1   | G     | 313 | ASN  | C-N-CA   | 5.34  | 126.28      | 120.83   |
| 1   | H     | 313 | ASN  | CA-C-N   | 5.33  | 126.27      | 120.83   |
| 1   | H     | 313 | ASN  | C-N-CA   | 5.33  | 126.27      | 120.83   |
| 1   | L     | 313 | ASN  | CA-C-N   | 5.33  | 126.27      | 120.83   |
| 1   | L     | 313 | ASN  | C-N-CA   | 5.33  | 126.27      | 120.83   |
| 1   | I     | 400 | PRO  | N-CA-C   | 5.32  | 117.19      | 110.70   |
| 1   | F     | 397 | TYR  | CA-CB-CG | 5.32  | 123.47      | 113.90   |
| 1   | C     | 397 | TYR  | CA-CB-CG | 5.31  | 123.46      | 113.90   |
| 1   | I     | 397 | TYR  | CA-CB-CG | 5.31  | 123.46      | 113.90   |
| 1   | H     | 397 | TYR  | CA-CB-CG | 5.31  | 123.45      | 113.90   |
| 1   | J     | 397 | TYR  | CA-CB-CG | 5.31  | 123.45      | 113.90   |
| 1   | A     | 397 | TYR  | CA-CB-CG | 5.30  | 123.45      | 113.90   |
| 1   | E     | 397 | TYR  | CA-CB-CG | 5.30  | 123.44      | 113.90   |
| 1   | K     | 397 | TYR  | CA-CB-CG | 5.30  | 123.44      | 113.90   |
| 1   | B     | 397 | TYR  | CA-CB-CG | 5.29  | 123.43      | 113.90   |
| 1   | L     | 397 | TYR  | CA-CB-CG | 5.29  | 123.42      | 113.90   |
| 1   | D     | 397 | TYR  | CA-CB-CG | 5.29  | 123.42      | 113.90   |
| 1   | G     | 397 | TYR  | CA-CB-CG | 5.28  | 123.41      | 113.90   |
| 1   | D     | 408 | PRO  | CB-CA-C  | 5.20  | 118.17      | 111.46   |
| 1   | F     | 408 | PRO  | CB-CA-C  | 5.20  | 118.17      | 111.46   |
| 1   | L     | 408 | PRO  | CB-CA-C  | 5.19  | 118.16      | 111.46   |
| 1   | H     | 408 | PRO  | CB-CA-C  | 5.19  | 118.16      | 111.46   |
| 1   | I     | 57  | TRP  | N-CA-C   | -5.19 | 106.90      | 114.12   |
| 1   | B     | 408 | PRO  | CB-CA-C  | 5.19  | 118.16      | 111.46   |
| 1   | I     | 408 | PRO  | CB-CA-C  | 5.19  | 118.16      | 111.46   |
| 1   | E     | 57  | TRP  | N-CA-C   | -5.19 | 106.91      | 114.12   |
| 1   | H     | 57  | TRP  | N-CA-C   | -5.19 | 106.91      | 114.12   |
| 1   | D     | 181 | PRO  | CA-N-CD  | -5.19 | 104.74      | 112.00   |
| 1   | K     | 181 | PRO  | CA-N-CD  | -5.19 | 104.74      | 112.00   |
| 1   | L     | 57  | TRP  | N-CA-C   | -5.19 | 106.91      | 114.12   |
| 1   | B     | 57  | TRP  | N-CA-C   | -5.18 | 106.92      | 114.12   |
| 1   | L     | 181 | PRO  | CA-N-CD  | -5.18 | 104.74      | 112.00   |
| 1   | A     | 408 | PRO  | CB-CA-C  | 5.18  | 118.14      | 111.46   |
| 1   | E     | 181 | PRO  | CA-N-CD  | -5.17 | 104.76      | 112.00   |
| 1   | J     | 181 | PRO  | CA-N-CD  | -5.17 | 104.75      | 112.00   |
| 1   | A     | 57  | TRP  | N-CA-C   | -5.17 | 106.93      | 114.12   |
| 1   | C     | 181 | PRO  | CA-N-CD  | -5.17 | 104.77      | 112.00   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 408 | PRO  | CB-CA-C | 5.17  | 118.12      | 111.46   |
| 1   | C     | 408 | PRO  | CB-CA-C | 5.17  | 118.12      | 111.46   |
| 1   | J     | 408 | PRO  | CB-CA-C | 5.17  | 118.12      | 111.46   |
| 1   | A     | 181 | PRO  | CA-N-CD | -5.16 | 104.77      | 112.00   |
| 1   | E     | 408 | PRO  | CB-CA-C | 5.16  | 118.12      | 111.46   |
| 1   | G     | 181 | PRO  | CA-N-CD | -5.16 | 104.77      | 112.00   |
| 1   | I     | 181 | PRO  | CA-N-CD | -5.16 | 104.78      | 112.00   |
| 1   | J     | 57  | TRP  | N-CA-C  | -5.16 | 106.95      | 114.12   |
| 1   | B     | 181 | PRO  | CA-N-CD | -5.16 | 104.78      | 112.00   |
| 1   | C     | 57  | TRP  | N-CA-C  | -5.16 | 106.95      | 114.12   |
| 1   | F     | 181 | PRO  | CA-N-CD | -5.16 | 104.78      | 112.00   |
| 1   | G     | 408 | PRO  | CB-CA-C | 5.15  | 118.11      | 111.46   |
| 1   | K     | 57  | TRP  | N-CA-C  | -5.15 | 106.96      | 114.12   |
| 1   | D     | 57  | TRP  | N-CA-C  | -5.15 | 106.96      | 114.12   |
| 1   | G     | 57  | TRP  | N-CA-C  | -5.15 | 106.97      | 114.12   |
| 1   | H     | 181 | PRO  | CA-N-CD | -5.14 | 104.80      | 112.00   |
| 1   | F     | 57  | TRP  | N-CA-C  | -5.13 | 106.98      | 114.12   |
| 1   | H     | 170 | GLY  | CA-C-N  | -5.03 | 115.32      | 122.77   |
| 1   | H     | 170 | GLY  | C-N-CA  | -5.03 | 115.32      | 122.77   |
| 1   | J     | 170 | GLY  | CA-C-N  | -5.02 | 115.34      | 122.77   |
| 1   | J     | 170 | GLY  | C-N-CA  | -5.02 | 115.34      | 122.77   |
| 1   | A     | 170 | GLY  | CA-C-N  | -5.02 | 115.34      | 122.77   |
| 1   | A     | 170 | GLY  | C-N-CA  | -5.02 | 115.34      | 122.77   |
| 1   | H     | 49  | PHE  | CA-C-N  | 5.01  | 131.72      | 123.25   |
| 1   | H     | 49  | PHE  | C-N-CA  | 5.01  | 131.72      | 123.25   |
| 1   | D     | 170 | GLY  | CA-C-N  | -5.01 | 115.35      | 122.77   |
| 1   | D     | 170 | GLY  | C-N-CA  | -5.01 | 115.35      | 122.77   |
| 1   | E     | 170 | GLY  | CA-C-N  | -5.01 | 115.35      | 122.77   |
| 1   | E     | 170 | GLY  | C-N-CA  | -5.01 | 115.35      | 122.77   |
| 1   | E     | 49  | PHE  | CA-C-N  | 5.00  | 131.71      | 123.25   |
| 1   | E     | 49  | PHE  | C-N-CA  | 5.00  | 131.71      | 123.25   |
| 1   | I     | 170 | GLY  | CA-C-N  | -5.00 | 115.36      | 122.77   |
| 1   | I     | 170 | GLY  | C-N-CA  | -5.00 | 115.36      | 122.77   |
| 1   | C     | 170 | GLY  | CA-C-N  | -5.00 | 115.37      | 122.77   |
| 1   | C     | 170 | GLY  | C-N-CA  | -5.00 | 115.37      | 122.77   |

