



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 01:41 AM EDT

PDB ID : 1T36  
Title : Crystal structure of E. coli carbamoyl phosphate synthetase small subunit mutant C248D complexed with uridine 5'-monophosphate  
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.  
Deposited on : 2004-04-24  
Resolution : 2.10 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

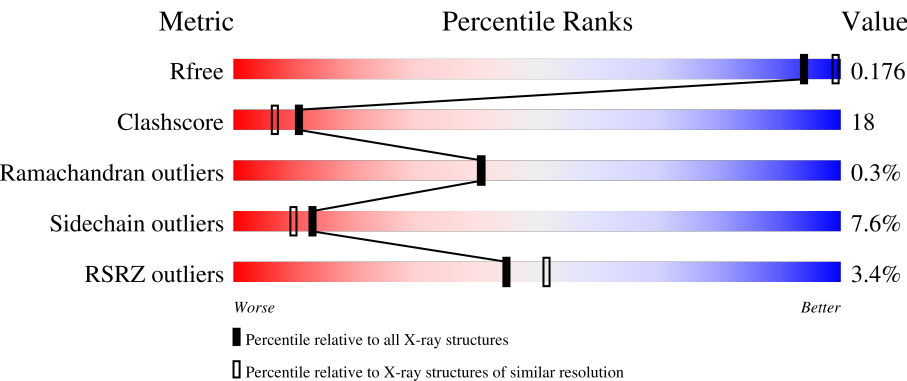
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R <sub>free</sub>     | 130704                      | 5197 (2.10-2.10)                                      |
| Clashscore            | 141614                      | 5710 (2.10-2.10)                                      |
| Ramachandran outliers | 138981                      | 5647 (2.10-2.10)                                      |
| Sidechain outliers    | 138945                      | 5648 (2.10-2.10)                                      |
| RSRZ outliers         | 127900                      | 5083 (2.10-2.10)                                      |

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     | 1073   | <div><div>2%</div><div>62%</div><div>30%</div><div>7%</div><div>.</div></div>  |
| 1   | C     | 1073   | <div><div>2%</div><div>58%</div><div>32%</div><div>7%</div><div>..</div></div> |
| 1   | E     | 1073   | <div><div>2%</div><div>65%</div><div>27%</div><div>6%</div><div>..</div></div> |
| 1   | G     | 1073   | <div><div>4%</div><div>52%</div><div>37%</div><div>9%</div><div>..</div></div> |
| 2   | B     | 382    | <div><div>4%</div><div>54%</div><div>35%</div><div>8%</div><div>..</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | D     | 382    |                  |
| 2   | F     | 382    |                  |
| 2   | H     | 382    |                  |

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   | PO4  | E     | 1078 | -         | X        | -       | -                |
| 5   | PO4  | G     | 1078 | -         | X        | -       | -                |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48757 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 Carbamoyl-phosphate synthase large chain.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1058     | Total | C    | N    | O    | S  | 0       | 9       | 0     |
|     |       |          | 8212  | 5155 | 1436 | 1575 | 46 |         |         |       |
| 1   | C     | 1058     | Total | C    | N    | O    | S  | 0       | 8       | 0     |
|     |       |          | 8197  | 5146 | 1426 | 1579 | 46 |         |         |       |
| 1   | E     | 1058     | Total | C    | N    | O    | S  | 0       | 5       | 0     |
|     |       |          | 8182  | 5137 | 1425 | 1575 | 45 |         |         |       |
| 1   | G     | 1058     | Total | C    | N    | O    | S  | 0       | 8       | 0     |
|     |       |          | 8206  | 5152 | 1432 | 1577 | 45 |         |         |       |

- Molecule 2 is a protein called Carbamoyl-phosphate synthase small chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 379      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2897  | 1826 | 508 | 554 | 9 |         |         |       |
| 2   | D     | 379      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2904  | 1830 | 511 | 554 | 9 |         |         |       |
| 2   | F     | 379      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2897  | 1826 | 508 | 554 | 9 |         |         |       |
| 2   | H     | 379      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2897  | 1826 | 508 | 554 | 9 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 248     | ASP      | CYS    | engineered mutation | UNP P00907 |
| D     | 248     | ASP      | CYS    | engineered mutation | UNP P00907 |
| F     | 248     | ASP      | CYS    | engineered mutation | UNP P00907 |
| H     | 248     | ASP      | CYS    | engineered mutation | UNP P00907 |

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | A     | 3        | Total Mn<br>3 3 | 0       | 0       |
| 3   | C     | 3        | Total Mn<br>3 3 | 0       | 0       |
| 3   | E     | 3        | Total Mn<br>3 3 | 0       | 0       |
| 3   | G     | 3        | Total Mn<br>3 3 | 0       | 0       |

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4   | A     | 4        | Total K<br>4 4 | 0       | 0       |
| 4   | B     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | C     | 4        | Total K<br>4 4 | 0       | 0       |
| 4   | D     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | E     | 5        | Total K<br>5 5 | 0       | 0       |
| 4   | F     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | G     | 5        | Total K<br>5 5 | 0       | 0       |
| 4   | H     | 1        | Total K<br>1 1 | 0       | 0       |

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

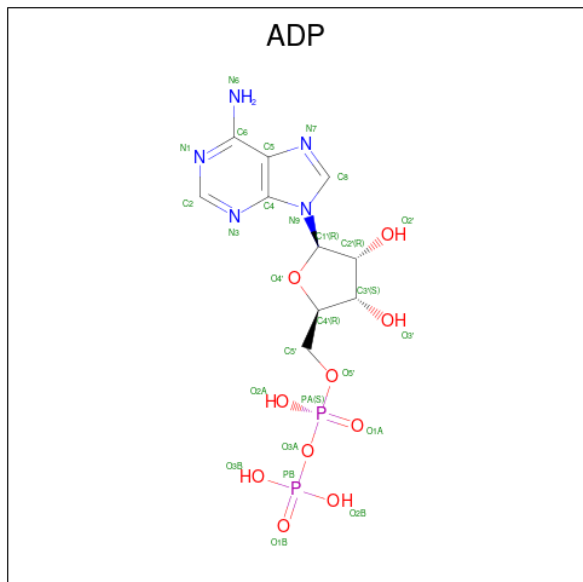


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

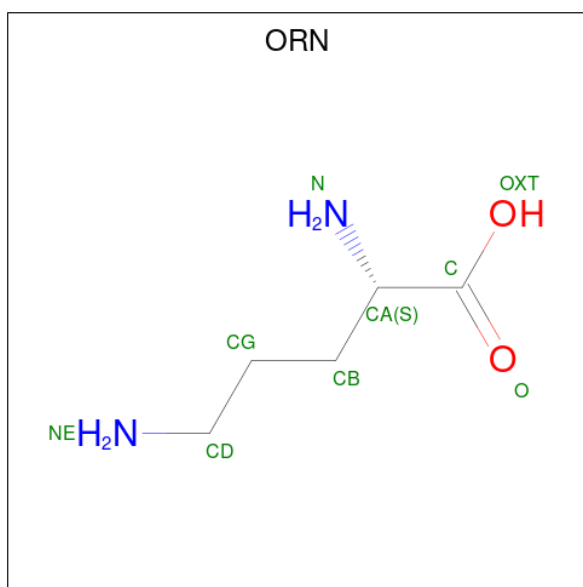
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 5        | Total | Cl | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 6   | C     | 6        | Total | Cl | 0       | 0       |
|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

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



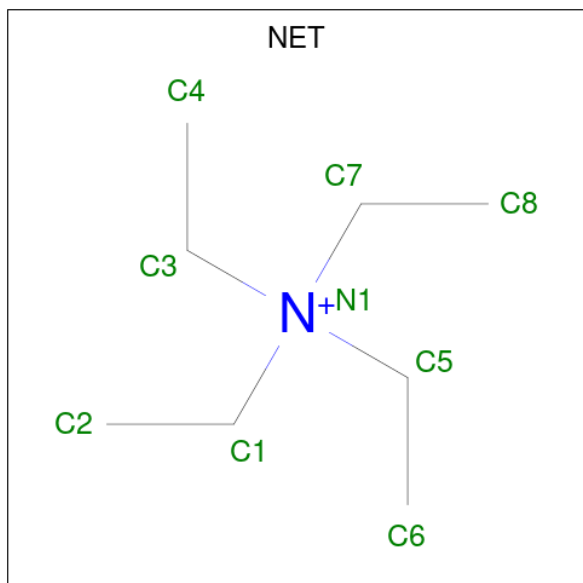
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 7   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 7   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 7   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 7   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 7   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 7   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 7   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 7   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

- Molecule 8 is L-ornithine (three-letter code: ORN) (formula:  $C_5H_{12}N_2O_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 8   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 5 | 2 | 2 |         |         |
| 8   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 5 | 2 | 2 |         |         |
| 8   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 5 | 2 | 2 |         |         |
| 8   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 5 | 2 | 2 |         |         |

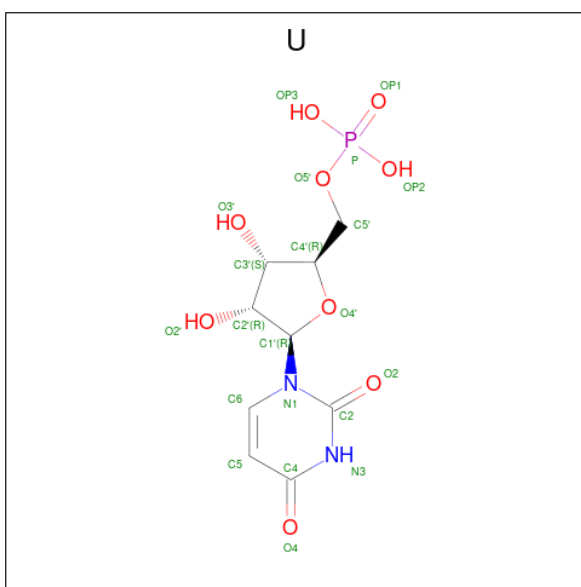
- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: C<sub>8</sub>H<sub>20</sub>N).





| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 9   | A     | 1        | Total C N<br>9 8 1 | 0       | 0       |
| 9   | C     | 1        | Total C N<br>9 8 1 | 0       | 0       |
| 9   | E     | 1        | Total C N<br>9 8 1 | 0       | 0       |
| 9   | G     | 1        | Total C N<br>9 8 1 | 0       | 0       |

- Molecule 10 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U) (formula:  $C_9H_{13}N_2O_9P$ ).



| Mol | Chain | Residues | Atoms                       | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------------|---------|---------|
| 10  | A     | 1        | Total C N O P<br>21 9 2 9 1 | 0       | 0       |
| 10  | C     | 1        | Total C N O P<br>21 9 2 9 1 | 0       | 0       |
| 10  | E     | 1        | Total C N O P<br>21 9 2 9 1 | 0       | 0       |
| 10  | G     | 1        | Total C N O P<br>21 9 2 9 1 | 0       | 0       |

- Molecule 11 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 11  | A     | 851      | Total O<br>851 851 | 0       | 0       |

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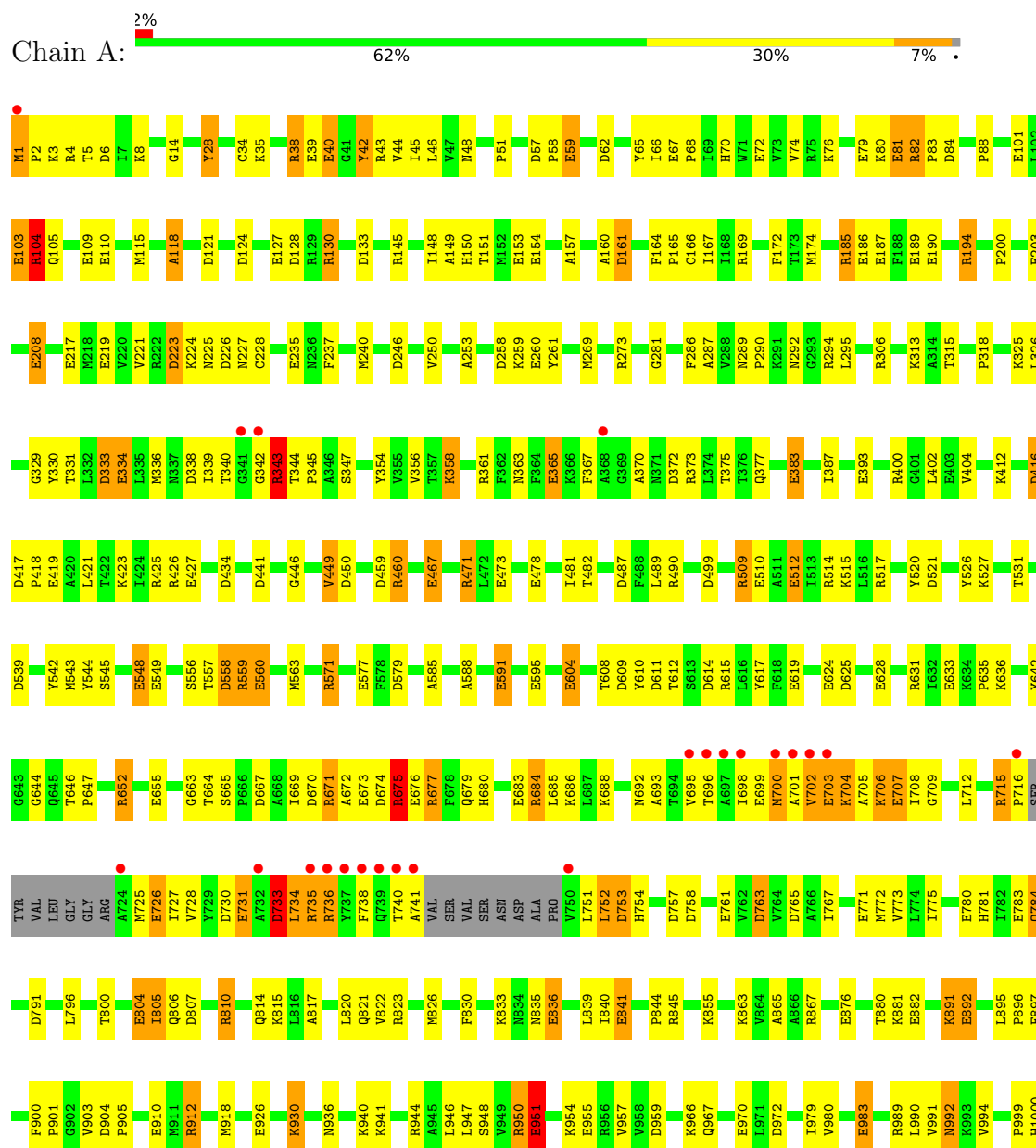
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 11  | B     | 161      | Total<br>161 | O<br>161 | 0       | 0       |
| 11  | C     | 819      | Total<br>819 | O<br>819 | 0       | 0       |
| 11  | D     | 221      | Total<br>221 | O<br>221 | 0       | 0       |
| 11  | E     | 832      | Total<br>832 | O<br>832 | 0       | 0       |
| 11  | F     | 200      | Total<br>200 | O<br>200 | 0       | 0       |
| 11  | G     | 705      | Total<br>705 | O<br>705 | 0       | 0       |
| 11  | H     | 118      | Total<br>118 | O<br>118 | 0       | 0       |

### 3 Residue-property plots

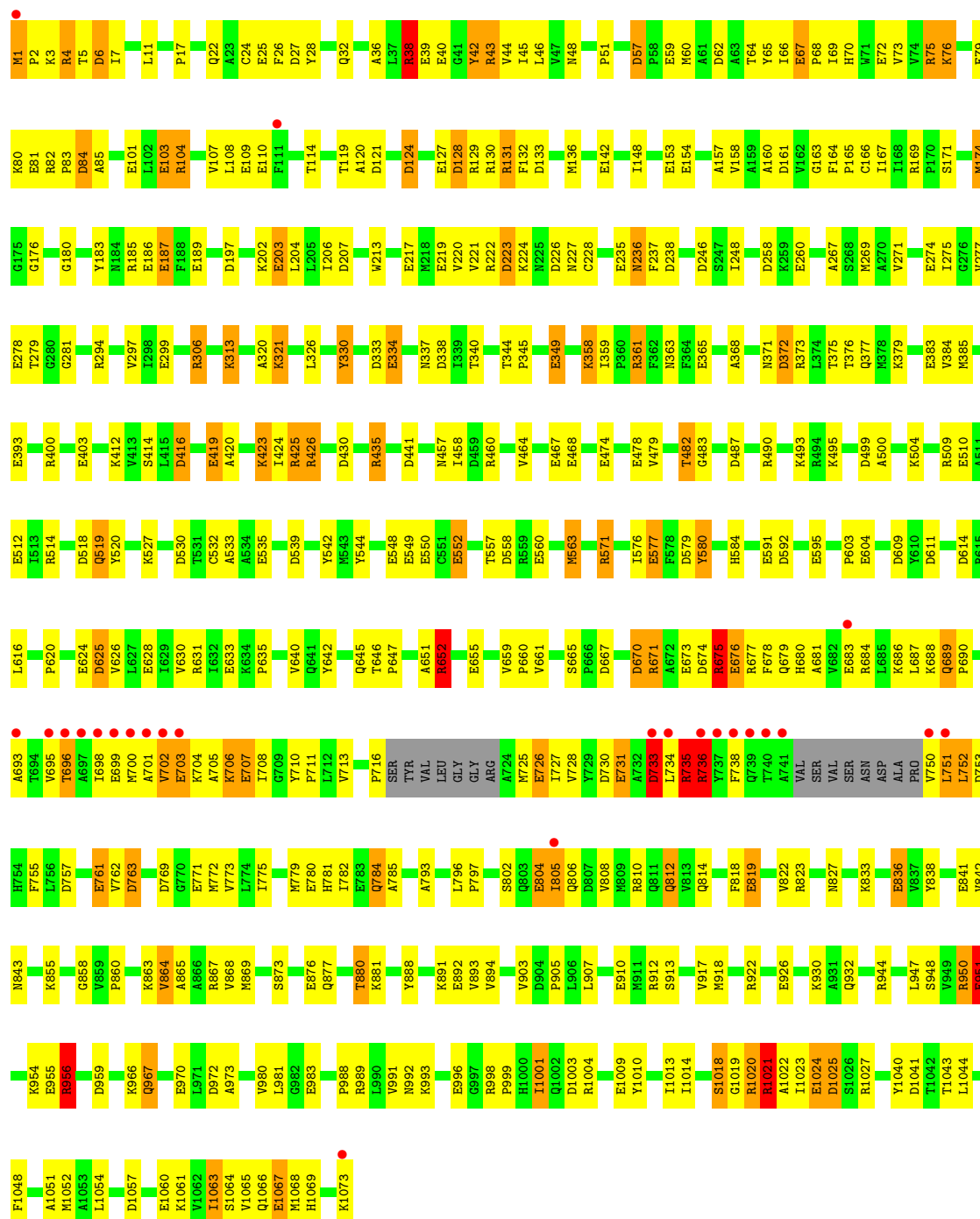
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Carbamoyl-phosphate synthase large chain

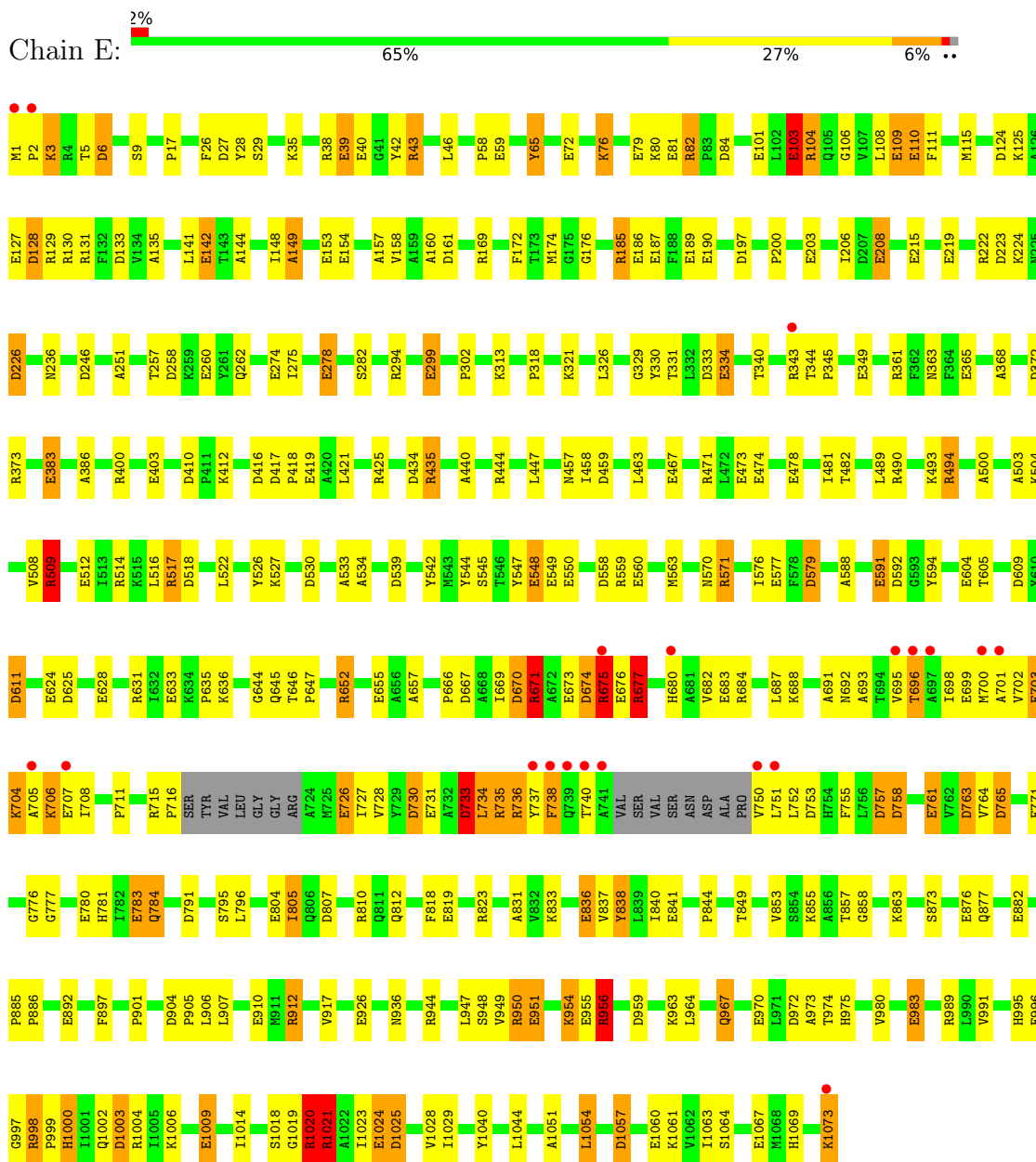




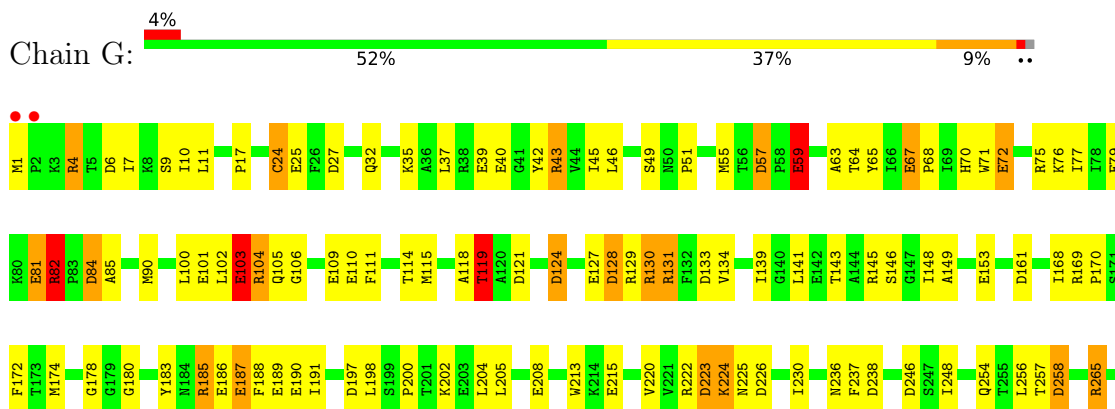
● Molecule 1: Carbamoyl-phosphate synthase large chain



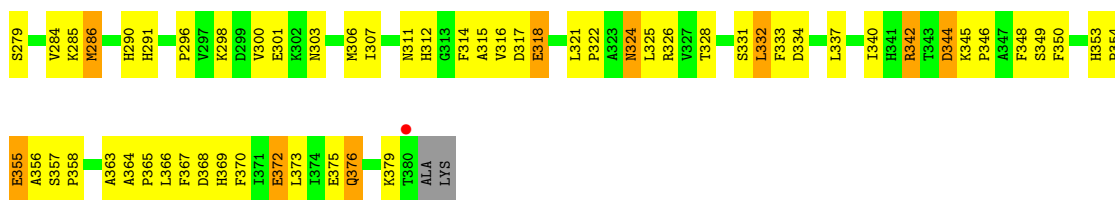
● Molecule 1: Carbamoyl-phosphate synthase large chain



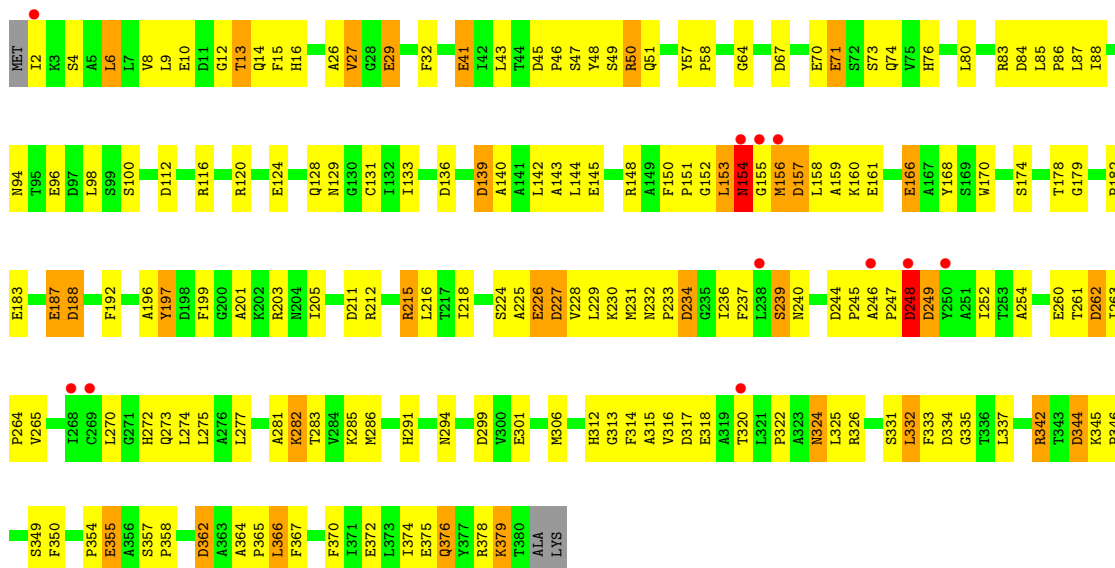
- Molecule 1: Carbamoyl-phosphate synthase large chain



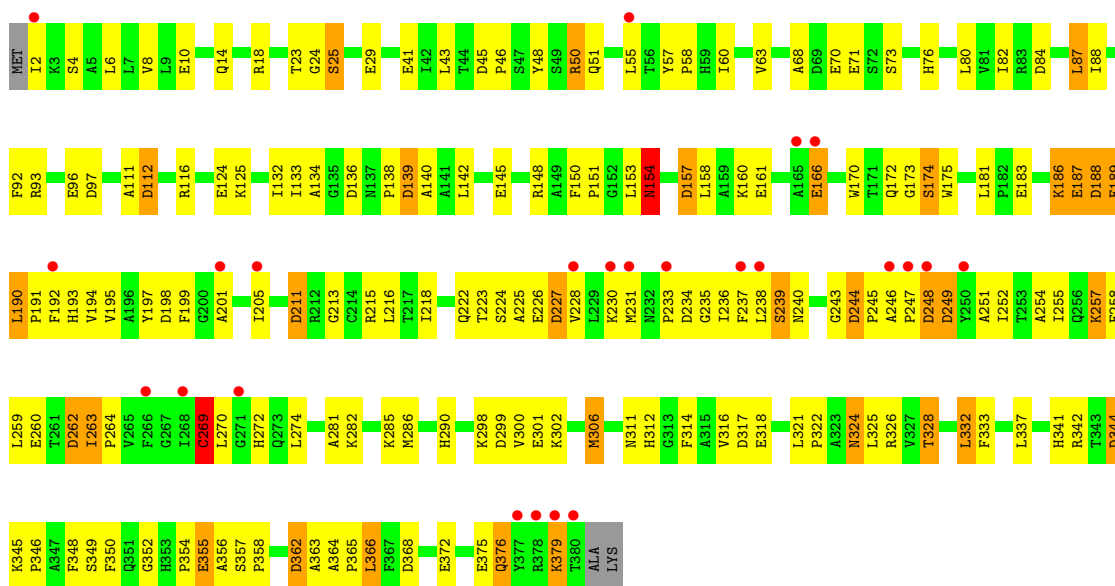




• Molecule 2: Carbamoyl-phosphate synthase small chain

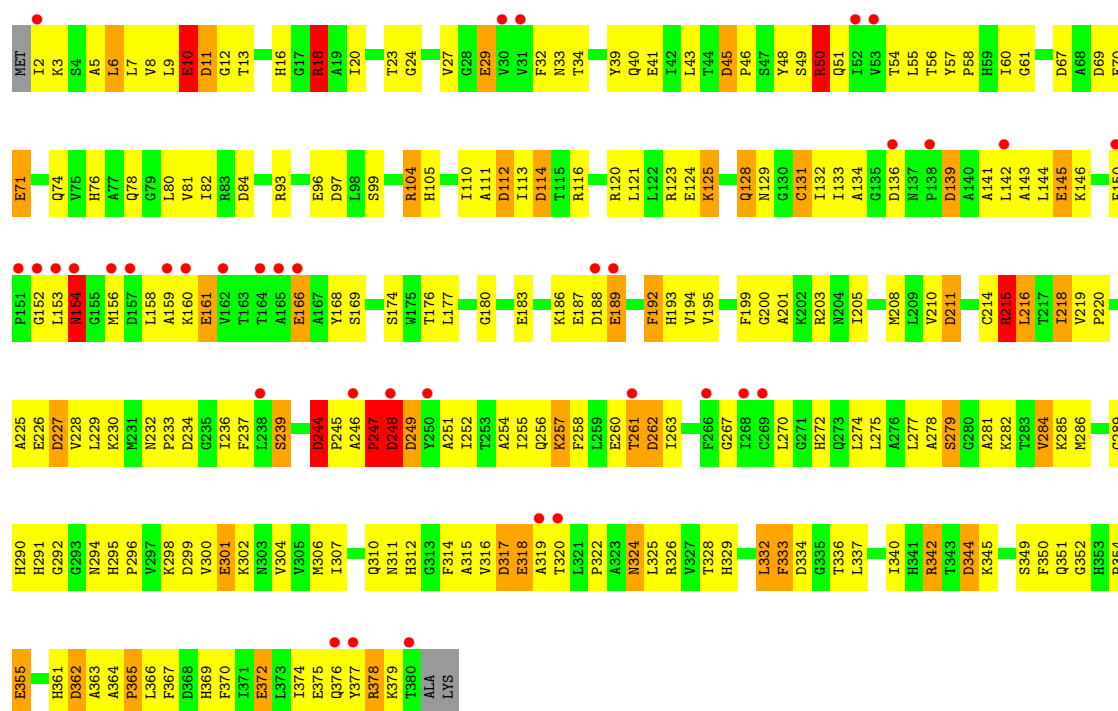


• Molecule 2: Carbamoyl-phosphate synthase small chain



• Molecule 2: Carbamoyl-phosphate synthase small chain

Chain H: 9% 41% 46% 11% ..





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 152.50Å 164.90Å 333.10Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 30.00 – 2.10<br>29.70 – 2.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.0 (30.00-2.10)<br>88.6 (29.70-2.10)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.05  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.88 (at 2.10Å)   | Xtriage          |
| Refinement program  | TNT   | Depositor        |
| R, $R_{free}$   | 0.176 , 0.209<br>0.175 , 0.176                              | Depositor<br>DCC |
| $R_{free}$ test set   | 42730 reflections (9.94%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 28.2  | Xtriage          |
| Anisotropy  | 0.072   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 120.0  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.96  | EDS              |
| Total number of atoms   | 48757   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 44.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: CL, NET, MN, K, ADP, ORN, PO4

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # $ Z  > 5$      | RMSZ        | # $ Z  > 5$      |
| 1   | A     | 1.05         | 68/8374 (0.8%)   | 1.50        | 137/11315 (1.2%) |
| 1   | C     | 1.06         | 81/8355 (1.0%)   | 1.48        | 127/11293 (1.1%) |
| 1   | E     | 1.06         | 74/8328 (0.9%)   | 1.50        | 128/11257 (1.1%) |
| 1   | G     | 1.05         | 74/8368 (0.9%)   | 1.50        | 148/11308 (1.3%) |
| 2   | B     | 0.94         | 19/2959 (0.6%)   | 1.46        | 43/4019 (1.1%)   |
| 2   | D     | 0.97         | 17/2970 (0.6%)   | 1.48        | 45/4033 (1.1%)   |
| 2   | F     | 0.97         | 19/2959 (0.6%)   | 1.45        | 41/4019 (1.0%)   |
| 2   | H     | 0.94         | 20/2959 (0.7%)   | 1.42        | 37/4019 (0.9%)   |
| All | All   | 1.03         | 372/45272 (0.8%) | 1.49        | 706/61263 (1.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 1                   | 0                   |
| 2   | D     | 1                   | 0                   |
| 2   | F     | 1                   | 0                   |
| All | All   | 3                   | 0                   |

All (372) bond length outliers are listed below:

| Mol | Chain | Res     | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|--------|------|-------------|----------|
| 2   | F     | 372     | GLU  | CD-OE2 | 8.39 | 1.34        | 1.25     |
| 2   | H     | 166     | GLU  | CD-OE2 | 8.34 | 1.34        | 1.25     |
| 2   | D     | 145     | GLU  | CD-OE2 | 8.28 | 1.34        | 1.25     |
| 1   | G     | 1009[A] | GLU  | CD-OE2 | 8.21 | 1.34        | 1.25     |
| 1   | G     | 1009[B] | GLU  | CD-OE2 | 8.21 | 1.34        | 1.25     |
| 1   | E     | 349     | GLU  | CD-OE2 | 8.21 | 1.34        | 1.25     |
| 2   | F     | 355     | GLU  | CD-OE2 | 8.16 | 1.34        | 1.25     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | B     | 183  | GLU  | CD-OE2 | 7.96 | 1.34        | 1.25     |
| 1   | E     | 190  | GLU  | CD-OE2 | 7.95 | 1.34        | 1.25     |
| 1   | A     | 109  | GLU  | CD-OE2 | 7.87 | 1.34        | 1.25     |
| 1   | E     | 655  | GLU  | CD-OE2 | 7.82 | 1.34        | 1.25     |
| 2   | H     | 145  | GLU  | CD-OE2 | 7.81 | 1.34        | 1.25     |
| 1   | E     | 1024 | GLU  | CD-OE2 | 7.80 | 1.34        | 1.25     |
| 1   | G     | 804  | GLU  | CD-OE2 | 7.73 | 1.34        | 1.25     |
| 1   | C     | 1024 | GLU  | CD-OE2 | 7.72 | 1.34        | 1.25     |
| 2   | H     | 226  | GLU  | CD-OE2 | 7.71 | 1.34        | 1.25     |
| 1   | A     | 1009 | GLU  | CD-OE2 | 7.63 | 1.34        | 1.25     |
| 1   | A     | 699  | GLU  | CD-OE2 | 7.62 | 1.34        | 1.25     |
| 2   | F     | 166  | GLU  | CD-OE2 | 7.60 | 1.34        | 1.25     |
| 2   | H     | 372  | GLU  | CD-OE2 | 7.59 | 1.34        | 1.25     |
| 1   | C     | 910  | GLU  | CD-OE2 | 7.59 | 1.34        | 1.25     |
| 2   | D     | 166  | GLU  | CD-OE2 | 7.55 | 1.33        | 1.25     |
| 2   | B     | 166  | GLU  | CD-OE2 | 7.54 | 1.33        | 1.25     |
| 2   | F     | 145  | GLU  | CD-OE2 | 7.54 | 1.33        | 1.25     |
| 1   | A     | 955  | GLU  | CD-OE2 | 7.53 | 1.33        | 1.25     |
| 1   | A     | 217  | GLU  | CD-OE2 | 7.49 | 1.33        | 1.25     |
| 1   | E     | 153  | GLU  | CD-OE2 | 7.44 | 1.33        | 1.25     |
| 2   | F     | 183  | GLU  | CD-OE2 | 7.41 | 1.33        | 1.25     |
| 1   | G     | 983  | GLU  | CD-OE2 | 7.40 | 1.33        | 1.25     |
| 2   | B     | 226  | GLU  | CD-OE2 | 7.38 | 1.33        | 1.25     |
| 1   | A     | 707  | GLU  | CD-OE2 | 7.36 | 1.33        | 1.25     |
| 1   | E     | 591  | GLU  | CD-OE2 | 7.32 | 1.33        | 1.25     |
| 1   | A     | 478  | GLU  | CD-OE2 | 7.29 | 1.33        | 1.25     |
| 1   | E     | 419  | GLU  | CD-OE2 | 7.28 | 1.33        | 1.25     |
| 1   | G     | 1024 | GLU  | CD-OE2 | 7.28 | 1.33        | 1.25     |
| 1   | E     | 983  | GLU  | CD-OE2 | 7.27 | 1.33        | 1.25     |
| 1   | C     | 771  | GLU  | CD-OE2 | 7.26 | 1.33        | 1.25     |
| 1   | C     | 217  | GLU  | CD-OE2 | 7.20 | 1.33        | 1.25     |
| 1   | E     | 1009 | GLU  | CD-OE2 | 7.17 | 1.33        | 1.25     |
| 1   | E     | 707  | GLU  | CD-OE2 | 7.14 | 1.33        | 1.25     |
| 1   | A     | 910  | GLU  | CD-OE2 | 7.13 | 1.33        | 1.25     |
| 1   | E     | 365  | GLU  | CD-OE2 | 7.13 | 1.33        | 1.25     |
| 1   | C     | 676  | GLU  | CD-OE2 | 7.12 | 1.33        | 1.25     |
| 2   | H     | 183  | GLU  | CD-OE2 | 7.12 | 1.33        | 1.25     |
| 1   | C     | 109  | GLU  | CD-OE2 | 7.10 | 1.33        | 1.25     |
| 1   | C     | 703  | GLU  | CD-OE2 | 7.09 | 1.33        | 1.25     |
| 2   | D     | 183  | GLU  | CD-OE2 | 7.08 | 1.33        | 1.25     |
| 1   | C     | 39   | GLU  | CD-OE2 | 7.08 | 1.33        | 1.25     |
| 1   | C     | 127  | GLU  | CD-OE2 | 7.08 | 1.33        | 1.25     |

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| Mol | Chain | Res    | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 1   | G     | 59     | GLU  | CD-OE2 | 7.08 | 1.33        | 1.25     |
| 1   | G     | 703    | GLU  | CD-OE2 | 7.07 | 1.33        | 1.25     |
| 1   | A     | 676    | GLU  | CD-OE2 | 7.06 | 1.33        | 1.25     |
| 1   | G     | 427    | GLU  | CD-OE2 | 7.04 | 1.33        | 1.25     |
| 2   | D     | 372    | GLU  | CD-OE2 | 7.02 | 1.33        | 1.25     |
| 1   | E     | 780    | GLU  | CD-OE2 | 6.98 | 1.33        | 1.25     |
| 1   | A     | 951    | GLU  | CD-OE2 | 6.97 | 1.33        | 1.25     |
| 2   | H     | 301    | GLU  | CD-OE2 | 6.97 | 1.33        | 1.25     |
| 1   | E     | 804    | GLU  | CD-OE2 | 6.97 | 1.33        | 1.25     |
| 1   | C     | 876    | GLU  | CD-OE2 | 6.96 | 1.33        | 1.25     |
| 1   | G     | 731    | GLU  | CD-OE2 | 6.96 | 1.33        | 1.25     |
| 1   | C     | 699    | GLU  | CD-OE2 | 6.96 | 1.33        | 1.25     |
| 1   | E     | 703    | GLU  | CD-OE2 | 6.95 | 1.33        | 1.25     |
| 1   | A     | 186    | GLU  | CD-OE2 | 6.93 | 1.33        | 1.25     |
| 1   | A     | 473    | GLU  | CD-OE2 | 6.89 | 1.33        | 1.25     |
| 2   | H     | 187    | GLU  | CD-OE2 | 6.87 | 1.33        | 1.25     |
| 1   | A     | 591    | GLU  | CD-OE2 | 6.87 | 1.33        | 1.25     |
| 1   | C     | 550    | GLU  | CD-OE2 | 6.86 | 1.33        | 1.25     |
| 2   | H     | 318    | GLU  | CD-OE2 | 6.86 | 1.33        | 1.25     |
| 1   | E     | 955    | GLU  | CD-OE2 | 6.86 | 1.33        | 1.25     |
| 1   | C     | 577    | GLU  | CD-OE2 | 6.84 | 1.33        | 1.25     |
| 1   | E     | 550    | GLU  | CD-OE2 | 6.83 | 1.33        | 1.25     |
| 1   | C     | 512    | GLU  | CD-OE2 | 6.83 | 1.33        | 1.25     |
| 2   | F     | 260    | GLU  | CD-OE2 | 6.82 | 1.33        | 1.25     |
| 2   | F     | 226    | GLU  | CD-OE2 | 6.81 | 1.33        | 1.25     |
| 2   | B     | 372    | GLU  | CD-OE2 | 6.79 | 1.33        | 1.25     |
| 1   | A     | 726    | GLU  | CD-OE2 | 6.79 | 1.33        | 1.25     |
| 1   | E     | 771    | GLU  | CD-OE2 | 6.78 | 1.33        | 1.25     |
| 1   | A     | 683    | GLU  | CD-OE2 | 6.77 | 1.33        | 1.25     |
| 1   | G     | 510    | GLU  | CD-OE2 | 6.77 | 1.33        | 1.25     |
| 2   | F     | 161    | GLU  | CD-OE2 | 6.76 | 1.33        | 1.25     |
| 1   | E     | 726    | GLU  | CD-OE2 | 6.76 | 1.33        | 1.25     |
| 2   | B     | 260    | GLU  | CD-OE2 | 6.75 | 1.33        | 1.25     |
| 1   | E     | 699    | GLU  | CD-OE2 | 6.74 | 1.33        | 1.25     |
| 2   | H     | 70     | GLU  | CD-OE2 | 6.74 | 1.33        | 1.25     |
| 1   | A     | 512[A] | GLU  | CD-OE2 | 6.73 | 1.33        | 1.25     |
| 1   | A     | 512[B] | GLU  | CD-OE2 | 6.73 | 1.33        | 1.25     |
| 1   | G     | 110    | GLU  | CD-OE2 | 6.73 | 1.33        | 1.25     |
| 1   | C     | 604    | GLU  | CD-OE2 | 6.71 | 1.33        | 1.25     |
| 2   | F     | 375    | GLU  | CD-OE2 | 6.70 | 1.33        | 1.25     |
| 1   | G     | 676    | GLU  | CD-OE2 | 6.67 | 1.32        | 1.25     |
| 2   | B     | 145    | GLU  | CD-OE2 | 6.67 | 1.32        | 1.25     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | H     | 355  | GLU  | CD-OE2 | 6.65  | 1.32        | 1.25     |
| 1   | A     | 467  | GLU  | CD-OE2 | 6.64  | 1.32        | 1.25     |
| 1   | A     | 780  | GLU  | CD-OE2 | 6.64  | 1.32        | 1.25     |
| 1   | G     | 215  | GLU  | CD-OE2 | 6.64  | 1.32        | 1.25     |
| 2   | D     | 96   | GLU  | CD-OE2 | 6.63  | 1.32        | 1.25     |
| 2   | D     | 226  | GLU  | CD-OE2 | 6.63  | 1.32        | 1.25     |
| 1   | E     | 836  | GLU  | CD-OE2 | 6.63  | 1.32        | 1.25     |
| 1   | G     | 699  | GLU  | CD-OE2 | 6.63  | 1.32        | 1.25     |
| 1   | G     | 683  | GLU  | CD-OE2 | 6.63  | 1.32        | 1.25     |
| 1   | E     | 951  | GLU  | CD-OE2 | 6.62  | 1.32        | 1.25     |
| 1   | E     | 783  | GLU  | CD-OE2 | 6.62  | 1.32        | 1.25     |
| 1   | A     | 203  | GLU  | CD-OE2 | 6.62  | 1.32        | 1.25     |
| 1   | C     | 560  | GLU  | CD-OE2 | 6.61  | 1.32        | 1.25     |
| 1   | G     | 673  | GLU  | CD-OE2 | 6.61  | 1.32        | 1.25     |
| 2   | D     | 355  | GLU  | CD-OE2 | 6.61  | 1.32        | 1.25     |
| 1   | E     | 683  | GLU  | CD-OE2 | 6.61  | 1.32        | 1.25     |
| 1   | G     | 109  | GLU  | CD-OE1 | -6.60 | 1.18        | 1.25     |
| 1   | E     | 910  | GLU  | CD-OE2 | 6.60  | 1.32        | 1.25     |
| 1   | G     | 771  | GLU  | CD-OE2 | 6.60  | 1.32        | 1.25     |
| 1   | C     | 349  | GLU  | CD-OE2 | 6.59  | 1.32        | 1.25     |
| 1   | C     | 1009 | GLU  | CD-OE2 | 6.59  | 1.32        | 1.25     |
| 1   | E     | 761  | GLU  | CD-OE2 | 6.59  | 1.32        | 1.25     |
| 1   | G     | 512  | GLU  | CD-OE2 | 6.58  | 1.32        | 1.25     |
| 1   | A     | 783  | GLU  | CD-OE2 | 6.57  | 1.32        | 1.25     |
| 2   | H     | 161  | GLU  | CD-OE2 | 6.55  | 1.32        | 1.25     |
| 1   | A     | 876  | GLU  | CD-OE2 | 6.54  | 1.32        | 1.25     |
| 1   | A     | 72   | GLU  | CD-OE2 | 6.54  | 1.32        | 1.25     |
| 1   | C     | 731  | GLU  | CD-OE2 | 6.53  | 1.32        | 1.25     |
| 1   | E     | 478  | GLU  | CD-OE2 | 6.53  | 1.32        | 1.25     |
| 1   | C     | 383  | GLU  | CD-OE2 | 6.52  | 1.32        | 1.25     |
| 1   | C     | 683  | GLU  | CD-OE2 | 6.51  | 1.32        | 1.25     |
| 1   | G     | 926  | GLU  | CD-OE2 | 6.51  | 1.32        | 1.25     |
| 1   | E     | 970  | GLU  | CD-OE2 | 6.51  | 1.32        | 1.25     |
| 1   | E     | 577  | GLU  | CD-OE2 | 6.49  | 1.32        | 1.25     |
| 1   | G     | 474  | GLU  | CD-OE2 | 6.48  | 1.32        | 1.25     |
| 1   | G     | 655  | GLU  | CD-OE2 | 6.47  | 1.32        | 1.25     |
| 1   | A     | 365  | GLU  | CD-OE2 | 6.47  | 1.32        | 1.25     |
| 1   | C     | 707  | GLU  | CD-OE2 | 6.47  | 1.32        | 1.25     |
| 1   | E     | 186  | GLU  | CD-OE2 | 6.46  | 1.32        | 1.25     |
| 2   | B     | 301  | GLU  | CD-OE2 | 6.45  | 1.32        | 1.25     |
| 1   | E     | 926  | GLU  | CD-OE2 | 6.45  | 1.32        | 1.25     |
| 1   | C     | 186  | GLU  | CD-OE2 | 6.44  | 1.32        | 1.25     |