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     | 3637  | 0        | 3542     | 186     | 0            |
| 1   | B     | 3637  | 0        | 3543     | 187     | 0            |
| 1   | C     | 3637  | 0        | 3543     | 189     | 0            |
| 1   | D     | 3637  | 0        | 3542     | 180     | 0            |
| 1   | E     | 3637  | 0        | 3543     | 177     | 0            |
| 1   | F     | 3637  | 0        | 3543     | 175     | 0            |
| 1   | G     | 3637  | 0        | 3542     | 182     | 0            |
| 1   | H     | 3637  | 0        | 3543     | 185     | 0            |
| 1   | I     | 3637  | 0        | 3542     | 190     | 0            |
| 1   | J     | 3637  | 0        | 3543     | 194     | 0            |
| 1   | K     | 3637  | 0        | 3543     | 188     | 0            |
| 1   | L     | 3637  | 0        | 3543     | 181     | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | J     | 2     | 0        | 0        | 0       | 0            |
| 2   | K     | 2     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 27    | 0        | 10       | 4       | 0            |
| 3   | B     | 27    | 0        | 10       | 4       | 0            |
| 3   | C     | 27    | 0        | 10       | 4       | 0            |
| 3   | D     | 27    | 0        | 10       | 4       | 0            |
| 3   | E     | 27    | 0        | 10       | 4       | 0            |
| 3   | F     | 27    | 0        | 10       | 4       | 0            |
| 3   | G     | 27    | 0        | 10       | 4       | 0            |
| 3   | H     | 27    | 0        | 10       | 4       | 0            |
| 3   | I     | 27    | 0        | 10       | 3       | 0            |
| 3   | J     | 27    | 0        | 10       | 4       | 0            |
| 3   | K     | 27    | 0        | 10       | 4       | 0            |
| 3   | L     | 27    | 0        | 10       | 4       | 0            |
| 4   | A     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | B     | 2     | 0        | 0        | 0       | 0            |
| 4   | C     | 2     | 0        | 0        | 0       | 0            |
| 4   | D     | 2     | 0        | 0        | 0       | 0            |
| 4   | E     | 2     | 0        | 0        | 0       | 0            |
| 4   | F     | 2     | 0        | 0        | 0       | 0            |
| 4   | G     | 2     | 0        | 0        | 0       | 0            |
| 4   | H     | 2     | 0        | 0        | 0       | 0            |
| 4   | I     | 2     | 0        | 0        | 0       | 0            |
| 4   | J     | 2     | 0        | 0        | 0       | 0            |
| 4   | K     | 2     | 0        | 0        | 0       | 0            |
| 4   | L     | 2     | 0        | 0        | 0       | 0            |
| 5   | A     | 8     | 0        | 14       | 28      | 0            |
| 5   | B     | 8     | 0        | 14       | 33      | 0            |
| 5   | C     | 8     | 0        | 14       | 32      | 0            |
| 5   | D     | 8     | 0        | 14       | 33      | 0            |
| 5   | E     | 8     | 0        | 14       | 28      | 0            |
| 5   | F     | 8     | 0        | 14       | 33      | 0            |
| 5   | G     | 8     | 0        | 14       | 30      | 0            |
| 5   | H     | 8     | 0        | 14       | 32      | 0            |
| 5   | I     | 8     | 0        | 14       | 34      | 0            |
| 5   | J     | 8     | 0        | 14       | 33      | 0            |
| 5   | K     | 8     | 0        | 14       | 32      | 0            |
| 5   | L     | 8     | 0        | 14       | 31      | 0            |
| 6   | A     | 120   | 0        | 0        | 7       | 0            |
| 6   | B     | 121   | 0        | 0        | 6       | 0            |
| 6   | C     | 119   | 0        | 0        | 5       | 0            |
| 6   | D     | 122   | 0        | 0        | 6       | 0            |
| 6   | E     | 122   | 0        | 0        | 7       | 0            |
| 6   | F     | 121   | 0        | 0        | 5       | 0            |
| 6   | G     | 122   | 0        | 0        | 6       | 0            |
| 6   | H     | 121   | 0        | 0        | 5       | 0            |
| 6   | I     | 122   | 0        | 0        | 6       | 0            |
| 6   | J     | 120   | 0        | 0        | 6       | 0            |
| 6   | K     | 123   | 0        | 0        | 6       | 0            |
| 6   | L     | 119   | 0        | 0        | 6       | 0            |
| All | All   | 45564 | 0        | 42800    | 2078    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2078) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 3:K:1481:ADP:N9 | 3:K:1481:ADP:C1' | 1.71                     | 1.54              |
| 3:I:1479:ADP:N9 | 3:I:1479:ADP:C1' | 1.71                     | 1.54              |
| 3:B:1472:ADP:N9 | 3:B:1472:ADP:C1' | 1.71                     | 1.52              |
| 3:F:1476:ADP:N9 | 3:F:1476:ADP:C1' | 1.71                     | 1.52              |
| 3:E:1475:ADP:N9 | 3:E:1475:ADP:C1' | 1.71                     | 1.51              |
| 3:H:1478:ADP:N9 | 3:H:1478:ADP:C1' | 1.71                     | 1.51              |
| 3:G:1477:ADP:N9 | 3:G:1477:ADP:C1' | 1.71                     | 1.51              |
| 3:C:1473:ADP:N9 | 3:C:1473:ADP:C1' | 1.71                     | 1.50              |
| 3:J:1480:ADP:N9 | 3:J:1480:ADP:C1' | 1.71                     | 1.50              |
| 3:D:1474:ADP:N9 | 3:D:1474:ADP:C1' | 1.71                     | 1.50              |
| 3:L:1482:ADP:N9 | 3:L:1482:ADP:C1' | 1.71                     | 1.49              |
| 3:A:1471:ADP:N9 | 3:A:1471:ADP:C1' | 1.71                     | 1.47              |
| 1:E:398:ASP:O   | 1:E:400:PRO:HD3  | 1.29                     | 1.33              |
| 1:J:398:ASP:O   | 1:J:400:PRO:HD3  | 1.29                     | 1.33              |
| 1:A:398:ASP:O   | 1:A:400:PRO:HD3  | 1.29                     | 1.33              |
| 1:B:398:ASP:O   | 1:B:400:PRO:HD3  | 1.29                     | 1.31              |
| 1:D:398:ASP:O   | 1:D:400:PRO:HD3  | 1.29                     | 1.30              |
| 1:L:398:ASP:O   | 1:L:400:PRO:HD3  | 1.29                     | 1.29              |
| 1:H:398:ASP:O   | 1:H:400:PRO:HD3  | 1.29                     | 1.27              |
| 1:K:398:ASP:O   | 1:K:400:PRO:HD3  | 1.29                     | 1.27              |
| 1:I:398:ASP:O   | 1:I:400:PRO:HD3  | 1.29                     | 1.26              |
| 1:C:398:ASP:O   | 1:C:400:PRO:HD3  | 1.29                     | 1.26              |
| 1:F:398:ASP:O   | 1:F:400:PRO:HD3  | 1.29                     | 1.24              |
| 1:G:398:ASP:O   | 1:G:400:PRO:HD3  | 1.29                     | 1.23              |
| 1:I:395:ASN:HB3 | 1:I:399:LEU:CD1  | 1.69                     | 1.23              |
| 1:B:395:ASN:HB3 | 1:B:399:LEU:CD1  | 1.69                     | 1.22              |
| 1:E:395:ASN:HB3 | 1:E:399:LEU:CD1  | 1.69                     | 1.22              |
| 1:C:395:ASN:HB3 | 1:C:399:LEU:CD1  | 1.69                     | 1.22              |
| 1:F:395:ASN:HB3 | 1:F:399:LEU:CD1  | 1.70                     | 1.22              |
| 1:K:395:ASN:HB3 | 1:K:399:LEU:CD1  | 1.69                     | 1.22              |
| 1:L:395:ASN:HB3 | 1:L:399:LEU:CD1  | 1.69                     | 1.22              |
| 1:A:395:ASN:HB3 | 1:A:399:LEU:CD1  | 1.69                     | 1.21              |
| 1:D:395:ASN:HB3 | 1:D:399:LEU:CD1  | 1.69                     | 1.21              |
| 1:J:395:ASN:HB3 | 1:J:399:LEU:CD1  | 1.69                     | 1.21              |
| 1:H:395:ASN:HB3 | 1:H:399:LEU:CD1  | 1.69                     | 1.20              |
| 1:G:395:ASN:HB3 | 1:G:399:LEU:CD1  | 1.70                     | 1.20              |
| 1:C:360:PHE:CD2 | 1:C:361:PRO:HD3  | 1.78                     | 1.19              |
| 1:A:360:PHE:CD2 | 1:A:361:PRO:HD3  | 1.78                     | 1.19              |
| 1:I:360:PHE:CD2 | 1:I:361:PRO:HD3  | 1.78                     | 1.19              |
| 1:H:360:PHE:CD2 | 1:H:361:PRO:HD3  | 1.78                     | 1.18              |
| 1:E:360:PHE:CD2 | 1:E:361:PRO:HD3  | 1.78                     | 1.18              |
| 1:L:360:PHE:CD2 | 1:L:361:PRO:HD3  | 1.78                     | 1.18              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:360:PHE:CD2  | 1:F:361:PRO:HD3  | 1.78                     | 1.18              |
| 1:K:360:PHE:CD2  | 1:K:361:PRO:HD3  | 1.78                     | 1.18              |
| 1:D:360:PHE:CD2  | 1:D:361:PRO:HD3  | 1.78                     | 1.17              |
| 1:G:360:PHE:CD2  | 1:G:361:PRO:HD3  | 1.78                     | 1.17              |
| 1:J:360:PHE:CD2  | 1:J:361:PRO:HD3  | 1.78                     | 1.17              |
| 1:B:360:PHE:CD2  | 1:B:361:PRO:HD3  | 1.78                     | 1.16              |
| 1:I:60:ILE:CG2   | 1:J:395:ASN:HD21 | 1.58                     | 1.14              |
| 1:G:60:ILE:CG2   | 1:H:395:ASN:HD21 | 1.63                     | 1.12              |
| 1:A:395:ASN:HD21 | 1:B:60:ILE:HG21  | 1.15                     | 1.10              |
| 1:A:395:ASN:HD21 | 1:B:60:ILE:CG2   | 1.65                     | 1.08              |
| 1:I:60:ILE:HG21  | 1:J:395:ASN:HD21 | 1.10                     | 1.08              |
| 1:C:395:ASN:HD21 | 1:D:60:ILE:CG2   | 1.67                     | 1.07              |
| 1:L:395:ASN:HB3  | 1:L:399:LEU:HD11 | 1.36                     | 1.06              |
| 1:F:82:ASP:H     | 5:F:1488:MPD:C1  | 1.69                     | 1.06              |
| 1:G:60:ILE:HG21  | 1:H:395:ASN:HD21 | 1.19                     | 1.06              |
| 1:J:395:ASN:HB3  | 1:J:399:LEU:HD11 | 1.36                     | 1.06              |
| 1:B:82:ASP:H     | 5:B:1484:MPD:C1  | 1.69                     | 1.06              |
| 1:H:82:ASP:H     | 5:H:1490:MPD:C1  | 1.69                     | 1.06              |
| 1:E:82:ASP:H     | 5:E:1487:MPD:C1  | 1.69                     | 1.06              |
| 1:D:82:ASP:H     | 5:D:1486:MPD:C1  | 1.69                     | 1.05              |
| 1:K:82:ASP:H     | 5:K:1493:MPD:C1  | 1.69                     | 1.05              |
| 1:C:82:ASP:H     | 5:C:1485:MPD:C1  | 1.69                     | 1.05              |
| 1:G:82:ASP:H     | 5:G:1489:MPD:C1  | 1.69                     | 1.05              |
| 1:C:395:ASN:HD21 | 1:D:60:ILE:HG21  | 1.20                     | 1.05              |
| 1:H:395:ASN:HB3  | 1:H:399:LEU:HD11 | 1.36                     | 1.05              |
| 1:B:395:ASN:HB3  | 1:B:399:LEU:HD11 | 1.36                     | 1.05              |
| 1:J:82:ASP:H     | 5:J:1492:MPD:C1  | 1.69                     | 1.05              |
| 1:I:82:ASP:H     | 5:I:1491:MPD:C1  | 1.69                     | 1.04              |
| 1:I:395:ASN:HB3  | 1:I:399:LEU:HD11 | 1.36                     | 1.04              |
| 1:L:82:ASP:H     | 5:L:1494:MPD:C1  | 1.69                     | 1.04              |
| 1:D:395:ASN:HB3  | 1:D:399:LEU:HD11 | 1.36                     | 1.04              |
| 1:A:82:ASP:H     | 5:A:1483:MPD:C1  | 1.69                     | 1.04              |
| 1:C:395:ASN:HB3  | 1:C:399:LEU:HD11 | 1.36                     | 1.03              |
| 1:F:395:ASN:HB3  | 1:F:399:LEU:HD11 | 1.36                     | 1.03              |
| 1:A:395:ASN:HB3  | 1:A:399:LEU:HD11 | 1.36                     | 1.03              |
| 1:K:395:ASN:HB3  | 1:K:399:LEU:HD11 | 1.36                     | 1.03              |
| 1:G:395:ASN:HB3  | 1:G:399:LEU:HD11 | 1.36                     | 1.02              |
| 1:E:395:ASN:HB3  | 1:E:399:LEU:HD11 | 1.36                     | 1.02              |
| 1:C:48:MET:HE2   | 1:C:66:VAL:HG22  | 1.43                     | 1.00              |
| 1:E:48:MET:HE2   | 1:E:66:VAL:HG22  | 1.43                     | 1.00              |
| 1:H:48:MET:HE2   | 1:H:66:VAL:HG22  | 1.43                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:48:MET:HE2   | 1:J:66:VAL:HG22  | 1.43                     | 1.00              |
| 1:L:48:MET:HE2   | 1:L:66:VAL:HG22  | 1.43                     | 1.00              |
| 1:A:48:MET:HE2   | 1:A:66:VAL:HG22  | 1.43                     | 1.00              |
| 1:J:60:ILE:CG2   | 1:K:395:ASN:HD21 | 1.74                     | 1.00              |
| 1:I:48:MET:HE2   | 1:I:66:VAL:HG22  | 1.43                     | 1.00              |
| 1:B:48:MET:HE2   | 1:B:66:VAL:HG22  | 1.43                     | 0.99              |
| 1:D:48:MET:HE2   | 1:D:66:VAL:HG22  | 1.43                     | 0.99              |
| 1:F:48:MET:HE2   | 1:F:66:VAL:HG22  | 1.43                     | 0.99              |
| 1:K:48:MET:HE2   | 1:K:66:VAL:HG22  | 1.43                     | 0.98              |
| 1:D:395:ASN:HD21 | 1:E:60:ILE:CG2   | 1.77                     | 0.97              |
| 1:G:48:MET:HE2   | 1:G:66:VAL:HG22  | 1.43                     | 0.96              |
| 1:G:395:ASN:HD21 | 1:L:60:ILE:HG21  | 1.28                     | 0.95              |
| 1:C:82:ASP:O     | 1:C:84:THR:HG22  | 1.68                     | 0.94              |
| 5:H:1490:MPD:H32 | 1:I:193:SER:CB   | 1.97                     | 0.94              |
| 1:A:82:ASP:O     | 1:A:84:THR:HG22  | 1.68                     | 0.94              |
| 1:E:82:ASP:O     | 1:E:84:THR:HG22  | 1.68                     | 0.94              |
| 1:J:82:ASP:O     | 1:J:84:THR:HG22  | 1.68                     | 0.94              |
| 1:C:80:PHE:HB3   | 5:C:1485:MPD:H11 | 1.50                     | 0.94              |
| 1:G:82:ASP:O     | 1:G:84:THR:HG22  | 1.68                     | 0.94              |
| 1:I:82:ASP:O     | 1:I:84:THR:HG22  | 1.68                     | 0.94              |
| 1:L:82:ASP:O     | 1:L:84:THR:HG22  | 1.68                     | 0.94              |
| 1:K:80:PHE:HB3   | 5:K:1493:MPD:H11 | 1.50                     | 0.94              |
| 1:A:80:PHE:HB3   | 5:A:1483:MPD:H11 | 1.50                     | 0.93              |
| 1:J:60:ILE:HG21  | 1:K:395:ASN:HD21 | 1.32                     | 0.93              |
| 1:D:395:ASN:HD21 | 1:E:60:ILE:HG21  | 1.33                     | 0.93              |
| 1:I:80:PHE:HB3   | 5:I:1491:MPD:H11 | 1.50                     | 0.93              |
| 1:F:80:PHE:HB3   | 5:F:1488:MPD:H11 | 1.50                     | 0.93              |
| 1:K:82:ASP:O     | 1:K:84:THR:HG22  | 1.68                     | 0.93              |
| 1:D:80:PHE:HB3   | 5:D:1486:MPD:H11 | 1.50                     | 0.93              |
| 1:H:80:PHE:HB3   | 5:H:1490:MPD:H11 | 1.50                     | 0.93              |
| 1:J:80:PHE:HB3   | 5:J:1492:MPD:H11 | 1.50                     | 0.93              |
| 1:A:395:ASN:HB3  | 1:A:399:LEU:HD12 | 1.50                     | 0.93              |
| 1:C:395:ASN:HB3  | 1:C:399:LEU:HD12 | 1.50                     | 0.92              |
| 1:G:80:PHE:HB3   | 5:G:1489:MPD:H11 | 1.50                     | 0.92              |
| 1:H:82:ASP:O     | 1:H:84:THR:HG22  | 1.68                     | 0.92              |
| 1:L:395:ASN:HB3  | 1:L:399:LEU:HD12 | 1.50                     | 0.92              |
| 1:C:52:SER:HB3   | 1:C:63:SER:HB3   | 1.51                     | 0.92              |
| 1:E:80:PHE:HB3   | 5:E:1487:MPD:H11 | 1.50                     | 0.92              |
| 1:F:82:ASP:O     | 1:F:84:THR:HG22  | 1.68                     | 0.92              |
| 1:I:395:ASN:HB3  | 1:I:399:LEU:HD12 | 1.50                     | 0.92              |
| 1:J:52:SER:HB3   | 1:J:63:SER:HB3   | 1.51                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:82:ASP:O     | 1:B:84:THR:HG22  | 1.68                     | 0.92              |
| 1:E:52:SER:HB3   | 1:E:63:SER:HB3   | 1.51                     | 0.92              |
| 1:A:52:SER:HB3   | 1:A:63:SER:HB3   | 1.51                     | 0.92              |
| 5:J:1492:MPD:H32 | 1:K:193:SER:CB   | 1.99                     | 0.92              |
| 1:C:1:SER:HA     | 1:C:71:ALA:CB    | 2.00                     | 0.92              |
| 1:H:52:SER:HB3   | 1:H:63:SER:HB3   | 1.51                     | 0.92              |
| 1:L:52:SER:HB3   | 1:L:63:SER:HB3   | 1.51                     | 0.92              |
| 1:L:80:PHE:HB3   | 5:L:1494:MPD:H11 | 1.50                     | 0.92              |
| 1:C:82:ASP:H     | 5:C:1485:MPD:H13 | 1.34                     | 0.92              |
| 1:D:1:SER:HA     | 1:D:71:ALA:CB    | 2.00                     | 0.92              |
| 1:G:82:ASP:H     | 5:G:1489:MPD:H13 | 1.34                     | 0.92              |
| 1:H:1:SER:HA     | 1:H:71:ALA:CB    | 2.00                     | 0.92              |
| 1:L:1:SER:HA     | 1:L:71:ALA:CB    | 2.00                     | 0.92              |
| 1:D:82:ASP:O     | 1:D:84:THR:HG22  | 1.68                     | 0.91              |
| 1:K:1:SER:HA     | 1:K:71:ALA:CB    | 2.00                     | 0.91              |
| 1:K:395:ASN:HB3  | 1:K:399:LEU:HD12 | 1.50                     | 0.91              |
| 1:D:395:ASN:HB3  | 1:D:399:LEU:HD12 | 1.50                     | 0.91              |
| 1:F:1:SER:HA     | 1:F:71:ALA:CB    | 2.00                     | 0.91              |
| 1:G:395:ASN:HD21 | 1:L:60:ILE:CG2   | 1.82                     | 0.91              |
| 1:B:52:SER:HB3   | 1:B:63:SER:HB3   | 1.51                     | 0.91              |
| 1:B:80:PHE:HB3   | 5:B:1484:MPD:H11 | 1.50                     | 0.91              |
| 1:B:395:ASN:HB3  | 1:B:399:LEU:HD12 | 1.50                     | 0.91              |
| 1:F:395:ASN:HB3  | 1:F:399:LEU:HD12 | 1.50                     | 0.91              |
| 1:H:395:ASN:HB3  | 1:H:399:LEU:HD12 | 1.50                     | 0.91              |
| 1:I:1:SER:HA     | 1:I:71:ALA:CB    | 2.00                     | 0.91              |
| 1:J:395:ASN:HB3  | 1:J:399:LEU:HD12 | 1.50                     | 0.91              |
| 1:K:52:SER:HB3   | 1:K:63:SER:HB3   | 1.51                     | 0.91              |
| 1:B:1:SER:HA     | 1:B:71:ALA:CB    | 2.00                     | 0.91              |
| 5:I:1491:MPD:H32 | 1:J:193:SER:CB   | 2.00                     | 0.91              |
| 1:J:1:SER:HA     | 1:J:71:ALA:CB    | 2.00                     | 0.91              |
| 1:L:82:ASP:H     | 5:L:1494:MPD:H13 | 1.34                     | 0.91              |
| 1:B:82:ASP:H     | 5:B:1484:MPD:H13 | 1.34                     | 0.91              |
| 1:A:1:SER:HA     | 1:A:71:ALA:CB    | 2.00                     | 0.90              |
| 1:B:193:SER:CB   | 5:C:1485:MPD:H32 | 2.00                     | 0.90              |
| 1:D:52:SER:HB3   | 1:D:63:SER:HB3   | 1.51                     | 0.90              |
| 1:G:52:SER:HB3   | 1:G:63:SER:HB3   | 1.51                     | 0.90              |
| 1:D:82:ASP:H     | 5:D:1486:MPD:H13 | 1.34                     | 0.90              |
| 1:H:82:ASP:H     | 5:H:1490:MPD:H13 | 1.34                     | 0.90              |
| 1:E:1:SER:HA     | 1:E:71:ALA:CB    | 2.00                     | 0.90              |
| 1:G:1:SER:HA     | 1:G:71:ALA:CB    | 2.00                     | 0.90              |
| 1:G:395:ASN:HB3  | 1:G:399:LEU:HD12 | 1.50                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:458:HIS:HD2  | 1:F:460:VAL:H    | 1.20                     | 0.90              |
| 1:G:193:SER:CB   | 5:L:1494:MPD:H32 | 2.02                     | 0.90              |
| 1:E:458:HIS:HD2  | 1:E:460:VAL:H    | 1.20                     | 0.89              |
| 1:C:458:HIS:HD2  | 1:C:460:VAL:H    | 1.20                     | 0.89              |
| 1:F:82:ASP:H     | 5:F:1488:MPD:H13 | 1.34                     | 0.89              |
| 1:J:458:HIS:HD2  | 1:J:460:VAL:H    | 1.20                     | 0.89              |
| 1:A:82:ASP:H     | 5:A:1483:MPD:H13 | 1.34                     | 0.89              |
| 1:E:193:SER:CB   | 5:F:1488:MPD:H32 | 2.01                     | 0.89              |
| 1:E:395:ASN:HB3  | 1:E:399:LEU:HD12 | 1.50                     | 0.89              |
| 1:A:60:ILE:CG2   | 1:F:395:ASN:HD21 | 1.85                     | 0.89              |
| 1:J:82:ASP:H     | 5:J:1492:MPD:H13 | 1.34                     | 0.89              |
| 1:E:82:ASP:H     | 5:E:1487:MPD:H13 | 1.34                     | 0.89              |
| 1:H:458:HIS:HD2  | 1:H:460:VAL:H    | 1.20                     | 0.89              |
| 1:I:82:ASP:H     | 5:I:1491:MPD:H13 | 1.34                     | 0.89              |
| 1:K:82:ASP:H     | 5:K:1493:MPD:H13 | 1.34                     | 0.89              |
| 1:L:458:HIS:HD2  | 1:L:460:VAL:H    | 1.20                     | 0.89              |
| 1:G:458:HIS:HD2  | 1:G:460:VAL:H    | 1.20                     | 0.89              |
| 1:B:458:HIS:HD2  | 1:B:460:VAL:H    | 1.20                     | 0.89              |
| 1:I:52:SER:HB3   | 1:I:63:SER:HB3   | 1.51                     | 0.89              |
| 1:D:401:PRO:HB3  | 1:D:404:ALA:HA   | 1.56                     | 0.88              |
| 1:F:52:SER:HB3   | 1:F:63:SER:HB3   | 1.51                     | 0.88              |
| 1:A:401:PRO:HB3  | 1:A:404:ALA:HA   | 1.56                     | 0.88              |
| 1:I:401:PRO:HB3  | 1:I:404:ALA:HA   | 1.56                     | 0.87              |
| 1:K:401:PRO:HB3  | 1:K:404:ALA:HA   | 1.56                     | 0.87              |
| 1:I:458:HIS:HD2  | 1:I:460:VAL:H    | 1.20                     | 0.87              |
| 1:A:193:SER:CB   | 5:B:1484:MPD:H32 | 2.05                     | 0.87              |
| 1:K:458:HIS:HD2  | 1:K:460:VAL:H    | 1.20                     | 0.87              |
| 1:B:401:PRO:HB3  | 1:B:404:ALA:HA   | 1.56                     | 0.86              |
| 1:B:395:ASN:HD21 | 1:C:60:ILE:CG2   | 1.88                     | 0.86              |
| 5:H:1490:MPD:HM3 | 1:I:190:ASP:OD2  | 1.75                     | 0.86              |
| 1:D:458:HIS:HD2  | 1:D:460:VAL:H    | 1.20                     | 0.86              |
| 1:G:401:PRO:HB3  | 1:G:404:ALA:HA   | 1.56                     | 0.86              |
| 1:C:401:PRO:HB3  | 1:C:404:ALA:HA   | 1.56                     | 0.86              |
| 1:H:401:PRO:HB3  | 1:H:404:ALA:HA   | 1.56                     | 0.86              |
| 1:E:401:PRO:HB3  | 1:E:404:ALA:HA   | 1.56                     | 0.86              |
| 1:L:401:PRO:HB3  | 1:L:404:ALA:HA   | 1.56                     | 0.86              |
| 1:A:224:ARG:HG2  | 1:A:224:ARG:HH21 | 1.41                     | 0.85              |
| 1:A:458:HIS:HD2  | 1:A:460:VAL:H    | 1.20                     | 0.85              |
| 1:G:190:ASP:OD2  | 5:L:1494:MPD:HM3 | 1.76                     | 0.85              |
| 1:L:224:ARG:HG2  | 1:L:224:ARG:HH21 | 1.41                     | 0.85              |
| 1:H:224:ARG:HH21 | 1:H:224:ARG:HG2  | 1.41                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:K:1493:MPD:HM3 | 1:L:190:ASP:OD2  | 1.74                     | 0.85              |
| 1:J:401:PRO:HB3  | 1:J:404:ALA:HA   | 1.56                     | 0.85              |
| 1:J:16:PHE:CD1   | 5:J:1492:MPD:H52 | 2.12                     | 0.85              |
| 1:B:224:ARG:HG2  | 1:B:224:ARG:HH21 | 1.42                     | 0.85              |
| 1:E:16:PHE:CD1   | 5:E:1487:MPD:H52 | 2.12                     | 0.85              |
| 1:F:16:PHE:CD1   | 5:F:1488:MPD:H52 | 2.12                     | 0.85              |
| 1:F:224:ARG:HH21 | 1:F:224:ARG:HG2  | 1.41                     | 0.85              |
| 1:L:16:PHE:CD1   | 5:L:1494:MPD:H52 | 2.12                     | 0.85              |
| 1:D:16:PHE:CD1   | 5:D:1486:MPD:H52 | 2.12                     | 0.85              |
| 1:I:60:ILE:HG21  | 1:J:395:ASN:ND2  | 1.89                     | 0.85              |
| 1:I:398:ASP:O    | 1:I:400:PRO:CD   | 2.22                     | 0.85              |
| 1:B:16:PHE:CD1   | 5:B:1484:MPD:H52 | 2.12                     | 0.85              |
| 1:E:224:ARG:HG2  | 1:E:224:ARG:HH21 | 1.41                     | 0.85              |
| 1:G:224:ARG:HG2  | 1:G:224:ARG:HH21 | 1.41                     | 0.85              |
| 1:C:224:ARG:HH21 | 1:C:224:ARG:HG2  | 1.41                     | 0.84              |
| 1:F:398:ASP:O    | 1:F:400:PRO:CD   | 2.22                     | 0.84              |
| 1:G:16:PHE:CD1   | 5:G:1489:MPD:H52 | 2.12                     | 0.84              |
| 1:J:224:ARG:HG2  | 1:J:224:ARG:HH21 | 1.42                     | 0.84              |
| 1:H:16:PHE:CD1   | 5:H:1490:MPD:H52 | 2.12                     | 0.84              |
| 1:C:16:PHE:CD1   | 5:C:1485:MPD:H52 | 2.12                     | 0.84              |
| 1:D:224:ARG:HG2  | 1:D:224:ARG:HH21 | 1.42                     | 0.84              |
| 1:A:398:ASP:O    | 1:A:400:PRO:CD   | 2.22                     | 0.84              |
| 1:F:401:PRO:HB3  | 1:F:404:ALA:HA   | 1.56                     | 0.84              |
| 1:K:16:PHE:CD1   | 5:K:1493:MPD:H52 | 2.12                     | 0.84              |
| 1:A:16:PHE:CD1   | 5:A:1483:MPD:H52 | 2.12                     | 0.84              |
| 1:I:224:ARG:HG2  | 1:I:224:ARG:HH21 | 1.41                     | 0.84              |
| 1:A:60:ILE:HG21  | 1:F:395:ASN:HD21 | 1.39                     | 0.83              |
| 1:I:16:PHE:CD1   | 5:I:1491:MPD:H52 | 2.12                     | 0.83              |
| 1:E:398:ASP:O    | 1:E:400:PRO:CD   | 2.22                     | 0.83              |
| 1:K:224:ARG:HH21 | 1:K:224:ARG:HG2  | 1.41                     | 0.83              |
| 1:K:398:ASP:O    | 1:K:400:PRO:CD   | 2.22                     | 0.83              |
| 1:H:82:ASP:H     | 5:H:1490:MPD:H12 | 1.44                     | 0.83              |
| 1:L:398:ASP:O    | 1:L:400:PRO:CD   | 2.22                     | 0.83              |
| 5:A:1483:MPD:HM3 | 1:F:190:ASP:OD2  | 1.78                     | 0.83              |
| 1:B:398:ASP:O    | 1:B:400:PRO:CD   | 2.22                     | 0.83              |
| 1:A:82:ASP:H     | 5:A:1483:MPD:H12 | 1.44                     | 0.82              |
| 1:A:395:ASN:ND2  | 1:B:60:ILE:HG21  | 1.94                     | 0.82              |
| 1:G:398:ASP:O    | 1:G:400:PRO:CD   | 2.22                     | 0.82              |
| 1:J:398:ASP:O    | 1:J:400:PRO:CD   | 2.22                     | 0.82              |
| 5:H:1490:MPD:H32 | 1:I:193:SER:HB2  | 1.61                     | 0.82              |
| 1:E:323:VAL:HG21 | 1:K:455:MET:HG2  | 1.60                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:398:ASP:O    | 1:D:400:PRO:CD   | 2.22                     | 0.82              |
| 5:K:1493:MPD:H32 | 1:L:193:SER:CB   | 2.08                     | 0.82              |
| 1:K:340:SER:HB3  | 1:K:396:LEU:HB3  | 1.62                     | 0.82              |
| 1:G:340:SER:HB3  | 1:G:396:LEU:HB3  | 1.62                     | 0.81              |
| 1:A:81:ALA:N     | 5:A:1483:MPD:H13 | 1.96                     | 0.81              |
| 1:A:340:SER:HB3  | 1:A:396:LEU:HB3  | 1.62                     | 0.81              |
| 1:D:395:ASN:CB   | 1:D:399:LEU:HD11 | 2.11                     | 0.81              |
| 1:G:395:ASN:CB   | 1:G:399:LEU:HD11 | 2.11                     | 0.81              |
| 1:C:81:ALA:N     | 5:C:1485:MPD:H13 | 1.96                     | 0.81              |
| 1:E:340:SER:HB3  | 1:E:396:LEU:HB3  | 1.62                     | 0.81              |
| 1:I:82:ASP:H     | 5:I:1491:MPD:H12 | 1.44                     | 0.81              |
| 1:J:81:ALA:N     | 5:J:1492:MPD:H13 | 1.96                     | 0.81              |
| 5:J:1492:MPD:O2  | 1:K:190:ASP:HA   | 1.80                     | 0.81              |
| 1:K:395:ASN:CB   | 1:K:399:LEU:HD11 | 2.10                     | 0.81              |
| 1:L:82:ASP:H     | 5:L:1494:MPD:H12 | 1.44                     | 0.81              |
| 1:A:395:ASN:CB   | 1:A:399:LEU:HD11 | 2.10                     | 0.81              |
| 1:E:81:ALA:N     | 5:E:1487:MPD:H13 | 1.96                     | 0.81              |
| 1:G:82:ASP:H     | 5:G:1489:MPD:H12 | 1.44                     | 0.81              |
| 1:K:81:ALA:N     | 5:K:1493:MPD:H13 | 1.96                     | 0.81              |
| 1:E:190:ASP:HA   | 5:F:1488:MPD:O2  | 1.81                     | 0.81              |
| 1:H:81:ALA:N     | 5:H:1490:MPD:H13 | 1.96                     | 0.81              |
| 1:J:395:ASN:CB   | 1:J:399:LEU:HD11 | 2.10                     | 0.81              |
| 1:K:82:ASP:H     | 5:K:1493:MPD:H12 | 1.44                     | 0.81              |
| 1:H:340:SER:HB3  | 1:H:396:LEU:HB3  | 1.62                     | 0.81              |
| 1:I:81:ALA:N     | 5:I:1491:MPD:H13 | 1.96                     | 0.81              |
| 1:L:340:SER:HB3  | 1:L:396:LEU:HB3  | 1.62                     | 0.81              |
| 1:H:395:ASN:CB   | 1:H:399:LEU:HD11 | 2.10                     | 0.81              |
| 1:J:82:ASP:H     | 5:J:1492:MPD:H12 | 1.44                     | 0.81              |
| 1:F:395:ASN:CB   | 1:F:399:LEU:HD11 | 2.10                     | 0.81              |
| 1:F:455:MET:HG2  | 1:L:323:VAL:HG21 | 1.62                     | 0.81              |
| 1:H:398:ASP:O    | 1:H:400:PRO:CD   | 2.22                     | 0.81              |
| 1:I:395:ASN:CB   | 1:I:399:LEU:HD11 | 2.10                     | 0.81              |
| 5:J:1492:MPD:H32 | 1:K:193:SER:HB2  | 1.62                     | 0.81              |
| 1:C:395:ASN:CB   | 1:C:399:LEU:HD11 | 2.10                     | 0.81              |
| 1:C:193:SER:CB   | 5:D:1486:MPD:H32 | 2.10                     | 0.80              |
| 1:C:398:ASP:O    | 1:C:400:PRO:CD   | 2.22                     | 0.80              |
| 1:L:81:ALA:N     | 5:L:1494:MPD:H13 | 1.96                     | 0.80              |
| 1:F:82:ASP:H     | 5:F:1488:MPD:H12 | 1.44                     | 0.80              |
| 1:C:340:SER:HB3  | 1:C:396:LEU:HB3  | 1.62                     | 0.80              |
| 1:L:395:ASN:CB   | 1:L:399:LEU:HD11 | 2.10                     | 0.80              |
| 1:D:82:ASP:H     | 5:D:1486:MPD:H12 | 1.44                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:190:ASP:OD2  | 5:D:1486:MPD:HM3 | 1.81                     | 0.80              |
| 1:B:81:ALA:N     | 5:B:1484:MPD:H13 | 1.96                     | 0.80              |
| 1:B:395:ASN:CB   | 1:B:399:LEU:HD11 | 2.10                     | 0.80              |
| 1:F:81:ALA:N     | 5:F:1488:MPD:H13 | 1.96                     | 0.80              |
| 1:F:340:SER:HB3  | 1:F:396:LEU:HB3  | 1.62                     | 0.80              |
| 1:G:190:ASP:HA   | 5:L:1494:MPD:O2  | 1.81                     | 0.80              |
| 1:I:340:SER:HB3  | 1:I:396:LEU:HB3  | 1.62                     | 0.80              |
| 1:B:340:SER:HB3  | 1:B:396:LEU:HB3  | 1.62                     | 0.80              |
| 1:D:81:ALA:N     | 5:D:1486:MPD:H13 | 1.96                     | 0.80              |
| 1:D:340:SER:HB3  | 1:D:396:LEU:HB3  | 1.62                     | 0.80              |
| 1:E:82:ASP:H     | 5:E:1487:MPD:H12 | 1.44                     | 0.80              |
| 1:F:402:GLU:HB2  | 1:F:405:LYS:HD3  | 1.64                     | 0.80              |
| 1:C:82:ASP:H     | 5:C:1485:MPD:H12 | 1.44                     | 0.79              |
| 1:G:193:SER:HB2  | 5:L:1494:MPD:H32 | 1.62                     | 0.79              |
| 1:L:402:GLU:HB2  | 1:L:405:LYS:HD3  | 1.64                     | 0.79              |
| 1:A:402:GLU:HB2  | 1:A:405:LYS:HD3  | 1.64                     | 0.79              |
| 1:B:82:ASP:H     | 5:B:1484:MPD:H12 | 1.44                     | 0.79              |
| 1:E:395:ASN:CB   | 1:E:399:LEU:HD11 | 2.10                     | 0.79              |
| 1:G:81:ALA:N     | 5:G:1489:MPD:H13 | 1.96                     | 0.79              |
| 1:J:340:SER:HB3  | 1:J:396:LEU:HB3  | 1.62                     | 0.79              |
| 1:A:323:VAL:HG21 | 1:G:455:MET:HG2  | 1.64                     | 0.78              |
| 1:G:402:GLU:HB2  | 1:G:405:LYS:HD3  | 1.64                     | 0.78              |
| 1:I:60:ILE:CG2   | 1:J:395:ASN:ND2  | 2.42                     | 0.78              |
| 5:I:1491:MPD:H32 | 1:J:193:SER:HB2  | 1.65                     | 0.78              |
| 1:J:402:GLU:HB2  | 1:J:405:LYS:HD3  | 1.64                     | 0.78              |
| 1:K:402:GLU:HB2  | 1:K:405:LYS:HD3  | 1.64                     | 0.78              |
| 1:L:52:SER:CB    | 1:L:63:SER:HB3   | 2.13                     | 0.78              |
| 1:D:52:SER:CB    | 1:D:63:SER:HB3   | 2.13                     | 0.78              |
| 1:J:52:SER:CB    | 1:J:63:SER:HB3   | 2.13                     | 0.78              |
| 1:K:52:SER:CB    | 1:K:63:SER:HB3   | 2.13                     | 0.78              |
| 1:K:60:ILE:CG2   | 1:L:395:ASN:HD21 | 1.96                     | 0.78              |
| 1:B:52:SER:CB    | 1:B:63:SER:HB3   | 2.13                     | 0.78              |
| 1:H:60:ILE:CG2   | 1:I:395:ASN:HD21 | 1.96                     | 0.78              |
| 1:H:395:ASN:CB   | 1:H:399:LEU:CD1  | 2.60                     | 0.78              |
| 1:I:52:SER:CB    | 1:I:63:SER:HB3   | 2.13                     | 0.78              |
| 1:I:402:GLU:HB2  | 1:I:405:LYS:HD3  | 1.64                     | 0.78              |
| 1:B:190:ASP:HA   | 5:C:1485:MPD:O2  | 1.84                     | 0.77              |
| 1:K:1:SER:HA     | 1:K:71:ALA:HB1   | 1.66                     | 0.77              |
| 1:C:402:GLU:HB2  | 1:C:405:LYS:HD3  | 1.64                     | 0.77              |
| 1:D:402:GLU:HB2  | 1:D:405:LYS:HD3  | 1.64                     | 0.77              |
| 1:A:1:SER:HA     | 1:A:71:ALA:HB1   | 1.66                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:402:GLU:HB2  | 1:E:405:LYS:HD3  | 1.64                     | 0.77              |
| 1:F:395:ASN:CB   | 1:F:399:LEU:CD1  | 2.60                     | 0.77              |
| 1:G:52:SER:CB    | 1:G:63:SER:HB3   | 2.13                     | 0.77              |
| 5:J:1492:MPD:HM3 | 1:K:190:ASP:OD2  | 1.82                     | 0.77              |
| 1:E:395:ASN:HD21 | 1:F:60:ILE:CG2   | 1.98                     | 0.77              |
| 1:F:1:SER:HA     | 1:F:71:ALA:HB1   | 1.66                     | 0.77              |
| 1:F:52:SER:CB    | 1:F:63:SER:HB3   | 2.13                     | 0.77              |
| 1:B:323:VAL:HG21 | 1:H:455:MET:HG2  | 1.66                     | 0.77              |
| 1:B:395:ASN:HD21 | 1:C:60:ILE:HG21  | 1.48                     | 0.77              |
| 1:B:402:GLU:HB2  | 1:B:405:LYS:HD3  | 1.64                     | 0.77              |
| 1:A:52:SER:CB    | 1:A:63:SER:HB3   | 2.13                     | 0.77              |
| 1:H:1:SER:HA     | 1:H:71:ALA:HB1   | 1.66                     | 0.77              |
| 1:H:52:SER:CB    | 1:H:63:SER:HB3   | 2.13                     | 0.77              |
| 1:H:402:GLU:HB2  | 1:H:405:LYS:HD3  | 1.64                     | 0.77              |
| 1:I:1:SER:HA     | 1:I:71:ALA:HB3   | 1.67                     | 0.77              |
| 1:A:190:ASP:HA   | 5:B:1484:MPD:O2  | 1.84                     | 0.77              |
| 1:E:1:SER:HA     | 1:E:71:ALA:HB1   | 1.66                     | 0.77              |
| 1:I:1:SER:HA     | 1:I:71:ALA:HB1   | 1.66                     | 0.77              |
| 1:B:1:SER:HA     | 1:B:71:ALA:HB3   | 1.67                     | 0.77              |
| 1:E:52:SER:CB    | 1:E:63:SER:HB3   | 2.13                     | 0.77              |
| 1:J:395:ASN:CB   | 1:J:399:LEU:CD1  | 2.60                     | 0.77              |
| 1:G:1:SER:HA     | 1:G:71:ALA:HB3   | 1.67                     | 0.76              |
| 1:J:1:SER:HA     | 1:J:71:ALA:HB1   | 1.66                     | 0.76              |
| 1:L:1:SER:HA     | 1:L:71:ALA:HB3   | 1.67                     | 0.76              |
| 1:C:52:SER:CB    | 1:C:63:SER:HB3   | 2.13                     | 0.76              |
| 5:G:1489:MPD:H32 | 1:H:193:SER:CB   | 2.14                     | 0.76              |
| 1:I:395:ASN:CB   | 1:I:399:LEU:CD1  | 2.60                     | 0.76              |
| 1:L:1:SER:HA     | 1:L:71:ALA:HB1   | 1.66                     | 0.76              |
| 1:A:52:SER:HB3   | 1:A:63:SER:CB    | 2.16                     | 0.76              |
| 1:C:455:MET:HG2  | 1:I:323:VAL:HG21 | 1.66                     | 0.76              |
| 1:B:1:SER:HA     | 1:B:71:ALA:HB1   | 1.66                     | 0.76              |
| 1:B:395:ASN:CB   | 1:B:399:LEU:CD1  | 2.60                     | 0.76              |
| 1:C:52:SER:HB3   | 1:C:63:SER:CB    | 2.16                     | 0.76              |
| 1:E:395:ASN:CB   | 1:E:399:LEU:CD1  | 2.60                     | 0.76              |
| 1:G:1:SER:HA     | 1:G:71:ALA:HB1   | 1.66                     | 0.76              |
| 1:J:1:SER:HA     | 1:J:71:ALA:HB3   | 1.67                     | 0.76              |
| 1:G:52:SER:HB3   | 1:G:63:SER:CB    | 2.16                     | 0.76              |
| 1:K:52:SER:HB3   | 1:K:63:SER:CB    | 2.16                     | 0.76              |
| 1:C:1:SER:HA     | 1:C:71:ALA:HB3   | 1.67                     | 0.76              |
| 1:E:52:SER:HB3   | 1:E:63:SER:CB    | 2.16                     | 0.76              |
| 1:B:190:ASP:OD2  | 5:C:1485:MPD:HM3 | 1.86                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:193:SER:HB2  | 5:C:1485:MPD:H32 | 1.67                     | 0.76              |
| 1:D:1:SER:HA     | 1:D:71:ALA:HB1   | 1.66                     | 0.76              |
| 1:D:323:VAL:HG21 | 1:J:455:MET:HG2  | 1.68                     | 0.76              |
| 1:C:395:ASN:ND2  | 1:D:60:ILE:HG21  | 2.00                     | 0.76              |
| 1:E:189:GLN:HG3  | 5:F:1488:MPD:HM1 | 1.68                     | 0.76              |
| 1:A:189:GLN:HG3  | 5:B:1484:MPD:HM1 | 1.68                     | 0.75              |
| 1:C:1:SER:HA     | 1:C:71:ALA:HB1   | 1.66                     | 0.75              |
| 3:A:1471:ADP:N9  | 3:A:1471:ADP:H1' | 1.99                     | 0.75              |
| 1:G:60:ILE:HG21  | 1:H:395:ASN:ND2  | 1.97                     | 0.75              |
| 3:H:1478:ADP:N9  | 3:H:1478:ADP:H1' | 1.99                     | 0.75              |
| 1:K:80:PHE:HB3   | 5:K:1493:MPD:C1  | 2.17                     | 0.75              |
| 5:I:1491:MPD:O2  | 1:J:190:ASP:HA   | 1.85                     | 0.75              |
| 1:A:80:PHE:HB3   | 5:A:1483:MPD:C1  | 2.17                     | 0.75              |
| 1:F:52:SER:HB3   | 1:F:63:SER:CB    | 2.16                     | 0.75              |
| 1:I:52:SER:HB3   | 1:I:63:SER:CB    | 2.16                     | 0.75              |
| 3:K:1481:ADP:N9  | 3:K:1481:ADP:H1' | 1.98                     | 0.75              |
| 1:B:52:SER:HB3   | 1:B:63:SER:CB    | 2.16                     | 0.75              |
| 1:D:1:SER:HA     | 1:D:71:ALA:HB3   | 1.67                     | 0.75              |
| 1:F:1:SER:HA     | 1:F:71:ALA:HB3   | 1.67                     | 0.75              |
| 1:G:323:VAL:O    | 1:G:325:GLY:N    | 2.20                     | 0.75              |
| 1:L:52:SER:HB3   | 1:L:63:SER:CB    | 2.16                     | 0.75              |
| 1:A:395:ASN:ND2  | 1:B:60:ILE:CG2   | 2.48                     | 0.75              |
| 1:F:80:PHE:HB3   | 5:F:1488:MPD:C1  | 2.17                     | 0.75              |
| 5:I:1491:MPD:HM3 | 1:J:190:ASP:OD2  | 1.87                     | 0.75              |
| 1:J:52:SER:HB3   | 1:J:63:SER:CB    | 2.16                     | 0.75              |
| 1:L:80:PHE:HB3   | 5:L:1494:MPD:C1  | 2.17                     | 0.75              |
| 1:A:323:VAL:O    | 1:A:325:GLY:N    | 2.20                     | 0.75              |
| 1:C:323:VAL:O    | 1:C:325:GLY:N    | 2.20                     | 0.75              |
| 1:D:190:ASP:OD2  | 5:E:1487:MPD:HM3 | 1.85                     | 0.75              |
| 1:E:193:SER:HB2  | 5:F:1488:MPD:H32 | 1.67                     | 0.75              |
| 1:I:80:PHE:HB3   | 5:I:1491:MPD:C1  | 2.17                     | 0.75              |
| 1:A:1:SER:HA     | 1:A:71:ALA:HB3   | 1.67                     | 0.75              |
| 1:D:80:PHE:HB3   | 5:D:1486:MPD:C1  | 2.17                     | 0.75              |
| 1:D:323:VAL:O    | 1:D:325:GLY:N    | 2.20                     | 0.75              |
| 1:E:1:SER:HA     | 1:E:71:ALA:HB3   | 1.67                     | 0.75              |
| 1:C:80:PHE:HB3   | 5:C:1485:MPD:C1  | 2.17                     | 0.74              |
| 1:D:52:SER:HB3   | 1:D:63:SER:CB    | 2.16                     | 0.74              |
| 1:I:323:VAL:O    | 1:I:325:GLY:N    | 2.20                     | 0.74              |
| 5:K:1493:MPD:H32 | 1:L:193:SER:HB2  | 1.69                     | 0.74              |
| 1:B:189:GLN:HG3  | 5:C:1485:MPD:HM1 | 1.69                     | 0.74              |
| 1:H:52:SER:HB3   | 1:H:63:SER:CB    | 2.16                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:1:SER:HA     | 1:K:71:ALA:HB3   | 1.67                     | 0.74              |
| 1:B:80:PHE:HB3   | 5:B:1484:MPD:C1  | 2.17                     | 0.74              |
| 1:C:190:ASP:HA   | 5:D:1486:MPD:O2  | 1.87                     | 0.74              |
| 3:C:1473:ADP:N9  | 3:C:1473:ADP:H1' | 1.99                     | 0.74              |
| 1:H:80:PHE:HB3   | 5:H:1490:MPD:C1  | 2.17                     | 0.74              |
| 1:J:323:VAL:O    | 1:J:325:GLY:N    | 2.20                     | 0.74              |
| 1:K:323:VAL:O    | 1:K:325:GLY:N    | 2.20                     | 0.74              |
| 1:L:323:VAL:O    | 1:L:325:GLY:N    | 2.20                     | 0.74              |
| 1:G:398:ASP:C    | 1:G:400:PRO:HD3  | 2.13                     | 0.74              |
| 1:H:179:TYR:O    | 1:H:181:PRO:CD   | 2.36                     | 0.74              |
| 1:H:323:VAL:O    | 1:H:325:GLY:N    | 2.20                     | 0.74              |
| 1:K:395:ASN:CB   | 1:K:399:LEU:CD1  | 2.60                     | 0.74              |
| 1:K:398:ASP:C    | 1:K:400:PRO:HD3  | 2.13                     | 0.74              |
| 1:E:179:TYR:O    | 1:E:181:PRO:CD   | 2.36                     | 0.74              |
| 1:E:323:VAL:O    | 1:E:325:GLY:N    | 2.20                     | 0.74              |
| 1:G:60:ILE:CG2   | 1:H:395:ASN:ND2  | 2.47                     | 0.74              |
| 1:L:179:TYR:O    | 1:L:181:PRO:CD   | 2.36                     | 0.74              |
| 1:A:179:TYR:O    | 1:A:181:PRO:CD   | 2.36                     | 0.74              |
| 1:B:455:MET:HG2  | 1:H:323:VAL:HG21 | 1.69                     | 0.74              |
| 1:H:1:SER:HA     | 1:H:71:ALA:HB3   | 1.67                     | 0.74              |
| 1:A:398:ASP:C    | 1:A:400:PRO:HD3  | 2.13                     | 0.74              |
| 1:J:80:PHE:HB3   | 5:J:1492:MPD:C1  | 2.17                     | 0.74              |
| 1:E:190:ASP:OD2  | 5:F:1488:MPD:HM3 | 1.86                     | 0.74              |
| 1:D:179:TYR:O    | 1:D:181:PRO:CD   | 2.36                     | 0.73              |
| 1:F:323:VAL:O    | 1:F:325:GLY:N    | 2.20                     | 0.73              |
| 1:G:179:TYR:O    | 1:G:181:PRO:CD   | 2.36                     | 0.73              |
| 1:C:179:TYR:O    | 1:C:181:PRO:CD   | 2.36                     | 0.73              |
| 1:E:80:PHE:HB3   | 5:E:1487:MPD:C1  | 2.17                     | 0.73              |
| 1:A:455:MET:HG2  | 1:G:323:VAL:HG21 | 1.69                     | 0.73              |
| 1:H:60:ILE:HG21  | 1:I:395:ASN:HD21 | 1.53                     | 0.73              |
| 1:I:398:ASP:C    | 1:I:400:PRO:HD3  | 2.13                     | 0.73              |
| 1:I:179:TYR:O    | 1:I:181:PRO:CD   | 2.36                     | 0.73              |
| 1:A:340:SER:CB   | 1:A:396:LEU:HB3  | 2.19                     | 0.73              |
| 1:C:398:ASP:C    | 1:C:400:PRO:HD3  | 2.13                     | 0.73              |
| 1:K:179:TYR:O    | 1:K:181:PRO:CD   | 2.36                     | 0.73              |
| 5:K:1493:MPD:O2  | 1:L:190:ASP:HA   | 1.87                     | 0.73              |
| 1:B:323:VAL:O    | 1:B:325:GLY:N    | 2.20                     | 0.73              |
| 5:G:1489:MPD:HM1 | 1:H:189:GLN:HG3  | 1.71                     | 0.73              |
| 1:B:179:TYR:O    | 1:B:181:PRO:CD   | 2.36                     | 0.73              |
| 3:E:1475:ADP:N9  | 3:E:1475:ADP:H1' | 1.98                     | 0.73              |
| 1:B:340:SER:CB   | 1:B:396:LEU:HB3  | 2.19                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:189:GLN:HG3  | 5:F:1488:MPD:CM  | 2.19                     | 0.73              |
| 1:E:340:SER:CB   | 1:E:396:LEU:HB3  | 2.19                     | 0.73              |
| 1:H:340:SER:CB   | 1:H:396:LEU:HB3  | 2.19                     | 0.73              |
| 1:K:340:SER:CB   | 1:K:396:LEU:HB3  | 2.19                     | 0.73              |
| 1:F:323:VAL:HG21 | 1:L:455:MET:HG2  | 1.71                     | 0.73              |
| 1:G:80:PHE:HB3   | 5:G:1489:MPD:C1  | 2.17                     | 0.73              |
| 1:A:395:ASN:CB   | 1:A:399:LEU:CD1  | 2.60                     | 0.72              |
| 1:J:179:TYR:O    | 1:J:181:PRO:CD   | 2.36                     | 0.72              |
| 1:L:398:ASP:C    | 1:L:400:PRO:HD3  | 2.13                     | 0.72              |
| 1:D:340:SER:CB   | 1:D:396:LEU:HB3  | 2.19                     | 0.72              |
| 1:E:398:ASP:C    | 1:E:400:PRO:HD3  | 2.13                     | 0.72              |
| 1:F:179:TYR:O    | 1:F:181:PRO:CD   | 2.36                     | 0.72              |
| 5:H:1490:MPD:O2  | 1:I:190:ASP:HA   | 1.87                     | 0.72              |
| 1:C:180:PHE:HB3  | 1:D:29:GLN:HB3   | 1.72                     | 0.72              |
| 1:C:340:SER:CB   | 1:C:396:LEU:HB3  | 2.19                     | 0.72              |
| 1:A:193:SER:HB2  | 5:B:1484:MPD:H32 | 1.70                     | 0.72              |
| 1:F:398:ASP:C    | 1:F:400:PRO:HD3  | 2.13                     | 0.72              |
| 1:I:29:GLN:HB3   | 1:J:180:PHE:HB3  | 1.71                     | 0.72              |
| 1:J:398:ASP:C    | 1:J:400:PRO:HD3  | 2.13                     | 0.72              |
| 1:E:395:ASN:HD21 | 1:F:60:ILE:HG21  | 1.55                     | 0.72              |
| 1:L:395:ASN:CB   | 1:L:399:LEU:CD1  | 2.60                     | 0.72              |
| 1:A:189:GLN:HG3  | 5:B:1484:MPD:CM  | 2.20                     | 0.72              |
| 1:E:334:TYR:CE2  | 1:E:391:PRO:HG3  | 2.25                     | 0.72              |
| 1:F:334:TYR:CE2  | 1:F:391:PRO:HG3  | 2.25                     | 0.72              |
| 1:F:340:SER:CB   | 1:F:396:LEU:HB3  | 2.19                     | 0.72              |
| 1:G:340:SER:CB   | 1:G:396:LEU:HB3  | 2.19                     | 0.72              |
| 1:I:340:SER:CB   | 1:I:396:LEU:HB3  | 2.19                     | 0.72              |
| 1:B:189:GLN:HG3  | 5:C:1485:MPD:CM  | 2.20                     | 0.71              |
| 1:F:1:SER:C      | 1:F:71:ALA:HB1   | 2.15                     | 0.71              |
| 1:L:340:SER:CB   | 1:L:396:LEU:HB3  | 2.19                     | 0.71              |
| 1:J:334:TYR:CE2  | 1:J:391:PRO:HG3  | 2.25                     | 0.71              |
| 3:J:1480:ADP:N9  | 3:J:1480:ADP:H1' | 1.99                     | 0.71              |
| 1:K:334:TYR:CE2  | 1:K:391:PRO:HG3  | 2.25                     | 0.71              |
| 1:C:395:ASN:CB   | 1:C:399:LEU:CD1  | 2.60                     | 0.71              |
| 1:G:1:SER:C      | 1:G:71:ALA:HB1   | 2.15                     | 0.71              |
| 1:G:334:TYR:CE2  | 1:G:391:PRO:HG3  | 2.25                     | 0.71              |
| 1:H:1:SER:C      | 1:H:71:ALA:HB1   | 2.15                     | 0.71              |
| 1:A:1:SER:C      | 1:A:71:ALA:HB1   | 2.15                     | 0.71              |
| 1:C:323:VAL:HG21 | 1:I:455:MET:HG2  | 1.70                     | 0.71              |
| 1:E:1:SER:C      | 1:E:71:ALA:HB1   | 2.15                     | 0.71              |
| 1:H:334:TYR:CE2  | 1:H:391:PRO:HG3  | 2.25                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:193:SER:HB2  | 5:D:1486:MPD:H32 | 1.72                     | 0.71              |
| 5:I:1491:MPD:HM1 | 1:J:189:GLN:HG3  | 1.71                     | 0.71              |
| 1:J:340:SER:CB   | 1:J:396:LEU:HB3  | 2.19                     | 0.71              |
| 1:B:334:TYR:CE2  | 1:B:391:PRO:HG3  | 2.25                     | 0.71              |
| 1:I:1:SER:C      | 1:I:71:ALA:HB1   | 2.15                     | 0.71              |
| 1:K:60:ILE:HG21  | 1:L:395:ASN:HD21 | 1.55                     | 0.71              |
| 1:B:398:ASP:C    | 1:B:400:PRO:HD3  | 2.13                     | 0.71              |
| 5:J:1492:MPD:HM1 | 1:K:189:GLN:HG3  | 1.73                     | 0.71              |
| 1:L:1:SER:C      | 1:L:71:ALA:HB1   | 2.15                     | 0.71              |
| 1:A:334:TYR:CE2  | 1:A:391:PRO:HG3  | 2.25                     | 0.71              |
| 1:I:334:TYR:CE2  | 1:I:391:PRO:HG3  | 2.25                     | 0.71              |
| 1:D:334:TYR:CE2  | 1:D:391:PRO:HG3  | 2.25                     | 0.71              |
| 1:G:395:ASN:CB   | 1:G:399:LEU:CD1  | 2.60                     | 0.71              |
| 1:H:398:ASP:C    | 1:H:400:PRO:HD3  | 2.13                     | 0.71              |
| 1:B:1:SER:C      | 1:B:71:ALA:HB1   | 2.15                     | 0.70              |
| 1:D:1:SER:C      | 1:D:71:ALA:HB1   | 2.15                     | 0.70              |
| 1:L:334:TYR:CE2  | 1:L:391:PRO:HG3  | 2.25                     | 0.70              |
| 1:C:334:TYR:CE2  | 1:C:391:PRO:HG3  | 2.25                     | 0.70              |
| 1:J:1:SER:C      | 1:J:71:ALA:HB1   | 2.15                     | 0.70              |
| 5:I:1491:MPD:CM  | 1:J:189:GLN:HG3  | 2.21                     | 0.70              |
| 1:K:1:SER:C      | 1:K:71:ALA:HB1   | 2.15                     | 0.70              |
| 1:A:190:ASP:OD2  | 5:B:1484:MPD:HM3 | 1.89                     | 0.70              |
| 1:C:1:SER:C      | 1:C:71:ALA:HB1   | 2.15                     | 0.70              |
| 1:D:455:MET:HG2  | 1:J:323:VAL:HG21 | 1.73                     | 0.70              |
| 5:G:1489:MPD:HM3 | 1:H:190:ASP:OD2  | 1.91                     | 0.70              |
| 5:G:1489:MPD:O2  | 1:H:190:ASP:HA   | 1.90                     | 0.70              |
| 3:I:1479:ADP:N9  | 3:I:1479:ADP:H1' | 1.99                     | 0.70              |
| 1:D:190:ASP:HA   | 5:E:1487:MPD:O2  | 1.91                     | 0.70              |
| 3:F:1476:ADP:N9  | 3:F:1476:ADP:H1' | 1.98                     | 0.70              |
| 1:E:455:MET:HG2  | 1:K:323:VAL:HG21 | 1.72                     | 0.69              |
| 1:D:398:ASP:C    | 1:D:400:PRO:HD3  | 2.13                     | 0.69              |
| 5:A:1483:MPD:O2  | 1:F:190:ASP:HA   | 1.92                     | 0.69              |
| 1:D:1:SER:CA     | 1:D:71:ALA:HB1   | 2.23                     | 0.69              |
| 1:F:1:SER:CA     | 1:F:71:ALA:HB1   | 2.23                     | 0.69              |
| 1:A:1:SER:CA     | 1:A:71:ALA:HB1   | 2.23                     | 0.69              |
| 1:A:211:HIS:HD2  | 1:A:212:GLU:O    | 1.76                     | 0.69              |
| 5:A:1483:MPD:H32 | 1:F:193:SER:CB   | 2.23                     | 0.69              |
| 1:B:1:SER:CA     | 1:B:71:ALA:HB1   | 2.23                     | 0.69              |
| 1:G:211:HIS:HD2  | 1:G:212:GLU:O    | 1.76                     | 0.69              |
| 1:H:1:SER:CA     | 1:H:71:ALA:HB1   | 2.23                     | 0.69              |
| 1:J:211:HIS:HD2  | 1:J:212:GLU:O    | 1.76                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:1472:ADP:N9  | 3:B:1472:ADP:H1' | 1.99                     | 0.69              |
| 1:E:211:HIS:HD2  | 1:E:212:GLU:O    | 1.76                     | 0.69              |
| 5:J:1492:MPD:CM  | 1:K:189:GLN:HG3  | 2.22                     | 0.69              |
| 1:F:211:HIS:HD2  | 1:F:212:GLU:O    | 1.76                     | 0.69              |
| 1:H:211:HIS:HD2  | 1:H:212:GLU:O    | 1.76                     | 0.69              |
| 1:J:1:SER:CA     | 1:J:71:ALA:HB1   | 2.23                     | 0.69              |
| 1:K:211:HIS:HD2  | 1:K:212:GLU:O    | 1.76                     | 0.69              |
| 1:C:1:SER:CA     | 1:C:71:ALA:HB1   | 2.23                     | 0.68              |
| 1:K:1:SER:CA     | 1:K:71:ALA:HB1   | 2.23                     | 0.68              |
| 1:L:1:SER:CA     | 1:L:71:ALA:HB1   | 2.23                     | 0.68              |
| 1:G:1:SER:CA     | 1:G:71:ALA:HB1   | 2.23                     | 0.68              |
| 1:I:1:SER:CA     | 1:I:71:ALA:HB1   | 2.23                     | 0.68              |
| 1:D:179:TYR:C    | 1:D:181:PRO:HD2  | 2.19                     | 0.68              |
| 1:F:179:TYR:C    | 1:F:181:PRO:HD2  | 2.19                     | 0.68              |
| 1:A:397:TYR:CE1  | 1:A:401:PRO:HD3  | 2.29                     | 0.68              |
| 1:C:211:HIS:HD2  | 1:C:212:GLU:O    | 1.76                     | 0.68              |
| 1:J:179:TYR:C    | 1:J:181:PRO:HD2  | 2.19                     | 0.68              |
| 1:J:397:TYR:CE1  | 1:J:401:PRO:HD3  | 2.29                     | 0.68              |
| 1:B:211:HIS:HD2  | 1:B:212:GLU:O    | 1.76                     | 0.68              |
| 1:C:397:TYR:CE1  | 1:C:401:PRO:HD3  | 2.29                     | 0.68              |
| 1:D:193:SER:CB   | 5:E:1487:MPD:H32 | 2.22                     | 0.68              |
| 1:D:395:ASN:CB   | 1:D:399:LEU:CD1  | 2.60                     | 0.68              |
| 1:D:397:TYR:CE1  | 1:D:401:PRO:HD3  | 2.29                     | 0.68              |
| 1:E:224:ARG:HH21 | 1:E:224:ARG:CG   | 2.07                     | 0.68              |
| 1:G:397:TYR:CE1  | 1:G:401:PRO:HD3  | 2.29                     | 0.68              |
| 1:I:211:HIS:HD2  | 1:I:212:GLU:O    | 1.76                     | 0.68              |
| 1:H:179:TYR:C    | 1:H:181:PRO:HD2  | 2.19                     | 0.68              |
| 1:C:179:TYR:C    | 1:C:181:PRO:HD2  | 2.19                     | 0.68              |
| 1:I:397:TYR:CE1  | 1:I:401:PRO:HD3  | 2.29                     | 0.68              |
| 1:K:179:TYR:C    | 1:K:181:PRO:HD2  | 2.19                     | 0.68              |
| 1:K:458:HIS:CD2  | 1:K:460:VAL:H    | 2.09                     | 0.68              |
| 1:L:211:HIS:HD2  | 1:L:212:GLU:O    | 1.76                     | 0.68              |
| 1:K:224:ARG:HH21 | 1:K:224:ARG:CG   | 2.07                     | 0.68              |
| 1:G:179:TYR:C    | 1:G:181:PRO:HD2  | 2.19                     | 0.68              |
| 5:G:1489:MPD:CM  | 1:H:189:GLN:HG3  | 2.24                     | 0.68              |
| 1:K:397:TYR:CE1  | 1:K:401:PRO:HD3  | 2.29                     | 0.68              |
| 1:B:179:TYR:C    | 1:B:181:PRO:HD2  | 2.19                     | 0.67              |
| 1:E:1:SER:CA     | 1:E:71:ALA:HB1   | 2.23                     | 0.67              |
| 1:L:179:TYR:C    | 1:L:181:PRO:HD2  | 2.19                     | 0.67              |
| 1:L:397:TYR:CE1  | 1:L:401:PRO:HD3  | 2.29                     | 0.67              |
| 1:D:129:GLU:OE2  | 1:D:269:HIS:HB2  | 1.95                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:211:HIS:HD2  | 1:D:212:GLU:O    | 1.76                     | 0.67              |
| 1:L:458:HIS:CD2  | 1:L:460:VAL:H    | 2.09                     | 0.67              |
| 3:L:1482:ADP:N9  | 3:L:1482:ADP:H1' | 1.99                     | 0.67              |
| 1:E:397:TYR:CE1  | 1:E:401:PRO:HD3  | 2.29                     | 0.67              |
| 1:I:179:TYR:C    | 1:I:181:PRO:HD2  | 2.19                     | 0.67              |
| 1:K:129:GLU:OE2  | 1:K:269:HIS:HB2  | 1.95                     | 0.67              |
| 3:D:1474:ADP:N9  | 3:D:1474:ADP:H1' | 1.99                     | 0.67              |
| 1:E:179:TYR:C    | 1:E:181:PRO:HD2  | 2.19                     | 0.67              |
| 1:I:129:GLU:OE2  | 1:I:269:HIS:HB2  | 1.95                     | 0.67              |
| 1:A:179:TYR:C    | 1:A:181:PRO:HD2  | 2.19                     | 0.67              |
| 1:A:224:ARG:HH21 | 1:A:224:ARG:CG   | 2.07                     | 0.67              |
| 1:B:224:ARG:HH21 | 1:B:224:ARG:CG   | 2.07                     | 0.67              |
| 1:G:129:GLU:OE2  | 1:G:269:HIS:HB2  | 1.95                     | 0.67              |
| 1:B:129:GLU:OE2  | 1:B:269:HIS:HB2  | 1.95                     | 0.67              |
| 1:F:397:TYR:CE1  | 1:F:401:PRO:HD3  | 2.29                     | 0.67              |
| 1:G:458:HIS:CD2  | 1:G:460:VAL:H    | 2.10                     | 0.67              |
| 1:J:129:GLU:OE2  | 1:J:269:HIS:HB2  | 1.95                     | 0.67              |
| 1:J:224:ARG:HH21 | 1:J:224:ARG:CG   | 2.07                     | 0.67              |
| 1:L:129:GLU:OE2  | 1:L:269:HIS:HB2  | 1.95                     | 0.67              |
| 1:D:224:ARG:HH21 | 1:D:224:ARG:CG   | 2.07                     | 0.67              |
| 1:F:129:GLU:OE2  | 1:F:269:HIS:HB2  | 1.95                     | 0.67              |
| 1:F:224:ARG:HH21 | 1:F:224:ARG:CG   | 2.07                     | 0.67              |
| 1:H:82:ASP:HB2   | 5:H:1490:MPD:H12 | 1.77                     | 0.67              |
| 1:H:224:ARG:HH21 | 1:H:224:ARG:CG   | 2.07                     | 0.67              |
| 1:C:129:GLU:OE2  | 1:C:269:HIS:HB2  | 1.95                     | 0.67              |
| 1:H:397:TYR:CE1  | 1:H:401:PRO:HD3  | 2.29                     | 0.67              |
| 1:J:82:ASP:HB2   | 5:J:1492:MPD:H12 | 1.77                     | 0.67              |
| 1:E:129:GLU:OE2  | 1:E:269:HIS:HB2  | 1.95                     | 0.66              |
| 1:H:458:HIS:CD2  | 1:H:460:VAL:H    | 2.09                     | 0.66              |
| 1:B:82:ASP:HB2   | 5:B:1484:MPD:H12 | 1.77                     | 0.66              |
| 1:D:82:ASP:HB2   | 5:D:1486:MPD:H12 | 1.77                     | 0.66              |
| 1:B:397:TYR:CE1  | 1:B:401:PRO:HD3  | 2.29                     | 0.66              |
| 1:C:458:HIS:CD2  | 1:C:460:VAL:H    | 2.09                     | 0.66              |
| 1:F:82:ASP:HB2   | 5:F:1488:MPD:H12 | 1.77                     | 0.66              |
| 1:G:180:PHE:HB3  | 1:L:29:GLN:HB3   | 1.77                     | 0.66              |
| 1:H:129:GLU:OE2  | 1:H:269:HIS:HB2  | 1.95                     | 0.66              |
| 1:C:224:ARG:HH21 | 1:C:224:ARG:CG   | 2.07                     | 0.66              |
| 1:E:458:HIS:CD2  | 1:E:460:VAL:H    | 2.10                     | 0.66              |
| 3:G:1477:ADP:N9  | 3:G:1477:ADP:H1' | 1.98                     | 0.66              |
| 1:L:403:GLU:O    | 1:L:403:GLU:HG2  | 1.96                     | 0.66              |
| 1:A:129:GLU:OE2  | 1:A:269:HIS:HB2  | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:29:GLN:HB3   | 1:K:180:PHE:HB3  | 1.77                     | 0.66              |
| 1:G:224:ARG:HH21 | 1:G:224:ARG:CG   | 2.07                     | 0.66              |
| 1:E:82:ASP:HB2   | 5:E:1487:MPD:H12 | 1.77                     | 0.66              |
| 1:C:82:ASP:HB2   | 5:C:1485:MPD:H12 | 1.77                     | 0.66              |
| 1:F:458:HIS:CD2  | 1:F:460:VAL:H    | 2.10                     | 0.66              |
| 1:I:397:TYR:HE1  | 1:I:401:PRO:HD3  | 1.61                     | 0.66              |
| 1:J:397:TYR:HE1  | 1:J:401:PRO:HD3  | 1.61                     | 0.66              |
| 1:L:224:ARG:HH21 | 1:L:224:ARG:CG   | 2.07                     | 0.66              |
| 1:L:397:TYR:HE1  | 1:L:401:PRO:HD3  | 1.61                     | 0.66              |
| 1:B:397:TYR:HE1  | 1:B:401:PRO:HD3  | 1.61                     | 0.66              |
| 1:F:397:TYR:HE1  | 1:F:401:PRO:HD3  | 1.61                     | 0.66              |
| 1:I:82:ASP:HB2   | 5:I:1491:MPD:H12 | 1.77                     | 0.66              |
| 1:F:403:GLU:O    | 1:F:403:GLU:HG2  | 1.96                     | 0.65              |
| 1:D:403:GLU:O    | 1:D:403:GLU:HG2  | 1.96                     | 0.65              |
| 1:I:224:ARG:HH21 | 1:I:224:ARG:CG   | 2.07                     | 0.65              |
| 1:L:82:ASP:HB2   | 5:L:1494:MPD:H12 | 1.77                     | 0.65              |
| 1:I:403:GLU:O    | 1:I:403:GLU:HG2  | 1.96                     | 0.65              |
| 1:A:82:ASP:HB2   | 5:A:1483:MPD:H12 | 1.77                     | 0.65              |
| 1:B:403:GLU:HG2  | 1:B:403:GLU:O    | 1.96                     | 0.65              |
| 1:J:60:ILE:HG21  | 1:K:395:ASN:ND2  | 2.08                     | 0.65              |
| 1:D:84:THR:HG21  | 5:D:1486:MPD:O4  | 1.97                     | 0.65              |
| 1:E:403:GLU:HG2  | 1:E:403:GLU:O    | 1.96                     | 0.65              |
| 1:A:403:GLU:O    | 1:A:403:GLU:HG2  | 1.96                     | 0.65              |
| 1:I:84:THR:HG21  | 5:I:1491:MPD:O4  | 1.97                     | 0.65              |
| 1:J:403:GLU:HG2  | 1:J:403:GLU:O    | 1.96                     | 0.65              |
| 1:C:397:TYR:HE1  | 1:C:401:PRO:HD3  | 1.61                     | 0.65              |
| 1:C:403:GLU:O    | 1:C:403:GLU:HG2  | 1.96                     | 0.65              |
| 1:G:155:GLU:OE1  | 1:G:211:HIS:HE1  | 1.80                     | 0.65              |
| 1:H:403:GLU:O    | 1:H:403:GLU:HG2  | 1.96                     | 0.65              |
| 1:K:82:ASP:HB2   | 5:K:1493:MPD:H12 | 1.77                     | 0.65              |
| 1:B:84:THR:HG21  | 5:B:1484:MPD:O4  | 1.97                     | 0.65              |
| 1:H:397:TYR:HE1  | 1:H:401:PRO:HD3  | 1.61                     | 0.65              |
| 1:C:180:PHE:O    | 1:D:29:GLN:HA    | 1.97                     | 0.64              |
| 1:E:84:THR:HG21  | 5:E:1487:MPD:O4  | 1.97                     | 0.64              |
| 1:C:155:GLU:OE1  | 1:C:211:HIS:HE1  | 1.80                     | 0.64              |
| 1:D:189:GLN:HG3  | 5:E:1487:MPD:HM1 | 1.79                     | 0.64              |
| 1:L:84:THR:HG21  | 5:L:1494:MPD:O4  | 1.97                     | 0.64              |
| 1:B:193:SER:OG   | 5:C:1485:MPD:H32 | 1.97                     | 0.64              |
| 1:D:155:GLU:OE1  | 1:D:211:HIS:HE1  | 1.80                     | 0.64              |
| 1:D:397:TYR:HE1  | 1:D:401:PRO:HD3  | 1.61                     | 0.64              |
| 1:G:84:THR:HG21  | 5:G:1489:MPD:O4  | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:395:ASN:ND2  | 1:L:60:ILE:HG21  | 2.07                     | 0.64              |
| 1:A:84:THR:HG21  | 5:A:1483:MPD:O4  | 1.97                     | 0.64              |
| 1:A:180:PHE:HB3  | 1:B:29:GLN:HB3   | 1.80                     | 0.64              |
| 1:G:403:GLU:HG2  | 1:G:403:GLU:O    | 1.96                     | 0.64              |
| 1:G:82:ASP:HB2   | 5:G:1489:MPD:H12 | 1.77                     | 0.64              |
| 1:G:360:PHE:CD2  | 1:G:361:PRO:CD   | 2.71                     | 0.64              |
| 1:J:84:THR:HG21  | 5:J:1492:MPD:O4  | 1.97                     | 0.64              |
| 1:A:155:GLU:OE1  | 1:A:211:HIS:HE1  | 1.80                     | 0.64              |
| 1:A:397:TYR:HE1  | 1:A:401:PRO:HD3  | 1.61                     | 0.64              |
| 1:B:458:HIS:CD2  | 1:B:460:VAL:H    | 2.10                     | 0.64              |
| 1:C:189:GLN:HG3  | 5:D:1486:MPD:HM1 | 1.79                     | 0.64              |
| 1:F:84:THR:HG21  | 5:F:1488:MPD:O4  | 1.97                     | 0.64              |
| 1:I:155:GLU:OE1  | 1:I:211:HIS:HE1  | 1.80                     | 0.64              |
| 1:F:155:GLU:OE1  | 1:F:211:HIS:HE1  | 1.80                     | 0.64              |
| 1:J:155:GLU:OE1  | 1:J:211:HIS:HE1  | 1.80                     | 0.64              |
| 1:C:84:THR:HG21  | 5:C:1485:MPD:O4  | 1.97                     | 0.64              |
| 1:H:29:GLN:HB3   | 1:I:180:PHE:HB3  | 1.79                     | 0.64              |
| 1:H:84:THR:HG21  | 5:H:1490:MPD:O4  | 1.97                     | 0.64              |
| 1:K:84:THR:HG21  | 5:K:1493:MPD:O4  | 1.97                     | 0.64              |
| 1:K:397:TYR:HE1  | 1:K:401:PRO:HD3  | 1.61                     | 0.64              |
| 1:E:155:GLU:OE1  | 1:E:211:HIS:HE1  | 1.80                     | 0.63              |
| 1:C:395:ASN:ND2  | 1:D:60:ILE:CG2   | 2.51                     | 0.63              |
| 1:L:360:PHE:CD2  | 1:L:361:PRO:CD   | 2.71                     | 0.63              |
| 1:B:155:GLU:OE1  | 1:B:211:HIS:HE1  | 1.80                     | 0.63              |
| 1:G:29:GLN:HB3   | 1:H:180:PHE:HB3  | 1.78                     | 0.63              |
| 1:G:397:TYR:HE1  | 1:G:401:PRO:HD3  | 1.61                     | 0.63              |
| 1:D:458:HIS:CD2  | 1:D:460:VAL:H    | 2.09                     | 0.63              |
| 5:G:1489:MPD:H32 | 1:H:193:SER:HB2  | 1.78                     | 0.63              |
| 1:K:403:GLU:O    | 1:K:403:GLU:HG2  | 1.96                     | 0.63              |
| 1:E:360:PHE:CD2  | 1:E:361:PRO:CD   | 2.71                     | 0.63              |
| 1:F:48:MET:HE2   | 1:F:66:VAL:CG2   | 2.26                     | 0.63              |
| 1:H:155:GLU:OE1  | 1:H:211:HIS:HE1  | 1.80                     | 0.63              |
| 1:A:458:HIS:CD2  | 1:A:460:VAL:H    | 2.10                     | 0.63              |
| 1:A:384:ASN:HD22 | 1:A:384:ASN:N    | 1.97                     | 0.63              |
| 1:D:384:ASN:HD22 | 1:D:384:ASN:N    | 1.97                     | 0.63              |
| 1:E:384:ASN:HD22 | 1:E:384:ASN:N    | 1.97                     | 0.63              |
| 1:K:155:GLU:OE1  | 1:K:211:HIS:HE1  | 1.80                     | 0.63              |
| 1:A:29:GLN:HB3   | 1:F:180:PHE:HB3  | 1.81                     | 0.63              |
| 1:E:397:TYR:HE1  | 1:E:401:PRO:HD3  | 1.61                     | 0.63              |
| 1:F:384:ASN:N    | 1:F:384:ASN:HD22 | 1.97                     | 0.63              |
| 1:G:189:GLN:HG3  | 5:L:1494:MPD:CM  | 2.28                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:189:GLN:HG3  | 5:L:1494:MPD:HM1 | 1.79                     | 0.63              |
| 1:H:384:ASN:HD22 | 1:H:384:ASN:N    | 1.97                     | 0.63              |
| 1:K:384:ASN:HD22 | 1:K:384:ASN:N    | 1.97                     | 0.63              |
| 1:K:48:MET:HE2   | 1:K:66:VAL:CG2   | 2.26                     | 0.62              |
| 1:B:384:ASN:HD22 | 1:B:384:ASN:N    | 1.97                     | 0.62              |
| 1:I:384:ASN:N    | 1:I:384:ASN:HD22 | 1.97                     | 0.62              |
| 1:C:179:TYR:O    | 1:C:181:PRO:HD2  | 2.00                     | 0.62              |
| 1:E:396:LEU:O    | 1:E:399:LEU:HB2  | 2.00                     | 0.62              |
| 1:I:29:GLN:HA    | 1:J:180:PHE:O    | 1.98                     | 0.62              |
| 1:I:360:PHE:CD2  | 1:I:361:PRO:CD   | 2.71                     | 0.62              |
| 1:K:396:LEU:O    | 1:K:399:LEU:HB2  | 2.00                     | 0.62              |
| 1:L:155:GLU:OE1  | 1:L:211:HIS:HE1  | 1.80                     | 0.62              |
| 1:C:384:ASN:HD22 | 1:C:384:ASN:N    | 1.97                     | 0.62              |
| 1:A:396:LEU:O    | 1:A:399:LEU:HB2  | 2.00                     | 0.62              |
| 1:I:396:LEU:O    | 1:I:399:LEU:HB2  | 2.00                     | 0.62              |
| 1:K:29:GLN:HB3   | 1:L:180:PHE:HB3  | 1.81                     | 0.62              |
| 1:C:396:LEU:O    | 1:C:399:LEU:HB2  | 2.00                     | 0.62              |
| 1:D:396:LEU:O    | 1:D:399:LEU:HB2  | 2.00                     | 0.62              |
| 1:E:193:SER:OG   | 5:F:1488:MPD:H32 | 1.99                     | 0.62              |
| 1:F:179:TYR:O    | 1:F:181:PRO:HD2  | 2.00                     | 0.62              |
| 1:J:179:TYR:O    | 1:J:181:PRO:HD2  | 2.00                     | 0.62              |
| 1:D:360:PHE:CD2  | 1:D:361:PRO:CD   | 2.71                     | 0.62              |
| 1:F:179:TYR:O    | 1:F:181:PRO:HD3  | 2.00                     | 0.62              |
| 1:G:179:TYR:O    | 1:G:181:PRO:HD3  | 2.00                     | 0.62              |
| 1:G:384:ASN:HD22 | 1:G:384:ASN:N    | 1.97                     | 0.62              |
| 5:H:1490:MPD:HM1 | 1:I:189:GLN:HG3  | 1.81                     | 0.62              |
| 1:J:60:ILE:CG2   | 1:K:395:ASN:ND2  | 2.57                     | 0.62              |
| 1:C:189:GLN:HG3  | 5:D:1486:MPD:CM  | 2.30                     | 0.62              |
| 1:F:396:LEU:O    | 1:F:399:LEU:HB2  | 2.00                     | 0.62              |
| 1:H:396:LEU:O    | 1:H:399:LEU:HB2  | 2.00                     | 0.62              |
| 1:K:179:TYR:O    | 1:K:181:PRO:HD3  | 2.00                     | 0.62              |
| 1:C:179:TYR:O    | 1:C:181:PRO:HD3  | 2.00                     | 0.62              |
| 1:G:179:TYR:O    | 1:G:181:PRO:HD2  | 2.00                     | 0.62              |
| 1:L:384:ASN:HD22 | 1:L:384:ASN:N    | 1.97                     | 0.62              |
| 1:A:179:TYR:O    | 1:A:181:PRO:HD3  | 2.00                     | 0.61              |
| 1:J:384:ASN:HD22 | 1:J:384:ASN:N    | 1.97                     | 0.61              |
| 5:A:1483:MPD:H32 | 1:F:193:SER:HB2  | 1.82                     | 0.61              |
| 1:C:58:LYS:HZ1   | 1:C:60:ILE:HD11  | 1.66                     | 0.61              |
| 1:G:396:LEU:O    | 1:G:399:LEU:HB2  | 2.00                     | 0.61              |
| 1:J:396:LEU:O    | 1:J:399:LEU:HB2  | 2.00                     | 0.61              |
| 1:L:48:MET:HE2   | 1:L:66:VAL:CG2   | 2.26                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:396:LEU:O    | 1:L:399:LEU:HB2  | 2.00                     | 0.61              |
| 1:B:396:LEU:O    | 1:B:399:LEU:HB2  | 2.00                     | 0.61              |
| 1:G:224:ARG:HG2  | 1:G:224:ARG:NH2  | 2.15                     | 0.61              |
| 5:H:1490:MPD:C3  | 1:I:193:SER:CB   | 2.77                     | 0.61              |
| 1:I:179:TYR:O    | 1:I:181:PRO:HD3  | 2.00                     | 0.61              |
| 1:J:179:TYR:O    | 1:J:181:PRO:HD3  | 2.00                     | 0.61              |
| 5:A:1483:MPD:CM  | 1:F:190:ASP:OD2  | 2.48                     | 0.61              |
| 1:F:360:PHE:CD2  | 1:F:361:PRO:CD   | 2.71                     | 0.61              |
| 3:H:1478:ADP:C1' | 3:H:1478:ADP:C8  | 2.81                     | 0.61              |
| 1:B:179:TYR:O    | 1:B:181:PRO:HD2  | 2.00                     | 0.61              |
| 5:I:1491:MPD:H32 | 1:J:193:SER:OG   | 2.00                     | 0.61              |
| 1:D:179:TYR:O    | 1:D:181:PRO:HD2  | 2.00                     | 0.61              |
| 1:G:48:MET:HE2   | 1:G:66:VAL:CG2   | 2.26                     | 0.61              |
| 1:B:193:SER:OG   | 5:C:1485:MPD:C3  | 2.48                     | 0.61              |
| 1:C:82:ASP:N     | 5:C:1485:MPD:H13 | 2.13                     | 0.61              |
| 1:E:179:TYR:O    | 1:E:181:PRO:HD3  | 2.00                     | 0.61              |
| 1:H:179:TYR:O    | 1:H:181:PRO:HD2  | 2.00                     | 0.61              |
| 1:A:179:TYR:O    | 1:A:181:PRO:HD2  | 2.00                     | 0.60              |
| 1:D:179:TYR:O    | 1:D:181:PRO:HD3  | 2.00                     | 0.60              |
| 1:D:180:PHE:HB3  | 1:E:29:GLN:HB3   | 1.83                     | 0.60              |
| 5:H:1490:MPD:CM  | 1:I:189:GLN:HG3  | 2.31                     | 0.60              |
| 1:I:179:TYR:O    | 1:I:181:PRO:HD2  | 2.00                     | 0.60              |
| 1:K:179:TYR:O    | 1:K:181:PRO:HD2  | 2.00                     | 0.60              |
| 1:L:179:TYR:O    | 1:L:181:PRO:HD3  | 2.00                     | 0.60              |
| 1:D:193:SER:HB2  | 5:E:1487:MPD:H32 | 1.84                     | 0.60              |
| 1:E:179:TYR:O    | 1:E:181:PRO:HD2  | 2.00                     | 0.60              |
| 1:H:179:TYR:O    | 1:H:181:PRO:HD3  | 2.00                     | 0.60              |
| 1:I:395:ASN:CB   | 1:I:399:LEU:HD12 | 2.29                     | 0.60              |
| 1:B:179:TYR:O    | 1:B:181:PRO:HD3  | 2.00                     | 0.60              |
| 1:G:58:LYS:HZ1   | 1:G:60:ILE:HD11  | 1.67                     | 0.60              |
| 1:G:82:ASP:CB    | 5:G:1489:MPD:H12 | 2.32                     | 0.60              |
| 1:A:82:ASP:CB    | 5:A:1483:MPD:H12 | 2.32                     | 0.60              |
| 1:B:82:ASP:CB    | 5:B:1484:MPD:H12 | 2.32                     | 0.60              |
| 1:D:58:LYS:HZ1   | 1:D:60:ILE:HD11  | 1.66                     | 0.60              |
| 1:E:48:MET:HE2   | 1:E:66:VAL:CG2   | 2.26                     | 0.60              |
| 1:G:82:ASP:N     | 5:G:1489:MPD:H12 | 2.17                     | 0.60              |
| 1:I:458:HIS:CD2  | 1:I:460:VAL:H    | 2.09                     | 0.60              |
| 1:J:82:ASP:CB    | 5:J:1492:MPD:H12 | 2.32                     | 0.60              |
| 1:A:82:ASP:N     | 5:A:1483:MPD:H13 | 2.13                     | 0.60              |
| 1:F:82:ASP:CB    | 5:F:1488:MPD:H12 | 2.32                     | 0.60              |
| 1:J:29:GLN:HA    | 1:K:180:PHE:O    | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:K:1493:MPD:HM1 | 1:L:189:GLN:HG3  | 1.84                     | 0.60              |
| 1:D:395:ASN:ND2  | 1:E:60:ILE:HG21  | 2.11                     | 0.60              |
| 5:I:1491:MPD:C3  | 1:J:193:SER:OG   | 2.49                     | 0.60              |
| 1:D:48:MET:HE2   | 1:D:66:VAL:CG2   | 2.26                     | 0.60              |
| 1:F:82:ASP:N     | 5:F:1488:MPD:H12 | 2.17                     | 0.60              |
| 1:H:82:ASP:N     | 5:H:1490:MPD:C1  | 2.54                     | 0.60              |
| 5:H:1490:MPD:C3  | 1:I:193:SER:OG   | 2.50                     | 0.60              |
| 1:L:179:TYR:O    | 1:L:181:PRO:HD2  | 2.00                     | 0.60              |
| 1:H:360:PHE:CD2  | 1:H:361:PRO:CD   | 2.71                     | 0.60              |
| 1:I:50:ASP:CG    | 6:I:1613:HOH:O   | 2.44                     | 0.60              |
| 3:L:1482:ADP:C1' | 3:L:1482:ADP:C8  | 2.81                     | 0.60              |
| 1:C:82:ASP:CB    | 5:C:1485:MPD:H12 | 2.32                     | 0.59              |
| 1:E:82:ASP:N     | 5:E:1487:MPD:H12 | 2.17                     | 0.59              |
| 1:I:82:ASP:CB    | 5:I:1491:MPD:H12 | 2.32                     | 0.59              |
| 1:F:82:ASP:N     | 5:F:1488:MPD:H13 | 2.13                     | 0.59              |
| 1:K:224:ARG:HG2  | 1:K:224:ARG:NH2  | 2.15                     | 0.59              |
| 1:L:395:ASN:CB   | 1:L:399:LEU:HD12 | 2.30                     | 0.59              |
| 1:B:180:PHE:N    | 1:B:180:PHE:CD1  | 2.70                     | 0.59              |
| 1:D:82:ASP:CB    | 5:D:1486:MPD:H12 | 2.32                     | 0.59              |
| 1:D:180:PHE:N    | 1:D:180:PHE:CD1  | 2.70                     | 0.59              |
| 1:D:189:GLN:HG3  | 5:E:1487:MPD:CM  | 2.32                     | 0.59              |
| 1:E:193:SER:OG   | 5:F:1488:MPD:C3  | 2.50                     | 0.59              |
| 1:J:82:ASP:N     | 5:J:1492:MPD:H12 | 2.17                     | 0.59              |
| 1:D:456:THR:O    | 1:J:458:HIS:HE1  | 1.86                     | 0.59              |
| 1:E:82:ASP:CB    | 5:E:1487:MPD:H12 | 2.32                     | 0.59              |
| 1:C:82:ASP:N     | 5:C:1485:MPD:C1  | 2.54                     | 0.59              |
| 1:E:180:PHE:N    | 1:E:180:PHE:CD1  | 2.70                     | 0.59              |
| 1:F:180:PHE:CD1  | 1:F:180:PHE:N    | 2.70                     | 0.59              |
| 1:K:82:ASP:N     | 5:K:1493:MPD:H13 | 2.13                     | 0.59              |
| 1:K:180:PHE:CD1  | 1:K:180:PHE:N    | 2.70                     | 0.59              |
| 1:L:58:LYS:HZ1   | 1:L:60:ILE:HD11  | 1.67                     | 0.59              |
| 1:L:82:ASP:CB    | 5:L:1494:MPD:H12 | 2.32                     | 0.59              |
| 1:E:179:TYR:HB2  | 6:E:1524:HOH:O   | 2.03                     | 0.59              |
| 5:J:1492:MPD:H32 | 1:K:193:SER:OG   | 2.01                     | 0.59              |
| 3:D:1474:ADP:C1' | 3:D:1474:ADP:C8  | 2.81                     | 0.59              |
| 5:J:1492:MPD:C3  | 1:K:193:SER:OG   | 2.50                     | 0.59              |
| 1:K:179:TYR:HB2  | 6:K:1534:HOH:O   | 2.03                     | 0.59              |
| 1:B:179:TYR:HB2  | 6:B:1521:HOH:O   | 2.03                     | 0.59              |
| 1:H:82:ASP:N     | 5:H:1490:MPD:H12 | 2.17                     | 0.59              |
| 1:D:82:ASP:N     | 5:D:1486:MPD:H13 | 2.13                     | 0.59              |
| 1:H:82:ASP:CB    | 5:H:1490:MPD:H12 | 2.32                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:179:TYR:HB2  | 6:A:1514:HOH:O   | 2.03                     | 0.58              |
| 1:C:180:PHE:CD1  | 1:C:180:PHE:N    | 2.70                     | 0.58              |
| 3:C:1473:ADP:C1' | 3:C:1473:ADP:C8  | 2.81                     | 0.58              |
| 1:F:82:ASP:N     | 5:F:1488:MPD:C1  | 2.54                     | 0.58              |
| 1:H:179:TYR:HB2  | 6:H:1528:HOH:O   | 2.03                     | 0.58              |
| 1:J:458:HIS:CD2  | 1:J:460:VAL:H    | 2.10                     | 0.58              |
| 1:L:82:ASP:N     | 5:L:1494:MPD:H12 | 2.17                     | 0.58              |
| 1:A:193:SER:OG   | 5:B:1484:MPD:H32 | 2.03                     | 0.58              |
| 1:A:58:LYS:HZ1   | 1:A:60:ILE:HD11  | 1.68                     | 0.58              |
| 1:G:82:ASP:N     | 5:G:1489:MPD:C1  | 2.54                     | 0.58              |
| 1:H:180:PHE:N    | 1:H:180:PHE:CD1  | 2.70                     | 0.58              |
| 1:K:82:ASP:CB    | 5:K:1493:MPD:H12 | 2.32                     | 0.58              |
| 1:D:179:TYR:HB2  | 6:D:1525:HOH:O   | 2.03                     | 0.58              |
| 1:E:82:ASP:N     | 5:E:1487:MPD:C1  | 2.54                     | 0.58              |
| 1:E:308:ILE:HG21 | 1:E:374:LEU:HD13 | 1.86                     | 0.58              |
| 1:G:180:PHE:N    | 1:G:180:PHE:CD1  | 2.70                     | 0.58              |
| 1:H:82:ASP:N     | 5:H:1490:MPD:H13 | 2.13                     | 0.58              |
| 1:A:29:GLN:HA    | 1:F:180:PHE:O    | 2.02                     | 0.58              |
| 1:A:308:ILE:HG21 | 1:A:374:LEU:HD13 | 1.86                     | 0.58              |
| 1:G:308:ILE:HG21 | 1:G:374:LEU:HD13 | 1.86                     | 0.58              |
| 1:K:308:ILE:HG21 | 1:K:374:LEU:HD13 | 1.86                     | 0.58              |
| 1:K:360:PHE:CD2  | 1:K:361:PRO:CD   | 2.71                     | 0.58              |
| 1:A:16:PHE:HB2   | 5:A:1483:MPD:H51 | 1.86                     | 0.58              |
| 1:D:397:TYR:C    | 1:D:399:LEU:N    | 2.60                     | 0.58              |
| 1:I:63:SER:HB2   | 1:J:339:ARG:HH22 | 1.69                     | 0.58              |
| 1:B:224:ARG:HG2  | 1:B:224:ARG:NH2  | 2.15                     | 0.58              |
| 1:G:326:TYR:CD2  | 1:G:326:TYR:N    | 2.72                     | 0.58              |
| 1:I:180:PHE:N    | 1:I:180:PHE:CD1  | 2.70                     | 0.58              |
| 1:F:179:TYR:HB2  | 6:F:1527:HOH:O   | 2.03                     | 0.58              |
| 5:H:1490:MPD:C3  | 1:I:193:SER:HB2  | 2.32                     | 0.58              |
| 1:J:179:TYR:HB2  | 6:J:1530:HOH:O   | 2.03                     | 0.58              |
| 3:A:1471:ADP:C1' | 3:A:1471:ADP:C8  | 2.81                     | 0.58              |
| 1:D:16:PHE:HB2   | 5:D:1486:MPD:H51 | 1.86                     | 0.58              |
| 1:F:16:PHE:CD1   | 5:F:1488:MPD:C5  | 2.87                     | 0.57              |
| 1:F:395:ASN:CB   | 1:F:399:LEU:HD12 | 2.30                     | 0.57              |
| 1:A:395:ASN:CB   | 1:A:399:LEU:HD12 | 2.30                     | 0.57              |
| 1:B:308:ILE:HG21 | 1:B:374:LEU:HD13 | 1.86                     | 0.57              |
| 1:G:29:GLN:HA    | 1:H:180:PHE:O    | 2.03                     | 0.57              |
| 1:G:180:PHE:O    | 1:L:29:GLN:HA    | 2.03                     | 0.57              |
| 1:K:326:TYR:N    | 1:K:326:TYR:CD2  | 2.72                     | 0.57              |
| 1:C:308:ILE:HG21 | 1:C:374:LEU:HD13 | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:326:TYR:N    | 1:C:326:TYR:CD2  | 2.72                     | 0.57              |
| 1:I:397:TYR:C    | 1:I:399:LEU:N    | 2.60                     | 0.57              |
| 1:A:82:ASP:N     | 5:A:1483:MPD:H12 | 2.17                     | 0.57              |
| 1:C:179:TYR:HB2  | 6:C:1523:HOH:O   | 2.03                     | 0.57              |
| 1:G:179:TYR:HB2  | 6:G:1528:HOH:O   | 2.03                     | 0.57              |
| 1:H:29:GLN:HA    | 1:I:180:PHE:O    | 2.03                     | 0.57              |
| 1:H:48:MET:HE2   | 1:H:66:VAL:CG2   | 2.26                     | 0.57              |
| 1:H:308:ILE:HG21 | 1:H:374:LEU:HD13 | 1.86                     | 0.57              |
| 1:K:16:PHE:HB2   | 5:K:1493:MPD:H51 | 1.86                     | 0.57              |
| 1:I:16:PHE:HB2   | 5:I:1491:MPD:H51 | 1.86                     | 0.57              |
| 1:J:180:PHE:N    | 1:J:180:PHE:CD1  | 2.70                     | 0.57              |
| 1:L:16:PHE:CD1   | 5:L:1494:MPD:C5  | 2.87                     | 0.57              |
| 1:B:82:ASP:N     | 5:B:1484:MPD:H12 | 2.17                     | 0.57              |
| 1:F:308:ILE:HG21 | 1:F:374:LEU:HD13 | 1.86                     | 0.57              |
| 1:L:179:TYR:HB2  | 6:L:1365:HOH:O   | 2.03                     | 0.57              |
| 1:B:180:PHE:HB3  | 1:C:29:GLN:HB3   | 1.85                     | 0.57              |
| 1:C:224:ARG:HG2  | 1:C:224:ARG:NH2  | 2.15                     | 0.57              |
| 1:D:326:TYR:CD2  | 1:D:326:TYR:N    | 2.72                     | 0.57              |
| 1:F:192:ARG:HD3  | 1:F:219:ASN:HD22 | 1.70                     | 0.57              |
| 5:H:1490:MPD:H32 | 1:I:193:SER:OG   | 2.04                     | 0.57              |
| 5:K:1493:MPD:CM  | 1:L:190:ASP:OD2  | 2.49                     | 0.57              |
| 1:L:16:PHE:HB2   | 5:L:1494:MPD:H51 | 1.86                     | 0.57              |
| 5:A:1483:MPD:HM1 | 1:F:189:GLN:HG3  | 1.86                     | 0.57              |
| 1:D:180:PHE:O    | 1:E:29:GLN:HA    | 2.05                     | 0.57              |
| 1:E:326:TYR:N    | 1:E:326:TYR:CD2  | 2.72                     | 0.57              |
| 1:E:395:ASN:CB   | 1:E:399:LEU:HD12 | 2.30                     | 0.57              |
| 1:G:192:ARG:HD3  | 1:G:219:ASN:HD22 | 1.70                     | 0.57              |
| 1:I:82:ASP:N     | 5:I:1491:MPD:H13 | 2.13                     | 0.57              |
| 1:I:308:ILE:HG21 | 1:I:374:LEU:HD13 | 1.86                     | 0.57              |
| 1:K:82:ASP:N     | 5:K:1493:MPD:C1  | 2.54                     | 0.57              |
| 1:A:193:SER:OG   | 5:B:1484:MPD:C3  | 2.53                     | 0.57              |
| 1:C:395:ASN:CB   | 1:C:399:LEU:HD12 | 2.30                     | 0.57              |
| 1:E:1:SER:CA     | 1:E:71:ALA:CB    | 2.80                     | 0.57              |
| 1:E:16:PHE:CD1   | 5:E:1487:MPD:C5  | 2.87                     | 0.57              |
| 1:I:179:TYR:HB2  | 6:I:1530:HOH:O   | 2.03                     | 0.57              |
| 1:I:192:ARG:HD3  | 1:I:219:ASN:HD22 | 1.70                     | 0.57              |
| 1:J:16:PHE:HB2   | 5:J:1492:MPD:H51 | 1.86                     | 0.57              |
| 3:J:1480:ADP:C1' | 3:J:1480:ADP:C8  | 2.81                     | 0.57              |
| 1:K:29:GLN:HA    | 1:L:180:PHE:O    | 2.04                     | 0.57              |
| 3:K:1481:ADP:C1' | 3:K:1481:ADP:C8  | 2.81                     | 0.57              |
| 1:L:180:PHE:N    | 1:L:180:PHE:CD1  | 2.70                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:16:PHE:CD1   | 5:A:1483:MPD:C5  | 2.87                     | 0.57              |
| 3:B:1472:ADP:C1' | 3:B:1472:ADP:C8  | 2.81                     | 0.57              |
| 1:D:458:HIS:HE1  | 1:J:456:THR:O    | 1.87                     | 0.57              |
| 1:A:82:ASP:N     | 5:A:1483:MPD:C1  | 2.54                     | 0.56              |
| 1:A:326:TYR:CD2  | 1:A:326:TYR:N    | 2.72                     | 0.56              |
| 1:E:58:LYS:HZ1   | 1:E:60:ILE:HD11  | 1.70                     | 0.56              |
| 1:H:16:PHE:HB2   | 5:H:1490:MPD:H51 | 1.86                     | 0.56              |
| 1:I:58:LYS:HZ1   | 1:I:60:ILE:HD11  | 1.70                     | 0.56              |
| 1:J:58:LYS:HZ1   | 1:J:60:ILE:HD11  | 1.70                     | 0.56              |
| 1:J:308:ILE:HG21 | 1:J:374:LEU:HD13 | 1.86                     | 0.56              |
| 1:B:360:PHE:CD2  | 1:B:361:PRO:CD   | 2.71                     | 0.56              |
| 3:E:1475:ADP:C1' | 3:E:1475:ADP:C8  | 2.81                     | 0.56              |
| 3:G:1477:ADP:C1' | 3:G:1477:ADP:C8  | 2.81                     | 0.56              |
| 1:H:16:PHE:CD1   | 5:H:1490:MPD:C5  | 2.87                     | 0.56              |
| 1:L:308:ILE:HG21 | 1:L:374:LEU:HD13 | 1.86                     | 0.56              |
| 1:A:180:PHE:N    | 1:A:180:PHE:CD1  | 2.70                     | 0.56              |
| 1:B:82:ASP:N     | 5:B:1484:MPD:H13 | 2.13                     | 0.56              |
| 1:C:48:MET:HE2   | 1:C:66:VAL:CG2   | 2.26                     | 0.56              |
| 1:C:82:ASP:N     | 5:C:1485:MPD:H12 | 2.17                     | 0.56              |
| 1:C:192:ARG:HD3  | 1:C:219:ASN:HD22 | 1.70                     | 0.56              |
| 1:D:82:ASP:N     | 5:D:1486:MPD:H12 | 2.17                     | 0.56              |
| 1:D:308:ILE:HG21 | 1:D:374:LEU:HD13 | 1.86                     | 0.56              |
| 1:E:455:MET:HE2  | 1:K:261:PHE:HE1  | 1.70                     | 0.56              |
| 1:I:63:SER:OG    | 1:J:339:ARG:NH2  | 2.39                     | 0.56              |
| 1:J:326:TYR:CD2  | 1:J:326:TYR:N    | 2.72                     | 0.56              |
| 5:K:1493:MPD:CM  | 1:L:189:GLN:HG3  | 2.35                     | 0.56              |
| 1:B:16:PHE:HB2   | 5:B:1484:MPD:H51 | 1.86                     | 0.56              |
| 1:C:16:PHE:HB2   | 5:C:1485:MPD:H51 | 1.86                     | 0.56              |
| 1:E:16:PHE:HB2   | 5:E:1487:MPD:H51 | 1.86                     | 0.56              |
| 1:G:16:PHE:HB2   | 5:G:1489:MPD:H51 | 1.86                     | 0.56              |
| 1:G:82:ASP:N     | 5:G:1489:MPD:H13 | 2.13                     | 0.56              |
| 1:G:193:SER:CB   | 5:L:1494:MPD:C3  | 2.82                     | 0.56              |
| 1:A:360:PHE:CD2  | 1:A:361:PRO:CD   | 2.71                     | 0.56              |
| 1:D:399:LEU:O    | 1:D:400:PRO:O    | 2.24                     | 0.56              |
| 1:G:193:SER:HB2  | 5:L:1494:MPD:C3  | 2.35                     | 0.56              |
| 1:H:192:ARG:HD3  | 1:H:219:ASN:HD22 | 1.70                     | 0.56              |
| 1:B:399:LEU:O    | 1:B:400:PRO:O    | 2.24                     | 0.56              |
| 1:B:456:THR:O    | 1:H:458:HIS:HE1  | 1.88                     | 0.56              |
| 1:C:397:TYR:C    | 1:C:399:LEU:N    | 2.60                     | 0.56              |
| 1:F:399:LEU:O    | 1:F:400:PRO:O    | 2.24                     | 0.56              |
| 1:I:48:MET:HE2   | 1:I:66:VAL:CG2   | 2.26                     | 0.56              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:82:ASP:N    | 5:I:1491:MPD:C1  | 2.54                     | 0.56              |
| 1:L:1:SER:CA    | 1:L:71:ALA:CB    | 2.80                     | 0.56              |
| 1:J:16:PHE:CD1  | 5:J:1492:MPD:C5  | 2.87                     | 0.56              |
| 1:K:399:LEU:O   | 1:K:400:PRO:O    | 2.24                     | 0.56              |
| 1:L:192:ARG:HD3 | 1:L:219:ASN:HD22 | 1.70                     | 0.56              |
| 1:E:118:THR:OG1 | 1:E:120:ILE:HG13 | 2.06                     | 0.56              |
| 1:J:397:TYR:C   | 1:J:399:LEU:N    | 2.60                     | 0.56              |
| 1:K:82:ASP:N    | 5:K:1493:MPD:H12 | 2.17                     | 0.56              |
| 1:B:192:ARG:HD3 | 1:B:219:ASN:HD22 | 1.70                     | 0.56              |
| 1:B:458:HIS:HE1 | 1:H:456:THR:O    | 1.89                     | 0.56              |
| 1:D:192:ARG:HD3 | 1:D:219:ASN:HD22 | 1.70                     | 0.56              |
| 1:E:224:ARG:HG2 | 1:E:224:ARG:NH2  | 2.15                     | 0.56              |
| 1:G:16:PHE:CD1  | 5:G:1489:MPD:C5  | 2.87                     | 0.56              |
| 1:H:399:LEU:O   | 1:H:400:PRO:O    | 2.24                     | 0.56              |
| 1:K:192:ARG:HD3 | 1:K:219:ASN:HD22 | 1.70                     | 0.56              |
| 1:F:16:PHE:HB2  | 5:F:1488:MPD:H51 | 1.86                     | 0.55              |
| 1:H:118:THR:OG1 | 1:H:120:ILE:HG13 | 2.06                     | 0.55              |
| 1:J:192:ARG:HD3 | 1:J:219:ASN:HD22 | 1.70                     | 0.55              |
| 1:K:16:PHE:CD1  | 5:K:1493:MPD:C5  | 2.87                     | 0.55              |
| 1:C:118:THR:OG1 | 1:C:120:ILE:HG13 | 2.06                     | 0.55              |
| 1:F:326:TYR:N   | 1:F:326:TYR:CD2  | 2.72                     | 0.55              |
| 1:A:192:ARG:HD3 | 1:A:219:ASN:HD22 | 1.70                     | 0.55              |
| 1:D:50:ASP:CG   | 6:D:1493:HOH:O   | 2.48                     | 0.55              |
| 1:F:1:SER:CA    | 1:F:71:ALA:CB    | 2.80                     | 0.55              |
| 1:H:395:ASN:CB  | 1:H:399:LEU:HD12 | 2.30                     | 0.55              |
| 1:J:118:THR:OG1 | 1:J:120:ILE:HG13 | 2.06                     | 0.55              |
| 1:L:224:ARG:HG2 | 1:L:224:ARG:NH2  | 2.15                     | 0.55              |
| 1:A:180:PHE:O   | 1:B:29:GLN:HA    | 2.06                     | 0.55              |
| 1:D:16:PHE:CD1  | 5:D:1486:MPD:C5  | 2.87                     | 0.55              |
| 1:E:192:ARG:HD3 | 1:E:219:ASN:HD22 | 1.70                     | 0.55              |
| 1:G:395:ASN:CB  | 1:G:399:LEU:HD12 | 2.30                     | 0.55              |
| 1:L:397:TYR:C   | 1:L:399:LEU:N    | 2.60                     | 0.55              |
| 1:B:118:THR:OG1 | 1:B:120:ILE:HG13 | 2.06                     | 0.55              |
| 1:C:400:PRO:CB  | 1:C:401:PRO:HD2  | 2.37                     | 0.55              |
| 1:I:326:TYR:CD2 | 1:I:326:TYR:N    | 2.72                     | 0.55              |
| 1:B:326:TYR:CD2 | 1:B:326:TYR:N    | 2.72                     | 0.55              |
| 1:B:395:ASN:CB  | 1:B:399:LEU:HD12 | 2.29                     | 0.55              |
| 1:C:16:PHE:CD1  | 5:C:1485:MPD:C5  | 2.87                     | 0.55              |
| 1:F:397:TYR:C   | 1:F:399:LEU:N    | 2.60                     | 0.55              |
| 1:J:1:SER:CA    | 1:J:71:ALA:CB    | 2.80                     | 0.55              |
| 1:L:118:THR:OG1 | 1:L:120:ILE:HG13 | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:399:LEU:O    | 1:E:400:PRO:O    | 2.24                     | 0.55              |
| 1:J:82:ASP:N     | 5:J:1492:MPD:H13 | 2.13                     | 0.55              |
| 1:L:399:LEU:O    | 1:L:400:PRO:O    | 2.24                     | 0.55              |
| 1:A:118:THR:OG1  | 1:A:120:ILE:HG13 | 2.06                     | 0.55              |
| 1:B:48:MET:HE2   | 1:B:66:VAL:CG2   | 2.26                     | 0.55              |
| 1:F:400:PRO:CB   | 1:F:401:PRO:HD2  | 2.37                     | 0.55              |
| 1:G:193:SER:OG   | 5:L:1494:MPD:C3  | 2.55                     | 0.55              |
| 1:G:395:ASN:ND2  | 1:L:60:ILE:CG2   | 2.63                     | 0.55              |
| 1:G:400:PRO:CB   | 1:G:401:PRO:HD2  | 2.37                     | 0.55              |
| 3:I:1479:ADP:C1' | 3:I:1479:ADP:C8  | 2.81                     | 0.55              |
| 1:J:360:PHE:CD2  | 1:J:361:PRO:CD   | 2.71                     | 0.55              |
| 1:J:395:ASN:CB   | 1:J:399:LEU:HD12 | 2.30                     | 0.55              |
| 1:K:395:ASN:CB   | 1:K:399:LEU:HD12 | 2.29                     | 0.55              |
| 1:L:326:TYR:CD2  | 1:L:326:TYR:N    | 2.72                     | 0.55              |
| 1:L:400:PRO:CB   | 1:L:401:PRO:HD2  | 2.37                     | 0.55              |
| 1:B:180:PHE:O    | 1:C:29:GLN:HA    | 2.06                     | 0.55              |
| 1:D:118:THR:OG1  | 1:D:120:ILE:HG13 | 2.06                     | 0.55              |
| 1:D:400:PRO:CB   | 1:D:401:PRO:HD2  | 2.37                     | 0.55              |
| 1:G:118:THR:OG1  | 1:G:120:ILE:HG13 | 2.06                     | 0.55              |
| 1:H:326:TYR:N    | 1:H:326:TYR:CD2  | 2.72                     | 0.55              |
| 1:I:118:THR:OG1  | 1:I:120:ILE:HG13 | 2.06                     | 0.55              |
| 1:I:400:PRO:CB   | 1:I:401:PRO:HD2  | 2.37                     | 0.55              |
| 1:J:399:LEU:O    | 1:J:400:PRO:O    | 2.24                     | 0.55              |
| 1:C:399:LEU:O    | 1:C:400:PRO:O    | 2.24                     | 0.55              |
| 1:E:397:TYR:C    | 1:E:399:LEU:N    | 2.60                     | 0.55              |
| 1:E:400:PRO:CB   | 1:E:401:PRO:HD2  | 2.37                     | 0.55              |
| 1:G:399:LEU:O    | 1:G:400:PRO:O    | 2.24                     | 0.55              |
| 1:K:400:PRO:CB   | 1:K:401:PRO:HD2  | 2.37                     | 0.55              |
| 1:A:399:LEU:O    | 1:A:400:PRO:O    | 2.24                     | 0.54              |
| 1:B:397:TYR:C    | 1:B:399:LEU:N    | 2.60                     | 0.54              |
| 1:J:82:ASP:N     | 5:J:1492:MPD:C1  | 2.54                     | 0.54              |
| 1:J:400:PRO:CB   | 1:J:401:PRO:HD2  | 2.37                     | 0.54              |
| 1:C:360:PHE:CD2  | 1:C:361:PRO:CD   | 2.71                     | 0.54              |
| 1:I:399:LEU:O    | 1:I:400:PRO:O    | 2.24                     | 0.54              |
| 1:K:118:THR:OG1  | 1:K:120:ILE:HG13 | 2.06                     | 0.54              |
| 1:D:360:PHE:CE2  | 1:D:361:PRO:HD3  | 2.39                     | 0.54              |
| 1:F:58:LYS:HZ1   | 1:F:60:ILE:HD11  | 1.73                     | 0.54              |
| 1:I:16:PHE:CD1   | 5:I:1491:MPD:C5  | 2.87                     | 0.54              |
| 1:B:400:PRO:CB   | 1:B:401:PRO:HD2  | 2.37                     | 0.54              |
| 1:D:82:ASP:N     | 5:D:1486:MPD:C1  | 2.54                     | 0.54              |
| 1:A:48:MET:HE2   | 1:A:66:VAL:CG2   | 2.26                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:1476:ADP:C1' | 3:F:1476:ADP:C8  | 2.81                     | 0.54              |
| 5:I:1491:MPD:C3  | 1:J:193:SER:HB2  | 2.37                     | 0.54              |
| 1:G:190:ASP:OD2  | 5:L:1494:MPD:CM  | 2.53                     | 0.54              |
| 1:B:82:ASP:N     | 5:B:1484:MPD:C1  | 2.54                     | 0.54              |
| 1:C:458:HIS:HE1  | 1:I:456:THR:O    | 1.90                     | 0.54              |
| 1:E:179:TYR:C    | 1:E:181:PRO:CD   | 2.81                     | 0.54              |
| 1:G:179:TYR:C    | 1:G:181:PRO:CD   | 2.81                     | 0.54              |
| 1:H:179:TYR:C    | 1:H:181:PRO:CD   | 2.80                     | 0.54              |
| 5:J:1492:MPD:C3  | 1:K:193:SER:HB2  | 2.36                     | 0.54              |
| 1:A:400:PRO:CB   | 1:A:401:PRO:HD2  | 2.37                     | 0.54              |
| 1:F:360:PHE:CE2  | 1:F:361:PRO:HD3  | 2.39                     | 0.54              |
| 1:F:458:HIS:HE1  | 1:L:456:THR:O    | 1.90                     | 0.54              |
| 1:I:82:ASP:N     | 5:I:1491:MPD:H12 | 2.17                     | 0.54              |
| 1:C:179:TYR:C    | 1:C:181:PRO:CD   | 2.81                     | 0.53              |
| 1:F:118:THR:OG1  | 1:F:120:ILE:HG13 | 2.06                     | 0.53              |
| 1:K:179:TYR:C    | 1:K:181:PRO:CD   | 2.81                     | 0.53              |
| 1:B:16:PHE:CD1   | 5:B:1484:MPD:C5  | 2.87                     | 0.53              |
| 1:B:193:SER:CB   | 5:C:1485:MPD:C3  | 2.81                     | 0.53              |
| 1:E:454:ARG:O    | 1:K:320:LYS:HG2  | 2.08                     | 0.53              |
| 5:H:1490:MPD:CM  | 1:I:190:ASP:OD2  | 2.53                     | 0.53              |
| 1:K:58:LYS:HZ1   | 1:K:60:ILE:HD11  | 1.72                     | 0.53              |
| 1:A:360:PHE:CE2  | 1:A:361:PRO:HD3  | 2.39                     | 0.53              |
| 1:H:400:PRO:CB   | 1:H:401:PRO:HD2  | 2.37                     | 0.53              |
| 1:J:179:TYR:C    | 1:J:181:PRO:CD   | 2.81                     | 0.53              |
| 1:C:456:THR:O    | 1:I:458:HIS:HE1  | 1.91                     | 0.53              |
| 1:D:302:ILE:HG23 | 1:D:332:LEU:HB3  | 1.91                     | 0.53              |
| 1:G:427:PHE:CE1  | 1:G:428:LEU:HD13 | 2.44                     | 0.53              |
| 5:I:1491:MPD:C3  | 1:J:193:SER:CB   | 2.80                     | 0.53              |
| 1:K:397:TYR:C    | 1:K:399:LEU:N    | 2.60                     | 0.53              |
| 1:E:82:ASP:N     | 5:E:1487:MPD:H13 | 2.13                     | 0.53              |
| 5:A:1483:MPD:CM  | 1:F:189:GLN:HG3  | 2.39                     | 0.53              |
| 1:B:360:PHE:CE2  | 1:B:361:PRO:HD3  | 2.39                     | 0.53              |
| 1:G:337:ARG:HG2  | 1:G:338:ASN:H    | 1.74                     | 0.53              |
| 1:H:302:ILE:HG23 | 1:H:332:LEU:HB3  | 1.91                     | 0.53              |
| 1:B:179:TYR:C    | 1:B:181:PRO:CD   | 2.81                     | 0.53              |
| 1:D:80:PHE:CG    | 5:D:1486:MPD:HM2 | 2.44                     | 0.53              |
| 1:H:427:PHE:CE1  | 1:H:428:LEU:HD13 | 2.44                     | 0.53              |
| 1:I:224:ARG:HG2  | 1:I:224:ARG:NH2  | 2.15                     | 0.53              |
| 1:I:337:ARG:HG2  | 1:I:338:ASN:H    | 1.74                     | 0.53              |
| 1:J:427:PHE:CE1  | 1:J:428:LEU:HD13 | 2.44                     | 0.53              |
| 1:L:80:PHE:CG    | 5:L:1494:MPD:HM2 | 2.44                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:80:PHE:CG    | 5:A:1483:MPD:HM2 | 2.44                     | 0.53              |
| 1:D:395:ASN:CB   | 1:D:399:LEU:HD12 | 2.30                     | 0.53              |
| 1:E:312:ALA:HB1  | 1:E:361:PRO:HG3  | 1.91                     | 0.53              |
| 1:H:337:ARG:HG2  | 1:H:338:ASN:H    | 1.74                     | 0.53              |
| 1:J:360:PHE:CE2  | 1:J:361:PRO:HD3  | 2.39                     | 0.53              |
| 1:K:80:PHE:CG    | 5:K:1493:MPD:HM2 | 2.44                     | 0.53              |
| 1:B:337:ARG:HG2  | 1:B:338:ASN:H    | 1.74                     | 0.53              |
| 1:C:427:PHE:CE1  | 1:C:428:LEU:HD13 | 2.44                     | 0.53              |
| 1:F:80:PHE:CG    | 5:F:1488:MPD:HM2 | 2.44                     | 0.53              |
| 1:F:337:ARG:HG2  | 1:F:338:ASN:H    | 1.74                     | 0.53              |
| 1:G:80:PHE:CG    | 5:G:1489:MPD:HM2 | 2.44                     | 0.53              |
| 1:I:427:PHE:CE1  | 1:I:428:LEU:HD13 | 2.44                     | 0.53              |
| 1:J:312:ALA:HB1  | 1:J:361:PRO:HG3  | 1.91                     | 0.53              |
| 5:J:1492:MPD:C3  | 1:K:193:SER:CB   | 2.81                     | 0.53              |
| 1:A:302:ILE:HG23 | 1:A:332:LEU:HB3  | 1.91                     | 0.52              |
| 1:C:312:ALA:HB1  | 1:C:361:PRO:HG3  | 1.91                     | 0.52              |
| 1:C:339:ARG:NH2  | 1:D:63:SER:OG    | 2.42                     | 0.52              |
| 1:D:427:PHE:CE1  | 1:D:428:LEU:HD13 | 2.44                     | 0.52              |
| 1:G:193:SER:OG   | 5:L:1494:MPD:H32 | 2.08                     | 0.52              |
| 1:H:80:PHE:CG    | 5:H:1490:MPD:HM2 | 2.44                     | 0.52              |
| 1:J:302:ILE:HG23 | 1:J:332:LEU:HB3  | 1.91                     | 0.52              |
| 1:L:427:PHE:CE1  | 1:L:428:LEU:HD13 | 2.44                     | 0.52              |
| 1:A:312:ALA:HB1  | 1:A:361:PRO:HG3  | 1.91                     | 0.52              |
| 1:B:427:PHE:CE1  | 1:B:428:LEU:HD13 | 2.44                     | 0.52              |
| 1:C:1:SER:CA     | 1:C:71:ALA:CB    | 2.80                     | 0.52              |
| 1:F:427:PHE:CE1  | 1:F:428:LEU:HD13 | 2.44                     | 0.52              |
| 1:G:169:LYS:O    | 1:L:252:THR:OG1  | 2.26                     | 0.52              |
| 1:L:312:ALA:HB1  | 1:L:361:PRO:HG3  | 1.91                     | 0.52              |
| 1:C:124:VAL:HG11 | 1:C:375:LEU:HG   | 1.92                     | 0.52              |
| 1:D:179:TYR:C    | 1:D:181:PRO:CD   | 2.81                     | 0.52              |
| 1:E:80:PHE:CG    | 5:E:1487:MPD:HM2 | 2.44                     | 0.52              |
| 1:E:180:PHE:HB3  | 1:F:29:GLN:HB3   | 1.92                     | 0.52              |
| 1:E:320:LYS:HG2  | 1:K:454:ARG:O    | 2.09                     | 0.52              |
| 1:E:427:PHE:CE1  | 1:E:428:LEU:HD13 | 2.44                     | 0.52              |
| 1:F:124:VAL:HG11 | 1:F:375:LEU:HG   | 1.92                     | 0.52              |
| 1:I:179:TYR:C    | 1:I:181:PRO:CD   | 2.81                     | 0.52              |
| 1:K:337:ARG:HG2  | 1:K:338:ASN:H    | 1.74                     | 0.52              |
| 1:B:80:PHE:CG    | 5:B:1484:MPD:HM2 | 2.44                     | 0.52              |
| 1:C:337:ARG:HG2  | 1:C:338:ASN:H    | 1.74                     | 0.52              |
| 1:D:312:ALA:HB1  | 1:D:361:PRO:HG3  | 1.91                     | 0.52              |
| 1:F:80:PHE:CD1   | 5:F:1488:MPD:O4  | 2.63                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:80:PHE:CD1   | 5:H:1490:MPD:O4  | 2.63                     | 0.52              |
| 1:H:360:PHE:CE2  | 1:H:361:PRO:HD3  | 2.39                     | 0.52              |
| 1:H:397:TYR:C    | 1:H:399:LEU:N    | 2.60                     | 0.52              |
| 1:K:427:PHE:CE1  | 1:K:428:LEU:HD13 | 2.44                     | 0.52              |
| 1:L:302:ILE:HG23 | 1:L:332:LEU:HB3  | 1.91                     | 0.52              |
| 1:B:80:PHE:CD1   | 5:B:1484:MPD:O4  | 2.63                     | 0.52              |
| 1:B:302:ILE:HG23 | 1:B:332:LEU:HB3  | 1.91                     | 0.52              |
| 1:F:179:TYR:C    | 1:F:181:PRO:CD   | 2.81                     | 0.52              |
| 1:F:302:ILE:HG23 | 1:F:332:LEU:HB3  | 1.91                     | 0.52              |
| 1:G:124:VAL:HG11 | 1:G:375:LEU:HG   | 1.92                     | 0.52              |
| 1:H:312:ALA:HB1  | 1:H:361:PRO:HG3  | 1.91                     | 0.52              |
| 1:I:80:PHE:CG    | 5:I:1491:MPD:HM2 | 2.44                     | 0.52              |
| 1:J:48:MET:HE2   | 1:J:66:VAL:CG2   | 2.26                     | 0.52              |
| 1:J:80:PHE:CG    | 5:J:1492:MPD:HM2 | 2.44                     | 0.52              |
| 1:A:80:PHE:CD1   | 5:A:1483:MPD:O4  | 2.63                     | 0.52              |
| 1:A:465:TYR:O    | 1:A:468:VAL:HB   | 2.10                     | 0.52              |
| 1:B:465:TYR:O    | 1:B:468:VAL:HB   | 2.10                     | 0.52              |
| 1:C:80:PHE:CD1   | 5:C:1485:MPD:O4  | 2.63                     | 0.52              |
| 1:C:465:TYR:O    | 1:C:468:VAL:HB   | 2.10                     | 0.52              |
| 1:E:124:VAL:HG11 | 1:E:375:LEU:HG   | 1.92                     | 0.52              |
| 1:G:50:ASP:CG    | 6:G:1609:HOH:O   | 2.53                     | 0.52              |
| 1:G:80:PHE:CD1   | 5:G:1489:MPD:O4  | 2.63                     | 0.52              |
| 1:I:465:TYR:O    | 1:I:468:VAL:HB   | 2.10                     | 0.52              |
| 1:K:80:PHE:CD1   | 5:K:1493:MPD:O4  | 2.63                     | 0.52              |
| 1:L:82:ASP:N     | 5:L:1494:MPD:H13 | 2.13                     | 0.52              |
| 1:L:124:VAL:HG11 | 1:L:375:LEU:HG   | 1.92                     | 0.52              |
| 1:B:124:VAL:HG11 | 1:B:375:LEU:HG   | 1.92                     | 0.52              |
| 1:C:302:ILE:HG23 | 1:C:332:LEU:HB3  | 1.91                     | 0.52              |
| 1:E:16:PHE:HB2   | 1:E:84:THR:HB    | 1.92                     | 0.52              |
| 1:F:456:THR:O    | 1:L:458:HIS:HE1  | 1.93                     | 0.52              |
| 1:G:360:PHE:CE2  | 1:G:361:PRO:HD3  | 2.39                     | 0.52              |
| 1:I:124:VAL:HG11 | 1:I:375:LEU:HG   | 1.92                     | 0.52              |
| 1:L:82:ASP:N     | 5:L:1494:MPD:C1  | 2.54                     | 0.52              |
| 1:A:60:ILE:HG21  | 1:F:395:ASN:ND2  | 2.18                     | 0.52              |
| 1:B:312:ALA:HB1  | 1:B:361:PRO:HG3  | 1.91                     | 0.52              |
| 1:F:312:ALA:HB1  | 1:F:361:PRO:HG3  | 1.91                     | 0.52              |
| 1:I:302:ILE:HG23 | 1:I:332:LEU:HB3  | 1.91                     | 0.52              |
| 1:I:312:ALA:HB1  | 1:I:361:PRO:HG3  | 1.91                     | 0.52              |
| 1:J:340:SER:OG   | 1:J:396:LEU:HB3  | 2.10                     | 0.52              |
| 1:K:16:PHE:HB2   | 1:K:84:THR:HB    | 1.92                     | 0.52              |
| 1:L:179:TYR:C    | 1:L:181:PRO:CD   | 2.81                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:180:PHE:N    | 1:L:180:PHE:HD1  | 2.08                     | 0.52              |
| 1:A:337:ARG:HG2  | 1:A:338:ASN:H    | 1.74                     | 0.52              |
| 1:C:80:PHE:CG    | 5:C:1485:MPD:HM2 | 2.44                     | 0.52              |
| 1:D:337:ARG:HG2  | 1:D:338:ASN:H    | 1.74                     | 0.52              |
| 1:D:465:TYR:O    | 1:D:468:VAL:HB   | 2.10                     | 0.52              |
| 1:E:337:ARG:HG2  | 1:E:338:ASN:H    | 1.74                     | 0.52              |
| 1:F:340:SER:OG   | 1:F:396:LEU:HB3  | 2.10                     | 0.52              |
| 1:K:124:VAL:HG11 | 1:K:375:LEU:HG   | 1.92                     | 0.52              |
| 1:L:80:PHE:CD1   | 5:L:1494:MPD:O4  | 2.63                     | 0.52              |
| 1:L:340:SER:OG   | 1:L:396:LEU:HB3  | 2.10                     | 0.52              |
| 1:F:465:TYR:O    | 1:F:468:VAL:HB   | 2.10                     | 0.52              |
| 1:I:80:PHE:CD1   | 5:I:1491:MPD:O4  | 2.63                     | 0.52              |
| 1:J:180:PHE:N    | 1:J:180:PHE:HD1  | 2.08                     | 0.52              |
| 1:K:360:PHE:CE2  | 1:K:361:PRO:HD3  | 2.39                     | 0.52              |
| 1:A:455:MET:HE2  | 1:G:261:PHE:HE1  | 1.75                     | 0.51              |
| 1:D:80:PHE:CD1   | 5:D:1486:MPD:O4  | 2.63                     | 0.51              |
| 1:D:340:SER:OG   | 1:D:396:LEU:HB3  | 2.10                     | 0.51              |
| 1:J:337:ARG:HG2  | 1:J:338:ASN:H    | 1.74                     | 0.51              |
| 1:K:302:ILE:HG23 | 1:K:332:LEU:HB3  | 1.91                     | 0.51              |
| 1:K:312:ALA:HB1  | 1:K:361:PRO:HG3  | 1.91                     | 0.51              |
| 1:K:465:TYR:O    | 1:K:468:VAL:HB   | 2.10                     | 0.51              |
| 1:B:16:PHE:HB2   | 1:B:84:THR:HB    | 1.92                     | 0.51              |
| 1:B:340:SER:OG   | 1:B:396:LEU:HB3  | 2.10                     | 0.51              |
| 1:E:80:PHE:CD1   | 5:E:1487:MPD:O4  | 2.63                     | 0.51              |
| 1:E:465:TYR:O    | 1:E:468:VAL:HB   | 2.10                     | 0.51              |
| 5:G:1489:MPD:H32 | 1:H:193:SER:OG   | 2.09                     | 0.51              |
| 1:H:124:VAL:HG11 | 1:H:375:LEU:HG   | 1.92                     | 0.51              |
| 1:H:180:PHE:N    | 1:H:180:PHE:HD1  | 2.08                     | 0.51              |
| 1:J:80:PHE:CD1   | 5:J:1492:MPD:O4  | 2.63                     | 0.51              |
| 1:A:179:TYR:C    | 1:A:181:PRO:CD   | 2.81                     | 0.51              |
| 1:G:312:ALA:HB1  | 1:G:361:PRO:HG3  | 1.91                     | 0.51              |
| 1:H:16:PHE:HB2   | 1:H:84:THR:HB    | 1.92                     | 0.51              |
| 1:A:340:SER:OG   | 1:A:396:LEU:HB3  | 2.10                     | 0.51              |
| 1:A:427:PHE:CE1  | 1:A:428:LEU:HD13 | 2.44                     | 0.51              |
| 1:C:180:PHE:N    | 1:C:180:PHE:HD1  | 2.08                     | 0.51              |
| 1:C:340:SER:OG   | 1:C:396:LEU:HB3  | 2.10                     | 0.51              |
| 1:E:360:PHE:CE2  | 1:E:361:PRO:HD3  | 2.39                     | 0.51              |
| 1:G:302:ILE:HG23 | 1:G:332:LEU:HB3  | 1.91                     | 0.51              |
| 1:J:465:TYR:O    | 1:J:468:VAL:HB   | 2.10                     | 0.51              |
| 1:L:337:ARG:HG2  | 1:L:338:ASN:H    | 1.74                     | 0.51              |
| 1:L:465:TYR:O    | 1:L:468:VAL:HB   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:193:SER:HB2  | 5:C:1485:MPD:C3 | 2.39                     | 0.51              |
| 1:G:16:PHE:HB2   | 1:G:84:THR:HB   | 1.92                     | 0.51              |
| 1:G:465:TYR:O    | 1:G:468:VAL:HB  | 2.10                     | 0.51              |
| 1:H:465:TYR:O    | 1:H:468:VAL:HB  | 2.10                     | 0.51              |
| 1:I:375:LEU:HD22 | 1:I:379:LEU:HG  | 1.93                     | 0.51              |
| 1:A:224:ARG:HG2  | 1:A:224:ARG:NH2 | 2.15                     | 0.51              |
| 1:F:49:PHE:CD2   | 1:F:49:PHE:N    | 2.79                     | 0.51              |
| 1:F:124:VAL:HG13 | 1:F:274:LEU:CD2 | 2.41                     | 0.51              |
| 1:I:16:PHE:HB2   | 1:I:84:THR:HB   | 1.92                     | 0.51              |
| 1:I:124:VAL:HG13 | 1:I:274:LEU:CD2 | 2.41                     | 0.51              |
| 1:I:340:SER:OG   | 1:I:396:LEU:HB3 | 2.10                     | 0.51              |
| 1:K:49:PHE:CD2   | 1:K:49:PHE:N    | 2.79                     | 0.51              |
| 1:A:180:PHE:N    | 1:A:180:PHE:HD1 | 2.08                     | 0.51              |
| 1:H:58:LYS:HZ1   | 1:H:60:ILE:HD11 | 1.74                     | 0.51              |
| 1:L:49:PHE:N     | 1:L:49:PHE:CD2  | 2.79                     | 0.51              |
| 1:A:16:PHE:HB2   | 1:A:84:THR:HB   | 1.92                     | 0.51              |
| 1:A:124:VAL:HG11 | 1:A:375:LEU:HG  | 1.92                     | 0.51              |
| 1:G:124:VAL:HG13 | 1:G:274:LEU:CD2 | 2.41                     | 0.51              |
| 1:I:180:PHE:N    | 1:I:180:PHE:HD1 | 2.08                     | 0.51              |
| 1:J:124:VAL:HG11 | 1:J:375:LEU:HG  | 1.92                     | 0.51              |
| 1:L:360:PHE:CE2  | 1:L:361:PRO:HD3 | 2.39                     | 0.51              |
| 1:B:180:PHE:N    | 1:B:180:PHE:HD1 | 2.08                     | 0.51              |
| 1:C:16:PHE:HB2   | 1:C:84:THR:HB   | 1.92                     | 0.51              |
| 1:C:124:VAL:HG13 | 1:C:274:LEU:CD2 | 2.41                     | 0.51              |
| 1:D:360:PHE:CG   | 1:D:361:PRO:HD3 | 2.42                     | 0.51              |
| 1:G:340:SER:OG   | 1:G:396:LEU:HB3 | 2.10                     | 0.51              |
| 1:H:49:PHE:CD2   | 1:H:49:PHE:N    | 2.79                     | 0.51              |
| 1:K:124:VAL:HG13 | 1:K:274:LEU:CD2 | 2.41                     | 0.51              |
| 1:D:375:LEU:HD22 | 1:D:379:LEU:HG  | 1.93                     | 0.51              |
| 1:E:302:ILE:HG23 | 1:E:332:LEU:HB3 | 1.91                     | 0.51              |
| 1:G:180:PHE:N    | 1:G:180:PHE:HD1 | 2.08                     | 0.51              |
| 1:J:124:VAL:HG13 | 1:J:274:LEU:CD2 | 2.41                     | 0.51              |
| 1:D:124:VAL:HG13 | 1:D:274:LEU:CD2 | 2.41                     | 0.50              |
| 1:E:49:PHE:CD2   | 1:E:49:PHE:N    | 2.79                     | 0.50              |
| 1:F:375:LEU:HD22 | 1:F:379:LEU:HG  | 1.93                     | 0.50              |
| 1:J:16:PHE:HB2   | 1:J:84:THR:HB   | 1.92                     | 0.50              |
| 1:J:58:LYS:O     | 1:J:58:LYS:HG2  | 2.12                     | 0.50              |
| 5:K:1493:MPD:C3  | 1:L:193:SER:HB2 | 2.41                     | 0.50              |
| 1:A:49:PHE:N     | 1:A:49:PHE:CD2  | 2.79                     | 0.50              |
| 1:A:124:VAL:HG13 | 1:A:274:LEU:CD2 | 2.41                     | 0.50              |
| 1:A:339:ARG:HH22 | 1:B:63:SER:HB2  | 1.76                     | 0.50              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:124:VAL:HG13 | 1:E:274:LEU:CD2 | 2.41                     | 0.50              |
| 1:F:16:PHE:HB2   | 1:F:84:THR:HB   | 1.92                     | 0.50              |
| 1:F:360:PHE:CG   | 1:F:361:PRO:HD3 | 2.43                     | 0.50              |
| 1:H:124:VAL:HG13 | 1:H:274:LEU:CD2 | 2.41                     | 0.50              |
| 1:L:124:VAL:HG13 | 1:L:274:LEU:CD2 | 2.41                     | 0.50              |
| 1:A:397:TYR:C    | 1:A:399:LEU:N   | 2.60                     | 0.50              |
| 1:B:375:LEU:HD22 | 1:B:379:LEU:HG  | 1.93                     | 0.50              |
| 1:D:124:VAL:HG11 | 1:D:375:LEU:HG  | 1.92                     | 0.50              |
| 1:B:49:PHE:N     | 1:B:49:PHE:CD2  | 2.79                     | 0.50              |
| 1:H:58:LYS:HG2   | 1:H:58:LYS:O    | 2.12                     | 0.50              |
| 1:H:340:SER:OG   | 1:H:396:LEU:HB3 | 2.10                     | 0.50              |
| 1:I:49:PHE:N     | 1:I:49:PHE:CD2  | 2.79                     | 0.50              |
| 1:B:50:ASP:CG    | 6:B:1490:HOH:O  | 2.54                     | 0.50              |
| 1:D:16:PHE:HB2   | 1:D:84:THR:HB   | 1.92                     | 0.50              |
| 1:E:58:LYS:HG2   | 1:E:58:LYS:O    | 2.12                     | 0.50              |
| 1:G:49:PHE:N     | 1:G:49:PHE:CD2  | 2.79                     | 0.50              |
| 1:G:375:LEU:HD22 | 1:G:379:LEU:HG  | 1.93                     | 0.50              |
| 1:K:375:LEU:HD22 | 1:K:379:LEU:HG  | 1.93                     | 0.50              |
| 1:A:360:PHE:CG   | 1:A:361:PRO:HD3 | 2.43                     | 0.50              |
| 1:A:398:ASP:C    | 1:A:400:PRO:CD  | 2.82                     | 0.50              |
| 1:B:49:PHE:N     | 1:B:49:PHE:HD2  | 2.10                     | 0.50              |
| 1:B:124:VAL:HG13 | 1:B:274:LEU:CD2 | 2.41                     | 0.50              |
| 1:C:397:TYR:OH   | 1:C:404:ALA:O   | 2.29                     | 0.50              |
| 1:D:401:PRO:CB   | 1:D:404:ALA:HA  | 2.37                     | 0.50              |
| 1:E:189:GLN:OE1  | 5:F:1488:MPD:H4 | 2.12                     | 0.50              |
| 1:F:224:ARG:HG2  | 1:F:224:ARG:NH2 | 2.15                     | 0.50              |
| 1:L:16:PHE:HB2   | 1:L:84:THR:HB   | 1.92                     | 0.50              |
| 1:L:58:LYS:O     | 1:L:58:LYS:HG2  | 2.12                     | 0.50              |
| 1:A:454:ARG:O    | 1:G:320:LYS:HG2 | 2.11                     | 0.50              |
| 1:G:84:THR:HG21  | 5:G:1489:MPD:C5 | 2.42                     | 0.50              |
| 1:I:84:THR:HG21  | 5:I:1491:MPD:C5 | 2.42                     | 0.50              |
| 1:K:340:SER:OG   | 1:K:396:LEU:HB3 | 2.10                     | 0.50              |
| 1:K:435:THR:HG23 | 6:K:1518:HOH:O  | 2.12                     | 0.50              |
| 1:B:58:LYS:HG2   | 1:B:58:LYS:O    | 2.12                     | 0.50              |
| 1:B:395:ASN:ND2  | 1:C:60:ILE:HG21 | 2.22                     | 0.50              |
| 1:D:49:PHE:N     | 1:D:49:PHE:CD2  | 2.79                     | 0.50              |
| 1:D:84:THR:HG21  | 5:D:1486:MPD:C5 | 2.42                     | 0.50              |
| 1:D:395:ASN:ND2  | 1:E:60:ILE:CG2  | 2.61                     | 0.50              |
| 1:H:49:PHE:N     | 1:H:49:PHE:HD2  | 2.10                     | 0.50              |
| 1:J:49:PHE:N     | 1:J:49:PHE:CD2  | 2.79                     | 0.50              |
| 1:K:84:THR:HG21  | 5:K:1493:MPD:C5 | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:PHE:N     | 1:A:49:PHE:HD2   | 2.10                     | 0.50              |
| 1:C:49:PHE:CD2   | 1:C:49:PHE:N     | 2.79                     | 0.50              |
| 1:C:360:PHE:CE2  | 1:C:361:PRO:HD3  | 2.39                     | 0.50              |
| 1:C:375:LEU:HD22 | 1:C:379:LEU:HG   | 1.93                     | 0.50              |
| 1:E:340:SER:OG   | 1:E:396:LEU:HB3  | 2.10                     | 0.50              |
| 1:D:180:PHE:N    | 1:D:180:PHE:HD1  | 2.08                     | 0.49              |
| 1:E:84:THR:HG21  | 5:E:1487:MPD:C5  | 2.42                     | 0.49              |
| 1:F:49:PHE:N     | 1:F:49:PHE:HD2   | 2.10                     | 0.49              |
| 5:G:1489:MPD:H4  | 1:H:189:GLN:OE1  | 2.12                     | 0.49              |
| 1:H:375:LEU:HD22 | 1:H:379:LEU:HG   | 1.93                     | 0.49              |
| 1:K:49:PHE:N     | 1:K:49:PHE:HD2   | 2.10                     | 0.49              |
| 1:A:58:LYS:O     | 1:A:58:LYS:HG2   | 2.12                     | 0.49              |
| 1:A:339:ARG:NH2  | 1:B:63:SER:OG    | 2.46                     | 0.49              |
| 1:J:375:LEU:HD22 | 1:J:379:LEU:HG   | 1.93                     | 0.49              |
| 1:J:435:THR:HG23 | 6:J:1514:HOH:O   | 2.12                     | 0.49              |
| 1:B:398:ASP:C    | 1:B:400:PRO:CD   | 2.82                     | 0.49              |
| 1:F:84:THR:HG21  | 5:F:1488:MPD:C5  | 2.42                     | 0.49              |
| 5:G:1489:MPD:C3  | 1:H:193:SER:OG   | 2.60                     | 0.49              |
| 1:I:34:PRO:HG2   | 1:J:206:VAL:O    | 2.12                     | 0.49              |
| 5:K:1493:MPD:C3  | 1:L:193:SER:CB   | 2.88                     | 0.49              |
| 1:L:375:LEU:HD22 | 1:L:379:LEU:HG   | 1.93                     | 0.49              |
| 1:A:435:THR:HG23 | 6:A:1498:HOH:O   | 2.12                     | 0.49              |
| 1:B:435:THR:HG23 | 6:B:1505:HOH:O   | 2.12                     | 0.49              |
| 1:E:375:LEU:HD22 | 1:E:379:LEU:HG   | 1.93                     | 0.49              |
| 1:F:180:PHE:N    | 1:F:180:PHE:HD1  | 2.08                     | 0.49              |
| 1:I:29:GLN:HB3   | 1:J:180:PHE:CB   | 2.41                     | 0.49              |
| 1:L:84:THR:HG21  | 5:L:1494:MPD:C5  | 2.42                     | 0.49              |
| 1:A:84:THR:HG21  | 5:A:1483:MPD:C5  | 2.42                     | 0.49              |
| 1:A:375:LEU:HD22 | 1:A:379:LEU:HG   | 1.93                     | 0.49              |
| 1:C:190:ASP:OD2  | 5:D:1486:MPD:CM  | 2.54                     | 0.49              |
| 1:C:193:SER:OG   | 5:D:1486:MPD:H32 | 2.13                     | 0.49              |
| 1:G:58:LYS:O     | 1:G:58:LYS:HG2   | 2.12                     | 0.49              |
| 1:I:33:ILE:CD1   | 1:J:208:ALA:HB2  | 2.42                     | 0.49              |
| 1:I:49:PHE:N     | 1:I:49:PHE:HD2   | 2.10                     | 0.49              |
| 1:B:84:THR:HG21  | 5:B:1484:MPD:C5  | 2.42                     | 0.49              |
| 1:D:1:SER:CA     | 1:D:71:ALA:CB    | 2.80                     | 0.49              |
| 1:I:1:SER:CA     | 1:I:71:ALA:CB    | 2.80                     | 0.49              |
| 1:I:33:ILE:HD11  | 1:J:208:ALA:HB2  | 1.94                     | 0.49              |
| 1:L:49:PHE:N     | 1:L:49:PHE:HD2   | 2.10                     | 0.49              |
| 1:B:58:LYS:HZ1   | 1:B:60:ILE:HD11  | 1.77                     | 0.49              |
| 1:D:49:PHE:N     | 1:D:49:PHE:HD2   | 2.10                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:190:ASP:OD2  | 5:E:1487:MPD:CM | 2.55                     | 0.49              |
| 1:E:49:PHE:N     | 1:E:49:PHE:HD2  | 2.10                     | 0.49              |
| 1:J:49:PHE:N     | 1:J:49:PHE:HD2  | 2.10                     | 0.49              |
| 1:C:84:THR:HG21  | 5:C:1485:MPD:C5 | 2.42                     | 0.49              |
| 1:D:58:LYS:O     | 1:D:58:LYS:HG2  | 2.12                     | 0.49              |
| 1:G:397:TYR:C    | 1:G:399:LEU:N   | 2.60                     | 0.49              |
| 1:A:192:ARG:HH21 | 1:A:219:ASN:ND2 | 2.11                     | 0.49              |
| 1:E:398:ASP:C    | 1:E:400:PRO:CD  | 2.82                     | 0.49              |
| 1:I:401:PRO:CB   | 1:I:404:ALA:HA  | 2.37                     | 0.49              |
| 1:I:435:THR:HG23 | 6:I:1514:HOH:O  | 2.12                     | 0.49              |
| 1:K:58:LYS:O     | 1:K:58:LYS:HG2  | 2.12                     | 0.49              |
| 1:C:193:SER:OG   | 5:D:1486:MPD:C3 | 2.61                     | 0.49              |
| 1:F:435:THR:HG23 | 6:F:1511:HOH:O  | 2.12                     | 0.49              |
| 1:J:60:ILE:HD13  | 1:J:60:ILE:HA   | 1.62                     | 0.49              |
| 1:J:192:ARG:HH21 | 1:J:219:ASN:ND2 | 2.11                     | 0.49              |
| 1:J:398:ASP:C    | 1:J:400:PRO:CD  | 2.82                     | 0.49              |
| 1:C:454:ARG:O    | 1:I:320:LYS:HG2 | 2.13                     | 0.48              |
| 1:D:435:THR:HG23 | 6:D:1509:HOH:O  | 2.12                     | 0.48              |
| 1:F:261:PHE:HE1  | 1:L:455:MET:HE2 | 1.78                     | 0.48              |
| 1:H:84:THR:HG21  | 5:H:1490:MPD:C5 | 2.42                     | 0.48              |
| 1:H:435:THR:HG23 | 6:H:1512:HOH:O  | 2.12                     | 0.48              |
| 1:I:192:ARG:HH21 | 1:I:219:ASN:ND2 | 2.11                     | 0.48              |
| 1:J:84:THR:HG21  | 5:J:1492:MPD:C5 | 2.42                     | 0.48              |
| 1:K:401:PRO:CB   | 1:K:404:ALA:HA  | 2.37                     | 0.48              |
| 1:B:189:GLN:OE1  | 5:C:1485:MPD:H4 | 2.13                     | 0.48              |
| 1:C:192:ARG:HH21 | 1:C:219:ASN:ND2 | 2.11                     | 0.48              |
| 1:F:287:TYR:O    | 1:F:290:LEU:HB2 | 2.14                     | 0.48              |
| 1:G:435:THR:HG23 | 6:G:1512:HOH:O  | 2.12                     | 0.48              |
| 1:K:192:ARG:HH21 | 1:K:219:ASN:ND2 | 2.11                     | 0.48              |
| 1:L:360:PHE:CG   | 1:L:361:PRO:HD3 | 2.43                     | 0.48              |
| 1:L:435:THR:HG23 | 6:L:1348:HOH:O  | 2.12                     | 0.48              |
| 1:A:320:LYS:HG2  | 1:G:454:ARG:O   | 2.13                     | 0.48              |
| 1:C:435:THR:HG23 | 6:C:1507:HOH:O  | 2.12                     | 0.48              |
| 1:D:287:TYR:O    | 1:D:290:LEU:HB2 | 2.14                     | 0.48              |
| 1:E:180:PHE:O    | 1:F:29:GLN:HA   | 2.13                     | 0.48              |
| 1:E:435:THR:HG23 | 6:E:1508:HOH:O  | 2.12                     | 0.48              |
| 1:F:58:LYS:O     | 1:F:58:LYS:HG2  | 2.12                     | 0.48              |
| 5:K:1493:MPD:H32 | 1:L:193:SER:OG  | 2.13                     | 0.48              |
| 1:L:287:TYR:O    | 1:L:290:LEU:HB2 | 2.14                     | 0.48              |
| 1:A:193:SER:CB   | 5:B:1484:MPD:C3 | 2.86                     | 0.48              |
| 1:C:49:PHE:N     | 1:C:49:PHE:HD2  | 2.10                     | 0.48              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:48:MET:CE    | 1:G:66:VAL:HG22 | 2.31                     | 0.48              |
| 1:G:49:PHE:N     | 1:G:49:PHE:HD2  | 2.10                     | 0.48              |
| 1:G:287:TYR:O    | 1:G:290:LEU:HB2 | 2.14                     | 0.48              |
| 1:H:397:TYR:OH   | 1:H:404:ALA:O   | 2.29                     | 0.48              |
| 1:I:287:TYR:O    | 1:I:290:LEU:HB2 | 2.14                     | 0.48              |
| 1:L:398:ASP:C    | 1:L:400:PRO:CD  | 2.82                     | 0.48              |
| 1:D:192:ARG:HH21 | 1:D:219:ASN:ND2 | 2.11                     | 0.48              |
| 1:J:224:ARG:HG2  | 1:J:224:ARG:NH2 | 2.15                     | 0.48              |
| 1:L:192:ARG:HH21 | 1:L:219:ASN:ND2 | 2.11                     | 0.48              |
| 1:C:58:LYS:O     | 1:C:58:LYS:HG2  | 2.12                     | 0.48              |
| 1:C:455:MET:HE2  | 1:I:261:PHE:HE1 | 1.77                     | 0.48              |
| 1:D:455:MET:HE2  | 1:J:261:PHE:HE1 | 1.77                     | 0.48              |
| 1:F:332:LEU:HB2  | 1:F:408:PRO:O   | 2.14                     | 0.48              |
| 1:I:58:LYS:O     | 1:I:58:LYS:HG2  | 2.12                     | 0.48              |
| 1:J:287:TYR:O    | 1:J:290:LEU:HB2 | 2.14                     | 0.48              |
| 1:H:192:ARG:HH21 | 1:H:219:ASN:ND2 | 2.11                     | 0.48              |
| 1:I:332:LEU:HB2  | 1:I:408:PRO:O   | 2.14                     | 0.48              |
| 1:K:1:SER:CA     | 1:K:71:ALA:CB   | 2.80                     | 0.48              |
| 5:K:1493:MPD:C3  | 1:L:193:SER:OG  | 2.61                     | 0.48              |
| 1:B:1:SER:CA     | 1:B:71:ALA:CB   | 2.80                     | 0.48              |
| 1:C:287:TYR:O    | 1:C:290:LEU:HB2 | 2.14                     | 0.48              |
| 1:C:332:LEU:HB2  | 1:C:408:PRO:O   | 2.14                     | 0.48              |
| 1:B:192:ARG:HH21 | 1:B:219:ASN:ND2 | 2.11                     | 0.48              |
| 1:E:180:PHE:N    | 1:E:180:PHE:HD1 | 2.08                     | 0.48              |
| 1:L:332:LEU:HB2  | 1:L:408:PRO:O   | 2.14                     | 0.48              |
| 1:D:443:ILE:O    | 1:D:447:ARG:HB2 | 2.14                     | 0.48              |
| 1:E:287:TYR:O    | 1:E:290:LEU:HB2 | 2.14                     | 0.48              |
| 1:G:60:ILE:HD13  | 1:G:60:ILE:HA   | 1.62                     | 0.48              |
| 1:G:332:LEU:HB2  | 1:G:408:PRO:O   | 2.14                     | 0.48              |
| 1:H:332:LEU:HB2  | 1:H:408:PRO:O   | 2.14                     | 0.48              |
| 1:A:332:LEU:HB2  | 1:A:408:PRO:O   | 2.14                     | 0.47              |
| 1:B:287:TYR:O    | 1:B:290:LEU:HB2 | 2.14                     | 0.47              |
| 1:D:395:ASN:HD22 | 1:D:395:ASN:HA  | 1.53                     | 0.47              |
| 1:E:332:LEU:HB2  | 1:E:408:PRO:O   | 2.14                     | 0.47              |
| 1:F:192:ARG:HH21 | 1:F:219:ASN:ND2 | 2.11                     | 0.47              |
| 1:K:180:PHE:N    | 1:K:180:PHE:HD1 | 2.08                     | 0.47              |
| 1:C:339:ARG:HH22 | 1:D:63:SER:HB2  | 1.78                     | 0.47              |
| 1:E:395:ASN:ND2  | 1:F:60:ILE:HG21 | 2.28                     | 0.47              |
| 1:J:311:LEU:HD22 | 1:J:369:LEU:HB3 | 1.97                     | 0.47              |
| 1:A:189:GLN:OE1  | 5:B:1484:MPD:H4 | 2.13                     | 0.47              |
| 1:A:443:ILE:O    | 1:A:447:ARG:HB2 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:189:GLN:OE1  | 5:E:1487:MPD:H4  | 2.13                     | 0.47              |
| 1:D:224:ARG:HG2  | 1:D:224:ARG:NH2  | 2.15                     | 0.47              |
| 1:D:332:LEU:HB2  | 1:D:408:PRO:O    | 2.14                     | 0.47              |
| 1:E:261:PHE:HE1  | 1:K:455:MET:HE2  | 1.80                     | 0.47              |
| 1:G:63:SER:HB2   | 1:H:339:ARG:HH22 | 1.79                     | 0.47              |
| 1:A:287:TYR:O    | 1:A:290:LEU:HB2  | 2.14                     | 0.47              |
| 1:F:18:ASP:OD2   | 1:F:30:HIS:HD2   | 1.98                     | 0.47              |
| 1:G:63:SER:OG    | 1:H:339:ARG:NH2  | 2.47                     | 0.47              |
| 1:G:311:LEU:HD22 | 1:G:369:LEU:HB3  | 1.97                     | 0.47              |
| 1:L:443:ILE:O    | 1:L:447:ARG:HB2  | 2.14                     | 0.47              |
| 1:E:48:MET:CE    | 1:E:66:VAL:HG22  | 2.31                     | 0.47              |
| 1:G:18:ASP:OD2   | 1:G:30:HIS:HD2   | 1.98                     | 0.47              |
| 1:G:401:PRO:CB   | 1:G:404:ALA:HA   | 2.37                     | 0.47              |
| 1:I:443:ILE:O    | 1:I:447:ARG:HB2  | 2.14                     | 0.47              |
| 1:J:18:ASP:OD2   | 1:J:30:HIS:HD2   | 1.98                     | 0.47              |
| 1:J:34:PRO:HG2   | 1:K:206:VAL:O    | 2.14                     | 0.47              |
| 1:L:401:PRO:CB   | 1:L:404:ALA:HA   | 2.37                     | 0.47              |
| 1:A:339:ARG:HD3  | 1:A:339:ARG:HA   | 1.71                     | 0.47              |
| 1:F:443:ILE:O    | 1:F:447:ARG:HB2  | 2.14                     | 0.47              |
| 1:H:287:TYR:O    | 1:H:290:LEU:HB2  | 2.14                     | 0.47              |
| 1:J:332:LEU:HB2  | 1:J:408:PRO:O    | 2.14                     | 0.47              |
| 1:J:443:ILE:O    | 1:J:447:ARG:HB2  | 2.14                     | 0.47              |
| 1:K:332:LEU:HB2  | 1:K:408:PRO:O    | 2.14                     | 0.47              |
| 1:B:443:ILE:O    | 1:B:447:ARG:HB2  | 2.14                     | 0.47              |
| 1:C:18:ASP:OD2   | 1:C:30:HIS:HD2   | 1.98                     | 0.47              |
| 1:D:18:ASP:OD2   | 1:D:30:HIS:HD2   | 1.98                     | 0.47              |
| 1:E:193:SER:CB   | 5:F:1488:MPD:C3  | 2.84                     | 0.47              |
| 1:F:311:LEU:HD22 | 1:F:369:LEU:HB3  | 1.97                     | 0.47              |
| 1:F:398:ASP:C    | 1:F:400:PRO:CD   | 2.82                     | 0.47              |
| 1:G:443:ILE:O    | 1:G:447:ARG:HB2  | 2.14                     | 0.47              |
| 1:H:1:SER:CA     | 1:H:71:ALA:CB    | 2.81                     | 0.47              |
| 1:K:60:ILE:HD13  | 1:K:60:ILE:HA    | 1.62                     | 0.47              |
| 1:A:397:TYR:OH   | 1:A:404:ALA:O    | 2.29                     | 0.47              |
| 1:B:360:PHE:CG   | 1:B:361:PRO:HD3  | 2.43                     | 0.47              |
| 1:B:455:MET:HE2  | 1:H:261:PHE:HE1  | 1.79                     | 0.47              |
| 1:C:193:SER:HB2  | 5:D:1486:MPD:C3  | 2.44                     | 0.47              |
| 1:E:456:THR:O    | 1:K:458:HIS:HE1  | 1.97                     | 0.47              |
| 1:G:192:ARG:HH21 | 1:G:219:ASN:ND2  | 2.11                     | 0.47              |
| 1:B:18:ASP:OD2   | 1:B:30:HIS:HD2   | 1.98                     | 0.47              |
| 1:B:311:LEU:HD22 | 1:B:369:LEU:HB3  | 1.97                     | 0.47              |
| 1:B:332:LEU:HB2  | 1:B:408:PRO:O    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:136:ASP:O    | 1:I:169:LYS:NZ   | 2.35                     | 0.47              |
| 1:A:400:PRO:HB3  | 1:A:401:PRO:HD2  | 1.97                     | 0.47              |
| 1:C:180:PHE:CB   | 1:D:29:GLN:HB3   | 2.43                     | 0.47              |
| 1:C:208:ALA:HB2  | 1:D:33:ILE:HD11  | 1.97                     | 0.47              |
| 1:C:311:LEU:HD22 | 1:C:369:LEU:HB3  | 1.97                     | 0.47              |
| 1:C:443:ILE:O    | 1:C:447:ARG:HB2  | 2.15                     | 0.47              |
| 1:E:192:ARG:HH21 | 1:E:219:ASN:ND2  | 2.11                     | 0.47              |
| 1:F:401:PRO:CB   | 1:F:404:ALA:HA   | 2.37                     | 0.47              |
| 1:I:398:ASP:C    | 1:I:400:PRO:CD   | 2.82                     | 0.47              |
| 5:J:1492:MPD:H4  | 1:K:189:GLN:OE1  | 2.15                     | 0.47              |
| 1:K:287:TYR:O    | 1:K:290:LEU:HB2  | 2.14                     | 0.47              |
| 1:K:398:ASP:C    | 1:K:400:PRO:CD   | 2.82                     | 0.47              |
| 1:C:261:PHE:HE1  | 1:I:455:MET:HE2  | 1.79                     | 0.46              |
| 1:E:401:PRO:CB   | 1:E:404:ALA:HA   | 2.37                     | 0.46              |
| 1:E:443:ILE:O    | 1:E:447:ARG:HB2  | 2.14                     | 0.46              |
| 1:G:81:ALA:H     | 5:G:1489:MPD:H13 | 1.80                     | 0.46              |
| 1:G:360:PHE:CG   | 1:G:361:PRO:HD3  | 2.43                     | 0.46              |
| 1:I:48:MET:CE    | 1:I:66:VAL:HG22  | 2.31                     | 0.46              |
| 1:K:443:ILE:O    | 1:K:447:ARG:HB2  | 2.14                     | 0.46              |
| 1:A:456:THR:O    | 1:G:458:HIS:HE1  | 1.98                     | 0.46              |
| 1:D:397:TYR:OH   | 1:D:404:ALA:O    | 2.29                     | 0.46              |
| 1:E:311:LEU:HD22 | 1:E:369:LEU:HB3  | 1.96                     | 0.46              |
| 1:I:18:ASP:OD2   | 1:I:30:HIS:HD2   | 1.98                     | 0.46              |
| 1:I:286:LYS:HE2  | 1:I:292:GLU:HB3  | 1.98                     | 0.46              |
| 1:I:360:PHE:CE2  | 1:I:361:PRO:HD3  | 2.39                     | 0.46              |
| 1:K:311:LEU:HD22 | 1:K:369:LEU:HB3  | 1.97                     | 0.46              |
| 1:C:286:LYS:HE2  | 1:C:292:GLU:HB3  | 1.98                     | 0.46              |
| 1:F:337:ARG:HD3  | 1:F:393:ASP:OD2  | 2.15                     | 0.46              |
| 1:H:443:ILE:O    | 1:H:447:ARG:HB2  | 2.14                     | 0.46              |
| 1:I:337:ARG:HD3  | 1:I:393:ASP:OD2  | 2.15                     | 0.46              |
| 1:K:360:PHE:CG   | 1:K:361:PRO:HD3  | 2.43                     | 0.46              |
| 1:L:311:LEU:HD22 | 1:L:369:LEU:HB3  | 1.97                     | 0.46              |
| 1:C:400:PRO:HB3  | 1:C:401:PRO:HD2  | 1.97                     | 0.46              |
| 1:D:398:ASP:C    | 1:D:400:PRO:CD   | 2.82                     | 0.46              |
| 1:F:286:LYS:HE2  | 1:F:292:GLU:HB3  | 1.98                     | 0.46              |
| 1:G:286:LYS:HE2  | 1:G:292:GLU:HB3  | 1.98                     | 0.46              |
| 1:I:311:LEU:HD22 | 1:I:369:LEU:HB3  | 1.97                     | 0.46              |
| 1:K:18:ASP:OD2   | 1:K:30:HIS:HD2   | 1.98                     | 0.46              |
| 1:A:18:ASP:OD2   | 1:A:30:HIS:HD2   | 1.98                     | 0.46              |
| 1:D:286:LYS:HE2  | 1:D:292:GLU:HB3  | 1.98                     | 0.46              |
| 1:F:454:ARG:O    | 1:L:320:LYS:HG2  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:124:VAL:HG13 | 1:G:274:LEU:HD21 | 1.98                     | 0.46              |
| 1:J:395:ASN:HD22 | 1:J:395:ASN:HA   | 1.53                     | 0.46              |
| 1:L:400:PRO:HB3  | 1:L:401:PRO:HD2  | 1.97                     | 0.46              |
| 1:B:60:ILE:HD13  | 1:B:60:ILE:HA    | 1.62                     | 0.46              |
| 1:B:395:ASN:ND2  | 1:C:60:ILE:CG2   | 2.69                     | 0.46              |
| 1:D:261:PHE:HE1  | 1:J:455:MET:HE2  | 1.80                     | 0.46              |
| 1:E:400:PRO:HB3  | 1:E:401:PRO:HD2  | 1.97                     | 0.46              |
| 1:F:403:GLU:C    | 1:F:405:LYS:H    | 2.23                     | 0.46              |
| 1:G:400:PRO:HB3  | 1:G:401:PRO:HD2  | 1.97                     | 0.46              |
| 1:H:398:ASP:C    | 1:H:400:PRO:CD   | 2.82                     | 0.46              |
| 1:I:33:ILE:HG13  | 1:J:207:GLU:O    | 2.14                     | 0.46              |
| 1:I:400:PRO:HB3  | 1:I:401:PRO:HD2  | 1.97                     | 0.46              |
| 1:K:296:TYR:CE2  | 1:K:385:LYS:HD3  | 2.51                     | 0.46              |
| 1:L:18:ASP:OD2   | 1:L:30:HIS:HD2   | 1.98                     | 0.46              |
| 1:L:28:GLU:OE1   | 1:L:88:ARG:NH1   | 2.48                     | 0.46              |
| 1:B:337:ARG:HD3  | 1:B:393:ASP:OD2  | 2.16                     | 0.46              |
| 1:C:124:VAL:HG13 | 1:C:274:LEU:HD21 | 1.98                     | 0.46              |
| 1:H:18:ASP:OD2   | 1:H:30:HIS:HD2   | 1.98                     | 0.46              |
| 1:L:296:TYR:CE2  | 1:L:385:LYS:HD3  | 2.51                     | 0.46              |
| 1:C:296:TYR:CE2  | 1:C:385:LYS:HD3  | 2.51                     | 0.46              |
| 1:E:18:ASP:OD2   | 1:E:30:HIS:HD2   | 1.98                     | 0.46              |
| 1:F:466:TYR:CE1  | 1:L:254:THR:HB   | 2.51                     | 0.46              |
| 1:H:296:TYR:CE2  | 1:H:385:LYS:HD3  | 2.51                     | 0.46              |
| 1:J:286:LYS:HE2  | 1:J:292:GLU:HB3  | 1.98                     | 0.46              |
| 1:A:311:LEU:HD22 | 1:A:369:LEU:HB3  | 1.97                     | 0.46              |
| 1:C:337:ARG:HD3  | 1:C:393:ASP:OD2  | 2.15                     | 0.46              |
| 1:D:93:GLU:HB3   | 1:D:96:THR:HG23  | 1.98                     | 0.46              |
| 1:D:311:LEU:HD22 | 1:D:369:LEU:HB3  | 1.97                     | 0.46              |
| 1:E:193:SER:HB2  | 5:F:1488:MPD:C3  | 2.40                     | 0.46              |
| 1:G:1:SER:CA     | 1:G:71:ALA:CB    | 2.80                     | 0.46              |
| 1:A:296:TYR:CE2  | 1:A:385:LYS:HD3  | 2.51                     | 0.46              |
| 1:A:463:GLU:HA   | 1:G:140:PHE:CE1  | 2.51                     | 0.46              |
| 1:B:177:GLY:C    | 1:B:179:TYR:H    | 2.25                     | 0.46              |
| 1:B:296:TYR:CE2  | 1:B:385:LYS:HD3  | 2.51                     | 0.46              |
| 1:B:403:GLU:C    | 1:B:405:LYS:H    | 2.24                     | 0.46              |
| 1:C:401:PRO:CB   | 1:C:404:ALA:HA   | 2.37                     | 0.46              |
| 1:I:93:GLU:HB3   | 1:I:96:THR:HG23  | 1.98                     | 0.46              |
| 1:I:296:TYR:CE2  | 1:I:385:LYS:HD3  | 2.51                     | 0.46              |
| 1:L:286:LYS:HE2  | 1:L:292:GLU:HB3  | 1.98                     | 0.46              |
| 1:A:93:GLU:HB3   | 1:A:96:THR:HG23  | 1.98                     | 0.45              |
| 1:A:286:LYS:HE2  | 1:A:292:GLU:HB3  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:337:ARG:HD3  | 1:A:393:ASP:OD2  | 2.15                     | 0.45              |
| 1:B:206:VAL:O    | 1:C:34:PRO:HG2   | 2.16                     | 0.45              |
| 1:B:320:LYS:HG2  | 1:H:454:ARG:O    | 2.16                     | 0.45              |
| 1:F:296:TYR:CE2  | 1:F:385:LYS:HD3  | 2.51                     | 0.45              |
| 1:G:398:ASP:C    | 1:G:400:PRO:CD   | 2.82                     | 0.45              |
| 1:G:403:GLU:C    | 1:G:405:LYS:H    | 2.23                     | 0.45              |
| 1:I:397:TYR:OH   | 1:I:404:ALA:O    | 2.29                     | 0.45              |
| 1:J:50:ASP:CG    | 6:J:1612:HOH:O   | 2.59                     | 0.45              |
| 1:J:296:TYR:CE2  | 1:J:385:LYS:HD3  | 2.51                     | 0.45              |
| 1:K:124:VAL:HG13 | 1:K:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:K:337:ARG:HD3  | 1:K:393:ASP:OD2  | 2.15                     | 0.45              |
| 1:L:337:ARG:HD3  | 1:L:393:ASP:OD2  | 2.15                     | 0.45              |
| 1:A:124:VAL:HG13 | 1:A:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:B:401:PRO:CB   | 1:B:404:ALA:HA   | 2.37                     | 0.45              |
| 1:C:398:ASP:C    | 1:C:400:PRO:CD   | 2.82                     | 0.45              |
| 1:C:403:GLU:C    | 1:C:405:LYS:H    | 2.23                     | 0.45              |
| 1:E:403:GLU:C    | 1:E:405:LYS:H    | 2.24                     | 0.45              |
| 1:F:400:PRO:HB3  | 1:F:401:PRO:HD2  | 1.97                     | 0.45              |
| 1:G:339:ARG:NH2  | 1:L:63:SER:OG    | 2.49                     | 0.45              |
| 1:I:124:VAL:HG13 | 1:I:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:J:337:ARG:HD3  | 1:J:393:ASP:OD2  | 2.16                     | 0.45              |
| 1:K:93:GLU:HB3   | 1:K:96:THR:HG23  | 1.98                     | 0.45              |
| 1:K:400:PRO:HB3  | 1:K:401:PRO:HD2  | 1.97                     | 0.45              |
| 1:A:48:MET:CE    | 1:A:66:VAL:HG22  | 2.31                     | 0.45              |
| 1:D:124:VAL:HG13 | 1:D:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:D:432:GLY:HA2  | 6:D:1602:HOH:O   | 2.17                     | 0.45              |
| 1:E:124:VAL:HG13 | 1:E:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:E:296:TYR:CE2  | 1:E:385:LYS:HD3  | 2.51                     | 0.45              |
| 1:H:286:LYS:HE2  | 1:H:292:GLU:HB3  | 1.98                     | 0.45              |
| 1:I:60:ILE:HD13  | 1:I:60:ILE:HA    | 1.62                     | 0.45              |
| 1:I:177:GLY:C    | 1:I:179:TYR:H    | 2.25                     | 0.45              |
| 1:J:177:GLY:C    | 1:J:179:TYR:H    | 2.24                     | 0.45              |
| 1:J:401:PRO:CB   | 1:J:404:ALA:HA   | 2.37                     | 0.45              |
| 1:K:48:MET:CE    | 1:K:66:VAL:HG22  | 2.31                     | 0.45              |
| 1:B:261:PHE:HE1  | 1:H:455:MET:HE2  | 1.81                     | 0.45              |
| 1:C:48:MET:CE    | 1:C:66:VAL:HG22  | 2.31                     | 0.45              |
| 1:E:286:LYS:HE2  | 1:E:292:GLU:HB3  | 1.98                     | 0.45              |
| 1:G:337:ARG:HD3  | 1:G:393:ASP:OD2  | 2.15                     | 0.45              |
| 1:J:33:ILE:HD11  | 1:K:208:ALA:HB2  | 1.98                     | 0.45              |
| 1:L:195:MET:O    | 1:L:199:MET:HG3  | 2.17                     | 0.45              |
| 1:L:339:ARG:HD3  | 1:L:339:ARG:HA   | 1.71                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:261:PHE:HE1  | 1:G:455:MET:HE2  | 1.82                     | 0.45              |
| 1:A:403:GLU:C    | 1:A:405:LYS:H    | 2.23                     | 0.45              |
| 1:F:124:VAL:HG13 | 1:F:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:H:311:LEU:HD22 | 1:H:369:LEU:HB3  | 1.97                     | 0.45              |
| 5:I:1491:MPD:H4  | 1:J:189:GLN:OE1  | 2.17                     | 0.45              |
| 1:J:400:PRO:HB3  | 1:J:401:PRO:HD2  | 1.98                     | 0.45              |
| 1:K:403:GLU:C    | 1:K:405:LYS:H    | 2.23                     | 0.45              |
| 1:L:432:GLY:HA2  | 6:L:1452:HOH:O   | 2.17                     | 0.45              |
| 1:A:195:MET:O    | 1:A:199:MET:HG3  | 2.17                     | 0.45              |
| 1:H:403:GLU:C    | 1:H:405:LYS:H    | 2.24                     | 0.45              |
| 1:K:395:ASN:HD22 | 1:K:395:ASN:HA   | 1.53                     | 0.45              |
| 1:A:289:GLY:O    | 1:A:354:ARG:HD2  | 2.17                     | 0.45              |
| 1:D:48:MET:CE    | 1:D:66:VAL:HG22  | 2.31                     | 0.45              |
| 1:D:195:MET:O    | 1:D:199:MET:HG3  | 2.17                     | 0.45              |
| 1:D:289:GLY:O    | 1:D:354:ARG:HD2  | 2.17                     | 0.45              |
| 1:D:337:ARG:HD3  | 1:D:393:ASP:OD2  | 2.15                     | 0.45              |
| 1:G:93:GLU:HB3   | 1:G:96:THR:HG23  | 1.98                     | 0.45              |
| 1:H:337:ARG:HD3  | 1:H:393:ASP:OD2  | 2.15                     | 0.45              |
| 1:H:395:ASN:HD22 | 1:H:395:ASN:HA   | 1.53                     | 0.45              |
| 1:I:195:MET:O    | 1:I:199:MET:HG3  | 2.17                     | 0.45              |
| 1:I:432:GLY:HA2  | 6:I:1606:HOH:O   | 2.17                     | 0.45              |
| 1:L:50:ASP:CG    | 6:L:838:HOH:O    | 2.60                     | 0.45              |
| 1:A:206:VAL:O    | 1:B:34:PRO:HG2   | 2.17                     | 0.45              |
| 1:B:84:THR:CG2   | 5:B:1484:MPD:C5  | 2.95                     | 0.45              |
| 1:B:124:VAL:HG13 | 1:B:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:C:193:SER:CB   | 5:D:1486:MPD:C3  | 2.90                     | 0.45              |
| 1:D:272:MET:O    | 1:D:355:ARG:HB2  | 2.17                     | 0.45              |
| 1:D:296:TYR:CE2  | 1:D:385:LYS:HD3  | 2.51                     | 0.45              |
| 1:D:339:ARG:HD3  | 1:D:339:ARG:HA   | 1.71                     | 0.45              |
| 1:G:289:GLY:O    | 1:G:354:ARG:HD2  | 2.17                     | 0.45              |
| 1:H:124:VAL:HG13 | 1:H:274:LEU:HD21 | 1.98                     | 0.45              |
| 1:H:272:MET:O    | 1:H:355:ARG:HB2  | 2.17                     | 0.45              |
| 1:J:33:ILE:CD1   | 1:K:208:ALA:HB2  | 2.47                     | 0.45              |
| 1:J:289:GLY:O    | 1:J:354:ARG:HD2  | 2.17                     | 0.45              |
| 1:J:432:GLY:HA2  | 6:J:1605:HOH:O   | 2.17                     | 0.45              |
| 1:K:272:MET:O    | 1:K:355:ARG:HB2  | 2.17                     | 0.45              |
| 1:B:432:GLY:HA2  | 6:B:1597:HOH:O   | 2.17                     | 0.45              |
| 1:C:93:GLU:HB3   | 1:C:96:THR:HG23  | 1.98                     | 0.45              |
| 1:E:289:GLY:O    | 1:E:354:ARG:HD2  | 2.17                     | 0.45              |
| 1:F:254:THR:HB   | 1:L:466:TYR:CE1  | 2.52                     | 0.45              |
| 1:F:432:GLY:HA2  | 6:F:1604:HOH:O   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:432:GLY:HA2  | 6:A:1590:HOH:O   | 2.17                     | 0.45              |
| 1:B:93:GLU:HB3   | 1:B:96:THR:HG23  | 1.98                     | 0.45              |
| 1:B:289:GLY:O    | 1:B:354:ARG:HD2  | 2.17                     | 0.45              |
| 1:D:400:PRO:HB3  | 1:D:401:PRO:HD2  | 1.97                     | 0.45              |
| 1:F:177:GLY:C    | 1:F:179:TYR:H    | 2.25                     | 0.45              |
| 1:G:190:ASP:N    | 5:L:1494:MPD:HM1 | 2.32                     | 0.45              |
| 1:G:296:TYR:CE2  | 1:G:385:LYS:HD3  | 2.51                     | 0.45              |
| 1:H:339:ARG:HD3  | 6:H:1602:HOH:O   | 2.17                     | 0.45              |
| 1:H:400:PRO:HB3  | 1:H:401:PRO:HD2  | 1.97                     | 0.45              |
| 1:I:84:THR:CG2   | 5:I:1491:MPD:C5  | 2.95                     | 0.45              |
| 1:I:403:GLU:C    | 1:I:405:LYS:H    | 2.24                     | 0.45              |
| 1:J:396:LEU:H    | 1:J:396:LEU:HG   | 1.54                     | 0.45              |
| 1:K:289:GLY:O    | 1:K:354:ARG:HD2  | 2.17                     | 0.45              |
| 1:L:93:GLU:HB3   | 1:L:96:THR:HG23  | 1.98                     | 0.45              |
| 1:D:28:GLU:OE1   | 1:D:88:ARG:NH1   | 2.48                     | 0.44              |
| 1:E:84:THR:CG2   | 5:E:1487:MPD:C5  | 2.95                     | 0.44              |
| 1:E:337:ARG:HD3  | 1:E:393:ASP:OD2  | 2.16                     | 0.44              |
| 1:F:195:MET:O    | 1:F:199:MET:HG3  | 2.17                     | 0.44              |
| 1:G:177:GLY:C    | 1:G:179:TYR:H    | 2.25                     | 0.44              |
| 1:G:339:ARG:HD3  | 6:G:1602:HOH:O   | 2.17                     | 0.44              |
| 1:H:34:PRO:HG2   | 1:I:206:VAL:O    | 2.17                     | 0.44              |
| 1:D:84:THR:CG2   | 5:D:1486:MPD:C5  | 2.95                     | 0.44              |
| 1:E:339:ARG:HD3  | 6:E:1597:HOH:O   | 2.17                     | 0.44              |
| 1:F:48:MET:CE    | 1:F:66:VAL:HG22  | 2.31                     | 0.44              |
| 1:G:84:THR:CG2   | 5:G:1489:MPD:C5  | 2.95                     | 0.44              |
| 1:H:93:GLU:HB3   | 1:H:96:THR:HG23  | 1.98                     | 0.44              |
| 1:I:289:GLY:O    | 1:I:354:ARG:HD2  | 2.17                     | 0.44              |
| 1:I:405:LYS:HA   | 1:I:405:LYS:HD2  | 1.84                     | 0.44              |
| 1:K:28:GLU:OE1   | 1:K:88:ARG:NH1   | 2.48                     | 0.44              |
| 1:K:286:LYS:HE2  | 1:K:292:GLU:HB3  | 1.98                     | 0.44              |
| 1:L:124:VAL:HG13 | 1:L:274:LEU:HD21 | 1.98                     | 0.44              |
| 1:A:114:TYR:CD2  | 1:A:431:GLY:HA3  | 2.53                     | 0.44              |
| 1:A:140:PHE:CE1  | 1:F:160:SER:HB2  | 2.53                     | 0.44              |
| 1:A:458:HIS:HE1  | 1:G:456:THR:O    | 2.00                     | 0.44              |
| 1:B:195:MET:O    | 1:B:199:MET:HG3  | 2.17                     | 0.44              |
| 1:B:286:LYS:HE2  | 1:B:292:GLU:HB3  | 1.98                     | 0.44              |
| 1:E:272:MET:O    | 1:E:355:ARG:HB2  | 2.17                     | 0.44              |
| 1:E:458:HIS:HE1  | 1:K:456:THR:O    | 2.00                     | 0.44              |
| 1:F:114:TYR:CD2  | 1:F:431:GLY:HA3  | 2.53                     | 0.44              |
| 1:H:432:GLY:HA2  | 6:H:1604:HOH:O   | 2.17                     | 0.44              |
| 1:B:4:HIS:O      | 1:B:7:THR:HB     | 2.18                     | 0.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:54:ILE:HG22  | 1:B:55:GLY:N    | 2.33                     | 0.44              |
| 1:B:114:TYR:CD2  | 1:B:431:GLY:HA3 | 2.53                     | 0.44              |
| 1:B:230:LYS:O    | 1:B:233:ASP:HB2 | 2.18                     | 0.44              |
| 1:C:177:GLY:C    | 1:C:179:TYR:H   | 2.25                     | 0.44              |
| 1:C:432:GLY:HA2  | 6:C:1597:HOH:O  | 2.17                     | 0.44              |
| 1:E:360:PHE:CG   | 1:E:361:PRO:HD3 | 2.42                     | 0.44              |
| 1:F:272:MET:O    | 1:F:355:ARG:HB2 | 2.17                     | 0.44              |
| 1:G:272:MET:O    | 1:G:355:ARG:HB2 | 2.17                     | 0.44              |
| 1:G:405:LYS:HD2  | 1:G:405:LYS:HA  | 1.84                     | 0.44              |
| 1:H:54:ILE:HG22  | 1:H:55:GLY:N    | 2.33                     | 0.44              |
| 1:L:54:ILE:HG22  | 1:L:55:GLY:N    | 2.33                     | 0.44              |
| 1:A:84:THR:CG2   | 5:A:1483:MPD:C5 | 2.95                     | 0.44              |
| 1:B:28:GLU:OE1   | 1:B:88:ARG:NH1  | 2.48                     | 0.44              |
| 1:B:272:MET:O    | 1:B:355:ARG:HB2 | 2.17                     | 0.44              |
| 1:B:454:ARG:O    | 1:H:320:LYS:HG2 | 2.17                     | 0.44              |
| 1:E:54:ILE:HG22  | 1:E:55:GLY:N    | 2.33                     | 0.44              |
| 1:F:84:THR:CG2   | 5:F:1488:MPD:C5 | 2.95                     | 0.44              |
| 1:H:289:GLY:O    | 1:H:354:ARG:HD2 | 2.17                     | 0.44              |
| 1:J:4:HIS:O      | 1:J:7:THR:HB    | 2.18                     | 0.44              |
| 1:J:114:TYR:CD2  | 1:J:431:GLY:HA3 | 2.53                     | 0.44              |
| 5:J:1492:MPD:HM1 | 1:K:190:ASP:N   | 2.33                     | 0.44              |
| 1:K:195:MET:O    | 1:K:199:MET:HG3 | 2.17                     | 0.44              |
| 1:L:400:PRO:CB   | 1:L:401:PRO:CD  | 2.96                     | 0.44              |
| 1:A:28:GLU:OE1   | 1:A:88:ARG:NH1  | 2.48                     | 0.44              |
| 1:A:272:MET:O    | 1:A:355:ARG:HB2 | 2.17                     | 0.44              |
| 1:C:400:PRO:CB   | 1:C:401:PRO:CD  | 2.96                     | 0.44              |
| 1:F:54:ILE:HG22  | 1:F:55:GLY:N    | 2.33                     | 0.44              |
| 1:G:28:GLU:OE1   | 1:G:88:ARG:NH1  | 2.48                     | 0.44              |
| 5:G:1489:MPD:CM  | 1:H:190:ASP:OD2 | 2.64                     | 0.44              |
| 1:H:360:PHE:CG   | 1:H:361:PRO:HD3 | 2.43                     | 0.44              |
| 1:J:54:ILE:HG22  | 1:J:55:GLY:N    | 2.33                     | 0.44              |
| 1:J:84:THR:CG2   | 5:J:1492:MPD:C5 | 2.95                     | 0.44              |
| 1:J:403:GLU:C    | 1:J:405:LYS:H   | 2.23                     | 0.44              |
| 1:K:54:ILE:HG22  | 1:K:55:GLY:N    | 2.33                     | 0.44              |
| 1:K:177:GLY:C    | 1:K:179:TYR:H   | 2.25                     | 0.44              |
| 1:L:68:MET:HA    | 1:L:69:PRO:HD2  | 1.89                     | 0.44              |
| 1:L:114:TYR:CD2  | 1:L:431:GLY:HA3 | 2.53                     | 0.44              |
| 1:B:400:PRO:CB   | 1:B:401:PRO:CD  | 2.96                     | 0.44              |
| 1:B:400:PRO:HB3  | 1:B:401:PRO:HD2 | 1.97                     | 0.44              |
| 1:C:54:ILE:HG22  | 1:C:55:GLY:N    | 2.33                     | 0.44              |
| 1:C:114:TYR:CD2  | 1:C:431:GLY:HA3 | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:195:MET:O    | 1:C:199:MET:HG3  | 2.17                     | 0.44              |
| 1:D:4:HIS:O      | 1:D:7:THR:HB     | 2.18                     | 0.44              |
| 1:D:81:ALA:H     | 5:D:1486:MPD:H13 | 1.79                     | 0.44              |
| 1:D:339:ARG:HD3  | 6:D:1600:HOH:O   | 2.17                     | 0.44              |
| 1:F:230:LYS:O    | 1:F:233:ASP:HB2  | 2.18                     | 0.44              |
| 1:G:195:MET:O    | 1:G:199:MET:HG3  | 2.17                     | 0.44              |
| 1:G:230:LYS:O    | 1:G:233:ASP:HB2  | 2.18                     | 0.44              |
| 1:J:93:GLU:HB3   | 1:J:96:THR:HG23  | 1.98                     | 0.44              |
| 1:J:195:MET:O    | 1:J:199:MET:HG3  | 2.17                     | 0.44              |
| 1:K:230:LYS:O    | 1:K:233:ASP:HB2  | 2.18                     | 0.44              |
| 1:K:339:ARG:HD3  | 6:K:1607:HOH:O   | 2.17                     | 0.44              |
| 1:L:84:THR:CG2   | 5:L:1494:MPD:C5  | 2.95                     | 0.44              |
| 1:L:177:GLY:C    | 1:L:179:TYR:H    | 2.25                     | 0.44              |
| 1:D:114:TYR:CD2  | 1:D:431:GLY:HA3  | 2.53                     | 0.44              |
| 1:E:195:MET:O    | 1:E:199:MET:HG3  | 2.17                     | 0.44              |
| 1:G:114:TYR:CD2  | 1:G:431:GLY:HA3  | 2.53                     | 0.44              |
| 1:H:224:ARG:HG2  | 1:H:224:ARG:NH2  | 2.15                     | 0.44              |
| 1:I:400:PRO:CB   | 1:I:401:PRO:CD   | 2.96                     | 0.44              |
| 1:J:400:PRO:CB   | 1:J:401:PRO:CD   | 2.96                     | 0.44              |
| 1:L:289:GLY:O    | 1:L:354:ARG:HD2  | 2.17                     | 0.44              |
| 1:L:339:ARG:HD3  | 6:L:1450:HOH:O   | 2.17                     | 0.44              |
| 1:A:4:HIS:O      | 1:A:7:THR:HB     | 2.18                     | 0.44              |
| 1:B:339:ARG:HD3  | 6:B:1595:HOH:O   | 2.17                     | 0.44              |
| 1:D:177:GLY:C    | 1:D:179:TYR:H    | 2.25                     | 0.44              |
| 1:D:230:LYS:O    | 1:D:233:ASP:HB2  | 2.18                     | 0.44              |
| 1:E:93:GLU:HB3   | 1:E:96:THR:HG23  | 1.98                     | 0.44              |
| 1:E:114:TYR:CD2  | 1:E:431:GLY:HA3  | 2.53                     | 0.44              |
| 1:F:4:HIS:O      | 1:F:7:THR:HB     | 2.18                     | 0.44              |
| 1:F:60:ILE:HD13  | 1:F:60:ILE:HA    | 1.62                     | 0.44              |
| 1:F:289:GLY:O    | 1:F:354:ARG:HD2  | 2.17                     | 0.44              |
| 1:F:320:LYS:HG2  | 1:L:454:ARG:O    | 2.17                     | 0.44              |
| 1:F:339:ARG:HD3  | 6:F:1602:HOH:O   | 2.17                     | 0.44              |
| 1:G:432:GLY:HA2  | 6:G:1604:HOH:O   | 2.17                     | 0.44              |
| 1:H:195:MET:O    | 1:H:199:MET:HG3  | 2.17                     | 0.44              |
| 1:I:51:GLY:O     | 1:I:54:ILE:N     | 2.51                     | 0.44              |
| 1:I:80:PHE:CE2   | 1:J:189:GLN:HG2  | 2.53                     | 0.44              |
| 1:I:230:LYS:O    | 1:I:233:ASP:HB2  | 2.18                     | 0.44              |
| 1:I:272:MET:O    | 1:I:355:ARG:HB2  | 2.17                     | 0.44              |
| 1:I:337:ARG:HG2  | 1:I:338:ASN:N    | 2.33                     | 0.44              |
| 1:J:124:VAL:HG13 | 1:J:274:LEU:HD21 | 1.98                     | 0.44              |
| 1:K:84:THR:CG2   | 5:K:1493:MPD:C5  | 2.95                     | 0.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:4:HIS:O      | 1:C:7:THR:HB    | 2.18                     | 0.43              |
| 1:C:84:THR:CG2   | 5:C:1485:MPD:C5 | 2.95                     | 0.43              |
| 1:D:54:ILE:HG22  | 1:D:55:GLY:N    | 2.33                     | 0.43              |
| 1:E:432:GLY:HA2  | 6:E:1599:HOH:O  | 2.17                     | 0.43              |
| 1:E:463:GLU:HA   | 1:K:140:PHE:CE1 | 2.53                     | 0.43              |
| 1:F:93:GLU:HB3   | 1:F:96:THR:HG23 | 1.98                     | 0.43              |
| 1:G:4:HIS:O      | 1:G:7:THR:HB    | 2.18                     | 0.43              |
| 1:H:252:THR:OG1  | 1:I:169:LYS:O   | 2.26                     | 0.43              |
| 1:I:54:ILE:HG22  | 1:I:55:GLY:N    | 2.33                     | 0.43              |
| 1:K:432:GLY:HA2  | 6:K:1609:HOH:O  | 2.17                     | 0.43              |
| 1:L:4:HIS:O      | 1:L:7:THR:HB    | 2.18                     | 0.43              |
| 1:L:51:GLY:O     | 1:L:54:ILE:N    | 2.51                     | 0.43              |
| 1:L:272:MET:O    | 1:L:355:ARG:HB2 | 2.17                     | 0.43              |
| 1:L:337:ARG:HG2  | 1:L:338:ASN:N   | 2.33                     | 0.43              |
| 1:A:400:PRO:CB   | 1:A:401:PRO:CD  | 2.96                     | 0.43              |
| 1:B:395:ASN:HD22 | 1:B:395:ASN:HA  | 1.53                     | 0.43              |
| 1:C:289:GLY:O    | 1:C:354:ARG:HD2 | 2.17                     | 0.43              |
| 1:D:337:ARG:HG2  | 1:D:338:ASN:N   | 2.33                     | 0.43              |
| 1:D:403:GLU:C    | 1:D:405:LYS:H   | 2.23                     | 0.43              |
| 1:H:84:THR:CG2   | 5:H:1490:MPD:C5 | 2.95                     | 0.43              |
| 1:I:339:ARG:HD3  | 6:I:1604:HOH:O  | 2.17                     | 0.43              |
| 1:J:272:MET:O    | 1:J:355:ARG:HB2 | 2.17                     | 0.43              |
| 1:A:230:LYS:O    | 1:A:233:ASP:HB2 | 2.18                     | 0.43              |
| 1:A:384:ASN:N    | 1:A:384:ASN:ND2 | 2.66                     | 0.43              |
| 1:C:254:THR:HB   | 1:I:466:TYR:CE1 | 2.54                     | 0.43              |
| 1:C:320:LYS:HG2  | 1:I:454:ARG:O   | 2.18                     | 0.43              |
| 1:C:339:ARG:HD3  | 6:C:1595:HOH:O  | 2.17                     | 0.43              |
| 1:E:177:GLY:C    | 1:E:179:TYR:H   | 2.25                     | 0.43              |
| 1:F:337:ARG:HG2  | 1:F:338:ASN:N   | 2.33                     | 0.43              |
| 1:I:4:HIS:O      | 1:I:7:THR:HB    | 2.18                     | 0.43              |
| 1:J:339:ARG:HD3  | 6:J:1603:HOH:O  | 2.17                     | 0.43              |
| 1:L:230:LYS:O    | 1:L:233:ASP:HB2 | 2.18                     | 0.43              |
| 1:C:189:GLN:OE1  | 5:D:1486:MPD:H4 | 2.18                     | 0.43              |
| 1:C:210:HIS:HB3  | 1:D:31:VAL:HG23 | 2.01                     | 0.43              |
| 1:D:33:ILE:HA    | 1:D:34:PRO:HD3  | 1.92                     | 0.43              |
| 1:G:445:LEU:O    | 1:G:448:GLU:HG2 | 2.19                     | 0.43              |
| 1:H:28:GLU:OE1   | 1:H:88:ARG:NH1  | 2.48                     | 0.43              |
| 1:J:33:ILE:HG13  | 1:K:207:GLU:O   | 2.19                     | 0.43              |
| 1:K:400:PRO:CB   | 1:K:401:PRO:CD  | 2.96                     | 0.43              |
| 1:L:403:GLU:C    | 1:L:405:LYS:H   | 2.24                     | 0.43              |
| 1:A:445:LEU:O    | 1:A:448:GLU:HG2 | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:272:MET:O    | 1:C:355:ARG:HB2  | 2.17                     | 0.43              |
| 1:E:4:HIS:O      | 1:E:7:THR:HB     | 2.18                     | 0.43              |
| 1:E:230:LYS:O    | 1:E:233:ASP:HB2  | 2.18                     | 0.43              |
| 1:F:455:MET:HE2  | 1:L:261:PHE:HE1  | 1.83                     | 0.43              |
| 1:G:337:ARG:HG2  | 1:G:338:ASN:N    | 2.33                     | 0.43              |
| 1:G:400:PRO:CB   | 1:G:401:PRO:CD   | 2.96                     | 0.43              |
| 1:H:4:HIS:O      | 1:H:7:THR:HB     | 2.18                     | 0.43              |
| 1:J:81:ALA:H     | 5:J:1492:MPD:H13 | 1.79                     | 0.43              |
| 1:B:1:SER:O      | 1:B:2:ALA:C      | 2.62                     | 0.43              |
| 1:G:54:ILE:HG22  | 1:G:55:GLY:N     | 2.33                     | 0.43              |
| 1:H:114:TYR:CD2  | 1:H:431:GLY:HA3  | 2.53                     | 0.43              |
| 1:H:177:GLY:C    | 1:H:179:TYR:H    | 2.25                     | 0.43              |
| 1:H:400:PRO:CB   | 1:H:401:PRO:CD   | 2.96                     | 0.43              |
| 1:J:28:GLU:OE1   | 1:J:88:ARG:NH1   | 2.48                     | 0.43              |
| 1:J:230:LYS:O    | 1:J:233:ASP:HB2  | 2.18                     | 0.43              |
| 1:J:360:PHE:CG   | 1:J:361:PRO:HD3  | 2.43                     | 0.43              |
| 1:K:81:ALA:H     | 5:K:1493:MPD:H13 | 1.79                     | 0.43              |
| 1:L:48:MET:CE    | 1:L:66:VAL:HG22  | 2.31                     | 0.43              |
| 1:A:54:ILE:HG22  | 1:A:55:GLY:N     | 2.33                     | 0.43              |
| 1:A:193:SER:HB2  | 5:B:1484:MPD:C3  | 2.43                     | 0.43              |
| 1:B:337:ARG:HG2  | 1:B:338:ASN:N    | 2.33                     | 0.43              |
| 1:B:339:ARG:HD3  | 1:B:339:ARG:HA   | 1.71                     | 0.43              |
| 1:C:360:PHE:CG   | 1:C:361:PRO:HD3  | 2.43                     | 0.43              |
| 1:D:180:PHE:O    | 1:D:181:PRO:C    | 2.61                     | 0.43              |
| 1:D:445:LEU:O    | 1:D:448:GLU:HG2  | 2.19                     | 0.43              |
| 1:E:337:ARG:HG2  | 1:E:338:ASN:N    | 2.33                     | 0.43              |
| 1:F:445:LEU:O    | 1:F:448:GLU:HG2  | 2.19                     | 0.43              |
| 1:H:230:LYS:O    | 1:H:233:ASP:HB2  | 2.18                     | 0.43              |
| 1:H:401:PRO:CB   | 1:H:404:ALA:HA   | 2.37                     | 0.43              |
| 5:I:1491:MPD:HM2 | 1:J:189:GLN:HG3  | 2.00                     | 0.43              |
| 1:A:177:GLY:C    | 1:A:179:TYR:H    | 2.25                     | 0.43              |
| 1:A:208:ALA:HB2  | 1:B:33:ILE:HD11  | 2.01                     | 0.43              |
| 1:B:445:LEU:O    | 1:B:448:GLU:HG2  | 2.19                     | 0.43              |
| 1:C:384:ASN:N    | 1:C:384:ASN:ND2  | 2.66                     | 0.43              |
| 1:E:189:GLN:HG3  | 5:F:1488:MPD:HM2 | 2.00                     | 0.43              |
| 1:E:384:ASN:N    | 1:E:384:ASN:ND2  | 2.66                     | 0.43              |
| 1:F:400:PRO:CB   | 1:F:401:PRO:CD   | 2.96                     | 0.43              |
| 1:I:445:LEU:O    | 1:I:448:GLU:HG2  | 2.19                     | 0.43              |
| 1:K:314:PRO:HG3  | 1:K:365:ALA:HA   | 2.01                     | 0.43              |
| 1:L:445:LEU:O    | 1:L:448:GLU:HG2  | 2.19                     | 0.43              |
| 1:A:339:ARG:HD3  | 6:A:1588:HOH:O   | 2.17                     | 0.43              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:180:PHE:O   | 1:B:181:PRO:C   | 2.61                     | 0.43              |
| 1:D:400:PRO:CB  | 1:D:401:PRO:CD  | 2.96                     | 0.43              |
| 1:D:454:ARG:O   | 1:J:320:LYS:HG2 | 2.19                     | 0.43              |
| 1:E:396:LEU:O   | 1:E:399:LEU:CB  | 2.67                     | 0.43              |
| 1:E:400:PRO:CB  | 1:E:401:PRO:CD  | 2.96                     | 0.43              |
| 1:H:445:LEU:O   | 1:H:448:GLU:HG2 | 2.19                     | 0.43              |
| 1:I:114:TYR:CD2 | 1:I:431:GLY:HA3 | 2.53                     | 0.43              |
| 1:K:4:His:O     | 1:K:7:THR:HB    | 2.18                     | 0.43              |
| 1:K:114:TYR:CD2 | 1:K:431:GLY:HA3 | 2.53                     | 0.43              |
| 1:K:445:LEU:O   | 1:K:448:GLU:HG2 | 2.19                     | 0.43              |
| 1:A:208:ALA:HB2 | 1:B:33:ILE:CD1  | 2.49                     | 0.43              |
| 1:A:337:ARG:HG2 | 1:A:338:ASN:N   | 2.33                     | 0.43              |
| 5:A:1483:MPD:H4 | 1:F:189:GLN:OE1 | 2.19                     | 0.43              |
| 1:C:337:ARG:HG2 | 1:C:338:ASN:N   | 2.33                     | 0.43              |
| 1:E:28:GLU:OE1  | 1:E:88:ARG:NH1  | 2.48                     | 0.43              |
| 1:E:206:VAL:O   | 1:F:34:PRO:HG2  | 2.19                     | 0.43              |
| 1:E:339:ARG:HD3 | 1:E:339:ARG:HA  | 1.71                     | 0.43              |
| 1:G:339:ARG:HD3 | 1:G:339:ARG:HA  | 1.71                     | 0.43              |
| 1:H:1:SER:O     | 1:H:2:ALA:C     | 2.62                     | 0.43              |
| 1:H:33:ILE:HA   | 1:H:34:PRO:HD3  | 1.92                     | 0.43              |
| 1:A:426:GLU:HG2 | 6:A:1563:HOH:O  | 2.20                     | 0.42              |
| 1:B:396:LEU:O   | 1:B:399:LEU:CB  | 2.67                     | 0.42              |
| 1:C:445:LEU:O   | 1:C:448:GLU:HG2 | 2.19                     | 0.42              |
| 1:E:1:SER:O     | 1:E:2:ALA:C     | 2.62                     | 0.42              |
| 1:F:231:LYS:HD2 | 1:F:231:LYS:HA  | 1.82                     | 0.42              |
| 1:G:208:ALA:HB2 | 1:L:33:ILE:HD11 | 2.01                     | 0.42              |
| 1:G:314:PRO:HG3 | 1:G:365:ALA:HA  | 2.01                     | 0.42              |
| 1:H:314:PRO:HG3 | 1:H:365:ALA:HA  | 2.01                     | 0.42              |
| 1:J:405:LYS:HD2 | 1:J:405:LYS:HA  | 1.84                     | 0.42              |
| 1:K:337:ARG:HG2 | 1:K:338:ASN:N   | 2.34                     | 0.42              |
| 1:A:51:GLY:O    | 1:A:54:ILE:N    | 2.51                     | 0.42              |
| 1:E:254:THR:HB  | 1:K:466:TYR:CE1 | 2.54                     | 0.42              |
| 1:E:314:PRO:HG3 | 1:E:365:ALA:HA  | 2.01                     | 0.42              |
| 1:F:405:LYS:HA  | 1:F:405:LYS:HD2 | 1.85                     | 0.42              |
| 1:H:140:PHE:CE1 | 1:I:160:SER:HB2 | 2.54                     | 0.42              |
| 1:H:426:GLU:HG2 | 6:H:1577:HOH:O  | 2.20                     | 0.42              |
| 1:I:63:SER:CB   | 1:J:339:ARG:NH2 | 2.82                     | 0.42              |
| 1:B:314:PRO:HG3 | 1:B:365:ALA:HA  | 2.01                     | 0.42              |
| 1:K:180:PHE:O   | 1:K:181:PRO:C   | 2.61                     | 0.42              |
| 1:C:28:GLU:OE1  | 1:C:88:ARG:NH1  | 2.48                     | 0.42              |
| 1:E:68:MET:HA   | 1:E:69:PRO:HD2  | 1.89                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:397:TYR:OH  | 1:F:404:ALA:O    | 2.29                     | 0.42              |
| 1:G:180:PHE:O   | 1:G:181:PRO:C    | 2.61                     | 0.42              |
| 1:H:58:LYS:NZ   | 1:H:60:ILE:HD11  | 2.35                     | 0.42              |
| 1:J:314:PRO:HG3 | 1:J:365:ALA:HA   | 2.01                     | 0.42              |
| 1:A:405:LYS:HA  | 1:A:405:LYS:HD2  | 1.84                     | 0.42              |
| 1:C:33:ILE:HA   | 1:C:34:PRO:HD3   | 1.92                     | 0.42              |
| 1:C:81:ALA:H    | 5:C:1485:MPD:H13 | 1.79                     | 0.42              |
| 1:C:208:ALA:HB2 | 1:D:33:ILE:CD1   | 2.50                     | 0.42              |
| 1:F:1:SER:O     | 1:F:2:ALA:C      | 2.62                     | 0.42              |
| 1:F:28:GLU:OE1  | 1:F:88:ARG:NH1   | 2.48                     | 0.42              |
| 5:I:1491:MPD:CM | 1:J:190:ASP:OD2  | 2.63                     | 0.42              |
| 1:K:1:SER:O     | 1:K:2:ALA:C      | 2.62                     | 0.42              |
| 1:K:231:LYS:HD2 | 1:K:231:LYS:HA   | 1.82                     | 0.42              |
| 1:K:458:HIS:HD2 | 1:K:460:VAL:N    | 2.02                     | 0.42              |
| 1:C:396:LEU:O   | 1:C:399:LEU:CB   | 2.67                     | 0.42              |
| 1:D:426:GLU:HG2 | 6:D:1575:HOH:O   | 2.20                     | 0.42              |
| 1:E:383:LYS:C   | 1:E:384:ASN:HD22 | 2.28                     | 0.42              |
| 1:E:426:GLU:HG2 | 6:E:1572:HOH:O   | 2.19                     | 0.42              |
| 1:I:180:PHE:O   | 1:I:181:PRO:C    | 2.61                     | 0.42              |
| 1:K:397:TYR:OH  | 1:K:404:ALA:O    | 2.29                     | 0.42              |
| 1:B:383:LYS:C   | 1:B:384:ASN:HD22 | 2.28                     | 0.42              |
| 1:C:230:LYS:O   | 1:C:233:ASP:HB2  | 2.18                     | 0.42              |
| 1:D:320:LYS:HG2 | 1:J:454:ARG:O    | 2.18                     | 0.42              |
| 1:E:127:GLY:HA3 | 3:E:1475:ADP:H1' | 2.02                     | 0.42              |
| 1:F:396:LEU:O   | 1:F:399:LEU:CB   | 2.67                     | 0.42              |
| 1:A:401:PRO:CB  | 1:A:404:ALA:HA   | 2.37                     | 0.42              |
| 1:C:68:MET:HA   | 1:C:69:PRO:HD2   | 1.89                     | 0.42              |
| 1:H:337:ARG:HG2 | 1:H:338:ASN:N    | 2.33                     | 0.42              |
| 1:L:426:GLU:HG2 | 6:L:1421:HOH:O   | 2.20                     | 0.42              |
| 1:A:190:ASP:OD2 | 5:B:1484:MPD:CM  | 2.65                     | 0.42              |
| 1:A:383:LYS:C   | 1:A:384:ASN:HD22 | 2.28                     | 0.42              |
| 1:C:1:SER:O     | 1:C:2:ALA:C      | 2.62                     | 0.42              |
| 1:C:426:GLU:HG2 | 6:C:1571:HOH:O   | 2.20                     | 0.42              |
| 1:G:403:GLU:O   | 1:G:404:ALA:HB3  | 2.20                     | 0.42              |
| 1:H:180:PHE:O   | 1:H:181:PRO:C    | 2.61                     | 0.42              |
| 1:I:28:GLU:OE1  | 1:I:88:ARG:NH1   | 2.48                     | 0.42              |
| 1:J:339:ARG:HD3 | 1:J:339:ARG:HA   | 1.71                     | 0.42              |
| 1:J:445:LEU:O   | 1:J:448:GLU:HG2  | 2.19                     | 0.42              |
| 1:K:127:GLY:HA3 | 3:K:1481:ADP:H1' | 2.02                     | 0.42              |
| 1:A:31:VAL:HG23 | 1:F:210:HIS:HB3  | 2.02                     | 0.42              |
| 1:A:180:PHE:O   | 1:A:181:PRO:C    | 2.61                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:230:LYS:HE3 | 1:A:230:LYS:HB2  | 1.89                     | 0.42              |
| 1:B:127:GLY:HA3 | 3:B:1472:ADP:H1' | 2.02                     | 0.42              |
| 1:E:445:LEU:O   | 1:E:448:GLU:HG2  | 2.19                     | 0.42              |
| 1:F:426:GLU:HG2 | 6:F:1577:HOH:O   | 2.19                     | 0.42              |
| 1:G:383:LYS:C   | 1:G:384:ASN:HD22 | 2.28                     | 0.42              |
| 1:H:68:MET:HA   | 1:H:69:PRO:HD2   | 1.89                     | 0.42              |
| 1:H:80:PHE:CZ   | 1:I:189:GLN:HG2  | 2.55                     | 0.42              |
| 1:I:314:PRO:HG3 | 1:I:365:ALA:HA   | 2.01                     | 0.42              |
| 1:J:403:GLU:O   | 1:J:404:ALA:HB3  | 2.20                     | 0.42              |
| 1:K:426:GLU:HG2 | 6:K:1582:HOH:O   | 2.20                     | 0.42              |
| 1:L:405:LYS:HA  | 1:L:405:LYS:HD2  | 1.84                     | 0.42              |
| 1:A:1:SER:O     | 1:A:2:ALA:C      | 2.62                     | 0.41              |
| 1:A:82:ASP:O    | 1:A:84:THR:CG2   | 2.55                     | 0.41              |
| 1:A:314:PRO:HG3 | 1:A:365:ALA:HA   | 2.01                     | 0.41              |
| 1:B:81:ALA:H    | 5:B:1484:MPD:H13 | 1.79                     | 0.41              |
| 1:C:314:PRO:HG3 | 1:C:365:ALA:HA   | 2.01                     | 0.41              |
| 1:C:339:ARG:HD3 | 1:C:339:ARG:HA   | 1.71                     | 0.41              |
| 1:D:328:ALA:HA  | 1:D:329:PRO:HD2  | 1.93                     | 0.41              |
| 1:D:396:LEU:O   | 1:D:399:LEU:CB   | 2.67                     | 0.41              |
| 1:G:426:GLU:HG2 | 6:G:1577:HOH:O   | 2.19                     | 0.41              |
| 1:H:51:GLY:O    | 1:H:54:ILE:N     | 2.51                     | 0.41              |
| 1:H:127:GLY:HA3 | 3:H:1478:ADP:H1' | 2.02                     | 0.41              |
| 1:I:383:LYS:C   | 1:I:384:ASN:HD22 | 2.28                     | 0.41              |
| 5:J:1492:MPD:CM | 1:K:190:ASP:OD2  | 2.59                     | 0.41              |
| 1:K:58:LYS:NZ   | 1:K:60:ILE:HD11  | 2.35                     | 0.41              |
| 1:A:396:LEU:O   | 1:A:399:LEU:CB   | 2.67                     | 0.41              |
| 1:C:390:GLU:HA  | 1:C:391:PRO:HD3  | 1.95                     | 0.41              |
| 1:C:403:GLU:O   | 1:C:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:D:58:LYS:NZ   | 1:D:60:ILE:HD11  | 2.35                     | 0.41              |
| 1:E:50:ASP:CG   | 6:E:1493:HOH:O   | 2.63                     | 0.41              |
| 1:G:396:LEU:O   | 1:G:399:LEU:CB   | 2.67                     | 0.41              |
| 1:I:1:SER:O     | 1:I:2:ALA:C      | 2.62                     | 0.41              |
| 1:J:48:MET:CE   | 1:J:66:VAL:HG22  | 2.31                     | 0.41              |
| 1:J:51:GLY:O    | 1:J:54:ILE:N     | 2.51                     | 0.41              |
| 1:L:230:LYS:HE3 | 1:L:230:LYS:HB2  | 1.89                     | 0.41              |
| 1:L:383:LYS:C   | 1:L:384:ASN:HD22 | 2.28                     | 0.41              |
| 1:A:127:GLY:HA3 | 3:A:1471:ADP:H1' | 2.02                     | 0.41              |
| 1:B:189:GLN:HG3 | 5:C:1485:MPD:HM2 | 2.00                     | 0.41              |
| 1:C:383:LYS:C   | 1:C:384:ASN:HD22 | 2.28                     | 0.41              |
| 1:D:383:LYS:C   | 1:D:384:ASN:HD22 | 2.28                     | 0.41              |
| 1:F:340:SER:OG  | 1:F:396:LEU:CB   | 2.69                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:1:SER:O      | 1:G:2:ALA:C      | 2.62                     | 0.41              |
| 1:G:127:GLY:HA3  | 3:G:1477:ADP:H1' | 2.02                     | 0.41              |
| 1:J:80:PHE:CE2   | 1:K:189:GLN:HG2  | 2.55                     | 0.41              |
| 1:J:337:ARG:HG2  | 1:J:338:ASN:N    | 2.33                     | 0.41              |
| 1:J:383:LYS:C    | 1:J:384:ASN:HD22 | 2.28                     | 0.41              |
| 1:J:426:GLU:HG2  | 6:J:1578:HOH:O   | 2.20                     | 0.41              |
| 1:K:31:VAL:HG23  | 1:L:210:HIS:HB3  | 2.03                     | 0.41              |
| 1:L:328:ALA:HA   | 1:L:329:PRO:HD2  | 1.93                     | 0.41              |
| 1:F:339:ARG:HD3  | 1:F:339:ARG:HA   | 1.71                     | 0.41              |
| 1:G:340:SER:OG   | 1:G:396:LEU:CB   | 2.69                     | 0.41              |
| 1:H:231:LYS:HD2  | 1:H:231:LYS:HA   | 1.82                     | 0.41              |
| 1:I:81:ALA:H     | 5:I:1491:MPD:H13 | 1.79                     | 0.41              |
| 1:K:339:ARG:HD3  | 1:K:339:ARG:HA   | 1.71                     | 0.41              |
| 1:K:403:GLU:O    | 1:K:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:B:254:THR:HB   | 1:H:466:TYR:CE1  | 2.55                     | 0.41              |
| 1:B:426:GLU:HG2  | 6:B:1570:HOH:O   | 2.20                     | 0.41              |
| 1:C:398:ASP:C    | 1:C:400:PRO:N    | 2.78                     | 0.41              |
| 1:D:16:PHE:CG    | 5:D:1486:MPD:H52 | 2.55                     | 0.41              |
| 1:E:51:GLY:O     | 1:E:54:ILE:N     | 2.51                     | 0.41              |
| 1:F:180:PHE:O    | 1:F:181:PRO:C    | 2.61                     | 0.41              |
| 1:H:49:PHE:O     | 1:H:64:ASP:OD2   | 2.39                     | 0.41              |
| 5:H:1490:MPD:HM1 | 1:I:190:ASP:N    | 2.35                     | 0.41              |
| 1:J:340:SER:OG   | 1:J:396:LEU:CB   | 2.69                     | 0.41              |
| 1:K:405:LYS:HD2  | 1:K:405:LYS:HA   | 1.84                     | 0.41              |
| 1:L:1:SER:O      | 1:L:2:ALA:C      | 2.62                     | 0.41              |
| 1:L:49:PHE:O     | 1:L:64:ASP:OD2   | 2.39                     | 0.41              |
| 1:L:180:PHE:O    | 1:L:181:PRO:C    | 2.61                     | 0.41              |
| 1:A:1:SER:CA     | 1:A:71:ALA:CB    | 2.80                     | 0.41              |
| 1:A:16:PHE:CG    | 5:A:1483:MPD:H52 | 2.55                     | 0.41              |
| 1:A:49:PHE:O     | 1:A:64:ASP:OD2   | 2.39                     | 0.41              |
| 1:B:403:GLU:O    | 1:B:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:C:127:GLY:HA3  | 3:C:1473:ADP:H1' | 2.02                     | 0.41              |
| 1:D:314:PRO:HG3  | 1:D:365:ALA:HA   | 2.01                     | 0.41              |
| 1:H:383:LYS:C    | 1:H:384:ASN:HD22 | 2.28                     | 0.41              |
| 1:H:403:GLU:O    | 1:H:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:H:405:LYS:HA   | 1:H:405:LYS:HD2  | 1.85                     | 0.41              |
| 1:I:398:ASP:C    | 1:I:400:PRO:N    | 2.79                     | 0.41              |
| 1:J:396:LEU:O    | 1:J:399:LEU:CB   | 2.67                     | 0.41              |
| 1:B:51:GLY:O     | 1:B:54:ILE:N     | 2.51                     | 0.41              |
| 1:B:398:ASP:C    | 1:B:400:PRO:N    | 2.79                     | 0.41              |
| 1:C:49:PHE:O     | 1:C:64:ASP:OD2   | 2.39                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:58:LYS:HZ1   | 1:C:60:ILE:CD1   | 2.32                     | 0.41              |
| 1:C:82:ASP:O     | 1:C:84:THR:CG2   | 2.55                     | 0.41              |
| 1:C:340:SER:OG   | 1:C:396:LEU:CB   | 2.69                     | 0.41              |
| 1:F:284:GLY:HA3  | 1:F:291:SER:HA   | 2.03                     | 0.41              |
| 1:F:314:PRO:HG3  | 1:F:365:ALA:HA   | 2.01                     | 0.41              |
| 1:G:206:VAL:O    | 1:L:34:PRO:HG2   | 2.21                     | 0.41              |
| 1:I:396:LEU:H    | 1:I:396:LEU:HG   | 1.54                     | 0.41              |
| 1:J:1:SER:O      | 1:J:2:ALA:C      | 2.62                     | 0.41              |
| 1:J:49:PHE:O     | 1:J:64:ASP:OD2   | 2.39                     | 0.41              |
| 1:K:140:PHE:CE1  | 1:L:160:SER:HB2  | 2.56                     | 0.41              |
| 1:K:396:LEU:H    | 1:K:396:LEU:HG   | 1.54                     | 0.41              |
| 1:C:51:GLY:O     | 1:C:54:ILE:N     | 2.51                     | 0.41              |
| 1:C:396:LEU:H    | 1:C:396:LEU:HG   | 1.54                     | 0.41              |
| 1:C:466:TYR:CE1  | 1:I:254:THR:HB   | 2.56                     | 0.41              |
| 1:D:284:GLY:HA3  | 1:D:291:SER:HA   | 2.03                     | 0.41              |
| 1:E:81:ALA:H     | 5:E:1487:MPD:H13 | 1.79                     | 0.41              |
| 1:E:190:ASP:N    | 5:F:1488:MPD:HM1 | 2.36                     | 0.41              |
| 1:H:384:ASN:N    | 1:H:384:ASN:ND2  | 2.66                     | 0.41              |
| 1:I:426:GLU:HG2  | 6:I:1579:HOH:O   | 2.20                     | 0.41              |
| 1:L:314:PRO:HG3  | 1:L:365:ALA:HA   | 2.01                     | 0.41              |
| 1:L:398:ASP:C    | 1:L:400:PRO:N    | 2.79                     | 0.41              |
| 1:A:68:MET:HA    | 1:A:69:PRO:HD2   | 1.89                     | 0.41              |
| 1:A:281:LEU:HD23 | 1:A:293:GLN:OE1  | 2.21                     | 0.41              |
| 1:A:403:GLU:O    | 1:A:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:B:49:PHE:O     | 1:B:64:ASP:OD2   | 2.39                     | 0.41              |
| 1:B:58:LYS:NZ    | 1:B:60:ILE:HD11  | 2.35                     | 0.41              |
| 1:B:58:LYS:HZ2   | 1:B:60:ILE:HD13  | 1.85                     | 0.41              |
| 1:C:458:HIS:HD2  | 1:C:460:VAL:N    | 2.02                     | 0.41              |
| 1:D:1:SER:O      | 1:D:2:ALA:C      | 2.62                     | 0.41              |
| 1:D:49:PHE:O     | 1:D:64:ASP:OD2   | 2.39                     | 0.41              |
| 1:E:340:SER:OG   | 1:E:396:LEU:CB   | 2.69                     | 0.41              |
| 1:E:350:SER:HA   | 1:E:351:PRO:HD3  | 1.98                     | 0.41              |
| 1:F:51:GLY:O     | 1:F:54:ILE:N     | 2.51                     | 0.41              |
| 1:F:58:LYS:NZ    | 1:F:60:ILE:HD11  | 2.35                     | 0.41              |
| 1:F:383:LYS:C    | 1:F:384:ASN:HD22 | 2.28                     | 0.41              |
| 1:F:403:GLU:O    | 1:F:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:G:284:GLY:HA3  | 1:G:291:SER:HA   | 2.03                     | 0.41              |
| 1:H:48:MET:CE    | 1:H:66:VAL:HG22  | 2.31                     | 0.41              |
| 1:H:80:PHE:CE2   | 1:I:189:GLN:HG2  | 2.55                     | 0.41              |
| 1:H:281:LEU:HD23 | 1:H:293:GLN:OE1  | 2.21                     | 0.41              |
| 1:I:68:MET:HA    | 1:I:69:PRO:HD2   | 1.89                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:340:SER:OG   | 1:I:396:LEU:CB   | 2.69                     | 0.41              |
| 1:I:396:LEU:O    | 1:I:399:LEU:CB   | 2.67                     | 0.41              |
| 1:I:403:GLU:O    | 1:I:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:J:31:VAL:HG23  | 1:K:210:HIS:HB3  | 2.03                     | 0.41              |
| 1:K:128:PRO:HD2  | 6:K:1507:HOH:O   | 2.21                     | 0.41              |
| 1:L:127:GLY:HA3  | 3:L:1482:ADP:H1' | 2.02                     | 0.41              |
| 1:L:403:GLU:O    | 1:L:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:A:207:GLU:O    | 1:B:33:ILE:HG13  | 2.20                     | 0.41              |
| 1:B:340:SER:OG   | 1:B:396:LEU:CB   | 2.69                     | 0.41              |
| 1:C:281:LEU:HD23 | 1:C:293:GLN:OE1  | 2.21                     | 0.41              |
| 1:C:284:GLY:HA3  | 1:C:291:SER:HA   | 2.03                     | 0.41              |
| 1:D:127:GLY:HA3  | 3:D:1474:ADP:H1' | 2.02                     | 0.41              |
| 1:E:180:PHE:O    | 1:E:181:PRO:C    | 2.61                     | 0.41              |
| 1:E:403:GLU:O    | 1:E:404:ALA:HB3  | 2.20                     | 0.41              |
| 1:F:398:ASP:C    | 1:F:400:PRO:N    | 2.79                     | 0.41              |
| 1:G:281:LEU:HD23 | 1:G:293:GLN:OE1  | 2.21                     | 0.41              |
| 1:H:16:PHE:CG    | 5:H:1490:MPD:H52 | 2.55                     | 0.41              |
| 1:I:16:PHE:CG    | 5:I:1491:MPD:H52 | 2.55                     | 0.41              |
| 1:I:360:PHE:CG   | 1:I:361:PRO:HD3  | 2.43                     | 0.41              |
| 1:J:284:GLY:HA3  | 1:J:291:SER:HA   | 2.03                     | 0.41              |
| 1:L:284:GLY:HA3  | 1:L:291:SER:HA   | 2.03                     | 0.41              |
| 1:B:466:TYR:CE1  | 1:H:254:THR:HB   | 2.56                     | 0.40              |
| 1:E:398:ASP:C    | 1:E:400:PRO:N    | 2.79                     | 0.40              |
| 1:F:16:PHE:CG    | 5:F:1488:MPD:H52 | 2.55                     | 0.40              |
| 1:I:281:LEU:HD23 | 1:I:293:GLN:OE1  | 2.21                     | 0.40              |
| 1:J:33:ILE:HA    | 1:J:34:PRO:HD3   | 1.92                     | 0.40              |
| 1:J:231:LYS:HD2  | 1:J:231:LYS:HA   | 1.82                     | 0.40              |
| 1:K:33:ILE:HA    | 1:K:34:PRO:HD3   | 1.92                     | 0.40              |
| 1:K:51:GLY:O     | 1:K:54:ILE:N     | 2.51                     | 0.40              |
| 1:K:383:LYS:C    | 1:K:384:ASN:HD22 | 2.28                     | 0.40              |
| 1:K:396:LEU:O    | 1:K:399:LEU:CB   | 2.67                     | 0.40              |
| 1:K:398:ASP:C    | 1:K:400:PRO:N    | 2.78                     | 0.40              |
| 1:A:50:ASP:CG    | 6:A:1596:HOH:O   | 2.64                     | 0.40              |
| 1:A:128:PRO:HD2  | 6:A:1487:HOH:O   | 2.21                     | 0.40              |
| 1:B:16:PHE:CG    | 5:B:1484:MPD:H52 | 2.55                     | 0.40              |
| 1:B:189:GLN:HG2  | 1:C:80:PHE:CE2   | 2.57                     | 0.40              |
| 1:D:403:GLU:O    | 1:D:404:ALA:HB3  | 2.20                     | 0.40              |
| 1:E:49:PHE:O     | 1:E:64:ASP:OD2   | 2.39                     | 0.40              |
| 1:E:128:PRO:HD2  | 6:E:1497:HOH:O   | 2.21                     | 0.40              |
| 1:F:127:GLY:HA3  | 3:F:1476:ADP:H1' | 2.02                     | 0.40              |
| 1:F:384:ASN:N    | 1:F:384:ASN:ND2  | 2.66                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:340:SER:OG   | 1:H:396:LEU:CB   | 2.69                     | 0.40              |
| 1:H:398:ASP:C    | 1:H:400:PRO:N    | 2.79                     | 0.40              |
| 1:J:127:GLY:HA3  | 3:J:1480:ADP:H1' | 2.02                     | 0.40              |
| 1:L:340:SER:OG   | 1:L:396:LEU:CB   | 2.69                     | 0.40              |
| 1:B:204:LEU:HD23 | 1:B:223:THR:HG21 | 2.04                     | 0.40              |
| 1:D:82:ASP:O     | 1:D:84:THR:CG2   | 2.55                     | 0.40              |
| 1:G:189:GLN:HG2  | 1:L:80:PHE:CE2   | 2.57                     | 0.40              |
| 1:G:323:VAL:O    | 1:G:324:PRO:C    | 2.64                     | 0.40              |
| 1:H:339:ARG:HD3  | 1:H:339:ARG:HA   | 1.71                     | 0.40              |
| 1:H:396:LEU:O    | 1:H:399:LEU:CB   | 2.67                     | 0.40              |
| 1:I:230:LYS:HE3  | 1:I:230:LYS:HB2  | 1.89                     | 0.40              |
| 1:K:281:LEU:HD23 | 1:K:293:GLN:OE1  | 2.21                     | 0.40              |
| 1:A:284:GLY:HA3  | 1:A:291:SER:HA   | 2.03                     | 0.40              |
| 1:D:230:LYS:HE3  | 1:D:230:LYS:HB2  | 1.89                     | 0.40              |
| 1:D:281:LEU:HD23 | 1:D:293:GLN:OE1  | 2.21                     | 0.40              |
| 1:F:281:LEU:HD23 | 1:F:293:GLN:OE1  | 2.21                     | 0.40              |
| 1:J:281:LEU:HD23 | 1:J:293:GLN:OE1  | 2.21                     | 0.40              |
| 5:K:1493:MPD:H4  | 1:L:189:GLN:OE1  | 2.21                     | 0.40              |
| 1:A:180:PHE:CB   | 1:B:29:GLN:HB3   | 2.50                     | 0.40              |
| 1:B:384:ASN:N    | 1:B:384:ASN:ND2  | 2.66                     | 0.40              |
| 1:D:254:THR:HB   | 1:J:466:TYR:CE1  | 2.57                     | 0.40              |
| 1:G:58:LYS:NZ    | 1:G:60:ILE:HD11  | 2.35                     | 0.40              |
| 1:G:398:ASP:C    | 1:G:400:PRO:N    | 2.79                     | 0.40              |
| 1:H:284:GLY:HA3  | 1:H:291:SER:HA   | 2.03                     | 0.40              |
| 1:J:419:ASN:O    | 1:J:422:ASP:HB3  | 2.22                     | 0.40              |
| 1:K:49:PHE:O     | 1:K:64:ASP:OD2   | 2.39                     | 0.40              |
| 1:L:384:ASN:N    | 1:L:384:ASN:ND2  | 2.66                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | B     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | C     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | D     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | E     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | F     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | G     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | H     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | I     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | J     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | K     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| 1   | L     | 466/468 (100%)   | 429 (92%)  | 28 (6%)  | 9 (2%)   | 6           | 15 |
| All | All   | 5592/5616 (100%) | 5148 (92%) | 336 (6%) | 108 (2%) | 6           | 15 |