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| Mol | Chain | Res    | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 1   | C     | 955    | GLU  | CD-OE2 | 6.44 | 1.32        | 1.25     |
| 1   | C     | 478    | GLU  | CD-OE2 | 6.42 | 1.32        | 1.25     |
| 1   | C     | 951    | GLU  | CD-OE2 | 6.42 | 1.32        | 1.25     |
| 1   | G     | 383    | GLU  | CD-OE2 | 6.41 | 1.32        | 1.25     |
| 1   | G     | 103    | GLU  | CD-OE2 | 6.41 | 1.32        | 1.25     |
| 1   | A     | 983    | GLU  | CD-OE2 | 6.39 | 1.32        | 1.25     |
| 1   | A     | 771    | GLU  | CD-OE2 | 6.39 | 1.32        | 1.25     |
| 1   | G     | 955    | GLU  | CD-OE2 | 6.39 | 1.32        | 1.25     |
| 1   | G     | 190    | GLU  | CD-OE2 | 6.37 | 1.32        | 1.25     |
| 1   | A     | 153    | GLU  | CD-OE2 | 6.36 | 1.32        | 1.25     |
| 1   | C     | 72     | GLU  | CD-OE2 | 6.36 | 1.32        | 1.25     |
| 1   | E     | 110    | GLU  | CD-OE2 | 6.36 | 1.32        | 1.25     |
| 1   | G     | 467    | GLU  | CD-OE2 | 6.35 | 1.32        | 1.25     |
| 1   | A     | 219    | GLU  | CD-OE2 | 6.35 | 1.32        | 1.25     |
| 1   | A     | 804    | GLU  | CD-OE2 | 6.35 | 1.32        | 1.25     |
| 1   | A     | 334    | GLU  | CD-OE2 | 6.34 | 1.32        | 1.25     |
| 1   | C     | 419    | GLU  | CD-OE2 | 6.33 | 1.32        | 1.25     |
| 1   | A     | 577    | GLU  | CD-OE2 | 6.33 | 1.32        | 1.25     |
| 1   | C     | 110    | GLU  | CD-OE2 | 6.31 | 1.32        | 1.25     |
| 1   | C     | 274    | GLU  | CD-OE2 | 6.31 | 1.32        | 1.25     |
| 1   | E     | 189    | GLU  | CD-OE2 | 6.27 | 1.32        | 1.25     |
| 1   | G     | 334    | GLU  | CD-OE2 | 6.27 | 1.32        | 1.25     |
| 1   | E     | 549    | GLU  | CD-OE2 | 6.26 | 1.32        | 1.25     |
| 1   | E     | 731    | GLU  | CD-OE2 | 6.26 | 1.32        | 1.25     |
| 1   | G     | 591    | GLU  | CD-OE2 | 6.25 | 1.32        | 1.25     |
| 2   | B     | 375    | GLU  | CD-OE2 | 6.25 | 1.32        | 1.25     |
| 1   | A     | 633    | GLU  | CD-OE2 | 6.24 | 1.32        | 1.25     |
| 1   | C     | 260    | GLU  | CD-OE2 | 6.23 | 1.32        | 1.25     |
| 2   | F     | 189    | GLU  | CD-OE2 | 6.23 | 1.32        | 1.25     |
| 1   | G     | 153[A] | GLU  | CD-OE2 | 6.21 | 1.32        | 1.25     |
| 1   | G     | 153[B] | GLU  | CD-OE2 | 6.21 | 1.32        | 1.25     |
| 1   | G     | 186    | GLU  | CD-OE2 | 6.21 | 1.32        | 1.25     |
| 1   | C     | 624    | GLU  | CD-OE2 | 6.21 | 1.32        | 1.25     |
| 1   | E     | 676    | GLU  | CD-OE2 | 6.20 | 1.32        | 1.25     |
| 1   | C     | 299    | GLU  | CD-OE2 | 6.19 | 1.32        | 1.25     |
| 1   | A     | 970    | GLU  | CD-OE2 | 6.19 | 1.32        | 1.25     |
| 1   | E     | 72     | GLU  | CD-OE2 | 6.18 | 1.32        | 1.25     |
| 1   | C     | 726    | GLU  | CD-OE2 | 6.18 | 1.32        | 1.25     |
| 1   | E     | 876    | GLU  | CD-OE2 | 6.15 | 1.32        | 1.25     |
| 1   | G     | 633    | GLU  | CD-OE2 | 6.14 | 1.32        | 1.25     |
| 1   | G     | 707    | GLU  | CD-OE2 | 6.14 | 1.32        | 1.25     |
| 1   | C     | 467    | GLU  | CD-OE2 | 6.13 | 1.32        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | E     | 187 | GLU  | CD-OE2 | 6.13 | 1.32        | 1.25     |
| 1   | G     | 419 | GLU  | CD-OE2 | 6.12 | 1.32        | 1.25     |
| 1   | A     | 110 | GLU  | CD-OE2 | 6.12 | 1.32        | 1.25     |
| 2   | B     | 161 | GLU  | CD-OE2 | 6.12 | 1.32        | 1.25     |
| 2   | D     | 29  | GLU  | CD-OE2 | 6.12 | 1.32        | 1.25     |
| 1   | C     | 841 | GLU  | CD-OE2 | 6.12 | 1.32        | 1.25     |
| 1   | C     | 996 | GLU  | CD-OE2 | 6.11 | 1.32        | 1.25     |
| 1   | E     | 215 | GLU  | CD-OE2 | 6.11 | 1.32        | 1.25     |
| 2   | H     | 375 | GLU  | CD-OE2 | 6.09 | 1.32        | 1.25     |
| 1   | C     | 983 | GLU  | CD-OE2 | 6.08 | 1.32        | 1.25     |
| 2   | F     | 96  | GLU  | CD-OE2 | 6.07 | 1.32        | 1.25     |
| 1   | C     | 474 | GLU  | CD-OE2 | 6.07 | 1.32        | 1.25     |
| 1   | A     | 510 | GLU  | CD-OE2 | 6.07 | 1.32        | 1.25     |
| 1   | A     | 703 | GLU  | CD-OE2 | 6.07 | 1.32        | 1.25     |
| 1   | G     | 187 | GLU  | CD-OE2 | 6.06 | 1.32        | 1.25     |
| 1   | G     | 892 | GLU  | CD-OE2 | 6.05 | 1.32        | 1.25     |
| 2   | D     | 318 | GLU  | CD-OE2 | 6.03 | 1.32        | 1.25     |
| 1   | G     | 208 | GLU  | CD-OE2 | 6.03 | 1.32        | 1.25     |
| 1   | C     | 655 | GLU  | CD-OE2 | 6.02 | 1.32        | 1.25     |
| 1   | E     | 208 | GLU  | CD-OE2 | 6.02 | 1.32        | 1.25     |
| 1   | A     | 624 | GLU  | CD-OE2 | 6.01 | 1.32        | 1.25     |
| 2   | H     | 124 | GLU  | CD-OE2 | 6.01 | 1.32        | 1.25     |
| 2   | F     | 70  | GLU  | CD-OE2 | 6.00 | 1.32        | 1.25     |
| 2   | F     | 301 | GLU  | CD-OE2 | 6.00 | 1.32        | 1.25     |
| 1   | G     | 478 | GLU  | CD-OE2 | 5.98 | 1.32        | 1.25     |
| 1   | G     | 274 | GLU  | CD-OE2 | 5.98 | 1.32        | 1.25     |
| 1   | G     | 549 | GLU  | CD-OE2 | 5.98 | 1.32        | 1.25     |
| 1   | C     | 403 | GLU  | CD-OE2 | 5.97 | 1.32        | 1.25     |
| 1   | E     | 109 | GLU  | CD-OE2 | 5.96 | 1.32        | 1.25     |
| 1   | E     | 103 | GLU  | CD-OE2 | 5.95 | 1.32        | 1.25     |
| 1   | A     | 892 | GLU  | CD-OE2 | 5.95 | 1.32        | 1.25     |
| 1   | C     | 549 | GLU  | CD-OE2 | 5.95 | 1.32        | 1.25     |
| 1   | G     | 836 | GLU  | CD-OE2 | 5.95 | 1.32        | 1.25     |
| 2   | B     | 318 | GLU  | CD-OE2 | 5.94 | 1.32        | 1.25     |
| 1   | C     | 468 | GLU  | CD-OE2 | 5.94 | 1.32        | 1.25     |
| 1   | G     | 560 | GLU  | CD-OE2 | 5.93 | 1.32        | 1.25     |
| 1   | G     | 876 | GLU  | CD-OE2 | 5.93 | 1.32        | 1.25     |
| 1   | G     | 577 | GLU  | CD-OE2 | 5.92 | 1.32        | 1.25     |
| 1   | C     | 510 | GLU  | CD-OE2 | 5.92 | 1.32        | 1.25     |
| 1   | E     | 673 | GLU  | CD-OE2 | 5.92 | 1.32        | 1.25     |
| 1   | A     | 655 | GLU  | CD-OE2 | 5.91 | 1.32        | 1.25     |
| 1   | E     | 474 | GLU  | CD-OE2 | 5.90 | 1.32        | 1.25     |

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| Mol | Chain | Res    | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 2   | B     | 10     | GLU  | CD-OE2 | 5.89 | 1.32        | 1.25     |
| 2   | B     | 41     | GLU  | CD-OE2 | 5.89 | 1.32        | 1.25     |
| 2   | B     | 189    | GLU  | CD-OE2 | 5.88 | 1.32        | 1.25     |
| 1   | A     | 1024   | GLU  | CD-OE2 | 5.86 | 1.32        | 1.25     |
| 1   | G     | 299    | GLU  | CD-OE2 | 5.85 | 1.32        | 1.25     |
| 1   | E     | 154    | GLU  | CD-OE2 | 5.85 | 1.32        | 1.25     |
| 2   | D     | 260    | GLU  | CD-OE2 | 5.83 | 1.32        | 1.25     |
| 1   | G     | 628    | GLU  | CD-OE2 | 5.83 | 1.32        | 1.25     |
| 1   | A     | 59     | GLU  | CD-OE2 | 5.82 | 1.32        | 1.25     |
| 2   | F     | 29     | GLU  | CD-OE2 | 5.80 | 1.32        | 1.25     |
| 1   | C     | 628    | GLU  | CD-OE2 | 5.80 | 1.32        | 1.25     |
| 2   | H     | 10     | GLU  | CD-OE2 | 5.79 | 1.32        | 1.25     |
| 1   | G     | 189    | GLU  | CD-OE2 | 5.79 | 1.32        | 1.25     |
| 1   | A     | 1067   | GLU  | CD-OE2 | 5.79 | 1.32        | 1.25     |
| 1   | C     | 633    | GLU  | CD-OE2 | 5.79 | 1.32        | 1.25     |
| 2   | B     | 71     | GLU  | CD-OE2 | 5.78 | 1.32        | 1.25     |
| 2   | D     | 375    | GLU  | CD-OE2 | 5.78 | 1.32        | 1.25     |
| 1   | A     | 549[A] | GLU  | CD-OE2 | 5.78 | 1.32        | 1.25     |
| 1   | A     | 549[B] | GLU  | CD-OE2 | 5.78 | 1.32        | 1.25     |
| 1   | E     | 39[A]  | GLU  | CD-OE2 | 5.77 | 1.31        | 1.25     |
| 1   | E     | 39[B]  | GLU  | CD-OE2 | 5.77 | 1.31        | 1.25     |
| 1   | C     | 535    | GLU  | CD-OE2 | 5.77 | 1.31        | 1.25     |
| 1   | C     | 1067   | GLU  | CD-OE2 | 5.76 | 1.31        | 1.25     |
| 1   | C     | 1060   | GLU  | CD-OE2 | 5.76 | 1.31        | 1.25     |
| 1   | G     | 726    | GLU  | CD-OE2 | 5.76 | 1.31        | 1.25     |
| 1   | G     | 783    | GLU  | CD-OE2 | 5.76 | 1.31        | 1.25     |
| 2   | F     | 187    | GLU  | CD-OE2 | 5.75 | 1.31        | 1.25     |
| 1   | G     | 996    | GLU  | CD-OE2 | 5.75 | 1.31        | 1.25     |
| 1   | A     | 841    | GLU  | CD-OE2 | 5.74 | 1.31        | 1.25     |
| 1   | E     | 996    | GLU  | CD-OE2 | 5.74 | 1.31        | 1.25     |
| 1   | A     | 731    | GLU  | CD-OE2 | 5.74 | 1.31        | 1.25     |
| 2   | D     | 70     | GLU  | CD-OE2 | 5.73 | 1.31        | 1.25     |
| 2   | H     | 260    | GLU  | CD-OE2 | 5.71 | 1.31        | 1.25     |
| 1   | A     | 628    | GLU  | CD-OE2 | 5.71 | 1.31        | 1.25     |
| 1   | C     | 79     | GLU  | CD-OE2 | 5.70 | 1.31        | 1.25     |
| 1   | E     | 512    | GLU  | CD-OE2 | 5.68 | 1.31        | 1.25     |
| 1   | C     | 780    | GLU  | CD-OE2 | 5.67 | 1.31        | 1.25     |
| 1   | C     | 101    | GLU  | CD-OE2 | 5.67 | 1.31        | 1.25     |
| 1   | E     | 467    | GLU  | CD-OE2 | 5.67 | 1.31        | 1.25     |
| 1   | G     | 127    | GLU  | CD-OE2 | 5.66 | 1.31        | 1.25     |
| 1   | E     | 560    | GLU  | CD-OE2 | 5.64 | 1.31        | 1.25     |
| 1   | E     | 819    | GLU  | CD-OE2 | 5.64 | 1.31        | 1.25     |

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| Mol | Chain | Res    | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 1   | C     | 535    | GLU  | CD-OE1 | -5.63 | 1.19        | 1.25     |
| 1   | A     | 560    | GLU  | CD-OE2 | 5.63  | 1.31        | 1.25     |
| 2   | H     | 96     | GLU  | CD-OE2 | 5.62  | 1.31        | 1.25     |
| 2   | H     | 71     | GLU  | CD-OE2 | 5.60  | 1.31        | 1.25     |
| 1   | G     | 67     | GLU  | CD-OE2 | 5.60  | 1.31        | 1.25     |
| 1   | G     | 1060   | GLU  | CD-OE2 | 5.59  | 1.31        | 1.25     |
| 1   | G     | 535    | GLU  | CD-OE2 | 5.58  | 1.31        | 1.25     |
| 1   | E     | 628    | GLU  | CD-OE2 | 5.55  | 1.31        | 1.25     |
| 1   | E     | 40     | GLU  | CD-OE2 | 5.55  | 1.31        | 1.25     |
| 1   | E     | 299    | GLU  | CD-OE2 | 5.54  | 1.31        | 1.25     |
| 1   | C     | 59     | GLU  | CD-OE2 | 5.54  | 1.31        | 1.25     |
| 1   | A     | 836    | GLU  | CD-OE2 | 5.53  | 1.31        | 1.25     |
| 1   | C     | 219    | GLU  | CD-OE2 | 5.53  | 1.31        | 1.25     |
| 1   | A     | 673    | GLU  | CD-OE2 | 5.52  | 1.31        | 1.25     |
| 1   | A     | 190    | GLU  | CD-OE2 | 5.52  | 1.31        | 1.25     |
| 1   | A     | 189    | GLU  | CD-OE2 | 5.52  | 1.31        | 1.25     |
| 1   | A     | 926    | GLU  | CD-OE2 | 5.52  | 1.31        | 1.25     |
| 1   | C     | 153    | GLU  | CD-OE2 | 5.52  | 1.31        | 1.25     |
| 1   | G     | 841    | GLU  | CD-OE2 | 5.51  | 1.31        | 1.25     |
| 2   | D     | 41     | GLU  | CD-OE2 | 5.51  | 1.31        | 1.25     |
| 1   | A     | 419    | GLU  | CD-OE2 | 5.51  | 1.31        | 1.25     |
| 1   | G     | 39     | GLU  | CD-OE2 | 5.51  | 1.31        | 1.25     |
| 2   | B     | 355    | GLU  | CD-OE2 | 5.51  | 1.31        | 1.25     |
| 2   | F     | 10     | GLU  | CD-OE2 | 5.50  | 1.31        | 1.25     |
| 1   | E     | 260    | GLU  | CD-OE2 | 5.49  | 1.31        | 1.25     |
| 1   | C     | 673    | GLU  | CD-OE2 | 5.49  | 1.31        | 1.25     |
| 1   | E     | 473    | GLU  | CD-OE2 | 5.49  | 1.31        | 1.25     |
| 2   | H     | 189    | GLU  | CD-OE2 | 5.49  | 1.31        | 1.25     |
| 1   | A     | 260    | GLU  | CD-OE2 | 5.47  | 1.31        | 1.25     |
| 1   | C     | 550    | GLU  | CD-OE1 | -5.45 | 1.19        | 1.25     |
| 1   | C     | 67     | GLU  | CD-OE2 | 5.44  | 1.31        | 1.25     |
| 1   | G     | 951    | GLU  | CD-OE2 | 5.43  | 1.31        | 1.25     |
| 1   | A     | 187    | GLU  | CD-OE2 | 5.42  | 1.31        | 1.25     |
| 1   | E     | 219    | GLU  | CD-OE2 | 5.42  | 1.31        | 1.25     |
| 1   | C     | 591[A] | GLU  | CD-OE2 | 5.42  | 1.31        | 1.25     |
| 1   | C     | 591[B] | GLU  | CD-OE2 | 5.42  | 1.31        | 1.25     |
| 1   | E     | 892    | GLU  | CD-OE2 | 5.41  | 1.31        | 1.25     |
| 2   | D     | 301    | GLU  | CD-OE2 | 5.41  | 1.31        | 1.25     |
| 1   | A     | 393    | GLU  | CD-OE2 | 5.40  | 1.31        | 1.25     |
| 1   | E     | 548    | GLU  | CD-OE2 | 5.40  | 1.31        | 1.25     |
| 1   | A     | 127    | GLU  | CD-OE2 | 5.39  | 1.31        | 1.25     |
| 2   | D     | 71     | GLU  | CD-OE2 | 5.39  | 1.31        | 1.25     |

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| Mol | Chain | Res    | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 1   | C     | 203    | GLU  | CD-OE2 | 5.39  | 1.31        | 1.25     |
| 1   | E     | 79     | GLU  | CD-OE2 | 5.39  | 1.31        | 1.25     |
| 1   | A     | 619    | GLU  | CD-OE2 | 5.36  | 1.31        | 1.25     |
| 1   | C     | 334    | GLU  | CD-OE2 | 5.36  | 1.31        | 1.25     |
| 1   | C     | 804[A] | GLU  | CD-OE2 | 5.35  | 1.31        | 1.25     |
| 1   | C     | 804[B] | GLU  | CD-OE2 | 5.35  | 1.31        | 1.25     |
| 2   | B     | 96     | GLU  | CD-OE2 | 5.35  | 1.31        | 1.25     |
| 1   | C     | 926    | GLU  | CD-OE2 | 5.35  | 1.31        | 1.25     |
| 1   | A     | 103    | GLU  | CD-OE2 | 5.34  | 1.31        | 1.25     |
| 1   | G     | 624    | GLU  | CD-OE2 | 5.34  | 1.31        | 1.25     |
| 1   | A     | 79     | GLU  | CD-OE2 | 5.34  | 1.31        | 1.25     |
| 1   | C     | 819    | GLU  | CD-OE2 | 5.33  | 1.31        | 1.25     |
| 1   | C     | 142    | GLU  | CD-OE2 | 5.33  | 1.31        | 1.25     |
| 1   | E     | 142    | GLU  | CD-OE2 | 5.33  | 1.31        | 1.25     |
| 2   | B     | 29     | GLU  | CD-OE2 | 5.32  | 1.31        | 1.25     |
| 1   | C     | 836    | GLU  | CD-OE2 | 5.32  | 1.31        | 1.25     |
| 1   | G     | 468    | GLU  | CD-OE2 | 5.31  | 1.31        | 1.25     |
| 1   | C     | 187    | GLU  | CD-OE2 | 5.31  | 1.31        | 1.25     |
| 1   | G     | 619    | GLU  | CD-OE2 | 5.31  | 1.31        | 1.25     |
| 1   | E     | 383    | GLU  | CD-OE1 | -5.31 | 1.19        | 1.25     |
| 2   | B     | 124    | GLU  | CD-OE2 | 5.30  | 1.31        | 1.25     |
| 1   | E     | 278    | GLU  | CD-OE2 | 5.30  | 1.31        | 1.25     |
| 1   | A     | 383    | GLU  | CD-OE2 | 5.29  | 1.31        | 1.25     |
| 1   | A     | 81     | GLU  | CD-OE2 | 5.28  | 1.31        | 1.25     |
| 1   | G     | 761    | GLU  | CD-OE2 | 5.28  | 1.31        | 1.25     |
| 1   | E     | 624    | GLU  | CD-OE2 | 5.27  | 1.31        | 1.25     |
| 1   | C     | 189    | GLU  | CD-OE2 | 5.26  | 1.31        | 1.25     |
| 1   | C     | 39     | GLU  | CD-OE1 | -5.26 | 1.19        | 1.25     |
| 1   | G     | 278    | GLU  | CD-OE2 | 5.26  | 1.31        | 1.25     |
| 1   | G     | 550    | GLU  | CD-OE2 | 5.25  | 1.31        | 1.25     |
| 1   | E     | 1067   | GLU  | CD-OE2 | 5.25  | 1.31        | 1.25     |
| 1   | A     | 604    | GLU  | CD-OE2 | 5.23  | 1.31        | 1.25     |
| 2   | F     | 124    | GLU  | CD-OE2 | 5.22  | 1.31        | 1.25     |
| 1   | C     | 154    | GLU  | CD-OE2 | 5.22  | 1.31        | 1.25     |
| 1   | C     | 278    | GLU  | CD-OE2 | 5.21  | 1.31        | 1.25     |
| 1   | C     | 552    | GLU  | CD-OE1 | -5.20 | 1.20        | 1.25     |
| 1   | G     | 819    | GLU  | CD-OE2 | 5.20  | 1.31        | 1.25     |
| 1   | G     | 595    | GLU  | CD-OE2 | 5.19  | 1.31        | 1.25     |
| 2   | D     | 187    | GLU  | CD-OE2 | 5.19  | 1.31        | 1.25     |
| 2   | H     | 41     | GLU  | CD-OE2 | 5.19  | 1.31        | 1.25     |
| 2   | F     | 318    | GLU  | CD-OE2 | 5.19  | 1.31        | 1.25     |
| 1   | C     | 235    | GLU  | CD-OE2 | 5.15  | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 127 | GLU  | CD-OE2 | 5.14  | 1.31        | 1.25     |
| 2   | D     | 124 | GLU  | CD-OE2 | 5.14  | 1.31        | 1.25     |
| 1   | C     | 970 | GLU  | CD-OE2 | 5.14  | 1.31        | 1.25     |
| 2   | H     | 29  | GLU  | CD-OE2 | 5.12  | 1.31        | 1.25     |
| 1   | G     | 780 | GLU  | CD-OE2 | 5.12  | 1.31        | 1.25     |
| 1   | C     | 365 | GLU  | CD-OE2 | 5.11  | 1.31        | 1.25     |
| 1   | E     | 203 | GLU  | CD-OE2 | 5.11  | 1.31        | 1.25     |
| 1   | G     | 970 | GLU  | CD-OE2 | 5.11  | 1.31        | 1.25     |
| 1   | C     | 761 | GLU  | CD-OE2 | 5.11  | 1.31        | 1.25     |
| 1   | E     | 882 | GLU  | CD-OE2 | 5.11  | 1.31        | 1.25     |
| 1   | A     | 427 | GLU  | CD-OE2 | 5.10  | 1.31        | 1.25     |
| 1   | C     | 393 | GLU  | CD-OE2 | 5.09  | 1.31        | 1.25     |
| 1   | G     | 910 | GLU  | CD-OE2 | 5.09  | 1.31        | 1.25     |
| 1   | A     | 39  | GLU  | CD-OE2 | 5.08  | 1.31        | 1.25     |
| 1   | G     | 25  | GLU  | CD-OE2 | 5.08  | 1.31        | 1.25     |
| 1   | E     | 624 | GLU  | CD-OE1 | -5.07 | 1.20        | 1.25     |
| 1   | G     | 393 | GLU  | CD-OE2 | 5.06  | 1.31        | 1.25     |
| 1   | G     | 916 | GLU  | CD-OE2 | 5.06  | 1.31        | 1.25     |
| 1   | E     | 403 | GLU  | CD-OE2 | 5.06  | 1.31        | 1.25     |
| 1   | A     | 208 | GLU  | CD-OE2 | 5.06  | 1.31        | 1.25     |
| 1   | E     | 633 | GLU  | CD-OE2 | 5.06  | 1.31        | 1.25     |
| 1   | E     | 841 | GLU  | CD-OE2 | 5.05  | 1.31        | 1.25     |
| 2   | F     | 71  | GLU  | CD-OE2 | 5.05  | 1.31        | 1.25     |
| 1   | G     | 72  | GLU  | CD-OE2 | 5.04  | 1.31        | 1.25     |
| 1   | E     | 101 | GLU  | CD-OE2 | 5.04  | 1.31        | 1.25     |
| 1   | G     | 101 | GLU  | CD-OE2 | 5.03  | 1.31        | 1.25     |
| 1   | C     | 595 | GLU  | CD-OE2 | 5.02  | 1.31        | 1.25     |
| 1   | A     | 595 | GLU  | CD-OE2 | 5.02  | 1.31        | 1.25     |
| 2   | B     | 187 | GLU  | CD-OE2 | 5.00  | 1.31        | 1.25     |

All (706) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | E     | 514 | ARG  | NE-CZ-NH2 | -15.12 | 112.74      | 120.30   |
| 1   | A     | 944 | ARG  | NE-CZ-NH1 | 14.25  | 127.42      | 120.30   |
| 1   | C     | 514 | ARG  | NE-CZ-NH2 | -14.00 | 113.30      | 120.30   |
| 1   | A     | 104 | ARG  | NE-CZ-NH1 | 13.43  | 127.02      | 120.30   |
| 1   | A     | 652 | ARG  | NE-CZ-NH1 | 13.13  | 126.87      | 120.30   |
| 1   | E     | 810 | ARG  | NE-CZ-NH1 | 12.83  | 126.72      | 120.30   |
| 1   | C     | 43  | ARG  | NE-CZ-NH1 | 12.53  | 126.56      | 120.30   |
| 1   | G     | 82  | ARG  | NE-CZ-NH1 | 11.39  | 126.00      | 120.30   |
| 1   | G     | 75  | ARG  | NE-CZ-NH1 | 11.24  | 125.92      | 120.30   |

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| Mol | Chain | Res    | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|--------|-------------|----------|
| 1   | E     | 514    | ARG  | NE-CZ-NH1 | 11.07  | 125.84      | 120.30   |
| 1   | G     | 42     | TYR  | CB-CG-CD1 | -10.98 | 114.41      | 121.00   |
| 1   | A     | 104    | ARG  | NE-CZ-NH2 | -10.93 | 114.83      | 120.30   |
| 1   | E     | 400    | ARG  | NE-CZ-NH1 | 10.80  | 125.70      | 120.30   |
| 1   | A     | 471    | ARG  | NE-CZ-NH1 | 10.55  | 125.58      | 120.30   |
| 1   | E     | 104    | ARG  | NE-CZ-NH1 | 10.38  | 125.49      | 120.30   |
| 1   | E     | 517    | ARG  | NE-CZ-NH1 | 10.36  | 125.48      | 120.30   |
| 1   | C     | 425    | ARG  | NE-CZ-NH1 | 10.28  | 125.44      | 120.30   |
| 1   | C     | 514    | ARG  | NE-CZ-NH1 | 10.26  | 125.43      | 120.30   |
| 1   | A     | 736    | ARG  | NE-CZ-NH2 | -10.05 | 115.27      | 120.30   |
| 1   | G     | 389    | ARG  | NE-CZ-NH1 | 10.05  | 125.33      | 120.30   |
| 1   | A     | 400    | ARG  | NE-CZ-NH1 | 10.04  | 125.32      | 120.30   |
| 1   | G     | 265    | ARG  | NE-CZ-NH1 | 10.02  | 125.31      | 120.30   |
| 1   | C     | 518    | ASP  | CB-CG-OD2 | -9.92  | 109.37      | 118.30   |
| 1   | A     | 677    | ARG  | NE-CZ-NH1 | 9.73   | 125.16      | 120.30   |
| 1   | A     | 130[A] | ARG  | NE-CZ-NH1 | 9.66   | 125.13      | 120.30   |
| 1   | A     | 130[B] | ARG  | NE-CZ-NH1 | 9.66   | 125.13      | 120.30   |
| 1   | A     | 736    | ARG  | NE-CZ-NH1 | 9.62   | 125.11      | 120.30   |
| 1   | A     | 43     | ARG  | NE-CZ-NH2 | -9.59  | 115.51      | 120.30   |
| 1   | G     | 671    | ARG  | NE-CZ-NH1 | 9.47   | 125.03      | 120.30   |
| 1   | A     | 684    | ARG  | NE-CZ-NH2 | -9.36  | 115.62      | 120.30   |
| 1   | A     | 652    | ARG  | CD-NE-CZ  | 9.35   | 136.69      | 123.60   |
| 1   | E     | 1021   | ARG  | NE-CZ-NH1 | 9.34   | 124.97      | 120.30   |
| 1   | C     | 769    | ASP  | CB-CG-OD2 | -9.24  | 109.99      | 118.30   |
| 1   | E     | 38     | ARG  | NE-CZ-NH1 | 9.20   | 124.90      | 120.30   |
| 1   | G     | 75     | ARG  | NE-CZ-NH2 | -9.15  | 115.72      | 120.30   |
| 1   | C     | 838    | TYR  | CB-CG-CD1 | -9.10  | 115.54      | 121.00   |
| 2   | H     | 93     | ARG  | NE-CZ-NH2 | -9.07  | 115.77      | 120.30   |
| 1   | G     | 670    | ASP  | CB-CG-OD2 | -9.05  | 110.15      | 118.30   |
| 1   | E     | 912    | ARG  | NE-CZ-NH1 | 9.04   | 124.82      | 120.30   |
| 1   | E     | 912    | ARG  | NE-CZ-NH2 | -8.94  | 115.83      | 120.30   |
| 2   | H     | 342    | ARG  | NE-CZ-NH1 | 8.89   | 124.75      | 120.30   |
| 1   | E     | 1020   | ARG  | NE-CZ-NH1 | 8.87   | 124.73      | 120.30   |
| 1   | G     | 625    | ASP  | CB-CG-OD2 | -8.87  | 110.32      | 118.30   |
| 1   | A     | 579    | ASP  | CB-CG-OD1 | 8.86   | 126.27      | 118.30   |
| 1   | E     | 956    | ARG  | NE-CZ-NH2 | -8.85  | 115.88      | 120.30   |
| 1   | G     | 460    | ARG  | NE-CZ-NH1 | 8.80   | 124.70      | 120.30   |
| 1   | C     | 518    | ASP  | CB-CG-OD1 | 8.79   | 126.21      | 118.30   |
| 1   | G     | 671    | ARG  | NE-CZ-NH2 | -8.69  | 115.96      | 120.30   |
| 1   | E     | 131    | ARG  | NE-CZ-NH1 | 8.66   | 124.63      | 120.30   |
| 1   | G     | 131    | ARG  | NE-CZ-NH1 | 8.60   | 124.60      | 120.30   |
| 2   | F     | 188    | ASP  | CB-CG-OD1 | 8.59   | 126.03      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | E     | 509  | ARG  | NE-CZ-NH1 | 8.59  | 124.59      | 120.30   |
| 1   | C     | 128  | ASP  | CB-CG-OD2 | -8.57 | 110.59      | 118.30   |
| 2   | B     | 112  | ASP  | CB-CG-OD1 | 8.56  | 126.00      | 118.30   |
| 1   | E     | 1020 | ARG  | NE-CZ-NH2 | -8.52 | 116.04      | 120.30   |
| 1   | G     | 972  | ASP  | CB-CG-OD2 | -8.52 | 110.63      | 118.30   |
| 1   | C     | 43   | ARG  | NE-CZ-NH2 | -8.51 | 116.05      | 120.30   |
| 2   | H     | 97   | ASP  | CB-CG-OD2 | -8.46 | 110.68      | 118.30   |
| 1   | G     | 956  | ARG  | NE-CZ-NH2 | -8.43 | 116.09      | 120.30   |
| 1   | A     | 43   | ARG  | NE-CZ-NH1 | 8.42  | 124.51      | 120.30   |
| 1   | A     | 373  | ARG  | NE-CZ-NH2 | -8.41 | 116.09      | 120.30   |
| 1   | G     | 517  | ARG  | NE-CZ-NH1 | 8.38  | 124.49      | 120.30   |
| 1   | C     | 652  | ARG  | NE-CZ-NH1 | 8.36  | 124.48      | 120.30   |
| 1   | C     | 128  | ASP  | CB-CG-OD1 | 8.35  | 125.82      | 118.30   |
| 2   | B     | 262  | ASP  | CB-CG-OD2 | -8.35 | 110.79      | 118.30   |
| 1   | A     | 579  | ASP  | CB-CG-OD2 | -8.32 | 110.81      | 118.30   |
| 1   | C     | 425  | ARG  | NE-CZ-NH2 | -8.32 | 116.14      | 120.30   |
| 1   | C     | 972  | ASP  | CB-CG-OD2 | -8.32 | 110.81      | 118.30   |
| 1   | C     | 609  | ASP  | CB-CG-OD2 | -8.31 | 110.82      | 118.30   |
| 1   | E     | 372  | ASP  | CB-CG-OD2 | -8.31 | 110.82      | 118.30   |
| 1   | E     | 944  | ARG  | NE-CZ-NH1 | 8.31  | 124.45      | 120.30   |
| 1   | G     | 579  | ASP  | CB-CG-OD2 | -8.27 | 110.86      | 118.30   |
| 1   | E     | 223  | ASP  | CB-CG-OD2 | -8.27 | 110.86      | 118.30   |
| 1   | E     | 810  | ARG  | NE-CZ-NH2 | -8.27 | 116.17      | 120.30   |
| 1   | G     | 416  | ASP  | CB-CG-OD2 | -8.25 | 110.88      | 118.30   |
| 1   | E     | 753  | ASP  | CB-CG-OD2 | -8.24 | 110.88      | 118.30   |
| 1   | A     | 416  | ASP  | CB-CG-OD1 | 8.23  | 125.71      | 118.30   |
| 1   | A     | 611  | ASP  | CB-CG-OD2 | -8.22 | 110.91      | 118.30   |
| 1   | G     | 104  | ARG  | NE-CZ-NH1 | 8.20  | 124.40      | 120.30   |
| 1   | G     | 223  | ASP  | CB-CG-OD1 | 8.16  | 125.64      | 118.30   |
| 2   | B     | 136  | ASP  | CB-CG-OD2 | -8.11 | 111.00      | 118.30   |
| 1   | A     | 42   | TYR  | CB-CG-CD1 | -8.10 | 116.14      | 121.00   |
| 2   | D     | 342  | ARG  | NE-CZ-NH1 | 8.09  | 124.34      | 120.30   |
| 1   | G     | 222  | ARG  | NE-CZ-NH1 | 8.05  | 124.32      | 120.30   |
| 1   | E     | 558  | ASP  | N-CA-CB   | -8.04 | 96.12       | 110.60   |
| 1   | E     | 671  | ARG  | NE-CZ-NH1 | 8.02  | 124.31      | 120.30   |
| 1   | C     | 1004 | ARG  | NE-CZ-NH1 | 7.99  | 124.30      | 120.30   |
| 2   | D     | 136  | ASP  | CB-CG-OD2 | -7.99 | 111.11      | 118.30   |
| 1   | C     | 733  | ASP  | CB-CG-OD2 | -7.96 | 111.13      | 118.30   |
| 1   | A     | 223  | ASP  | CB-CG-OD2 | -7.95 | 111.14      | 118.30   |
| 1   | C     | 6    | ASP  | CB-CG-OD2 | -7.94 | 111.15      | 118.30   |
| 2   | D     | 248  | ASP  | N-CA-CB   | -7.94 | 96.31       | 110.60   |
| 1   | G     | 6    | ASP  | CB-CG-OD2 | -7.93 | 111.16      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | G     | 306  | ARG  | NE-CZ-NH1 | 7.93  | 124.27      | 120.30   |
| 2   | H     | 50   | ARG  | NE-CZ-NH1 | 7.91  | 124.25      | 120.30   |
| 1   | G     | 6    | ASP  | CB-CG-OD1 | 7.90  | 125.41      | 118.30   |
| 1   | A     | 128  | ASP  | CB-CG-OD1 | 7.90  | 125.41      | 118.30   |
| 2   | B     | 227  | ASP  | CB-CG-OD1 | 7.89  | 125.40      | 118.30   |
| 1   | E     | 459  | ASP  | CB-CG-OD2 | -7.87 | 111.22      | 118.30   |
| 1   | E     | 670  | ASP  | CB-CG-OD1 | 7.86  | 125.38      | 118.30   |
| 2   | H     | 378  | ARG  | NE-CZ-NH1 | 7.86  | 124.23      | 120.30   |
| 1   | E     | 609  | ASP  | CB-CG-OD2 | -7.86 | 111.23      | 118.30   |
| 1   | E     | 223  | ASP  | CB-CG-OD1 | 7.86  | 125.37      | 118.30   |
| 1   | G     | 57   | ASP  | CB-CG-OD2 | -7.86 | 111.23      | 118.30   |
| 1   | C     | 1021 | ARG  | NE-CZ-NH1 | 7.85  | 124.23      | 120.30   |
| 2   | B     | 50   | ARG  | NE-CZ-NH1 | 7.84  | 124.22      | 120.30   |
| 1   | E     | 998  | ARG  | NE-CZ-NH1 | 7.84  | 124.22      | 120.30   |
| 1   | A     | 867  | ARG  | NE-CZ-NH1 | 7.83  | 124.21      | 120.30   |
| 2   | D     | 248  | ASP  | CB-CG-OD2 | -7.82 | 111.27      | 118.30   |
| 1   | G     | 223  | ASP  | CB-CG-OD2 | -7.82 | 111.26      | 118.30   |
| 2   | D     | 112  | ASP  | CB-CG-OD2 | -7.80 | 111.28      | 118.30   |
| 1   | E     | 558  | ASP  | CB-CG-OD2 | -7.79 | 111.29      | 118.30   |
| 1   | E     | 631  | ARG  | NE-CZ-NH1 | 7.77  | 124.19      | 120.30   |
| 1   | E     | 38   | ARG  | NE-CZ-NH2 | -7.76 | 116.42      | 120.30   |
| 2   | F     | 326  | ARG  | NE-CZ-NH2 | -7.75 | 116.42      | 120.30   |
| 2   | F     | 188  | ASP  | CB-CG-OD2 | -7.75 | 111.33      | 118.30   |
| 2   | B     | 211  | ASP  | CB-CG-OD2 | -7.74 | 111.34      | 118.30   |
| 2   | D     | 227  | ASP  | CB-CG-OD2 | -7.74 | 111.34      | 118.30   |
| 2   | H     | 342  | ARG  | NE-CZ-NH2 | -7.74 | 116.43      | 120.30   |
| 1   | G     | 912  | ARG  | NE-CZ-NH1 | 7.72  | 124.16      | 120.30   |
| 1   | G     | 372  | ASP  | CB-CG-OD2 | -7.71 | 111.36      | 118.30   |
| 1   | E     | 674  | ASP  | CB-CG-OD2 | -7.71 | 111.37      | 118.30   |
| 2   | B     | 212  | ARG  | NE-CZ-NH2 | -7.70 | 116.45      | 120.30   |
| 1   | A     | 42   | TYR  | CB-CG-CD2 | 7.69  | 125.62      | 121.00   |
| 1   | C     | 736  | ARG  | NE-CZ-NH1 | 7.69  | 124.15      | 120.30   |
| 1   | G     | 579  | ASP  | CB-CG-OD1 | 7.69  | 125.22      | 118.30   |
| 1   | E     | 459  | ASP  | CB-CG-OD1 | 7.68  | 125.21      | 118.30   |
| 1   | A     | 611  | ASP  | CB-CG-OD1 | 7.66  | 125.19      | 118.30   |
| 1   | E     | 1054 | LEU  | N-CA-CB   | -7.66 | 95.08       | 110.40   |
| 2   | F     | 249  | ASP  | CB-CG-OD2 | -7.65 | 111.42      | 118.30   |
| 2   | H     | 112  | ASP  | CB-CG-OD2 | -7.64 | 111.42      | 118.30   |
| 2   | B     | 11   | ASP  | CB-CG-OD2 | -7.60 | 111.46      | 118.30   |
| 1   | C     | 631  | ARG  | NE-CZ-NH1 | 7.60  | 124.10      | 120.30   |
| 2   | D     | 317  | ASP  | CB-CG-OD1 | 7.59  | 125.14      | 118.30   |
| 1   | G     | 1021 | ARG  | NE-CZ-NH1 | 7.59  | 124.09      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | C     | 959  | ASP  | CB-CG-OD2 | -7.58 | 111.47      | 118.30   |
| 1   | C     | 306  | ARG  | NE-CZ-NH1 | 7.58  | 124.09      | 120.30   |
| 1   | E     | 609  | ASP  | CB-CG-OD1 | 7.57  | 125.11      | 118.30   |
| 1   | C     | 922  | ARG  | NE-CZ-NH2 | -7.56 | 116.52      | 120.30   |
| 1   | A     | 959  | ASP  | CB-CG-OD2 | -7.56 | 111.50      | 118.30   |
| 1   | G     | 753  | ASP  | CB-CG-OD2 | -7.52 | 111.53      | 118.30   |
| 1   | E     | 736  | ARG  | NE-CZ-NH1 | 7.52  | 124.06      | 120.30   |
| 1   | C     | 490  | ARG  | NE-CZ-NH1 | 7.51  | 124.05      | 120.30   |
| 2   | B     | 262  | ASP  | CB-CG-OD1 | 7.50  | 125.05      | 118.30   |
| 1   | G     | 736  | ARG  | NE-CZ-NH1 | 7.50  | 124.05      | 120.30   |
| 1   | C     | 730  | ASP  | CB-CG-OD2 | -7.49 | 111.56      | 118.30   |
| 1   | G     | 922  | ARG  | NE-CZ-NH1 | 7.49  | 124.04      | 120.30   |
| 1   | E     | 579  | ASP  | CB-CG-OD2 | -7.47 | 111.57      | 118.30   |
| 1   | E     | 1021 | ARG  | NE-CZ-NH2 | -7.47 | 116.56      | 120.30   |
| 1   | A     | 161  | ASP  | CB-CG-OD2 | -7.47 | 111.58      | 118.30   |
| 2   | H     | 317  | ASP  | CB-CG-OD2 | -7.45 | 111.59      | 118.30   |
| 1   | A     | 124  | ASP  | CB-CG-OD1 | 7.45  | 125.01      | 118.30   |
| 1   | A     | 520  | TYR  | CB-CG-CD2 | -7.44 | 116.54      | 121.00   |
| 2   | D     | 15   | PHE  | CB-CG-CD2 | 7.43  | 126.00      | 120.80   |
| 1   | E     | 807  | ASP  | CB-CG-OD2 | -7.43 | 111.61      | 118.30   |
| 1   | E     | 959  | ASP  | CB-CG-OD2 | -7.43 | 111.62      | 118.30   |
| 1   | C     | 989  | ARG  | NE-CZ-NH1 | 7.41  | 124.00      | 120.30   |
| 1   | E     | 6    | ASP  | CB-CG-OD1 | 7.41  | 124.97      | 118.30   |
| 2   | H     | 211  | ASP  | CB-CG-OD2 | -7.41 | 111.63      | 118.30   |
| 1   | A     | 609  | ASP  | CB-CG-OD1 | 7.39  | 124.96      | 118.30   |
| 1   | A     | 487  | ASP  | CB-CG-OD2 | -7.39 | 111.65      | 118.30   |
| 2   | B     | 227  | ASP  | CB-CG-OD2 | -7.35 | 111.69      | 118.30   |
| 2   | F     | 136  | ASP  | CB-CG-OD2 | -7.34 | 111.69      | 118.30   |
| 2   | F     | 227  | ASP  | CB-CG-OD2 | -7.34 | 111.69      | 118.30   |
| 1   | E     | 579  | ASP  | CB-CG-OD1 | 7.34  | 124.90      | 118.30   |
| 1   | G     | 128  | ASP  | CB-CG-OD1 | 7.33  | 124.90      | 118.30   |
| 1   | C     | 558  | ASP  | CB-CG-OD2 | -7.33 | 111.71      | 118.30   |
| 1   | G     | 944  | ARG  | NE-CZ-NH1 | 7.33  | 123.96      | 120.30   |
| 1   | A     | 867  | ARG  | NE-CZ-NH2 | -7.32 | 116.64      | 120.30   |
| 1   | A     | 652  | ARG  | NE-CZ-NH2 | -7.32 | 116.64      | 120.30   |
| 1   | E     | 197  | ASP  | CB-CG-OD2 | -7.32 | 111.72      | 118.30   |
| 1   | G     | 614  | ASP  | CB-CG-OD2 | -7.32 | 111.72      | 118.30   |
| 2   | F     | 248  | ASP  | CB-CG-OD2 | -7.31 | 111.72      | 118.30   |
| 1   | G     | 226  | ASP  | CB-CG-OD1 | 7.31  | 124.88      | 118.30   |
| 1   | G     | 959  | ASP  | CB-CG-OD2 | -7.28 | 111.75      | 118.30   |
| 2   | D     | 136  | ASP  | CB-CG-OD1 | 7.27  | 124.84      | 118.30   |
| 1   | E     | 6    | ASP  | CB-CG-OD2 | -7.27 | 111.76      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | E     | 611  | ASP  | CB-CG-OD1 | 7.26  | 124.84      | 118.30   |
| 1   | A     | 558  | ASP  | CB-CG-OD1 | 7.25  | 124.83      | 118.30   |
| 1   | A     | 194  | ARG  | NE-CZ-NH2 | -7.25 | 116.67      | 120.30   |
| 1   | C     | 530  | ASP  | CB-CG-OD2 | -7.24 | 111.78      | 118.30   |
| 2   | H     | 116  | ARG  | NE-CZ-NH1 | 7.24  | 123.92      | 120.30   |
| 2   | D     | 362  | ASP  | CB-CG-OD2 | -7.23 | 111.79      | 118.30   |
| 2   | F     | 326  | ARG  | NE-CZ-NH1 | 7.23  | 123.91      | 120.30   |
| 1   | E     | 611  | ASP  | CB-CG-OD2 | -7.22 | 111.80      | 118.30   |
| 1   | C     | 487  | ASP  | CB-CG-OD2 | -7.22 | 111.80      | 118.30   |
| 1   | G     | 558  | ASP  | CB-CG-OD2 | -7.21 | 111.81      | 118.30   |
| 1   | E     | 27   | ASP  | CB-CG-OD1 | 7.19  | 124.77      | 118.30   |
| 1   | A     | 1030 | ARG  | NE-CZ-NH1 | 7.18  | 123.89      | 120.30   |
| 1   | G     | 84   | ASP  | CB-CG-OD2 | -7.18 | 111.84      | 118.30   |
| 1   | G     | 124  | ASP  | CB-CG-OD2 | -7.16 | 111.85      | 118.30   |
| 1   | E     | 416  | ASP  | CB-CG-OD2 | -7.16 | 111.86      | 118.30   |
| 1   | C     | 670  | ASP  | CB-CG-OD2 | -7.16 | 111.86      | 118.30   |
| 1   | C     | 769  | ASP  | CB-CG-OD1 | 7.14  | 124.73      | 118.30   |
| 1   | E     | 765  | ASP  | CB-CG-OD1 | 7.14  | 124.73      | 118.30   |
| 2   | H     | 249  | ASP  | CB-CG-OD2 | -7.14 | 111.87      | 118.30   |
| 1   | C     | 838  | TYR  | CB-CG-CD2 | 7.14  | 125.28      | 121.00   |
| 1   | E     | 333  | ASP  | CB-CG-OD2 | -7.14 | 111.88      | 118.30   |
| 1   | E     | 675  | ARG  | NE-CZ-NH1 | 7.13  | 123.86      | 120.30   |
| 1   | C     | 361  | ARG  | NE-CZ-NH1 | 7.13  | 123.86      | 120.30   |
| 2   | F     | 50   | ARG  | NE-CZ-NH2 | -7.11 | 116.75      | 120.30   |
| 1   | A     | 223  | ASP  | CB-CG-OD1 | 7.09  | 124.68      | 118.30   |
| 1   | G     | 501  | ARG  | NE-CZ-NH2 | -7.07 | 116.76      | 120.30   |
| 1   | G     | 667  | ASP  | CB-CG-OD2 | -7.07 | 111.93      | 118.30   |
| 1   | G     | 471  | ARG  | NE-CZ-NH1 | 7.07  | 123.83      | 120.30   |
| 1   | G     | 246  | ASP  | CB-CG-OD1 | 7.06  | 124.65      | 118.30   |
| 2   | B     | 97   | ASP  | CB-CG-OD2 | -7.05 | 111.96      | 118.30   |
| 2   | F     | 262  | ASP  | CB-CG-OD2 | -7.05 | 111.96      | 118.30   |
| 1   | C     | 490  | ARG  | NE-CZ-NH2 | -7.05 | 116.78      | 120.30   |
| 2   | B     | 114  | ASP  | CB-CG-OD2 | -7.04 | 111.96      | 118.30   |
| 2   | D     | 83   | ARG  | NE-CZ-NH2 | -7.03 | 116.78      | 120.30   |
| 1   | A     | 237  | PHE  | CB-CG-CD1 | -7.03 | 115.88      | 120.80   |
| 1   | A     | 845  | ARG  | NE-CZ-NH1 | 7.03  | 123.81      | 120.30   |
| 1   | G     | 333  | ASP  | CB-CG-OD2 | -7.03 | 111.97      | 118.30   |
| 1   | A     | 82   | ARG  | NE-CZ-NH1 | -7.00 | 116.80      | 120.30   |
| 2   | D     | 15   | PHE  | CB-CG-CD1 | -6.99 | 115.91      | 120.80   |
| 1   | G     | 509  | ARG  | NE-CZ-NH1 | 6.99  | 123.80      | 120.30   |
| 1   | E     | 129  | ARG  | NE-CZ-NH1 | 6.99  | 123.79      | 120.30   |
| 2   | B     | 188  | ASP  | CB-CG-OD1 | 6.98  | 124.58      | 118.30   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 2   | F     | 262    | ASP  | CB-CG-OD1 | 6.96  | 124.56      | 118.30   |
| 2   | B     | 342    | ARG  | NE-CZ-NH1 | 6.95  | 123.78      | 120.30   |
| 1   | A     | 675    | ARG  | NE-CZ-NH1 | 6.93  | 123.77      | 120.30   |
| 1   | G     | 43     | ARG  | NE-CZ-NH1 | 6.93  | 123.76      | 120.30   |
| 1   | E     | 625    | ASP  | CB-CG-OD1 | 6.91  | 124.52      | 118.30   |
| 1   | A     | 715    | ARG  | NE-CZ-NH1 | 6.88  | 123.74      | 120.30   |
| 2   | B     | 212    | ARG  | NE-CZ-NH1 | 6.87  | 123.74      | 120.30   |
| 1   | G     | 43     | ARG  | NE-CZ-NH2 | -6.87 | 116.86      | 120.30   |
| 1   | A     | 471    | ARG  | NE-CZ-NH2 | -6.86 | 116.87      | 120.30   |
| 1   | A     | 460    | ARG  | NE-CZ-NH2 | -6.86 | 116.87      | 120.30   |
| 1   | A     | 558    | ASP  | CB-CG-OD2 | -6.86 | 112.13      | 118.30   |
| 1   | G     | 733    | ASP  | CB-CG-OD2 | -6.85 | 112.13      | 118.30   |
| 1   | C     | 223    | ASP  | CB-CG-OD1 | 6.85  | 124.46      | 118.30   |
| 1   | A     | 670    | ASP  | CB-CG-OD2 | -6.84 | 112.14      | 118.30   |
| 1   | G     | 131    | ARG  | NE-CZ-NH2 | -6.84 | 116.88      | 120.30   |
| 2   | F     | 97     | ASP  | CB-CG-OD2 | -6.83 | 112.15      | 118.30   |
| 1   | E     | 82     | ARG  | NE-CZ-NH1 | 6.82  | 123.71      | 120.30   |
| 1   | A     | 490[A] | ARG  | NE-CZ-NH1 | 6.82  | 123.71      | 120.30   |
| 1   | A     | 490[B] | ARG  | NE-CZ-NH1 | 6.82  | 123.71      | 120.30   |
| 1   | C     | 956    | ARG  | NE-CZ-NH2 | -6.82 | 116.89      | 120.30   |
| 2   | H     | 215    | ARG  | NE-CZ-NH1 | 6.82  | 123.71      | 120.30   |
| 1   | E     | 435    | ARG  | NE-CZ-NH2 | -6.81 | 116.89      | 120.30   |
| 2   | H     | 67     | ASP  | CB-CG-OD1 | 6.81  | 124.43      | 118.30   |
| 2   | F     | 50     | ARG  | NE-CZ-NH1 | 6.81  | 123.70      | 120.30   |
| 1   | E     | 517    | ARG  | NE-CZ-NH2 | -6.80 | 116.90      | 120.30   |
| 2   | F     | 317    | ASP  | CB-CG-OD2 | -6.79 | 112.19      | 118.30   |
| 1   | C     | 757    | ASP  | CB-CG-OD1 | 6.76  | 124.39      | 118.30   |
| 1   | A     | 124    | ASP  | CB-CG-OD2 | -6.74 | 112.24      | 118.30   |
| 1   | C     | 330    | TYR  | CB-CG-CD2 | -6.73 | 116.96      | 121.00   |
| 2   | H     | 227    | ASP  | CB-CG-OD2 | -6.73 | 112.24      | 118.30   |
| 1   | G     | 848    | ARG  | NE-CZ-NH1 | 6.72  | 123.66      | 120.30   |
| 1   | A     | 763    | ASP  | CB-CG-OD2 | -6.72 | 112.25      | 118.30   |
| 1   | G     | 460    | ARG  | NE-CZ-NH2 | -6.71 | 116.94      | 120.30   |
| 1   | G     | 133    | ASP  | CB-CG-OD2 | -6.71 | 112.26      | 118.30   |
| 1   | C     | 223    | ASP  | CB-CG-OD2 | -6.71 | 112.26      | 118.30   |
| 2   | F     | 211    | ASP  | CB-CG-OD2 | -6.71 | 112.26      | 118.30   |
| 1   | C     | 609    | ASP  | CB-CG-OD1 | 6.68  | 124.32      | 118.30   |
| 1   | E     | 490    | ARG  | NE-CZ-NH1 | 6.68  | 123.64      | 120.30   |
| 2   | B     | 97     | ASP  | CB-CG-OD1 | 6.67  | 124.31      | 118.30   |
| 2   | D     | 334    | ASP  | CB-CG-OD2 | -6.67 | 112.30      | 118.30   |
| 1   | G     | 434    | ASP  | CB-CG-OD2 | -6.67 | 112.30      | 118.30   |
| 1   | A     | 333    | ASP  | CB-CG-OD2 | -6.67 | 112.30      | 118.30   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | G     | 330    | TYR  | CB-CG-CD2 | -6.67 | 117.00      | 121.00   |
| 2   | F     | 198    | ASP  | CB-CG-OD1 | 6.66  | 124.30      | 118.30   |
| 1   | G     | 238    | ASP  | CB-CG-OD2 | -6.66 | 112.31      | 118.30   |
| 2   | B     | 342    | ARG  | NE-CZ-NH2 | -6.66 | 116.97      | 120.30   |
| 1   | A     | 810    | ARG  | NE-CZ-NH2 | -6.65 | 116.97      | 120.30   |
| 1   | C     | 84     | ASP  | CB-CG-OD2 | -6.65 | 112.31      | 118.30   |
| 1   | G     | 625    | ASP  | CB-CG-OD1 | 6.64  | 124.28      | 118.30   |
| 1   | E     | 246    | ASP  | CB-CG-OD1 | 6.62  | 124.26      | 118.30   |
| 1   | C     | 124    | ASP  | CB-CG-OD2 | -6.62 | 112.35      | 118.30   |
| 1   | E     | 128    | ASP  | CB-CG-OD1 | 6.62  | 124.25      | 118.30   |
| 1   | C     | 104    | ARG  | NE-CZ-NH1 | 6.61  | 123.61      | 120.30   |
| 2   | B     | 188    | ASP  | CB-CG-OD2 | -6.61 | 112.36      | 118.30   |
| 1   | C     | 579    | ASP  | CB-CG-OD2 | -6.61 | 112.36      | 118.30   |
| 2   | D     | 262    | ASP  | CB-CG-OD2 | -6.61 | 112.36      | 118.30   |
| 1   | E     | 372    | ASP  | CB-CG-OD1 | 6.60  | 124.24      | 118.30   |
| 2   | F     | 139    | ASP  | CB-CG-OD2 | -6.60 | 112.36      | 118.30   |
| 1   | A     | 128    | ASP  | CB-CG-OD2 | -6.59 | 112.37      | 118.30   |
| 2   | F     | 227    | ASP  | CB-CG-OD1 | 6.59  | 124.23      | 118.30   |
| 2   | D     | 148[A] | ARG  | NE-CZ-NH1 | 6.59  | 123.59      | 120.30   |
| 2   | D     | 148[B] | ARG  | NE-CZ-NH1 | 6.59  | 123.59      | 120.30   |
| 1   | E     | 471    | ARG  | NE-CZ-NH2 | -6.59 | 117.01      | 120.30   |
| 1   | G     | 246    | ASP  | CB-CG-OD2 | -6.58 | 112.38      | 118.30   |
| 1   | C     | 530    | ASP  | CB-CG-OD1 | 6.58  | 124.22      | 118.30   |
| 1   | E     | 715    | ARG  | NE-CZ-NH2 | 6.57  | 123.58      | 120.30   |
| 2   | F     | 269    | CYS  | CA-CB-SG  | 6.55  | 125.79      | 114.00   |
| 1   | G     | 426[A] | ARG  | NE-CZ-NH2 | -6.55 | 117.03      | 120.30   |
| 1   | G     | 426[B] | ARG  | NE-CZ-NH2 | -6.55 | 117.03      | 120.30   |
| 1   | A     | 169    | ARG  | NE-CZ-NH1 | 6.55  | 123.57      | 120.30   |
| 1   | C     | 1027   | ARG  | NE-CZ-NH1 | 6.54  | 123.57      | 120.30   |
| 1   | A     | 459    | ASP  | CB-CG-OD2 | -6.54 | 112.41      | 118.30   |
| 1   | A     | 287    | ALA  | N-CA-CB   | 6.54  | 119.26      | 110.10   |
| 1   | A     | 343    | ARG  | NE-CZ-NH1 | 6.54  | 123.57      | 120.30   |
| 1   | G     | 258    | ASP  | CB-CG-OD2 | -6.54 | 112.42      | 118.30   |
| 1   | G     | 294    | ARG  | NE-CZ-NH2 | -6.53 | 117.03      | 120.30   |
| 1   | G     | 757    | ASP  | CB-CG-OD1 | 6.53  | 124.17      | 118.30   |
| 1   | A     | 667    | ASP  | CB-CG-OD2 | -6.52 | 112.43      | 118.30   |
| 1   | A     | 460    | ARG  | NE-CZ-NH1 | 6.52  | 123.56      | 120.30   |
| 2   | D     | 67     | ASP  | CB-CG-OD2 | -6.51 | 112.44      | 118.30   |
| 1   | G     | 226    | ASP  | CB-CG-OD2 | -6.51 | 112.44      | 118.30   |
| 2   | B     | 317    | ASP  | CB-CG-OD1 | 6.50  | 124.15      | 118.30   |
| 1   | C     | 57     | ASP  | CB-CG-OD2 | -6.50 | 112.45      | 118.30   |
| 1   | C     | 258    | ASP  | CB-CG-OD1 | 6.49  | 124.14      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | G     | 670  | ASP  | CB-CG-OD1  | 6.49  | 124.14      | 118.30   |
| 1   | A     | 614  | ASP  | CB-CG-OD1  | 6.49  | 124.14      | 118.30   |
| 1   | A     | 1041 | ASP  | CB-CG-OD1  | 6.48  | 124.13      | 118.30   |
| 2   | F     | 317  | ASP  | CB-CG-OD1  | 6.47  | 124.13      | 118.30   |
| 1   | G     | 642  | TYR  | CB-CG-CD2  | -6.47 | 117.12      | 121.00   |
| 1   | G     | 539  | ASP  | CB-CG-OD2  | -6.47 | 112.48      | 118.30   |
| 1   | G     | 258  | ASP  | CB-CG-OD1  | 6.46  | 124.12      | 118.30   |
| 1   | G     | 410  | ASP  | CB-CG-OD1  | 6.46  | 124.11      | 118.30   |
| 1   | A     | 944  | ARG  | NH1-CZ-NH2 | -6.45 | 112.30      | 119.40   |
| 1   | E     | 1025 | ASP  | CB-CG-OD1  | 6.45  | 124.10      | 118.30   |
| 2   | H     | 84   | ASP  | CB-CG-OD1  | 6.45  | 124.10      | 118.30   |
| 1   | E     | 791  | ASP  | CB-CG-OD1  | 6.44  | 124.10      | 118.30   |
| 1   | E     | 373  | ARG  | NE-CZ-NH1  | 6.44  | 123.52      | 120.30   |
| 2   | D     | 84   | ASP  | CB-CG-OD2  | -6.43 | 112.51      | 118.30   |
| 2   | D     | 50   | ARG  | NE-CZ-NH2  | -6.43 | 117.08      | 120.30   |
| 1   | E     | 410  | ASP  | CB-CG-OD1  | 6.43  | 124.09      | 118.30   |
| 1   | C     | 736  | ARG  | NE-CZ-NH2  | -6.41 | 117.09      | 120.30   |
| 2   | D     | 84   | ASP  | CB-CG-OD1  | 6.41  | 124.07      | 118.30   |
| 2   | D     | 192  | PHE  | CB-CG-CD1  | -6.41 | 116.31      | 120.80   |
| 1   | E     | 972  | ASP  | CB-CG-OD2  | -6.41 | 112.53      | 118.30   |
| 1   | G     | 991  | VAL  | CA-CB-CG1  | 6.41  | 120.51      | 110.90   |
| 1   | A     | 631  | ARG  | NE-CZ-NH1  | 6.40  | 123.50      | 120.30   |
| 1   | G     | 1025 | ASP  | CB-CG-OD1  | 6.38  | 124.04      | 118.30   |
| 1   | E     | 592  | ASP  | CB-CG-OD2  | -6.37 | 112.56      | 118.30   |
| 1   | E     | 124  | ASP  | CB-CG-OD1  | 6.36  | 124.03      | 118.30   |
| 1   | E     | 43   | ARG  | NE-CZ-NH2  | -6.36 | 117.12      | 120.30   |
| 1   | A     | 294  | ARG  | NE-CZ-NH1  | 6.35  | 123.47      | 120.30   |
| 1   | G     | 989  | ARG  | NE-CZ-NH2  | -6.35 | 117.12      | 120.30   |
| 1   | C     | 944  | ARG  | NE-CZ-NH1  | 6.34  | 123.47      | 120.30   |
| 1   | E     | 333  | ASP  | CB-CG-OD1  | 6.34  | 124.01      | 118.30   |
| 1   | A     | 763  | ASP  | CB-CG-OD1  | 6.34  | 124.01      | 118.30   |
| 2   | H     | 188  | ASP  | CB-CG-OD1  | 6.34  | 124.00      | 118.30   |
| 1   | A     | 57   | ASP  | CB-CG-OD2  | -6.33 | 112.60      | 118.30   |
| 1   | E     | 1025 | ASP  | CB-CG-OD2  | -6.32 | 112.61      | 118.30   |
| 1   | G     | 757  | ASP  | CB-CG-OD2  | -6.32 | 112.61      | 118.30   |
| 1   | E     | 494  | ARG  | NE-CZ-NH1  | 6.31  | 123.45      | 120.30   |
| 1   | C     | 667  | ASP  | CB-CG-OD2  | -6.30 | 112.63      | 118.30   |
| 1   | C     | 753  | ASP  | CB-CG-OD2  | -6.30 | 112.63      | 118.30   |
| 1   | E     | 733  | ASP  | CB-CG-OD2  | -6.30 | 112.63      | 118.30   |
| 1   | C     | 735  | ARG  | NE-CZ-NH2  | -6.30 | 117.15      | 120.30   |
| 1   | E     | 149  | ALA  | N-CA-CB    | 6.28  | 118.90      | 110.10   |
| 1   | C     | 57   | ASP  | CB-CG-OD1  | 6.28  | 123.95      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 161 | ASP  | CB-CG-OD2 | -6.28 | 112.65      | 118.30   |
| 1   | C     | 226 | ASP  | CB-CG-OD1 | 6.28  | 123.95      | 118.30   |
| 2   | B     | 317 | ASP  | CB-CG-OD2 | -6.27 | 112.66      | 118.30   |
| 2   | H     | 262 | ASP  | CB-CG-OD2 | -6.27 | 112.66      | 118.30   |
| 2   | D     | 112 | ASP  | CB-CG-OD1 | 6.26  | 123.94      | 118.30   |
| 2   | D     | 249 | ASP  | CB-CG-OD2 | -6.26 | 112.67      | 118.30   |
| 2   | F     | 249 | ASP  | CB-CG-OD1 | 6.26  | 123.93      | 118.30   |
| 1   | G     | 434 | ASP  | CB-CG-OD1 | 6.26  | 123.93      | 118.30   |
| 1   | G     | 807 | ASP  | CB-CG-OD1 | 6.25  | 123.92      | 118.30   |
| 1   | A     | 441 | ASP  | CB-CG-OD1 | 6.25  | 123.92      | 118.30   |
| 1   | C     | 460 | ARG  | NE-CZ-NH1 | 6.25  | 123.42      | 120.30   |
| 1   | A     | 521 | ASP  | CB-CG-OD2 | -6.23 | 112.69      | 118.30   |
| 1   | C     | 169 | ARG  | NE-CZ-NH1 | 6.22  | 123.41      | 120.30   |
| 1   | E     | 807 | ASP  | CB-CG-OD1 | 6.21  | 123.89      | 118.30   |
| 1   | G     | 27  | ASP  | CB-CG-OD2 | -6.20 | 112.72      | 118.30   |
| 2   | D     | 211 | ASP  | CB-CG-OD1 | 6.19  | 123.88      | 118.30   |
| 1   | A     | 261 | TYR  | CB-CG-CD2 | -6.19 | 117.28      | 121.00   |
| 1   | A     | 609 | ASP  | CB-CG-OD2 | -6.19 | 112.73      | 118.30   |
| 1   | C     | 539 | ASP  | CB-CG-OD2 | -6.19 | 112.73      | 118.30   |
| 2   | D     | 227 | ASP  | CB-CG-OD1 | 6.18  | 123.86      | 118.30   |
| 1   | G     | 130 | ARG  | NE-CZ-NH1 | 6.18  | 123.39      | 120.30   |
| 1   | G     | 956 | ARG  | NE-CZ-NH1 | 6.18  | 123.39      | 120.30   |
| 1   | G     | 674 | ASP  | CB-CG-OD2 | -6.17 | 112.74      | 118.30   |
| 1   | A     | 757 | ASP  | CB-CG-OD1 | 6.17  | 123.85      | 118.30   |
| 2   | B     | 249 | ASP  | CB-CG-OD2 | -6.17 | 112.75      | 118.30   |
| 1   | A     | 6   | ASP  | CB-CG-OD2 | -6.14 | 112.77      | 118.30   |
| 1   | A     | 416 | ASP  | CB-CG-OD2 | -6.14 | 112.78      | 118.30   |
| 1   | C     | 460 | ARG  | NE-CZ-NH2 | -6.13 | 117.23      | 120.30   |
| 2   | F     | 148 | ARG  | NE-CZ-NH2 | -6.13 | 117.23      | 120.30   |
| 2   | D     | 211 | ASP  | CB-CG-OD2 | -6.13 | 112.78      | 118.30   |
| 1   | A     | 670 | ASP  | CB-CG-OD1 | 6.12  | 123.81      | 118.30   |
| 1   | E     | 161 | ASP  | CB-CG-OD2 | -6.11 | 112.80      | 118.30   |
| 1   | G     | 716 | PRO  | N-CA-CB   | 6.11  | 110.64      | 103.30   |
| 1   | G     | 991 | VAL  | CA-CB-CG2 | 6.11  | 120.07      | 110.90   |
| 1   | G     | 959 | ASP  | CB-CG-OD1 | 6.11  | 123.80      | 118.30   |
| 1   | C     | 6   | ASP  | CB-CG-OD1 | 6.11  | 123.80      | 118.30   |
| 1   | C     | 197 | ASP  | CB-CG-OD1 | 6.11  | 123.80      | 118.30   |
| 1   | C     | 416 | ASP  | CB-CG-OD2 | -6.11 | 112.81      | 118.30   |
| 1   | G     | 769 | ASP  | CB-CG-OD2 | -6.09 | 112.82      | 118.30   |
| 1   | A     | 959 | ASP  | CB-CG-OD1 | 6.09  | 123.78      | 118.30   |
| 1   | A     | 400 | ARG  | NE-CZ-NH2 | -6.09 | 117.26      | 120.30   |
| 1   | C     | 558 | ASP  | N-CA-CB   | -6.08 | 99.65       | 110.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | E     | 197  | ASP  | CB-CG-OD1 | 6.08  | 123.77      | 118.30   |
| 1   | C     | 592  | ASP  | CB-CG-OD2 | -6.08 | 112.83      | 118.30   |
| 1   | E     | 539  | ASP  | CB-CG-OD1 | 6.07  | 123.77      | 118.30   |
| 1   | A     | 246  | ASP  | CB-CG-OD2 | -6.07 | 112.84      | 118.30   |
| 2   | B     | 211  | ASP  | CB-CG-OD1 | 6.07  | 123.76      | 118.30   |
| 1   | E     | 128  | ASP  | CB-CG-OD2 | -6.05 | 112.85      | 118.30   |
| 1   | E     | 539  | ASP  | CB-CG-OD2 | -6.05 | 112.85      | 118.30   |
| 1   | G     | 197  | ASP  | CB-CG-OD2 | -6.05 | 112.85      | 118.30   |
| 1   | A     | 294  | ARG  | NE-CZ-NH2 | -6.05 | 117.28      | 120.30   |
| 2   | B     | 69   | ASP  | CB-CG-OD1 | 6.05  | 123.74      | 118.30   |
| 1   | A     | 758  | ASP  | CB-CG-OD1 | 6.04  | 123.74      | 118.30   |
| 1   | E     | 671  | ARG  | NE-CZ-NH2 | -6.04 | 117.28      | 120.30   |
| 1   | C     | 333  | ASP  | CB-CG-OD1 | 6.04  | 123.73      | 118.30   |
| 1   | C     | 238  | ASP  | CB-CG-OD1 | 6.02  | 123.72      | 118.30   |
| 1   | C     | 652  | ARG  | CD-NE-CZ  | 6.02  | 132.03      | 123.60   |
| 1   | C     | 670  | ASP  | CB-CG-OD1 | 6.02  | 123.72      | 118.30   |
| 1   | G     | 169  | ARG  | NE-CZ-NH1 | 6.02  | 123.31      | 120.30   |
| 1   | C     | 757  | ASP  | CB-CG-OD2 | -6.01 | 112.89      | 118.30   |
| 1   | G     | 42   | TYR  | CB-CG-CD2 | 6.00  | 124.60      | 121.00   |
| 1   | A     | 28   | TYR  | CB-CG-CD2 | -5.99 | 117.41      | 121.00   |
| 1   | A     | 333  | ASP  | CB-CG-OD1 | 5.99  | 123.69      | 118.30   |
| 1   | C     | 487  | ASP  | CB-CG-OD1 | 5.97  | 123.67      | 118.30   |
| 1   | C     | 1010 | TYR  | CB-CG-CD2 | -5.97 | 117.42      | 121.00   |
| 1   | C     | 810  | ARG  | NE-CZ-NH1 | 5.95  | 123.28      | 120.30   |
| 1   | G     | 559  | ARG  | NE-CZ-NH2 | -5.95 | 117.33      | 120.30   |
| 1   | A     | 499  | ASP  | CB-CG-OD1 | 5.95  | 123.65      | 118.30   |
| 2   | B     | 105  | HIS  | CA-CB-CG  | -5.95 | 103.49      | 113.60   |
| 1   | A     | 1057 | ASP  | CB-CG-OD1 | 5.94  | 123.65      | 118.30   |
| 1   | A     | 499  | ASP  | CB-CG-OD2 | -5.94 | 112.95      | 118.30   |
| 2   | F     | 136  | ASP  | CB-CG-OD1 | 5.94  | 123.64      | 118.30   |
| 1   | A     | 539  | ASP  | CB-CG-OD2 | -5.93 | 112.96      | 118.30   |
| 2   | H     | 139  | ASP  | CB-CG-OD2 | -5.93 | 112.96      | 118.30   |
| 2   | H     | 114  | ASP  | CB-CG-OD1 | 5.92  | 123.63      | 118.30   |
| 2   | D     | 299  | ASP  | CB-CG-OD2 | -5.92 | 112.97      | 118.30   |
| 1   | G     | 82   | ARG  | NE-CZ-NH2 | -5.92 | 117.34      | 120.30   |
| 1   | G     | 758  | ASP  | CB-CG-OD1 | 5.92  | 123.62      | 118.30   |
| 2   | F     | 344  | ASP  | CB-CG-OD2 | -5.91 | 112.98      | 118.30   |
| 1   | E     | 84   | ASP  | CB-CG-OD2 | -5.90 | 112.99      | 118.30   |
| 1   | A     | 517  | ARG  | NE-CZ-NH1 | 5.90  | 123.25      | 120.30   |
| 1   | A     | 810  | ARG  | NE-CZ-NH1 | 5.90  | 123.25      | 120.30   |
| 1   | E     | 823  | ARG  | NE-CZ-NH1 | 5.90  | 123.25      | 120.30   |
| 2   | B     | 344  | ASP  | CB-CG-OD2 | -5.89 | 113.00      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | G     | 128  | ASP  | CB-CG-OD2 | -5.89 | 113.00      | 118.30   |
| 1   | C     | 42   | TYR  | CB-CG-CD1 | -5.89 | 117.47      | 121.00   |
| 1   | E     | 974  | THR  | CA-CB-CG2 | -5.88 | 104.16      | 112.40   |
| 1   | C     | 441  | ASP  | CB-CG-OD2 | -5.88 | 113.00      | 118.30   |
| 1   | C     | 557  | THR  | C-N-CA    | 5.88  | 136.41      | 121.70   |
| 1   | G     | 338  | ASP  | CB-CG-OD2 | -5.88 | 113.01      | 118.30   |
| 2   | D     | 299  | ASP  | CB-CG-OD1 | 5.88  | 123.59      | 118.30   |
| 1   | G     | 1025 | ASP  | CB-CG-OD2 | -5.87 | 113.01      | 118.30   |
| 1   | G     | 238  | ASP  | CB-CG-OD1 | 5.87  | 123.58      | 118.30   |
| 2   | H     | 215  | ARG  | N-CA-CB   | -5.87 | 100.04      | 110.60   |
| 2   | F     | 84   | ASP  | CB-CG-OD1 | 5.86  | 123.58      | 118.30   |
| 1   | G     | 521  | ASP  | CB-CG-OD1 | 5.86  | 123.58      | 118.30   |
| 1   | E     | 959  | ASP  | CB-CG-OD1 | 5.85  | 123.57      | 118.30   |
| 1   | C     | 161  | ASP  | CB-CG-OD2 | -5.84 | 113.04      | 118.30   |
| 1   | A     | 449  | VAL  | CA-CB-CG2 | -5.83 | 102.15      | 110.90   |
| 1   | E     | 944  | ARG  | NE-CZ-NH2 | -5.83 | 117.39      | 120.30   |
| 1   | C     | 1025 | ASP  | CB-CG-OD1 | 5.83  | 123.55      | 118.30   |
| 1   | C     | 372  | ASP  | CB-CG-OD2 | -5.83 | 113.06      | 118.30   |
| 2   | F     | 211  | ASP  | CB-CG-OD1 | 5.83  | 123.54      | 118.30   |
| 1   | G     | 57   | ASP  | CB-CG-OD1 | 5.83  | 123.54      | 118.30   |
| 1   | C     | 226  | ASP  | CB-CG-OD2 | -5.82 | 113.06      | 118.30   |
| 1   | C     | 674  | ASP  | CB-CG-OD1 | 5.82  | 123.54      | 118.30   |
| 1   | A     | 4    | ARG  | NE-CZ-NH1 | 5.81  | 123.21      | 120.30   |
| 1   | E     | 334  | GLU  | CB-CA-C   | -5.81 | 98.78       | 110.40   |
| 1   | E     | 251  | ALA  | N-CA-CB   | 5.81  | 118.23      | 110.10   |
| 2   | F     | 248  | ASP  | CB-CG-OD1 | 5.80  | 123.52      | 118.30   |
| 1   | A     | 1057 | ASP  | CB-CG-OD2 | -5.79 | 113.09      | 118.30   |
| 1   | E     | 791  | ASP  | CB-CG-OD2 | -5.79 | 113.09      | 118.30   |
| 1   | E     | 730  | ASP  | CB-CG-OD2 | -5.78 | 113.09      | 118.30   |
| 1   | G     | 430  | ASP  | CB-CG-OD2 | -5.78 | 113.10      | 118.30   |
| 1   | C     | 430  | ASP  | CB-CG-OD2 | -5.78 | 113.10      | 118.30   |
| 1   | C     | 131  | ARG  | NE-CZ-NH2 | -5.77 | 117.41      | 120.30   |
| 1   | C     | 716  | PRO  | N-CA-CB   | 5.77  | 110.23      | 103.30   |
| 1   | A     | 441  | ASP  | CB-CG-OD2 | -5.77 | 113.11      | 118.30   |
| 1   | G     | 758  | ASP  | CB-CG-OD2 | -5.76 | 113.11      | 118.30   |
| 1   | G     | 807  | ASP  | CB-CG-OD2 | -5.76 | 113.11      | 118.30   |
| 1   | G     | 904  | ASP  | CB-CG-OD1 | 5.76  | 123.49      | 118.30   |
| 1   | C     | 207  | ASP  | CB-CG-OD2 | -5.76 | 113.12      | 118.30   |
| 2   | H     | 112  | ASP  | CB-CG-OD1 | 5.76  | 123.48      | 118.30   |
| 1   | C     | 625  | ASP  | CB-CG-OD1 | 5.75  | 123.48      | 118.30   |
| 1   | G     | 974  | THR  | CA-CB-CG2 | -5.75 | 104.35      | 112.40   |
| 1   | A     | 684  | ARG  | NE-CZ-NH1 | 5.75  | 123.17      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | D     | 128  | GLN  | CB-CA-C   | -5.75 | 98.91       | 110.40   |
| 1   | C     | 642  | TYR  | CB-CG-CD2 | -5.74 | 117.56      | 121.00   |
| 2   | H     | 136  | ASP  | CB-CG-OD2 | -5.74 | 113.14      | 118.30   |
| 1   | E     | 131  | ARG  | NE-CZ-NH2 | -5.73 | 117.44      | 120.30   |
| 2   | H     | 244  | ASP  | CB-CG-OD1 | 5.72  | 123.45      | 118.30   |
| 2   | D     | 362  | ASP  | CB-CG-OD1 | 5.71  | 123.44      | 118.30   |
| 1   | A     | 912  | ARG  | NE-CZ-NH1 | 5.71  | 123.16      | 120.30   |
| 1   | A     | 677  | ARG  | NE-CZ-NH2 | -5.71 | 117.45      | 120.30   |
| 1   | G     | 129  | ARG  | NE-CZ-NH1 | 5.70  | 123.15      | 120.30   |
| 1   | G     | 950  | ARG  | NE-CZ-NH2 | -5.70 | 117.45      | 120.30   |
| 1   | A     | 434  | ASP  | CB-CG-OD2 | -5.70 | 113.17      | 118.30   |
| 1   | E     | 1020 | ARG  | CD-NE-CZ  | 5.69  | 131.57      | 123.60   |
| 1   | G     | 912  | ARG  | CD-NE-CZ  | 5.69  | 131.57      | 123.60   |
| 1   | A     | 84   | ASP  | CB-CG-OD2 | -5.68 | 113.19      | 118.30   |
| 2   | B     | 154  | ASN  | N-CA-CB   | 5.67  | 120.81      | 110.60   |
| 1   | C     | 129  | ARG  | NE-CZ-NH2 | -5.67 | 117.47      | 120.30   |
| 1   | A     | 674  | ASP  | CB-CG-OD2 | -5.66 | 113.20      | 118.30   |
| 1   | G     | 373  | ARG  | NE-CZ-NH1 | 5.66  | 123.13      | 120.30   |
| 1   | E     | 730  | ASP  | CB-CG-OD1 | 5.65  | 123.38      | 118.30   |
| 1   | G     | 558  | ASP  | CB-CG-OD1 | 5.64  | 123.38      | 118.30   |
| 1   | G     | 133  | ASP  | CB-CG-OD1 | 5.64  | 123.38      | 118.30   |
| 1   | E     | 133  | ASP  | CB-CG-OD1 | 5.64  | 123.38      | 118.30   |
| 1   | G     | 273  | ARG  | NE-CZ-NH2 | -5.64 | 117.48      | 120.30   |
| 2   | H     | 67   | ASP  | CB-CG-OD2 | -5.64 | 113.22      | 118.30   |
| 1   | C     | 667  | ASP  | CB-CG-OD1 | 5.64  | 123.37      | 118.30   |
| 2   | B     | 127  | ALA  | N-CA-CB   | 5.63  | 117.99      | 110.10   |
| 2   | F     | 198  | ASP  | CB-CG-OD2 | -5.62 | 113.24      | 118.30   |
| 2   | F     | 362  | ASP  | CB-CG-OD2 | -5.62 | 113.24      | 118.30   |
| 1   | E     | 998  | ARG  | NE-CZ-NH2 | -5.62 | 117.49      | 120.30   |
| 1   | G     | 501  | ARG  | NE-CZ-NH1 | 5.62  | 123.11      | 120.30   |
| 1   | G     | 558  | ASP  | N-CA-CB   | -5.62 | 100.48      | 110.60   |
| 1   | A     | 121  | ASP  | CB-CG-OD2 | -5.62 | 113.25      | 118.30   |
| 1   | E     | 716  | PRO  | N-CA-CB   | 5.61  | 110.04      | 103.30   |
| 2   | B     | 84   | ASP  | CB-CG-OD1 | 5.61  | 123.35      | 118.30   |
| 1   | C     | 579  | ASP  | CB-CG-OD1 | 5.61  | 123.35      | 118.30   |
| 1   | G     | 609  | ASP  | CB-CG-OD2 | -5.61 | 113.25      | 118.30   |
| 2   | B     | 154  | ASN  | CB-CA-C   | 5.60  | 121.61      | 110.40   |
| 1   | A     | 716  | PRO  | N-CA-CB   | 5.60  | 110.02      | 103.30   |
| 1   | G     | 373  | ARG  | NE-CZ-NH2 | -5.59 | 117.50      | 120.30   |
| 1   | C     | 133  | ASP  | CB-CG-OD2 | -5.59 | 113.27      | 118.30   |
| 1   | G     | 82   | ARG  | CD-NE-CZ  | 5.59  | 131.42      | 123.60   |
| 2   | D     | 45   | ASP  | CB-CG-OD2 | -5.58 | 113.28      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | G     | 487  | ASP  | CB-CG-OD2 | -5.58 | 113.28      | 118.30   |
| 1   | A     | 169  | ARG  | NE-CZ-NH2 | -5.58 | 117.51      | 120.30   |
| 2   | D     | 249  | ASP  | CB-CG-OD1 | 5.58  | 123.32      | 118.30   |
| 1   | E     | 386  | ALA  | N-CA-CB   | 5.58  | 117.91      | 110.10   |
| 1   | A     | 625  | ASP  | CB-CG-OD1 | 5.57  | 123.32      | 118.30   |
| 1   | E     | 684  | ARG  | NE-CZ-NH1 | 5.57  | 123.09      | 120.30   |
| 1   | G     | 119  | THR  | CA-CB-CG2 | -5.57 | 104.60      | 112.40   |
| 2   | D     | 159  | ALA  | CB-CA-C   | 5.56  | 118.44      | 110.10   |
| 1   | A     | 557  | THR  | C-N-CA    | 5.56  | 135.59      | 121.70   |
| 1   | G     | 609  | ASP  | CB-CG-OD1 | 5.54  | 123.29      | 118.30   |
| 2   | H     | 139  | ASP  | CB-CG-OD1 | 5.54  | 123.29      | 118.30   |
| 1   | E     | 625  | ASP  | CB-CG-OD2 | -5.54 | 113.31      | 118.30   |
| 2   | H     | 344  | ASP  | CB-CG-OD2 | -5.54 | 113.31      | 118.30   |
| 1   | A     | 258  | ASP  | CB-CG-OD1 | 5.54  | 123.28      | 118.30   |
| 2   | B     | 326  | ARG  | NE-CZ-NH1 | 5.53  | 123.07      | 120.30   |
| 2   | B     | 139  | ASP  | CB-CG-OD2 | -5.53 | 113.32      | 118.30   |
| 1   | G     | 39   | GLU  | CB-CA-C   | -5.53 | 99.35       | 110.40   |
| 2   | H     | 378  | ARG  | NE-CZ-NH2 | -5.53 | 117.54      | 120.30   |
| 1   | C     | 121  | ASP  | CB-CG-OD1 | 5.52  | 123.27      | 118.30   |
| 2   | B     | 368  | ASP  | CB-CG-OD1 | 5.52  | 123.26      | 118.30   |
| 1   | C     | 625  | ASP  | CB-CG-OD2 | -5.52 | 113.34      | 118.30   |
| 1   | E     | 410  | ASP  | CB-CG-OD2 | -5.50 | 113.34      | 118.30   |
| 2   | B     | 198  | ASP  | CB-CG-OD2 | -5.50 | 113.35      | 118.30   |
| 2   | H     | 377  | TYR  | CB-CG-CD2 | -5.50 | 117.70      | 121.00   |
| 1   | C     | 84   | ASP  | CB-CG-OD1 | 5.50  | 123.25      | 118.30   |
| 1   | C     | 435  | ARG  | NE-CZ-NH1 | 5.50  | 123.05      | 120.30   |
| 1   | A     | 1025 | ASP  | CB-CG-OD1 | 5.50  | 123.25      | 118.30   |
| 2   | D     | 197  | TYR  | CB-CG-CD2 | 5.50  | 124.30      | 121.00   |
| 1   | G     | 972  | ASP  | CB-CG-OD1 | 5.50  | 123.25      | 118.30   |
| 2   | D     | 13   | THR  | CA-CB-CG2 | -5.50 | 104.70      | 112.40   |
| 2   | F     | 97   | ASP  | CB-CG-OD1 | 5.49  | 123.24      | 118.30   |
| 1   | G     | 338  | ASP  | CB-CG-OD1 | 5.49  | 123.24      | 118.30   |
| 1   | A     | 133  | ASP  | CB-CG-OD1 | 5.49  | 123.24      | 118.30   |
| 1   | C     | 867  | ARG  | NE-CZ-NH1 | 5.49  | 123.05      | 120.30   |
| 1   | C     | 520  | TYR  | CB-CG-CD2 | -5.48 | 117.71      | 121.00   |
| 1   | G     | 631  | ARG  | NE-CZ-NH1 | 5.48  | 123.04      | 120.30   |
| 1   | E     | 478  | GLU  | CB-CG-CD  | -5.47 | 99.42       | 114.20   |
| 1   | E     | 594  | TYR  | CB-CG-CD2 | -5.47 | 117.72      | 121.00   |
| 1   | A     | 1025 | ASP  | CB-CG-OD2 | -5.47 | 113.38      | 118.30   |
| 1   | G     | 521  | ASP  | CB-CG-OD2 | -5.47 | 113.38      | 118.30   |
| 1   | A     | 237  | PHE  | CB-CG-CD2 | 5.46  | 124.63      | 120.80   |
| 1   | C     | 888  | TYR  | CB-CG-CD1 | -5.46 | 117.72      | 121.00   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 2   | H     | 93     | ARG  | NE-CZ-NH1 | 5.46  | 123.03      | 120.30   |
| 1   | A     | 667    | ASP  | CB-CG-OD1 | 5.46  | 123.22      | 118.30   |
| 1   | E     | 457    | ASN  | N-CA-CB   | 5.46  | 120.43      | 110.60   |
| 2   | F     | 344    | ASP  | CB-CG-OD1 | 5.46  | 123.21      | 118.30   |
| 1   | A     | 118    | ALA  | N-CA-CB   | 5.45  | 117.73      | 110.10   |
| 1   | C     | 38     | ARG  | NE-CZ-NH1 | 5.45  | 123.02      | 120.30   |
| 2   | B     | 248    | ASP  | CB-CG-OD1 | 5.44  | 123.20      | 118.30   |
| 2   | F     | 362    | ASP  | CB-CG-OD1 | 5.44  | 123.20      | 118.30   |
| 1   | A     | 459    | ASP  | CB-CG-OD1 | 5.44  | 123.19      | 118.30   |
| 2   | D     | 234    | ASP  | CB-CG-OD2 | -5.44 | 113.41      | 118.30   |
| 1   | G     | 121    | ASP  | CB-CG-OD2 | -5.43 | 113.41      | 118.30   |
| 2   | D     | 247    | PRO  | C-N-CA    | 5.43  | 135.28      | 121.70   |
| 1   | G     | 471    | ARG  | NE-CZ-NH2 | -5.43 | 117.58      | 120.30   |
| 1   | G     | 791    | ASP  | CB-CG-OD1 | 5.43  | 123.19      | 118.30   |
| 1   | G     | 389    | ARG  | NE-CZ-NH2 | -5.43 | 117.58      | 120.30   |
| 1   | A     | 338    | ASP  | CB-CG-OD2 | -5.42 | 113.42      | 118.30   |
| 1   | A     | 130[A] | ARG  | NE-CZ-NH2 | -5.42 | 117.59      | 120.30   |
| 1   | A     | 130[B] | ARG  | NE-CZ-NH2 | -5.42 | 117.59      | 120.30   |
| 2   | F     | 157    | ASP  | CB-CG-OD1 | 5.42  | 123.18      | 118.30   |
| 1   | G     | 922    | ARG  | NE-CZ-NH2 | -5.42 | 117.59      | 120.30   |
| 2   | H     | 45     | ASP  | CB-CG-OD1 | 5.41  | 123.17      | 118.30   |
| 1   | C     | 1003   | ASP  | CB-CG-OD2 | -5.41 | 113.44      | 118.30   |
| 2   | D     | 139    | ASP  | CB-CG-OD2 | -5.41 | 113.44      | 118.30   |
| 1   | C     | 361    | ARG  | NE-CZ-NH2 | -5.40 | 117.60      | 120.30   |
| 2   | H     | 18     | ARG  | NE-CZ-NH2 | -5.40 | 117.60      | 120.30   |
| 1   | G     | 887    | TYR  | CB-CG-CD1 | -5.39 | 117.76      | 121.00   |
| 1   | A     | 82     | ARG  | CD-NE-CZ  | -5.38 | 116.07      | 123.60   |
| 2   | B     | 157    | ASP  | CB-CG-OD1 | 5.38  | 123.14      | 118.30   |
| 1   | A     | 757    | ASP  | CB-CG-OD2 | -5.37 | 113.46      | 118.30   |
| 1   | A     | 904    | ASP  | CB-CG-OD1 | 5.37  | 123.13      | 118.30   |
| 1   | E     | 763    | ASP  | CB-CA-C   | -5.37 | 99.66       | 110.40   |
| 1   | G     | 416    | ASP  | CB-CG-OD1 | 5.37  | 123.13      | 118.30   |
| 1   | G     | 494    | ARG  | NE-CZ-NH2 | -5.37 | 117.61      | 120.30   |
| 1   | G     | 330    | TYR  | CB-CG-CD1 | 5.37  | 124.22      | 121.00   |
| 1   | C     | 763    | ASP  | CB-CG-OD2 | -5.37 | 113.47      | 118.30   |
| 2   | B     | 286    | MET  | CG-SD-CE  | -5.36 | 91.62       | 100.20   |
| 2   | H     | 362    | ASP  | CB-CG-OD2 | -5.35 | 113.48      | 118.30   |
| 1   | G     | 1031   | ARG  | NE-CZ-NH1 | 5.35  | 122.97      | 120.30   |
| 1   | E     | 972    | ASP  | N-CA-CB   | 5.34  | 120.22      | 110.60   |
| 1   | A     | 614    | ASP  | CB-CG-OD2 | -5.34 | 113.49      | 118.30   |
| 1   | C     | 400    | ARG  | NE-CZ-NH1 | 5.34  | 122.97      | 120.30   |
| 1   | G     | 674    | ASP  | CB-CG-OD1 | 5.33  | 123.10      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | C     | 297  | VAL  | CA-CB-CG1 | -5.33 | 102.91      | 110.90   |
| 1   | E     | 1003 | ASP  | CB-CG-OD2 | -5.33 | 113.51      | 118.30   |
| 2   | D     | 344  | ASP  | CB-CG-OD2 | -5.33 | 113.51      | 118.30   |
| 1   | G     | 559  | ARG  | NE-CZ-NH1 | 5.32  | 122.96      | 120.30   |
| 1   | A     | 830  | PHE  | CB-CA-C   | -5.31 | 99.78       | 110.40   |
| 1   | C     | 922  | ARG  | NE-CZ-NH1 | 5.31  | 122.96      | 120.30   |
| 1   | C     | 1003 | ASP  | CB-CG-OD1 | 5.31  | 123.08      | 118.30   |
| 1   | C     | 333  | ASP  | CB-CG-OD2 | -5.30 | 113.53      | 118.30   |
| 1   | E     | 124  | ASP  | CB-CG-OD2 | -5.30 | 113.53      | 118.30   |
| 1   | C     | 75   | ARG  | NE-CZ-NH1 | 5.30  | 122.95      | 120.30   |
| 1   | G     | 372  | ASP  | CB-CG-OD1 | 5.29  | 123.06      | 118.30   |
| 2   | D     | 197  | TYR  | CB-CG-CD1 | -5.29 | 117.83      | 121.00   |
| 1   | E     | 652  | ARG  | NE-CZ-NH2 | -5.29 | 117.66      | 120.30   |
| 1   | E     | 27   | ASP  | CB-CG-OD2 | -5.29 | 113.54      | 118.30   |
| 2   | H     | 216  | LEU  | CA-C-N    | -5.29 | 105.57      | 117.20   |
| 1   | A     | 57   | ASP  | CB-CG-OD1 | 5.28  | 123.05      | 118.30   |
| 2   | B     | 136  | ASP  | CB-CG-OD1 | 5.28  | 123.05      | 118.30   |
| 1   | E     | 226  | ASP  | CB-CG-OD2 | -5.28 | 113.55      | 118.30   |
| 1   | A     | 733  | ASP  | CB-CG-OD2 | -5.28 | 113.55      | 118.30   |
| 1   | G     | 353  | ASP  | CB-CG-OD1 | 5.28  | 123.05      | 118.30   |
| 2   | D     | 157  | ASP  | CB-CG-OD1 | 5.27  | 123.05      | 118.30   |
| 1   | C     | 204  | LEU  | CB-CA-C   | -5.27 | 100.19      | 110.20   |
| 2   | F     | 244  | ASP  | CB-CG-OD2 | -5.27 | 113.56      | 118.30   |
| 1   | G     | 487  | ASP  | CB-CG-OD1 | 5.26  | 123.04      | 118.30   |
| 1   | A     | 608  | THR  | CA-CB-CG2 | -5.25 | 105.05      | 112.40   |
| 1   | A     | 807  | ASP  | CB-CG-OD2 | -5.25 | 113.58      | 118.30   |
| 2   | B     | 247  | PRO  | C-N-CA    | 5.24  | 134.79      | 121.70   |
| 1   | E     | 757  | ASP  | CB-CG-OD2 | -5.24 | 113.59      | 118.30   |
| 1   | A     | 807  | ASP  | CB-CG-OD1 | 5.23  | 123.01      | 118.30   |
| 1   | C     | 614  | ASP  | CB-CG-OD2 | -5.23 | 113.59      | 118.30   |
| 1   | A     | 758  | ASP  | CB-CG-OD2 | -5.22 | 113.60      | 118.30   |
| 1   | C     | 675  | ARG  | NE-CZ-NH1 | 5.22  | 122.91      | 120.30   |
| 1   | G     | 333  | ASP  | CB-CG-OD1 | 5.22  | 123.00      | 118.30   |
| 1   | G     | 27   | ASP  | CB-CG-OD1 | 5.22  | 123.00      | 118.30   |
| 1   | C     | 371  | ASN  | O-C-N     | -5.21 | 114.36      | 122.70   |
| 2   | D     | 154  | ASN  | N-CA-C    | 5.21  | 125.07      | 111.00   |
| 1   | A     | 40   | GLU  | CG-CD-OE2 | -5.21 | 107.88      | 118.30   |
| 1   | C     | 1041 | ASP  | CB-CG-OD1 | 5.21  | 122.99      | 118.30   |
| 1   | C     | 1025 | ASP  | CB-CG-OD2 | -5.21 | 113.61      | 118.30   |
| 2   | F     | 112  | ASP  | CB-CG-OD1 | 5.21  | 122.99      | 118.30   |
| 1   | C     | 730  | ASP  | CB-CG-OD1 | 5.21  | 122.98      | 118.30   |
| 1   | E     | 757  | ASP  | CB-CG-OD1 | 5.20  | 122.98      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | C     | 246  | ASP  | CB-CG-OD2 | -5.20 | 113.62      | 118.30   |
| 2   | F     | 157  | ASP  | CB-CG-OD2 | -5.20 | 113.62      | 118.30   |
| 1   | C     | 864  | VAL  | CA-CB-CG2 | -5.20 | 103.11      | 110.90   |
| 1   | E     | 667  | ASP  | CB-CG-OD1 | 5.19  | 122.97      | 118.30   |
| 1   | E     | 133  | ASP  | CB-CG-OD2 | -5.19 | 113.63      | 118.30   |
| 1   | E     | 677  | ARG  | NE-CZ-NH1 | 5.19  | 122.89      | 120.30   |
| 1   | E     | 758  | ASP  | CB-CG-OD1 | 5.18  | 122.96      | 118.30   |
| 1   | G     | 81   | GLU  | CG-CD-OE2 | -5.18 | 107.94      | 118.30   |
| 2   | H     | 247  | PRO  | C-N-CA    | 5.18  | 134.65      | 121.70   |
| 1   | C     | 1057 | ASP  | CB-CG-OD1 | 5.17  | 122.95      | 118.30   |
| 2   | B     | 50   | ARG  | NE-CZ-NH2 | -5.17 | 117.72      | 120.30   |
| 1   | E     | 989  | ARG  | NE-CZ-NH2 | -5.16 | 117.72      | 120.30   |
| 1   | G     | 24   | CYS  | CA-CB-SG  | -5.16 | 104.71      | 114.00   |
| 1   | C     | 539  | ASP  | CB-CG-OD1 | 5.15  | 122.94      | 118.30   |
| 1   | A     | 306  | ARG  | NE-CZ-NH2 | 5.15  | 122.88      | 120.30   |
| 1   | A     | 615  | ARG  | NE-CZ-NH1 | 5.15  | 122.88      | 120.30   |
| 1   | G     | 450  | ASP  | CB-CG-OD2 | -5.15 | 113.67      | 118.30   |
| 1   | C     | 580  | TYR  | CB-CG-CD1 | -5.14 | 117.92      | 121.00   |
| 1   | C     | 684  | ARG  | NE-CZ-NH2 | -5.13 | 117.73      | 120.30   |
| 1   | G     | 528  | ARG  | NE-CZ-NH1 | 5.13  | 122.86      | 120.30   |
| 1   | A     | 517  | ARG  | NE-CZ-NH2 | -5.12 | 117.74      | 120.30   |
| 1   | E     | 65   | TYR  | CB-CG-CD1 | -5.12 | 117.92      | 121.00   |
| 1   | C     | 959  | ASP  | CB-CG-OD1 | 5.12  | 122.91      | 118.30   |
| 1   | A     | 765  | ASP  | CB-CG-OD1 | 5.12  | 122.90      | 118.30   |
| 1   | A     | 904  | ASP  | CB-CG-OD2 | -5.11 | 113.70      | 118.30   |
| 1   | G     | 294  | ARG  | NE-CZ-NH1 | 5.11  | 122.85      | 120.30   |
| 2   | D     | 188  | ASP  | CB-CG-OD2 | -5.10 | 113.71      | 118.30   |
| 2   | D     | 326  | ARG  | NE-CZ-NH1 | 5.10  | 122.85      | 120.30   |
| 2   | H     | 154  | ASN  | CB-CA-C   | 5.10  | 120.60      | 110.40   |
| 2   | B     | 15   | PHE  | CB-CG-CD1 | -5.09 | 117.24      | 120.80   |
| 2   | B     | 50   | ARG  | CB-CA-C   | -5.09 | 100.22      | 110.40   |
| 1   | C     | 1057 | ASP  | N-CA-CB   | 5.09  | 119.77      | 110.60   |
| 2   | F     | 84   | ASP  | CB-CG-OD2 | -5.08 | 113.72      | 118.30   |
| 2   | H     | 97   | ASP  | CB-CG-OD1 | 5.08  | 122.88      | 118.30   |
| 2   | F     | 154  | ASN  | N-CA-CB   | 5.08  | 119.75      | 110.60   |
| 1   | A     | 372  | ASP  | CB-CG-OD2 | -5.08 | 113.73      | 118.30   |
| 1   | A     | 559  | ARG  | NE-CZ-NH2 | -5.08 | 117.76      | 120.30   |
| 2   | B     | 306  | MET  | CG-SD-CE  | -5.08 | 92.08       | 100.20   |
| 2   | D     | 6    | LEU  | N-CA-CB   | -5.07 | 100.25      | 110.40   |
| 1   | E     | 104  | ARG  | NE-CZ-NH2 | -5.07 | 117.76      | 120.30   |
| 1   | E     | 416  | ASP  | CB-CG-OD1 | 5.07  | 122.86      | 118.30   |
| 1   | G     | 557  | THR  | C-N-CA    | 5.07  | 134.38      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | G     | 885  | PRO  | N-CA-CB   | 5.07  | 109.38      | 103.30   |
| 1   | A     | 402  | LEU  | CB-CG-CD2 | -5.06 | 102.39      | 111.00   |
| 1   | C     | 27   | ASP  | CB-CG-OD1 | 5.06  | 122.86      | 118.30   |
| 1   | E     | 530  | ASP  | CB-CG-OD2 | -5.06 | 113.75      | 118.30   |
| 1   | E     | 1054 | LEU  | CB-CA-C   | -5.06 | 100.59      | 110.20   |
| 2   | F     | 88   | ILE  | CB-CA-C   | -5.06 | 101.49      | 111.60   |
| 2   | F     | 269  | CYS  | N-CA-CB   | 5.05  | 119.70      | 110.60   |
| 1   | C     | 614  | ASP  | CB-CG-OD1 | 5.05  | 122.85      | 118.30   |
| 1   | E     | 1000 | HIS  | CA-CB-CG  | -5.05 | 105.01      | 113.60   |
| 1   | E     | 471  | ARG  | NE-CZ-NH1 | 5.05  | 122.82      | 120.30   |
| 2   | F     | 328  | THR  | N-CA-CB   | 5.05  | 119.89      | 110.30   |
| 1   | G     | 161  | ASP  | CB-CG-OD1 | 5.05  | 122.84      | 118.30   |
| 1   | G     | 386  | ALA  | N-CA-CB   | 5.05  | 117.17      | 110.10   |
| 1   | E     | 278  | GLU  | CB-CA-C   | -5.04 | 100.32      | 110.40   |
| 1   | G     | 304  | VAL  | CA-CB-CG1 | -5.04 | 103.34      | 110.90   |
| 2   | B     | 344  | ASP  | CB-CG-OD1 | 5.03  | 122.83      | 118.30   |
| 1   | A     | 912  | ARG  | NE-CZ-NH2 | -5.03 | 117.79      | 120.30   |
| 1   | C     | 279  | THR  | CA-CB-CG2 | -5.03 | 105.36      | 112.40   |
| 1   | C     | 338  | ASP  | CB-CG-OD2 | -5.03 | 113.78      | 118.30   |
| 1   | E     | 818  | PHE  | CB-CG-CD1 | 5.02  | 124.32      | 120.80   |
| 2   | H     | 248  | ASP  | CB-CG-OD1 | 5.01  | 122.81      | 118.30   |
| 1   | A     | 226  | ASP  | CB-CG-OD1 | 5.01  | 122.81      | 118.30   |
| 1   | A     | 791  | ASP  | CB-CG-OD2 | -5.00 | 113.80      | 118.30   |
| 1   | E     | 657  | ALA  | C-N-CA    | -5.00 | 111.80      | 122.30   |
| 1   | E     | 1057 | ASP  | CB-CG-OD1 | 5.00  | 122.80      | 118.30   |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | B     | 154 | ASN  | CA   |
| 2   | D     | 154 | ASN  | CA   |
| 2   | F     | 154 | ASN  | CA   |