All (108) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 52  | SER  |
| 1   | A     | 62  | GLU  |
| 1   | A     | 180 | PHE  |
| 1   | A     | 399 | LEU  |
| 1   | A     | 400 | PRO  |
| 1   | A     | 401 | PRO  |
| 1   | B     | 52  | SER  |
| 1   | B     | 62  | GLU  |
| 1   | B     | 180 | PHE  |
| 1   | B     | 399 | LEU  |
| 1   | B     | 400 | PRO  |
| 1   | B     | 401 | PRO  |
| 1   | C     | 52  | SER  |
| 1   | C     | 62  | GLU  |
| 1   | C     | 180 | PHE  |
| 1   | C     | 399 | LEU  |
| 1   | C     | 400 | PRO  |
| 1   | C     | 401 | PRO  |
| 1   | D     | 52  | SER  |
| 1   | D     | 62  | GLU  |
| 1   | D     | 180 | PHE  |
| 1   | D     | 399 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 400 | PRO  |
| 1   | D     | 401 | PRO  |
| 1   | E     | 52  | SER  |
| 1   | E     | 62  | GLU  |
| 1   | E     | 180 | PHE  |
| 1   | E     | 399 | LEU  |
| 1   | E     | 400 | PRO  |
| 1   | E     | 401 | PRO  |
| 1   | F     | 52  | SER  |
| 1   | F     | 62  | GLU  |
| 1   | F     | 180 | PHE  |
| 1   | F     | 399 | LEU  |
| 1   | F     | 400 | PRO  |
| 1   | F     | 401 | PRO  |
| 1   | G     | 52  | SER  |
| 1   | G     | 62  | GLU  |
| 1   | G     | 180 | PHE  |
| 1   | G     | 399 | LEU  |
| 1   | G     | 400 | PRO  |
| 1   | G     | 401 | PRO  |
| 1   | H     | 52  | SER  |
| 1   | H     | 62  | GLU  |
| 1   | H     | 180 | PHE  |
| 1   | H     | 399 | LEU  |
| 1   | H     | 400 | PRO  |
| 1   | H     | 401 | PRO  |
| 1   | I     | 52  | SER  |
| 1   | I     | 62  | GLU  |
| 1   | I     | 180 | PHE  |
| 1   | I     | 399 | LEU  |
| 1   | I     | 400 | PRO  |
| 1   | I     | 401 | PRO  |
| 1   | J     | 52  | SER  |
| 1   | J     | 62  | GLU  |
| 1   | J     | 180 | PHE  |
| 1   | J     | 399 | LEU  |
| 1   | J     | 400 | PRO  |
| 1   | J     | 401 | PRO  |
| 1   | K     | 52  | SER  |
| 1   | K     | 62  | GLU  |
| 1   | K     | 180 | PHE  |
| 1   | K     | 399 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 400 | PRO  |
| 1   | K     | 401 | PRO  |
| 1   | L     | 52  | SER  |
| 1   | L     | 62  | GLU  |
| 1   | L     | 180 | PHE  |
| 1   | L     | 399 | LEU  |
| 1   | L     | 400 | PRO  |
| 1   | L     | 401 | PRO  |
| 1   | A     | 324 | PRO  |
| 1   | A     | 396 | LEU  |
| 1   | B     | 324 | PRO  |
| 1   | B     | 396 | LEU  |
| 1   | C     | 324 | PRO  |
| 1   | C     | 396 | LEU  |
| 1   | D     | 324 | PRO  |
| 1   | D     | 396 | LEU  |
| 1   | E     | 324 | PRO  |
| 1   | E     | 396 | LEU  |
| 1   | F     | 324 | PRO  |
| 1   | F     | 396 | LEU  |
| 1   | G     | 324 | PRO  |
| 1   | G     | 396 | LEU  |
| 1   | H     | 324 | PRO  |
| 1   | H     | 396 | LEU  |
| 1   | I     | 324 | PRO  |
| 1   | I     | 396 | LEU  |
| 1   | J     | 324 | PRO  |
| 1   | J     | 396 | LEU  |
| 1   | K     | 324 | PRO  |
| 1   | K     | 396 | LEU  |
| 1   | L     | 324 | PRO  |
| 1   | L     | 396 | LEU  |
| 1   | A     | 349 | ALA  |
| 1   | B     | 349 | ALA  |
| 1   | C     | 349 | ALA  |
| 1   | D     | 349 | ALA  |
| 1   | E     | 349 | ALA  |
| 1   | F     | 349 | ALA  |
| 1   | G     | 349 | ALA  |
| 1   | H     | 349 | ALA  |
| 1   | I     | 349 | ALA  |
| 1   | J     | 349 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 349 | ALA  |
| 1   | L     | 349 | ALA  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|------------------|------------|-----------|-------------|----|
| 1   | A     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | B     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | C     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | D     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | E     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | F     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | G     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | H     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | I     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | J     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | K     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| 1   | L     | 384/384 (100%)   | 339 (88%)  | 45 (12%)  | 5           | 12 |
| All | All   | 4608/4608 (100%) | 4068 (88%) | 540 (12%) | 5           | 12 |

All (540) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | SER  |
| 1   | A     | 6   | LEU  |
| 1   | A     | 15  | LYS  |
| 1   | A     | 19  | LEU  |
| 1   | A     | 33  | ILE  |
| 1   | A     | 49  | PHE  |
| 1   | A     | 50  | ASP  |
| 1   | A     | 60  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 62  | GLU  |
| 1   | A     | 63  | SER  |
| 1   | A     | 64  | ASP  |
| 1   | A     | 84  | THR  |
| 1   | A     | 96  | THR  |
| 1   | A     | 102 | ARG  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 124 | VAL  |
| 1   | A     | 125 | LEU  |
| 1   | A     | 147 | SER  |
| 1   | A     | 179 | TYR  |
| 1   | A     | 181 | PRO  |
| 1   | A     | 207 | GLU  |
| 1   | A     | 209 | HIS  |
| 1   | A     | 224 | ARG  |
| 1   | A     | 248 | ARG  |
| 1   | A     | 264 | ASN  |
| 1   | A     | 290 | LEU  |
| 1   | A     | 323 | VAL  |
| 1   | A     | 326 | TYR  |
| 1   | A     | 332 | LEU  |
| 1   | A     | 337 | ARG  |
| 1   | A     | 340 | SER  |
| 1   | A     | 344 | ARG  |
| 1   | A     | 355 | ARG  |
| 1   | A     | 374 | LEU  |
| 1   | A     | 375 | LEU  |
| 1   | A     | 384 | ASN  |
| 1   | A     | 395 | ASN  |
| 1   | A     | 396 | LEU  |
| 1   | A     | 403 | GLU  |
| 1   | A     | 419 | ASN  |
| 1   | A     | 428 | LEU  |
| 1   | A     | 447 | ARG  |
| 1   | A     | 459 | PRO  |
| 1   | A     | 464 | LEU  |
| 1   | A     | 468 | VAL  |
| 1   | B     | 1   | SER  |
| 1   | B     | 6   | LEU  |
| 1   | B     | 15  | LYS  |
| 1   | B     | 19  | LEU  |
| 1   | B     | 33  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 49  | PHE  |
| 1   | B     | 50  | ASP  |
| 1   | B     | 60  | ILE  |
| 1   | B     | 62  | GLU  |
| 1   | B     | 63  | SER  |
| 1   | B     | 64  | ASP  |
| 1   | B     | 84  | THR  |
| 1   | B     | 96  | THR  |
| 1   | B     | 102 | ARG  |
| 1   | B     | 115 | LEU  |
| 1   | B     | 124 | VAL  |
| 1   | B     | 125 | LEU  |
| 1   | B     | 147 | SER  |
| 1   | B     | 179 | TYR  |
| 1   | B     | 181 | PRO  |
| 1   | B     | 207 | GLU  |
| 1   | B     | 209 | HIS  |
| 1   | B     | 224 | ARG  |
| 1   | B     | 248 | ARG  |
| 1   | B     | 264 | ASN  |
| 1   | B     | 290 | LEU  |
| 1   | B     | 323 | VAL  |
| 1   | B     | 326 | TYR  |
| 1   | B     | 332 | LEU  |
| 1   | B     | 337 | ARG  |
| 1   | B     | 340 | SER  |
| 1   | B     | 344 | ARG  |
| 1   | B     | 355 | ARG  |
| 1   | B     | 374 | LEU  |
| 1   | B     | 375 | LEU  |
| 1   | B     | 384 | ASN  |
| 1   | B     | 395 | ASN  |
| 1   | B     | 396 | LEU  |
| 1   | B     | 403 | GLU  |
| 1   | B     | 419 | ASN  |
| 1   | B     | 428 | LEU  |
| 1   | B     | 447 | ARG  |
| 1   | B     | 459 | PRO  |
| 1   | B     | 464 | LEU  |
| 1   | B     | 468 | VAL  |
| 1   | C     | 1   | SER  |
| 1   | C     | 6   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 15  | LYS  |
| 1   | C     | 19  | LEU  |
| 1   | C     | 33  | ILE  |
| 1   | C     | 49  | PHE  |
| 1   | C     | 50  | ASP  |
| 1   | C     | 60  | ILE  |
| 1   | C     | 62  | GLU  |
| 1   | C     | 63  | SER  |
| 1   | C     | 64  | ASP  |
| 1   | C     | 84  | THR  |
| 1   | C     | 96  | THR  |
| 1   | C     | 102 | ARG  |
| 1   | C     | 115 | LEU  |
| 1   | C     | 124 | VAL  |
| 1   | C     | 125 | LEU  |
| 1   | C     | 147 | SER  |
| 1   | C     | 179 | TYR  |
| 1   | C     | 181 | PRO  |
| 1   | C     | 207 | GLU  |
| 1   | C     | 209 | HIS  |
| 1   | C     | 224 | ARG  |
| 1   | C     | 248 | ARG  |
| 1   | C     | 264 | ASN  |
| 1   | C     | 290 | LEU  |
| 1   | C     | 323 | VAL  |
| 1   | C     | 326 | TYR  |
| 1   | C     | 332 | LEU  |
| 1   | C     | 337 | ARG  |
| 1   | C     | 340 | SER  |
| 1   | C     | 344 | ARG  |
| 1   | C     | 355 | ARG  |
| 1   | C     | 374 | LEU  |
| 1   | C     | 375 | LEU  |
| 1   | C     | 384 | ASN  |
| 1   | C     | 395 | ASN  |
| 1   | C     | 396 | LEU  |
| 1   | C     | 403 | GLU  |
| 1   | C     | 419 | ASN  |
| 1   | C     | 428 | LEU  |
| 1   | C     | 447 | ARG  |
| 1   | C     | 459 | PRO  |
| 1   | C     | 464 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 468 | VAL  |
| 1   | D     | 1   | SER  |
| 1   | D     | 6   | LEU  |
| 1   | D     | 15  | LYS  |
| 1   | D     | 19  | LEU  |
| 1   | D     | 33  | ILE  |
| 1   | D     | 49  | PHE  |
| 1   | D     | 50  | ASP  |
| 1   | D     | 60  | ILE  |
| 1   | D     | 62  | GLU  |
| 1   | D     | 63  | SER  |
| 1   | D     | 64  | ASP  |
| 1   | D     | 84  | THR  |
| 1   | D     | 96  | THR  |
| 1   | D     | 102 | ARG  |
| 1   | D     | 115 | LEU  |
| 1   | D     | 124 | VAL  |
| 1   | D     | 125 | LEU  |
| 1   | D     | 147 | SER  |
| 1   | D     | 179 | TYR  |
| 1   | D     | 181 | PRO  |
| 1   | D     | 207 | GLU  |
| 1   | D     | 209 | HIS  |
| 1   | D     | 224 | ARG  |
| 1   | D     | 248 | ARG  |
| 1   | D     | 264 | ASN  |
| 1   | D     | 290 | LEU  |
| 1   | D     | 323 | VAL  |
| 1   | D     | 326 | TYR  |
| 1   | D     | 332 | LEU  |
| 1   | D     | 337 | ARG  |
| 1   | D     | 340 | SER  |
| 1   | D     | 344 | ARG  |
| 1   | D     | 355 | ARG  |
| 1   | D     | 374 | LEU  |
| 1   | D     | 375 | LEU  |
| 1   | D     | 384 | ASN  |
| 1   | D     | 395 | ASN  |
| 1   | D     | 396 | LEU  |
| 1   | D     | 403 | GLU  |
| 1   | D     | 419 | ASN  |
| 1   | D     | 428 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 447 | ARG  |
| 1   | D     | 459 | PRO  |
| 1   | D     | 464 | LEU  |
| 1   | D     | 468 | VAL  |
| 1   | E     | 1   | SER  |
| 1   | E     | 6   | LEU  |
| 1   | E     | 15  | LYS  |
| 1   | E     | 19  | LEU  |
| 1   | E     | 33  | ILE  |
| 1   | E     | 49  | PHE  |
| 1   | E     | 50  | ASP  |
| 1   | E     | 60  | ILE  |
| 1   | E     | 62  | GLU  |
| 1   | E     | 63  | SER  |
| 1   | E     | 64  | ASP  |
| 1   | E     | 84  | THR  |
| 1   | E     | 96  | THR  |
| 1   | E     | 102 | ARG  |
| 1   | E     | 115 | LEU  |
| 1   | E     | 124 | VAL  |
| 1   | E     | 125 | LEU  |
| 1   | E     | 147 | SER  |
| 1   | E     | 179 | TYR  |
| 1   | E     | 181 | PRO  |
| 1   | E     | 207 | GLU  |
| 1   | E     | 209 | HIS  |
| 1   | E     | 224 | ARG  |
| 1   | E     | 248 | ARG  |
| 1   | E     | 264 | ASN  |
| 1   | E     | 290 | LEU  |
| 1   | E     | 323 | VAL  |
| 1   | E     | 326 | TYR  |
| 1   | E     | 332 | LEU  |
| 1   | E     | 337 | ARG  |
| 1   | E     | 340 | SER  |
| 1   | E     | 344 | ARG  |
| 1   | E     | 355 | ARG  |
| 1   | E     | 374 | LEU  |
| 1   | E     | 375 | LEU  |
| 1   | E     | 384 | ASN  |
| 1   | E     | 395 | ASN  |
| 1   | E     | 396 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 403 | GLU  |
| 1   | E     | 419 | ASN  |
| 1   | E     | 428 | LEU  |
| 1   | E     | 447 | ARG  |
| 1   | E     | 459 | PRO  |
| 1   | E     | 464 | LEU  |
| 1   | E     | 468 | VAL  |
| 1   | F     | 1   | SER  |
| 1   | F     | 6   | LEU  |
| 1   | F     | 15  | LYS  |
| 1   | F     | 19  | LEU  |
| 1   | F     | 33  | ILE  |
| 1   | F     | 49  | PHE  |
| 1   | F     | 50  | ASP  |
| 1   | F     | 60  | ILE  |
| 1   | F     | 62  | GLU  |
| 1   | F     | 63  | SER  |
| 1   | F     | 64  | ASP  |
| 1   | F     | 84  | THR  |
| 1   | F     | 96  | THR  |
| 1   | F     | 102 | ARG  |
| 1   | F     | 115 | LEU  |
| 1   | F     | 124 | VAL  |
| 1   | F     | 125 | LEU  |
| 1   | F     | 147 | SER  |
| 1   | F     | 179 | TYR  |
| 1   | F     | 181 | PRO  |
| 1   | F     | 207 | GLU  |
| 1   | F     | 209 | HIS  |
| 1   | F     | 224 | ARG  |
| 1   | F     | 248 | ARG  |
| 1   | F     | 264 | ASN  |
| 1   | F     | 290 | LEU  |
| 1   | F     | 323 | VAL  |
| 1   | F     | 326 | TYR  |
| 1   | F     | 332 | LEU  |
| 1   | F     | 337 | ARG  |
| 1   | F     | 340 | SER  |
| 1   | F     | 344 | ARG  |
| 1   | F     | 355 | ARG  |
| 1   | F     | 374 | LEU  |
| 1   | F     | 375 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 384 | ASN  |
| 1   | F     | 395 | ASN  |
| 1   | F     | 396 | LEU  |
| 1   | F     | 403 | GLU  |
| 1   | F     | 419 | ASN  |
| 1   | F     | 428 | LEU  |
| 1   | F     | 447 | ARG  |
| 1   | F     | 459 | PRO  |
| 1   | F     | 464 | LEU  |
| 1   | F     | 468 | VAL  |
| 1   | G     | 1   | SER  |
| 1   | G     | 6   | LEU  |
| 1   | G     | 15  | LYS  |
| 1   | G     | 19  | LEU  |
| 1   | G     | 33  | ILE  |
| 1   | G     | 49  | PHE  |
| 1   | G     | 50  | ASP  |
| 1   | G     | 60  | ILE  |
| 1   | G     | 62  | GLU  |
| 1   | G     | 63  | SER  |
| 1   | G     | 64  | ASP  |
| 1   | G     | 84  | THR  |
| 1   | G     | 96  | THR  |
| 1   | G     | 102 | ARG  |
| 1   | G     | 115 | LEU  |
| 1   | G     | 124 | VAL  |
| 1   | G     | 125 | LEU  |
| 1   | G     | 147 | SER  |
| 1   | G     | 179 | TYR  |
| 1   | G     | 181 | PRO  |
| 1   | G     | 207 | GLU  |
| 1   | G     | 209 | HIS  |
| 1   | G     | 224 | ARG  |
| 1   | G     | 248 | ARG  |
| 1   | G     | 264 | ASN  |
| 1   | G     | 290 | LEU  |
| 1   | G     | 323 | VAL  |
| 1   | G     | 326 | TYR  |
| 1   | G     | 332 | LEU  |
| 1   | G     | 337 | ARG  |
| 1   | G     | 340 | SER  |
| 1   | G     | 344 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 355 | ARG  |
| 1   | G     | 374 | LEU  |
| 1   | G     | 375 | LEU  |
| 1   | G     | 384 | ASN  |
| 1   | G     | 395 | ASN  |
| 1   | G     | 396 | LEU  |
| 1   | G     | 403 | GLU  |
| 1   | G     | 419 | ASN  |
| 1   | G     | 428 | LEU  |
| 1   | G     | 447 | ARG  |
| 1   | G     | 459 | PRO  |
| 1   | G     | 464 | LEU  |
| 1   | G     | 468 | VAL  |
| 1   | H     | 1   | SER  |
| 1   | H     | 6   | LEU  |
| 1   | H     | 15  | LYS  |
| 1   | H     | 19  | LEU  |
| 1   | H     | 33  | ILE  |
| 1   | H     | 49  | PHE  |
| 1   | H     | 50  | ASP  |
| 1   | H     | 60  | ILE  |
| 1   | H     | 62  | GLU  |
| 1   | H     | 63  | SER  |
| 1   | H     | 64  | ASP  |
| 1   | H     | 84  | THR  |
| 1   | H     | 96  | THR  |
| 1   | H     | 102 | ARG  |
| 1   | H     | 115 | LEU  |
| 1   | H     | 124 | VAL  |
| 1   | H     | 125 | LEU  |
| 1   | H     | 147 | SER  |
| 1   | H     | 179 | TYR  |
| 1   | H     | 181 | PRO  |
| 1   | H     | 207 | GLU  |
| 1   | H     | 209 | HIS  |
| 1   | H     | 224 | ARG  |
| 1   | H     | 248 | ARG  |
| 1   | H     | 264 | ASN  |
| 1   | H     | 290 | LEU  |
| 1   | H     | 323 | VAL  |
| 1   | H     | 326 | TYR  |
| 1   | H     | 332 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 337 | ARG  |
| 1   | H     | 340 | SER  |
| 1   | H     | 344 | ARG  |
| 1   | H     | 355 | ARG  |
| 1   | H     | 374 | LEU  |
| 1   | H     | 375 | LEU  |
| 1   | H     | 384 | ASN  |
| 1   | H     | 395 | ASN  |
| 1   | H     | 396 | LEU  |
| 1   | H     | 403 | GLU  |
| 1   | H     | 419 | ASN  |
| 1   | H     | 428 | LEU  |
| 1   | H     | 447 | ARG  |
| 1   | H     | 459 | PRO  |
| 1   | H     | 464 | LEU  |
| 1   | H     | 468 | VAL  |
| 1   | I     | 1   | SER  |
| 1   | I     | 6   | LEU  |
| 1   | I     | 15  | LYS  |
| 1   | I     | 19  | LEU  |
| 1   | I     | 33  | ILE  |
| 1   | I     | 49  | PHE  |
| 1   | I     | 50  | ASP  |
| 1   | I     | 60  | ILE  |
| 1   | I     | 62  | GLU  |
| 1   | I     | 63  | SER  |
| 1   | I     | 64  | ASP  |
| 1   | I     | 84  | THR  |
| 1   | I     | 96  | THR  |
| 1   | I     | 102 | ARG  |
| 1   | I     | 115 | LEU  |
| 1   | I     | 124 | VAL  |
| 1   | I     | 125 | LEU  |
| 1   | I     | 147 | SER  |
| 1   | I     | 179 | TYR  |
| 1   | I     | 181 | PRO  |
| 1   | I     | 207 | GLU  |
| 1   | I     | 209 | HIS  |
| 1   | I     | 224 | ARG  |
| 1   | I     | 248 | ARG  |
| 1   | I     | 264 | ASN  |
| 1   | I     | 290 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 323 | VAL  |
| 1   | I     | 326 | TYR  |
| 1   | I     | 332 | LEU  |
| 1   | I     | 337 | ARG  |
| 1   | I     | 340 | SER  |
| 1   | I     | 344 | ARG  |
| 1   | I     | 355 | ARG  |
| 1   | I     | 374 | LEU  |
| 1   | I     | 375 | LEU  |
| 1   | I     | 384 | ASN  |
| 1   | I     | 395 | ASN  |
| 1   | I     | 396 | LEU  |
| 1   | I     | 403 | GLU  |
| 1   | I     | 419 | ASN  |
| 1   | I     | 428 | LEU  |
| 1   | I     | 447 | ARG  |
| 1   | I     | 459 | PRO  |
| 1   | I     | 464 | LEU  |
| 1   | I     | 468 | VAL  |
| 1   | J     | 1   | SER  |
| 1   | J     | 6   | LEU  |
| 1   | J     | 15  | LYS  |
| 1   | J     | 19  | LEU  |
| 1   | J     | 33  | ILE  |
| 1   | J     | 49  | PHE  |
| 1   | J     | 50  | ASP  |
| 1   | J     | 60  | ILE  |
| 1   | J     | 62  | GLU  |
| 1   | J     | 63  | SER  |
| 1   | J     | 64  | ASP  |
| 1   | J     | 84  | THR  |
| 1   | J     | 96  | THR  |
| 1   | J     | 102 | ARG  |
| 1   | J     | 115 | LEU  |
| 1   | J     | 124 | VAL  |
| 1   | J     | 125 | LEU  |
| 1   | J     | 147 | SER  |
| 1   | J     | 179 | TYR  |
| 1   | J     | 181 | PRO  |
| 1   | J     | 207 | GLU  |
| 1   | J     | 209 | HIS  |
| 1   | J     | 224 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 248 | ARG  |
| 1   | J     | 264 | ASN  |
| 1   | J     | 290 | LEU  |
| 1   | J     | 323 | VAL  |
| 1   | J     | 326 | TYR  |
| 1   | J     | 332 | LEU  |
| 1   | J     | 337 | ARG  |
| 1   | J     | 340 | SER  |
| 1   | J     | 344 | ARG  |
| 1   | J     | 355 | ARG  |
| 1   | J     | 374 | LEU  |
| 1   | J     | 375 | LEU  |
| 1   | J     | 384 | ASN  |
| 1   | J     | 395 | ASN  |
| 1   | J     | 396 | LEU  |
| 1   | J     | 403 | GLU  |
| 1   | J     | 419 | ASN  |
| 1   | J     | 428 | LEU  |
| 1   | J     | 447 | ARG  |
| 1   | J     | 459 | PRO  |
| 1   | J     | 464 | LEU  |
| 1   | J     | 468 | VAL  |
| 1   | K     | 1   | SER  |
| 1   | K     | 6   | LEU  |
| 1   | K     | 15  | LYS  |
| 1   | K     | 19  | LEU  |
| 1   | K     | 33  | ILE  |
| 1   | K     | 49  | PHE  |
| 1   | K     | 50  | ASP  |
| 1   | K     | 60  | ILE  |
| 1   | K     | 62  | GLU  |
| 1   | K     | 63  | SER  |
| 1   | K     | 64  | ASP  |
| 1   | K     | 84  | THR  |
| 1   | K     | 96  | THR  |
| 1   | K     | 102 | ARG  |
| 1   | K     | 115 | LEU  |
| 1   | K     | 124 | VAL  |
| 1   | K     | 125 | LEU  |
| 1   | K     | 147 | SER  |
| 1   | K     | 179 | TYR  |
| 1   | K     | 181 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 207 | GLU  |
| 1   | K     | 209 | HIS  |
| 1   | K     | 224 | ARG  |
| 1   | K     | 248 | ARG  |
| 1   | K     | 264 | ASN  |
| 1   | K     | 290 | LEU  |
| 1   | K     | 323 | VAL  |
| 1   | K     | 326 | TYR  |
| 1   | K     | 332 | LEU  |
| 1   | K     | 337 | ARG  |
| 1   | K     | 340 | SER  |
| 1   | K     | 344 | ARG  |
| 1   | K     | 355 | ARG  |
| 1   | K     | 374 | LEU  |
| 1   | K     | 375 | LEU  |
| 1   | K     | 384 | ASN  |
| 1   | K     | 395 | ASN  |
| 1   | K     | 396 | LEU  |
| 1   | K     | 403 | GLU  |
| 1   | K     | 419 | ASN  |
| 1   | K     | 428 | LEU  |
| 1   | K     | 447 | ARG  |
| 1   | K     | 459 | PRO  |
| 1   | K     | 464 | LEU  |
| 1   | K     | 468 | VAL  |
| 1   | L     | 1   | SER  |
| 1   | L     | 6   | LEU  |
| 1   | L     | 15  | LYS  |
| 1   | L     | 19  | LEU  |
| 1   | L     | 33  | ILE  |
| 1   | L     | 49  | PHE  |
| 1   | L     | 50  | ASP  |
| 1   | L     | 60  | ILE  |
| 1   | L     | 62  | GLU  |
| 1   | L     | 63  | SER  |
| 1   | L     | 64  | ASP  |
| 1   | L     | 84  | THR  |
| 1   | L     | 96  | THR  |
| 1   | L     | 102 | ARG  |
| 1   | L     | 115 | LEU  |
| 1   | L     | 124 | VAL  |
| 1   | L     | 125 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 147 | SER  |
| 1   | L     | 179 | TYR  |
| 1   | L     | 181 | PRO  |
| 1   | L     | 207 | GLU  |
| 1   | L     | 209 | HIS  |
| 1   | L     | 224 | ARG  |
| 1   | L     | 248 | ARG  |
| 1   | L     | 264 | ASN  |
| 1   | L     | 290 | LEU  |
| 1   | L     | 323 | VAL  |
| 1   | L     | 326 | TYR  |
| 1   | L     | 332 | LEU  |
| 1   | L     | 337 | ARG  |
| 1   | L     | 340 | SER  |
| 1   | L     | 344 | ARG  |
| 1   | L     | 355 | ARG  |
| 1   | L     | 374 | LEU  |
| 1   | L     | 375 | LEU  |
| 1   | L     | 384 | ASN  |
| 1   | L     | 395 | ASN  |
| 1   | L     | 396 | LEU  |
| 1   | L     | 403 | GLU  |
| 1   | L     | 419 | ASN  |
| 1   | L     | 428 | LEU  |
| 1   | L     | 447 | ARG  |
| 1   | L     | 459 | PRO  |
| 1   | L     | 464 | LEU  |
| 1   | L     | 468 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | ASN  |
| 1   | A     | 61  | ASN  |
| 1   | A     | 211 | HIS  |
| 1   | A     | 218 | GLN  |
| 1   | A     | 219 | ASN  |
| 1   | A     | 244 | ASN  |
| 1   | A     | 313 | ASN  |
| 1   | A     | 338 | ASN  |
| 1   | A     | 384 | ASN  |
| 1   | A     | 395 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 409 | GLN  |
| 1   | A     | 458 | HIS  |
| 1   | B     | 10  | ASN  |
| 1   | B     | 61  | ASN  |
| 1   | B     | 211 | HIS  |
| 1   | B     | 218 | GLN  |
| 1   | B     | 219 | ASN  |
| 1   | B     | 244 | ASN  |
| 1   | B     | 313 | ASN  |
| 1   | B     | 338 | ASN  |
| 1   | B     | 384 | ASN  |
| 1   | B     | 395 | ASN  |
| 1   | B     | 409 | GLN  |
| 1   | B     | 458 | HIS  |
| 1   | C     | 10  | ASN  |
| 1   | C     | 61  | ASN  |
| 1   | C     | 211 | HIS  |
| 1   | C     | 218 | GLN  |
| 1   | C     | 219 | ASN  |
| 1   | C     | 244 | ASN  |
| 1   | C     | 313 | ASN  |
| 1   | C     | 338 | ASN  |
| 1   | C     | 384 | ASN  |
| 1   | C     | 395 | ASN  |
| 1   | C     | 409 | GLN  |
| 1   | C     | 458 | HIS  |
| 1   | D     | 10  | ASN  |
| 1   | D     | 61  | ASN  |
| 1   | D     | 211 | HIS  |
| 1   | D     | 218 | GLN  |
| 1   | D     | 219 | ASN  |
| 1   | D     | 244 | ASN  |
| 1   | D     | 313 | ASN  |
| 1   | D     | 338 | ASN  |
| 1   | D     | 384 | ASN  |
| 1   | D     | 395 | ASN  |
| 1   | D     | 409 | GLN  |
| 1   | D     | 458 | HIS  |
| 1   | E     | 10  | ASN  |
| 1   | E     | 61  | ASN  |
| 1   | E     | 211 | HIS  |
| 1   | E     | 218 | GLN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 219 | ASN  |
| 1   | E     | 244 | ASN  |
| 1   | E     | 313 | ASN  |
| 1   | E     | 338 | ASN  |
| 1   | E     | 384 | ASN  |
| 1   | E     | 395 | ASN  |
| 1   | E     | 409 | GLN  |
| 1   | E     | 458 | HIS  |
| 1   | F     | 10  | ASN  |
| 1   | F     | 61  | ASN  |
| 1   | F     | 211 | HIS  |
| 1   | F     | 218 | GLN  |
| 1   | F     | 219 | ASN  |
| 1   | F     | 244 | ASN  |
| 1   | F     | 313 | ASN  |
| 1   | F     | 338 | ASN  |
| 1   | F     | 384 | ASN  |
| 1   | F     | 395 | ASN  |
| 1   | F     | 409 | GLN  |
| 1   | F     | 458 | HIS  |
| 1   | G     | 10  | ASN  |
| 1   | G     | 61  | ASN  |
| 1   | G     | 211 | HIS  |
| 1   | G     | 218 | GLN  |
| 1   | G     | 219 | ASN  |
| 1   | G     | 244 | ASN  |
| 1   | G     | 313 | ASN  |
| 1   | G     | 338 | ASN  |
| 1   | G     | 384 | ASN  |
| 1   | G     | 395 | ASN  |
| 1   | G     | 409 | GLN  |
| 1   | G     | 458 | HIS  |
| 1   | H     | 10  | ASN  |
| 1   | H     | 61  | ASN  |
| 1   | H     | 211 | HIS  |
| 1   | H     | 218 | GLN  |
| 1   | H     | 219 | ASN  |
| 1   | H     | 244 | ASN  |
| 1   | H     | 313 | ASN  |
| 1   | H     | 338 | ASN  |
| 1   | H     | 384 | ASN  |
| 1   | H     | 395 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 409 | GLN  |
| 1   | H     | 458 | HIS  |
| 1   | I     | 10  | ASN  |
| 1   | I     | 61  | ASN  |
| 1   | I     | 211 | HIS  |
| 1   | I     | 218 | GLN  |
| 1   | I     | 219 | ASN  |
| 1   | I     | 244 | ASN  |
| 1   | I     | 313 | ASN  |
| 1   | I     | 338 | ASN  |
| 1   | I     | 384 | ASN  |
| 1   | I     | 395 | ASN  |
| 1   | I     | 409 | GLN  |
| 1   | I     | 458 | HIS  |
| 1   | J     | 10  | ASN  |
| 1   | J     | 61  | ASN  |
| 1   | J     | 211 | HIS  |
| 1   | J     | 218 | GLN  |
| 1   | J     | 219 | ASN  |
| 1   | J     | 244 | ASN  |
| 1   | J     | 313 | ASN  |
| 1   | J     | 338 | ASN  |
| 1   | J     | 384 | ASN  |
| 1   | J     | 395 | ASN  |
| 1   | J     | 409 | GLN  |
| 1   | J     | 458 | HIS  |
| 1   | K     | 10  | ASN  |
| 1   | K     | 61  | ASN  |
| 1   | K     | 211 | HIS  |
| 1   | K     | 218 | GLN  |
| 1   | K     | 219 | ASN  |
| 1   | K     | 244 | ASN  |
| 1   | K     | 313 | ASN  |
| 1   | K     | 338 | ASN  |
| 1   | K     | 384 | ASN  |
| 1   | K     | 395 | ASN  |
| 1   | K     | 409 | GLN  |
| 1   | K     | 458 | HIS  |
| 1   | L     | 10  | ASN  |
| 1   | L     | 61  | ASN  |
| 1   | L     | 211 | HIS  |
| 1   | L     | 218 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 219 | ASN  |
| 1   | L     | 244 | ASN  |
| 1   | L     | 313 | ASN  |
| 1   | L     | 338 | ASN  |
| 1   | L     | 384 | ASN  |
| 1   | L     | 395 | ASN  |
| 1   | L     | 409 | GLN  |
| 1   | L     | 458 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 48 are monoatomic - leaving 24 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | MPD  | L     | 1494 | -    | 7,7,7        | 1.17 | 0           | 9,10,10     | 0.73 | 0           |
| 3   | ADP  | I     | 1479 | -    | 28,29,29     | 3.43 | 12 (42%)    | 43,45,45    | 3.02 | 16 (37%)    |
| 3   | ADP  | G     | 1477 | -    | 28,29,29     | 3.42 | 12 (42%)    | 43,45,45    | 3.02 | 16 (37%)    |
| 5   | MPD  | G     | 1489 | -    | 7,7,7        | 1.17 | 0           | 9,10,10     | 0.72 | 0           |
| 3   | ADP  | B     | 1472 | -    | 28,29,29     | 3.42 | 12 (42%)    | 43,45,45    | 3.02 | 16 (37%)    |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ADP  | J     | 1480 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 5   | MPD  | C     | 1485 | -    | 7,7,7        | 1.18 | 0        | 9,10,10     | 0.72 | 0        |
| 3   | ADP  | C     | 1473 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 5   | MPD  | A     | 1483 | -    | 7,7,7        | 1.17 | 0        | 9,10,10     | 0.73 | 0        |
| 3   | ADP  | E     | 1475 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 5   | MPD  | H     | 1490 | -    | 7,7,7        | 1.18 | 0        | 9,10,10     | 0.72 | 0        |
| 5   | MPD  | K     | 1493 | -    | 7,7,7        | 1.17 | 0        | 9,10,10     | 0.72 | 0        |
| 3   | ADP  | L     | 1482 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 3   | ADP  | D     | 1474 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 5   | MPD  | J     | 1492 | -    | 7,7,7        | 1.17 | 0        | 9,10,10     | 0.72 | 0        |
| 3   | ADP  | H     | 1478 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 5   | MPD  | F     | 1488 | -    | 7,7,7        | 1.18 | 0        | 9,10,10     | 0.73 | 0        |
| 5   | MPD  | D     | 1486 | -    | 7,7,7        | 1.17 | 0        | 9,10,10     | 0.72 | 0        |
| 5   | MPD  | I     | 1491 | -    | 7,7,7        | 1.17 | 0        | 9,10,10     | 0.72 | 0        |
| 3   | ADP  | A     | 1471 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 3   | ADP  | F     | 1476 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 3   | ADP  | K     | 1481 | -    | 28,29,29     | 3.42 | 12 (42%) | 43,45,45    | 3.02 | 16 (37%) |
| 5   | MPD  | B     | 1484 | -    | 7,7,7        | 1.17 | 0        | 9,10,10     | 0.72 | 0        |
| 5   | MPD  | E     | 1487 | -    | 7,7,7        | 1.16 | 0        | 9,10,10     | 0.73 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 5   | MPD  | L     | 1494 | -    | -       | 3/5/5/5    | -       |
| 3   | ADP  | I     | 1479 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 3   | ADP  | G     | 1477 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 5   | MPD  | G     | 1489 | -    | -       | 3/5/5/5    | -       |
| 3   | ADP  | B     | 1472 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 3   | ADP  | J     | 1480 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 5   | MPD  | C     | 1485 | -    | -       | 3/5/5/5    | -       |
| 3   | ADP  | C     | 1473 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 5   | MPD  | A     | 1483 | -    | -       | 3/5/5/5    | -       |
| 3   | ADP  | E     | 1475 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 5   | MPD  | H     | 1490 | -    | -       | 3/5/5/5    | -       |
| 5   | MPD  | K     | 1493 | -    | -       | 3/5/5/5    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | ADP  | L     | 1482 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 3   | ADP  | D     | 1474 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 5   | MPD  | J     | 1492 | -    | -       | 3/5/5/5    | -       |
| 3   | ADP  | H     | 1478 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 5   | MPD  | F     | 1488 | -    | -       | 3/5/5/5    | -       |
| 5   | MPD  | D     | 1486 | -    | -       | 3/5/5/5    | -       |
| 5   | MPD  | I     | 1491 | -    | -       | 3/5/5/5    | -       |
| 3   | ADP  | A     | 1471 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 3   | ADP  | F     | 1476 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 3   | ADP  | K     | 1481 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 5   | MPD  | B     | 1484 | -    | -       | 3/5/5/5    | -       |
| 5   | MPD  | E     | 1487 | -    | -       | 3/5/5/5    | -       |