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     | 8212  | 0        | 8255     | 231     | 0            |
| 1   | C     | 8197  | 0        | 8225     | 254     | 0            |
| 1   | E     | 8182  | 0        | 8216     | 209     | 0            |
| 1   | G     | 8206  | 0        | 8247     | 340     | 0            |
| 2   | B     | 2897  | 0        | 2860     | 147     | 0            |
| 2   | D     | 2904  | 0        | 2869     | 133     | 0            |
| 2   | F     | 2897  | 0        | 2860     | 128     | 0            |
| 2   | H     | 2897  | 0        | 2860     | 213     | 0            |
| 3   | A     | 3     | 0        | 0        | 0       | 0            |
| 3   | C     | 3     | 0        | 0        | 0       | 0            |
| 3   | E     | 3     | 0        | 0        | 0       | 0            |
| 3   | G     | 3     | 0        | 0        | 0       | 0            |
| 4   | A     | 4     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 4     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 5     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 5     | 0        | 0        | 0       | 0            |
| 4   | H     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 5     | 0        | 0        | 0       | 0            |
| 5   | C     | 10    | 0        | 0        | 1       | 0            |
| 5   | E     | 5     | 0        | 0        | 0       | 0            |
| 5   | G     | 5     | 0        | 0        | 0       | 0            |
| 6   | A     | 5     | 0        | 0        | 1       | 0            |
| 6   | C     | 6     | 0        | 0        | 0       | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 6   | E     | 6     | 0        | 0        | 1       | 0            |
| 6   | F     | 1     | 0        | 0        | 0       | 0            |
| 6   | G     | 6     | 0        | 0        | 2       | 0            |
| 6   | H     | 2     | 0        | 0        | 0       | 0            |
| 7   | A     | 54    | 0        | 24       | 2       | 0            |
| 7   | C     | 54    | 0        | 24       | 0       | 0            |
| 7   | E     | 54    | 0        | 24       | 3       | 0            |
| 7   | G     | 54    | 0        | 24       | 0       | 0            |
| 8   | A     | 9     | 0        | 11       | 0       | 0            |
| 8   | C     | 9     | 0        | 11       | 1       | 0            |
| 8   | E     | 9     | 0        | 11       | 2       | 0            |
| 8   | G     | 9     | 0        | 11       | 1       | 0            |
| 9   | A     | 9     | 0        | 20       | 1       | 0            |
| 9   | C     | 9     | 0        | 20       | 1       | 0            |
| 9   | E     | 9     | 0        | 20       | 2       | 0            |
| 9   | G     | 9     | 0        | 20       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | A     | 21    | 0        | 11       | 1       | 0            |
| 10  | C     | 21    | 0        | 11       | 2       | 0            |
| 10  | E     | 21    | 0        | 11       | 2       | 0            |
| 10  | G     | 21    | 0        | 11       | 1       | 0            |
| 11  | A     | 851   | 0        | 0        | 29      | 1            |
| 11  | B     | 161   | 0        | 0        | 5       | 0            |
| 11  | C     | 819   | 0        | 0        | 23      | 1            |
| 11  | D     | 221   | 0        | 0        | 5       | 0            |
| 11  | E     | 832   | 0        | 0        | 24      | 0            |
| 11  | F     | 200   | 0        | 0        | 2       | 0            |
| 11  | G     | 705   | 0        | 0        | 28      | 0            |
| 11  | H     | 118   | 0        | 0        | 5       | 0            |
| All | All   | 48757 | 0        | 44656    | 1643    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1643) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:27:VAL:HG22  | 2:H:131:CYS:HB2  | 1.13                     | 1.10              |
| 2:D:227:ASP:HA   | 2:D:230:LYS:HD2  | 1.25                     | 1.07              |
| 1:G:784:GLN:NE2  | 1:G:784:GLN:H    | 1.53                     | 1.05              |
| 2:H:133:ILE:HD12 | 2:H:143:ALA:HB2  | 1.41                     | 1.03              |
| 1:A:38:ARG:HG3   | 1:A:38:ARG:HH11  | 1.25                     | 1.00              |
| 2:H:354:PRO:HG3  | 2:H:366:LEU:HD22 | 1.45                     | 0.99              |
| 2:H:324:ASN:N    | 2:H:324:ASN:HD22 | 1.55                     | 0.98              |
| 2:D:133:ILE:HD12 | 2:D:143:ALA:HB2  | 1.44                     | 0.98              |
| 2:B:245:PRO:HD3  | 2:B:270:LEU:HD11 | 1.47                     | 0.97              |
| 2:H:245:PRO:HD3  | 2:H:270:LEU:HD11 | 1.46                     | 0.97              |
| 2:H:324:ASN:HD22 | 2:H:324:ASN:H    | 0.96                     | 0.95              |
| 2:D:324:ASN:H    | 2:D:324:ASN:HD22 | 0.99                     | 0.94              |
| 2:B:187:GLU:HG2  | 2:B:215:ARG:HD2  | 1.50                     | 0.94              |
| 1:C:695:VAL:HG21 | 1:C:701:ALA:HA   | 1.49                     | 0.93              |
| 1:G:1:MET:HB2    | 1:G:224:LYS:HZ2  | 1.33                     | 0.93              |
| 1:C:728:VAL:HG12 | 1:C:733:ASP:HB3  | 1.50                     | 0.92              |
| 1:C:38:ARG:HG3   | 1:C:38:ARG:HH11  | 1.33                     | 0.92              |
| 1:G:695:VAL:HG11 | 1:G:701:ALA:HB2  | 1.52                     | 0.92              |
| 2:H:322:PRO:HB2  | 2:H:324:ASN:HD21 | 1.33                     | 0.91              |
| 1:G:784:GLN:HE21 | 1:G:784:GLN:N    | 1.67                     | 0.91              |
| 2:D:245:PRO:HD3  | 2:D:270:LEU:HD11 | 1.51                     | 0.91              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:F:245:PRO:HD3    | 2:F:270:LEU:HD11 | 1.51                     | 0.91              |
| 2:D:322:PRO:HB2    | 2:D:324:ASN:HD21 | 1.35                     | 0.91              |
| 1:E:1002:GLN:HE22  | 1:E:1006:LYS:HE3 | 1.34                     | 0.91              |
| 2:D:322:PRO:HB2    | 2:D:324:ASN:ND2  | 1.87                     | 0.90              |
| 2:H:195:VAL:HG23   | 2:H:233:PRO:HB3  | 1.54                     | 0.90              |
| 1:G:1:MET:HB2      | 1:G:224:LYS:NZ   | 1.86                     | 0.90              |
| 2:H:322:PRO:HB2    | 2:H:324:ASN:ND2  | 1.87                     | 0.90              |
| 2:H:324:ASN:H      | 2:H:324:ASN:ND2  | 1.65                     | 0.89              |
| 2:B:285:LYS:HG3    | 2:B:314:PHE:CE1  | 2.08                     | 0.89              |
| 1:G:339:ILE:HD12   | 1:G:530:ASP:HA   | 1.55                     | 0.88              |
| 1:A:695:VAL:HG13   | 1:A:700:MET:HB3  | 1.55                     | 0.87              |
| 1:G:728:VAL:CG1    | 1:G:733:ASP:HB3  | 2.05                     | 0.87              |
| 1:C:670:ASP:HB3    | 1:C:677:ARG:HH21 | 1.39                     | 0.86              |
| 1:C:695:VAL:HG13   | 1:C:700:MET:HB3  | 1.57                     | 0.86              |
| 2:B:50:ARG:HG3     | 2:B:50:ARG:HH11  | 1.40                     | 0.86              |
| 2:H:245:PRO:CD     | 2:H:270:LEU:HD11 | 2.05                     | 0.86              |
| 2:D:285:LYS:HG3    | 2:D:314:PHE:CE1  | 2.12                     | 0.85              |
| 2:D:324:ASN:HD22   | 2:D:324:ASN:N    | 1.67                     | 0.85              |
| 1:E:728:VAL:HG13   | 1:E:733:ASP:HB3  | 1.57                     | 0.85              |
| 1:G:509:ARG:HH11   | 1:G:509:ARG:HB2  | 1.42                     | 0.84              |
| 1:C:687:LEU:HD13   | 1:C:812:GLN:HG2  | 1.57                     | 0.84              |
| 2:B:57:TYR:CD1     | 2:B:58:PRO:HD2   | 2.13                     | 0.84              |
| 1:G:708:ILE:HG22   | 1:G:712:LEU:HD11 | 1.59                     | 0.83              |
| 1:C:728:VAL:CG1    | 1:C:733:ASP:HB3  | 2.08                     | 0.83              |
| 1:E:695:VAL:HG21   | 1:E:701:ALA:HA   | 1.59                     | 0.83              |
| 1:E:698:ILE:HD12   | 1:E:698:ILE:H    | 1.42                     | 0.83              |
| 1:A:40:GLU:CG      | 1:A:325:LYS:HE2  | 2.07                     | 0.83              |
| 1:A:728:VAL:HG13   | 1:A:733:ASP:HB3  | 1.58                     | 0.83              |
| 1:E:695:VAL:HG11   | 1:E:701:ALA:HB2  | 1.60                     | 0.83              |
| 1:G:784:GLN:H      | 1:G:784:GLN:HE21 | 0.86                     | 0.83              |
| 2:D:324:ASN:H      | 2:D:324:ASN:ND2  | 1.77                     | 0.83              |
| 2:H:6:LEU:HD11     | 2:H:8:VAL:CG2    | 2.08                     | 0.83              |
| 2:H:6:LEU:HD11     | 2:H:8:VAL:HG23   | 1.58                     | 0.83              |
| 2:H:27:VAL:CG2     | 2:H:131:CYS:HB2  | 2.05                     | 0.83              |
| 1:A:130[A]:ARG:HB2 | 1:A:148:ILE:HG13 | 1.60                     | 0.82              |
| 2:D:227:ASP:HA     | 2:D:230:LYS:CD   | 2.08                     | 0.82              |
| 2:F:322:PRO:HD2    | 2:F:325:LEU:HD12 | 1.62                     | 0.82              |
| 1:A:990:LEU:HD23   | 1:G:979:ILE:HG12 | 1.62                     | 0.82              |
| 1:G:475[B]:LYS:HD2 | 1:G:488:PHE:CZ   | 2.14                     | 0.82              |
| 2:H:247:PRO:HA     | 2:H:252:ILE:HD13 | 1.61                     | 0.82              |
| 1:G:563:MET:CE     | 1:G:635:PRO:HG3  | 2.10                     | 0.81              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:C:693:ALA:HB2     | 1:C:708:ILE:HD11  | 1.61                     | 0.81              |
| 1:E:967[B]:GLN:HE21 | 1:E:1054:LEU:HD13 | 1.43                     | 0.81              |
| 1:G:768:CYS:HB2     | 1:G:773:VAL:HG22  | 1.63                     | 0.80              |
| 2:H:272:HIS:HA      | 2:H:349:SER:HB2   | 1.63                     | 0.80              |
| 1:G:872:LYS:HG2     | 1:G:877:GLN:HG2   | 1.64                     | 0.80              |
| 2:D:228:VAL:HA      | 2:D:231:MET:CE    | 2.11                     | 0.80              |
| 1:A:130[B]:ARG:HB2  | 1:A:148:ILE:HG13  | 1.64                     | 0.80              |
| 1:A:1073:LYS:HD2    | 1:A:1073:LYS:N    | 1.95                     | 0.80              |
| 1:G:708:ILE:CG2     | 1:G:712:LEU:HD11  | 2.12                     | 0.79              |
| 1:G:991:VAL:HB      | 11:G:1721:HOH:O   | 1.83                     | 0.79              |
| 1:G:225:ASN:ND2     | 1:G:331:THR:HG21  | 1.97                     | 0.79              |
| 1:C:695:VAL:HG11    | 1:C:701:ALA:HB2   | 1.64                     | 0.78              |
| 1:E:509:ARG:CB      | 1:E:509:ARG:HH11  | 1.97                     | 0.78              |
| 2:F:263:ILE:HG22    | 2:F:264:PRO:HD2   | 1.65                     | 0.78              |
| 2:H:57:TYR:CD1      | 2:H:58:PRO:HD2    | 2.19                     | 0.78              |
| 2:F:187:GLU:HG2     | 2:F:215:ARG:CD    | 2.14                     | 0.77              |
| 1:G:728:VAL:HG12    | 1:G:733:ASP:HB3   | 1.66                     | 0.77              |
| 2:F:322:PRO:HB2     | 2:F:324:ASN:ND2   | 1.99                     | 0.77              |
| 1:G:479:VAL:CG2     | 1:G:483:GLY:HA3   | 2.14                     | 0.77              |
| 1:G:726:GLU:HG3     | 1:G:727:ILE:N     | 2.00                     | 0.77              |
| 1:A:784:GLN:HE21    | 1:A:784:GLN:H     | 1.33                     | 0.77              |
| 1:A:1020:ARG:O      | 1:A:1024:GLU:HG3  | 1.85                     | 0.77              |
| 2:D:133:ILE:CD1     | 2:D:143:ALA:HB2   | 2.15                     | 0.77              |
| 1:G:563:MET:HE1     | 1:G:635:PRO:HG3   | 1.66                     | 0.77              |
| 1:A:725:MET:HE3     | 11:A:1609:HOH:O   | 1.84                     | 0.77              |
| 2:B:194:VAL:HB      | 2:B:216:LEU:HD23  | 1.65                     | 0.77              |
| 1:C:652:ARG:HG2     | 1:C:652:ARG:HH11  | 1.47                     | 0.76              |
| 2:F:57:TYR:CD1      | 2:F:58:PRO:HD2    | 2.19                     | 0.76              |
| 2:D:27:VAL:HG13     | 2:D:131:CYS:HB2   | 1.68                     | 0.76              |
| 1:G:1020:ARG:O      | 1:G:1024:GLU:HG3  | 1.85                     | 0.76              |
| 2:F:154:ASN:HD21    | 2:F:314:PHE:HZ    | 1.34                     | 0.76              |
| 2:B:324:ASN:HD22    | 2:B:324:ASN:N     | 1.81                     | 0.76              |
| 1:G:1001:ILE:HD12   | 1:G:1029:ILE:HG12 | 1.67                     | 0.76              |
| 2:F:259:LEU:O       | 2:F:345:LYS:HE3   | 1.86                     | 0.76              |
| 1:G:1017:THR:HG21   | 1:G:1023:ILE:HA   | 1.65                     | 0.76              |
| 1:C:967[A]:GLN:HG3  | 1:C:1054:LEU:HD13 | 1.68                     | 0.76              |
| 1:E:157:ALA:HA      | 11:E:1237:HOH:O   | 1.84                     | 0.76              |
| 2:F:324:ASN:H       | 2:F:324:ASN:HD22  | 1.34                     | 0.76              |
| 1:A:228:CYS:SG      | 1:A:269:MET:HG2   | 2.26                     | 0.76              |
| 2:D:345:LYS:HB3     | 2:D:346:PRO:HD2   | 1.68                     | 0.76              |
| 1:E:1020:ARG:O      | 1:E:1024:GLU:HG3  | 1.85                     | 0.76              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:E:103:GLU:HG3    | 1:E:104:ARG:N     | 2.01                     | 0.76              |
| 2:H:215:ARG:HH11   | 2:H:215:ARG:HG2   | 1.51                     | 0.76              |
| 1:E:3:LYS:HB2      | 1:E:42:TYR:OH     | 1.85                     | 0.75              |
| 2:H:39:TYR:CZ      | 2:H:61:GLY:HA2    | 2.21                     | 0.75              |
| 2:H:71:GLU:O       | 2:H:203:ARG:HG3   | 1.87                     | 0.75              |
| 1:G:57:ASP:HB3     | 1:G:59:GLU:OE1    | 1.86                     | 0.75              |
| 2:B:322:PRO:HG2    | 2:B:324:ASN:HD21  | 1.51                     | 0.75              |
| 1:C:3:LYS:HB3      | 1:C:330:TYR:CE1   | 2.22                     | 0.75              |
| 1:C:675:ARG:H      | 1:C:675:ARG:CD    | 1.99                     | 0.75              |
| 2:D:227:ASP:CA     | 2:D:230:LYS:HD2   | 2.12                     | 0.75              |
| 1:E:693:ALA:HB3    | 1:E:708:ILE:HD11  | 1.68                     | 0.75              |
| 1:A:726:GLU:HG3    | 1:A:727:ILE:N     | 2.00                     | 0.74              |
| 2:D:50:ARG:HD2     | 2:D:50:ARG:N      | 2.01                     | 0.74              |
| 1:G:695:VAL:HG13   | 1:G:700:MET:HB3   | 1.69                     | 0.74              |
| 9:E:1092:NET:H22   | 9:E:1092:NET:H42  | 1.66                     | 0.74              |
| 1:C:693:ALA:CB     | 1:C:708:ILE:HD11  | 2.16                     | 0.74              |
| 1:C:1020:ARG:O     | 1:C:1024:GLU:HG3  | 1.87                     | 0.74              |
| 2:B:324:ASN:HD22   | 2:B:324:ASN:H     | 1.36                     | 0.74              |
| 2:D:8:VAL:HG22     | 2:D:14:GLN:HG2    | 1.70                     | 0.74              |
| 1:A:563:MET:HE3    | 1:A:635:PRO:HG3   | 1.69                     | 0.74              |
| 2:D:228:VAL:HA     | 2:D:231:MET:HE2   | 1.68                     | 0.74              |
| 2:D:282:LYS:HG3    | 2:D:320:THR:HG21  | 1.68                     | 0.74              |
| 1:A:675:ARG:CD     | 1:A:675:ARG:H     | 1.99                     | 0.73              |
| 1:A:1001:ILE:HD12  | 1:A:1002:GLN:N    | 2.03                     | 0.73              |
| 2:B:139:ASP:OD2    | 2:B:142:LEU:HB2   | 1.89                     | 0.73              |
| 1:G:64:THR:O       | 1:G:1065:VAL:HG23 | 1.88                     | 0.73              |
| 1:A:449:VAL:N      | 11:A:1435:HOH:O   | 2.21                     | 0.73              |
| 2:D:226:GLU:O      | 2:D:230:LYS:HG3   | 1.87                     | 0.73              |
| 2:H:16:HIS:O       | 2:H:113:ILE:HG22  | 1.88                     | 0.73              |
| 1:C:967[B]:GLN:HG2 | 1:C:1054:LEU:HD13 | 1.69                     | 0.73              |
| 2:D:150:PHE:CE1    | 2:D:152:GLY:HA2   | 2.24                     | 0.73              |
| 1:G:423:LYS:HB3    | 11:G:1397:HOH:O   | 1.89                     | 0.73              |
| 2:H:50:ARG:HG3     | 2:H:50:ARG:HH11   | 1.52                     | 0.73              |
| 1:E:331:THR:OG1    | 1:E:334:GLU:HG3   | 1.89                     | 0.72              |
| 2:F:154:ASN:ND2    | 2:F:285:LYS:HE2   | 2.04                     | 0.72              |
| 1:G:858:GLY:HA2    | 1:G:1069:HIS:CE1  | 2.24                     | 0.72              |
| 1:E:734:LEU:HD12   | 1:E:734:LEU:O     | 1.89                     | 0.72              |
| 1:A:344:THR:HB     | 1:A:345:PRO:HD2   | 1.71                     | 0.72              |
| 1:C:698:ILE:HD12   | 1:C:698:ILE:H     | 1.53                     | 0.72              |
| 2:B:316:VAL:HG12   | 2:B:337:LEU:HD23  | 1.71                     | 0.72              |
| 1:C:38:ARG:HG3     | 1:C:38:ARG:NH1    | 2.03                     | 0.72              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:B:261:THR:OG1    | 2:B:263:ILE:HG13    | 1.89                     | 0.72              |
| 1:C:772:MET:SD     | 1:C:880:THR:HG22    | 2.30                     | 0.72              |
| 2:H:33:ASN:HA      | 2:H:291:HIS:O       | 1.90                     | 0.72              |
| 1:C:905:PRO:HB2    | 1:C:1040:TYR:OH     | 1.90                     | 0.72              |
| 2:B:50:ARG:HG3     | 2:B:50:ARG:NH1      | 2.03                     | 0.72              |
| 2:D:263:ILE:HG22   | 2:D:264:PRO:HD2     | 1.72                     | 0.72              |
| 2:B:324:ASN:H      | 2:B:324:ASN:ND2     | 1.87                     | 0.71              |
| 2:H:299:ASP:OD1    | 2:H:302:LYS:HD2     | 1.91                     | 0.71              |
| 1:G:1004:ARG:HD3   | 1:G:1009[B]:GLU:OE2 | 1.91                     | 0.71              |
| 2:B:286:MET:HE1    | 2:B:315:ALA:HB2     | 1.73                     | 0.71              |
| 1:G:1001:ILE:HD12  | 1:G:1029:ILE:CG1    | 2.21                     | 0.71              |
| 2:B:246:ALA:HB1    | 2:B:248:ASP:CG      | 2.12                     | 0.70              |
| 1:C:321:LYS:HE3    | 11:C:1621:HOH:O     | 1.91                     | 0.70              |
| 1:E:967[B]:GLN:NE2 | 1:E:1054:LEU:HB3    | 2.06                     | 0.70              |
| 2:F:286:MET:HG2    | 11:F:1893:HOH:O     | 1.91                     | 0.70              |
| 2:F:376:GLN:HA     | 2:F:379:LYS:HZ2     | 1.56                     | 0.70              |
| 1:C:670:ASP:HB3    | 1:C:677:ARG:NH2     | 2.05                     | 0.70              |
| 1:G:671:ARG:HG2    | 1:G:677:ARG:NH1     | 2.06                     | 0.70              |
| 2:B:205:ILE:HG13   | 2:B:355:GLU:HG3     | 1.74                     | 0.70              |
| 2:F:187:GLU:HG2    | 2:F:215:ARG:HD2     | 1.72                     | 0.70              |
| 1:E:1:MET:HB2      | 1:E:224:LYS:NZ      | 2.07                     | 0.70              |
| 1:C:1:MET:HB2      | 1:C:224:LYS:NZ      | 2.05                     | 0.70              |
| 1:E:734:LEU:HD11   | 1:E:738:PHE:CE2     | 2.27                     | 0.70              |
| 1:A:930:LYS:HE3    | 11:A:1156:HOH:O     | 1.92                     | 0.69              |
| 1:G:668:ALA:O      | 1:G:671:ARG:HB2     | 1.92                     | 0.69              |
| 1:C:873:SER:O      | 1:C:877:GLN:HG3     | 1.93                     | 0.69              |
| 1:A:38:ARG:HG3     | 1:A:38:ARG:NH1      | 2.00                     | 0.69              |
| 2:B:190:LEU:HD13   | 2:B:214:CYS:O       | 1.91                     | 0.69              |
| 2:H:285:LYS:HG3    | 2:H:314:PHE:CE1     | 2.27                     | 0.69              |
| 1:G:726:GLU:HG3    | 1:G:727:ILE:H       | 1.57                     | 0.69              |
| 2:B:324:ASN:O      | 2:B:342:ARG:HD2     | 1.91                     | 0.69              |
| 2:F:324:ASN:O      | 2:F:342:ARG:HD2     | 1.93                     | 0.69              |
| 2:B:279:SER:O      | 2:B:322:PRO:HG3     | 1.93                     | 0.69              |
| 1:C:1063:ILE:HG12  | 1:C:1067:GLU:OE2    | 1.93                     | 0.69              |
| 2:H:326:ARG:O      | 2:H:340:ILE:HG22    | 1.93                     | 0.69              |
| 2:F:254:ALA:O      | 2:F:257:LYS:HB2     | 1.92                     | 0.68              |
| 1:G:901:PRO:HD2    | 6:G:1086:CL:CL      | 2.30                     | 0.68              |
| 1:E:644:GLY:O      | 1:E:647:PRO:HD2     | 1.92                     | 0.68              |
| 1:E:726:GLU:HG3    | 1:E:727:ILE:H       | 1.56                     | 0.68              |
| 2:H:334:ASP:OD2    | 2:H:336:THR:HG23    | 1.94                     | 0.68              |
| 1:A:784:GLN:H      | 1:A:784:GLN:NE2     | 1.90                     | 0.68              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:G:652[A]:ARG:NH1 | 1:G:667:ASP:HA    | 2.09                     | 0.68              |
| 2:H:150:PHE:CE1    | 2:H:152:GLY:HA2   | 2.27                     | 0.68              |
| 1:A:695:VAL:HG21   | 1:A:701:ALA:HA    | 1.76                     | 0.68              |
| 1:C:833:LYS:O      | 1:C:836:GLU:HB2   | 1.94                     | 0.68              |
| 1:C:228:CYS:SG     | 1:C:269:MET:HG2   | 2.34                     | 0.67              |
| 1:G:1027:ARG:HE    | 1:G:1031:ARG:HD3  | 1.59                     | 0.67              |
| 2:H:133:ILE:HD12   | 2:H:143:ALA:CB    | 2.22                     | 0.67              |
| 1:A:1:MET:HG3      | 1:A:2:PRO:HD2     | 1.75                     | 0.67              |
| 1:C:43:ARG:NH2     | 1:C:81:GLU:OE2    | 2.28                     | 0.67              |
| 1:G:967[A]:GLN:HG3 | 1:G:1054:LEU:HD13 | 1.76                     | 0.67              |
| 1:A:703:GLU:O      | 1:A:706:LYS:HB2   | 1.94                     | 0.67              |
| 2:B:322:PRO:CG     | 2:B:324:ASN:HD21  | 2.08                     | 0.67              |
| 2:D:227:ASP:O      | 2:D:230:LYS:HB2   | 1.95                     | 0.67              |
| 1:A:343:ARG:HD3    | 11:A:1715:HOH:O   | 1.92                     | 0.67              |
| 2:F:157:ASP:HB3    | 2:F:160:LYS:HE2   | 1.76                     | 0.67              |
| 2:B:50:ARG:N       | 2:B:50:ARG:HD2    | 1.99                     | 0.67              |
| 2:D:50:ARG:HG3     | 2:D:50:ARG:HH11   | 1.58                     | 0.67              |
| 1:E:1021:ARG:HD3   | 1:E:1025:ASP:OD2  | 1.94                     | 0.67              |
| 1:C:1:MET:HG3      | 1:C:2:PRO:HD2     | 1.77                     | 0.67              |
| 1:G:716:PRO:HA     | 1:G:750:VAL:HG22  | 1.77                     | 0.67              |
| 1:A:40:GLU:HG2     | 1:A:325:LYS:HE2   | 1.77                     | 0.67              |
| 2:B:225:ALA:O      | 2:B:228:VAL:HB    | 1.94                     | 0.67              |
| 2:B:228:VAL:HA     | 2:B:231:MET:CE    | 2.25                     | 0.67              |
| 1:E:905:PRO:HB2    | 1:E:1040:TYR:OH   | 1.95                     | 0.67              |
| 2:B:263:ILE:HG22   | 2:B:264:PRO:HD2   | 1.77                     | 0.67              |
| 2:B:322:PRO:HB2    | 2:B:324:ASN:ND2   | 2.09                     | 0.67              |
| 2:D:282:LYS:HG3    | 2:D:320:THR:CG2   | 2.24                     | 0.67              |
| 2:H:192:PHE:O      | 2:H:215:ARG:HB3   | 1.95                     | 0.67              |
| 2:B:222:GLN:HB2    | 11:B:3567:HOH:O   | 1.95                     | 0.66              |
| 1:G:172:PHE:HB3    | 1:G:200:PRO:HG2   | 1.77                     | 0.66              |
| 1:G:479:VAL:HG23   | 1:G:483:GLY:HA3   | 1.77                     | 0.66              |
| 1:G:687:LEU:HD13   | 1:G:812:GLN:HG2   | 1.76                     | 0.66              |
| 2:B:228:VAL:HA     | 2:B:231:MET:HE2   | 1.77                     | 0.66              |
| 1:C:726:GLU:HG3    | 1:C:727:ILE:H     | 1.59                     | 0.66              |
| 1:G:728:VAL:HG13   | 1:G:733:ASP:HB3   | 1.76                     | 0.66              |
| 1:G:863:LYS:O      | 1:G:866:ALA:HB3   | 1.94                     | 0.66              |
| 2:B:153:LEU:O      | 2:B:156:MET:HB2   | 1.95                     | 0.66              |
| 2:B:228:VAL:HG11   | 2:B:258:PHE:CE1   | 2.30                     | 0.66              |
| 1:C:419:GLU:HG2    | 11:C:1718:HOH:O   | 1.95                     | 0.66              |
| 2:D:139:ASP:OD2    | 2:D:142:LEU:HB2   | 1.96                     | 0.66              |
| 1:E:563:MET:HE3    | 1:E:635:PRO:HG3   | 1.77                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:695:VAL:HG11   | 1:A:701:ALA:HB2    | 1.76                     | 0.66              |
| 2:B:286:MET:HG2    | 11:B:3570:HOH:O    | 1.94                     | 0.66              |
| 1:G:735:ARG:O      | 1:G:738:PHE:N      | 2.29                     | 0.66              |
| 1:E:757:ASP:O      | 1:E:833:LYS:NZ     | 2.28                     | 0.66              |
| 1:A:672:ALA:HB3    | 1:A:844:PRO:HG3    | 1.78                     | 0.66              |
| 1:C:482:THR:HB     | 11:C:1747:HOH:O    | 1.96                     | 0.66              |
| 2:D:50:ARG:HG3     | 2:D:50:ARG:NH1     | 2.11                     | 0.66              |
| 1:G:695:VAL:HG11   | 1:G:701:ALA:CB     | 2.23                     | 0.66              |
| 1:G:803:GLN:HG3    | 1:G:807:ASP:OD1    | 1.96                     | 0.66              |
| 1:E:698:ILE:H      | 1:E:698:ILE:CD1    | 2.09                     | 0.66              |
| 1:E:907:LEU:HD11   | 8:E:1091:ORN:HD3   | 1.76                     | 0.66              |
| 2:H:40:GLN:OE1     | 2:H:69:ASP:HB2     | 1.95                     | 0.66              |
| 1:C:956:ARG:HB3    | 1:C:1044:LEU:CD2   | 2.27                     | 0.65              |
| 2:B:228:VAL:HG12   | 2:B:229:LEU:N      | 2.10                     | 0.65              |
| 2:F:244:ASP:OD2    | 2:F:245:PRO:HD2    | 1.97                     | 0.65              |
| 1:E:43:ARG:NH2     | 1:E:81:GLU:OE2     | 2.30                     | 0.65              |
| 1:G:873:SER:O      | 1:G:877:GLN:HG3    | 1.97                     | 0.65              |
| 1:G:475[C]:LYS:HD3 | 1:G:488:PHE:CZ     | 2.32                     | 0.65              |
| 1:A:509:ARG:NH1    | 1:A:512[A]:GLU:OE1 | 2.29                     | 0.65              |
| 1:A:735:ARG:O      | 1:A:738:PHE:N      | 2.29                     | 0.65              |
| 1:A:814:GLN:NE2    | 11:A:1532:HOH:O    | 2.30                     | 0.65              |
| 1:C:671:ARG:NH2    | 1:C:819:GLU:O      | 2.30                     | 0.65              |
| 1:C:703:GLU:O      | 1:C:706:LYS:HB2    | 1.97                     | 0.65              |
| 1:E:674:ASP:HB3    | 1:E:677:ARG:HG3    | 1.79                     | 0.65              |
| 1:A:289:ASN:HB3    | 1:A:292:ASN:OD1    | 1.97                     | 0.65              |
| 1:G:24:CYS:HB2     | 1:G:604:GLU:HB2    | 1.79                     | 0.65              |
| 1:A:905:PRO:HB2    | 1:A:1040:TYR:OH    | 1.96                     | 0.65              |
| 2:H:33:ASN:OD1     | 2:H:292:GLY:HA2    | 1.97                     | 0.65              |
| 1:E:726:GLU:OE1    | 1:E:1020:ARG:NE    | 2.30                     | 0.64              |
| 1:G:475[A]:LYS:HD3 | 1:G:488:PHE:CZ     | 2.32                     | 0.64              |
| 2:D:228:VAL:HG22   | 2:D:231:MET:CE     | 2.27                     | 0.64              |
| 1:E:3:LYS:HB3      | 1:E:330:TYR:CE1    | 2.32                     | 0.64              |
| 1:G:954:LYS:O      | 1:G:957:VAL:HG12   | 1.96                     | 0.64              |
| 2:H:262:ASP:OD1    | 2:H:345:LYS:NZ     | 2.31                     | 0.64              |
| 1:A:696:THR:HB     | 1:A:700:MET:SD     | 2.37                     | 0.64              |
| 1:E:703:GLU:O      | 1:E:706:LYS:HB2    | 1.97                     | 0.64              |
| 2:B:71:GLU:O       | 2:B:203:ARG:HG3    | 1.96                     | 0.64              |
| 1:G:4:ARG:HD3      | 1:G:7:ILE:HD12     | 1.79                     | 0.64              |
| 1:G:417:ASP:OD1    | 1:G:423:LYS:NZ     | 2.29                     | 0.64              |
| 2:H:34:THR:HA      | 2:H:56:THR:OG1     | 1.97                     | 0.64              |
| 2:H:139:ASP:OD2    | 2:H:142:LEU:HB2    | 1.97                     | 0.64              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:344:THR:HB     | 1:A:345:PRO:CD   | 2.27                     | 0.64              |
| 2:B:228:VAL:HG11   | 2:B:258:PHE:CZ   | 2.33                     | 0.64              |
| 1:G:781:HIS:CE1    | 1:G:789:SER:HB2  | 2.33                     | 0.64              |
| 9:G:1092:NET:H22   | 9:G:1092:NET:H42 | 1.79                     | 0.64              |
| 1:A:946:LEU:C      | 1:A:947:LEU:HD12 | 2.18                     | 0.64              |
| 1:G:738:PHE:O      | 1:G:741:ALA:HB3  | 1.97                     | 0.64              |
| 2:H:248:ASP:OD2    | 2:H:248:ASP:N    | 2.29                     | 0.64              |
| 1:E:1:MET:HB2      | 1:E:224:LYS:HE3  | 1.80                     | 0.64              |
| 1:G:321:LYS:NZ     | 1:G:611:ASP:OD1  | 2.30                     | 0.64              |
| 1:G:702:VAL:HG11   | 1:G:735:ARG:NH2  | 2.13                     | 0.64              |
| 2:H:286:MET:HE1    | 2:H:312:HIS:HE1  | 1.62                     | 0.64              |
| 2:D:158:LEU:O      | 2:D:161:GLU:HB2  | 1.98                     | 0.64              |
| 1:A:172:PHE:HB3    | 1:A:200:PRO:HG2  | 1.78                     | 0.64              |
| 1:G:1:MET:HB2      | 1:G:224:LYS:CE   | 2.28                     | 0.64              |
| 1:G:950:ARG:NH1    | 11:G:1675:HOH:O  | 2.31                     | 0.64              |
| 1:A:425[B]:ARG:NH2 | 11:A:1745:HOH:O  | 2.31                     | 0.63              |
| 1:C:687:LEU:CD1    | 1:C:812:GLN:HG2  | 2.27                     | 0.63              |
| 1:E:321:LYS:NZ     | 1:E:611:ASP:OD1  | 2.30                     | 0.63              |
| 1:G:339:ILE:HD11   | 1:G:531:THR:HG23 | 1.79                     | 0.63              |
| 2:H:215:ARG:HG2    | 2:H:215:ARG:NH1  | 2.13                     | 0.63              |
| 2:D:120:ARG:NH2    | 11:D:2337:HOH:O  | 2.29                     | 0.63              |
| 2:D:201:ALA:HB2    | 2:D:239:SER:CB   | 2.28                     | 0.63              |
| 2:F:322:PRO:HB2    | 2:F:324:ASN:HD21 | 1.61                     | 0.63              |
| 1:A:375:THR:HG23   | 1:A:377:GLN:H    | 1.63                     | 0.63              |
| 1:A:1001:ILE:HD12  | 1:A:1002:GLN:HB2 | 1.79                     | 0.63              |
| 2:B:344:ASP:O      | 2:B:345:LYS:HD3  | 1.99                     | 0.63              |
| 2:F:194:VAL:HG13   | 2:F:235:GLY:O    | 1.98                     | 0.63              |
| 1:G:981:LEU:HD12   | 1:G:988:PRO:HG3  | 1.79                     | 0.63              |
| 1:C:693:ALA:HB1    | 1:C:704:LYS:HG2  | 1.81                     | 0.63              |
| 1:E:1:MET:N        | 11:E:1623:HOH:O  | 2.30                     | 0.63              |
| 2:F:8:VAL:HG22     | 2:F:14:GLN:HG2   | 1.80                     | 0.63              |
| 1:A:698:ILE:HD12   | 1:A:698:ILE:H    | 1.63                     | 0.63              |
| 2:H:46:PRO:HG2     | 2:H:200:GLY:O    | 1.99                     | 0.63              |
| 1:E:1:MET:HB2      | 1:E:224:LYS:CE   | 2.29                     | 0.63              |
| 1:E:698:ILE:O      | 1:E:702:VAL:HG23 | 1.98                     | 0.63              |
| 1:C:495:LYS:NZ     | 11:C:1740:HOH:O  | 2.27                     | 0.63              |
| 2:H:74:GLN:HA      | 11:H:475:HOH:O   | 1.98                     | 0.63              |
| 1:C:32:GLN:OE1     | 1:C:320:ALA:HB3  | 1.98                     | 0.62              |
| 2:D:286:MET:HB2    | 2:D:313:GLY:O    | 1.98                     | 0.62              |
| 2:F:195:VAL:HG23   | 2:F:233:PRO:HB3  | 1.81                     | 0.62              |
| 2:B:353:HIS:ND1    | 2:B:355:GLU:OE1  | 2.30                     | 0.62              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:D:153:LEU:O       | 2:D:156:MET:HB2  | 1.99                     | 0.62              |
| 1:E:493:LYS:HE2     | 1:E:517:ARG:HD3  | 1.82                     | 0.62              |
| 1:E:812:GLN:NE2     | 11:E:1791:HOH:O  | 2.27                     | 0.62              |
| 2:D:228:VAL:HA      | 2:D:231:MET:HE3  | 1.80                     | 0.62              |
| 2:F:324:ASN:HD22    | 2:F:324:ASN:N    | 1.97                     | 0.62              |
| 1:C:65:TYR:OH       | 1:C:80:LYS:HE2   | 1.99                     | 0.62              |
| 1:E:858:GLY:HA2     | 1:E:1069:HIS:CE1 | 2.33                     | 0.62              |
| 1:G:974:THR:O       | 1:G:975:HIS:C    | 2.38                     | 0.62              |
| 2:H:46:PRO:HA       | 2:H:76:HIS:CG    | 2.35                     | 0.62              |
| 1:A:67:GLU:HB3      | 1:A:68:PRO:HD2   | 1.82                     | 0.62              |
| 1:C:698:ILE:O       | 1:C:702:VAL:HG23 | 1.99                     | 0.62              |
| 1:C:702:VAL:HG11    | 1:C:735:ARG:NH2  | 2.13                     | 0.62              |
| 2:F:263:ILE:CG2     | 2:F:264:PRO:HD2  | 2.30                     | 0.62              |
| 1:G:762:VAL:HG13    | 1:G:779:MET:O    | 2.00                     | 0.62              |
| 1:G:1037:LYS:HE2    | 11:G:1756:HOH:O  | 1.98                     | 0.62              |
| 2:H:5:ALA:CB        | 2:H:110:ILE:HG13 | 2.30                     | 0.62              |
| 1:E:997:GLY:O       | 1:E:1000:HIS:HB3 | 2.00                     | 0.62              |
| 2:F:251:ALA:O       | 2:F:252:ILE:C    | 2.38                     | 0.62              |
| 2:H:27:VAL:HG22     | 2:H:131:CYS:CB   | 2.08                     | 0.62              |
| 1:A:563:MET:CE      | 1:A:635:PRO:HG3  | 2.30                     | 0.62              |
| 1:G:488:PHE:O       | 1:G:491:GLN:N    | 2.33                     | 0.62              |
| 2:H:5:ALA:HB3       | 2:H:110:ILE:HG13 | 1.82                     | 0.62              |
| 2:H:286:MET:CE      | 2:H:315:ALA:HB2  | 2.29                     | 0.62              |
| 2:B:245:PRO:HD3     | 2:B:270:LEU:CD1  | 2.27                     | 0.62              |
| 2:D:26:ALA:O        | 2:D:131:CYS:HA   | 2.00                     | 0.62              |
| 2:D:228:VAL:O       | 2:D:231:MET:HG3  | 2.00                     | 0.62              |
| 1:E:675:ARG:CD      | 1:E:675:ARG:H    | 2.12                     | 0.62              |
| 1:E:698:ILE:HD12    | 1:E:698:ILE:N    | 2.14                     | 0.61              |
| 1:E:784:GLN:H       | 1:E:784:GLN:NE2  | 1.98                     | 0.61              |
| 1:G:76:LYS:HE3      | 11:G:1740:HOH:O  | 1.99                     | 0.61              |
| 1:G:400:ARG:HD3     | 11:G:1373:HOH:O  | 2.00                     | 0.61              |
| 2:B:247:PRO:HA      | 2:B:252:ILE:CD1  | 2.30                     | 0.61              |
| 1:C:761:GLU:HG2     | 1:C:781:HIS:CE1  | 2.34                     | 0.61              |
| 1:G:734:LEU:HD11    | 1:G:738:PHE:CE2  | 2.35                     | 0.61              |
| 2:H:144:LEU:HD12    | 2:H:144:LEU:O    | 2.00                     | 0.61              |
| 2:F:48:TYR:HA       | 2:F:51:GLN:HE21  | 1.63                     | 0.61              |
| 1:G:1063:ILE:HG13   | 1:G:1067:GLU:OE2 | 1.99                     | 0.61              |
| 1:A:728:VAL:CG1     | 1:A:733:ASP:HB3  | 2.29                     | 0.61              |
| 1:A:738:PHE:O       | 1:A:741:ALA:HB3  | 2.01                     | 0.61              |
| 1:E:967[B]:GLN:HE21 | 1:E:1054:LEU:CD1 | 2.13                     | 0.61              |
| 1:G:354:TYR:HB2     | 1:G:388:GLY:O    | 2.01                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:236:ILE:HD12 | 2:H:263:ILE:HG21  | 1.82                     | 0.61              |
| 1:C:44:VAL:N     | 1:C:62:ASP:OD2    | 2.29                     | 0.61              |
| 1:C:698:ILE:HD12 | 1:C:698:ILE:N     | 2.14                     | 0.61              |
| 1:G:65:TYR:CG    | 1:G:77:ILE:HD13   | 2.36                     | 0.61              |
| 2:H:195:VAL:CG2  | 2:H:233:PRO:HB3   | 2.28                     | 0.61              |
| 1:C:998:ARG:CB   | 1:C:999:PRO:HA    | 2.30                     | 0.61              |
| 1:G:617:TYR:CG   | 1:G:629:ILE:HD13  | 2.35                     | 0.61              |
| 1:E:1002:GLN:NE2 | 1:E:1006:LYS:HE3  | 2.12                     | 0.61              |
| 1:A:1000:HIS:CD2 | 1:A:1003:ASP:H    | 2.19                     | 0.60              |
| 1:E:1000:HIS:CD2 | 1:E:1003:ASP:H    | 2.19                     | 0.60              |
| 1:G:804:GLU:O    | 1:G:808:VAL:HG23  | 2.00                     | 0.60              |
| 2:H:324:ASN:N    | 2:H:324:ASN:ND2   | 2.30                     | 0.60              |
| 1:C:17:PRO:HG3   | 1:C:917:VAL:HG13  | 1.83                     | 0.60              |
| 1:E:509:ARG:HH11 | 1:E:509:ARG:HB3   | 1.66                     | 0.60              |
| 1:G:946:LEU:CD1  | 1:G:991:VAL:HG11  | 2.31                     | 0.60              |
| 2:H:342:ARG:HB3  | 2:H:344:ASP:OD2   | 2.01                     | 0.60              |
| 2:B:34:THR:HA    | 2:B:56:THR:OG1    | 2.02                     | 0.60              |
| 1:C:956:ARG:HB3  | 1:C:1044:LEU:HD21 | 1.82                     | 0.60              |
| 1:C:1020:ARG:O   | 1:C:1020:ARG:HG3  | 2.01                     | 0.60              |
| 1:G:471:ARG:HD2  | 11:G:1643:HOH:O   | 2.00                     | 0.60              |
| 1:G:1021:ARG:HG3 | 1:G:1021:ARG:HH11 | 1.66                     | 0.60              |
| 1:C:822:VAL:O    | 1:C:823:ARG:HD3   | 2.01                     | 0.60              |
| 1:E:1000:HIS:HD2 | 1:E:1003:ASP:H    | 1.48                     | 0.60              |
| 1:E:527:LYS:HD2  | 2:F:116:ARG:HD3   | 1.84                     | 0.60              |
| 2:B:246:ALA:HB1  | 2:B:248:ASP:OD2   | 2.01                     | 0.60              |
| 2:B:237:PHE:HE1  | 2:B:268:ILE:HG13  | 1.66                     | 0.60              |
| 2:D:178:THR:HG22 | 2:D:179:GLY:N     | 2.15                     | 0.60              |
| 2:B:232:ASN:N    | 2:B:233:PRO:HD3   | 2.16                     | 0.60              |
| 2:B:245:PRO:CG   | 2:B:274:LEU:HD21  | 2.32                     | 0.60              |
| 1:C:907:LEU:HD11 | 8:C:1091:ORN:HD3  | 1.84                     | 0.60              |
| 2:F:247:PRO:HA   | 2:F:252:ILE:HD13  | 1.82                     | 0.60              |
| 2:H:104:ARG:HG2  | 2:H:105:HIS:CD2   | 2.36                     | 0.60              |
| 2:H:367:PHE:O    | 2:H:370:PHE:HB3   | 2.01                     | 0.60              |
| 1:A:948:SER:OG   | 10:A:1091:U:H5"   | 2.01                     | 0.60              |
| 1:E:257:THR:HG22 | 2:F:63:VAL:HG21   | 1.84                     | 0.60              |
| 1:G:728:VAL:HG11 | 1:G:734:LEU:HA    | 1.84                     | 0.60              |
| 1:G:772:MET:HE2  | 1:G:880:THR:HA    | 1.82                     | 0.60              |
| 1:A:994:VAL:HG23 | 1:A:1001:ILE:HD11 | 1.82                     | 0.59              |
| 1:E:344:THR:HB   | 1:E:345:PRO:HD2   | 1.83                     | 0.59              |
| 2:F:300:VAL:HG22 | 2:F:328:THR:O     | 2.01                     | 0.59              |
| 2:H:29:GLU:CD    | 2:H:153:LEU:HD22  | 2.22                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:50:ARG:HD2    | 2:H:50:ARG:N     | 2.17                     | 0.59              |
| 2:H:232:ASN:N     | 2:H:233:PRO:HD3  | 2.17                     | 0.59              |
| 1:C:698:ILE:H     | 1:C:698:ILE:CD1  | 2.14                     | 0.59              |
| 1:E:1021:ARG:HH11 | 1:E:1021:ARG:CG  | 2.15                     | 0.59              |
| 1:G:620:PRO:HB2   | 1:G:622:THR:HG23 | 1.83                     | 0.59              |
| 1:A:695:VAL:CG1   | 1:A:700:MET:HB3  | 2.30                     | 0.59              |
| 1:E:1073:LYS:N    | 1:E:1073:LYS:HD2 | 2.17                     | 0.59              |
| 2:B:78:GLN:HG2    | 11:B:3896:HOH:O  | 2.03                     | 0.59              |
| 1:C:519:GLN:NE2   | 11:C:1768:HOH:O  | 2.32                     | 0.59              |
| 1:C:552:GLU:HB3   | 11:C:1775:HOH:O  | 2.01                     | 0.59              |
| 2:D:157:ASP:OD2   | 2:D:160:LYS:HG2  | 2.03                     | 0.59              |
| 2:D:282:LYS:HG3   | 2:D:320:THR:CB   | 2.32                     | 0.59              |
| 2:F:41:GLU:CB     | 2:F:358:PRO:HD3  | 2.33                     | 0.59              |
| 2:B:269:CYS:O     | 2:B:272:HIS:HB3  | 2.02                     | 0.59              |
| 1:C:237:PHE:CE2   | 1:C:458:ILE:HD13 | 2.38                     | 0.59              |
| 1:G:905:PRO:HB2   | 1:G:1040:TYR:OH  | 2.02                     | 0.59              |
| 1:A:693:ALA:HB2   | 1:A:708:ILE:HD11 | 1.84                     | 0.59              |
| 1:A:1000:HIS:HD2  | 1:A:1003:ASP:H   | 1.49                     | 0.59              |
| 1:C:784:GLN:H     | 1:C:784:GLN:HE21 | 1.50                     | 0.59              |
| 1:C:784:GLN:HE22  | 1:C:1043:THR:HB  | 1.68                     | 0.59              |
| 1:G:734:LEU:HD12  | 1:G:734:LEU:O    | 2.02                     | 0.59              |
| 2:H:215:ARG:HH11  | 2:H:215:ARG:CG   | 2.16                     | 0.59              |
| 1:A:115:MET:HG2   | 1:A:118:ALA:O    | 2.01                     | 0.59              |
| 1:G:597:ILE:HG12  | 1:G:615:ARG:HB2  | 1.85                     | 0.59              |
| 1:C:713:VAL:HG23  | 1:C:755:PHE:HB2  | 1.84                     | 0.58              |
| 2:D:57:TYR:CD1    | 2:D:58:PRO:HD2   | 2.39                     | 0.58              |
| 1:E:904:ASP:O     | 1:E:906:LEU:N    | 2.36                     | 0.58              |
| 2:F:345:LYS:HB3   | 2:F:346:PRO:HD2  | 1.85                     | 0.58              |
| 1:C:1:MET:N       | 1:C:224:LYS:HE3  | 2.17                     | 0.58              |
| 1:C:1021:ARG:HH11 | 1:C:1021:ARG:HG3 | 1.67                     | 0.58              |
| 2:B:245:PRO:HG2   | 2:B:274:LEU:CD2  | 2.34                     | 0.58              |
| 2:F:376:GLN:HA    | 2:F:379:LYS:NZ   | 2.18                     | 0.58              |
| 1:G:698:ILE:O     | 1:G:702:VAL:HG23 | 2.03                     | 0.58              |
| 1:A:417:ASP:OD1   | 1:A:423:LYS:NZ   | 2.30                     | 0.58              |
| 1:C:17:PRO:HG3    | 1:C:917:VAL:CG1  | 2.33                     | 0.58              |
| 2:F:92:PHE:CE1    | 2:F:93:ARG:HG2   | 2.38                     | 0.58              |
| 2:F:322:PRO:CD    | 2:F:325:LEU:HD12 | 2.33                     | 0.58              |
| 2:H:247:PRO:HA    | 2:H:252:ILE:CD1  | 2.31                     | 0.58              |
| 1:G:676:GLU:O     | 1:G:680:HIS:ND1  | 2.36                     | 0.58              |
| 1:G:761:GLU:HG2   | 1:G:781:HIS:CE1  | 2.39                     | 0.58              |
| 1:G:1000:HIS:CD2  | 1:G:1002:GLN:HB3 | 2.38                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:153:LEU:O     | 2:H:156:MET:HB2   | 2.03                     | 0.58              |
| 2:B:272:HIS:ND1   | 2:B:349:SER:OG    | 2.32                     | 0.58              |
| 1:C:646:THR:HB    | 1:C:647:PRO:HD3   | 1.86                     | 0.58              |
| 1:G:773:VAL:HG21  | 1:G:817:ALA:CB    | 2.33                     | 0.58              |
| 1:A:761:GLU:HB3   | 1:A:781:HIS:ND1   | 2.19                     | 0.58              |
| 1:E:440:ALA:O     | 1:E:444:ARG:HG3   | 2.03                     | 0.58              |
| 1:G:79:GLU:HG2    | 1:G:111:PHE:CE2   | 2.38                     | 0.58              |
| 2:B:345:LYS:HB3   | 2:B:346:PRO:HD2   | 1.84                     | 0.58              |
| 1:C:1:MET:H3      | 1:C:224:LYS:HE3   | 1.69                     | 0.58              |
| 2:D:275:LEU:HD23  | 2:D:349:SER:OG    | 2.04                     | 0.58              |
| 2:F:186:LYS:HB2   | 2:F:189:GLU:OE2   | 2.04                     | 0.58              |
| 1:G:481:ILE:HA    | 1:G:484:LEU:HD12  | 1.86                     | 0.58              |
| 1:E:172:PHE:HB3   | 1:E:200:PRO:HG2   | 1.85                     | 0.58              |
| 1:E:735:ARG:O     | 1:E:738:PHE:N     | 2.37                     | 0.58              |
| 1:G:784:GLN:NE2   | 1:G:784:GLN:N     | 2.36                     | 0.58              |
| 1:C:858:GLY:HA2   | 1:C:1069:HIS:CE1  | 2.38                     | 0.57              |
| 2:B:46:PRO:HA     | 2:B:76:HIS:CG     | 2.39                     | 0.57              |
| 1:C:60[B]:MET:HE3 | 11:C:1146:HOH:O   | 2.04                     | 0.57              |
| 1:E:947:LEU:HG    | 1:E:1014:ILE:CG2  | 2.34                     | 0.57              |
| 2:H:201:ALA:HB2   | 2:H:239:SER:CB    | 2.34                     | 0.57              |
| 1:C:814:GLN:HG3   | 1:C:818:PHE:HE2   | 1.69                     | 0.57              |
| 1:E:340:THR:O     | 1:E:343:ARG:HB2   | 2.04                     | 0.57              |
| 1:G:118:ALA:HA    | 11:G:1763:HOH:O   | 2.03                     | 0.57              |
| 1:G:32:GLN:OE1    | 1:G:320:ALA:HB3   | 2.04                     | 0.57              |
| 1:G:702:VAL:O     | 1:G:706:LYS:HD2   | 2.05                     | 0.57              |
| 1:G:902:GLY:O     | 1:G:1027:ARG:NH2  | 2.38                     | 0.57              |
| 1:A:726:GLU:HG3   | 1:A:727:ILE:H     | 1.67                     | 0.57              |
| 1:A:1072:ILE:C    | 1:A:1073:LYS:HD2  | 2.24                     | 0.57              |
| 1:C:157:ALA:O     | 1:C:160:ALA:HB3   | 2.05                     | 0.57              |
| 1:C:678:PHE:CE1   | 1:C:842:VAL:HG23  | 2.40                     | 0.57              |
| 1:G:168:ILE:CG2   | 1:G:204:LEU:HD22  | 2.34                     | 0.57              |
| 1:G:1021:ARG:HH11 | 1:G:1021:ARG:CG   | 2.17                     | 0.57              |
| 11:G:1440:HOH:O   | 2:H:123:ARG:HD2   | 2.02                     | 0.57              |
| 2:H:272:HIS:HA    | 2:H:349:SER:CB    | 2.32                     | 0.57              |
| 2:H:361:HIS:ND1   | 11:H:399:HOH:O    | 2.30                     | 0.57              |
| 1:C:419:GLU:HB3   | 1:C:423[B]:LYS:NZ | 2.18                     | 0.57              |
| 1:C:761:GLU:HB3   | 1:C:781:HIS:ND1   | 2.19                     | 0.57              |
| 2:H:142:LEU:O     | 2:H:146:LYS:HG3   | 2.05                     | 0.57              |
| 2:H:369:HIS:O     | 2:H:372:GLU:HB2   | 2.05                     | 0.57              |
| 1:C:24:CYS:SG     | 1:C:576:ILE:HD12  | 2.44                     | 0.57              |
| 2:D:225:ALA:HB2   | 2:D:254:ALA:HB1   | 1.87                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:E:1006:LYS:HG3   | 1:E:1006:LYS:O    | 2.04                     | 0.57              |
| 1:G:702:VAL:HG13   | 1:G:731:GLU:HG3   | 1.86                     | 0.57              |
| 1:G:105:GLN:NE2    | 1:G:105:GLN:HA    | 2.20                     | 0.57              |
| 1:G:516:LEU:HD11   | 1:G:520:TYR:CZ    | 2.40                     | 0.57              |
| 1:G:965:LEU:HG     | 1:G:971:LEU:HD11  | 1.87                     | 0.57              |
| 1:A:460:ARG:HG3    | 11:A:1299:HOH:O   | 2.04                     | 0.57              |
| 1:A:936:ASN:HB2    | 11:A:1109:HOH:O   | 2.04                     | 0.57              |
| 1:E:947:LEU:HD12   | 1:E:947:LEU:N     | 2.20                     | 0.57              |
| 1:G:695:VAL:CG1    | 1:G:700:MET:HB3   | 2.34                     | 0.57              |
| 1:E:158:VAL:HG11   | 1:E:206:ILE:HB    | 1.86                     | 0.56              |
| 2:H:286:MET:HE2    | 2:H:315:ALA:HB2   | 1.87                     | 0.56              |
| 2:B:324:ASN:N      | 2:B:324:ASN:ND2   | 2.45                     | 0.56              |
| 1:A:1001:ILE:O     | 1:A:1005:ILE:HG13 | 2.06                     | 0.56              |
| 2:B:150:PHE:CE1    | 2:B:152:GLY:HA2   | 2.40                     | 0.56              |
| 2:B:237:PHE:CE1    | 2:B:268:ILE:HG13  | 2.41                     | 0.56              |
| 2:B:322:PRO:HB2    | 2:B:324:ASN:HD21  | 1.69                     | 0.56              |
| 1:C:51:PRO:HG3     | 1:C:918:MET:HB2   | 1.86                     | 0.56              |
| 1:C:814:GLN:HG3    | 1:C:818:PHE:CE2   | 2.39                     | 0.56              |
| 2:D:201:ALA:HA     | 2:D:240:ASN:OD1   | 2.05                     | 0.56              |
| 1:E:417:ASP:OD2    | 1:E:418:PRO:HD2   | 2.04                     | 0.56              |
| 1:A:730:ASP:H      | 1:A:733:ASP:HB2   | 1.71                     | 0.56              |
| 1:E:503:ALA:HB1    | 1:E:508:VAL:O     | 2.06                     | 0.56              |
| 2:H:342:ARG:NH2    | 2:H:344:ASP:OD1   | 2.33                     | 0.56              |
| 1:E:950:ARG:HD3    | 11:E:1593:HOH:O   | 2.04                     | 0.56              |
| 2:F:290:HIS:HB2    | 2:F:312:HIS:CD2   | 2.40                     | 0.56              |
| 1:C:423[A]:LYS:HE2 | 11:C:1420:HOH:O   | 2.04                     | 0.56              |
| 1:E:142:GLU:OE2    | 1:E:294:ARG:NH2   | 2.38                     | 0.56              |
| 2:H:133:ILE:HD11   | 2:H:143:ALA:HA    | 1.87                     | 0.56              |
| 2:F:201:ALA:HB2    | 2:F:239:SER:HB2   | 1.87                     | 0.56              |
| 1:G:695:VAL:HG11   | 1:G:701:ALA:N     | 2.21                     | 0.56              |
| 1:A:698:ILE:O      | 1:A:702:VAL:HG23  | 2.06                     | 0.56              |
| 1:G:698:ILE:HD12   | 1:G:698:ILE:N     | 2.20                     | 0.56              |
| 2:H:295:HIS:HD2    | 2:H:296:PRO:O     | 1.89                     | 0.56              |
| 1:E:1057:ASP:HB3   | 1:E:1060:GLU:HB2  | 1.87                     | 0.56              |
| 1:G:703:GLU:HA     | 1:G:706:LYS:HD3   | 1.88                     | 0.56              |
| 1:C:695:VAL:HG21   | 1:C:701:ALA:CA    | 2.28                     | 0.55              |
| 2:D:48:TYR:HA      | 2:D:51:GLN:HE21   | 1.70                     | 0.55              |
| 2:D:345:LYS:HB3    | 2:D:346:PRO:CD    | 2.35                     | 0.55              |
| 1:E:995:HIS:ND1    | 11:E:1847:HOH:O   | 2.33                     | 0.55              |
| 1:G:223:ASP:OD1    | 1:G:225:ASN:N     | 2.39                     | 0.55              |