All (144) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 3   | I     | 1479 | ADP  | C1'-N9 | 9.00 | 1.71        | 1.46     |
| 3   | L     | 1482 | ADP  | C1'-N9 | 8.99 | 1.71        | 1.46     |
| 3   | H     | 1478 | ADP  | C1'-N9 | 8.98 | 1.71        | 1.46     |
| 3   | D     | 1474 | ADP  | C1'-N9 | 8.98 | 1.71        | 1.46     |
| 3   | C     | 1473 | ADP  | C1'-N9 | 8.98 | 1.71        | 1.46     |
| 3   | A     | 1471 | ADP  | C1'-N9 | 8.98 | 1.71        | 1.46     |
| 3   | B     | 1472 | ADP  | C1'-N9 | 8.97 | 1.71        | 1.46     |
| 3   | F     | 1476 | ADP  | C1'-N9 | 8.97 | 1.71        | 1.46     |
| 3   | J     | 1480 | ADP  | C1'-N9 | 8.97 | 1.71        | 1.46     |
| 3   | E     | 1475 | ADP  | C1'-N9 | 8.96 | 1.71        | 1.46     |
| 3   | G     | 1477 | ADP  | C1'-N9 | 8.95 | 1.71        | 1.46     |
| 3   | K     | 1481 | ADP  | C1'-N9 | 8.95 | 1.71        | 1.46     |
| 3   | J     | 1480 | ADP  | PA-O3A | 8.38 | 1.68        | 1.59     |
| 3   | I     | 1479 | ADP  | PA-O3A | 8.37 | 1.68        | 1.59     |
| 3   | D     | 1474 | ADP  | PA-O3A | 8.35 | 1.68        | 1.59     |
| 3   | B     | 1472 | ADP  | PA-O3A | 8.34 | 1.68        | 1.59     |
| 3   | L     | 1482 | ADP  | PA-O3A | 8.34 | 1.68        | 1.59     |
| 3   | A     | 1471 | ADP  | PA-O3A | 8.33 | 1.68        | 1.59     |
| 3   | C     | 1473 | ADP  | PA-O3A | 8.31 | 1.68        | 1.59     |
| 3   | F     | 1476 | ADP  | PA-O3A | 8.30 | 1.68        | 1.59     |
| 3   | G     | 1477 | ADP  | PA-O3A | 8.30 | 1.68        | 1.59     |
| 3   | E     | 1475 | ADP  | PA-O3A | 8.29 | 1.68        | 1.59     |
| 3   | K     | 1481 | ADP  | PA-O3A | 8.29 | 1.68        | 1.59     |
| 3   | H     | 1478 | ADP  | PA-O3A | 8.26 | 1.68        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | G     | 1477 | ADP  | C8-N9   | 5.73  | 1.47        | 1.37     |
| 3   | L     | 1482 | ADP  | C8-N9   | 5.71  | 1.47        | 1.37     |
| 3   | C     | 1473 | ADP  | C8-N9   | 5.71  | 1.47        | 1.37     |
| 3   | H     | 1478 | ADP  | C8-N9   | 5.70  | 1.47        | 1.37     |
| 3   | E     | 1475 | ADP  | C8-N9   | 5.69  | 1.47        | 1.37     |
| 3   | K     | 1481 | ADP  | C8-N9   | 5.69  | 1.47        | 1.37     |
| 3   | I     | 1479 | ADP  | C8-N9   | 5.68  | 1.47        | 1.37     |
| 3   | F     | 1476 | ADP  | C8-N9   | 5.68  | 1.47        | 1.37     |
| 3   | B     | 1472 | ADP  | C8-N9   | 5.68  | 1.47        | 1.37     |
| 3   | A     | 1471 | ADP  | C8-N9   | 5.67  | 1.47        | 1.37     |
| 3   | D     | 1474 | ADP  | C8-N9   | 5.67  | 1.47        | 1.37     |
| 3   | J     | 1480 | ADP  | C8-N9   | 5.67  | 1.47        | 1.37     |
| 3   | L     | 1482 | ADP  | C4-N3   | 4.69  | 1.43        | 1.34     |
| 3   | K     | 1481 | ADP  | C4-N3   | 4.66  | 1.43        | 1.34     |
| 3   | B     | 1472 | ADP  | C4-N3   | 4.66  | 1.43        | 1.34     |
| 3   | D     | 1474 | ADP  | C4-N3   | 4.65  | 1.43        | 1.34     |
| 3   | A     | 1471 | ADP  | C4-N3   | 4.65  | 1.43        | 1.34     |
| 3   | H     | 1478 | ADP  | C4-N3   | 4.64  | 1.43        | 1.34     |
| 3   | E     | 1475 | ADP  | C4-N3   | 4.63  | 1.43        | 1.34     |
| 3   | G     | 1477 | ADP  | C4-N3   | 4.63  | 1.43        | 1.34     |
| 3   | C     | 1473 | ADP  | C4-N3   | 4.63  | 1.43        | 1.34     |
| 3   | F     | 1476 | ADP  | C4-N3   | 4.63  | 1.43        | 1.34     |
| 3   | J     | 1480 | ADP  | C4-N3   | 4.62  | 1.43        | 1.34     |
| 3   | I     | 1479 | ADP  | C4-N3   | 4.62  | 1.43        | 1.34     |
| 3   | K     | 1481 | ADP  | C6-N6   | -4.24 | 1.23        | 1.34     |
| 3   | K     | 1481 | ADP  | O4'-C1' | 4.24  | 1.51        | 1.42     |
| 3   | G     | 1477 | ADP  | O4'-C1' | 4.24  | 1.51        | 1.42     |
| 3   | I     | 1479 | ADP  | C6-N6   | -4.24 | 1.23        | 1.34     |
| 3   | D     | 1474 | ADP  | C6-N6   | -4.24 | 1.23        | 1.34     |
| 3   | G     | 1477 | ADP  | C6-N6   | -4.24 | 1.23        | 1.34     |
| 3   | C     | 1473 | ADP  | C6-N6   | -4.23 | 1.23        | 1.34     |
| 3   | H     | 1478 | ADP  | O4'-C1' | 4.23  | 1.51        | 1.42     |
| 3   | I     | 1479 | ADP  | O4'-C1' | 4.23  | 1.51        | 1.42     |
| 3   | L     | 1482 | ADP  | O4'-C1' | 4.23  | 1.51        | 1.42     |
| 3   | E     | 1475 | ADP  | O4'-C1' | 4.22  | 1.51        | 1.42     |
| 3   | A     | 1471 | ADP  | C6-N6   | -4.22 | 1.23        | 1.34     |
| 3   | J     | 1480 | ADP  | C6-N6   | -4.22 | 1.23        | 1.34     |
| 3   | B     | 1472 | ADP  | O4'-C1' | 4.22  | 1.51        | 1.42     |
| 3   | D     | 1474 | ADP  | O4'-C1' | 4.22  | 1.51        | 1.42     |
| 3   | A     | 1471 | ADP  | O4'-C1' | 4.22  | 1.51        | 1.42     |
| 3   | J     | 1480 | ADP  | O4'-C1' | 4.21  | 1.51        | 1.42     |
| 3   | H     | 1478 | ADP  | C6-N6   | -4.21 | 1.23        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | E     | 1475 | ADP  | C6-N6   | -4.21 | 1.23        | 1.34     |
| 3   | L     | 1482 | ADP  | C6-N6   | -4.21 | 1.23        | 1.34     |
| 3   | C     | 1473 | ADP  | O4'-C1' | 4.20  | 1.51        | 1.42     |
| 3   | B     | 1472 | ADP  | C6-N6   | -4.20 | 1.23        | 1.34     |
| 3   | F     | 1476 | ADP  | C6-N6   | -4.20 | 1.23        | 1.34     |
| 3   | F     | 1476 | ADP  | O4'-C1' | 4.19  | 1.51        | 1.42     |
| 3   | B     | 1472 | ADP  | O4'-C4' | 4.05  | 1.54        | 1.45     |
| 3   | C     | 1473 | ADP  | O4'-C4' | 4.05  | 1.54        | 1.45     |
| 3   | I     | 1479 | ADP  | O4'-C4' | 4.04  | 1.54        | 1.45     |
| 3   | J     | 1480 | ADP  | O4'-C4' | 4.04  | 1.54        | 1.45     |
| 3   | K     | 1481 | ADP  | O4'-C4' | 4.03  | 1.54        | 1.45     |
| 3   | F     | 1476 | ADP  | O4'-C4' | 4.03  | 1.54        | 1.45     |
| 3   | H     | 1478 | ADP  | O4'-C4' | 4.03  | 1.53        | 1.45     |
| 3   | A     | 1471 | ADP  | O4'-C4' | 4.02  | 1.53        | 1.45     |
| 3   | G     | 1477 | ADP  | O4'-C4' | 4.02  | 1.53        | 1.45     |
| 3   | E     | 1475 | ADP  | O4'-C4' | 4.01  | 1.53        | 1.45     |
| 3   | L     | 1482 | ADP  | O4'-C4' | 4.01  | 1.53        | 1.45     |
| 3   | D     | 1474 | ADP  | O4'-C4' | 3.99  | 1.53        | 1.45     |
| 3   | E     | 1475 | ADP  | C4-N9   | 3.91  | 1.45        | 1.37     |
| 3   | F     | 1476 | ADP  | C4-N9   | 3.90  | 1.45        | 1.37     |
| 3   | H     | 1478 | ADP  | C4-N9   | 3.90  | 1.45        | 1.37     |
| 3   | I     | 1479 | ADP  | C4-N9   | 3.89  | 1.45        | 1.37     |
| 3   | K     | 1481 | ADP  | C4-N9   | 3.89  | 1.45        | 1.37     |
| 3   | J     | 1480 | ADP  | C4-N9   | 3.89  | 1.45        | 1.37     |
| 3   | A     | 1471 | ADP  | C4-N9   | 3.89  | 1.45        | 1.37     |
| 3   | B     | 1472 | ADP  | C4-N9   | 3.89  | 1.45        | 1.37     |
| 3   | C     | 1473 | ADP  | C4-N9   | 3.88  | 1.45        | 1.37     |
| 3   | G     | 1477 | ADP  | C4-N9   | 3.87  | 1.45        | 1.37     |
| 3   | L     | 1482 | ADP  | C4-N9   | 3.87  | 1.45        | 1.37     |
| 3   | D     | 1474 | ADP  | C4-N9   | 3.86  | 1.45        | 1.37     |
| 3   | K     | 1481 | ADP  | C5-C4   | 3.81  | 1.45        | 1.39     |
| 3   | E     | 1475 | ADP  | C5-C4   | 3.81  | 1.45        | 1.39     |
| 3   | G     | 1477 | ADP  | C5-C4   | 3.81  | 1.45        | 1.39     |
| 3   | F     | 1476 | ADP  | C5-C4   | 3.81  | 1.45        | 1.39     |
| 3   | A     | 1471 | ADP  | C5-C4   | 3.78  | 1.45        | 1.39     |
| 3   | C     | 1473 | ADP  | C5-C4   | 3.78  | 1.45        | 1.39     |
| 3   | D     | 1474 | ADP  | C5-C4   | 3.78  | 1.45        | 1.39     |
| 3   | I     | 1479 | ADP  | C5-C4   | 3.78  | 1.45        | 1.39     |
| 3   | J     | 1480 | ADP  | C5-C4   | 3.78  | 1.45        | 1.39     |
| 3   | L     | 1482 | ADP  | C5-C4   | 3.77  | 1.45        | 1.39     |
| 3   | H     | 1478 | ADP  | C5-C4   | 3.76  | 1.45        | 1.39     |
| 3   | B     | 1472 | ADP  | C5-C4   | 3.76  | 1.45        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | G     | 1477 | ADP  | PB-O3B  | 3.61  | 1.68        | 1.54     |
| 3   | J     | 1480 | ADP  | PB-O3B  | 3.60  | 1.68        | 1.54     |
| 3   | B     | 1472 | ADP  | PB-O3B  | 3.58  | 1.68        | 1.54     |
| 3   | A     | 1471 | ADP  | PB-O3B  | 3.58  | 1.68        | 1.54     |
| 3   | F     | 1476 | ADP  | PB-O3B  | 3.58  | 1.68        | 1.54     |
| 3   | K     | 1481 | ADP  | PB-O3B  | 3.58  | 1.68        | 1.54     |
| 3   | D     | 1474 | ADP  | PB-O3B  | 3.58  | 1.68        | 1.54     |
| 3   | L     | 1482 | ADP  | PB-O3B  | 3.58  | 1.68        | 1.54     |
| 3   | H     | 1478 | ADP  | PB-O3B  | 3.58  | 1.68        | 1.54     |
| 3   | I     | 1479 | ADP  | PB-O3B  | 3.57  | 1.68        | 1.54     |
| 3   | C     | 1473 | ADP  | PB-O3B  | 3.57  | 1.68        | 1.54     |
| 3   | E     | 1475 | ADP  | PB-O3B  | 3.57  | 1.68        | 1.54     |
| 3   | J     | 1480 | ADP  | C2-N3   | 2.78  | 1.38        | 1.33     |
| 3   | K     | 1481 | ADP  | C2-N3   | 2.77  | 1.38        | 1.33     |
| 3   | E     | 1475 | ADP  | C2-N3   | 2.77  | 1.38        | 1.33     |
| 3   | I     | 1479 | ADP  | C2-N3   | 2.76  | 1.38        | 1.33     |
| 3   | C     | 1473 | ADP  | C2-N3   | 2.76  | 1.38        | 1.33     |
| 3   | F     | 1476 | ADP  | C2-N3   | 2.75  | 1.38        | 1.33     |
| 3   | G     | 1477 | ADP  | C2-N3   | 2.75  | 1.38        | 1.33     |
| 3   | A     | 1471 | ADP  | C2-N3   | 2.75  | 1.38        | 1.33     |
| 3   | L     | 1482 | ADP  | C2-N3   | 2.75  | 1.38        | 1.33     |
| 3   | B     | 1472 | ADP  | C2-N3   | 2.75  | 1.38        | 1.33     |
| 3   | H     | 1478 | ADP  | C3'-C4' | -2.74 | 1.46        | 1.53     |
| 3   | J     | 1480 | ADP  | C3'-C4' | -2.74 | 1.46        | 1.53     |
| 3   | K     | 1481 | ADP  | C3'-C4' | -2.74 | 1.46        | 1.53     |
| 3   | H     | 1478 | ADP  | C2-N3   | 2.74  | 1.38        | 1.33     |
| 3   | G     | 1477 | ADP  | C3'-C4' | -2.74 | 1.46        | 1.53     |
| 3   | D     | 1474 | ADP  | C2-N3   | 2.73  | 1.38        | 1.33     |
| 3   | E     | 1475 | ADP  | C3'-C4' | -2.73 | 1.46        | 1.53     |
| 3   | L     | 1482 | ADP  | C3'-C4' | -2.73 | 1.46        | 1.53     |
| 3   | F     | 1476 | ADP  | C3'-C4' | -2.73 | 1.46        | 1.53     |
| 3   | A     | 1471 | ADP  | C3'-C4' | -2.73 | 1.46        | 1.53     |
| 3   | I     | 1479 | ADP  | C3'-C4' | -2.72 | 1.46        | 1.53     |
| 3   | D     | 1474 | ADP  | C3'-C4' | -2.72 | 1.46        | 1.53     |
| 3   | B     | 1472 | ADP  | C3'-C4' | -2.71 | 1.46        | 1.53     |
| 3   | C     | 1473 | ADP  | C3'-C4' | -2.70 | 1.46        | 1.53     |