| 1:C:571:ARG:HD3    | 1:C:571:ARG:N     | 2.21                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:G:695:VAL:HG21   | 1:G:701:ALA:HA    | 1.88                     | 0.55              |
| 1:A:40:GLU:HG3     | 1:A:325:LYS:HE2   | 1.88                     | 0.55              |
| 2:D:201:ALA:HB2    | 2:D:239:SER:HB2   | 1.87                     | 0.55              |
| 1:E:703:GLU:HA     | 1:E:706:LYS:HD3   | 1.89                     | 0.55              |
| 1:E:967[B]:GLN:NE2 | 1:E:1054:LEU:HD13 | 2.17                     | 0.55              |
| 1:E:494:ARG:HG2    | 1:E:547:TYR:HB2   | 1.89                     | 0.55              |
| 1:G:874:LEU:HB3    | 1:G:879:VAL:O     | 2.05                     | 0.55              |
| 2:H:218:ILE:N      | 2:H:218:ILE:HD13  | 2.21                     | 0.55              |
| 2:H:363:ALA:O      | 2:H:366:LEU:HD13  | 2.06                     | 0.55              |
| 2:B:298:LYS:HE2    | 2:B:303:ASN:OD1   | 2.06                     | 0.55              |
| 1:E:956:ARG:HB3    | 1:E:1044:LEU:CD2  | 2.36                     | 0.55              |
| 1:G:950:ARG:HG2    | 1:G:1016:THR:OG1  | 2.07                     | 0.55              |
| 2:F:153:LEU:HG     | 2:F:158:LEU:HD11  | 1.88                     | 0.55              |
| 2:B:168:TYR:O      | 2:B:218:ILE:N     | 2.29                     | 0.55              |
| 1:C:423[B]:LYS:NZ  | 11:C:1420:HOH:O   | 2.38                     | 0.55              |
| 1:E:108:LEU:HB2    | 11:E:1179:HOH:O   | 2.07                     | 0.55              |
| 1:E:1061:LYS:NZ    | 11:E:1828:HOH:O   | 2.39                     | 0.55              |
| 2:F:259:LEU:HD13   | 2:F:342:ARG:HH12  | 1.72                     | 0.55              |
| 1:G:274:GLU:HB2    | 11:G:1205:HOH:O   | 2.06                     | 0.55              |
| 1:G:802:SER:O      | 1:G:806:GLN:HG3   | 2.07                     | 0.55              |
| 1:A:130[A]:ARG:NE  | 11:A:1197:HOH:O   | 2.38                     | 0.55              |
| 2:F:224:SER:OG     | 2:F:227:ASP:HB2   | 2.07                     | 0.55              |
| 1:G:645[A]:GLN:HG3 | 1:G:649:LYS:HE3   | 1.89                     | 0.55              |
| 1:A:76:LYS:HD3     | 11:A:1163:HOH:O   | 2.07                     | 0.55              |
| 2:B:263:ILE:CG2    | 2:B:264:PRO:HD2   | 2.36                     | 0.55              |
| 1:C:1:MET:HB2      | 1:C:224:LYS:HZ1   | 1.72                     | 0.55              |
| 1:C:509:ARG:HD3    | 11:C:1763:HOH:O   | 2.07                     | 0.55              |
| 1:A:1001:ILE:HD12  | 1:A:1002:GLN:H    | 1.69                     | 0.55              |
| 2:B:172:GLN:O      | 2:B:207:ARG:HA    | 2.07                     | 0.55              |
| 1:E:3:LYS:NZ       | 11:E:1094:HOH:O   | 2.39                     | 0.55              |
| 1:G:128:ASP:CG     | 1:G:131:ARG:HG3   | 2.27                     | 0.55              |
| 1:G:948:SER:OG     | 10:G:1093:U:H5"   | 2.07                     | 0.55              |
| 1:A:336:MET:HB3    | 1:A:342:GLY:HA2   | 1.89                     | 0.54              |
| 1:A:446:GLY:O      | 1:E:447:LEU:HD23  | 2.07                     | 0.54              |
| 1:C:64:THR:O       | 1:C:1065:VAL:HG23 | 2.07                     | 0.54              |
| 1:G:213:TRP:CZ3    | 1:G:296:ILE:HD12  | 2.42                     | 0.54              |
| 1:C:321:LYS:NZ     | 1:C:611:ASP:OD1   | 2.40                     | 0.54              |
| 2:H:186:LYS:O      | 2:H:189:GLU:HB2   | 2.06                     | 0.54              |
| 2:H:350:PHE:CG     | 2:H:366:LEU:HD21  | 2.42                     | 0.54              |
| 1:A:588:ALA:HB2    | 1:A:863:LYS:HG2   | 1.90                     | 0.54              |
| 1:A:701:ALA:O      | 1:A:705:ALA:N     | 2.30                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:C:46:LEU:HD12    | 1:C:46:LEU:C      | 2.28                     | 0.54              |
| 2:D:205:ILE:HG13   | 2:D:355:GLU:HG3   | 1.89                     | 0.54              |
| 1:E:1:MET:N        | 1:E:224:LYS:HE3   | 2.21                     | 0.54              |
| 1:G:788:HIS:ND1    | 1:G:911:MET:HB2   | 2.23                     | 0.54              |
| 1:A:646:THR:HB     | 1:A:647:PRO:HD3   | 1.88                     | 0.54              |
| 1:C:661:VAL:HB     | 11:C:1801:HOH:O   | 2.08                     | 0.54              |
| 1:E:695:VAL:HG13   | 1:E:700:MET:HB3   | 1.89                     | 0.54              |
| 1:G:1001:ILE:HD11  | 11:G:1537:HOH:O   | 2.07                     | 0.54              |
| 2:H:334:ASP:CG     | 2:H:336:THR:HG23  | 2.28                     | 0.54              |
| 1:A:167:ILE:HD12   | 1:A:167:ILE:N     | 2.21                     | 0.54              |
| 2:B:322:PRO:CB     | 2:B:324:ASN:HD21  | 2.21                     | 0.54              |
| 2:F:342:ARG:HB3    | 2:F:345:LYS:H     | 1.71                     | 0.54              |
| 1:G:294:ARG:HD2    | 6:G:1085:CL:CL    | 2.45                     | 0.54              |
| 1:A:833:LYS:O      | 1:A:836:GLU:HB2   | 2.08                     | 0.54              |
| 2:D:324:ASN:ND2    | 2:D:324:ASN:N     | 2.41                     | 0.54              |
| 2:F:228:VAL:O      | 2:F:231:MET:HG3   | 2.08                     | 0.54              |
| 1:G:563:MET:HE3    | 1:G:635:PRO:HG3   | 1.89                     | 0.54              |
| 2:B:201:ALA:HB2    | 2:B:239:SER:CB    | 2.38                     | 0.54              |
| 2:B:355:GLU:OE2    | 2:B:355:GLU:N     | 2.30                     | 0.54              |
| 2:B:364:ALA:N      | 2:B:365:PRO:HD2   | 2.23                     | 0.54              |
| 1:E:670:ASP:HB2    | 11:E:1785:HOH:O   | 2.08                     | 0.54              |
| 2:F:50:ARG:HD2     | 2:F:50:ARG:N      | 2.21                     | 0.54              |
| 1:G:991:VAL:HG21   | 1:G:1001:ILE:HG22 | 1.89                     | 0.54              |
| 2:H:257:LYS:O      | 2:H:261:THR:HG23  | 2.06                     | 0.54              |
| 1:C:762:VAL:HG13   | 1:C:779:MET:O     | 2.08                     | 0.54              |
| 1:C:905:PRO:HB2    | 1:C:1040:TYR:HH   | 1.70                     | 0.54              |
| 2:D:10:GLU:OE2     | 2:D:129:ASN:N     | 2.29                     | 0.54              |
| 1:E:185:ARG:NH2    | 11:E:1238:HOH:O   | 2.40                     | 0.54              |
| 1:G:967[B]:GLN:HG2 | 1:G:1054:LEU:HD13 | 1.90                     | 0.54              |
| 2:H:132:ILE:HG22   | 2:H:133:ILE:N     | 2.23                     | 0.54              |
| 1:C:43:ARG:HA      | 1:C:62:ASP:OD2    | 2.08                     | 0.54              |
| 2:F:50:ARG:HG2     | 2:F:158:LEU:HD22  | 1.90                     | 0.54              |
| 2:H:69:ASP:HA      | 11:H:500:HOH:O    | 2.07                     | 0.54              |
| 2:D:277:LEU:HD23   | 2:D:281:ALA:O     | 2.08                     | 0.54              |
| 1:E:125:LYS:NZ     | 11:E:1188:HOH:O   | 2.41                     | 0.54              |
| 1:E:144:ALA:HB1    | 1:E:208:GLU:CG    | 2.38                     | 0.54              |
| 1:E:901:PRO:HD2    | 6:E:1086:CL:CL    | 2.45                     | 0.54              |
| 1:G:1067:GLU:O     | 1:G:1068:MET:C    | 2.46                     | 0.53              |
| 9:A:1090:NET:H82   | 9:A:1090:NET:H62  | 1.91                     | 0.53              |
| 2:B:6:LEU:HD12     | 2:B:7:LEU:N       | 2.23                     | 0.53              |
| 1:C:827:ASN:HB3    | 1:C:843:ASN:HB2   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:D:262:ASP:HB2   | 11:D:2882:HOH:O    | 2.08                     | 0.53              |
| 2:D:272:HIS:HA    | 2:D:349:SER:HB2    | 1.88                     | 0.53              |
| 1:E:1:MET:HB2     | 1:E:224:LYS:HZ2    | 1.73                     | 0.53              |
| 1:G:698:ILE:HD12  | 1:G:698:ILE:H      | 1.73                     | 0.53              |
| 2:H:275:LEU:HD23  | 2:H:349:SER:CB     | 2.39                     | 0.53              |
| 2:H:363:ALA:C     | 2:H:365:PRO:HD2    | 2.28                     | 0.53              |
| 1:A:941:LYS:NZ    | 1:A:1056:ALA:O     | 2.33                     | 0.53              |
| 1:E:1051:ALA:O    | 1:E:1054:LEU:HB2   | 2.08                     | 0.53              |
| 2:F:197:TYR:HB3   | 2:F:199:PHE:CZ     | 2.44                     | 0.53              |
| 1:G:622:THR:O     | 1:G:626:VAL:HG23   | 2.08                     | 0.53              |
| 1:A:772[B]:MET:SD | 1:A:880:THR:HG22   | 2.49                     | 0.53              |
| 1:E:482:THR:HB    | 11:E:1442:HOH:O    | 2.08                     | 0.53              |
| 1:E:734:LEU:HD12  | 1:E:734:LEU:C      | 2.28                     | 0.53              |
| 2:F:43:LEU:HD21   | 2:F:80:LEU:HD13    | 1.90                     | 0.53              |
| 2:F:350:PHE:HB2   | 2:F:366:LEU:CD2    | 2.39                     | 0.53              |
| 1:G:139:ILE:HD11  | 1:G:141:LEU:HD12   | 1.90                     | 0.53              |
| 1:A:709:GLY:O     | 1:A:754:HIS:ND1    | 2.41                     | 0.53              |
| 1:C:171:SER:HB2   | 1:C:203:GLU:HB3    | 1.90                     | 0.53              |
| 1:C:1019:GLY:O    | 1:C:1023:ILE:HD12  | 2.08                     | 0.53              |
| 1:E:675:ARG:H     | 1:E:675:ARG:HD3    | 1.72                     | 0.53              |
| 1:E:954:LYS:O     | 1:E:980:VAL:HG11   | 2.09                     | 0.53              |
| 1:G:710:TYR:HB3   | 1:G:729:TYR:O      | 2.07                     | 0.53              |
| 2:H:45:ASP:HB3    | 2:H:48:TYR:HD2     | 1.74                     | 0.53              |
| 2:H:236:ILE:HD12  | 2:H:263:ILE:CG2    | 2.38                     | 0.53              |
| 1:A:70:HIS:O      | 1:A:74:VAL:HG23    | 2.09                     | 0.53              |
| 2:B:322:PRO:HG2   | 2:B:324:ASN:ND2    | 2.21                     | 0.53              |
| 2:F:41:GLU:HB2    | 2:F:358:PRO:HD3    | 1.91                     | 0.53              |
| 1:G:423:LYS:HA    | 1:G:426[B]:ARG:NH2 | 2.24                     | 0.53              |
| 1:G:946:LEU:HD11  | 1:G:991:VAL:HG11   | 1.89                     | 0.53              |
| 2:H:236:ILE:CD1   | 2:H:263:ILE:HG21   | 2.39                     | 0.53              |
| 2:H:275:LEU:HD23  | 2:H:349:SER:OG     | 2.09                     | 0.53              |
| 2:F:201:ALA:HB2   | 2:F:239:SER:CB     | 2.38                     | 0.53              |
| 2:H:8:VAL:HG12    | 2:H:9:LEU:N        | 2.24                     | 0.53              |
| 2:H:205:ILE:HG13  | 2:H:355:GLU:HG3    | 1.90                     | 0.53              |
| 1:A:979:ILE:O     | 1:A:983:GLU:HG3    | 2.08                     | 0.53              |
| 2:B:49:SER:O      | 2:B:50:ARG:HB2     | 2.08                     | 0.53              |
| 1:C:1051:ALA:O    | 1:C:1054:LEU:HB2   | 2.07                     | 0.53              |
| 1:G:272:LEU:HD21  | 1:G:282:SER:HB2    | 1.89                     | 0.53              |
| 2:H:279:SER:OG    | 2:H:342:ARG:NH1    | 2.30                     | 0.53              |
| 1:A:3:LYS:HB2     | 1:A:42:TYR:OH      | 2.08                     | 0.53              |
| 1:A:289:ASN:OD1   | 1:A:290:PRO:HD2    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:665:SER:O    | 1:A:669:ILE:HG13   | 2.09                     | 0.53              |
| 2:B:367:PHE:O    | 2:B:370:PHE:HB3    | 2.08                     | 0.53              |
| 1:C:1:MET:CG     | 1:C:2:PRO:HD2      | 2.39                     | 0.53              |
| 1:C:728:VAL:HG11 | 1:C:734:LEU:HA     | 1.91                     | 0.53              |
| 2:D:188:ASP:OD2  | 2:D:188:ASP:N      | 2.31                     | 0.53              |
| 1:G:100:LEU:N    | 1:G:100:LEU:HD12   | 2.24                     | 0.53              |
| 2:B:50:ARG:HH11  | 2:B:50:ARG:CG      | 2.18                     | 0.52              |
| 2:B:247:PRO:HA   | 2:B:252:ILE:HD12   | 1.90                     | 0.52              |
| 1:G:751:LEU:O    | 1:G:752:LEU:HD12   | 2.08                     | 0.52              |
| 1:A:695:VAL:HG12 | 1:A:696:THR:N      | 2.22                     | 0.52              |
| 1:E:956:ARG:HB3  | 1:E:1044:LEU:HD21  | 1.90                     | 0.52              |
| 2:H:48:TYR:O     | 2:H:51:GLN:HB2     | 2.09                     | 0.52              |
| 1:C:992:ASN:ND2  | 1:E:975:HIS:NE2    | 2.57                     | 0.52              |
| 2:F:41:GLU:HB3   | 2:F:358:PRO:HD3    | 1.92                     | 0.52              |
| 1:G:17:PRO:HG3   | 1:G:917:VAL:HG13   | 1.90                     | 0.52              |
| 1:G:237:PHE:HB3  | 1:G:248:ILE:HB     | 1.91                     | 0.52              |
| 1:E:278:GLU:HG2  | 11:E:1310:HOH:O    | 2.09                     | 0.52              |
| 1:E:726:GLU:HG3  | 1:E:727:ILE:N      | 2.24                     | 0.52              |
| 1:G:1:MET:HB2    | 1:G:224:LYS:HE3    | 1.90                     | 0.52              |
| 1:G:178:GLY:HA3  | 1:G:198:LEU:HD23   | 1.91                     | 0.52              |
| 1:A:28:TYR:CZ    | 1:A:313:LYS:HE3    | 2.43                     | 0.52              |
| 2:B:350:PHE:HB2  | 2:B:366:LEU:CD2    | 2.40                     | 0.52              |
| 1:C:419:GLU:CB   | 1:C:423[B]:LYS:NZ  | 2.73                     | 0.52              |
| 2:F:193:HIS:O    | 2:F:234:ASP:HB2    | 2.10                     | 0.52              |
| 1:G:384:VAL:HG22 | 1:G:385:MET:N      | 2.24                     | 0.52              |
| 2:H:176:THR:O    | 2:H:180:GLY:N      | 2.37                     | 0.52              |
| 1:A:685:LEU:O    | 1:A:686:LYS:HB2    | 2.09                     | 0.52              |
| 1:A:822:VAL:O    | 1:A:823:ARG:HD3    | 2.10                     | 0.52              |
| 1:C:420:ALA:HA   | 1:C:423[B]:LYS:HD2 | 1.91                     | 0.52              |
| 1:C:542:TYR:CD1  | 1:C:616:LEU:HD23   | 2.45                     | 0.52              |
| 2:F:259:LEU:HD13 | 2:F:342:ARG:NH1    | 2.24                     | 0.52              |
| 1:G:1035:GLN:NE2 | 11:G:1544:HOH:O    | 2.43                     | 0.52              |
| 1:A:954:LYS:O    | 1:A:957:VAL:HG12   | 2.10                     | 0.52              |
| 1:C:3:LYS:HB3    | 1:C:330:TYR:CZ     | 2.44                     | 0.52              |
| 1:A:671:ARG:HG3  | 1:A:677:ARG:NH1    | 2.24                     | 0.52              |
| 1:C:998:ARG:HB3  | 1:C:999:PRO:HA     | 1.91                     | 0.52              |
| 2:D:228:VAL:HG22 | 2:D:231:MET:HE1    | 1.91                     | 0.52              |
| 2:D:245:PRO:HD3  | 2:D:270:LEU:CD1    | 2.33                     | 0.52              |
| 2:D:282:LYS:HG3  | 2:D:320:THR:HB     | 1.92                     | 0.52              |
| 1:G:708:ILE:HG21 | 1:G:712:LEU:HD11   | 1.92                     | 0.52              |
| 2:H:54:THR:HG23  | 2:H:81:VAL:HG12    | 1.90                     | 0.52              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:B:316:VAL:CG1    | 2:B:337:LEU:HD23 | 2.38                     | 0.52              |
| 2:F:199:PHE:HB3    | 2:F:270:LEU:HD23 | 1.92                     | 0.52              |
| 1:A:370:ALA:HB2    | 1:A:903:VAL:CG2  | 2.40                     | 0.52              |
| 1:A:891:LYS:HG2    | 1:A:892:GLU:N    | 2.25                     | 0.52              |
| 2:B:50:ARG:HG2     | 2:B:158:LEU:CD2  | 2.40                     | 0.52              |
| 2:D:46:PRO:HA      | 2:D:76:HIS:CG    | 2.45                     | 0.52              |
| 1:E:517:ARG:HG2    | 1:E:522:LEU:HD23 | 1.91                     | 0.52              |
| 1:A:223:ASP:OD1    | 1:A:227:ASN:HB2  | 2.10                     | 0.51              |
| 2:D:362:ASP:OD2    | 2:D:362:ASP:N    | 2.41                     | 0.51              |
| 2:F:247:PRO:HD2    | 2:F:248:ASP:OD1  | 2.10                     | 0.51              |
| 1:G:10:ILE:HD13    | 1:G:37:LEU:HD13  | 1.90                     | 0.51              |
| 2:B:340:ILE:O      | 2:B:348:PHE:HB2  | 2.10                     | 0.51              |
| 1:C:174:MET:HB2    | 5:C:1078:PO4:O1  | 2.09                     | 0.51              |
| 2:D:196:ALA:HA     | 2:D:237:PHE:O    | 2.10                     | 0.51              |
| 1:E:873:SER:O      | 1:E:877:GLN:HG3  | 2.09                     | 0.51              |
| 1:G:701:ALA:O      | 1:G:705:ALA:N    | 2.33                     | 0.51              |
| 2:H:160:LYS:HE3    | 2:H:161:GLU:OE2  | 2.09                     | 0.51              |
| 1:A:663:GLY:O      | 1:A:664:THR:C    | 2.48                     | 0.51              |
| 1:C:426:ARG:HD3    | 1:C:426:ARG:C    | 2.30                     | 0.51              |
| 1:E:967[B]:GLN:NE2 | 1:E:1054:LEU:CB  | 2.74                     | 0.51              |
| 1:E:998:ARG:CB     | 1:E:999:PRO:HA   | 2.40                     | 0.51              |
| 1:G:784:GLN:HB3    | 11:G:1480:HOH:O  | 2.11                     | 0.51              |
| 2:H:286:MET:HE1    | 2:H:312:HIS:CE1  | 2.44                     | 0.51              |
| 2:H:317:ASP:HB3    | 2:H:320:THR:HG23 | 1.92                     | 0.51              |
| 1:A:224:LYS:HE2    | 1:A:329:GLY:O    | 2.10                     | 0.51              |
| 1:A:450:ASP:N      | 11:A:1435:HOH:O  | 2.27                     | 0.51              |
| 2:B:83:ARG:HH11    | 2:B:83:ARG:HG3   | 1.75                     | 0.51              |
| 1:G:225:ASN:ND2    | 11:G:1296:HOH:O  | 2.42                     | 0.51              |
| 1:G:762:VAL:HG12   | 1:G:763:ASP:N    | 2.25                     | 0.51              |
| 2:H:50:ARG:HG3     | 2:H:50:ARG:NH1   | 2.16                     | 0.51              |
| 2:H:317:ASP:OD2    | 2:H:319:ALA:HB3  | 2.09                     | 0.51              |
| 1:C:344:THR:HB     | 1:C:345:PRO:HD2  | 1.93                     | 0.51              |
| 1:C:998:ARG:HA     | 1:C:999:PRO:C    | 2.28                     | 0.51              |
| 1:C:7:ILE:HG23     | 1:C:84:ASP:HB2   | 1.91                     | 0.51              |
| 1:C:784:GLN:H      | 1:C:784:GLN:NE2  | 2.08                     | 0.51              |
| 1:E:500:ALA:O      | 1:E:504:LYS:HG3  | 2.10                     | 0.51              |
| 1:G:526:TYR:CE1    | 1:G:545:SER:HB3  | 2.46                     | 0.51              |
| 2:H:6:LEU:HD12     | 2:H:7:LEU:N      | 2.25                     | 0.51              |
| 1:A:228:CYS:HB2    | 1:A:273:ARG:NH2  | 2.26                     | 0.51              |
| 1:C:167:ILE:HD12   | 1:C:167:ILE:N    | 2.25                     | 0.51              |
| 1:C:973:ALA:O      | 1:C:991:VAL:HG12 | 2.10                     | 0.51              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:E:361:ARG:CZ      | 1:E:571:ARG:HG2    | 2.41                     | 0.51              |
| 1:E:682:VAL:HG13    | 1:E:687:LEU:HB2    | 1.90                     | 0.51              |
| 1:E:796:LEU:C       | 1:E:796:LEU:HD23   | 2.31                     | 0.51              |
| 2:F:255:ILE:HA      | 2:F:258:PHE:HD2    | 1.76                     | 0.51              |
| 1:G:773:VAL:HG21    | 1:G:817:ALA:HB3    | 1.91                     | 0.51              |
| 1:G:1000:HIS:CD2    | 1:G:1003:ASP:H     | 2.28                     | 0.51              |
| 1:C:69:ILE:O        | 1:C:69:ILE:HG22    | 2.10                     | 0.51              |
| 1:G:695:VAL:CG2     | 1:G:752:LEU:HD22   | 2.40                     | 0.51              |
| 1:A:730:ASP:OD2     | 1:A:733:ASP:HB2    | 2.11                     | 0.51              |
| 1:A:948:SER:O       | 1:A:1015:ASN:HA    | 2.11                     | 0.51              |
| 1:A:991:VAL:HG22    | 1:A:992:ASN:N      | 2.26                     | 0.51              |
| 2:B:248:ASP:OD2     | 2:B:248:ASP:N      | 2.41                     | 0.51              |
| 1:C:385:MET:HB2     | 1:C:603:PRO:HG3    | 1.92                     | 0.51              |
| 2:D:277:LEU:HD21    | 2:D:283:THR:HG23   | 1.93                     | 0.51              |
| 1:E:258:ASP:O       | 1:E:262:GLN:HG2    | 2.10                     | 0.51              |
| 1:E:526:TYR:CE1     | 1:E:545:SER:HB3    | 2.46                     | 0.51              |
| 9:E:1092:NET:H42    | 9:E:1092:NET:C2    | 2.33                     | 0.51              |
| 1:A:772[A]:MET:SD   | 1:A:880:THR:HG22   | 2.51                     | 0.51              |
| 1:A:1027[B]:ARG:HB3 | 1:A:1027[B]:ARG:CZ | 2.40                     | 0.51              |
| 2:D:174:SER:O       | 2:D:182:PRO:HD3    | 2.11                     | 0.51              |
| 1:E:973:ALA:O       | 1:E:991:VAL:HG12   | 2.10                     | 0.51              |
| 1:G:143:THR:HA      | 1:G:296:ILE:HG23   | 1.93                     | 0.51              |
| 1:G:146:SER:HB2     | 1:G:205:LEU:HD11   | 1.93                     | 0.51              |
| 1:G:479:VAL:HG21    | 1:G:483:GLY:HA3    | 1.92                     | 0.51              |
| 1:G:891:LYS:NZ      | 11:G:1678:HOH:O    | 2.43                     | 0.51              |
| 2:B:72:SER:HB2      | 11:B:3543:HOH:O    | 2.10                     | 0.50              |
| 2:B:194:VAL:HB      | 2:B:216:LEU:CD2    | 2.38                     | 0.50              |
| 2:F:190:LEU:HD23    | 2:F:213:GLY:HA2    | 1.93                     | 0.50              |
| 1:G:43:ARG:NH2      | 1:G:81:GLU:OE2     | 2.39                     | 0.50              |
| 1:G:119:THR:HG23    | 11:G:1763:HOH:O    | 2.11                     | 0.50              |
| 2:H:244:ASP:OD2     | 2:H:245:PRO:HD2    | 2.11                     | 0.50              |
| 1:C:1048:PHE:O      | 1:C:1052:MET:HG3   | 2.11                     | 0.50              |
| 1:G:770:GLY:HA2     | 1:G:823:ARG:NH1    | 2.26                     | 0.50              |
| 2:H:9:LEU:O         | 2:H:10:GLU:C       | 2.49                     | 0.50              |
| 2:H:141:ALA:O       | 2:H:145:GLU:N      | 2.39                     | 0.50              |
| 1:A:951:GLU:HA      | 1:A:951:GLU:OE1    | 2.06                     | 0.50              |
| 2:D:116:ARG:O       | 2:D:120:ARG:HG3    | 2.11                     | 0.50              |
| 2:F:306:MET:HB3     | 2:F:362:ASP:HB3    | 1.92                     | 0.50              |
| 1:G:1:MET:O         | 1:G:334:GLU:OE1    | 2.29                     | 0.50              |
| 2:H:82:ILE:O        | 2:H:111:ALA:HA     | 2.12                     | 0.50              |
| 1:A:333:ASP:OD1     | 1:A:333:ASP:N      | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:245:PRO:HG2  | 2:B:274:LEU:HD21 | 1.93                     | 0.50              |
| 2:D:246:ALA:HB1  | 2:D:248:ASP:HB2  | 1.94                     | 0.50              |
| 1:G:577:GLU:O    | 1:G:580:TYR:HB3  | 2.12                     | 0.50              |
| 2:H:49:SER:O     | 2:H:50:ARG:HB2   | 2.11                     | 0.50              |
| 2:H:316:VAL:HG12 | 2:H:337:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:715:ARG:NH2  | 7:A:1088:ADP:O1A | 2.44                     | 0.50              |
| 2:B:6:LEU:HD11   | 2:B:8:VAL:CG2    | 2.41                     | 0.50              |
| 2:B:318:GLU:HA   | 2:B:321:LEU:HD13 | 1.91                     | 0.50              |
| 1:C:951:GLU:HA   | 1:C:954:LYS:HD2  | 1.93                     | 0.50              |
| 2:D:316:VAL:CG1  | 2:D:337:LEU:HD23 | 2.41                     | 0.50              |
| 1:G:814:GLN:CG   | 1:G:818:PHE:HE2  | 2.25                     | 0.50              |
| 2:H:10:GLU:HB2   | 2:H:128:GLN:HG2  | 1.94                     | 0.50              |
| 2:H:121:LEU:CD1  | 2:H:125:LYS:HD3  | 2.42                     | 0.50              |
| 2:H:225:ALA:HA   | 2:H:258:PHE:CZ   | 2.47                     | 0.50              |
| 2:B:6:LEU:HD11   | 2:B:8:VAL:HG23   | 1.94                     | 0.50              |
| 1:C:948:SER:OG   | 10:C:1093:U:H5'' | 2.11                     | 0.50              |
| 2:D:12:GLY:HA2   | 2:D:144:LEU:HD13 | 1.92                     | 0.50              |
| 2:F:246:ALA:C    | 2:F:248:ASP:H    | 2.13                     | 0.50              |
| 1:G:40:GLU:OE1   | 1:G:325:LYS:HE2  | 2.12                     | 0.50              |
| 1:G:796:LEU:HD23 | 1:G:797:PRO:N    | 2.27                     | 0.50              |
| 1:A:101:GLU:OE2  | 1:A:104:ARG:NH2  | 2.41                     | 0.50              |
| 1:A:467:GLU:O    | 1:A:471:ARG:HG2  | 2.12                     | 0.50              |
| 2:B:285:LYS:HG3  | 2:B:314:PHE:CD1  | 2.47                     | 0.50              |
| 1:C:1:MET:HB2    | 1:C:224:LYS:HZ2  | 1.76                     | 0.50              |
| 1:C:675:ARG:H    | 1:C:675:ARG:HD3  | 1.77                     | 0.50              |
| 1:C:802:SER:O    | 1:C:806:GLN:HG3  | 2.12                     | 0.50              |
| 1:E:682:VAL:CG1  | 1:E:687:LEU:HB2  | 2.42                     | 0.50              |
| 1:G:358:LYS:HG2  | 1:G:359:ILE:N    | 2.19                     | 0.50              |
| 2:H:324:ASN:O    | 2:H:342:ARG:HA   | 2.10                     | 0.50              |
| 1:C:372:ASP:N    | 11:C:1371:HOH:O  | 2.30                     | 0.50              |
| 1:E:425:ARG:HD3  | 11:E:1422:HOH:O  | 2.11                     | 0.50              |
| 2:F:154:ASN:ND2  | 2:F:314:PHE:HZ   | 2.08                     | 0.50              |
| 1:G:339:ILE:CD1  | 1:G:530:ASP:HA   | 2.36                     | 0.50              |
| 1:G:579:ASP:OD1  | 1:G:605:THR:HB   | 2.12                     | 0.50              |
| 1:A:527:LYS:HB2  | 1:A:544:TYR:CZ   | 2.46                     | 0.50              |
| 1:C:349:GLU:O    | 2:D:294:ASN:HB2  | 2.12                     | 0.50              |
| 1:C:563:MET:HE3  | 1:C:635:PRO:HG3  | 1.94                     | 0.50              |
| 2:F:23:THR:HG22  | 2:F:24:GLY:N     | 2.25                     | 0.50              |
| 2:F:342:ARG:NE   | 2:F:344:ASP:OD2  | 2.45                     | 0.50              |
| 2:H:32:PHE:HA    | 2:H:54:THR:O     | 2.11                     | 0.50              |
| 2:H:161:GLU:OE1  | 2:H:161:GLU:HA   | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:6:LEU:HD13   | 2:D:16:HIS:CE1   | 2.47                     | 0.49              |
| 2:D:9:LEU:HD12   | 2:D:13:THR:HB    | 1.94                     | 0.49              |
| 2:F:281:ALA:HB2  | 2:F:322:PRO:HD3  | 1.94                     | 0.49              |
| 1:G:9:SER:O      | 1:G:84:ASP:HB2   | 2.11                     | 0.49              |
| 1:G:180:GLY:HA2  | 1:G:376:THR:OG1  | 2.11                     | 0.49              |
| 1:G:439:ILE:O    | 1:G:442:ALA:HB3  | 2.12                     | 0.49              |
| 1:A:421:LEU:HB3  | 1:E:421:LEU:HD13 | 1.94                     | 0.49              |
| 1:C:930:LYS:HE3  | 11:C:1159:HOH:O  | 2.11                     | 0.49              |
| 1:C:1066:GLN:HB2 | 11:C:1156:HOH:O  | 2.12                     | 0.49              |
| 1:G:569:PRO:O    | 1:G:571:ARG:HD2  | 2.13                     | 0.49              |
| 1:A:416:ASP:N    | 1:A:416:ASP:OD2  | 2.34                     | 0.49              |
| 1:G:697:ALA:HB3  | 1:G:700:MET:HB2  | 1.95                     | 0.49              |
| 2:H:48:TYR:CZ    | 2:H:311:ASN:ND2  | 2.80                     | 0.49              |
| 1:A:145:ARG:HH12 | 1:A:161:ASP:CG   | 2.16                     | 0.49              |
| 1:C:702:VAL:O    | 1:C:706:LYS:HD3  | 2.12                     | 0.49              |
| 1:E:735:ARG:O    | 1:E:738:PHE:HB2  | 2.13                     | 0.49              |
| 1:C:951:GLU:O    | 1:C:954:LYS:HB2  | 2.13                     | 0.49              |
| 2:F:154:ASN:HD22 | 2:F:285:LYS:HE2  | 1.76                     | 0.49              |
| 1:G:735:ARG:O    | 1:G:738:PHE:HB2  | 2.12                     | 0.49              |
| 1:A:59:GLU:HG3   | 11:A:1503:HOH:O  | 2.13                     | 0.49              |
| 2:B:157:ASP:OD1  | 2:B:160:LYS:HD3  | 2.13                     | 0.49              |
| 2:B:186:LYS:O    | 2:B:187:GLU:C    | 2.50                     | 0.49              |
| 1:C:1:MET:CB     | 1:C:2:PRO:HD2    | 2.43                     | 0.49              |
| 1:C:223:ASP:OD2  | 1:C:227:ASN:HB2  | 2.12                     | 0.49              |
| 2:D:263:ILE:HG22 | 2:D:264:PRO:CD   | 2.40                     | 0.49              |
| 2:D:370:PHE:O    | 2:D:374:ILE:HG13 | 2.12                     | 0.49              |
| 2:F:255:ILE:HA   | 2:F:258:PHE:CD2  | 2.48                     | 0.49              |
| 1:A:240:MET:HE3  | 7:A:1087:ADP:C4  | 2.46                     | 0.49              |
| 1:C:337:ASN:HB3  | 1:C:340:THR:OG1  | 2.13                     | 0.49              |
| 2:D:2:ILE:HD11   | 11:D:2829:HOH:O  | 2.12                     | 0.49              |
| 1:E:559:ARG:NH1  | 11:E:1893:HOH:O  | 2.44                     | 0.49              |
| 1:E:691:ALA:HB3  | 1:E:708:ILE:HG23 | 1.95                     | 0.49              |
| 1:E:695:VAL:HG21 | 1:E:701:ALA:CA   | 2.37                     | 0.49              |
| 1:G:702:VAL:CG1  | 1:G:731:GLU:HG3  | 2.43                     | 0.49              |
| 1:G:781:HIS:HE1  | 1:G:789:SER:HB2  | 1.76                     | 0.49              |
| 1:A:1:MET:O      | 1:A:334:GLU:OE1  | 2.30                     | 0.49              |
| 1:A:365:GLU:OE2  | 1:A:365:GLU:N    | 2.39                     | 0.49              |
| 1:A:767:ILE:CD1  | 1:A:865:ALA:HB2  | 2.42                     | 0.49              |
| 1:C:686:LYS:O    | 1:C:687:LEU:HD23 | 2.13                     | 0.49              |
| 1:C:950:ARG:HD3  | 11:C:1583:HOH:O  | 2.12                     | 0.49              |
| 1:E:157:ALA:O    | 1:E:160:ALA:HB3  | 2.12                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:1017:THR:HG21  | 1:G:1023:ILE:CA    | 2.40                     | 0.49              |
| 1:A:358:LYS:HE3    | 11:A:1128:HOH:O    | 2.11                     | 0.49              |
| 2:B:199:PHE:O      | 2:B:241:GLY:HA3    | 2.13                     | 0.49              |
| 2:B:376:GLN:O      | 2:B:376:GLN:HG3    | 2.13                     | 0.49              |
| 1:G:79:GLU:HG2     | 1:G:111:PHE:CZ     | 2.48                     | 0.49              |
| 1:G:672:ALA:CB     | 1:G:844:PRO:HG3    | 2.42                     | 0.49              |
| 1:G:695:VAL:HG11   | 1:G:701:ALA:CA     | 2.43                     | 0.49              |
| 2:H:310:GLN:OE1    | 2:H:312:HIS:NE2    | 2.46                     | 0.49              |
| 2:H:350:PHE:HD2    | 2:H:354:PRO:HD3    | 1.77                     | 0.49              |
| 1:A:150:HIS:N      | 1:A:154:GLU:OE2    | 2.30                     | 0.49              |
| 1:A:225:ASN:ND2    | 1:A:331:THR:HG21   | 2.28                     | 0.49              |
| 1:A:675:ARG:H      | 1:A:675:ARG:HD3    | 1.76                     | 0.49              |
| 1:A:1006:LYS:O     | 1:A:1006:LYS:HG3   | 2.12                     | 0.49              |
| 2:B:345:LYS:HB3    | 2:B:346:PRO:CD     | 2.43                     | 0.49              |
| 1:C:420:ALA:HA     | 1:C:423[A]:LYS:HD2 | 1.95                     | 0.49              |
| 1:E:967[A]:GLN:HG3 | 1:E:1054:LEU:HD13  | 1.94                     | 0.49              |
| 2:F:133:ILE:HG22   | 2:F:138:PRO:HB3    | 1.94                     | 0.49              |
| 1:E:58:PRO:HD2     | 1:E:59:GLU:OE2     | 2.13                     | 0.48              |
| 1:E:110:GLU:HG2    | 1:E:111:PHE:CD1    | 2.47                     | 0.48              |
| 1:E:493:LYS:HE2    | 1:E:517:ARG:CD     | 2.43                     | 0.48              |
| 1:E:693:ALA:CB     | 1:E:708:ILE:HD11   | 2.38                     | 0.48              |
| 2:F:170:TRP:HB3    | 2:F:216:LEU:HB2    | 1.95                     | 0.48              |
| 1:G:170:PRO:HA     | 1:G:204:LEU:HD23   | 1.94                     | 0.48              |
| 1:G:354:TYR:CD2    | 1:G:387:ILE:HG23   | 2.48                     | 0.48              |
| 1:G:1021:ARG:O     | 1:G:1025:ASP:OD2   | 2.31                     | 0.48              |
| 2:H:275:LEU:HD23   | 2:H:349:SER:HB3    | 1.95                     | 0.48              |
| 2:H:286:MET:HE3    | 2:H:315:ALA:HB2    | 1.95                     | 0.48              |
| 1:A:347:SER:O      | 2:B:296:PRO:HB3    | 2.12                     | 0.48              |
| 6:A:1083:CL:CL     | 11:A:1622:HOH:O    | 2.57                     | 0.48              |
| 1:G:315:THR:O      | 1:G:531:THR:HG22   | 2.12                     | 0.48              |
| 1:G:493:LYS:NZ     | 1:G:499:ASP:OD2    | 2.34                     | 0.48              |
| 2:H:298:LYS:O      | 2:H:329:HIS:HA     | 2.14                     | 0.48              |
| 1:A:65:TYR:OH      | 1:A:80[A]:LYS:HE3  | 2.14                     | 0.48              |
| 1:A:515:LYS:HG3    | 11:A:1774:HOH:O    | 2.12                     | 0.48              |
| 1:C:68:PRO:HG3     | 1:C:930:LYS:O      | 2.13                     | 0.48              |
| 1:C:479:VAL:HB     | 1:C:483:GLY:HA3    | 1.95                     | 0.48              |
| 1:C:527:LYS:HB2    | 1:C:544:TYR:CZ     | 2.48                     | 0.48              |
| 1:G:460:ARG:HG3    | 11:G:1283:HOH:O    | 2.11                     | 0.48              |
| 1:G:1000:HIS:HD2   | 1:G:1003:ASP:H     | 1.61                     | 0.48              |
| 2:H:355:GLU:OE2    | 2:H:355:GLU:N      | 2.42                     | 0.48              |
| 1:A:101:GLU:O      | 1:A:105:GLN:HG2    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:284:VAL:O     | 2:B:314:PHE:HA    | 2.14                     | 0.48              |
| 1:C:228:CYS:O     | 1:C:269:MET:HE1   | 2.14                     | 0.48              |
| 1:E:509:ARG:HH11  | 1:E:509:ARG:HB2   | 1.75                     | 0.48              |
| 1:E:636:LYS:HD3   | 11:E:1773:HOH:O   | 2.12                     | 0.48              |
| 1:E:853:VAL:O     | 1:E:857:THR:HG23  | 2.13                     | 0.48              |
| 1:C:751:LEU:O     | 1:C:752:LEU:HD12  | 2.13                     | 0.48              |
| 1:C:772:MET:HE2   | 1:C:880:THR:HA    | 1.96                     | 0.48              |
| 1:E:1004:ARG:NH1  | 1:E:1009:GLU:OE1  | 2.41                     | 0.48              |
| 2:H:43:LEU:HD21   | 2:H:80:LEU:HD13   | 1.95                     | 0.48              |
| 2:H:227:ASP:HA    | 2:H:230:LYS:HD2   | 1.95                     | 0.48              |
| 1:C:174:MET:HB3   | 11:C:1191:HOH:O   | 2.13                     | 0.48              |
| 1:C:361:ARG:NH2   | 1:C:571:ARG:HG2   | 2.28                     | 0.48              |
| 1:C:726:GLU:HG3   | 1:C:727:ILE:N     | 2.27                     | 0.48              |
| 2:D:187:GLU:HG2   | 2:D:215:ARG:HD2   | 1.96                     | 0.48              |
| 1:E:2:PRO:O       | 1:E:3:LYS:C       | 2.48                     | 0.48              |
| 1:E:128:ASP:OD1   | 1:E:130:ARG:HB3   | 2.14                     | 0.48              |
| 1:E:1021:ARG:HH11 | 1:E:1021:ARG:HG3  | 1.79                     | 0.48              |
| 2:F:45:ASP:OD2    | 2:F:46:PRO:HD2    | 2.13                     | 0.48              |
| 1:G:730:ASP:O     | 1:G:733:ASP:HB2   | 2.12                     | 0.48              |
| 1:A:775:ILE:HG13  | 1:A:810:ARG:HG2   | 1.94                     | 0.48              |
| 2:B:290:HIS:NE2   | 2:B:334:ASP:OD1   | 2.46                     | 0.48              |
| 1:C:626:VAL:O     | 1:C:630:VAL:HG23  | 2.13                     | 0.48              |
| 2:D:342:ARG:NH2   | 2:D:344:ASP:OD1   | 2.30                     | 0.48              |
| 1:E:35:LYS:O      | 1:E:39[B]:GLU:HB2 | 2.13                     | 0.48              |
| 2:F:25:SER:HA     | 2:F:132:ILE:O     | 2.14                     | 0.48              |
| 1:A:151:THR:OG1   | 1:A:154:GLU:HG3   | 2.13                     | 0.48              |
| 1:A:340:THR:O     | 1:A:343:ARG:HB2   | 2.14                     | 0.48              |
| 1:C:267:ALA:O     | 1:C:271:VAL:HG23  | 2.14                     | 0.48              |
| 1:C:784:GLN:O     | 1:C:784:GLN:HG2   | 2.13                     | 0.48              |
| 2:F:158:LEU:HD12  | 2:F:243:GLY:HA3   | 1.95                     | 0.48              |
| 2:B:50:ARG:HG2    | 2:B:158:LEU:HD22  | 1.95                     | 0.48              |
| 2:D:153:LEU:O     | 2:D:155:GLY:N     | 2.47                     | 0.48              |
| 2:F:6:LEU:HD21    | 2:F:140:ALA:HA    | 1.94                     | 0.48              |
| 2:F:263:ILE:HG22  | 2:F:264:PRO:CD    | 2.40                     | 0.48              |
| 1:G:183:TYR:HB2   | 1:G:187:GLU:OE1   | 2.14                     | 0.48              |
| 2:H:18:ARG:NH1    | 2:H:20:ILE:HG22   | 2.29                     | 0.48              |
| 2:H:295:HIS:NE2   | 2:H:333:PHE:HB2   | 2.29                     | 0.48              |
| 1:A:703:GLU:HA    | 1:A:703:GLU:OE2   | 2.14                     | 0.48              |
| 1:A:704:LYS:O     | 1:A:707:GLU:HB2   | 2.13                     | 0.48              |
| 2:D:154:ASN:ND2   | 2:D:314:PHE:HZ    | 2.12                     | 0.48              |
| 1:E:950:ARG:HH11  | 1:E:950:ARG:HD2   | 1.55                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:342:ARG:NH2  | 2:F:344:ASP:OD1  | 2.47                     | 0.48              |
| 1:G:530:ASP:C    | 1:G:531:THR:HG23 | 2.35                     | 0.48              |
| 1:G:563:MET:HB2  | 1:G:638:VAL:HG22 | 1.96                     | 0.48              |
| 1:G:1027:ARG:NE  | 1:G:1031:ARG:HD3 | 2.28                     | 0.48              |
| 1:A:509:ARG:HB2  | 1:A:509:ARG:CZ   | 2.44                     | 0.47              |
| 1:E:494:ARG:HG2  | 1:E:547:TYR:CB   | 2.44                     | 0.47              |
| 1:E:736:ARG:O    | 1:E:740:THR:HG23 | 2.13                     | 0.47              |
| 2:F:186:LYS:HB3  | 2:F:188:ASP:OD2  | 2.13                     | 0.47              |
| 2:H:237:PHE:CE2  | 2:H:239:SER:HA   | 2.48                     | 0.47              |
| 1:A:101:GLU:OE2  | 1:A:101:GLU:HA   | 2.14                     | 0.47              |
| 1:A:315:THR:O    | 1:A:531:THR:HG22 | 2.14                     | 0.47              |
| 2:F:68:ALA:HA    | 2:F:181:LEU:HD11 | 1.96                     | 0.47              |
| 1:G:563:MET:CB   | 1:G:638:VAL:HG22 | 2.44                     | 0.47              |
| 2:H:296:PRO:HB2  | 2:H:332:LEU:HB2  | 1.97                     | 0.47              |
| 1:A:361:ARG:CZ   | 1:A:571:ARG:HG2  | 2.45                     | 0.47              |
| 1:C:70:HIS:O     | 1:C:73:VAL:N     | 2.45                     | 0.47              |
| 1:C:130:ARG:HG3  | 1:C:148:ILE:HG13 | 1.96                     | 0.47              |
| 1:C:772:MET:CE   | 1:C:880:THR:HG22 | 2.44                     | 0.47              |
| 2:D:170:TRP:HB3  | 2:D:216:LEU:HB2  | 1.96                     | 0.47              |
| 2:H:32:PHE:O     | 2:H:291:HIS:HB2  | 2.15                     | 0.47              |
| 1:A:1:MET:HB2    | 1:A:224:LYS:HE3  | 1.95                     | 0.47              |
| 1:E:224:LYS:NZ   | 11:E:1624:HOH:O  | 2.42                     | 0.47              |
| 1:E:897:PHE:HB3  | 11:E:1557:HOH:O  | 2.14                     | 0.47              |
| 1:G:49:SER:O     | 1:G:51:PRO:HD3   | 2.15                     | 0.47              |
| 1:G:956:ARG:HB3  | 1:G:1044:LEU:CD2 | 2.44                     | 0.47              |
| 1:A:67:GLU:HB3   | 1:A:68:PRO:CD    | 2.45                     | 0.47              |
| 1:C:67:GLU:HB3   | 1:C:68:PRO:HD2   | 1.96                     | 0.47              |
| 1:C:860:PRO:HB2  | 1:C:863:LYS:HB2  | 1.97                     | 0.47              |
| 2:D:272:HIS:HA   | 2:D:349:SER:CB   | 2.44                     | 0.47              |
| 1:G:168:ILE:HG23 | 1:G:204:LEU:HD22 | 1.96                     | 0.47              |
| 1:G:349:GLU:O    | 2:H:294:ASN:HB2  | 2.15                     | 0.47              |
| 1:G:698:ILE:H    | 1:G:698:ILE:CD1  | 2.27                     | 0.47              |
| 1:G:943:GLY:O    | 1:G:969:PHE:HA   | 2.14                     | 0.47              |
| 2:H:325:LEU:HA   | 2:H:325:LEU:HD23 | 1.35                     | 0.47              |
| 1:A:548:GLU:OE1  | 2:B:114:ASP:HA   | 2.14                     | 0.47              |
| 1:A:947:LEU:HD12 | 1:A:947:LEU:N    | 2.30                     | 0.47              |
| 2:B:272:HIS:HA   | 2:B:349:SER:HB2  | 1.95                     | 0.47              |
| 2:D:197:TYR:HB3  | 2:D:199:PHE:CZ   | 2.50                     | 0.47              |
| 2:D:286:MET:HG2  | 11:D:2883:HOH:O  | 2.13                     | 0.47              |
| 2:D:316:VAL:HG12 | 2:D:337:LEU:CD2  | 2.44                     | 0.47              |
| 1:E:368:ALA:HA   | 11:E:1708:HOH:O  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:363:ALA:C    | 2:F:365:PRO:HD2   | 2.34                     | 0.47              |
| 1:G:772:MET:SD   | 1:G:880:THR:HG22  | 2.54                     | 0.47              |
| 2:H:251:ALA:O    | 2:H:255:ILE:HG13  | 2.15                     | 0.47              |
| 2:H:370:PHE:CZ   | 2:H:374:ILE:HD11  | 2.49                     | 0.47              |
| 1:A:950:ARG:HD3  | 11:A:1597:HOH:O   | 2.14                     | 0.47              |
| 2:B:48:TYR:HA    | 2:B:51:GLN:HE21   | 1.80                     | 0.47              |
| 2:B:291:HIS:HD2  | 2:B:311:ASN:OD1   | 1.98                     | 0.47              |
| 1:C:3:LYS:HB2    | 1:C:42:TYR:OH     | 2.15                     | 0.47              |
| 1:C:25:GLU:HG3   | 1:C:306:ARG:HA    | 1.96                     | 0.47              |
| 1:C:640:VAL:HG21 | 1:C:651:ALA:HB2   | 1.97                     | 0.47              |
| 1:C:676:GLU:O    | 1:C:680:HIS:ND1   | 2.48                     | 0.47              |
| 2:D:245:PRO:CG   | 2:D:274:LEU:HD21  | 2.44                     | 0.47              |
| 2:F:174:SER:HB2  | 2:F:211:ASP:OD2   | 2.13                     | 0.47              |
| 1:G:527:LYS:HB2  | 1:G:544:TYR:CZ    | 2.49                     | 0.47              |
| 1:G:675:ARG:CD   | 1:G:675:ARG:H     | 2.26                     | 0.47              |
| 1:G:947:LEU:HA   | 1:G:1014:ILE:HG23 | 1.95                     | 0.47              |
| 2:H:45:ASP:OD2   | 2:H:46:PRO:HD2    | 2.14                     | 0.47              |
| 2:H:55:LEU:HD13  | 2:H:60:ILE:HD12   | 1.95                     | 0.47              |
| 2:H:363:ALA:HB1  | 2:H:366:LEU:HD13  | 1.97                     | 0.47              |
| 1:A:259:LYS:HD3  | 2:B:175:TRP:CE3   | 2.50                     | 0.47              |
| 1:C:124:ASP:OD1  | 1:C:131:ARG:HD3   | 2.15                     | 0.47              |
| 2:D:205:ILE:HG21 | 2:D:237:PHE:CZ    | 2.49                     | 0.47              |
| 1:E:144:ALA:HB1  | 1:E:208:GLU:HG2   | 1.96                     | 0.47              |
| 2:F:298:LYS:HG2  | 2:F:299:ASP:N     | 2.30                     | 0.47              |
| 1:G:670:ASP:HB3  | 1:G:677:ARG:NH2   | 2.29                     | 0.47              |
| 1:G:699:GLU:OE2  | 1:G:699:GLU:HA    | 2.15                     | 0.47              |
| 1:A:767:ILE:HD13 | 1:A:865:ALA:HB2   | 1.97                     | 0.47              |
| 1:C:75:ARG:HG3   | 1:C:107:VAL:CG1   | 2.45                     | 0.47              |
| 1:C:158:VAL:HG11 | 1:C:206:ILE:HB    | 1.96                     | 0.47              |
| 1:C:702:VAL:CG1  | 1:C:731:GLU:HG3   | 2.45                     | 0.47              |
| 1:C:773:VAL:HG23 | 1:C:818:PHE:CZ    | 2.50                     | 0.47              |
| 1:C:1018:SER:O   | 1:C:1022:ALA:HB3  | 2.14                     | 0.47              |
| 1:E:836:GLU:HB2  | 1:E:838:TYR:CE2   | 2.50                     | 0.47              |
| 2:F:187:GLU:CG   | 2:F:215:ARG:HD2   | 2.43                     | 0.47              |
| 2:H:111:ALA:O    | 2:H:112:ASP:HB2   | 2.15                     | 0.47              |
| 2:H:267:GLY:O    | 2:H:349:SER:HA    | 2.14                     | 0.47              |
| 1:A:692:ASN:HA   | 1:A:752:LEU:O     | 2.15                     | 0.47              |
| 1:C:695:VAL:HG23 | 1:C:752:LEU:HD22  | 1.97                     | 0.47              |
| 1:E:1051:ALA:HA  | 1:E:1054:LEU:HD12 | 1.96                     | 0.47              |
| 2:F:55:LEU:HD13  | 2:F:60:ILE:HD12   | 1.95                     | 0.47              |
| 1:G:185:ARG:O    | 1:G:188:PHE:HB3   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:G:1004:ARG:O   | 1:G:1009[B]:GLU:HB2 | 2.14                     | 0.47              |
| 1:A:612:THR:HG22 | 1:A:612:THR:O       | 2.15                     | 0.46              |
| 2:B:209:LEU:HD23 | 2:B:209:LEU:HA      | 1.81                     | 0.46              |
| 1:E:1019:GLY:O   | 1:E:1023:ILE:HG13   | 2.15                     | 0.46              |
| 2:H:318:GLU:HG2  | 2:H:318:GLU:O       | 2.14                     | 0.46              |
| 2:D:98:LEU:HD12  | 2:D:98:LEU:O        | 2.16                     | 0.46              |
| 1:E:109:GLU:O    | 1:E:110:GLU:C       | 2.50                     | 0.46              |
| 1:E:481:ILE:HG23 | 1:E:482:THR:N       | 2.29                     | 0.46              |
| 2:F:324:ASN:ND2  | 2:F:324:ASN:H       | 2.07                     | 0.46              |
| 1:G:90:MET:HA    | 1:G:304:VAL:HG22    | 1.96                     | 0.46              |
| 1:G:423:LYS:H    | 1:G:423:LYS:HG3     | 1.50                     | 0.46              |
| 1:G:435:ARG:O    | 1:G:436:ILE:C       | 2.52                     | 0.46              |
| 1:A:514:ARG:HD3  | 11:A:1461:HOH:O     | 2.14                     | 0.46              |
| 1:C:532:CYS:O    | 1:C:533:ALA:HB3     | 2.16                     | 0.46              |
| 1:G:103:GLU:HG3  | 1:G:104:ARG:N       | 2.19                     | 0.46              |
| 1:G:131:ARG:HD2  | 11:G:1750:HOH:O     | 2.15                     | 0.46              |
| 2:D:252:ILE:HD13 | 2:D:277:LEU:HB3     | 1.97                     | 0.46              |
| 2:D:376:GLN:HA   | 2:D:379:LYS:NZ      | 2.30                     | 0.46              |
| 2:H:254:ALA:O    | 2:H:257:LYS:HB2     | 2.15                     | 0.46              |
| 2:H:301:GLU:OE1  | 2:H:328:THR:HG22    | 2.15                     | 0.46              |
| 1:A:992:ASN:HB2  | 1:A:999:PRO:O       | 2.14                     | 0.46              |
| 1:E:998:ARG:HA   | 1:E:999:PRO:C       | 2.33                     | 0.46              |
| 2:F:379:LYS:NZ   | 2:F:379:LYS:HB2     | 2.30                     | 0.46              |
| 1:G:486:ALA:HB2  | 1:G:520:TYR:CG      | 2.51                     | 0.46              |
| 1:G:734:LEU:HD11 | 1:G:738:PHE:HE2     | 1.79                     | 0.46              |
| 1:A:972:ASP:OD1  | 1:A:989:ARG:HB3     | 2.15                     | 0.46              |
| 2:B:41:GLU:HG3   | 2:B:69:ASP:O        | 2.16                     | 0.46              |
| 2:D:263:ILE:CG2  | 2:D:264:PRO:HD2     | 2.42                     | 0.46              |
| 1:G:124:ASP:OD1  | 1:G:131:ARG:HD3     | 2.16                     | 0.46              |
| 1:G:484:LEU:HD22 | 1:G:489:LEU:HD13    | 1.98                     | 0.46              |
| 1:G:665:SER:HB2  | 11:G:1668:HOH:O     | 2.16                     | 0.46              |
| 1:G:726:GLU:OE1  | 1:G:1020:ARG:NE     | 2.36                     | 0.46              |
| 1:A:693:ALA:CB   | 1:A:708:ILE:HD11    | 2.45                     | 0.46              |
| 1:A:805:ILE:HG22 | 1:A:806:GLN:N       | 2.29                     | 0.46              |
| 1:C:119:THR:O    | 1:C:120:ALA:C       | 2.53                     | 0.46              |
| 1:E:176:GLY:N    | 7:E:1089:ADP:O2B    | 2.41                     | 0.46              |
| 1:E:318:PRO:HB2  | 1:E:321:LYS:HB2     | 1.97                     | 0.46              |
| 1:G:685:LEU:O    | 1:G:686:LYS:HB2     | 2.15                     | 0.46              |
| 2:H:10:GLU:O     | 2:H:12:GLY:N        | 2.48                     | 0.46              |
| 2:B:46:PRO:HA    | 2:B:76:HIS:CB       | 2.46                     | 0.46              |
| 1:C:236:ASN:N    | 1:C:236:ASN:HD22    | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:286:MET:HE1  | 2:D:315:ALA:HB2  | 1.98                     | 0.46              |
| 2:D:331:SER:O    | 2:D:335:GLY:HA2  | 2.15                     | 0.46              |
| 1:E:28:TYR:CZ    | 1:E:313:LYS:HE3  | 2.51                     | 0.46              |
| 1:G:625:ASP:O    | 1:G:629:ILE:HG13 | 2.15                     | 0.46              |
| 1:A:157:ALA:O    | 1:A:160:ALA:HB3  | 2.16                     | 0.46              |
| 1:A:992:ASN:ND2  | 1:G:975:HIS:HE2  | 2.14                     | 0.46              |
| 2:B:286:MET:CE   | 2:B:312:HIS:ND1  | 2.79                     | 0.46              |
| 1:C:782:ILE:HD13 | 1:C:793:ALA:C    | 2.36                     | 0.46              |
| 1:E:783:GLU:OE1  | 8:E:1091:ORN:NE  | 2.49                     | 0.46              |
| 1:G:734:LEU:CD1  | 1:G:738:PHE:CE2  | 2.99                     | 0.46              |
| 8:G:1091:ORN:N   | 11:G:1554:HOH:O  | 2.36                     | 0.46              |
| 2:H:45:ASP:HB3   | 2:H:48:TYR:CD2   | 2.50                     | 0.46              |
| 2:H:169:SER:HA   | 2:H:216:LEU:O    | 2.16                     | 0.46              |
| 2:H:364:ALA:O    | 2:H:366:LEU:N    | 2.48                     | 0.46              |
| 1:A:367:PHE:HB3  | 1:A:903:VAL:HG21 | 1.98                     | 0.46              |
| 2:D:154:ASN:ND2  | 2:D:314:PHE:CZ   | 2.84                     | 0.46              |
| 2:D:364:ALA:N    | 2:D:365:PRO:CD   | 2.79                     | 0.46              |
| 1:E:169:ARG:HG2  | 11:E:1874:HOH:O  | 2.15                     | 0.46              |
| 1:G:417:ASP:HB3  | 1:G:420:ALA:HB2  | 1.97                     | 0.46              |
| 1:G:674:ASP:HB3  | 1:G:677:ARG:HG3  | 1.98                     | 0.46              |
| 1:G:806:GLN:HB3  | 1:G:810:ARG:NH1  | 2.31                     | 0.46              |
| 2:H:27:VAL:O     | 2:H:78:GLN:HG2   | 2.16                     | 0.46              |
| 2:H:344:ASP:OD2  | 2:H:345:LYS:N    | 2.48                     | 0.46              |
| 1:A:585:ALA:HB2  | 1:A:642:TYR:CE2  | 2.52                     | 0.45              |
| 2:B:263:ILE:HG22 | 2:B:264:PRO:CD   | 2.45                     | 0.45              |
| 1:C:11:LEU:HA    | 1:C:45:ILE:O     | 2.17                     | 0.45              |
| 2:D:286:MET:CE   | 2:D:312:HIS:ND1  | 2.79                     | 0.45              |
| 1:G:597:ILE:HA   | 1:G:615:ARG:O    | 2.15                     | 0.45              |
| 2:H:218:ILE:N    | 2:H:218:ILE:CD1  | 2.79                     | 0.45              |
| 2:B:364:ALA:N    | 2:B:365:PRO:CD   | 2.79                     | 0.45              |
| 1:C:891:LYS:HG2  | 1:C:892:GLU:N    | 2.30                     | 0.45              |
| 2:D:286:MET:HE1  | 2:D:312:HIS:ND1  | 2.31                     | 0.45              |
| 1:E:489:LEU:HD22 | 1:E:516:LEU:HD23 | 1.98                     | 0.45              |
| 1:E:579:ASP:OD1  | 1:E:605:THR:HB   | 2.16                     | 0.45              |
| 2:F:222:GLN:HB2  | 11:F:1487:HOH:O  | 2.16                     | 0.45              |
| 1:G:775:ILE:CD1  | 1:G:813:VAL:HG11 | 2.46                     | 0.45              |
| 2:H:8:VAL:CG1    | 2:H:9:LEU:N      | 2.80                     | 0.45              |
| 2:H:153:LEU:O    | 2:H:154:ASN:C    | 2.54                     | 0.45              |
| 1:A:671:ARG:CG   | 1:A:677:ARG:NH1  | 2.80                     | 0.45              |
| 2:B:205:ILE:HG13 | 2:B:355:GLU:CG   | 2.46                     | 0.45              |
| 1:C:726:GLU:CG   | 1:C:727:ILE:N    | 2.79                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:383:GLU:OE2   | 1:E:604:GLU:OE1  | 2.34                     | 0.45              |
| 1:G:339:ILE:O     | 1:G:538:THR:OG1  | 2.29                     | 0.45              |
| 1:G:688:LYS:HD2   | 1:G:838:TYR:CE1  | 2.52                     | 0.45              |
| 2:H:11:ASP:OD2    | 2:H:13:THR:OG1   | 2.30                     | 0.45              |
| 2:H:272:HIS:CA    | 2:H:349:SER:HB2  | 2.41                     | 0.45              |
| 1:A:3:LYS:HB3     | 1:A:330:TYR:CE1  | 2.52                     | 0.45              |
| 1:A:38:ARG:HH11   | 1:A:38:ARG:CG    | 2.12                     | 0.45              |
| 1:C:220:VAL:O     | 1:C:281:GLY:HA2  | 2.16                     | 0.45              |
| 2:F:272:HIS:HA    | 2:F:349:SER:OG   | 2.15                     | 0.45              |
| 1:G:502:LEU:O     | 1:G:505:LEU:HB2  | 2.17                     | 0.45              |
| 2:H:50:ARG:HH12   | 2:H:156:MET:CE   | 2.30                     | 0.45              |
| 2:H:246:ALA:O     | 2:H:248:ASP:N    | 2.50                     | 0.45              |
| 2:H:352:GLY:O     | 2:H:354:PRO:HD3  | 2.16                     | 0.45              |
| 2:H:364:ALA:N     | 2:H:365:PRO:HD2  | 2.31                     | 0.45              |
| 1:A:286:PHE:CD1   | 1:A:295:LEU:HD11 | 2.51                     | 0.45              |
| 1:A:695:VAL:CG1   | 1:A:696:THR:N    | 2.80                     | 0.45              |
| 1:G:102:LEU:HD23  | 1:G:102:LEU:HA   | 1.82                     | 0.45              |
| 1:G:770:GLY:CA    | 1:G:823:ARG:NH1  | 2.80                     | 0.45              |
| 1:G:941:LYS:HE3   | 11:G:1704:HOH:O  | 2.15                     | 0.45              |
| 2:H:284:VAL:O     | 2:H:315:ALA:N    | 2.45                     | 0.45              |
| 1:A:644:GLY:O     | 1:A:647:PRO:HD2  | 2.17                     | 0.45              |
| 1:A:947:LEU:N     | 1:A:947:LEU:CD1  | 2.80                     | 0.45              |
| 1:C:103:GLU:HG3   | 1:C:104:ARG:N    | 2.31                     | 0.45              |
| 1:C:103:GLU:HB2   | 1:C:108:LEU:HD12 | 1.99                     | 0.45              |
| 1:C:176:GLY:HA3   | 1:C:377:GLN:HA   | 1.98                     | 0.45              |
| 1:C:577:GLU:O     | 1:C:580:TYR:HB3  | 2.17                     | 0.45              |
| 1:C:802:SER:OG    | 1:C:805:ILE:HB   | 2.16                     | 0.45              |
| 1:C:865:ALA:O     | 1:C:869:MET:HG3  | 2.16                     | 0.45              |
| 1:C:1001:ILE:HD11 | 11:C:1576:HOH:O  | 2.16                     | 0.45              |
| 2:D:316:VAL:HB    | 2:D:337:LEU:HD23 | 1.97                     | 0.45              |
| 2:H:350:PHE:CD1   | 2:H:366:LEU:HD21 | 2.51                     | 0.45              |
| 2:B:224:SER:O     | 2:B:225:ALA:C    | 2.51                     | 0.45              |
| 1:C:695:VAL:CG1   | 1:C:696:THR:N    | 2.80                     | 0.45              |
| 1:C:1064:SER:O    | 1:C:1068:MET:HG3 | 2.17                     | 0.45              |
| 1:E:141:LEU:HD23  | 1:E:141:LEU:HA   | 1.69                     | 0.45              |
| 1:E:963:LYS:O     | 1:E:964:LEU:C    | 2.53                     | 0.45              |
| 1:E:1021:ARG:O    | 1:E:1025:ASP:OD2 | 2.34                     | 0.45              |
| 2:F:272:HIS:HA    | 2:F:349:SER:CB   | 2.47                     | 0.45              |
| 1:G:813:VAL:HA    | 1:G:816:LEU:HD12 | 1.98                     | 0.45              |
| 2:H:121:LEU:HD11  | 2:H:125:LYS:HD3  | 1.99                     | 0.45              |
| 1:A:223:ASP:CG    | 1:A:227:ASN:HB2  | 2.36                     | 0.45              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:481:ILE:HG22 | 11:A:1762:HOH:O    | 2.16                     | 0.45              |
| 1:C:213:TRP:HH2  | 1:C:294:ARG:HD2    | 1.82                     | 0.45              |
| 1:C:344:THR:HB   | 1:C:345:PRO:CD     | 2.47                     | 0.45              |
| 1:C:1013:ILE:O   | 1:C:1040:TYR:HA    | 2.17                     | 0.45              |
| 2:F:82:ILE:O     | 2:F:111:ALA:HA     | 2.17                     | 0.45              |
| 2:F:223:THR:CG2  | 2:F:228:VAL:HG23   | 2.47                     | 0.45              |
| 1:G:254:GLN:NE2  | 2:H:57:TYR:OH      | 2.50                     | 0.45              |
| 2:H:23:THR:HG22  | 2:H:24:GLY:N       | 2.31                     | 0.45              |
| 1:A:35:LYS:HA    | 11:A:1142:HOH:O    | 2.17                     | 0.45              |
| 2:B:6:LEU:HD12   | 2:B:7:LEU:H        | 1.81                     | 0.45              |
| 2:B:369:HIS:O    | 2:B:373:LEU:HG     | 2.16                     | 0.45              |
| 1:E:726:GLU:CG   | 1:E:727:ILE:N      | 2.80                     | 0.45              |
| 2:F:111:ALA:O    | 2:F:112:ASP:HB2    | 2.17                     | 0.45              |
| 1:G:333:ASP:OD1  | 1:G:333:ASP:N      | 2.49                     | 0.45              |
| 1:G:703:GLU:O    | 1:G:706:LYS:HB2    | 2.17                     | 0.45              |
| 1:G:883:VAL:CG1  | 1:G:884:ILE:N      | 2.80                     | 0.45              |
| 2:H:153:LEU:N    | 2:H:153:LEU:CD1    | 2.79                     | 0.45              |
| 2:H:274:LEU:O    | 2:H:275:LEU:C      | 2.55                     | 0.45              |
| 1:A:167:ILE:N    | 1:A:167:ILE:CD1    | 2.80                     | 0.45              |
| 1:A:882:GLU:HB3  | 11:A:1828:HOH:O    | 2.17                     | 0.45              |
| 1:C:735:ARG:O    | 1:C:738:PHE:HB2    | 2.17                     | 0.45              |
| 2:D:50:ARG:NH1   | 2:D:156:MET:CE     | 2.80                     | 0.45              |
| 1:E:282:SER:OG   | 1:E:302:PRO:HA     | 2.17                     | 0.45              |
| 2:F:364:ALA:N    | 2:F:365:PRO:CD     | 2.80                     | 0.45              |
| 1:G:65:TYR:CE2   | 1:G:77:ILE:HG23    | 2.52                     | 0.45              |
| 1:G:265:ARG:O    | 1:G:269:MET:HG3    | 2.16                     | 0.45              |
| 2:H:232:ASN:N    | 2:H:233:PRO:CD     | 2.80                     | 0.45              |
| 1:A:148:ILE:CG2  | 1:A:149:ALA:N      | 2.80                     | 0.44              |
| 2:B:83:ARG:HG3   | 2:B:83:ARG:NH1     | 2.32                     | 0.44              |
| 1:C:419:GLU:CB   | 1:C:423[B]:LYS:HZ3 | 2.29                     | 0.44              |
| 2:D:232:ASN:N    | 2:D:233:PRO:HD3    | 2.33                     | 0.44              |
| 2:F:225:ALA:HB2  | 2:F:254:ALA:HB1    | 1.99                     | 0.44              |
| 1:G:561:LYS:HG2  | 1:G:595:GLU:OE2    | 2.17                     | 0.44              |
| 2:H:364:ALA:N    | 2:H:365:PRO:CD     | 2.80                     | 0.44              |
| 1:A:76:LYS:HA    | 1:A:76:LYS:HD2     | 1.80                     | 0.44              |
| 1:A:82:ARG:N     | 1:A:83:PRO:CD      | 2.81                     | 0.44              |
| 1:A:526:TYR:CE1  | 1:A:545:SER:HB3    | 2.52                     | 0.44              |
| 2:B:199:PHE:HB3  | 2:B:270:LEU:HD23   | 1.99                     | 0.44              |
| 2:B:350:PHE:CG   | 2:B:366:LEU:CD2    | 3.00                     | 0.44              |
| 1:E:730:ASP:OD2  | 1:E:733:ASP:HB2    | 2.17                     | 0.44              |
| 1:E:1028:VAL:CG1 | 1:E:1029:ILE:N     | 2.79                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:299:ASP:OD1  | 2:F:302:LYS:HD2   | 2.17                     | 0.44              |
| 1:G:866:ALA:O    | 1:G:869:MET:HB2   | 2.17                     | 0.44              |
| 1:G:1021:ARG:CG  | 1:G:1021:ARG:NH1  | 2.80                     | 0.44              |
| 2:H:18:ARG:NH1   | 11:H:502:HOH:O    | 2.50                     | 0.44              |
| 2:H:246:ALA:C    | 2:H:248:ASP:H     | 2.21                     | 0.44              |
| 2:H:281:ALA:HB2  | 2:H:322:PRO:HD3   | 2.00                     | 0.44              |
| 1:A:34:CYS:SG    | 1:A:46:LEU:HD22   | 2.58                     | 0.44              |
| 2:B:272:HIS:HA   | 2:B:349:SER:CB    | 2.48                     | 0.44              |
| 1:E:148:ILE:CG2  | 1:E:149:ALA:N     | 2.80                     | 0.44              |
| 2:F:332:LEU:HA   | 2:F:332:LEU:HD12  | 1.59                     | 0.44              |
| 1:G:436:ILE:HG22 | 11:G:1304:HOH:O   | 2.16                     | 0.44              |
| 1:G:730:ASP:H    | 1:G:733:ASP:HB2   | 1.83                     | 0.44              |
| 2:H:50:ARG:NH1   | 2:H:156:MET:CE    | 2.80                     | 0.44              |
| 2:H:286:MET:CE   | 2:H:312:HIS:CE1   | 3.00                     | 0.44              |
| 2:B:149:ALA:O    | 2:B:151:PRO:HD3   | 2.17                     | 0.44              |
| 2:B:176:THR:O    | 2:B:180:GLY:N     | 2.39                     | 0.44              |
| 2:B:354:PRO:HB2  | 2:B:367:PHE:CE2   | 2.53                     | 0.44              |
| 1:C:659:VAL:HG13 | 1:C:660:PRO:HD2   | 2.00                     | 0.44              |
| 1:C:736:ARG:CZ   | 1:C:736:ARG:HB3   | 2.47                     | 0.44              |
| 1:E:692:ASN:HA   | 1:E:752:LEU:O     | 2.17                     | 0.44              |
| 1:E:734:LEU:O    | 1:E:737:TYR:HB3   | 2.16                     | 0.44              |
| 1:G:473:GLU:HG2  | 1:G:505:LEU:HD11  | 1.98                     | 0.44              |
| 1:G:1026:SER:HB2 | 1:G:1030:ARG:HH12 | 1.82                     | 0.44              |
| 1:A:702:VAL:O    | 1:A:706:LYS:HD3   | 2.17                     | 0.44              |
| 1:C:464:VAL:HG21 | 2:D:88:ILE:HG12   | 2.00                     | 0.44              |
| 1:C:620:PRO:O    | 1:C:625:ASP:HB2   | 2.18                     | 0.44              |
| 2:D:205:ILE:HG21 | 2:D:237:PHE:CE2   | 2.52                     | 0.44              |
| 2:D:212:ARG:HG3  | 2:D:212:ARG:HH11  | 1.83                     | 0.44              |
| 1:E:344:THR:HB   | 1:E:345:PRO:CD    | 2.46                     | 0.44              |
| 1:E:588:ALA:HB2  | 1:E:863:LYS:HG2   | 1.99                     | 0.44              |
| 1:E:755:PHE:CE1  | 7:E:1090:ADP:C2   | 3.05                     | 0.44              |
| 2:F:172:GLN:HG2  | 2:F:173:GLY:N     | 2.29                     | 0.44              |
| 1:G:70:HIS:HE1   | 1:G:72:GLU:HG3    | 1.82                     | 0.44              |
| 1:G:796:LEU:HD23 | 1:G:797:PRO:CA    | 2.48                     | 0.44              |
| 1:A:735:ARG:O    | 1:A:736:ARG:C     | 2.54                     | 0.44              |
| 2:D:6:LEU:HD21   | 2:D:140:ALA:HB2   | 1.99                     | 0.44              |
| 2:D:342:ARG:HE   | 2:D:344:ASP:CG    | 2.19                     | 0.44              |
| 1:E:222:ARG:NE   | 1:E:226:ASP:OD2   | 2.49                     | 0.44              |
| 1:E:784:GLN:H    | 1:E:784:GLN:HE21  | 1.66                     | 0.44              |
| 2:F:23:THR:CG2   | 2:F:24:GLY:N      | 2.81                     | 0.44              |
| 2:F:150:PHE:HA   | 2:F:151:PRO:HD2   | 1.88                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:F:352:GLY:O      | 2:F:354:PRO:HD3   | 2.17                     | 0.44              |
| 2:F:365:PRO:O      | 2:F:368:ASP:N     | 2.49                     | 0.44              |
| 1:G:45:ILE:HA      | 1:G:63:ALA:O      | 2.18                     | 0.44              |
| 1:G:412:LYS:HE2    | 1:G:434:ASP:CG    | 2.37                     | 0.44              |
| 2:H:120:ARG:HD2    | 11:H:413:HOH:O    | 2.18                     | 0.44              |
| 2:H:153:LEU:CD1    | 2:H:153:LEU:H     | 2.30                     | 0.44              |
| 1:A:331:THR:OG1    | 1:A:334:GLU:HG3   | 2.18                     | 0.44              |
| 1:A:560:GLU:OE1    | 1:A:636:LYS:HD2   | 2.18                     | 0.44              |
| 1:A:703:GLU:OE2    | 1:A:706:LYS:NZ    | 2.36                     | 0.44              |
| 2:B:342:ARG:HD2    | 2:B:342:ARG:HA    | 1.88                     | 0.44              |
| 2:B:350:PHE:CG     | 2:B:366:LEU:HD22  | 2.53                     | 0.44              |
| 1:C:1:MET:O        | 1:C:334:GLU:OE1   | 2.36                     | 0.44              |
| 2:D:332:LEU:HA     | 2:D:332:LEU:HD12  | 1.68                     | 0.44              |
| 1:E:755:PHE:CD1    | 7:E:1090:ADP:C2   | 3.06                     | 0.44              |
| 1:G:1052:MET:O     | 1:G:1055:ASN:HB2  | 2.18                     | 0.44              |
| 2:H:50:ARG:HH12    | 2:H:156:MET:HE1   | 1.82                     | 0.44              |
| 1:A:250:VAL:HA     | 1:A:356:VAL:O     | 2.18                     | 0.44              |
| 1:A:900:PHE:N      | 1:A:901:PRO:HD3   | 2.33                     | 0.44              |
| 1:A:994:VAL:CG2    | 1:A:1001:ILE:HD11 | 2.48                     | 0.44              |
| 2:B:29:GLU:HB2     | 2:B:153:LEU:HD22  | 1.99                     | 0.44              |
| 2:H:50:ARG:NH1     | 2:H:156:MET:HE2   | 2.33                     | 0.44              |
| 2:H:104:ARG:HG2    | 2:H:105:HIS:HD2   | 1.82                     | 0.44              |
| 1:C:60[A]:MET:HE2  | 11:C:1495:HOH:O   | 2.17                     | 0.44              |
| 1:C:221:VAL:O      | 1:C:228:CYS:HA    | 2.17                     | 0.44              |
| 1:C:361:ARG:CZ     | 1:C:571:ARG:HG2   | 2.48                     | 0.44              |
| 2:D:379:LYS:HB3    | 2:D:379:LYS:HE2   | 1.75                     | 0.44              |
| 1:G:35:LYS:HD2     | 11:G:1144:HOH:O   | 2.17                     | 0.44              |
| 1:G:670:ASP:HB3    | 1:G:677:ARG:HH21  | 1.83                     | 0.44              |
| 1:G:713:VAL:HG23   | 1:G:755:PHE:HB2   | 2.00                     | 0.44              |
| 1:G:796:LEU:HD23   | 1:G:796:LEU:C     | 2.38                     | 0.44              |
| 1:G:873:SER:OG     | 1:G:876:GLU:HB2   | 2.18                     | 0.44              |
| 1:G:1027:ARG:HE    | 1:G:1031:ARG:CD   | 2.29                     | 0.44              |
| 2:H:350:PHE:CG     | 2:H:366:LEU:CD2   | 3.01                     | 0.44              |
| 1:A:1001:ILE:HD12  | 1:A:1002:GLN:CB   | 2.47                     | 0.43              |
| 2:B:228:VAL:HA     | 2:B:231:MET:HE3   | 2.00                     | 0.43              |
| 2:B:244:ASP:OD2    | 2:B:245:PRO:HD2   | 2.18                     | 0.43              |
| 1:C:82:ARG:N       | 1:C:83:PRO:CD     | 2.80                     | 0.43              |
| 1:C:894:VAL:O      | 1:C:913:SER:HB2   | 2.17                     | 0.43              |
| 1:E:691:ALA:CB     | 1:E:708:ILE:HG23  | 2.47                     | 0.43              |
| 1:E:967[B]:GLN:NE2 | 1:E:1054:LEU:CD1  | 2.78                     | 0.43              |
| 2:F:223:THR:HG22   | 2:F:228:VAL:HG23  | 1.98                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:245:PRO:CG   | 2:F:274:LEU:HD21 | 2.48                     | 0.43              |
| 1:G:664:THR:HG22 | 1:G:668:ALA:HB3  | 2.00                     | 0.43              |
| 2:H:27:VAL:HG21  | 2:H:146:LYS:HB3  | 2.00                     | 0.43              |
| 2:B:58:PRO:HA    | 2:B:83:ARG:HB3   | 2.00                     | 0.43              |
| 1:C:24:CYS:CB    | 1:C:576:ILE:HD12 | 2.48                     | 0.43              |
| 1:C:695:VAL:HG12 | 1:C:696:THR:N    | 2.33                     | 0.43              |
| 1:C:981:LEU:HD12 | 1:C:988:PRO:HG3  | 1.99                     | 0.43              |
| 2:D:244:ASP:OD2  | 2:D:245:PRO:HD2  | 2.18                     | 0.43              |
| 1:E:711:PRO:HG2  | 1:E:755:PHE:HD2  | 1.83                     | 0.43              |
| 2:F:48:TYR:HA    | 2:F:51:GLN:NE2   | 2.30                     | 0.43              |
| 1:G:530:ASP:O    | 1:G:531:THR:OG1  | 2.29                     | 0.43              |
| 1:G:560:GLU:OE1  | 1:G:636:LYS:HE3  | 2.17                     | 0.43              |
| 1:G:738:PHE:HA   | 1:G:741:ALA:HB3  | 2.00                     | 0.43              |
| 1:G:762:VAL:CG1  | 1:G:763:ASP:N    | 2.81                     | 0.43              |
| 9:G:1092:NET:H22 | 9:G:1092:NET:C4  | 2.43                     | 0.43              |
| 1:A:45:ILE:HD13  | 1:A:81:GLU:HB3   | 2.01                     | 0.43              |
| 1:A:145:ARG:HB3  | 1:A:208:GLU:CD   | 2.39                     | 0.43              |
| 1:A:235:GLU:HB2  | 1:A:253:ALA:HA   | 2.01                     | 0.43              |
| 1:A:571:ARG:NH2  | 11:A:1415:HOH:O  | 2.27                     | 0.43              |
| 2:B:307:ILE:N    | 2:B:307:ILE:HD13 | 2.33                     | 0.43              |
| 1:C:701:ALA:O    | 1:C:705:ALA:N    | 2.40                     | 0.43              |
| 1:C:702:VAL:HG11 | 1:C:735:ARG:HH21 | 1.79                     | 0.43              |
| 2:D:43:LEU:HD21  | 2:D:80:LEU:HD13  | 2.00                     | 0.43              |
| 1:E:533:ALA:O    | 1:E:534:ALA:HB3  | 2.18                     | 0.43              |
| 1:E:936:ASN:ND2  | 11:E:1156:HOH:O  | 2.52                     | 0.43              |
| 1:G:257:THR:O    | 1:G:258:ASP:C    | 2.56                     | 0.43              |
| 1:G:1000:HIS:NE2 | 1:G:1002:GLN:HB3 | 2.34                     | 0.43              |
| 2:H:195:VAL:HG11 | 2:H:228:VAL:HG13 | 1.99                     | 0.43              |
| 2:H:270:LEU:HA   | 2:H:270:LEU:HD12 | 1.57                     | 0.43              |
| 2:B:150:PHE:CD2  | 2:B:151:PRO:HD2  | 2.53                     | 0.43              |
| 1:C:704:LYS:O    | 1:C:707:GLU:HB2  | 2.19                     | 0.43              |
| 1:C:735:ARG:O    | 1:C:738:PHE:N    | 2.50                     | 0.43              |
| 9:C:1092:NET:H83 | 9:C:1092:NET:H11 | 1.80                     | 0.43              |
| 2:D:364:ALA:N    | 2:D:365:PRO:HD2  | 2.34                     | 0.43              |
| 2:F:195:VAL:HG21 | 2:F:231:MET:HE3  | 2.00                     | 0.43              |
| 1:G:178:GLY:CA   | 1:G:198:LEU:HD23 | 2.48                     | 0.43              |
| 1:G:488:PHE:O    | 1:G:489:LEU:C    | 2.55                     | 0.43              |
| 1:G:692:ASN:C    | 1:G:708:ILE:HD11 | 2.39                     | 0.43              |
| 1:G:709:GLY:O    | 1:G:754:HIS:ND1  | 2.50                     | 0.43              |
| 2:H:132:ILE:CG2  | 2:H:133:ILE:N    | 2.81                     | 0.43              |
| 2:H:193:HIS:O    | 2:H:234:ASP:HB2  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:426:ARG:HD3  | 1:A:426:ARG:C     | 2.39                     | 0.43              |
| 1:C:424:ILE:HD13 | 1:C:424:ILE:HG21  | 1.83                     | 0.43              |
| 1:C:693:ALA:HB3  | 1:C:752:LEU:HB2   | 2.01                     | 0.43              |
| 2:D:74:GLN:HB2   | 11:D:2853:HOH:O   | 2.18                     | 0.43              |
| 2:D:199:PHE:CE2  | 2:D:274:LEU:HD12  | 2.53                     | 0.43              |
| 2:D:354:PRO:HB2  | 2:D:367:PHE:CE2   | 2.54                     | 0.43              |
| 1:E:831:ALA:HB2  | 1:E:840:ILE:HD11  | 2.01                     | 0.43              |
| 1:E:949:VAL:O    | 1:E:954:LYS:NZ    | 2.41                     | 0.43              |
| 2:F:190:LEU:HA   | 2:F:191:PRO:HD2   | 1.80                     | 0.43              |
| 2:H:16:HIS:CD2   | 2:H:16:HIS:N      | 2.86                     | 0.43              |
| 2:H:199:PHE:CE2  | 2:H:274:LEU:CD1   | 3.02                     | 0.43              |
| 2:H:354:PRO:HB3  | 2:H:363:ALA:O     | 2.17                     | 0.43              |
| 1:A:740:THR:H    | 1:A:740:THR:HG23  | 1.51                     | 0.43              |
| 1:A:784:GLN:HE22 | 1:A:1043:THR:HB   | 1.83                     | 0.43              |
| 2:D:350:PHE:HB2  | 2:D:366:LEU:CD2   | 2.48                     | 0.43              |
| 1:E:563:MET:CE   | 1:E:635:PRO:HG3   | 2.45                     | 0.43              |
| 1:E:998:ARG:HG2  | 1:E:999:PRO:HA    | 2.01                     | 0.43              |
| 2:F:342:ARG:HD2  | 2:F:342:ARG:HA    | 1.79                     | 0.43              |
| 2:F:364:ALA:N    | 2:F:365:PRO:HD2   | 2.32                     | 0.43              |
| 1:G:814:GLN:O    | 1:G:815:LYS:C     | 2.54                     | 0.43              |
| 1:G:1019:GLY:O   | 1:G:1023:ILE:HG13 | 2.18                     | 0.43              |
| 2:H:210:VAL:O    | 2:H:211:ASP:C     | 2.57                     | 0.43              |
| 2:B:285:LYS:HG3  | 2:B:314:PHE:CZ    | 2.52                     | 0.43              |
| 1:C:163:GLY:O    | 1:C:166:CYS:HB3   | 2.18                     | 0.43              |
| 2:D:50:ARG:HH12  | 2:D:156:MET:CE    | 2.32                     | 0.43              |
| 1:E:17:PRO:HG3   | 1:E:917:VAL:HG13  | 2.00                     | 0.43              |
| 1:E:704:LYS:O    | 1:E:705:ALA:C     | 2.56                     | 0.43              |
| 2:F:195:VAL:CG2  | 2:F:231:MET:HE3   | 2.49                     | 0.43              |
| 1:G:106:GLY:HA2  | 11:G:1176:HOH:O   | 2.18                     | 0.43              |
| 1:G:548:GLU:OE1  | 2:H:114:ASP:HA    | 2.19                     | 0.43              |
| 1:G:814:GLN:HG3  | 1:G:818:PHE:CE2   | 2.53                     | 0.43              |
| 1:A:194:ARG:NH2  | 11:A:1266:HOH:O   | 2.30                     | 0.43              |
| 1:A:891:LYS:NZ   | 11:A:1825:HOH:O   | 2.51                     | 0.43              |
| 2:B:350:PHE:CD1  | 2:B:366:LEU:HD21  | 2.53                     | 0.43              |
| 1:C:28:TYR:CE1   | 1:C:313:LYS:HE3   | 2.53                     | 0.43              |
| 1:C:678:PHE:O    | 1:C:681:ALA:N     | 2.52                     | 0.43              |
| 2:D:6:LEU:HD13   | 2:D:16:HIS:ND1    | 2.34                     | 0.43              |
| 2:D:41:GLU:HB2   | 2:D:358:PRO:HD3   | 2.01                     | 0.43              |
| 2:D:168:TYR:O    | 2:D:218:ILE:N     | 2.43                     | 0.43              |
| 2:D:272:HIS:HB2  | 2:D:349:SER:HB2   | 2.01                     | 0.43              |
| 1:E:761:GLU:HG2  | 1:E:781:HIS:CE1   | 2.54                     | 0.43              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 2:F:46:PRO:HA       | 2:F:76:HIS:CG     | 2.53                     | 0.43              |
| 2:H:300:VAL:HG22    | 2:H:328:THR:O     | 2.19                     | 0.43              |
| 1:C:373:ARG:O       | 1:C:379:LYS:NZ    | 2.40                     | 0.43              |
| 1:C:375:THR:HG23    | 1:C:377:GLN:H     | 1.84                     | 0.43              |
| 2:D:201:ALA:CB      | 2:D:239:SER:HB2   | 2.48                     | 0.43              |
| 1:E:885:PRO:HA      | 1:E:886:PRO:HD3   | 1.65                     | 0.43              |
| 1:G:472:LEU:O       | 1:G:476:VAL:HG23  | 2.18                     | 0.43              |
| 1:G:883:VAL:HG12    | 1:G:884:ILE:N     | 2.33                     | 0.43              |
| 2:H:201:ALA:HB2     | 2:H:239:SER:HB2   | 2.01                     | 0.43              |
| 2:H:332:LEU:HA      | 2:H:332:LEU:HD12  | 1.59                     | 0.43              |
| 2:B:49:SER:HA       | 2:B:76:HIS:O      | 2.18                     | 0.43              |
| 2:B:201:ALA:HB2     | 2:B:239:SER:HB2   | 1.99                     | 0.43              |
| 1:C:28:TYR:CZ       | 1:C:313:LYS:HE3   | 2.54                     | 0.43              |
| 1:C:358:LYS:HG2     | 1:C:359:ILE:N     | 2.32                     | 0.43              |
| 1:C:891:LYS:HE3     | 1:C:893:VAL:HG12  | 2.01                     | 0.43              |
| 1:C:947:LEU:HG      | 1:C:1014:ILE:CG2  | 2.49                     | 0.43              |
| 2:D:234:ASP:CG      | 2:D:378:ARG:HH11  | 2.22                     | 0.43              |
| 1:E:805:ILE:CD1     | 1:E:837:VAL:HG23  | 2.48                     | 0.43              |
| 2:H:54:THR:HG23     | 2:H:81:VAL:CG1    | 2.48                     | 0.43              |
| 1:A:702:VAL:HG11    | 1:A:735:ARG:NH2   | 2.34                     | 0.42              |
| 2:B:342:ARG:NE      | 2:B:344:ASP:OD2   | 2.51                     | 0.42              |
| 1:E:493:LYS:HD2     | 1:E:493:LYS:HA    | 1.74                     | 0.42              |
| 1:E:646:THR:HB      | 1:E:647:PRO:HD3   | 2.00                     | 0.42              |
| 1:E:836:GLU:HG3     | 11:E:1817:HOH:O   | 2.18                     | 0.42              |
| 1:E:948:SER:OG      | 10:E:1093:U:H5''  | 2.18                     | 0.42              |
| 2:F:87:LEU:HD12     | 2:F:87:LEU:HA     | 1.69                     | 0.42              |
| 1:G:82:ARG:NH1      | 11:G:1744:HOH:O   | 2.52                     | 0.42              |
| 1:G:692:ASN:HB3     | 1:G:753:ASP:OD2   | 2.19                     | 0.42              |
| 2:H:210:VAL:HA      | 2:H:214:CYS:O     | 2.19                     | 0.42              |
| 1:A:425[A]:ARG:NH1  | 11:A:1430:HOH:O   | 2.32                     | 0.42              |
| 1:A:796:LEU:HD23    | 1:A:796:LEU:C     | 2.40                     | 0.42              |
| 2:B:268:ILE:HD13    | 2:B:354:PRO:HD2   | 2.00                     | 0.42              |
| 1:C:223:ASP:CG      | 1:C:227:ASN:HB2   | 2.39                     | 0.42              |
| 1:C:956:ARG:HB3     | 1:C:1044:LEU:HD23 | 2.00                     | 0.42              |
| 2:D:157:ASP:CG      | 2:D:160:LYS:HG2   | 2.40                     | 0.42              |
| 1:E:458:ILE:O       | 1:E:463:LEU:HD11  | 2.19                     | 0.42              |
| 1:E:1021:ARG:CG     | 1:E:1021:ARG:NH1  | 2.80                     | 0.42              |
| 2:F:379:LYS:NZ      | 2:F:379:LYS:CB    | 2.82                     | 0.42              |
| 1:G:652[A]:ARG:HH12 | 1:G:667:ASP:HA    | 1.81                     | 0.42              |
| 1:G:885:PRO:HA      | 1:G:886:PRO:HD3   | 1.66                     | 0.42              |
| 2:H:5:ALA:HB1       | 2:H:110:ILE:HG13  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:219:VAL:HG23 | 2:H:220:PRO:O    | 2.19                     | 0.42              |
| 1:A:67:GLU:OE1   | 1:A:1062:VAL:HA  | 2.19                     | 0.42              |
| 1:A:840:ILE:O    | 1:A:841:GLU:HB3  | 2.19                     | 0.42              |
| 2:B:255:ILE:HD13 | 2:B:274:LEU:HB3  | 2.01                     | 0.42              |
| 1:C:775:ILE:HD13 | 1:C:775:ILE:HA   | 1.84                     | 0.42              |
| 1:E:26:PHE:HA    | 1:E:29[B]:SER:OG | 2.19                     | 0.42              |
| 2:F:139:ASP:OD2  | 2:F:142:LEU:HB2  | 2.19                     | 0.42              |
| 1:G:671:ARG:NH2  | 1:G:819:GLU:O    | 2.52                     | 0.42              |
| 2:H:168:TYR:CD1  | 2:H:168:TYR:N    | 2.87                     | 0.42              |
| 1:A:446:GLY:C    | 1:E:447:LEU:HD23 | 2.40                     | 0.42              |
| 2:B:369:HIS:O    | 2:B:372:GLU:HB2  | 2.20                     | 0.42              |
| 1:C:710:TYR:HA   | 1:C:711:PRO:C    | 2.39                     | 0.42              |
| 1:C:864:VAL:O    | 1:C:868:VAL:HG23 | 2.19                     | 0.42              |
| 2:F:23:THR:HG23  | 2:F:134:ALA:O    | 2.19                     | 0.42              |
| 2:F:286:MET:CE   | 2:F:312:HIS:ND1  | 2.82                     | 0.42              |
| 2:H:29:GLU:HA    | 2:H:129:ASN:HA   | 1.99                     | 0.42              |
| 2:H:256:GLN:HG3  | 2:H:278:ALA:HB1  | 2.01                     | 0.42              |
| 1:C:435:ARG:HB2  | 11:C:1376:HOH:O  | 2.20                     | 0.42              |
| 2:D:29:GLU:CD    | 2:D:153:LEU:HD22 | 2.39                     | 0.42              |
| 2:F:218:ILE:HD13 | 2:F:218:ILE:N    | 2.34                     | 0.42              |
| 1:G:105:GLN:NE2  | 1:G:105:GLN:CA   | 2.82                     | 0.42              |
| 1:G:421:LEU:HD21 | 1:G:445:ALA:HB1  | 2.00                     | 0.42              |
| 1:G:479:VAL:HG23 | 1:G:480:GLY:O    | 2.19                     | 0.42              |
| 1:G:734:LEU:O    | 1:G:737:TYR:HB3  | 2.18                     | 0.42              |
| 1:G:772:MET:CE   | 1:G:880:THR:HA   | 2.49                     | 0.42              |
| 2:H:45:ASP:O     | 2:H:76:HIS:HB2   | 2.18                     | 0.42              |
| 2:H:275:LEU:CD2  | 2:H:349:SER:HB3  | 2.48                     | 0.42              |
| 1:A:1031:ARG:HE  | 1:A:1031:ARG:HB3 | 1.62                     | 0.42              |
| 1:C:932:GLN:HG3  | 11:C:1554:HOH:O  | 2.19                     | 0.42              |
| 2:D:50:ARG:NH1   | 2:D:156:MET:HE1  | 2.35                     | 0.42              |
| 2:D:325:LEU:HA   | 2:D:325:LEU:HD23 | 1.52                     | 0.42              |
| 1:E:1:MET:O      | 1:E:329:GLY:O    | 2.38                     | 0.42              |
| 1:E:6:ASP:OD2    | 1:E:6:ASP:N      | 2.42                     | 0.42              |
| 1:E:434:ASP:O    | 1:E:435:ARG:C    | 2.57                     | 0.42              |
| 2:F:188:ASP:OD2  | 2:F:188:ASP:N    | 2.52                     | 0.42              |
| 1:G:1:MET:CB     | 1:G:224:LYS:HZ2  | 2.17                     | 0.42              |
| 1:G:630:VAL:HG13 | 1:G:635:PRO:CD   | 2.50                     | 0.42              |
| 2:B:172:GLN:HA   | 11:B:3559:HOH:O  | 2.18                     | 0.42              |
| 2:D:71:GLU:O     | 2:D:203:ARG:HG3  | 2.20                     | 0.42              |
| 2:F:6:LEU:HD23   | 2:F:138:PRO:HB2  | 2.02                     | 0.42              |
| 2:F:205:ILE:HG12 | 2:F:355:GLU:HG3  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:130:ARG:O    | 1:G:134:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:339:ILE:HD13 | 1:A:339:ILE:HG21 | 1.79                     | 0.42              |
| 1:C:980:VAL:HG13 | 11:C:1568:HOH:O  | 2.20                     | 0.42              |
| 2:D:236:ILE:HB   | 2:D:265:VAL:HG22 | 2.00                     | 0.42              |
| 1:E:764:VAL:HA   | 1:E:777:GLY:O    | 2.20                     | 0.42              |
| 1:G:318:PRO:HB2  | 1:G:321:LYS:HB2  | 2.01                     | 0.42              |
| 1:G:762:VAL:CG2  | 1:G:801:LEU:HD11 | 2.49                     | 0.42              |
| 2:H:208:MET:SD   | 2:H:355:GLU:HA   | 2.59                     | 0.42              |
| 1:A:954:LYS:HB3  | 1:A:980:VAL:HG21 | 2.01                     | 0.42              |
| 1:A:992:ASN:HD21 | 1:G:975:HIS:HE2  | 1.68                     | 0.42              |
| 1:C:183:TYR:N    | 1:C:187:GLU:OE1  | 2.33                     | 0.42              |
| 1:C:689:GLN:O    | 1:C:690:PRO:C    | 2.58                     | 0.42              |
| 1:C:695:VAL:HG11 | 1:C:701:ALA:CB   | 2.41                     | 0.42              |
| 1:C:827:ASN:N    | 1:C:843:ASN:O    | 2.51                     | 0.42              |
| 1:C:954:LYS:HG2  | 1:C:980:VAL:HG21 | 2.01                     | 0.42              |
| 2:D:85:LEU:HD12  | 2:D:86:PRO:HD2   | 2.02                     | 0.42              |
| 1:E:757:ASP:O    | 1:E:758:ASP:C    | 2.58                     | 0.42              |
| 2:F:195:VAL:HG11 | 2:F:231:MET:CE   | 2.50                     | 0.42              |
| 2:F:274:LEU:HD23 | 2:F:274:LEU:HA   | 1.61                     | 0.42              |
| 1:G:948:SER:O    | 1:G:1015:ASN:HA  | 2.19                     | 0.42              |
| 2:H:158:LEU:O    | 2:H:161:GLU:HB2  | 2.19                     | 0.42              |
| 2:H:318:GLU:HA   | 2:H:337:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:44:VAL:O     | 1:A:62:ASP:HB2   | 2.20                     | 0.42              |
| 1:A:185:ARG:HH11 | 1:A:185:ARG:HD3  | 1.73                     | 0.42              |
| 1:A:370:ALA:HB2  | 1:A:903:VAL:HG23 | 2.00                     | 0.42              |
| 1:A:897:PHE:HB3  | 11:A:1561:HOH:O  | 2.20                     | 0.42              |
| 1:C:132:PHE:O    | 1:C:136:MET:HG2  | 2.20                     | 0.42              |
| 1:E:65:TYR:OH    | 1:E:80:LYS:HE3   | 2.20                     | 0.42              |
| 1:G:37:LEU:HD23  | 1:G:37:LEU:HA    | 1.81                     | 0.42              |
| 1:G:256:LEU:HD23 | 1:G:256:LEU:HA   | 1.91                     | 0.42              |
| 1:G:509:ARG:HB2  | 1:G:509:ARG:NH1  | 2.23                     | 0.42              |
| 1:G:698:ILE:N    | 1:G:698:ILE:CD1  | 2.83                     | 0.42              |
| 1:G:893:VAL:HA   | 1:G:916:GLU:HA   | 2.02                     | 0.42              |
| 2:H:193:HIS:HD2  | 2:H:194:VAL:N    | 2.18                     | 0.42              |
| 2:H:272:HIS:HE1  | 2:H:340:ILE:HG12 | 1.83                     | 0.42              |
| 1:A:14:GLY:HA2   | 11:A:1098:HOH:O  | 2.20                     | 0.41              |
| 1:A:804:GLU:HB3  | 11:A:1837:HOH:O  | 2.19                     | 0.41              |
| 1:A:817:ALA:HB2  | 1:A:826:MET:SD   | 2.60                     | 0.41              |
| 2:B:29:GLU:CB    | 2:B:153:LEU:HD22 | 2.50                     | 0.41              |
| 1:E:76:LYS:HA    | 1:E:76:LYS:HD2   | 1.91                     | 0.41              |
| 1:E:677:ARG:O    | 1:E:680:HIS:HB2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:239:SER:OG   | 2:F:240:ASN:O     | 2.38                     | 0.41              |
| 1:G:425:ARG:NH1  | 11:G:1403:HOH:O   | 2.50                     | 0.41              |
| 2:H:289:GLY:O    | 2:H:290:HIS:HD2   | 2.03                     | 0.41              |
| 2:H:307:ILE:O    | 2:H:362:ASP:HB2   | 2.20                     | 0.41              |
| 1:A:318:PRO:HG3  | 1:A:610:TYR:OH    | 2.20                     | 0.41              |
| 1:A:990:LEU:HD21 | 1:G:975:HIS:CE1   | 2.55                     | 0.41              |
| 2:B:190:LEU:HD12 | 2:B:215:ARG:HB2   | 2.02                     | 0.41              |
| 2:B:325:LEU:HA   | 2:B:325:LEU:HD23  | 1.57                     | 0.41              |
| 2:B:363:ALA:C    | 2:B:365:PRO:HD2   | 2.41                     | 0.41              |
| 1:C:222:ARG:HD3  | 1:C:277:VAL:O     | 2.20                     | 0.41              |
| 1:C:679:GLN:HG3  | 1:C:689:GLN:HE22  | 1.84                     | 0.41              |
| 1:C:956:ARG:HD3  | 1:C:1044:LEU:HD23 | 2.02                     | 0.41              |
| 1:E:652:ARG:HD3  | 1:E:666:PRO:HB2   | 2.01                     | 0.41              |
| 2:F:345:LYS:HB3  | 2:F:346:PRO:CD    | 2.50                     | 0.41              |
| 1:G:686:LYS:O    | 1:G:687:LEU:HD23  | 2.21                     | 0.41              |
| 1:G:735:ARG:O    | 1:G:736:ARG:C     | 2.58                     | 0.41              |
| 1:G:761:GLU:HB3  | 1:G:781:HIS:ND1   | 2.34                     | 0.41              |
| 2:H:299:ASP:HB3  | 2:H:304:VAL:HG22  | 2.01                     | 0.41              |
| 2:H:354:PRO:HA   | 2:H:363:ALA:HB3   | 2.03                     | 0.41              |
| 1:A:221:VAL:HA   | 1:A:281:GLY:HA2   | 2.01                     | 0.41              |
| 1:A:672:ALA:CB   | 1:A:844:PRO:HG3   | 2.48                     | 0.41              |
| 2:B:228:VAL:CG1  | 2:B:258:PHE:CE1   | 3.00                     | 0.41              |
| 2:B:355:GLU:O    | 2:B:356:ALA:C     | 2.58                     | 0.41              |
| 1:C:6:ASP:OD2    | 1:C:6:ASP:N       | 2.43                     | 0.41              |
| 1:C:57:ASP:OD1   | 1:C:584:HIS:NE2   | 2.46                     | 0.41              |
| 1:C:384:VAL:HG22 | 1:C:385:MET:N     | 2.35                     | 0.41              |
| 1:E:81:GLU:O     | 1:E:82:ARG:C      | 2.57                     | 0.41              |
| 1:E:106:GLY:HA2  | 11:E:1178:HOH:O   | 2.20                     | 0.41              |
| 1:G:1001:ILE:CD1 | 1:G:1029:ILE:HD11 | 2.51                     | 0.41              |
| 2:H:154:ASN:C    | 2:H:154:ASN:HD22  | 2.24                     | 0.41              |
| 1:A:166:CYS:C    | 1:A:167:ILE:HD12  | 2.41                     | 0.41              |
| 1:A:563:MET:HE3  | 1:A:563:MET:HB2   | 1.90                     | 0.41              |
| 1:A:734:LEU:HD11 | 1:A:738:PHE:CE2   | 2.55                     | 0.41              |
| 2:D:8:VAL:HG12   | 2:D:9:LEU:O       | 2.20                     | 0.41              |
| 2:D:324:ASN:O    | 2:D:342:ARG:HA    | 2.20                     | 0.41              |
| 1:E:734:LEU:CD1  | 1:E:738:PHE:CE2   | 3.00                     | 0.41              |
| 2:F:225:ALA:HA   | 2:F:258:PHE:CZ    | 2.56                     | 0.41              |
| 1:G:402:LEU:O    | 1:G:403:GLU:HB2   | 2.20                     | 0.41              |
| 1:G:656:ALA:C    | 1:G:658:GLY:H     | 2.24                     | 0.41              |
| 1:G:728:VAL:HG11 | 1:G:734:LEU:CA    | 2.49                     | 0.41              |
| 1:G:992:ASN:HA   | 1:G:996:GLU:OE1   | 2.19                     | 0.41              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:H:272:HIS:HD2    | 2:H:351:GLN:NE2  | 2.19                     | 0.41              |
| 1:A:543:MET:CE     | 1:A:617:TYR:CZ   | 3.03                     | 0.41              |
| 1:A:895:LEU:HA     | 1:A:896:PRO:HD3  | 1.90                     | 0.41              |
| 2:B:141:ALA:O      | 2:B:145:GLU:HB2  | 2.20                     | 0.41              |
| 1:C:48:ASN:O       | 1:C:66:ILE:HA    | 2.20                     | 0.41              |
| 1:C:176:GLY:HA3    | 1:C:376:THR:O    | 2.20                     | 0.41              |
| 1:C:180:GLY:HA2    | 1:C:376:THR:OG1  | 2.20                     | 0.41              |
| 1:C:457:ASN:ND2    | 11:C:1288:HOH:O  | 2.53                     | 0.41              |
| 1:C:493:LYS:NZ     | 1:C:499:ASP:OD2  | 2.51                     | 0.41              |
| 2:D:48:TYR:HA      | 2:D:51:GLN:NE2   | 2.35                     | 0.41              |
| 1:E:1:MET:CB       | 1:E:224:LYS:NZ   | 2.80                     | 0.41              |
| 1:E:527:LYS:HB2    | 1:E:544:TYR:CZ   | 2.55                     | 0.41              |
| 1:E:671:ARG:CG     | 1:E:677:ARG:NH1  | 2.84                     | 0.41              |
| 2:F:237:PHE:CE2    | 2:F:239:SER:HA   | 2.56                     | 0.41              |
| 2:F:270:LEU:HD12   | 2:F:270:LEU:HA   | 1.79                     | 0.41              |
| 2:F:325:LEU:HD23   | 2:F:325:LEU:HA   | 1.83                     | 0.41              |
| 1:G:637:GLY:HA2    | 1:G:660:PRO:O    | 2.20                     | 0.41              |
| 1:G:992:ASN:ND2    | 1:G:996:GLU:HB3  | 2.35                     | 0.41              |
| 1:A:367:PHE:O      | 1:A:370:ALA:HB3  | 2.20                     | 0.41              |
| 2:B:357:SER:HA     | 2:B:358:PRO:HA   | 1.76                     | 0.41              |
| 1:C:761:GLU:OE2    | 1:C:785:ALA:HA   | 2.20                     | 0.41              |
| 2:D:245:PRO:HG2    | 2:D:274:LEU:CD2  | 2.50                     | 0.41              |
| 1:E:954:LYS:NZ     | 10:E:1093:U:OP3  | 2.30                     | 0.41              |
| 1:G:804:GLU:HB3    | 11:G:1688:HOH:O  | 2.21                     | 0.41              |
| 1:G:853:VAL:HG12   | 1:G:861:LEU:HD11 | 2.03                     | 0.41              |
| 1:G:1065:VAL:O     | 1:G:1068:MET:HB2 | 2.21                     | 0.41              |
| 2:H:23:THR:HG23    | 2:H:134:ALA:O    | 2.21                     | 0.41              |
| 2:H:158:LEU:HD23   | 2:H:158:LEU:HA   | 1.70                     | 0.41              |
| 1:A:692:ASN:HB3    | 1:A:753:ASP:CG   | 2.41                     | 0.41              |
| 1:A:1001:ILE:CD1   | 1:A:1002:GLN:N   | 2.80                     | 0.41              |
| 2:B:300:VAL:HG22   | 2:B:328:THR:O    | 2.20                     | 0.41              |
| 1:C:75:ARG:HG3     | 1:C:107:VAL:HG11 | 2.02                     | 0.41              |
| 1:C:903:VAL:HG22   | 11:C:1369:HOH:O  | 2.20                     | 0.41              |
| 1:E:761:GLU:HB3    | 1:E:781:HIS:ND1  | 2.36                     | 0.41              |
| 2:F:269:CYS:O      | 2:F:270:LEU:C    | 2.59                     | 0.41              |
| 2:F:324:ASN:O      | 2:F:342:ARG:HA   | 2.21                     | 0.41              |
| 1:G:11:LEU:HA      | 1:G:45:ILE:O     | 2.21                     | 0.41              |
| 1:G:362:PHE:CE1    | 1:G:380:SER:HB3  | 2.55                     | 0.41              |
| 1:G:805:ILE:HD13   | 1:G:832:VAL:HG11 | 2.02                     | 0.41              |
| 2:H:20:ILE:O       | 2:H:99:SER:OG    | 2.35                     | 0.41              |
| 1:A:130[B]:ARG:HD2 | 11:A:1197:HOH:O  | 2.19                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:164:PHE:HA   | 1:A:165:PRO:C     | 2.40                     | 0.41              |
| 1:A:259:LYS:HD3  | 2:B:175:TRP:CD2   | 2.55                     | 0.41              |
| 2:B:13:THR:HG22  | 2:B:15:PHE:CE2    | 2.56                     | 0.41              |
| 2:B:255:ILE:CD1  | 2:B:274:LEU:HB3   | 2.50                     | 0.41              |
| 2:B:332:LEU:HA   | 2:B:332:LEU:HD12  | 1.76                     | 0.41              |
| 1:C:761:GLU:CG   | 1:C:781:HIS:CE1   | 3.03                     | 0.41              |
| 1:G:115:MET:HG2  | 1:G:118:ALA:O     | 2.21                     | 0.41              |
| 2:H:23:THR:CG2   | 2:H:24:GLY:N      | 2.84                     | 0.41              |
| 2:H:247:PRO:CA   | 2:H:252:ILE:CD1   | 2.99                     | 0.41              |
| 2:H:350:PHE:CD2  | 2:H:354:PRO:HD3   | 2.56                     | 0.41              |
| 2:H:374:ILE:O    | 2:H:378:ARG:HG3   | 2.20                     | 0.41              |
| 1:A:773:VAL:CG2  | 1:A:814:GLN:HG3   | 2.51                     | 0.41              |
| 2:B:133:ILE:HD13 | 2:B:133:ILE:HG21  | 1.73                     | 0.41              |
| 2:B:187:GLU:O    | 2:B:189:GLU:N     | 2.53                     | 0.41              |
| 2:B:350:PHE:HB2  | 2:B:366:LEU:HD23  | 2.01                     | 0.41              |
| 1:C:750:VAL:HG12 | 1:C:752:LEU:CD1   | 2.51                     | 0.41              |
| 2:D:64:GLY:HA3   | 2:D:94:ASN:OD1    | 2.21                     | 0.41              |
| 1:E:669:ILE:HA   | 1:E:844:PRO:HG2   | 2.01                     | 0.41              |
| 1:E:1063:ILE:CG1 | 1:E:1064:SER:N    | 2.84                     | 0.41              |
| 2:F:341:HIS:CD2  | 2:F:348:PHE:HB3   | 2.56                     | 0.41              |
| 1:G:187:GLU:O    | 1:G:191:ILE:HG13  | 2.20                     | 0.41              |
| 1:G:812:GLN:O    | 1:G:816:LEU:HD12  | 2.21                     | 0.41              |
| 1:G:830:PHE:CE1  | 1:G:839:LEU:CD1   | 3.04                     | 0.41              |
| 1:G:875:ALA:HB2  | 11:G:1504:HOH:O   | 2.21                     | 0.41              |
| 2:H:245:PRO:HG3  | 2:H:274:LEU:HG    | 2.02                     | 0.41              |
| 1:A:361:ARG:CZ   | 1:A:404:VAL:HG12  | 2.51                     | 0.41              |
| 1:A:677:ARG:HD2  | 11:A:1807:HOH:O   | 2.21                     | 0.41              |
| 1:A:820:LEU:O    | 1:A:821:GLN:HB2   | 2.20                     | 0.41              |
| 1:C:1051:ALA:HA  | 1:C:1054:LEU:HD12 | 2.03                     | 0.41              |
| 2:D:228:VAL:HG12 | 2:D:229:LEU:N     | 2.34                     | 0.41              |
| 1:E:570:ASN:HB2  | 11:E:1629:HOH:O   | 2.21                     | 0.41              |
| 1:E:576:ILE:HD13 | 1:E:576:ILE:HG21  | 1.88                     | 0.41              |
| 2:F:356:ALA:O    | 2:F:357:SER:HB3   | 2.21                     | 0.41              |
| 1:G:148:ILE:HG22 | 1:G:149:ALA:N     | 2.36                     | 0.41              |
| 1:G:524:PRO:CG   | 1:G:628:GLU:HG3   | 2.50                     | 0.41              |
| 1:G:814:GLN:CG   | 1:G:818:PHE:CE2   | 3.03                     | 0.41              |
| 1:G:947:LEU:HD12 | 1:G:947:LEU:N     | 2.36                     | 0.41              |
| 2:H:158:LEU:O    | 2:H:159:ALA:C     | 2.58                     | 0.41              |
| 1:C:164:PHE:HA   | 1:C:165:PRO:C     | 2.42                     | 0.40              |
| 1:C:500:ALA:O    | 1:C:504:LYS:HG3   | 2.21                     | 0.40              |
| 1:C:796:LEU:HA   | 1:C:797:PRO:HA    | 1.94                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:32:PHE:O      | 2:D:291:HIS:HB2   | 2.21                     | 0.40              |
| 2:D:150:PHE:HA    | 2:D:151:PRO:HD3   | 1.76                     | 0.40              |
| 1:G:70:HIS:O      | 1:G:71:TRP:C      | 2.59                     | 0.40              |
| 1:G:339:ILE:HG22  | 1:G:540:THR:OG1   | 2.21                     | 0.40              |
| 1:G:561:LYS:HE2   | 1:G:595:GLU:OE2   | 2.21                     | 0.40              |
| 1:G:1001:ILE:HG21 | 1:G:1001:ILE:HD13 | 1.69                     | 0.40              |
| 1:A:48:ASN:O      | 1:A:66:ILE:HA     | 2.21                     | 0.40              |
| 1:A:999:PRO:HD2   | 1:G:983:GLU:OE1   | 2.20                     | 0.40              |
| 1:C:85:ALA:HA     | 1:C:114:THR:O     | 2.21                     | 0.40              |
| 1:C:424:ILE:O     | 1:C:425:ARG:C     | 2.58                     | 0.40              |
| 1:C:1021:ARG:O    | 1:C:1025:ASP:OD2  | 2.39                     | 0.40              |
| 2:D:246:ALA:CB    | 2:D:248:ASP:HB2   | 2.51                     | 0.40              |
| 2:D:270:LEU:O     | 2:D:273:GLN:HB2   | 2.20                     | 0.40              |
| 1:E:9:SER:HA      | 1:E:43:ARG:O      | 2.20                     | 0.40              |
| 1:E:135:ALA:HB1   | 1:E:274:GLU:CG    | 2.51                     | 0.40              |
| 1:G:67:GLU:HB3    | 1:G:68:PRO:HD2    | 2.02                     | 0.40              |
| 1:G:479:VAL:HG23  | 1:G:483:GLY:CA    | 2.48                     | 0.40              |
| 1:G:734:LEU:HD12  | 1:G:734:LEU:C     | 2.41                     | 0.40              |
| 1:G:775:ILE:HD11  | 1:G:813:VAL:HG11  | 2.02                     | 0.40              |
| 1:G:991:VAL:HG22  | 1:G:1001:ILE:HG23 | 2.03                     | 0.40              |
| 2:H:199:PHE:CE2   | 2:H:274:LEU:HD12  | 2.56                     | 0.40              |
| 1:A:51:PRO:HG3    | 1:A:918:MET:HB2   | 2.02                     | 0.40              |
| 1:A:354:TYR:CD2   | 1:A:387:ILE:HG23  | 2.56                     | 0.40              |
| 1:A:489:LEU:HD12  | 1:A:489:LEU:HA    | 1.87                     | 0.40              |
| 1:A:726:GLU:CG    | 1:A:727:ILE:N     | 2.79                     | 0.40              |
| 2:B:286:MET:HE1   | 2:B:312:HIS:ND1   | 2.37                     | 0.40              |
| 1:C:22:GLN:HG3    | 1:C:26:PHE:CE2    | 2.57                     | 0.40              |
| 1:C:36:ALA:O      | 1:C:40:GLU:HG2    | 2.21                     | 0.40              |
| 1:C:237:PHE:HB3   | 1:C:248:ILE:O     | 2.20                     | 0.40              |
| 1:C:796:LEU:HD23  | 1:C:796:LEU:C     | 2.42                     | 0.40              |
| 1:G:972:ASP:HA    | 1:G:989:ARG:O     | 2.21                     | 0.40              |
| 1:A:58:PRO:HD2    | 1:A:59:GLU:OE2    | 2.22                     | 0.40              |
| 1:A:383:GLU:OE2   | 1:A:604:GLU:OE1   | 2.39                     | 0.40              |
| 1:A:930:LYS:NZ    | 1:A:1058:ALA:O    | 2.51                     | 0.40              |
| 1:A:992:ASN:O     | 1:A:1000:HIS:HA   | 2.22                     | 0.40              |
| 1:A:1054:LEU:HD23 | 1:A:1054:LEU:HA   | 1.97                     | 0.40              |
| 2:B:186:LYS:HB3   | 2:B:188:ASP:OD2   | 2.22                     | 0.40              |
| 1:C:4:ARG:NE      | 1:C:7:ILE:HD12    | 2.37                     | 0.40              |
| 1:C:76:LYS:HA     | 1:C:76:LYS:HD2    | 1.96                     | 0.40              |
| 1:E:765:ASP:O     | 1:E:776:GLY:N     | 2.49                     | 0.40              |
| 2:F:316:VAL:HB    | 2:F:337:LEU:HD23  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:540:THR:HG22 | 1:G:541:ALA:N    | 2.36                     | 0.40              |
| 1:G:695:VAL:HG23 | 1:G:752:LEU:HD22 | 2.03                     | 0.40              |
| 1:G:998:ARG:HA   | 1:G:999:PRO:C    | 2.40                     | 0.40              |
| 2:H:176:THR:O    | 2:H:177:LEU:C    | 2.57                     | 0.40              |
| 2:H:225:ALA:O    | 2:H:229:LEU:HD12 | 2.22                     | 0.40              |
| 2:H:277:LEU:HD23 | 2:H:277:LEU:HA   | 1.95                     | 0.40              |
| 1:A:702:VAL:CG1  | 1:A:731:GLU:CG   | 2.99                     | 0.40              |
| 2:B:274:LEU:HD23 | 2:B:274:LEU:HA   | 1.66                     | 0.40              |
| 1:C:124:ASP:O    | 1:C:128:ASP:HB3  | 2.22                     | 0.40              |
| 1:C:677:ARG:O    | 1:C:680:HIS:HB2  | 2.22                     | 0.40              |
| 1:C:678:PHE:O    | 1:C:679:GLN:C    | 2.59                     | 0.40              |
| 1:C:993:LYS:HG2  | 10:C:1093:U:C5   | 2.56                     | 0.40              |
| 1:E:361:ARG:NH2  | 1:E:571:ARG:HG2  | 2.37                     | 0.40              |
| 1:E:695:VAL:CG1  | 1:E:696:THR:N    | 2.84                     | 0.40              |
| 2:F:365:PRO:O    | 2:F:366:LEU:C    | 2.59                     | 0.40              |
| 1:G:85:ALA:HA    | 1:G:114:THR:O    | 2.22                     | 0.40              |
| 1:G:220:VAL:O    | 1:G:281:GLY:HA2  | 2.22                     | 0.40              |
| 1:G:812:GLN:O    | 1:G:813:VAL:C    | 2.60                     | 0.40              |