All (192) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 3   | K     | 1481 | ADP  | O5'-C5'-C4' | 8.10 | 136.58      | 108.99   |
| 3   | J     | 1480 | ADP  | O5'-C5'-C4' | 8.10 | 136.56      | 108.99   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 1475 | ADP  | O5'-C5'-C4' | 8.10  | 136.56      | 108.99   |
| 3   | D     | 1474 | ADP  | O5'-C5'-C4' | 8.10  | 136.56      | 108.99   |
| 3   | L     | 1482 | ADP  | O5'-C5'-C4' | 8.10  | 136.56      | 108.99   |
| 3   | A     | 1471 | ADP  | O5'-C5'-C4' | 8.09  | 136.54      | 108.99   |
| 3   | H     | 1478 | ADP  | O5'-C5'-C4' | 8.09  | 136.53      | 108.99   |
| 3   | C     | 1473 | ADP  | O5'-C5'-C4' | 8.09  | 136.53      | 108.99   |
| 3   | I     | 1479 | ADP  | O5'-C5'-C4' | 8.08  | 136.52      | 108.99   |
| 3   | F     | 1476 | ADP  | O5'-C5'-C4' | 8.08  | 136.52      | 108.99   |
| 3   | B     | 1472 | ADP  | O5'-C5'-C4' | 8.08  | 136.51      | 108.99   |
| 3   | G     | 1477 | ADP  | O5'-C5'-C4' | 8.08  | 136.50      | 108.99   |
| 3   | D     | 1474 | ADP  | O4'-C1'-C2' | -8.06 | 89.36       | 106.62   |
| 3   | G     | 1477 | ADP  | O4'-C1'-C2' | -8.06 | 89.38       | 106.62   |
| 3   | K     | 1481 | ADP  | O4'-C1'-C2' | -8.05 | 89.38       | 106.62   |
| 3   | B     | 1472 | ADP  | O4'-C1'-C2' | -8.05 | 89.39       | 106.62   |
| 3   | E     | 1475 | ADP  | O4'-C1'-C2' | -8.05 | 89.40       | 106.62   |
| 3   | I     | 1479 | ADP  | O4'-C1'-C2' | -8.04 | 89.40       | 106.62   |
| 3   | J     | 1480 | ADP  | O4'-C1'-C2' | -8.04 | 89.40       | 106.62   |
| 3   | F     | 1476 | ADP  | O4'-C1'-C2' | -8.04 | 89.41       | 106.62   |
| 3   | A     | 1471 | ADP  | O4'-C1'-C2' | -8.04 | 89.41       | 106.62   |
| 3   | C     | 1473 | ADP  | O4'-C1'-C2' | -8.03 | 89.42       | 106.62   |
| 3   | H     | 1478 | ADP  | O4'-C1'-C2' | -8.03 | 89.42       | 106.62   |
| 3   | L     | 1482 | ADP  | O4'-C1'-C2' | -8.03 | 89.43       | 106.62   |
| 3   | E     | 1475 | ADP  | O4'-C1'-N9  | 6.36  | 120.30      | 108.09   |
| 3   | D     | 1474 | ADP  | O4'-C1'-N9  | 6.35  | 120.29      | 108.09   |
| 3   | G     | 1477 | ADP  | O4'-C1'-N9  | 6.35  | 120.28      | 108.09   |
| 3   | K     | 1481 | ADP  | O4'-C1'-N9  | 6.35  | 120.28      | 108.09   |
| 3   | B     | 1472 | ADP  | O4'-C1'-N9  | 6.34  | 120.27      | 108.09   |
| 3   | F     | 1476 | ADP  | O4'-C1'-N9  | 6.34  | 120.27      | 108.09   |
| 3   | A     | 1471 | ADP  | O4'-C1'-N9  | 6.34  | 120.26      | 108.09   |
| 3   | J     | 1480 | ADP  | O4'-C1'-N9  | 6.34  | 120.26      | 108.09   |
| 3   | H     | 1478 | ADP  | O4'-C1'-N9  | 6.33  | 120.24      | 108.09   |
| 3   | C     | 1473 | ADP  | O4'-C1'-N9  | 6.32  | 120.23      | 108.09   |
| 3   | L     | 1482 | ADP  | O4'-C1'-N9  | 6.32  | 120.23      | 108.09   |
| 3   | I     | 1479 | ADP  | O4'-C1'-N9  | 6.31  | 120.22      | 108.09   |
| 3   | H     | 1478 | ADP  | C4-N9-C8    | -6.06 | 99.38       | 105.74   |
| 3   | K     | 1481 | ADP  | C4-N9-C8    | -6.04 | 99.40       | 105.74   |
| 3   | L     | 1482 | ADP  | C4-N9-C8    | -6.03 | 99.40       | 105.74   |
| 3   | G     | 1477 | ADP  | C4-N9-C8    | -6.03 | 99.40       | 105.74   |
| 3   | J     | 1480 | ADP  | C4-N9-C8    | -6.03 | 99.41       | 105.74   |
| 3   | C     | 1473 | ADP  | C4-N9-C8    | -6.03 | 99.41       | 105.74   |
| 3   | E     | 1475 | ADP  | C4-N9-C8    | -6.02 | 99.42       | 105.74   |
| 3   | A     | 1471 | ADP  | C4-N9-C8    | -6.01 | 99.42       | 105.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 1474 | ADP  | C4-N9-C8    | -6.01 | 99.43       | 105.74   |
| 3   | F     | 1476 | ADP  | C4-N9-C8    | -6.00 | 99.43       | 105.74   |
| 3   | B     | 1472 | ADP  | C4-N9-C8    | -6.00 | 99.44       | 105.74   |
| 3   | I     | 1479 | ADP  | C4-N9-C8    | -5.99 | 99.45       | 105.74   |
| 3   | D     | 1474 | ADP  | O4'-C4'-C5' | 4.98  | 125.27      | 109.33   |
| 3   | C     | 1473 | ADP  | O4'-C4'-C5' | 4.97  | 125.25      | 109.33   |
| 3   | E     | 1475 | ADP  | O4'-C4'-C5' | 4.97  | 125.25      | 109.33   |
| 3   | F     | 1476 | ADP  | O4'-C4'-C5' | 4.97  | 125.24      | 109.33   |
| 3   | A     | 1471 | ADP  | O4'-C4'-C5' | 4.96  | 125.22      | 109.33   |
| 3   | B     | 1472 | ADP  | O4'-C4'-C5' | 4.96  | 125.22      | 109.33   |
| 3   | G     | 1477 | ADP  | O4'-C4'-C5' | 4.96  | 125.22      | 109.33   |
| 3   | J     | 1480 | ADP  | O4'-C4'-C5' | 4.95  | 125.20      | 109.33   |
| 3   | K     | 1481 | ADP  | O4'-C4'-C5' | 4.95  | 125.19      | 109.33   |
| 3   | L     | 1482 | ADP  | O4'-C4'-C5' | 4.95  | 125.19      | 109.33   |
| 3   | I     | 1479 | ADP  | O4'-C4'-C5' | 4.95  | 125.18      | 109.33   |
| 3   | H     | 1478 | ADP  | O4'-C4'-C5' | 4.95  | 125.18      | 109.33   |
| 3   | H     | 1478 | ADP  | C4'-O4'-C1' | -4.19 | 100.22      | 109.47   |
| 3   | L     | 1482 | ADP  | C4'-O4'-C1' | -4.18 | 100.24      | 109.47   |
| 3   | I     | 1479 | ADP  | C4'-O4'-C1' | -4.18 | 100.24      | 109.47   |
| 3   | J     | 1480 | ADP  | C4'-O4'-C1' | -4.17 | 100.27      | 109.47   |
| 3   | B     | 1472 | ADP  | C4'-O4'-C1' | -4.16 | 100.28      | 109.47   |
| 3   | K     | 1481 | ADP  | C4'-O4'-C1' | -4.16 | 100.28      | 109.47   |
| 3   | A     | 1471 | ADP  | C4'-O4'-C1' | -4.16 | 100.28      | 109.47   |
| 3   | C     | 1473 | ADP  | C4'-O4'-C1' | -4.16 | 100.29      | 109.47   |
| 3   | E     | 1475 | ADP  | C4'-O4'-C1' | -4.15 | 100.30      | 109.47   |
| 3   | F     | 1476 | ADP  | C4'-O4'-C1' | -4.15 | 100.30      | 109.47   |
| 3   | G     | 1477 | ADP  | C4'-O4'-C1' | -4.15 | 100.30      | 109.47   |
| 3   | D     | 1474 | ADP  | C4'-O4'-C1' | -4.13 | 100.34      | 109.47   |
| 3   | L     | 1482 | ADP  | C4-N9-C1'   | 4.13  | 136.30      | 126.63   |
| 3   | C     | 1473 | ADP  | C4-N9-C1'   | 4.13  | 136.29      | 126.63   |
| 3   | G     | 1477 | ADP  | C4-N9-C1'   | 4.13  | 136.29      | 126.63   |
| 3   | H     | 1478 | ADP  | C4-N9-C1'   | 4.12  | 136.28      | 126.63   |
| 3   | J     | 1480 | ADP  | C4-N9-C1'   | 4.12  | 136.26      | 126.63   |
| 3   | B     | 1472 | ADP  | C4-N9-C1'   | 4.12  | 136.26      | 126.63   |
| 3   | D     | 1474 | ADP  | C4-N9-C1'   | 4.12  | 136.26      | 126.63   |
| 3   | K     | 1481 | ADP  | C4-N9-C1'   | 4.12  | 136.26      | 126.63   |
| 3   | A     | 1471 | ADP  | C4-N9-C1'   | 4.11  | 136.25      | 126.63   |
| 3   | E     | 1475 | ADP  | C4-N9-C1'   | 4.11  | 136.25      | 126.63   |
| 3   | I     | 1479 | ADP  | C4-N9-C1'   | 4.11  | 136.24      | 126.63   |
| 3   | F     | 1476 | ADP  | C4-N9-C1'   | 4.09  | 136.21      | 126.63   |
| 3   | I     | 1479 | ADP  | C5'-C4'-C3' | -3.95 | 101.00      | 115.21   |
| 3   | H     | 1478 | ADP  | N9-C8-N7    | 3.95  | 119.53      | 113.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | G     | 1477 | ADP  | C5'-C4'-C3' | -3.94 | 101.01      | 115.21   |
| 3   | A     | 1471 | ADP  | C5'-C4'-C3' | -3.94 | 101.02      | 115.21   |
| 3   | L     | 1482 | ADP  | C5'-C4'-C3' | -3.94 | 101.03      | 115.21   |
| 3   | B     | 1472 | ADP  | C5'-C4'-C3' | -3.94 | 101.03      | 115.21   |
| 3   | F     | 1476 | ADP  | C5'-C4'-C3' | -3.94 | 101.03      | 115.21   |
| 3   | H     | 1478 | ADP  | C5'-C4'-C3' | -3.94 | 101.03      | 115.21   |
| 3   | C     | 1473 | ADP  | N9-C8-N7    | 3.94  | 119.52      | 113.94   |
| 3   | J     | 1480 | ADP  | N9-C8-N7    | 3.94  | 119.52      | 113.94   |
| 3   | K     | 1481 | ADP  | N9-C8-N7    | 3.94  | 119.52      | 113.94   |
| 3   | J     | 1480 | ADP  | C5'-C4'-C3' | -3.94 | 101.04      | 115.21   |
| 3   | D     | 1474 | ADP  | C5'-C4'-C3' | -3.94 | 101.05      | 115.21   |
| 3   | C     | 1473 | ADP  | C5'-C4'-C3' | -3.93 | 101.05      | 115.21   |
| 3   | E     | 1475 | ADP  | C5'-C4'-C3' | -3.93 | 101.08      | 115.21   |
| 3   | K     | 1481 | ADP  | C5'-C4'-C3' | -3.93 | 101.08      | 115.21   |
| 3   | F     | 1476 | ADP  | N9-C8-N7    | 3.93  | 119.51      | 113.94   |
| 3   | E     | 1475 | ADP  | N9-C8-N7    | 3.92  | 119.50      | 113.94   |
| 3   | A     | 1471 | ADP  | N9-C8-N7    | 3.92  | 119.50      | 113.94   |
| 3   | G     | 1477 | ADP  | N9-C8-N7    | 3.91  | 119.49      | 113.94   |
| 3   | L     | 1482 | ADP  | N9-C8-N7    | 3.91  | 119.49      | 113.94   |
| 3   | B     | 1472 | ADP  | N9-C8-N7    | 3.91  | 119.48      | 113.94   |
| 3   | D     | 1474 | ADP  | N9-C8-N7    | 3.91  | 119.48      | 113.94   |
| 3   | I     | 1479 | ADP  | N9-C8-N7    | 3.89  | 119.46      | 113.94   |
| 3   | C     | 1473 | ADP  | O2'-C2'-C1' | 3.51  | 122.20      | 110.10   |
| 3   | G     | 1477 | ADP  | O2'-C2'-C1' | 3.51  | 122.19      | 110.10   |
| 3   | B     | 1472 | ADP  | O2'-C2'-C1' | 3.51  | 122.19      | 110.10   |
| 3   | H     | 1478 | ADP  | O2'-C2'-C1' | 3.51  | 122.19      | 110.10   |
| 3   | L     | 1482 | ADP  | O2'-C2'-C1' | 3.51  | 122.19      | 110.10   |
| 3   | A     | 1471 | ADP  | O2'-C2'-C1' | 3.51  | 122.19      | 110.10   |
| 3   | I     | 1479 | ADP  | O2'-C2'-C1' | 3.51  | 122.18      | 110.10   |
| 3   | J     | 1480 | ADP  | O2'-C2'-C1' | 3.50  | 122.17      | 110.10   |
| 3   | D     | 1474 | ADP  | O2'-C2'-C1' | 3.50  | 122.17      | 110.10   |
| 3   | K     | 1481 | ADP  | O2'-C2'-C1' | 3.50  | 122.16      | 110.10   |
| 3   | F     | 1476 | ADP  | O2'-C2'-C1' | 3.50  | 122.15      | 110.10   |
| 3   | E     | 1475 | ADP  | O2'-C2'-C1' | 3.50  | 122.14      | 110.10   |
| 3   | H     | 1478 | ADP  | C4-C5-N7    | 3.22  | 114.26      | 110.58   |
| 3   | B     | 1472 | ADP  | C4-C5-N7    | 3.21  | 114.25      | 110.58   |
| 3   | J     | 1480 | ADP  | C4-C5-N7    | 3.20  | 114.24      | 110.58   |
| 3   | I     | 1479 | ADP  | C4-C5-N7    | 3.20  | 114.24      | 110.58   |
| 3   | C     | 1473 | ADP  | C4-C5-N7    | 3.19  | 114.23      | 110.58   |
| 3   | A     | 1471 | ADP  | C4-C5-N7    | 3.19  | 114.22      | 110.58   |
| 3   | G     | 1477 | ADP  | C4-C5-N7    | 3.19  | 114.22      | 110.58   |
| 3   | D     | 1474 | ADP  | C4-C5-N7    | 3.18  | 114.22      | 110.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | F     | 1476 | ADP  | C4-C5-N7    | 3.18  | 114.22      | 110.58   |
| 3   | L     | 1482 | ADP  | C4-C5-N7    | 3.17  | 114.20      | 110.58   |
| 3   | E     | 1475 | ADP  | C4-C5-N7    | 3.16  | 114.19      | 110.58   |
| 3   | K     | 1481 | ADP  | C4-C5-N7    | 3.16  | 114.19      | 110.58   |
| 3   | J     | 1480 | ADP  | O3'-C3'-C2' | 2.98  | 121.38      | 111.82   |
| 3   | E     | 1475 | ADP  | O3'-C3'-C2' | 2.98  | 121.36      | 111.82   |
| 3   | K     | 1481 | ADP  | O3'-C3'-C2' | 2.98  | 121.36      | 111.82   |
| 3   | I     | 1479 | ADP  | O3'-C3'-C2' | 2.97  | 121.35      | 111.82   |
| 3   | D     | 1474 | ADP  | O3'-C3'-C2' | 2.97  | 121.35      | 111.82   |
| 3   | F     | 1476 | ADP  | O3'-C3'-C2' | 2.97  | 121.35      | 111.82   |
| 3   | L     | 1482 | ADP  | O3'-C3'-C2' | 2.97  | 121.34      | 111.82   |
| 3   | B     | 1472 | ADP  | O3'-C3'-C2' | 2.97  | 121.34      | 111.82   |
| 3   | C     | 1473 | ADP  | O3'-C3'-C2' | 2.97  | 121.33      | 111.82   |
| 3   | A     | 1471 | ADP  | O3'-C3'-C2' | 2.97  | 121.33      | 111.82   |
| 3   | G     | 1477 | ADP  | O3'-C3'-C2' | 2.96  | 121.30      | 111.82   |
| 3   | H     | 1478 | ADP  | O3'-C3'-C2' | 2.96  | 121.29      | 111.82   |
| 3   | J     | 1480 | ADP  | PA-O5'-C5'  | 2.94  | 138.20      | 121.35   |
| 3   | I     | 1479 | ADP  | PA-O5'-C5'  | 2.94  | 138.19      | 121.35   |
| 3   | K     | 1481 | ADP  | PA-O5'-C5'  | 2.94  | 138.19      | 121.35   |
| 3   | B     | 1472 | ADP  | PA-O5'-C5'  | 2.94  | 138.18      | 121.35   |
| 3   | F     | 1476 | ADP  | PA-O5'-C5'  | 2.94  | 138.18      | 121.35   |
| 3   | D     | 1474 | ADP  | PA-O5'-C5'  | 2.94  | 138.18      | 121.35   |
| 3   | A     | 1471 | ADP  | PA-O5'-C5'  | 2.94  | 138.18      | 121.35   |
| 3   | C     | 1473 | ADP  | PA-O5'-C5'  | 2.94  | 138.17      | 121.35   |
| 3   | E     | 1475 | ADP  | PA-O5'-C5'  | 2.94  | 138.17      | 121.35   |
| 3   | G     | 1477 | ADP  | PA-O5'-C5'  | 2.93  | 138.16      | 121.35   |
| 3   | L     | 1482 | ADP  | PA-O5'-C5'  | 2.93  | 138.15      | 121.35   |
| 3   | J     | 1480 | ADP  | O2B-PB-O3A  | 2.93  | 114.47      | 104.64   |
| 3   | B     | 1472 | ADP  | O2B-PB-O3A  | 2.93  | 114.46      | 104.64   |
| 3   | L     | 1482 | ADP  | O2B-PB-O3A  | 2.93  | 114.46      | 104.64   |
| 3   | H     | 1478 | ADP  | PA-O5'-C5'  | 2.93  | 138.14      | 121.35   |
| 3   | C     | 1473 | ADP  | O2B-PB-O3A  | 2.93  | 114.45      | 104.64   |
| 3   | G     | 1477 | ADP  | O2B-PB-O3A  | 2.92  | 114.44      | 104.64   |
| 3   | D     | 1474 | ADP  | O2B-PB-O3A  | 2.92  | 114.44      | 104.64   |
| 3   | E     | 1475 | ADP  | O2B-PB-O3A  | 2.92  | 114.44      | 104.64   |
| 3   | K     | 1481 | ADP  | O2B-PB-O3A  | 2.92  | 114.44      | 104.64   |
| 3   | A     | 1471 | ADP  | O2B-PB-O3A  | 2.92  | 114.43      | 104.64   |
| 3   | I     | 1479 | ADP  | O2B-PB-O3A  | 2.92  | 114.43      | 104.64   |
| 3   | H     | 1478 | ADP  | O2B-PB-O3A  | 2.92  | 114.42      | 104.64   |
| 3   | F     | 1476 | ADP  | O2B-PB-O3A  | 2.90  | 114.36      | 104.64   |
| 3   | L     | 1482 | ADP  | C5-C4-N3    | -2.22 | 123.66      | 126.72   |
| 3   | K     | 1481 | ADP  | C5-C4-N3    | -2.22 | 123.66      | 126.72   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | B     | 1472 | ADP  | C5-C4-N3 | -2.21 | 123.67      | 126.72   |
| 3   | G     | 1477 | ADP  | C5-C4-N3 | -2.21 | 123.67      | 126.72   |
| 3   | D     | 1474 | ADP  | C5-C4-N3 | -2.20 | 123.68      | 126.72   |
| 3   | A     | 1471 | ADP  | C5-C4-N3 | -2.20 | 123.68      | 126.72   |
| 3   | C     | 1473 | ADP  | C5-C4-N3 | -2.20 | 123.68      | 126.72   |
| 3   | H     | 1478 | ADP  | C5-C4-N3 | -2.20 | 123.69      | 126.72   |
| 3   | J     | 1480 | ADP  | C5-C4-N3 | -2.19 | 123.69      | 126.72   |
| 3   | F     | 1476 | ADP  | C5-C4-N3 | -2.19 | 123.70      | 126.72   |
| 3   | E     | 1475 | ADP  | C5-C4-N3 | -2.18 | 123.71      | 126.72   |
| 3   | I     | 1479 | ADP  | C5-C4-N3 | -2.18 | 123.72      | 126.72   |
| 3   | E     | 1475 | ADP  | C5-C6-N6 | -2.10 | 118.10      | 123.29   |
| 3   | B     | 1472 | ADP  | C5-C6-N6 | -2.09 | 118.11      | 123.29   |
| 3   | D     | 1474 | ADP  | C5-C6-N6 | -2.08 | 118.12      | 123.29   |
| 3   | G     | 1477 | ADP  | C5-C6-N6 | -2.08 | 118.13      | 123.29   |
| 3   | F     | 1476 | ADP  | C5-C6-N6 | -2.08 | 118.13      | 123.29   |
| 3   | A     | 1471 | ADP  | C5-C6-N6 | -2.08 | 118.13      | 123.29   |
| 3   | H     | 1478 | ADP  | C5-C6-N6 | -2.08 | 118.14      | 123.29   |
| 3   | I     | 1479 | ADP  | C5-C6-N6 | -2.08 | 118.14      | 123.29   |
| 3   | K     | 1481 | ADP  | C5-C6-N6 | -2.08 | 118.15      | 123.29   |
| 3   | L     | 1482 | ADP  | C5-C6-N6 | -2.07 | 118.15      | 123.29   |
| 3   | J     | 1480 | ADP  | C5-C6-N6 | -2.07 | 118.17      | 123.29   |
| 3   | C     | 1473 | ADP  | C5-C6-N6 | -2.06 | 118.19      | 123.29   |

There are no chirality outliers.