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

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 11:A:1848:HOH:O | 11:C:1912:HOH:O[4_555] | 2.14                     | 0.06              |

## 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     | 1061/1073 (99%) | 1015 (96%) | 44 (4%) | 2 (0%)   | 47 49       |
| 1   | C     | 1060/1073 (99%) | 1005 (95%) | 54 (5%) | 1 (0%)   | 51 54       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | E     | 1057/1073 (98%) | 1013 (96%) | 42 (4%)  | 2 (0%)   | 47          | 49 |
| 1   | G     | 1061/1073 (99%) | 996 (94%)  | 59 (6%)  | 6 (1%)   | 25          | 21 |
| 2   | B     | 377/382 (99%)   | 348 (92%)  | 26 (7%)  | 3 (1%)   | 19          | 15 |
| 2   | D     | 378/382 (99%)   | 354 (94%)  | 23 (6%)  | 1 (0%)   | 41          | 41 |
| 2   | F     | 377/382 (99%)   | 355 (94%)  | 21 (6%)  | 1 (0%)   | 41          | 41 |
| 2   | H     | 377/382 (99%)   | 346 (92%)  | 27 (7%)  | 4 (1%)   | 14          | 9  |
| All | All   | 5748/5820 (99%) | 5432 (94%) | 296 (5%) | 20 (0%)  | 41          | 41 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 154 | ASN  |
| 2   | D     | 154 | ASN  |
| 1   | E     | 738 | PHE  |
| 1   | G     | 485 | ASN  |
| 1   | G     | 975 | HIS  |
| 2   | H     | 11  | ASP  |
| 1   | A     | 558 | ASP  |
| 2   | F     | 311 | ASN  |
| 2   | H     | 247 | PRO  |
| 1   | G     | 798 | ALA  |
| 2   | B     | 188 | ASP  |
| 1   | C     | 368 | ALA  |
| 1   | E     | 954 | LYS  |
| 1   | G     | 739 | GLN  |
| 1   | G     | 736 | ARG  |
| 2   | H     | 10  | GLU  |
| 2   | H     | 365 | PRO  |
| 1   | A     | 88  | PRO  |
| 2   | B     | 191 | PRO  |
| 1   | G     | 871 | GLY  |

### 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     | 874/878 (100%)  | 811 (93%)  | 63 (7%)  | 14          | 11 |
| 1   | C     | 873/878 (99%)   | 809 (93%)  | 64 (7%)  | 14          | 11 |
| 1   | E     | 870/878 (99%)   | 818 (94%)  | 52 (6%)  | 19          | 16 |
| 1   | G     | 874/878 (100%)  | 800 (92%)  | 74 (8%)  | 10          | 7  |
| 2   | B     | 308/310 (99%)   | 283 (92%)  | 25 (8%)  | 11          | 8  |
| 2   | D     | 309/310 (100%)  | 283 (92%)  | 26 (8%)  | 11          | 7  |
| 2   | F     | 308/310 (99%)   | 276 (90%)  | 32 (10%) | 7           | 4  |
| 2   | H     | 308/310 (99%)   | 278 (90%)  | 30 (10%) | 8           | 5  |
| All | All   | 4724/4752 (99%) | 4358 (92%) | 366 (8%) | 13          | 9  |