All (120) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 3   | A     | 1471 | ADP  | PA-O3A-PB-O3B |
| 3   | B     | 1472 | ADP  | PA-O3A-PB-O3B |
| 3   | C     | 1473 | ADP  | PA-O3A-PB-O3B |
| 3   | D     | 1474 | ADP  | PA-O3A-PB-O3B |
| 3   | E     | 1475 | ADP  | PA-O3A-PB-O3B |
| 3   | F     | 1476 | ADP  | PA-O3A-PB-O3B |
| 3   | G     | 1477 | ADP  | PA-O3A-PB-O3B |
| 3   | H     | 1478 | ADP  | PA-O3A-PB-O3B |
| 3   | I     | 1479 | ADP  | PA-O3A-PB-O3B |
| 3   | J     | 1480 | ADP  | PA-O3A-PB-O3B |
| 3   | K     | 1481 | ADP  | PA-O3A-PB-O3B |
| 3   | L     | 1482 | ADP  | PA-O3A-PB-O3B |
| 5   | A     | 1483 | MPD  | C2-C3-C4-C5   |
| 5   | B     | 1484 | MPD  | C2-C3-C4-C5   |
| 5   | C     | 1485 | MPD  | C2-C3-C4-C5   |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 5   | D     | 1486 | MPD  | C2-C3-C4-C5    |
| 5   | E     | 1487 | MPD  | C2-C3-C4-C5    |
| 5   | F     | 1488 | MPD  | C2-C3-C4-C5    |
| 5   | G     | 1489 | MPD  | C2-C3-C4-C5    |
| 5   | H     | 1490 | MPD  | C2-C3-C4-C5    |
| 5   | I     | 1491 | MPD  | C2-C3-C4-C5    |
| 5   | J     | 1492 | MPD  | C2-C3-C4-C5    |
| 5   | K     | 1493 | MPD  | C2-C3-C4-C5    |
| 5   | L     | 1494 | MPD  | C2-C3-C4-C5    |
| 3   | A     | 1471 | ADP  | C2'-C1'-N9-C4  |
| 3   | B     | 1472 | ADP  | C2'-C1'-N9-C4  |
| 3   | C     | 1473 | ADP  | C2'-C1'-N9-C4  |
| 3   | D     | 1474 | ADP  | C2'-C1'-N9-C4  |
| 3   | E     | 1475 | ADP  | C2'-C1'-N9-C4  |
| 3   | F     | 1476 | ADP  | C2'-C1'-N9-C4  |
| 3   | G     | 1477 | ADP  | C2'-C1'-N9-C4  |
| 3   | H     | 1478 | ADP  | C2'-C1'-N9-C4  |
| 3   | I     | 1479 | ADP  | C2'-C1'-N9-C4  |
| 3   | J     | 1480 | ADP  | C2'-C1'-N9-C4  |
| 3   | K     | 1481 | ADP  | C2'-C1'-N9-C4  |
| 3   | L     | 1482 | ADP  | C2'-C1'-N9-C4  |
| 3   | A     | 1471 | ADP  | C2'-C1'-N9-C8  |
| 3   | B     | 1472 | ADP  | C2'-C1'-N9-C8  |
| 3   | C     | 1473 | ADP  | C2'-C1'-N9-C8  |
| 3   | D     | 1474 | ADP  | C2'-C1'-N9-C8  |
| 3   | E     | 1475 | ADP  | C2'-C1'-N9-C8  |
| 3   | F     | 1476 | ADP  | C2'-C1'-N9-C8  |
| 3   | G     | 1477 | ADP  | C2'-C1'-N9-C8  |
| 3   | H     | 1478 | ADP  | C2'-C1'-N9-C8  |
| 3   | I     | 1479 | ADP  | C2'-C1'-N9-C8  |
| 3   | J     | 1480 | ADP  | C2'-C1'-N9-C8  |
| 3   | K     | 1481 | ADP  | C2'-C1'-N9-C8  |
| 3   | L     | 1482 | ADP  | C2'-C1'-N9-C8  |
| 3   | A     | 1471 | ADP  | C5'-O5'-PA-O1A |
| 3   | A     | 1471 | ADP  | C5'-O5'-PA-O3A |
| 3   | B     | 1472 | ADP  | C5'-O5'-PA-O1A |
| 3   | B     | 1472 | ADP  | C5'-O5'-PA-O3A |
| 3   | C     | 1473 | ADP  | C5'-O5'-PA-O1A |
| 3   | C     | 1473 | ADP  | C5'-O5'-PA-O3A |
| 3   | D     | 1474 | ADP  | C5'-O5'-PA-O1A |
| 3   | D     | 1474 | ADP  | C5'-O5'-PA-O3A |
| 3   | E     | 1475 | ADP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | E     | 1475 | ADP  | C5'-O5'-PA-O3A |
| 3   | F     | 1476 | ADP  | C5'-O5'-PA-O1A |
| 3   | F     | 1476 | ADP  | C5'-O5'-PA-O3A |
| 3   | G     | 1477 | ADP  | C5'-O5'-PA-O1A |
| 3   | G     | 1477 | ADP  | C5'-O5'-PA-O3A |
| 3   | H     | 1478 | ADP  | C5'-O5'-PA-O1A |
| 3   | H     | 1478 | ADP  | C5'-O5'-PA-O3A |
| 3   | I     | 1479 | ADP  | C5'-O5'-PA-O1A |
| 3   | I     | 1479 | ADP  | C5'-O5'-PA-O3A |
| 3   | J     | 1480 | ADP  | C5'-O5'-PA-O1A |
| 3   | J     | 1480 | ADP  | C5'-O5'-PA-O3A |
| 3   | K     | 1481 | ADP  | C5'-O5'-PA-O1A |
| 3   | K     | 1481 | ADP  | C5'-O5'-PA-O3A |
| 3   | L     | 1482 | ADP  | C5'-O5'-PA-O1A |
| 3   | L     | 1482 | ADP  | C5'-O5'-PA-O3A |
| 3   | A     | 1471 | ADP  | PA-O3A-PB-O1B  |
| 3   | B     | 1472 | ADP  | PA-O3A-PB-O1B  |
| 3   | C     | 1473 | ADP  | PA-O3A-PB-O1B  |
| 3   | D     | 1474 | ADP  | PA-O3A-PB-O1B  |
| 3   | E     | 1475 | ADP  | PA-O3A-PB-O1B  |
| 3   | F     | 1476 | ADP  | PA-O3A-PB-O1B  |
| 3   | G     | 1477 | ADP  | PA-O3A-PB-O1B  |
| 3   | H     | 1478 | ADP  | PA-O3A-PB-O1B  |
| 3   | I     | 1479 | ADP  | PA-O3A-PB-O1B  |
| 3   | J     | 1480 | ADP  | PA-O3A-PB-O1B  |
| 3   | K     | 1481 | ADP  | PA-O3A-PB-O1B  |
| 3   | L     | 1482 | ADP  | PA-O3A-PB-O1B  |
| 3   | A     | 1471 | ADP  | O4'-C1'-N9-C8  |
| 3   | B     | 1472 | ADP  | O4'-C1'-N9-C8  |
| 3   | C     | 1473 | ADP  | O4'-C1'-N9-C8  |
| 3   | D     | 1474 | ADP  | O4'-C1'-N9-C8  |
| 3   | E     | 1475 | ADP  | O4'-C1'-N9-C8  |
| 3   | F     | 1476 | ADP  | O4'-C1'-N9-C8  |
| 3   | G     | 1477 | ADP  | O4'-C1'-N9-C8  |
| 3   | H     | 1478 | ADP  | O4'-C1'-N9-C8  |
| 3   | I     | 1479 | ADP  | O4'-C1'-N9-C8  |
| 3   | J     | 1480 | ADP  | O4'-C1'-N9-C8  |
| 3   | K     | 1481 | ADP  | O4'-C1'-N9-C8  |
| 3   | L     | 1482 | ADP  | O4'-C1'-N9-C8  |
| 5   | A     | 1483 | MPD  | O2-C2-C3-C4    |
| 5   | B     | 1484 | MPD  | O2-C2-C3-C4    |
| 5   | C     | 1485 | MPD  | O2-C2-C3-C4    |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 5   | D     | 1486 | MPD  | O2-C2-C3-C4 |
| 5   | E     | 1487 | MPD  | O2-C2-C3-C4 |
| 5   | F     | 1488 | MPD  | O2-C2-C3-C4 |
| 5   | G     | 1489 | MPD  | O2-C2-C3-C4 |
| 5   | H     | 1490 | MPD  | O2-C2-C3-C4 |
| 5   | I     | 1491 | MPD  | O2-C2-C3-C4 |
| 5   | J     | 1492 | MPD  | O2-C2-C3-C4 |
| 5   | K     | 1493 | MPD  | O2-C2-C3-C4 |
| 5   | L     | 1494 | MPD  | O2-C2-C3-C4 |
| 5   | A     | 1483 | MPD  | C2-C3-C4-O4 |
| 5   | B     | 1484 | MPD  | C2-C3-C4-O4 |
| 5   | C     | 1485 | MPD  | C2-C3-C4-O4 |
| 5   | D     | 1486 | MPD  | C2-C3-C4-O4 |
| 5   | E     | 1487 | MPD  | C2-C3-C4-O4 |
| 5   | F     | 1488 | MPD  | C2-C3-C4-O4 |
| 5   | G     | 1489 | MPD  | C2-C3-C4-O4 |
| 5   | H     | 1490 | MPD  | C2-C3-C4-O4 |
| 5   | I     | 1491 | MPD  | C2-C3-C4-O4 |
| 5   | J     | 1492 | MPD  | C2-C3-C4-O4 |
| 5   | K     | 1493 | MPD  | C2-C3-C4-O4 |
| 5   | L     | 1494 | MPD  | C2-C3-C4-O4 |

There are no ring outliers.

24 monomers are involved in 426 short contacts:

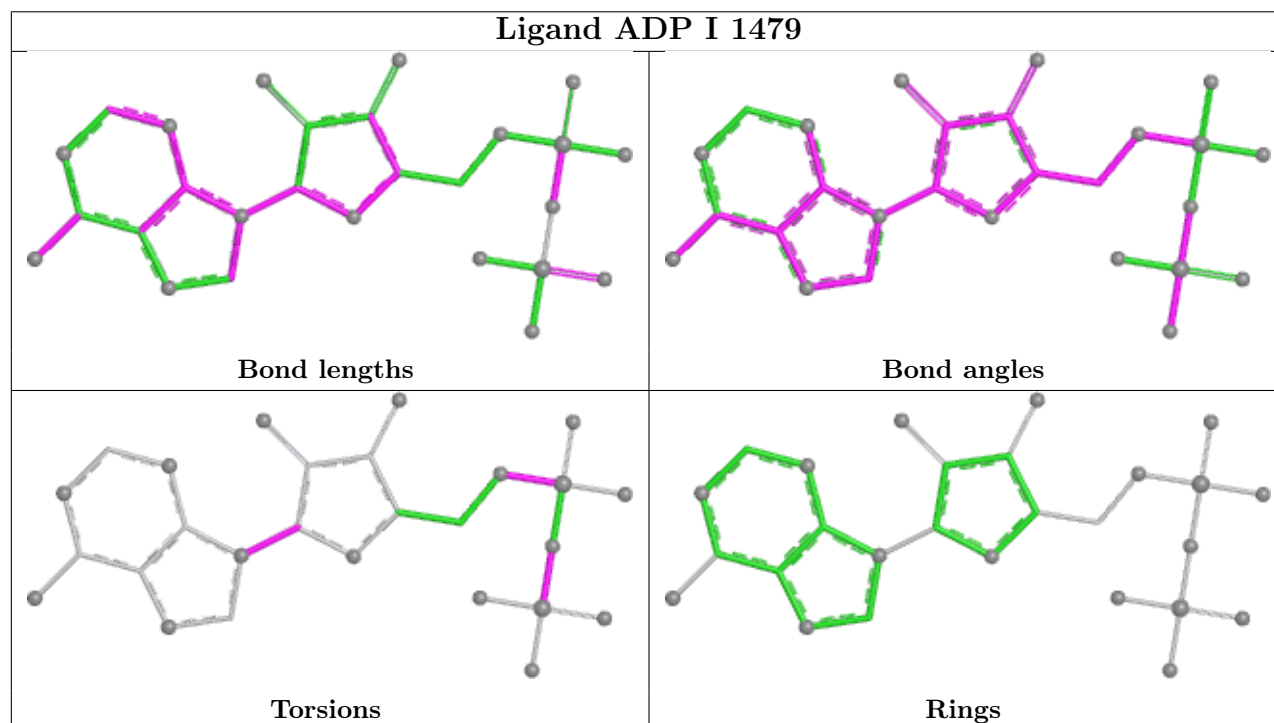
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | L     | 1494 | MPD  | 31      | 0            |
| 3   | I     | 1479 | ADP  | 3       | 0            |
| 3   | G     | 1477 | ADP  | 4       | 0            |
| 5   | G     | 1489 | MPD  | 30      | 0            |
| 3   | B     | 1472 | ADP  | 4       | 0            |
| 3   | J     | 1480 | ADP  | 4       | 0            |
| 5   | C     | 1485 | MPD  | 32      | 0            |
| 3   | C     | 1473 | ADP  | 4       | 0            |
| 5   | A     | 1483 | MPD  | 28      | 0            |
| 3   | E     | 1475 | ADP  | 4       | 0            |
| 5   | H     | 1490 | MPD  | 32      | 0            |
| 5   | K     | 1493 | MPD  | 32      | 0            |
| 3   | L     | 1482 | ADP  | 4       | 0            |
| 3   | D     | 1474 | ADP  | 4       | 0            |
| 5   | J     | 1492 | MPD  | 33      | 0            |
| 3   | H     | 1478 | ADP  | 4       | 0            |

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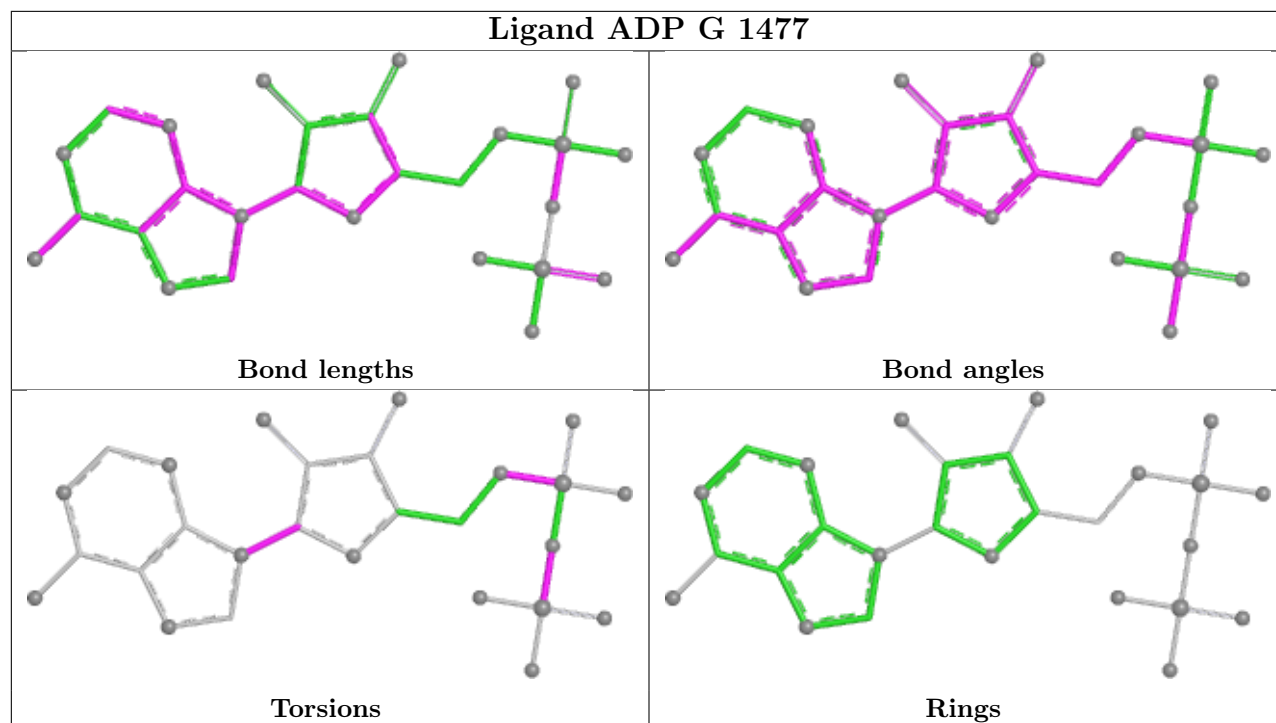
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | F     | 1488 | MPD  | 33      | 0            |
| 5   | D     | 1486 | MPD  | 33      | 0            |
| 5   | I     | 1491 | MPD  | 34      | 0            |
| 3   | A     | 1471 | ADP  | 4       | 0            |
| 3   | F     | 1476 | ADP  | 4       | 0            |
| 3   | K     | 1481 | ADP  | 4       | 0            |
| 5   | B     | 1484 | MPD  | 33      | 0            |
| 5   | E     | 1487 | MPD  | 28      | 0            |

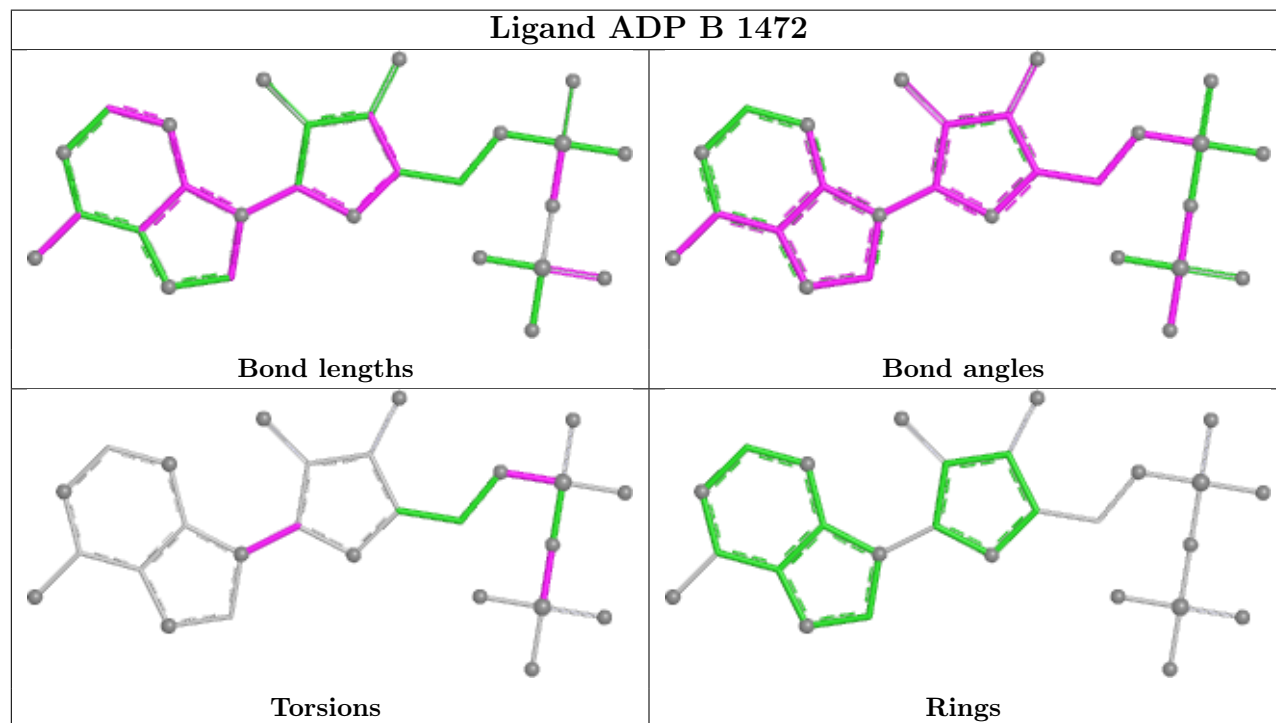
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

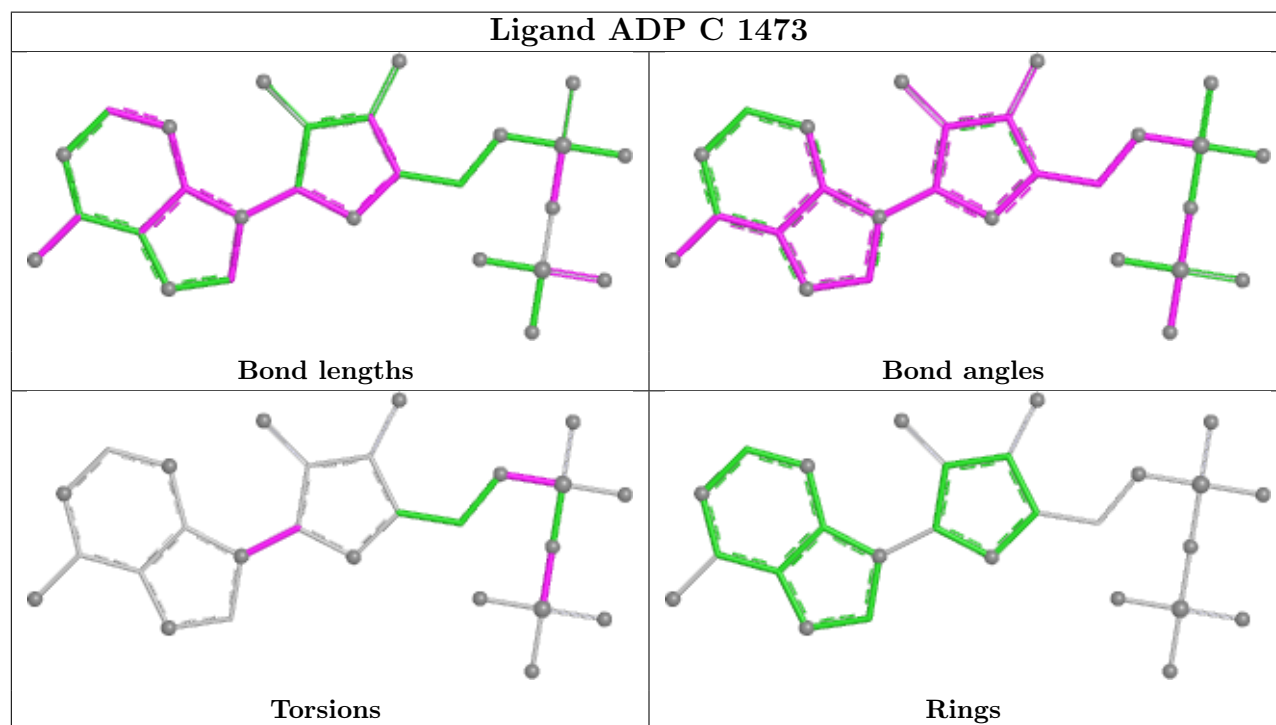
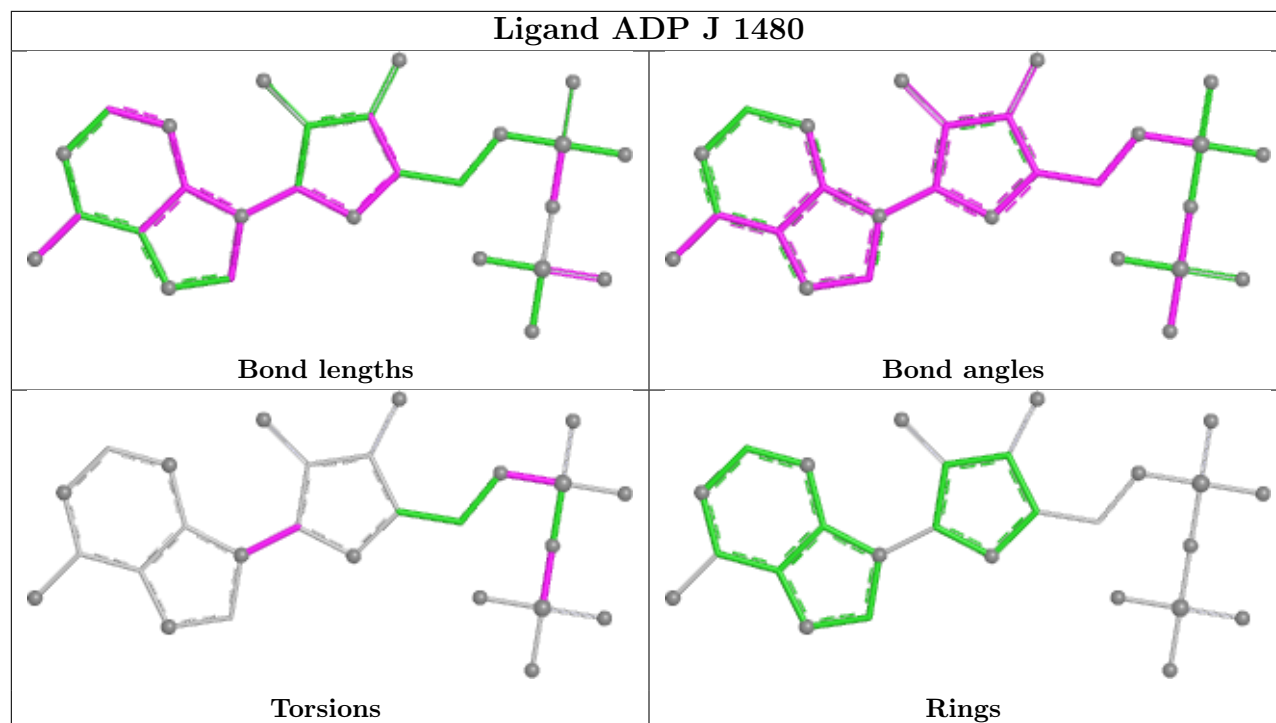


## Ligand ADP G 1477

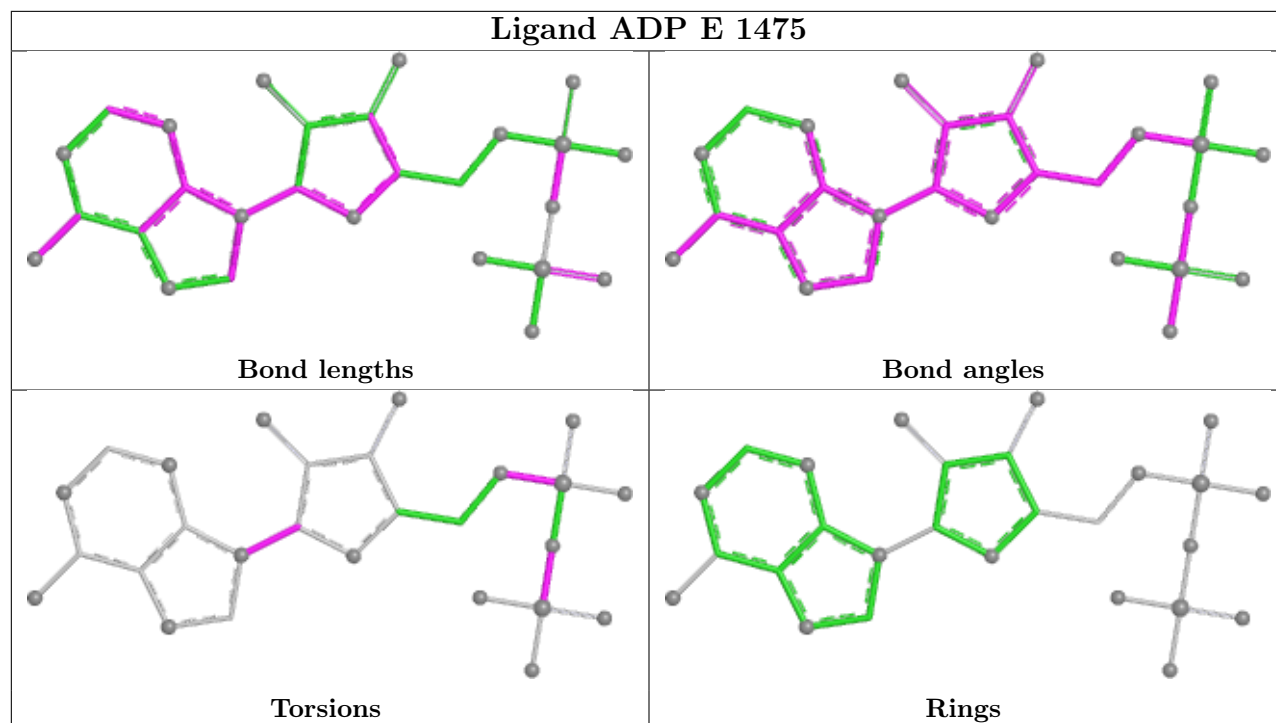


## Ligand ADP B 1472

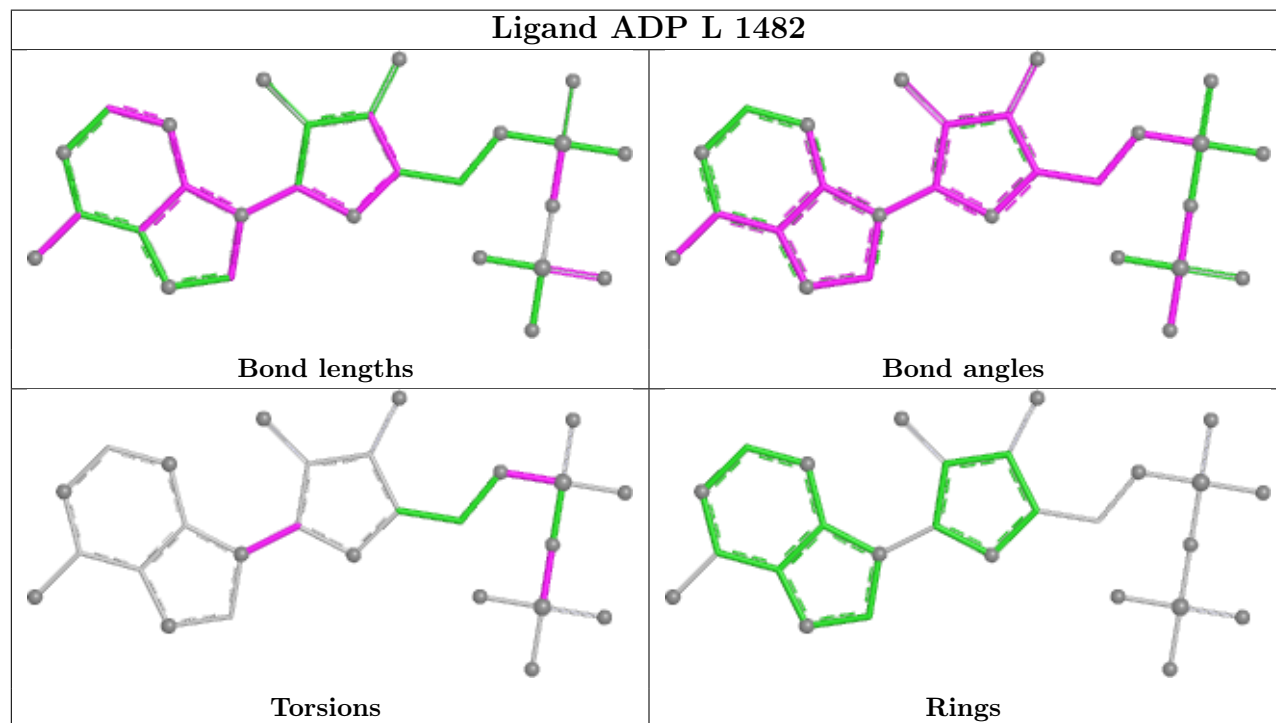




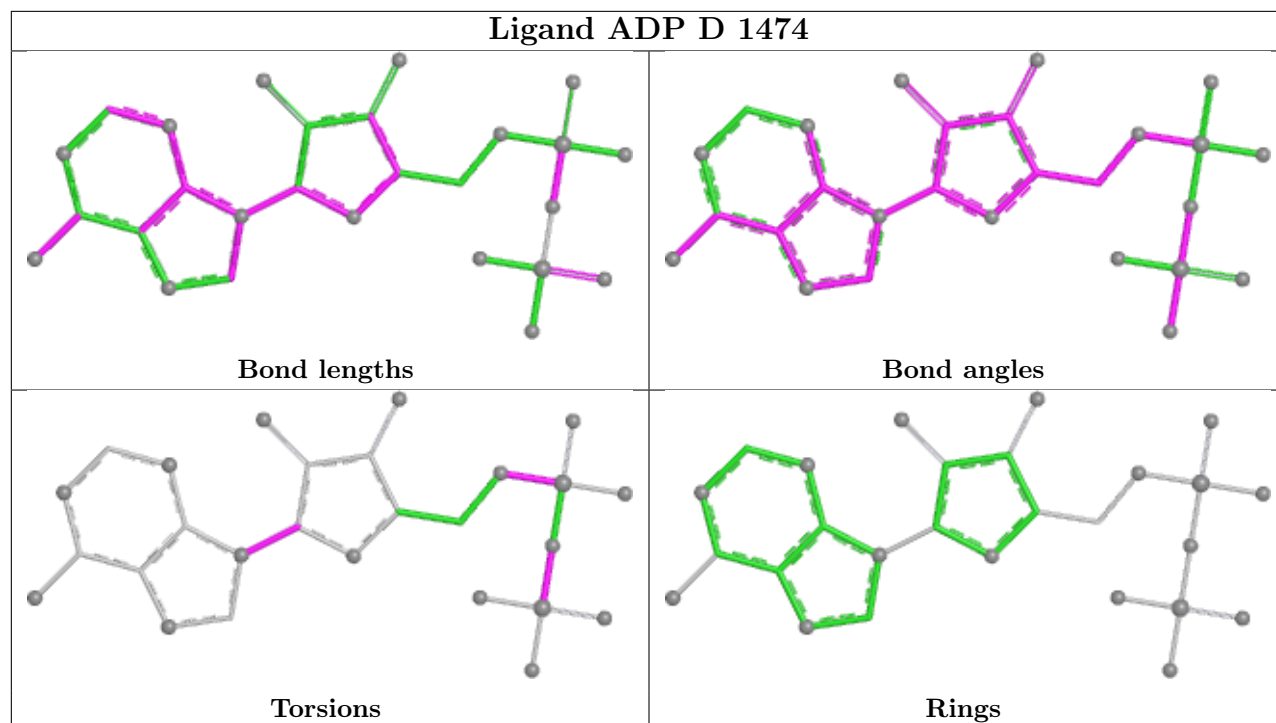
## Ligand ADP E 1475



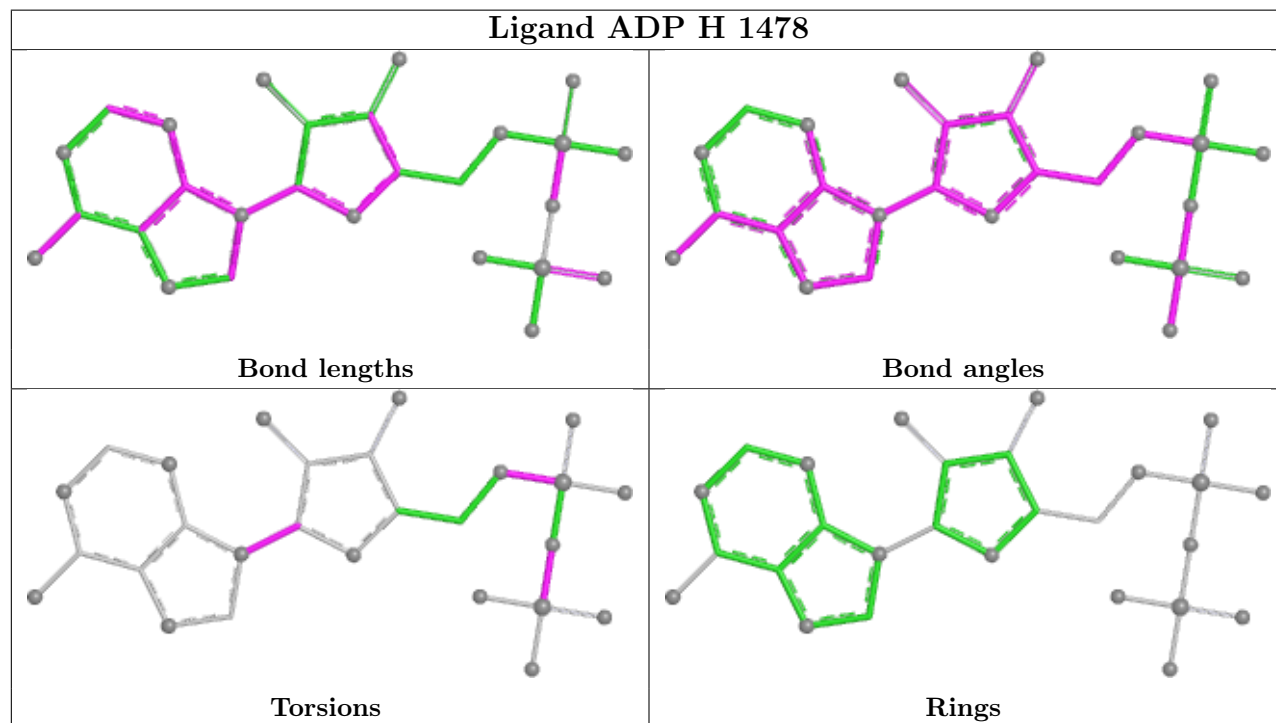
## Ligand ADP L 1482



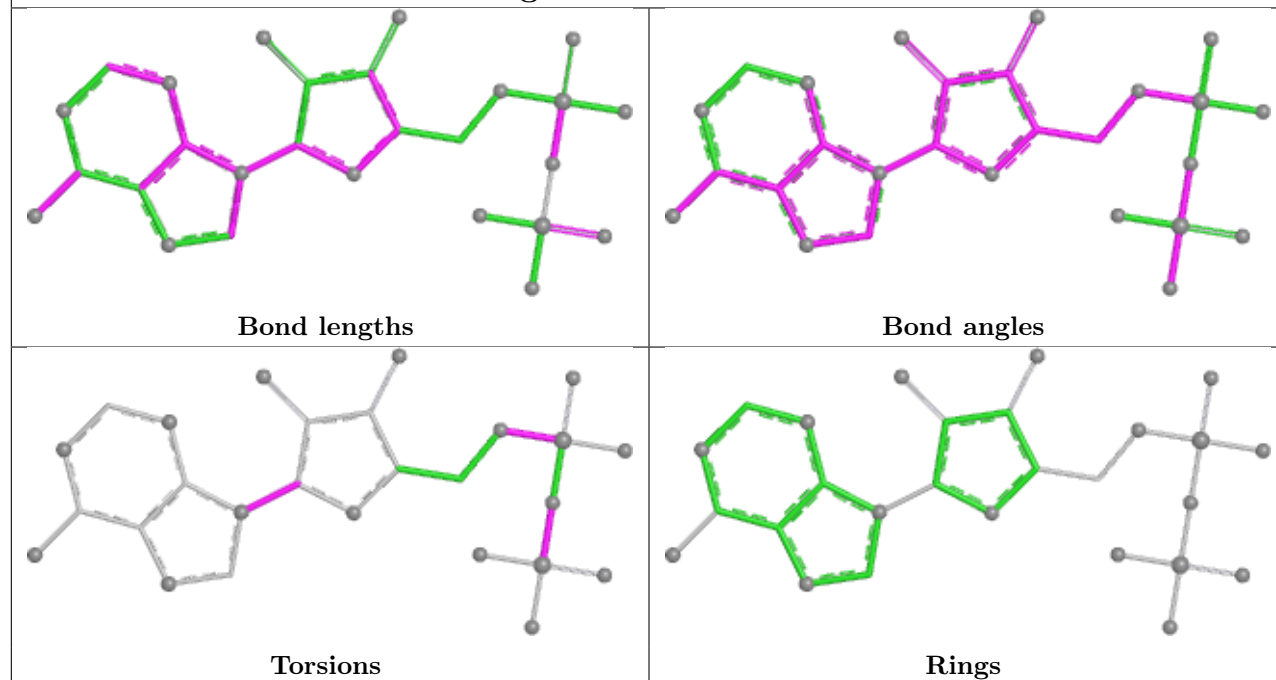
## Ligand ADP D 1474



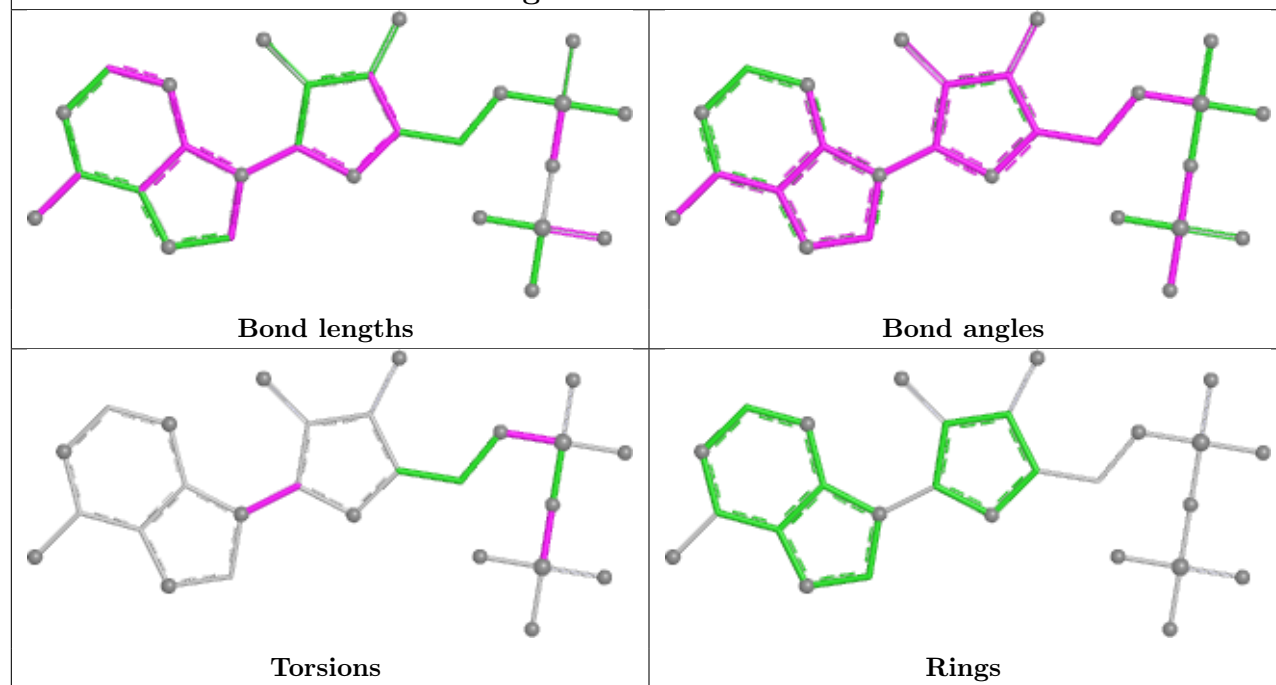
## Ligand ADP H 1478

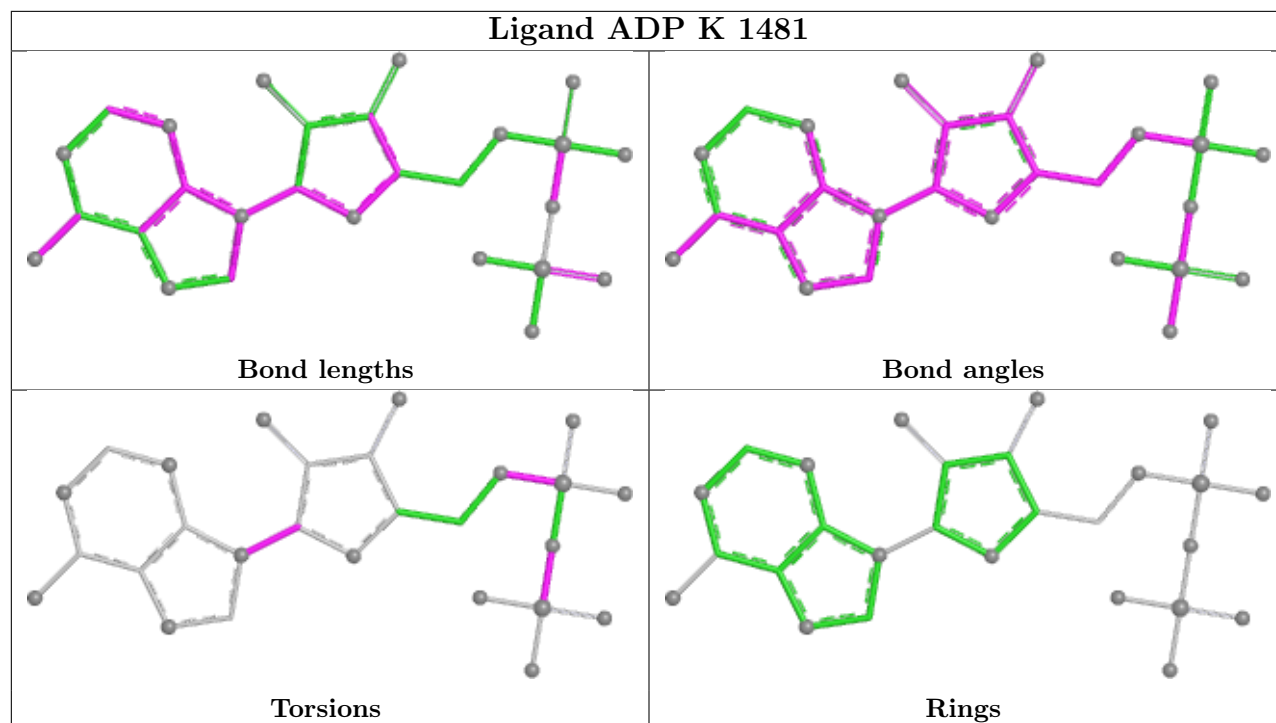


## Ligand ADP A 1471



## Ligand ADP F 1476





## 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     | 468/468 (100%)   | 0.90   | 80 (17%) 4 3   | 12, 39, 82, 100       | 29 (6%)  |
| 1   | B     | 468/468 (100%)   | 0.63   | 39 (8%) 17 14  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | C     | 468/468 (100%)   | 0.51   | 41 (8%) 15 13  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | D     | 468/468 (100%)   | 0.34   | 28 (5%) 27 24  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | E     | 468/468 (100%)   | 0.45   | 34 (7%) 21 18  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | F     | 468/468 (100%)   | 0.58   | 33 (7%) 22 18  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | G     | 468/468 (100%)   | 0.48   | 34 (7%) 21 18  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | H     | 468/468 (100%)   | 0.57   | 49 (10%) 11 9  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | I     | 468/468 (100%)   | 0.57   | 52 (11%) 10 8  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | J     | 468/468 (100%)   | 0.53   | 45 (9%) 13 11  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | K     | 468/468 (100%)   | 0.53   | 44 (9%) 14 12  | 12, 39, 82, 100       | 29 (6%)  |
| 1   | L     | 468/468 (100%)   | 0.65   | 54 (11%) 9 8   | 12, 39, 82, 100       | 29 (6%)  |
| All | All   | 5616/5616 (100%) | 0.56   | 533 (9%) 14 11 | 12, 39, 82, 100       | 348 (6%) |

All (533) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 179 | TYR  | 9.0  |
| 1   | K     | 50  | ASP  | 8.7  |
| 1   | G     | 50  | ASP  | 8.6  |
| 1   | I     | 51  | GLY  | 8.1  |
| 1   | B     | 53  | SER  | 7.9  |
| 1   | H     | 50  | ASP  | 7.8  |
| 1   | G     | 52  | SER  | 7.7  |
| 1   | B     | 51  | GLY  | 7.6  |
| 1   | A     | 52  | SER  | 7.6  |
| 1   | D     | 179 | TYR  | 7.4  |
| 1   | G     | 179 | TYR  | 7.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 50  | ASP  | 7.3  |
| 1   | H     | 179 | TYR  | 7.3  |
| 1   | F     | 179 | TYR  | 7.0  |
| 1   | L     | 50  | ASP  | 6.8  |
| 1   | I     | 54  | ILE  | 6.7  |
| 1   | H     | 52  | SER  | 6.7  |
| 1   | B     | 179 | TYR  | 6.6  |
| 1   | E     | 51  | GLY  | 6.6  |
| 1   | J     | 51  | GLY  | 6.5  |
| 1   | H     | 53  | SER  | 6.5  |
| 1   | K     | 179 | TYR  | 6.4  |
| 1   | A     | 51  | GLY  | 6.3  |
| 1   | J     | 50  | ASP  | 6.3  |
| 1   | L     | 51  | GLY  | 6.3  |
| 1   | D     | 53  | SER  | 6.2  |
| 1   | F     | 50  | ASP  | 6.2  |
| 1   | J     | 179 | TYR  | 6.0  |
| 1   | E     | 179 | TYR  | 6.0  |
| 1   | A     | 50  | ASP  | 5.9  |
| 1   | I     | 52  | SER  | 5.9  |
| 1   | C     | 179 | TYR  | 5.9  |
| 1   | F     | 51  | GLY  | 5.9  |
| 1   | H     | 397 | TYR  | 5.9  |
| 1   | A     | 328 | ALA  | 5.9  |
| 1   | F     | 52  | SER  | 5.8  |
| 1   | K     | 398 | ASP  | 5.7  |
| 1   | A     | 179 | TYR  | 5.7  |
| 1   | L     | 397 | TYR  | 5.6  |
| 1   | E     | 53  | SER  | 5.5  |
| 1   | G     | 51  | GLY  | 5.5  |
| 1   | A     | 296 | TYR  | 5.4  |
| 1   | D     | 51  | GLY  | 5.4  |
| 1   | D     | 50  | ASP  | 5.3  |
| 1   | A     | 273 | SER  | 5.3  |
| 1   | K     | 51  | GLY  | 5.3  |
| 1   | A     | 122 | ASP  | 5.2  |
| 1   | J     | 395 | ASN  | 5.2  |
| 1   | C     | 50  | ASP  | 5.2  |
| 1   | B     | 52  | SER  | 5.1  |
| 1   | J     | 52  | SER  | 5.0  |
| 1   | I     | 53  | SER  | 5.0  |
| 1   | L     | 395 | ASN  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 397 | TYR  | 4.9  |
| 1   | A     | 53  | SER  | 4.9  |
| 1   | H     | 51  | GLY  | 4.8  |
| 1   | D     | 52  | SER  | 4.8  |
| 1   | A     | 275 | ALA  | 4.8  |
| 1   | B     | 50  | ASP  | 4.8  |
| 1   | L     | 53  | SER  | 4.7  |
| 1   | G     | 54  | ILE  | 4.7  |
| 1   | D     | 285 | ASP  | 4.7  |
| 1   | I     | 179 | TYR  | 4.6  |
| 1   | I     | 404 | ALA  | 4.6  |
| 1   | A     | 59  | GLY  | 4.6  |
| 1   | A     | 334 | TYR  | 4.5  |
| 1   | E     | 63  | SER  | 4.5  |
| 1   | K     | 1   | SER  | 4.5  |
| 1   | H     | 8   | MET  | 4.5  |
| 1   | G     | 61  | ASN  | 4.4  |
| 1   | D     | 6   | LEU  | 4.4  |
| 1   | G     | 53  | SER  | 4.4  |
| 1   | H     | 1   | SER  | 4.4  |
| 1   | K     | 402 | GLU  | 4.4  |
| 1   | B     | 397 | TYR  | 4.4  |
| 1   | D     | 60  | ILE  | 4.4  |
| 1   | K     | 2   | ALA  | 4.4  |
| 1   | A     | 285 | ASP  | 4.2  |
| 1   | E     | 50  | ASP  | 4.2  |
| 1   | B     | 1   | SER  | 4.2  |
| 1   | F     | 63  | SER  | 4.2  |
| 1   | J     | 53  | SER  | 4.2  |
| 1   | K     | 44  | GLU  | 4.2  |
| 1   | A     | 279 | THR  | 4.2  |
| 1   | A     | 401 | PRO  | 4.1  |
| 1   | D     | 340 | SER  | 4.1  |
| 1   | J     | 54  | ILE  | 4.1  |
| 1   | C     | 53  | SER  | 4.1  |
| 1   | J     | 62  | GLU  | 4.1  |
| 1   | G     | 6   | LEU  | 4.1  |
| 1   | J     | 396 | LEU  | 4.1  |
| 1   | G     | 49  | PHE  | 4.0  |
| 1   | C     | 60  | ILE  | 4.0  |
| 1   | I     | 273 | SER  | 4.0  |
| 1   | A     | 278 | GLY  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 54  | ILE  | 4.0  |
| 1   | J     | 400 | PRO  | 4.0  |
| 1   | A     | 333 | ALA  | 3.9  |
| 1   | A     | 345 | ILE  | 3.9  |
| 1   | B     | 60  | ILE  | 3.9  |
| 1   | D     | 341 | ALA  | 3.9  |
| 1   | C     | 51  | GLY  | 3.9  |
| 1   | H     | 7   | THR  | 3.9  |
| 1   | A     | 326 | TYR  | 3.8  |
| 1   | K     | 63  | SER  | 3.8  |
| 1   | B     | 39  | ASN  | 3.8  |
| 1   | I     | 59  | GLY  | 3.8  |
| 1   | L     | 408 | PRO  | 3.8  |
| 1   | H     | 4   | HIS  | 3.8  |
| 1   | H     | 54  | ILE  | 3.7  |
| 1   | K     | 328 | ALA  | 3.7  |
| 1   | A     | 348 | VAL  | 3.7  |
| 1   | A     | 277 | ASN  | 3.7  |
| 1   | J     | 4   | HIS  | 3.7  |
| 1   | I     | 397 | TYR  | 3.7  |
| 1   | H     | 395 | ASN  | 3.7  |
| 1   | D     | 63  | SER  | 3.7  |
| 1   | L     | 52  | SER  | 3.7  |
| 1   | F     | 278 | GLY  | 3.6  |
| 1   | G     | 59  | GLY  | 3.6  |
| 1   | L     | 54  | ILE  | 3.6  |
| 1   | C     | 289 | GLY  | 3.6  |
| 1   | J     | 397 | TYR  | 3.6  |
| 1   | I     | 385 | LYS  | 3.6  |
| 1   | G     | 341 | ALA  | 3.6  |
| 1   | J     | 7   | THR  | 3.6  |
| 1   | L     | 49  | PHE  | 3.6  |
| 1   | H     | 328 | ALA  | 3.5  |
| 1   | K     | 326 | TYR  | 3.5  |
| 1   | L     | 63  | SER  | 3.5  |
| 1   | A     | 98  | GLN  | 3.5  |
| 1   | J     | 49  | PHE  | 3.5  |
| 1   | H     | 49  | PHE  | 3.5  |
| 1   | H     | 60  | ILE  | 3.5  |
| 1   | K     | 54  | ILE  | 3.5  |
| 1   | L     | 1   | SER  | 3.5  |
| 1   | L     | 405 | LYS  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 7   | THR  | 3.4  |
| 1   | I     | 170 | GLY  | 3.4  |
| 1   | I     | 3   | GLU  | 3.4  |
| 1   | L     | 333 | ALA  | 3.4  |
| 1   | K     | 60  | ILE  | 3.4  |
| 1   | L     | 296 | TYR  | 3.4  |
| 1   | A     | 351 | PRO  | 3.4  |
| 1   | F     | 53  | SER  | 3.3  |
| 1   | A     | 108 | ALA  | 3.3  |
| 1   | A     | 396 | LEU  | 3.3  |
| 1   | G     | 63  | SER  | 3.3  |
| 1   | J     | 1   | SER  | 3.3  |
| 1   | I     | 49  | PHE  | 3.3  |
| 1   | I     | 394 | LYS  | 3.3  |
| 1   | C     | 2   | ALA  | 3.3  |
| 1   | H     | 349 | ALA  | 3.3  |
| 1   | A     | 288 | ALA  | 3.2  |
| 1   | H     | 402 | GLU  | 3.2  |
| 1   | J     | 273 | SER  | 3.2  |
| 1   | E     | 328 | ALA  | 3.2  |
| 1   | L     | 7   | THR  | 3.2  |
| 1   | B     | 378 | GLY  | 3.2  |
| 1   | G     | 349 | ALA  | 3.2  |
| 1   | F     | 397 | TYR  | 3.2  |
| 1   | I     | 60  | ILE  | 3.2  |
| 1   | G     | 402 | GLU  | 3.2  |
| 1   | K     | 3   | GLU  | 3.2  |
| 1   | G     | 60  | ILE  | 3.2  |
| 1   | K     | 400 | PRO  | 3.1  |
| 1   | E     | 1   | SER  | 3.1  |
| 1   | E     | 52  | SER  | 3.1  |
| 1   | E     | 49  | PHE  | 3.1  |
| 1   | L     | 180 | PHE  | 3.1  |
| 1   | A     | 354 | ARG  | 3.1  |
| 1   | F     | 404 | ALA  | 3.1  |
| 1   | J     | 180 | PHE  | 3.1  |
| 1   | J     | 326 | TYR  | 3.1  |
| 1   | A     | 281 | LEU  | 3.1  |
| 1   | K     | 406 | GLU  | 3.1  |
| 1   | D     | 324 | PRO  | 3.1  |
| 1   | B     | 49  | PHE  | 3.1  |
| 1   | A     | 1   | SER  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 392 | MET  | 3.1  |
| 1   | H     | 324 | PRO  | 3.1  |
| 1   | J     | 328 | ALA  | 3.1  |
| 1   | G     | 395 | ASN  | 3.0  |
| 1   | B     | 54  | ILE  | 3.0  |
| 1   | H     | 178 | GLY  | 3.0  |
| 1   | H     | 63  | SER  | 3.0  |
| 1   | K     | 394 | LYS  | 3.0  |
| 1   | H     | 66  | VAL  | 3.0  |
| 1   | I     | 62  | GLU  | 3.0  |
| 1   | G     | 397 | TYR  | 3.0  |
| 1   | H     | 394 | LYS  | 3.0  |
| 1   | L     | 178 | GLY  | 3.0  |
| 1   | B     | 394 | LYS  | 3.0  |
| 1   | A     | 397 | TYR  | 3.0  |
| 1   | J     | 390 | GLU  | 2.9  |
| 1   | L     | 327 | GLU  | 2.9  |
| 1   | G     | 401 | PRO  | 2.9  |
| 1   | H     | 48  | MET  | 2.9  |
| 1   | A     | 99  | GLY  | 2.9  |
| 1   | K     | 180 | PHE  | 2.9  |
| 1   | L     | 6   | LEU  | 2.9  |
| 1   | H     | 327 | GLU  | 2.9  |
| 1   | L     | 392 | MET  | 2.9  |
| 1   | E     | 64  | ASP  | 2.9  |
| 1   | E     | 296 | TYR  | 2.9  |
| 1   | B     | 178 | GLY  | 2.9  |
| 1   | I     | 405 | LYS  | 2.9  |
| 1   | K     | 403 | GLU  | 2.9  |
| 1   | A     | 106 | SER  | 2.9  |
| 1   | K     | 296 | TYR  | 2.9  |
| 1   | E     | 341 | ALA  | 2.9  |
| 1   | K     | 327 | GLU  | 2.9  |
| 1   | G     | 324 | PRO  | 2.9  |
| 1   | A     | 63  | SER  | 2.9  |
| 1   | C     | 52  | SER  | 2.9  |
| 1   | C     | 397 | TYR  | 2.9  |
| 1   | G     | 326 | TYR  | 2.9  |
| 1   | B     | 38  | VAL  | 2.9  |
| 1   | B     | 396 | LEU  | 2.9  |
| 1   | G     | 328 | ALA  | 2.9  |
| 1   | J     | 5   | VAL  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 49  | PHE  | 2.9  |
| 1   | L     | 339 | ARG  | 2.8  |
| 1   | H     | 106 | SER  | 2.8  |
| 1   | E     | 396 | LEU  | 2.8  |
| 1   | L     | 60  | ILE  | 2.8  |
| 1   | L     | 394 | LYS  | 2.8  |
| 1   | C     | 325 | GLY  | 2.8  |
| 1   | J     | 398 | ASP  | 2.8  |
| 1   | D     | 49  | PHE  | 2.8  |
| 1   | C     | 386 | ILE  | 2.8  |
| 1   | I     | 407 | ILE  | 2.8  |
| 1   | E     | 395 | ASN  | 2.8  |
| 1   | D     | 64  | ASP  | 2.8  |
| 1   | D     | 326 | TYR  | 2.8  |
| 1   | A     | 346 | PRO  | 2.8  |
| 1   | G     | 339 | ARG  | 2.8  |
| 1   | C     | 293 | GLN  | 2.8  |
| 1   | A     | 349 | ALA  | 2.8  |
| 1   | H     | 347 | VAL  | 2.8  |
| 1   | L     | 328 | ALA  | 2.8  |
| 1   | A     | 126 | PHE  | 2.8  |
| 1   | I     | 339 | ARG  | 2.8  |
| 1   | K     | 340 | SER  | 2.7  |
| 1   | I     | 4   | HIS  | 2.7  |
| 1   | A     | 353 | ALA  | 2.7  |
| 1   | B     | 40  | ALA  | 2.7  |
| 1   | E     | 354 | ARG  | 2.7  |
| 1   | C     | 394 | LYS  | 2.7  |
| 1   | D     | 54  | ILE  | 2.7  |
| 1   | C     | 6   | LEU  | 2.7  |
| 1   | B     | 284 | GLY  | 2.7  |
| 1   | K     | 53  | SER  | 2.7  |
| 1   | K     | 325 | GLY  | 2.7  |
| 1   | K     | 64  | ASP  | 2.7  |
| 1   | K     | 399 | LEU  | 2.7  |
| 1   | K     | 431 | GLY  | 2.7  |
| 1   | B     | 377 | ALA  | 2.7  |
| 1   | A     | 391 | PRO  | 2.7  |
| 1   | G     | 351 | PRO  | 2.7  |
| 1   | L     | 326 | TYR  | 2.7  |
| 1   | L     | 332 | LEU  | 2.7  |
| 1   | A     | 284 | GLY  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 390 | GLU  | 2.7  |
| 1   | B     | 401 | PRO  | 2.7  |
| 1   | C     | 324 | PRO  | 2.7  |
| 1   | H     | 398 | ASP  | 2.7  |
| 1   | C     | 326 | TYR  | 2.6  |
| 1   | E     | 397 | TYR  | 2.6  |
| 1   | A     | 46  | GLY  | 2.6  |
| 1   | J     | 278 | GLY  | 2.6  |
| 1   | A     | 385 | LYS  | 2.6  |
| 1   | F     | 349 | ALA  | 2.6  |
| 1   | J     | 63  | SER  | 2.6  |
| 1   | H     | 401 | PRO  | 2.6  |
| 1   | L     | 361 | PRO  | 2.6  |
| 1   | L     | 285 | ASP  | 2.6  |
| 1   | H     | 396 | LEU  | 2.6  |
| 1   | A     | 112 | GLU  | 2.6  |
| 1   | H     | 383 | LYS  | 2.6  |
| 1   | A     | 111 | ALA  | 2.6  |
| 1   | B     | 2   | ALA  | 2.6  |
| 1   | C     | 404 | ALA  | 2.6  |
| 1   | G     | 404 | ALA  | 2.6  |
| 1   | J     | 285 | ASP  | 2.6  |
| 1   | E     | 60  | ILE  | 2.6  |
| 1   | B     | 6   | LEU  | 2.6  |
| 1   | D     | 296 | TYR  | 2.6  |
| 1   | I     | 326 | TYR  | 2.6  |
| 1   | I     | 396 | LEU  | 2.6  |
| 1   | B     | 344 | ARG  | 2.6  |
| 1   | B     | 327 | GLU  | 2.6  |
| 1   | A     | 378 | GLY  | 2.6  |
| 1   | C     | 328 | ALA  | 2.6  |
| 1   | E     | 2   | ALA  | 2.6  |
| 1   | H     | 400 | PRO  | 2.6  |
| 1   | C     | 7   | THR  | 2.6  |
| 1   | L     | 398 | ASP  | 2.6  |
| 1   | K     | 41  | GLU  | 2.6  |
| 1   | D     | 404 | ALA  | 2.6  |
| 1   | I     | 108 | ALA  | 2.6  |
| 1   | L     | 323 | VAL  | 2.6  |
| 1   | L     | 61  | ASN  | 2.6  |
| 1   | L     | 98  | GLN  | 2.6  |
| 1   | H     | 331 | MET  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 385 | LYS  | 2.5  |
| 1   | L     | 58  | LYS  | 2.5  |
| 1   | B     | 4   | HIS  | 2.5  |
| 1   | H     | 12  | HIS  | 2.5  |
| 1   | J     | 403 | GLU  | 2.5  |
| 1   | B     | 328 | ALA  | 2.5  |
| 1   | B     | 61  | ASN  | 2.5  |
| 1   | D     | 395 | ASN  | 2.5  |
| 1   | K     | 61  | ASN  | 2.5  |
| 1   | B     | 392 | MET  | 2.5  |
| 1   | H     | 393 | ASP  | 2.5  |
| 1   | I     | 64  | ASP  | 2.5  |
| 1   | A     | 274 | LEU  | 2.5  |
| 1   | A     | 327 | GLU  | 2.5  |
| 1   | C     | 327 | GLU  | 2.5  |
| 1   | E     | 62  | GLU  | 2.5  |
| 1   | I     | 403 | GLU  | 2.5  |
| 1   | I     | 401 | PRO  | 2.5  |
| 1   | I     | 328 | ALA  | 2.5  |
| 1   | A     | 123 | THR  | 2.5  |
| 1   | H     | 10  | ASN  | 2.5  |
| 1   | A     | 295 | LEU  | 2.5  |
| 1   | C     | 339 | ARG  | 2.5  |
| 1   | I     | 398 | ASP  | 2.5  |
| 1   | J     | 337 | ARG  | 2.5  |
| 1   | J     | 401 | PRO  | 2.5  |
| 1   | B     | 8   | MET  | 2.5  |
| 1   | J     | 98  | GLN  | 2.5  |
| 1   | J     | 404 | ALA  | 2.5  |
| 1   | B     | 7   | THR  | 2.5  |
| 1   | J     | 385 | LYS  | 2.5  |
| 1   | K     | 52  | SER  | 2.5  |
| 1   | A     | 4   | HIS  | 2.5  |
| 1   | F     | 3   | GLU  | 2.5  |
| 1   | C     | 381 | GLY  | 2.5  |
| 1   | L     | 351 | PRO  | 2.5  |
| 1   | A     | 49  | PHE  | 2.5  |
| 1   | A     | 276 | LYS  | 2.4  |
| 1   | A     | 356 | ILE  | 2.4  |
| 1   | I     | 165 | GLU  | 2.4  |
| 1   | K     | 13  | GLU  | 2.4  |
| 1   | K     | 178 | GLY  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 6   | LEU  | 2.4  |
| 1   | C     | 403 | GLU  | 2.4  |
| 1   | J     | 437 | GLU  | 2.4  |
| 1   | K     | 165 | GLU  | 2.4  |
| 1   | L     | 390 | GLU  | 2.4  |
| 1   | D     | 59  | GLY  | 2.4  |
| 1   | F     | 326 | TYR  | 2.4  |
| 1   | E     | 333 | ALA  | 2.4  |
| 1   | J     | 339 | ARG  | 2.4  |
| 1   | L     | 344 | ARG  | 2.4  |
| 1   | C     | 407 | ILE  | 2.4  |
| 1   | F     | 399 | LEU  | 2.4  |
| 1   | H     | 6   | LEU  | 2.4  |
| 1   | I     | 10  | ASN  | 2.4  |
| 1   | A     | 283 | SER  | 2.4  |
| 1   | L     | 403 | GLU  | 2.4  |
| 1   | L     | 401 | PRO  | 2.4  |
| 1   | G     | 5   | VAL  | 2.4  |
| 1   | A     | 43  | PHE  | 2.4  |
| 1   | I     | 341 | ALA  | 2.4  |
| 1   | D     | 396 | LEU  | 2.4  |
| 1   | I     | 63  | SER  | 2.4  |
| 1   | J     | 327 | GLU  | 2.4  |
| 1   | L     | 48  | MET  | 2.4  |
| 1   | B     | 35  | ALA  | 2.4  |
| 1   | C     | 349 | ALA  | 2.4  |
| 1   | A     | 125 | LEU  | 2.3  |
| 1   | D     | 4   | HIS  | 2.3  |
| 1   | G     | 398 | ASP  | 2.3  |
| 1   | B     | 372 | ALA  | 2.3  |
| 1   | C     | 282 | PHE  | 2.3  |
| 1   | F     | 180 | PHE  | 2.3  |
| 1   | F     | 364 | ALA  | 2.3  |
| 1   | G     | 396 | LEU  | 2.3  |
| 1   | L     | 407 | ILE  | 2.3  |
| 1   | E     | 10  | ASN  | 2.3  |
| 1   | G     | 293 | GLN  | 2.3  |
| 1   | H     | 5   | VAL  | 2.3  |
| 1   | D     | 328 | ALA  | 2.3  |
| 1   | A     | 54  | ILE  | 2.3  |
| 1   | G     | 296 | TYR  | 2.3  |
| 1   | A     | 437 | GLU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 64  | ASP  | 2.3  |
| 1   | H     | 64  | ASP  | 2.3  |
| 1   | I     | 1   | SER  | 2.3  |
| 1   | A     | 60  | ILE  | 2.3  |
| 1   | F     | 288 | ALA  | 2.3  |
| 1   | K     | 48  | MET  | 2.3  |
| 1   | J     | 296 | TYR  | 2.3  |
| 1   | F     | 327 | GLU  | 2.3  |
| 1   | I     | 395 | ASN  | 2.3  |
| 1   | H     | 337 | ARG  | 2.3  |
| 1   | H     | 339 | ARG  | 2.3  |
| 1   | K     | 359 | ARG  | 2.3  |
| 1   | I     | 98  | GLN  | 2.3  |
| 1   | A     | 330 | VAL  | 2.3  |
| 1   | A     | 282 | PHE  | 2.3  |
| 1   | B     | 43  | PHE  | 2.3  |
| 1   | A     | 404 | ALA  | 2.2  |
| 1   | H     | 407 | ILE  | 2.2  |
| 1   | L     | 404 | ALA  | 2.2  |
| 1   | G     | 394 | LYS  | 2.2  |
| 1   | I     | 392 | MET  | 2.2  |
| 1   | B     | 390 | GLU  | 2.2  |
| 1   | L     | 402 | GLU  | 2.2  |
| 1   | F     | 296 | TYR  | 2.2  |
| 1   | A     | 325 | GLY  | 2.2  |
| 1   | F     | 358 | VAL  | 2.2  |
| 1   | I     | 6   | LEU  | 2.2  |
| 1   | A     | 91  | ILE  | 2.2  |
| 1   | D     | 180 | PHE  | 2.2  |
| 1   | H     | 180 | PHE  | 2.2  |
| 1   | F     | 353 | ALA  | 2.2  |
| 1   | J     | 8   | MET  | 2.2  |
| 1   | B     | 41  | GLU  | 2.2  |
| 1   | I     | 402 | GLU  | 2.2  |
| 1   | C     | 265 | GLY  | 2.2  |
| 1   | E     | 278 | GLY  | 2.2  |
| 1   | G     | 291 | SER  | 2.2  |
| 1   | J     | 178 | GLY  | 2.2  |
| 1   | B     | 290 | LEU  | 2.2  |
| 1   | C     | 405 | LYS  | 2.2  |
| 1   | G     | 286 | LYS  | 2.2  |
| 1   | F     | 331 | MET  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 60  | ILE  | 2.2  |
| 1   | K     | 392 | MET  | 2.2  |
| 1   | B     | 404 | ALA  | 2.2  |
| 1   | C     | 121 | ALA  | 2.2  |
| 1   | I     | 353 | ALA  | 2.2  |
| 1   | K     | 7   | THR  | 2.2  |
| 1   | C     | 391 | PRO  | 2.2  |
| 1   | A     | 389 | GLY  | 2.2  |
| 1   | C     | 389 | GLY  | 2.2  |
| 1   | E     | 378 | GLY  | 2.2  |
| 1   | C     | 1   | SER  | 2.2  |
| 1   | J     | 340 | SER  | 2.2  |
| 1   | I     | 331 | MET  | 2.2  |
| 1   | L     | 347 | VAL  | 2.2  |
| 1   | A     | 387 | HIS  | 2.2  |
| 1   | C     | 49  | PHE  | 2.2  |
| 1   | C     | 180 | PHE  | 2.2  |
| 1   | H     | 62  | GLU  | 2.2  |
| 1   | J     | 3   | GLU  | 2.2  |
| 1   | A     | 329 | PRO  | 2.2  |
| 1   | D     | 401 | PRO  | 2.2  |
| 1   | L     | 391 | PRO  | 2.2  |
| 1   | I     | 399 | LEU  | 2.2  |
| 1   | H     | 122 | ASP  | 2.2  |
| 1   | L     | 64  | ASP  | 2.2  |
| 1   | L     | 393 | ASP  | 2.2  |
| 1   | L     | 273 | SER  | 2.2  |
| 1   | E     | 307 | ALA  | 2.1  |
| 1   | F     | 108 | ALA  | 2.1  |
| 1   | F     | 112 | GLU  | 2.1  |
| 1   | K     | 45  | GLU  | 2.1  |
| 1   | C     | 58  | LYS  | 2.1  |
| 1   | A     | 399 | LEU  | 2.1  |
| 1   | A     | 124 | VAL  | 2.1  |
| 1   | A     | 398 | ASP  | 2.1  |
| 1   | L     | 2   | ALA  | 2.1  |
| 1   | E     | 3   | GLU  | 2.1  |
| 1   | A     | 332 | LEU  | 2.1  |
| 1   | B     | 399 | LEU  | 2.1  |
| 1   | F     | 338 | ASN  | 2.1  |
| 1   | L     | 338 | ASN  | 2.1  |
| 1   | B     | 325 | GLY  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 378 | GLY  | 2.1  |
| 1   | G     | 284 | GLY  | 2.1  |
| 1   | D     | 398 | ASP  | 2.1  |
| 1   | L     | 33  | ILE  | 2.1  |
| 1   | L     | 11  | GLU  | 2.1  |
| 1   | E     | 339 | ARG  | 2.1  |
| 1   | A     | 230 | LYS  | 2.1  |
| 1   | L     | 286 | LYS  | 2.1  |
| 1   | F     | 324 | PRO  | 2.1  |
| 1   | H     | 408 | PRO  | 2.1  |
| 1   | I     | 324 | PRO  | 2.1  |
| 1   | L     | 324 | PRO  | 2.1  |
| 1   | E     | 392 | MET  | 2.1  |
| 1   | K     | 98  | GLN  | 2.1  |
| 1   | I     | 334 | TYR  | 2.1  |
| 1   | K     | 59  | GLY  | 2.1  |
| 1   | E     | 386 | ILE  | 2.1  |
| 1   | F     | 54  | ILE  | 2.1  |
| 1   | A     | 117 | ALA  | 2.1  |
| 1   | C     | 63  | SER  | 2.1  |
| 1   | C     | 292 | GLU  | 2.1  |
| 1   | F     | 165 | GLU  | 2.1  |
| 1   | I     | 112 | GLU  | 2.1  |
| 1   | I     | 327 | GLU  | 2.1  |
| 1   | I     | 336 | ALA  | 2.1  |
| 1   | K     | 121 | ALA  | 2.1  |
| 1   | A     | 293 | GLN  | 2.1  |
| 1   | I     | 293 | GLN  | 2.1  |
| 1   | A     | 280 | ASN  | 2.1  |
| 1   | A     | 299 | GLY  | 2.1  |
| 1   | H     | 55  | GLY  | 2.1  |
| 1   | J     | 389 | GLY  | 2.1  |
| 1   | A     | 287 | TYR  | 2.1  |
| 1   | F     | 334 | TYR  | 2.1  |
| 1   | H     | 326 | TYR  | 2.1  |
| 1   | I     | 287 | TYR  | 2.1  |
| 1   | A     | 344 | ARG  | 2.0  |
| 1   | C     | 398 | ASP  | 2.0  |
| 1   | F     | 393 | ASP  | 2.0  |
| 1   | I     | 344 | ARG  | 2.0  |
| 1   | J     | 64  | ASP  | 2.0  |
| 1   | D     | 41  | GLU  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 1   | SER  | 2.0  |
| 1   | I     | 340 | SER  | 2.0  |
| 1   | F     | 388 | PRO  | 2.0  |
| 1   | C     | 54  | ILE  | 2.0  |
| 1   | H     | 296 | TYR  | 2.0  |
| 1   | A     | 355 | ARG  | 2.0  |
| 1   | E     | 282 | PHE  | 2.0  |
| 1   | J     | 344 | ARG  | 2.0  |
| 1   | E     | 292 | GLU  | 2.0  |
| 1   | E     | 58  | LYS  | 2.0  |
| 1   | F     | 394 | LYS  | 2.0  |
| 1   | G     | 2   | ALA  | 2.0  |
| 1   | I     | 393 | ASP  | 2.0  |
| 1   | J     | 341 | ALA  | 2.0  |
| 1   | H     | 9   | LEU  | 2.0  |
| 1   | A     | 432 | GLY  | 2.0  |
| 1   | F     | 325 | GLY  | 2.0  |
| 1   | K     | 344 | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | ADP  | F     | 1476 | 27/27 | 0.64 | 0.20 | 20,78,100,100               | 27    |
| 3   | ADP  | I     | 1479 | 27/27 | 0.66 | 0.23 | 20,78,100,100               | 27    |
| 3   | ADP  | L     | 1482 | 27/27 | 0.71 | 0.23 | 20,78,100,100               | 27    |
| 3   | ADP  | B     | 1472 | 27/27 | 0.72 | 0.21 | 20,78,100,100               | 27    |
| 3   | ADP  | C     | 1473 | 27/27 | 0.73 | 0.20 | 20,78,100,100               | 27    |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | ADP  | A     | 1471 | 27/27 | 0.74 | 0.20 | 20,78,100,100               | 27    |
| 3   | ADP  | E     | 1475 | 27/27 | 0.75 | 0.17 | 20,78,100,100               | 27    |
| 3   | ADP  | D     | 1474 | 27/27 | 0.75 | 0.23 | 20,78,100,100               | 27    |
| 4   | TL   | I     | 473  | 1/1   | 0.75 | 0.25 | 67,67,67,67                 | 1     |
| 3   | ADP  | K     | 1481 | 27/27 | 0.76 | 0.22 | 20,78,100,100               | 27    |
| 4   | TL   | L     | 473  | 1/1   | 0.77 | 0.21 | 67,67,67,67                 | 1     |
| 3   | ADP  | H     | 1478 | 27/27 | 0.78 | 0.21 | 20,78,100,100               | 27    |
| 5   | MPD  | B     | 1484 | 8/8   | 0.81 | 0.32 | 16,43,64,74                 | 8     |
| 4   | TL   | J     | 474  | 1/1   | 0.82 | 0.10 | 75,75,75,75                 | 1     |
| 3   | ADP  | G     | 1477 | 27/27 | 0.83 | 0.20 | 20,78,100,100               | 27    |
| 3   | ADP  | J     | 1480 | 27/27 | 0.83 | 0.23 | 20,78,100,100               | 27    |
| 4   | TL   | A     | 473  | 1/1   | 0.84 | 0.19 | 67,67,67,67                 | 1     |
| 4   | TL   | K     | 473  | 1/1   | 0.84 | 0.12 | 67,67,67,67                 | 1     |
| 4   | TL   | F     | 473  | 1/1   | 0.85 | 0.14 | 67,67,67,67                 | 1     |
| 5   | MPD  | D     | 1486 | 8/8   | 0.86 | 0.32 | 16,43,64,74                 | 8     |
| 5   | MPD  | I     | 1491 | 8/8   | 0.86 | 0.28 | 16,43,64,74                 | 8     |
| 5   | MPD  | A     | 1483 | 8/8   | 0.87 | 0.32 | 16,43,64,74                 | 8     |
| 4   | TL   | C     | 474  | 1/1   | 0.87 | 0.08 | 75,75,75,75                 | 1     |
| 4   | TL   | H     | 473  | 1/1   | 0.88 | 0.18 | 67,67,67,67                 | 1     |
| 5   | MPD  | C     | 1485 | 8/8   | 0.88 | 0.27 | 16,43,64,74                 | 8     |
| 5   | MPD  | E     | 1487 | 8/8   | 0.90 | 0.25 | 16,43,64,74                 | 8     |
| 5   | MPD  | H     | 1490 | 8/8   | 0.91 | 0.26 | 16,43,64,74                 | 8     |
| 5   | MPD  | F     | 1488 | 8/8   | 0.91 | 0.23 | 16,43,64,74                 | 8     |
| 4   | TL   | A     | 474  | 1/1   | 0.92 | 0.07 | 75,75,75,75                 | 1     |
| 5   | MPD  | G     | 1489 | 8/8   | 0.92 | 0.29 | 16,43,64,74                 | 8     |
| 5   | MPD  | J     | 1492 | 8/8   | 0.92 | 0.28 | 16,43,64,74                 | 8     |
| 5   | MPD  | K     | 1493 | 8/8   | 0.92 | 0.23 | 16,43,64,74                 | 8     |
| 4   | TL   | E     | 473  | 1/1   | 0.93 | 0.09 | 67,67,67,67                 | 1     |
| 5   | MPD  | L     | 1494 | 8/8   | 0.93 | 0.24 | 16,43,64,74                 | 8     |
| 2   | MN   | F     | 470  | 1/1   | 0.94 | 0.08 | 41,41,41,41                 | 0     |
| 4   | TL   | G     | 474  | 1/1   | 0.94 | 0.08 | 75,75,75,75                 | 1     |
| 4   | TL   | D     | 473  | 1/1   | 0.94 | 0.07 | 67,67,67,67                 | 1     |
| 4   | TL   | H     | 474  | 1/1   | 0.94 | 0.06 | 75,75,75,75                 | 1     |
| 4   | TL   | B     | 473  | 1/1   | 0.94 | 0.08 | 67,67,67,67                 | 1     |
| 4   | TL   | J     | 473  | 1/1   | 0.94 | 0.22 | 67,67,67,67                 | 1     |
| 4   | TL   | E     | 474  | 1/1   | 0.94 | 0.07 | 75,75,75,75                 | 1     |
| 4   | TL   | D     | 474  | 1/1   | 0.95 | 0.06 | 75,75,75,75                 | 1     |
| 4   | TL   | B     | 474  | 1/1   | 0.95 | 0.06 | 75,75,75,75                 | 1     |
| 2   | MN   | A     | 469  | 1/1   | 0.95 | 0.08 | 34,34,34,34                 | 0     |
| 2   | MN   | B     | 469  | 1/1   | 0.95 | 0.06 | 34,34,34,34                 | 0     |
| 4   | TL   | G     | 473  | 1/1   | 0.96 | 0.09 | 67,67,67,67                 | 1     |
| 4   | TL   | I     | 474  | 1/1   | 0.96 | 0.07 | 75,75,75,75                 | 1     |

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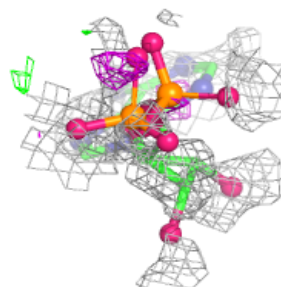
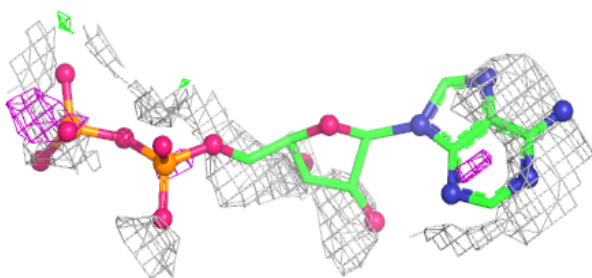
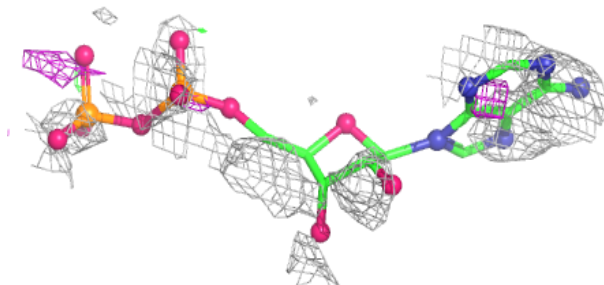
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | MN   | A     | 470 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 4   | TL   | L     | 474 | 1/1   | 0.96 | 0.07 | 75,75,75,75                 | 1     |
| 2   | MN   | C     | 469 | 1/1   | 0.97 | 0.05 | 34,34,34,34                 | 0     |
| 4   | TL   | F     | 474 | 1/1   | 0.97 | 0.06 | 75,75,75,75                 | 1     |
| 4   | TL   | C     | 473 | 1/1   | 0.97 | 0.12 | 67,67,67,67                 | 1     |
| 4   | TL   | K     | 474 | 1/1   | 0.97 | 0.05 | 75,75,75,75                 | 1     |
| 2   | MN   | H     | 469 | 1/1   | 0.97 | 0.03 | 34,34,34,34                 | 0     |
| 2   | MN   | I     | 470 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 2   | MN   | C     | 470 | 1/1   | 0.97 | 0.04 | 41,41,41,41                 | 0     |
| 2   | MN   | D     | 470 | 1/1   | 0.97 | 0.04 | 41,41,41,41                 | 0     |
| 2   | MN   | F     | 469 | 1/1   | 0.97 | 0.07 | 34,34,34,34                 | 0     |
| 2   | MN   | E     | 469 | 1/1   | 0.98 | 0.04 | 34,34,34,34                 | 0     |
| 2   | MN   | G     | 470 | 1/1   | 0.98 | 0.07 | 41,41,41,41                 | 0     |
| 2   | MN   | E     | 470 | 1/1   | 0.98 | 0.03 | 41,41,41,41                 | 0     |
| 2   | MN   | B     | 470 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 2   | MN   | J     | 469 | 1/1   | 0.98 | 0.07 | 34,34,34,34                 | 0     |
| 2   | MN   | J     | 470 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |
| 2   | MN   | K     | 469 | 1/1   | 0.98 | 0.05 | 34,34,34,34                 | 0     |
| 2   | MN   | L     | 470 | 1/1   | 0.98 | 0.11 | 41,41,41,41                 | 0     |
| 2   | MN   | G     | 469 | 1/1   | 0.99 | 0.03 | 34,34,34,34                 | 0     |
| 2   | MN   | H     | 470 | 1/1   | 0.99 | 0.04 | 41,41,41,41                 | 0     |
| 2   | MN   | I     | 469 | 1/1   | 0.99 | 0.02 | 34,34,34,34                 | 0     |
| 2   | MN   | K     | 470 | 1/1   | 0.99 | 0.10 | 41,41,41,41                 | 0     |
| 2   | MN   | L     | 469 | 1/1   | 0.99 | 0.04 | 34,34,34,34                 | 0     |
| 2   | MN   | D     | 469 | 1/1   | 0.99 | 0.02 | 34,34,34,34                 | 0     |

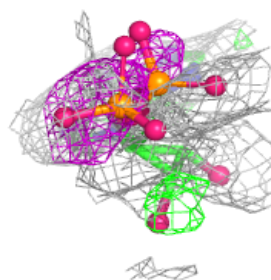
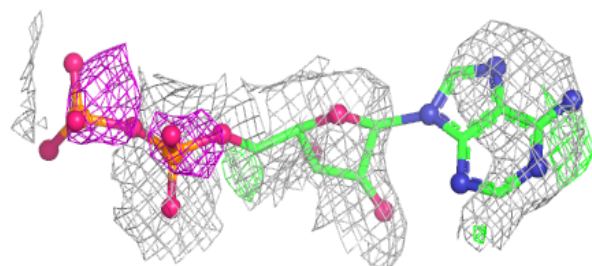
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP F 1476:**

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

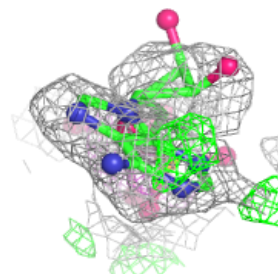
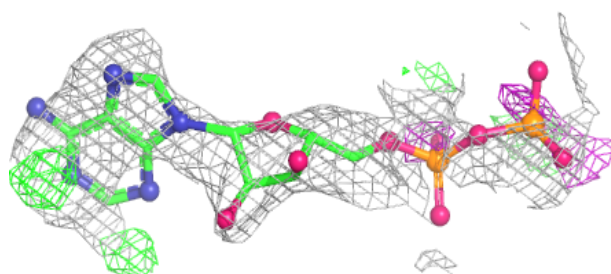
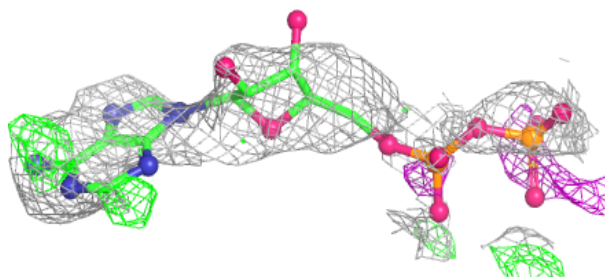
**Electron density around ADP I 1479:**

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

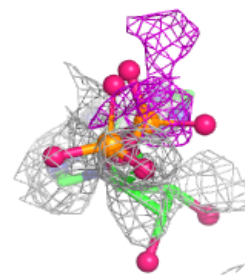
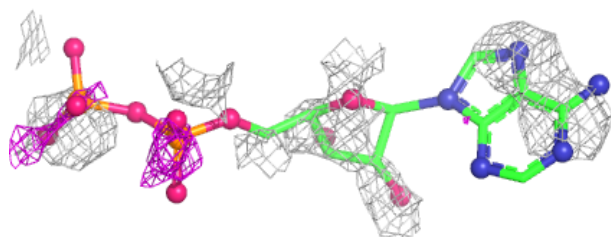
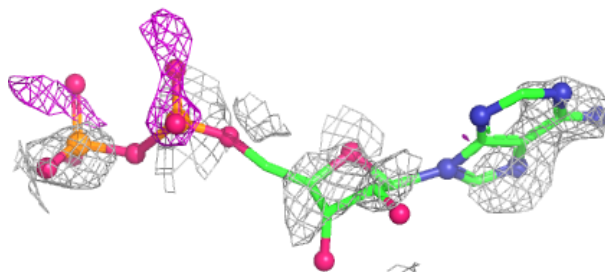


**Electron density around ADP L 1482:**

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

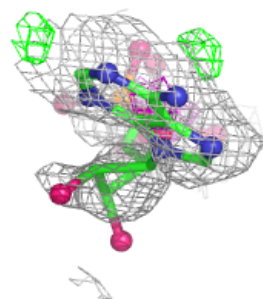
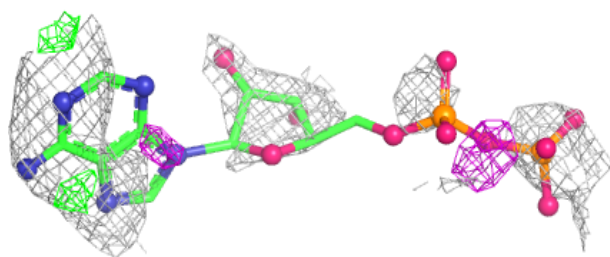
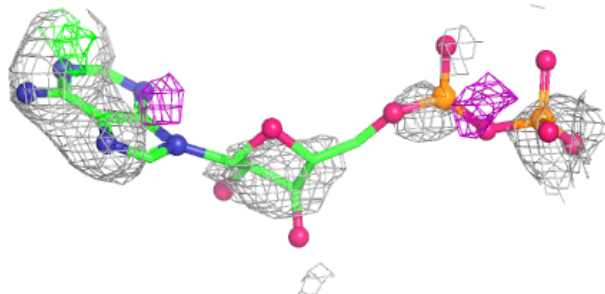
**Electron density around ADP B 1472:**

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

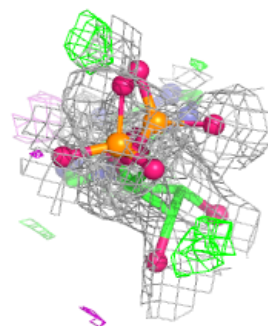
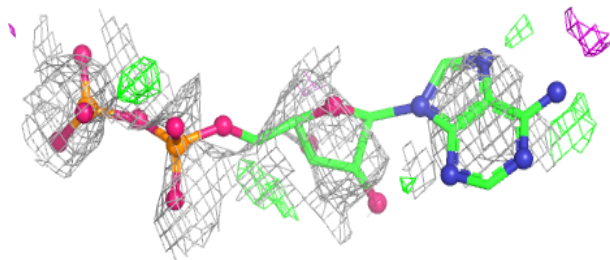
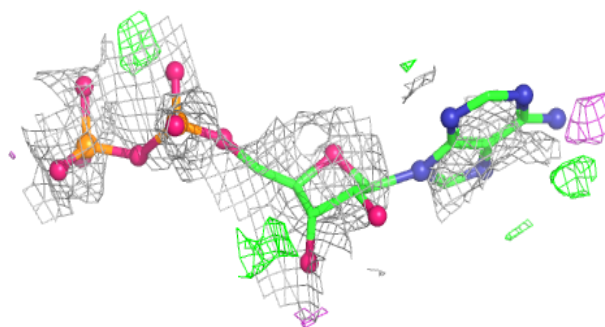


**Electron density around ADP C 1473:**

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

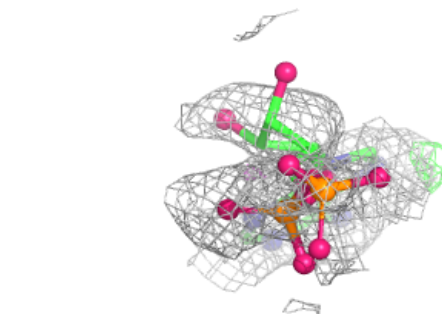
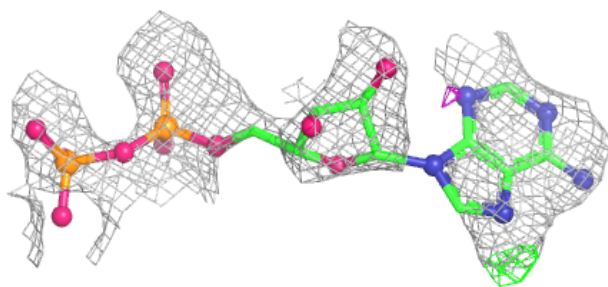
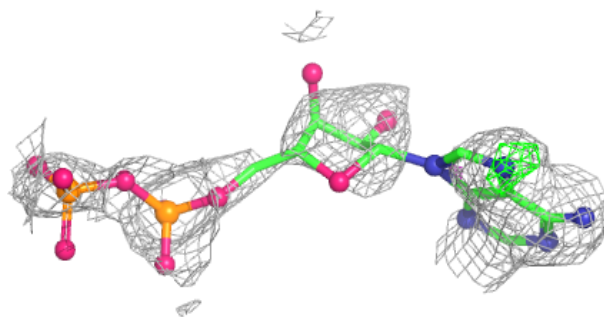
**Electron density around ADP A 1471:**

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

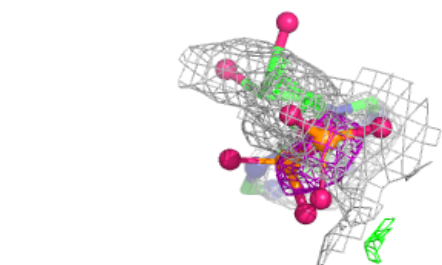
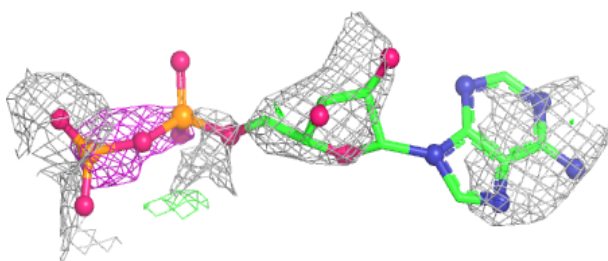
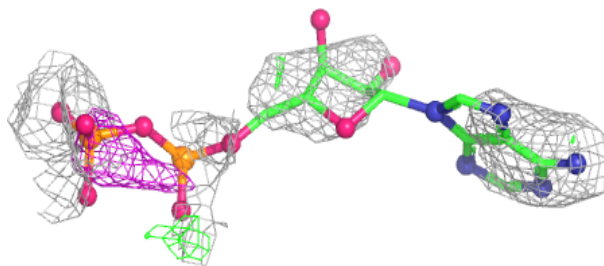


**Electron density around ADP E 1475:**

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

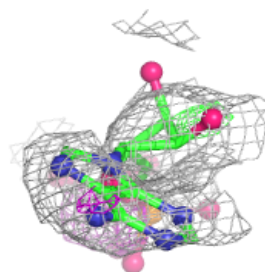
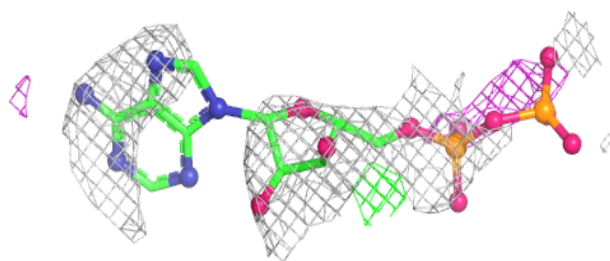
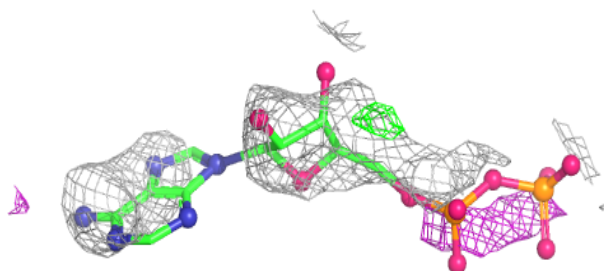
**Electron density around ADP D 1474:**

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

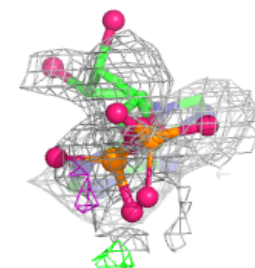
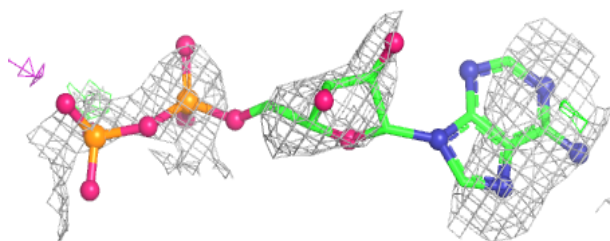
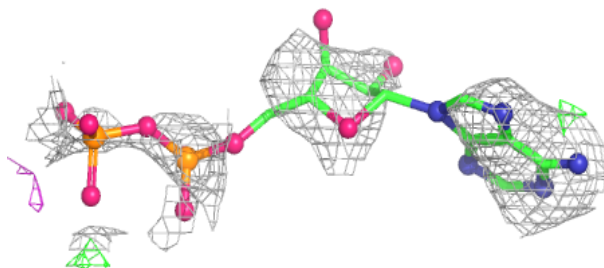


**Electron density around ADP K 1481:**

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

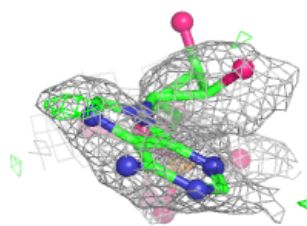
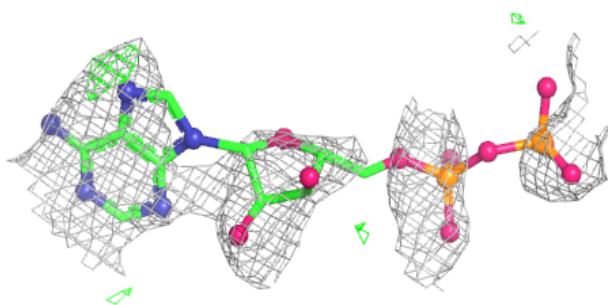
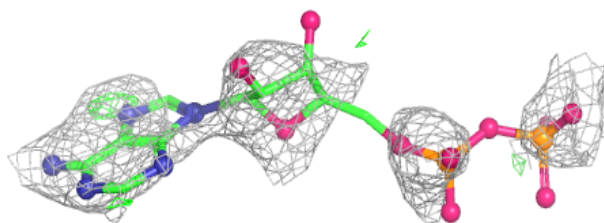
**Electron density around ADP H 1478:**

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

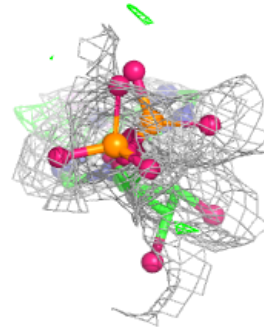
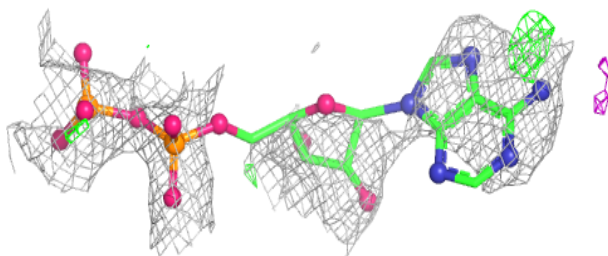
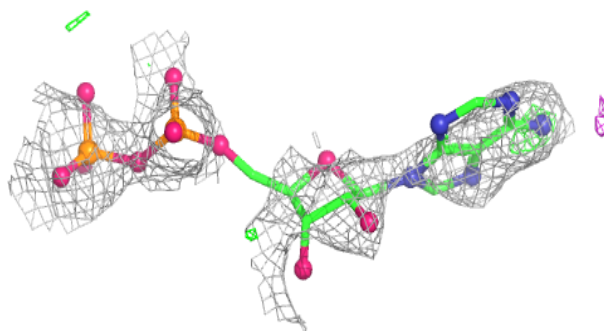


**Electron density around ADP G 1477:**

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

**Electron density around ADP J 1480:**

$2mF_o-DF_c$  (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.