All (366) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 5   | THR  |
| 1   | A     | 8   | LYS  |
| 1   | A     | 38  | ARG  |
| 1   | A     | 103 | GLU  |
| 1   | A     | 104 | ARG  |
| 1   | A     | 174 | MET  |
| 1   | A     | 185 | ARG  |
| 1   | A     | 326 | LEU  |
| 1   | A     | 343 | ARG  |
| 1   | A     | 358 | LYS  |
| 1   | A     | 363 | ASN  |
| 1   | A     | 412 | LYS  |
| 1   | A     | 418 | PRO  |
| 1   | A     | 482 | THR  |
| 1   | A     | 509 | ARG  |
| 1   | A     | 542 | TYR  |
| 1   | A     | 548 | GLU  |
| 1   | A     | 556 | SER  |
| 1   | A     | 559 | ARG  |
| 1   | A     | 571 | ARG  |
| 1   | A     | 591 | GLU  |
| 1   | A     | 652 | ARG  |
| 1   | A     | 671 | ARG  |
| 1   | A     | 675 | ARG  |
| 1   | A     | 679 | GLN  |
| 1   | A     | 680 | HIS  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 684    | ARG  |
| 1   | A     | 688    | LYS  |
| 1   | A     | 700    | MET  |
| 1   | A     | 702    | VAL  |
| 1   | A     | 704    | LYS  |
| 1   | A     | 706    | LYS  |
| 1   | A     | 712    | LEU  |
| 1   | A     | 733    | ASP  |
| 1   | A     | 734    | LEU  |
| 1   | A     | 735    | ARG  |
| 1   | A     | 751    | LEU  |
| 1   | A     | 752    | LEU  |
| 1   | A     | 753    | ASP  |
| 1   | A     | 763    | ASP  |
| 1   | A     | 784    | GLN  |
| 1   | A     | 800    | THR  |
| 1   | A     | 805    | ILE  |
| 1   | A     | 815    | LYS  |
| 1   | A     | 835    | ASN  |
| 1   | A     | 839    | LEU  |
| 1   | A     | 855    | LYS  |
| 1   | A     | 881    | LYS  |
| 1   | A     | 891    | LYS  |
| 1   | A     | 912    | ARG  |
| 1   | A     | 930    | LYS  |
| 1   | A     | 940    | LYS  |
| 1   | A     | 950    | ARG  |
| 1   | A     | 951    | GLU  |
| 1   | A     | 966    | LYS  |
| 1   | A     | 967[A] | GLN  |
| 1   | A     | 967[B] | GLN  |
| 1   | A     | 992    | ASN  |
| 1   | A     | 1006   | LYS  |
| 1   | A     | 1018   | SER  |
| 1   | A     | 1020   | ARG  |
| 1   | A     | 1073   | LYS  |
| 2   | B     | 2      | ILE  |
| 2   | B     | 6      | LEU  |
| 2   | B     | 18     | ARG  |
| 2   | B     | 49     | SER  |
| 2   | B     | 50     | ARG  |
| 2   | B     | 78     | GLN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | B     | 87     | LEU  |
| 2   | B     | 125    | LYS  |
| 2   | B     | 142    | LEU  |
| 2   | B     | 153    | LEU  |
| 2   | B     | 154    | ASN  |
| 2   | B     | 192    | PHE  |
| 2   | B     | 215    | ARG  |
| 2   | B     | 227    | ASP  |
| 2   | B     | 239    | SER  |
| 2   | B     | 248    | ASP  |
| 2   | B     | 249    | ASP  |
| 2   | B     | 261    | THR  |
| 2   | B     | 263    | ILE  |
| 2   | B     | 324    | ASN  |
| 2   | B     | 331    | SER  |
| 2   | B     | 332    | LEU  |
| 2   | B     | 333    | PHE  |
| 2   | B     | 376    | GLN  |
| 2   | B     | 379    | LYS  |
| 1   | C     | 1      | MET  |
| 1   | C     | 4      | ARG  |
| 1   | C     | 5      | THR  |
| 1   | C     | 38     | ARG  |
| 1   | C     | 76     | LYS  |
| 1   | C     | 103    | GLU  |
| 1   | C     | 174    | MET  |
| 1   | C     | 185    | ARG  |
| 1   | C     | 202    | LYS  |
| 1   | C     | 236    | ASN  |
| 1   | C     | 275    | ILE  |
| 1   | C     | 313    | LYS  |
| 1   | C     | 321    | LYS  |
| 1   | C     | 326    | LEU  |
| 1   | C     | 358    | LYS  |
| 1   | C     | 363    | ASN  |
| 1   | C     | 412    | LYS  |
| 1   | C     | 414    | SER  |
| 1   | C     | 416    | ASP  |
| 1   | C     | 423[A] | LYS  |
| 1   | C     | 423[B] | LYS  |
| 1   | C     | 426    | ARG  |
| 1   | C     | 482    | THR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | C     | 519    | GLN  |
| 1   | C     | 548    | GLU  |
| 1   | C     | 563    | MET  |
| 1   | C     | 571    | ARG  |
| 1   | C     | 645    | GLN  |
| 1   | C     | 652    | ARG  |
| 1   | C     | 665    | SER  |
| 1   | C     | 671    | ARG  |
| 1   | C     | 675    | ARG  |
| 1   | C     | 688    | LYS  |
| 1   | C     | 689    | GLN  |
| 1   | C     | 696    | THR  |
| 1   | C     | 702    | VAL  |
| 1   | C     | 706    | LYS  |
| 1   | C     | 725    | MET  |
| 1   | C     | 733    | ASP  |
| 1   | C     | 735    | ARG  |
| 1   | C     | 736    | ARG  |
| 1   | C     | 751    | LEU  |
| 1   | C     | 752    | LEU  |
| 1   | C     | 763    | ASP  |
| 1   | C     | 784    | GLN  |
| 1   | C     | 805    | ILE  |
| 1   | C     | 812    | GLN  |
| 1   | C     | 855    | LYS  |
| 1   | C     | 880    | THR  |
| 1   | C     | 881    | LYS  |
| 1   | C     | 912    | ARG  |
| 1   | C     | 950    | ARG  |
| 1   | C     | 951    | GLU  |
| 1   | C     | 956    | ARG  |
| 1   | C     | 966    | LYS  |
| 1   | C     | 967[A] | GLN  |
| 1   | C     | 967[B] | GLN  |
| 1   | C     | 1001   | ILE  |
| 1   | C     | 1018   | SER  |
| 1   | C     | 1020   | ARG  |
| 1   | C     | 1021   | ARG  |
| 1   | C     | 1061   | LYS  |
| 1   | C     | 1063   | ILE  |
| 1   | C     | 1073   | LYS  |
| 2   | D     | 4      | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 27  | VAL  |
| 2   | D     | 47  | SER  |
| 2   | D     | 49  | SER  |
| 2   | D     | 73  | SER  |
| 2   | D     | 87  | LEU  |
| 2   | D     | 100 | SER  |
| 2   | D     | 153 | LEU  |
| 2   | D     | 154 | ASN  |
| 2   | D     | 156 | MET  |
| 2   | D     | 166 | GLU  |
| 2   | D     | 215 | ARG  |
| 2   | D     | 224 | SER  |
| 2   | D     | 239 | SER  |
| 2   | D     | 248 | ASP  |
| 2   | D     | 249 | ASP  |
| 2   | D     | 261 | THR  |
| 2   | D     | 282 | LYS  |
| 2   | D     | 306 | MET  |
| 2   | D     | 324 | ASN  |
| 2   | D     | 332 | LEU  |
| 2   | D     | 333 | PHE  |
| 2   | D     | 357 | SER  |
| 2   | D     | 366 | LEU  |
| 2   | D     | 376 | GLN  |
| 2   | D     | 379 | LYS  |
| 1   | E     | 3   | LYS  |
| 1   | E     | 5   | THR  |
| 1   | E     | 46  | LEU  |
| 1   | E     | 76  | LYS  |
| 1   | E     | 103 | GLU  |
| 1   | E     | 115 | MET  |
| 1   | E     | 174 | MET  |
| 1   | E     | 185 | ARG  |
| 1   | E     | 236 | ASN  |
| 1   | E     | 275 | ILE  |
| 1   | E     | 299 | GLU  |
| 1   | E     | 326 | LEU  |
| 1   | E     | 363 | ASN  |
| 1   | E     | 412 | LYS  |
| 1   | E     | 509 | ARG  |
| 1   | E     | 518 | ASP  |
| 1   | E     | 542 | TYR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | E     | 548    | GLU  |
| 1   | E     | 571    | ARG  |
| 1   | E     | 591    | GLU  |
| 1   | E     | 645[A] | GLN  |
| 1   | E     | 645[B] | GLN  |
| 1   | E     | 671    | ARG  |
| 1   | E     | 675    | ARG  |
| 1   | E     | 677    | ARG  |
| 1   | E     | 688    | LYS  |
| 1   | E     | 696    | THR  |
| 1   | E     | 704    | LYS  |
| 1   | E     | 706    | LYS  |
| 1   | E     | 733    | ASP  |
| 1   | E     | 734    | LEU  |
| 1   | E     | 735    | ARG  |
| 1   | E     | 750    | VAL  |
| 1   | E     | 751    | LEU  |
| 1   | E     | 763    | ASP  |
| 1   | E     | 784    | GLN  |
| 1   | E     | 795    | SER  |
| 1   | E     | 805    | ILE  |
| 1   | E     | 838    | TYR  |
| 1   | E     | 849    | THR  |
| 1   | E     | 855    | LYS  |
| 1   | E     | 912    | ARG  |
| 1   | E     | 950    | ARG  |
| 1   | E     | 951    | GLU  |
| 1   | E     | 956    | ARG  |
| 1   | E     | 967[A] | GLN  |
| 1   | E     | 967[B] | GLN  |
| 1   | E     | 983    | GLU  |
| 1   | E     | 1018   | SER  |
| 1   | E     | 1020   | ARG  |
| 1   | E     | 1021   | ARG  |
| 1   | E     | 1073   | LYS  |
| 2   | F     | 2      | ILE  |
| 2   | F     | 4      | SER  |
| 2   | F     | 18     | ARG  |
| 2   | F     | 25     | SER  |
| 2   | F     | 73     | SER  |
| 2   | F     | 87     | LEU  |
| 2   | F     | 125    | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 154 | ASN  |
| 2   | F     | 166 | GLU  |
| 2   | F     | 174 | SER  |
| 2   | F     | 175 | TRP  |
| 2   | F     | 186 | LYS  |
| 2   | F     | 190 | LEU  |
| 2   | F     | 192 | PHE  |
| 2   | F     | 230 | LYS  |
| 2   | F     | 236 | ILE  |
| 2   | F     | 238 | LEU  |
| 2   | F     | 239 | SER  |
| 2   | F     | 249 | ASP  |
| 2   | F     | 257 | LYS  |
| 2   | F     | 262 | ASP  |
| 2   | F     | 263 | ILE  |
| 2   | F     | 269 | CYS  |
| 2   | F     | 282 | LYS  |
| 2   | F     | 306 | MET  |
| 2   | F     | 321 | LEU  |
| 2   | F     | 324 | ASN  |
| 2   | F     | 332 | LEU  |
| 2   | F     | 333 | PHE  |
| 2   | F     | 366 | LEU  |
| 2   | F     | 376 | GLN  |
| 2   | F     | 379 | LYS  |
| 1   | G     | 4   | ARG  |
| 1   | G     | 46  | LEU  |
| 1   | G     | 55  | MET  |
| 1   | G     | 59  | GLU  |
| 1   | G     | 82  | ARG  |
| 1   | G     | 103 | GLU  |
| 1   | G     | 119 | THR  |
| 1   | G     | 145 | ARG  |
| 1   | G     | 174 | MET  |
| 1   | G     | 185 | ARG  |
| 1   | G     | 202 | LYS  |
| 1   | G     | 224 | LYS  |
| 1   | G     | 230 | ILE  |
| 1   | G     | 236 | ASN  |
| 1   | G     | 282 | SER  |
| 1   | G     | 303 | ARG  |
| 1   | G     | 307 | SER  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | G     | 313    | LYS  |
| 1   | G     | 317    | PHE  |
| 1   | G     | 326    | LEU  |
| 1   | G     | 344    | THR  |
| 1   | G     | 428    | LEU  |
| 1   | G     | 479    | VAL  |
| 1   | G     | 493    | LYS  |
| 1   | G     | 509    | ARG  |
| 1   | G     | 519    | GLN  |
| 1   | G     | 542    | TYR  |
| 1   | G     | 548    | GLU  |
| 1   | G     | 571    | ARG  |
| 1   | G     | 591    | GLU  |
| 1   | G     | 645[A] | GLN  |
| 1   | G     | 645[B] | GLN  |
| 1   | G     | 648    | LEU  |
| 1   | G     | 652[A] | ARG  |
| 1   | G     | 652[B] | ARG  |
| 1   | G     | 675    | ARG  |
| 1   | G     | 688    | LYS  |
| 1   | G     | 692    | ASN  |
| 1   | G     | 696    | THR  |
| 1   | G     | 700    | MET  |
| 1   | G     | 706    | LYS  |
| 1   | G     | 708    | ILE  |
| 1   | G     | 712    | LEU  |
| 1   | G     | 733    | ASP  |
| 1   | G     | 735    | ARG  |
| 1   | G     | 751    | LEU  |
| 1   | G     | 763    | ASP  |
| 1   | G     | 774    | LEU  |
| 1   | G     | 784    | GLN  |
| 1   | G     | 810    | ARG  |
| 1   | G     | 849    | THR  |
| 1   | G     | 855    | LYS  |
| 1   | G     | 880    | THR  |
| 1   | G     | 884    | ILE  |
| 1   | G     | 891    | LYS  |
| 1   | G     | 912    | ARG  |
| 1   | G     | 940    | LYS  |
| 1   | G     | 951    | GLU  |
| 1   | G     | 955    | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | G     | 956    | ARG  |
| 1   | G     | 967[A] | GLN  |
| 1   | G     | 967[B] | GLN  |
| 1   | G     | 987    | ASN  |
| 1   | G     | 991    | VAL  |
| 1   | G     | 999    | PRO  |
| 1   | G     | 1006   | LYS  |
| 1   | G     | 1014   | ILE  |
| 1   | G     | 1018   | SER  |
| 1   | G     | 1020   | ARG  |
| 1   | G     | 1021   | ARG  |
| 1   | G     | 1027   | ARG  |
| 1   | G     | 1031   | ARG  |
| 1   | G     | 1061   | LYS  |
| 1   | G     | 1073   | LYS  |
| 2   | H     | 2      | ILE  |
| 2   | H     | 3      | LYS  |
| 2   | H     | 6      | LEU  |
| 2   | H     | 18     | ARG  |
| 2   | H     | 50     | ARG  |
| 2   | H     | 104    | ARG  |
| 2   | H     | 125    | LYS  |
| 2   | H     | 128    | GLN  |
| 2   | H     | 131    | CYS  |
| 2   | H     | 154    | ASN  |
| 2   | H     | 166    | GLU  |
| 2   | H     | 174    | SER  |
| 2   | H     | 192    | PHE  |
| 2   | H     | 215    | ARG  |
| 2   | H     | 218    | ILE  |
| 2   | H     | 239    | SER  |
| 2   | H     | 244    | ASP  |
| 2   | H     | 248    | ASP  |
| 2   | H     | 249    | ASP  |
| 2   | H     | 257    | LYS  |
| 2   | H     | 261    | THR  |
| 2   | H     | 279    | SER  |
| 2   | H     | 282    | LYS  |
| 2   | H     | 284    | VAL  |
| 2   | H     | 306    | MET  |
| 2   | H     | 324    | ASN  |
| 2   | H     | 332    | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 333 | PHE  |
| 2   | H     | 376 | GLN  |
| 2   | H     | 379 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 105  | GLN  |
| 1   | A     | 266  | ASN  |
| 1   | A     | 457  | ASN  |
| 1   | A     | 679  | GLN  |
| 1   | A     | 689  | GLN  |
| 1   | A     | 784  | GLN  |
| 1   | A     | 803  | GLN  |
| 1   | A     | 812  | GLN  |
| 1   | A     | 814  | GLN  |
| 1   | A     | 835  | ASN  |
| 1   | A     | 936  | ASN  |
| 1   | A     | 987  | ASN  |
| 1   | A     | 992  | ASN  |
| 1   | A     | 1000 | HIS  |
| 1   | A     | 1035 | GLN  |
| 1   | A     | 1055 | ASN  |
| 1   | A     | 1071 | GLN  |
| 2   | B     | 51   | GLN  |
| 2   | B     | 154  | ASN  |
| 2   | B     | 324  | ASN  |
| 1   | C     | 105  | GLN  |
| 1   | C     | 266  | ASN  |
| 1   | C     | 457  | ASN  |
| 1   | C     | 679  | GLN  |
| 1   | C     | 689  | GLN  |
| 1   | C     | 784  | GLN  |
| 1   | C     | 942  | HIS  |
| 1   | C     | 992  | ASN  |
| 1   | C     | 1000 | HIS  |
| 1   | C     | 1035 | GLN  |
| 1   | C     | 1055 | ASN  |
| 1   | C     | 1071 | GLN  |
| 2   | D     | 51   | GLN  |
| 2   | D     | 78   | GLN  |
| 2   | D     | 291  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 324  | ASN  |
| 1   | E     | 105  | GLN  |
| 1   | E     | 266  | ASN  |
| 1   | E     | 679  | GLN  |
| 1   | E     | 689  | GLN  |
| 1   | E     | 784  | GLN  |
| 1   | E     | 803  | GLN  |
| 1   | E     | 936  | ASN  |
| 1   | E     | 987  | ASN  |
| 1   | E     | 992  | ASN  |
| 1   | E     | 1000 | HIS  |
| 1   | E     | 1002 | GLN  |
| 1   | E     | 1035 | GLN  |
| 1   | E     | 1055 | ASN  |
| 1   | E     | 1071 | GLN  |
| 2   | F     | 51   | GLN  |
| 2   | F     | 78   | GLN  |
| 2   | F     | 154  | ASN  |
| 2   | F     | 273  | GLN  |
| 2   | F     | 324  | ASN  |
| 2   | F     | 351  | GLN  |
| 1   | G     | 105  | GLN  |
| 1   | G     | 266  | ASN  |
| 1   | G     | 523  | HIS  |
| 1   | G     | 679  | GLN  |
| 1   | G     | 689  | GLN  |
| 1   | G     | 784  | GLN  |
| 1   | G     | 803  | GLN  |
| 1   | G     | 814  | GLN  |
| 1   | G     | 835  | ASN  |
| 1   | G     | 936  | ASN  |
| 1   | G     | 987  | ASN  |
| 1   | G     | 992  | ASN  |
| 1   | G     | 1000 | HIS  |
| 1   | G     | 1035 | GLN  |
| 1   | G     | 1055 | ASN  |
| 1   | G     | 1071 | GLN  |
| 2   | H     | 51   | GLN  |
| 2   | H     | 78   | GLN  |
| 2   | H     | 154  | ASN  |
| 2   | H     | 291  | HIS  |
| 2   | H     | 311  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 324 | ASN  |

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 61 are monoatomic - leaving 25 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 |
| 7   | ADP  | A     | 1087 | 3    | 24,29,29     | 1.14 | 2 (8%)   | 29,45,45    | 1.05 | 3 (10%)  |
| 7   | ADP  | G     | 1090 | 3    | 24,29,29     | 1.22 | 3 (12%)  | 29,45,45    | 1.15 | 4 (13%)  |
| 10  | U    | A     | 1091 | -    | 18,22,22     | 1.51 | 4 (22%)  | 21,33,33    | 1.28 | 1 (4%)   |
| 7   | ADP  | C     | 1089 | 3    | 24,29,29     | 1.21 | 2 (8%)   | 29,45,45    | 1.39 | 4 (13%)  |
| 8   | ORN  | C     | 1091 | -    | 4,8,8        | 0.59 | 0        | 3,9,9       | 0.60 | 0        |
| 9   | NET  | A     | 1090 | -    | 8,8,8        | 0.72 | 0        | 10,10,10    | 0.65 | 0        |
| 10  | U    | E     | 1093 | -    | 18,22,22     | 1.55 | 4 (22%)  | 21,33,33    | 2.21 | 6 (28%)  |
| 5   | PO4  | E     | 1078 | 3    | 4,4,4        | 2.51 | 3 (75%)  | 6,6,6       | 1.33 | 1 (16%)  |
| 7   | ADP  | E     | 1089 | 3    | 24,29,29     | 1.16 | 2 (8%)   | 29,45,45    | 1.09 | 3 (10%)  |
| 8   | ORN  | G     | 1091 | -    | 4,8,8        | 0.49 | 0        | 3,9,9       | 0.30 | 0        |
| 5   | PO4  | C     | 1088 | -    | 4,4,4        | 2.51 | 3 (75%)  | 6,6,6       | 0.97 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | NET  | E     | 1092 | -    | 8,8,8        | 0.39 | 0        | 10,10,10    | 0.75 | 0        |
| 9   | NET  | G     | 1092 | -    | 8,8,8        | 0.71 | 0        | 10,10,10    | 0.46 | 0        |
| 10  | U    | G     | 1093 | -    | 18,22,22     | 1.57 | 4 (22%)  | 21,33,33    | 1.96 | 4 (19%)  |
| 5   | PO4  | G     | 1078 | 3    | 4,4,4        | 2.31 | 3 (75%)  | 6,6,6       | 1.20 | 1 (16%)  |
| 7   | ADP  | G     | 1089 | 3    | 24,29,29     | 1.27 | 3 (12%)  | 29,45,45    | 1.21 | 4 (13%)  |
| 5   | PO4  | A     | 1078 | 3    | 4,4,4        | 1.96 | 1 (25%)  | 6,6,6       | 1.37 | 1 (16%)  |
| 10  | U    | C     | 1093 | -    | 18,22,22     | 1.47 | 4 (22%)  | 21,33,33    | 1.37 | 1 (4%)   |
| 5   | PO4  | C     | 1078 | 3    | 4,4,4        | 2.29 | 3 (75%)  | 6,6,6       | 1.05 | 0        |
| 7   | ADP  | C     | 1090 | 3    | 24,29,29     | 1.01 | 1 (4%)   | 29,45,45    | 1.17 | 4 (13%)  |
| 8   | ORN  | E     | 1091 | -    | 4,8,8        | 0.71 | 0        | 3,9,9       | 0.21 | 0        |
| 8   | ORN  | A     | 1089 | -    | 4,8,8        | 0.73 | 0        | 3,9,9       | 0.49 | 0        |
| 9   | NET  | C     | 1092 | -    | 8,8,8        | 0.49 | 0        | 10,10,10    | 0.76 | 0        |
| 7   | ADP  | E     | 1090 | 3    | 24,29,29     | 1.21 | 3 (12%)  | 29,45,45    | 1.10 | 2 (6%)   |
| 7   | ADP  | A     | 1088 | 3    | 24,29,29     | 0.95 | 1 (4%)   | 29,45,45    | 1.23 | 2 (6%)   |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 7   | ADP  | A     | 1087 | 3    | -       | 1/12/32/32 | 0/3/3/3 |
| 7   | ADP  | G     | 1090 | 3    | -       | 1/12/32/32 | 0/3/3/3 |
| 10  | U    | A     | 1091 | -    | -       | 4/8/26/26  | 0/2/2/2 |
| 7   | ADP  | C     | 1089 | 3    | -       | 2/12/32/32 | 0/3/3/3 |
| 8   | ORN  | C     | 1091 | -    | -       | 4/4/8/8    | -       |
| 9   | NET  | A     | 1090 | -    | -       | 3/12/12/12 | -       |
| 10  | U    | E     | 1093 | -    | -       | 4/8/26/26  | 0/2/2/2 |
| 7   | ADP  | E     | 1089 | 3    | -       | 1/12/32/32 | 0/3/3/3 |
| 8   | ORN  | G     | 1091 | -    | -       | 4/4/8/8    | -       |
| 9   | NET  | E     | 1092 | -    | -       | 0/12/12/12 | -       |
| 9   | NET  | G     | 1092 | -    | -       | 0/12/12/12 | -       |
| 10  | U    | G     | 1093 | -    | -       | 4/8/26/26  | 0/2/2/2 |
| 7   | ADP  | G     | 1089 | 3    | -       | 0/12/32/32 | 0/3/3/3 |
| 10  | U    | C     | 1093 | -    | -       | 3/8/26/26  | 0/2/2/2 |
| 7   | ADP  | C     | 1090 | 3    | -       | 3/12/32/32 | 0/3/3/3 |
| 8   | ORN  | E     | 1091 | -    | -       | 3/4/8/8    | -       |
| 8   | ORN  | A     | 1089 | -    | -       | 4/4/8/8    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 9   | NET  | C     | 1092 | -    | -       | 0/12/12/12 | -       |
| 7   | ADP  | E     | 1090 | 3    | -       | 3/12/32/32 | 0/3/3/3 |
| 7   | ADP  | A     | 1088 | 3    | -       | 4/12/32/32 | 0/3/3/3 |

All (46) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | G     | 1093 | U    | C4-N3   | 3.94  | 1.39        | 1.33     |
| 10  | E     | 1093 | U    | C4-N3   | 3.79  | 1.39        | 1.33     |
| 10  | A     | 1091 | U    | C4-N3   | 3.79  | 1.39        | 1.33     |
| 10  | C     | 1093 | U    | C4-N3   | 3.78  | 1.39        | 1.33     |
| 5   | C     | 1088 | PO4  | P-O2    | -3.46 | 1.44        | 1.54     |
| 5   | E     | 1078 | PO4  | P-O3    | -3.27 | 1.44        | 1.54     |
| 7   | E     | 1090 | ADP  | O2'-C2' | 3.27  | 1.50        | 1.43     |
| 7   | C     | 1089 | ADP  | O2'-C2' | 3.13  | 1.50        | 1.43     |
| 7   | E     | 1090 | ADP  | O3'-C3' | 3.11  | 1.50        | 1.43     |
| 7   | G     | 1089 | ADP  | O2'-C2' | 3.08  | 1.50        | 1.43     |
| 5   | G     | 1078 | PO4  | P-O2    | -2.99 | 1.45        | 1.54     |
| 5   | C     | 1078 | PO4  | P-O2    | -2.97 | 1.45        | 1.54     |
| 5   | E     | 1078 | PO4  | P-O2    | -2.93 | 1.45        | 1.54     |
| 10  | A     | 1091 | U    | C6-C5   | -2.92 | 1.31        | 1.38     |
| 7   | G     | 1089 | ADP  | O4'-C1' | -2.88 | 1.37        | 1.41     |
| 10  | E     | 1093 | U    | P-OP3   | 2.88  | 1.65        | 1.54     |
| 10  | C     | 1093 | U    | P-OP3   | 2.88  | 1.65        | 1.54     |
| 7   | G     | 1090 | ADP  | O3'-C3' | 2.87  | 1.49        | 1.43     |
| 10  | E     | 1093 | U    | C6-C5   | -2.86 | 1.31        | 1.38     |
| 10  | C     | 1093 | U    | C6-C5   | -2.83 | 1.31        | 1.38     |
| 10  | A     | 1091 | U    | P-OP3   | 2.79  | 1.65        | 1.54     |
| 10  | G     | 1093 | U    | C6-N1   | 2.78  | 1.39        | 1.35     |
| 7   | E     | 1089 | ADP  | O3'-C3' | 2.78  | 1.49        | 1.43     |
| 10  | G     | 1093 | U    | C6-C5   | -2.77 | 1.32        | 1.38     |
| 7   | A     | 1087 | ADP  | O3'-C3' | 2.75  | 1.49        | 1.43     |
| 10  | G     | 1093 | U    | P-OP3   | 2.69  | 1.65        | 1.54     |
| 5   | C     | 1078 | PO4  | P-O3    | -2.65 | 1.46        | 1.54     |
| 7   | A     | 1087 | ADP  | C2-N1   | 2.58  | 1.38        | 1.33     |
| 5   | C     | 1088 | PO4  | P-O3    | -2.57 | 1.46        | 1.54     |
| 7   | C     | 1090 | ADP  | O3'-C3' | 2.56  | 1.49        | 1.43     |
| 7   | C     | 1089 | ADP  | C2-N1   | 2.52  | 1.38        | 1.33     |
| 10  | A     | 1091 | U    | C6-N1   | 2.49  | 1.38        | 1.35     |
| 5   | A     | 1078 | PO4  | P-O1    | -2.48 | 1.45        | 1.50     |
| 7   | E     | 1090 | ADP  | C2-N1   | 2.47  | 1.38        | 1.33     |
| 5   | G     | 1078 | PO4  | P-O3    | -2.44 | 1.47        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | C     | 1088 | PO4  | P-O4    | -2.41 | 1.47        | 1.54     |
| 7   | G     | 1090 | ADP  | O4'-C1' | -2.39 | 1.37        | 1.41     |
| 10  | E     | 1093 | U    | C6-N1   | 2.39  | 1.38        | 1.35     |
| 7   | G     | 1090 | ADP  | O2'-C2' | 2.31  | 1.48        | 1.43     |
| 7   | E     | 1089 | ADP  | O2'-C2' | 2.25  | 1.48        | 1.43     |
| 10  | C     | 1093 | U    | C6-N1   | 2.17  | 1.38        | 1.35     |
| 7   | G     | 1089 | ADP  | C2-N1   | 2.15  | 1.37        | 1.33     |
| 5   | G     | 1078 | PO4  | P-O4    | -2.12 | 1.48        | 1.54     |
| 5   | C     | 1078 | PO4  | P-O4    | -2.06 | 1.48        | 1.54     |
| 5   | E     | 1078 | PO4  | P-O4    | -2.05 | 1.48        | 1.54     |
| 7   | A     | 1088 | ADP  | O2'-C2' | 2.01  | 1.47        | 1.43     |

All (41) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | C     | 1089 | ADP  | C5-C6-N6    | 5.14  | 128.16      | 120.35   |
| 10  | E     | 1093 | U    | OP3-P-O5'   | -4.97 | 93.51       | 106.73   |
| 10  | E     | 1093 | U    | C5-C4-N3    | -4.84 | 112.66      | 123.31   |
| 10  | G     | 1093 | U    | C5-C4-N3    | -4.74 | 112.89      | 123.31   |
| 10  | C     | 1093 | U    | C5-C4-N3    | -4.71 | 112.95      | 123.31   |
| 10  | G     | 1093 | U    | OP3-P-O5'   | -4.36 | 95.14       | 106.73   |
| 10  | A     | 1091 | U    | C5-C4-N3    | -4.34 | 113.76      | 123.31   |
| 7   | A     | 1088 | ADP  | C5-C6-N6    | 4.02  | 126.47      | 120.35   |
| 10  | G     | 1093 | U    | OP2-P-O5'   | 3.26  | 115.41      | 106.73   |
| 7   | G     | 1089 | ADP  | N6-C6-N1    | 3.26  | 125.34      | 118.57   |
| 10  | E     | 1093 | U    | C3'-C2'-C1' | 2.92  | 105.38      | 100.98   |
| 7   | A     | 1087 | ADP  | C5-C6-N6    | 2.69  | 124.44      | 120.35   |
| 7   | C     | 1089 | ADP  | O2'-C2'-C3' | 2.69  | 120.51      | 111.82   |
| 7   | C     | 1090 | ADP  | O3'-C3'-C2' | 2.65  | 120.40      | 111.82   |
| 7   | A     | 1087 | ADP  | C3'-C2'-C1' | 2.62  | 104.92      | 100.98   |
| 7   | A     | 1087 | ADP  | C5-C6-N1    | -2.60 | 114.45      | 120.35   |
| 10  | G     | 1093 | U    | C3'-C2'-C1' | 2.59  | 104.87      | 100.98   |
| 10  | E     | 1093 | U    | O5'-P-OP1   | 2.58  | 113.71      | 106.47   |
| 5   | A     | 1078 | PO4  | O2-P-O1     | -2.57 | 101.49      | 110.89   |
| 10  | E     | 1093 | U    | OP2-P-O5'   | 2.45  | 113.24      | 106.73   |
| 7   | G     | 1090 | ADP  | C2'-C3'-C4' | -2.43 | 97.91       | 102.64   |
| 7   | C     | 1090 | ADP  | C5-C6-N6    | 2.42  | 124.03      | 120.35   |
| 7   | E     | 1090 | ADP  | C5-C6-N6    | 2.42  | 124.03      | 120.35   |
| 7   | C     | 1090 | ADP  | C3'-C2'-C1' | 2.42  | 104.62      | 100.98   |
| 10  | E     | 1093 | U    | O4'-C1'-C2' | -2.40 | 103.42      | 106.93   |
| 7   | G     | 1090 | ADP  | O4'-C4'-C5' | -2.37 | 101.57      | 109.37   |
| 7   | E     | 1089 | ADP  | C1'-N9-C4   | -2.31 | 122.58      | 126.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | E     | 1089 | ADP  | C3'-C2'-C1' | 2.31  | 104.45      | 100.98   |
| 7   | G     | 1090 | ADP  | C4-C5-N7    | 2.27  | 111.77      | 109.40   |
| 7   | G     | 1089 | ADP  | O3'-C3'-C2' | 2.26  | 119.14      | 111.82   |
| 7   | G     | 1090 | ADP  | O2'-C2'-C3' | 2.23  | 119.05      | 111.82   |
| 7   | E     | 1090 | ADP  | O3'-C3'-C2' | 2.18  | 118.89      | 111.82   |
| 7   | C     | 1089 | ADP  | N6-C6-N1    | -2.12 | 114.17      | 118.57   |
| 7   | G     | 1089 | ADP  | C4-C5-N7    | 2.12  | 111.61      | 109.40   |
| 7   | G     | 1089 | ADP  | C5-C6-N1    | -2.08 | 115.63      | 120.35   |
| 7   | E     | 1089 | ADP  | O3'-C3'-C2' | 2.08  | 118.54      | 111.82   |
| 7   | C     | 1089 | ADP  | C3'-C2'-C1' | 2.06  | 104.08      | 100.98   |
| 5   | E     | 1078 | PO4  | O2-P-O1     | -2.04 | 103.44      | 110.89   |
| 5   | G     | 1078 | PO4  | O4-P-O3     | 2.03  | 114.50      | 107.97   |
| 7   | A     | 1088 | ADP  | O2'-C2'-C3' | 2.02  | 118.37      | 111.82   |
| 7   | C     | 1090 | ADP  | O2B-PB-O3A  | 2.00  | 111.35      | 104.64   |

There are no chirality outliers.

All (48) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 7   | C     | 1090 | ADP  | PA-O3A-PB-O3B   |
| 7   | E     | 1090 | ADP  | PA-O3A-PB-O3B   |
| 8   | A     | 1089 | ORN  | N-CA-CB-CG      |
| 8   | A     | 1089 | ORN  | C-CA-CB-CG      |
| 8   | C     | 1091 | ORN  | N-CA-CB-CG      |
| 8   | C     | 1091 | ORN  | C-CA-CB-CG      |
| 8   | E     | 1091 | ORN  | N-CA-CB-CG      |
| 8   | E     | 1091 | ORN  | C-CA-CB-CG      |
| 8   | G     | 1091 | ORN  | N-CA-CB-CG      |
| 8   | G     | 1091 | ORN  | C-CA-CB-CG      |
| 10  | A     | 1091 | U    | O4'-C1'-N1-C6   |
| 10  | A     | 1091 | U    | C2'-C1'-N1-C6   |
| 10  | C     | 1093 | U    | O4'-C1'-N1-C6   |
| 10  | C     | 1093 | U    | C2'-C1'-N1-C6   |
| 10  | E     | 1093 | U    | O4'-C1'-N1-C6   |
| 10  | E     | 1093 | U    | C2'-C1'-N1-C6   |
| 10  | G     | 1093 | U    | O4'-C1'-N1-C6   |
| 10  | G     | 1093 | U    | C2'-C1'-N1-C6   |
| 10  | E     | 1093 | U    | O4'-C4'-C5'-O5' |
| 10  | G     | 1093 | U    | O4'-C4'-C5'-O5' |
| 8   | G     | 1091 | ORN  | CA-CB-CG-CD     |
| 10  | E     | 1093 | U    | C3'-C4'-C5'-O5' |
| 8   | E     | 1091 | ORN  | CA-CB-CG-CD     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 8   | C     | 1091 | ORN  | CA-CB-CG-CD     |
| 10  | G     | 1093 | U    | C3'-C4'-C5'-O5' |
| 8   | A     | 1089 | ORN  | NE-CD-CG-CB     |
| 8   | G     | 1091 | ORN  | NE-CD-CG-CB     |
| 7   | A     | 1088 | ADP  | PA-O3A-PB-O1B   |
| 7   | A     | 1088 | ADP  | PA-O3A-PB-O3B   |
| 7   | C     | 1089 | ADP  | PA-O3A-PB-O2B   |
| 7   | G     | 1090 | ADP  | C5'-O5'-PA-O3A  |
| 8   | A     | 1089 | ORN  | CA-CB-CG-CD     |
| 10  | A     | 1091 | U    | O4'-C4'-C5'-O5' |
| 7   | E     | 1090 | ADP  | PA-O3A-PB-O1B   |
| 9   | A     | 1090 | NET  | C8-C7-N1-C1     |
| 8   | C     | 1091 | ORN  | NE-CD-CG-CB     |
| 7   | A     | 1088 | ADP  | PB-O3A-PA-O2A   |
| 9   | A     | 1090 | NET  | C8-C7-N1-C5     |
| 7   | E     | 1090 | ADP  | PB-O3A-PA-O2A   |
| 10  | A     | 1091 | U    | C3'-C4'-C5'-O5' |
| 10  | C     | 1093 | U    | C5'-O5'-P-OP2   |
| 7   | C     | 1090 | ADP  | PA-O3A-PB-O1B   |
| 7   | A     | 1087 | ADP  | PB-O3A-PA-O2A   |
| 7   | A     | 1088 | ADP  | PB-O3A-PA-O1A   |
| 7   | C     | 1090 | ADP  | PB-O3A-PA-O2A   |
| 7   | C     | 1089 | ADP  | C5'-O5'-PA-O1A  |
| 7   | E     | 1089 | ADP  | C5'-O5'-PA-O1A  |
| 9   | A     | 1090 | NET  | C8-C7-N1-C3     |

There are no ring outliers.

16 monomers are involved in 22 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 7   | A     | 1087 | ADP  | 1       | 0            |
| 10  | A     | 1091 | U    | 1       | 0            |
| 8   | C     | 1091 | ORN  | 1       | 0            |
| 9   | A     | 1090 | NET  | 1       | 0            |
| 10  | E     | 1093 | U    | 2       | 0            |
| 7   | E     | 1089 | ADP  | 1       | 0            |
| 8   | G     | 1091 | ORN  | 1       | 0            |
| 9   | E     | 1092 | NET  | 2       | 0            |
| 9   | G     | 1092 | NET  | 2       | 0            |
| 10  | G     | 1093 | U    | 1       | 0            |
| 10  | C     | 1093 | U    | 2       | 0            |
| 5   | C     | 1078 | PO4  | 1       | 0            |

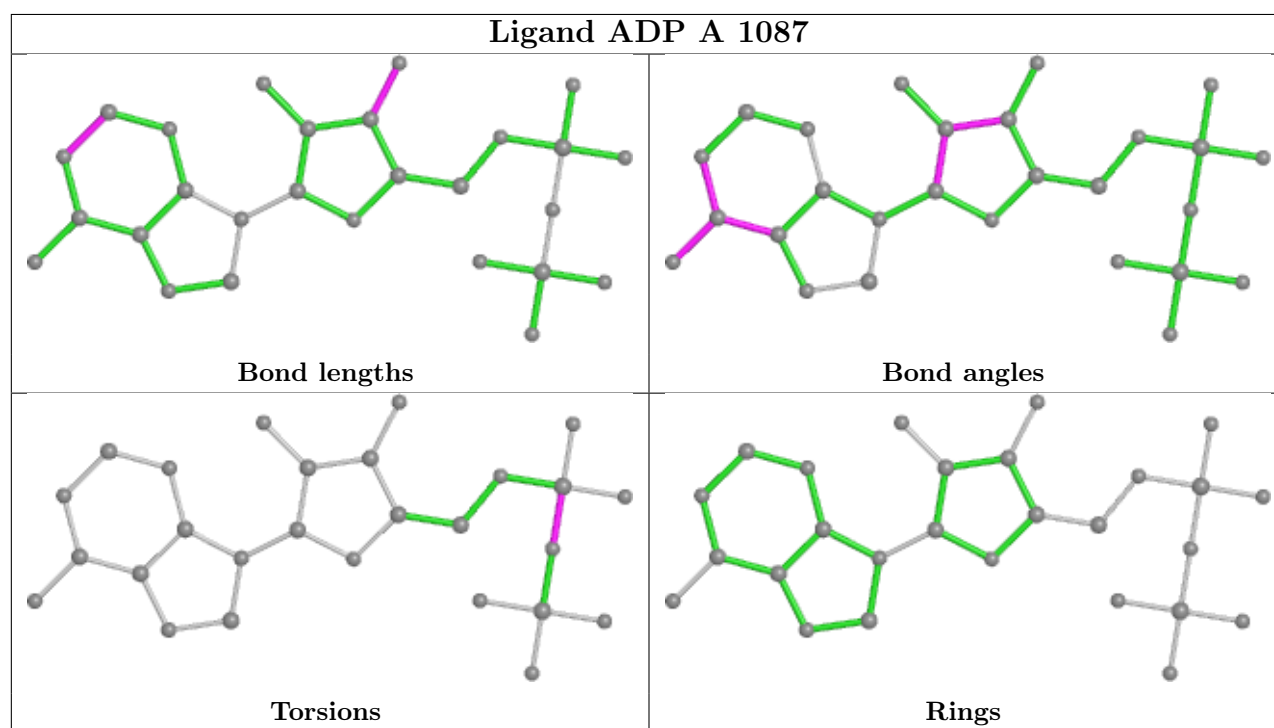
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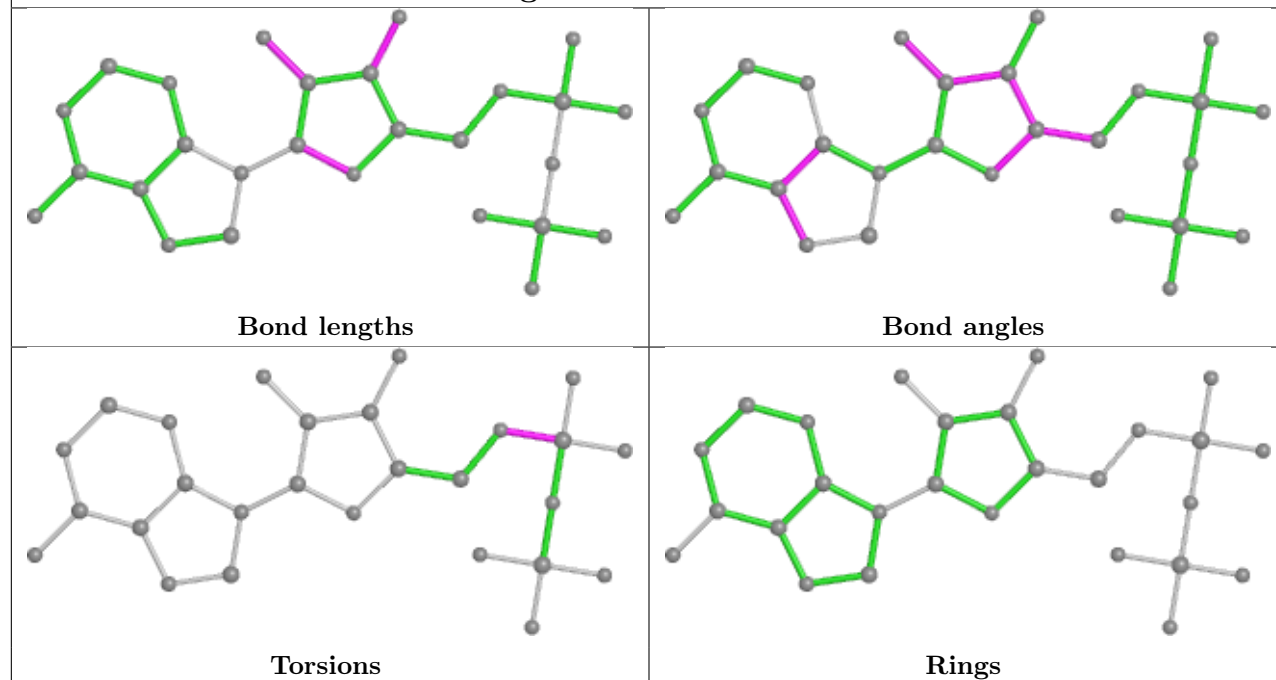
*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 8   | E     | 1091 | ORN  | 2       | 0            |
| 9   | C     | 1092 | NET  | 1       | 0            |
| 7   | E     | 1090 | ADP  | 2       | 0            |
| 7   | A     | 1088 | ADP  | 1       | 0            |

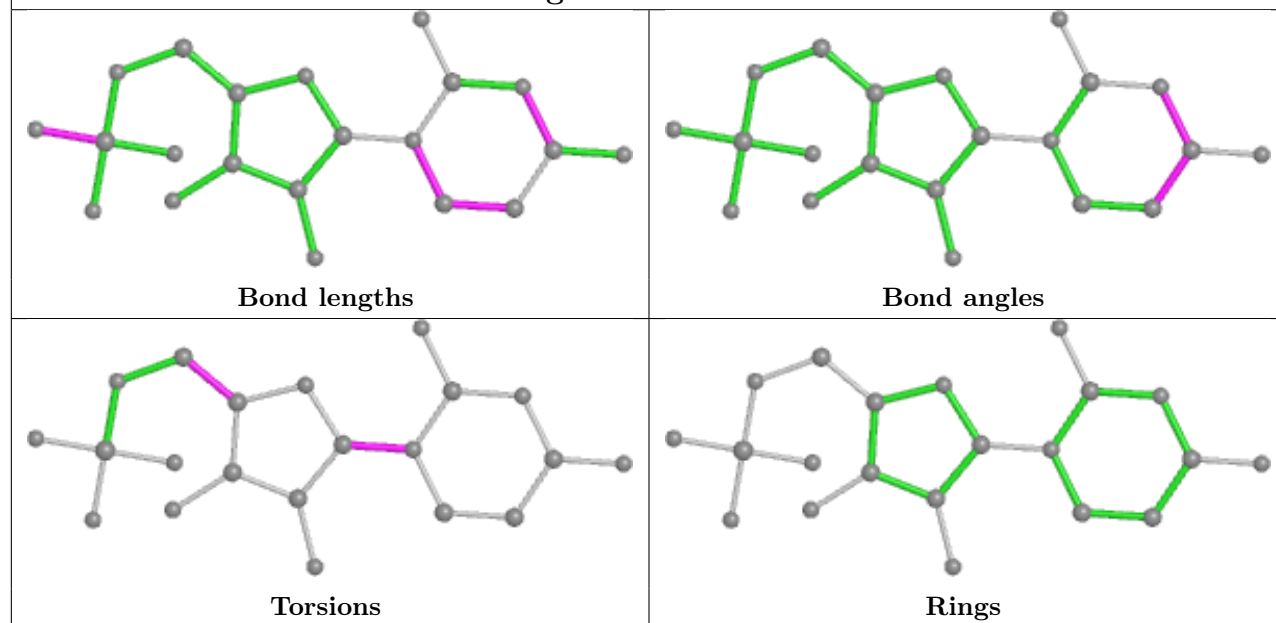
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



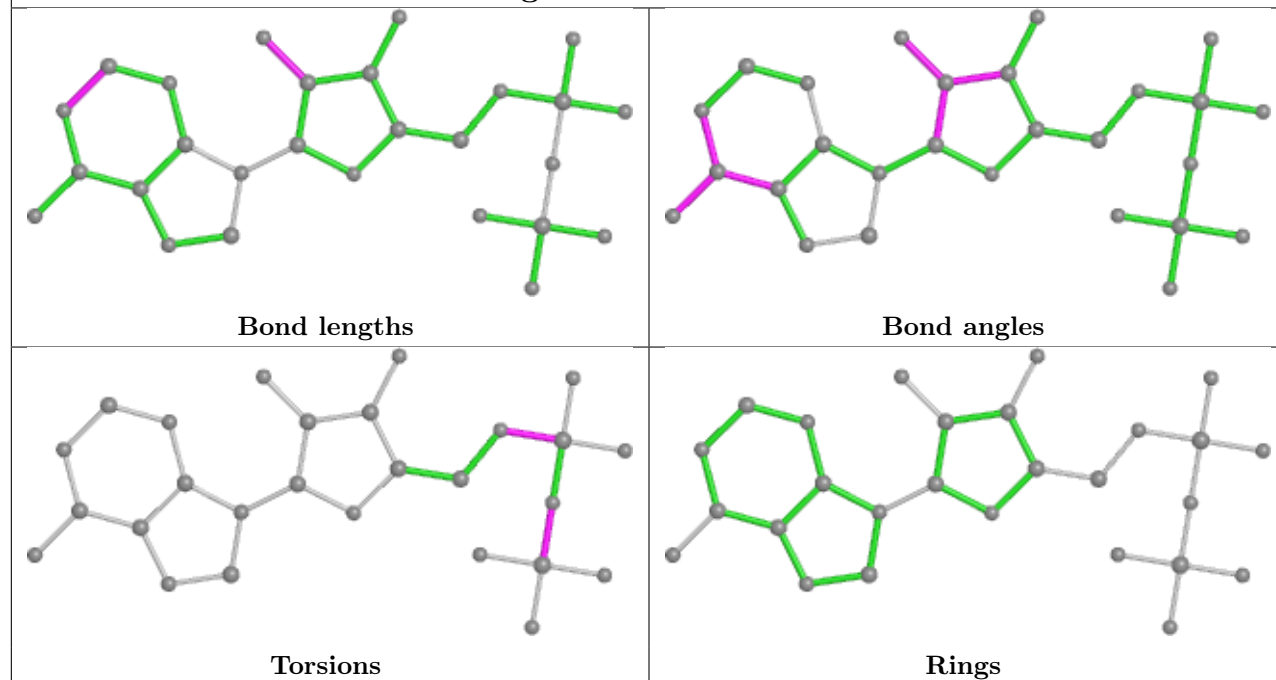
## Ligand ADP G 1090



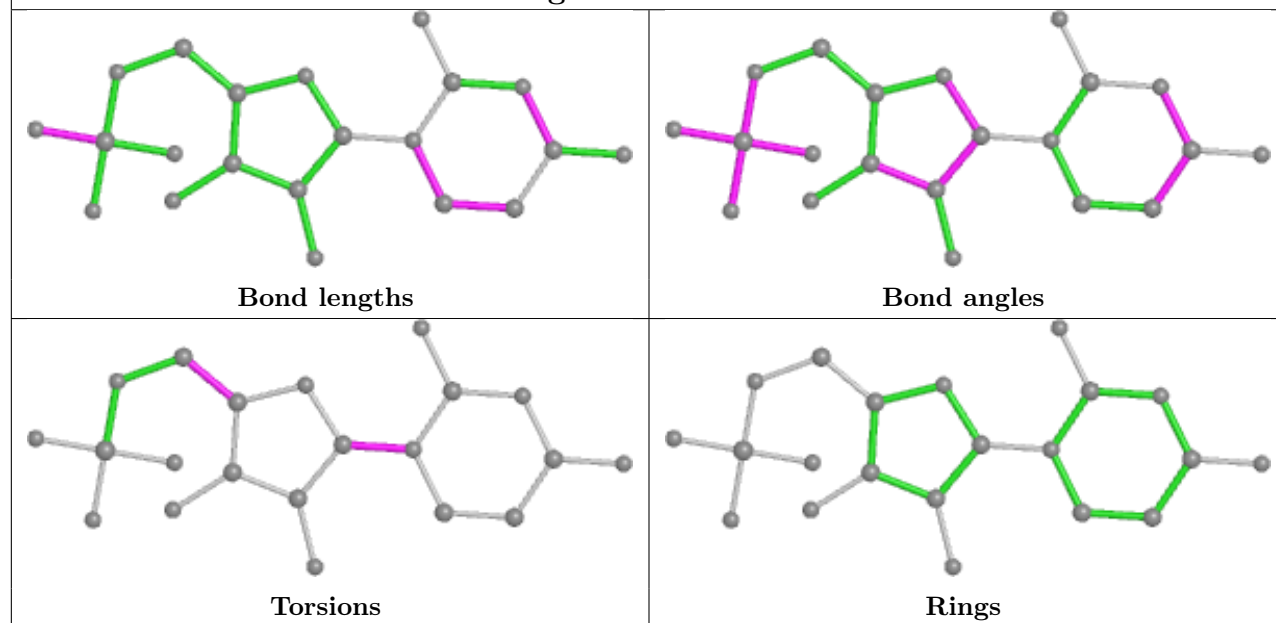
## Ligand U A 1091



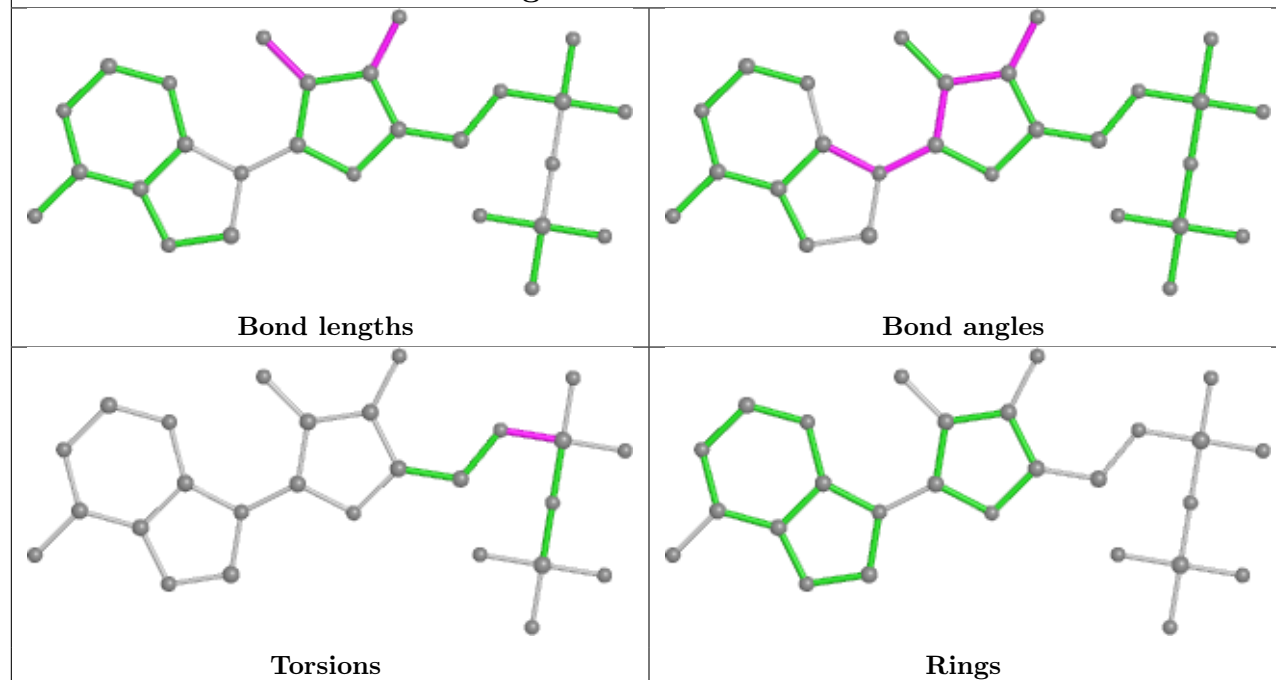
## Ligand ADP C 1089



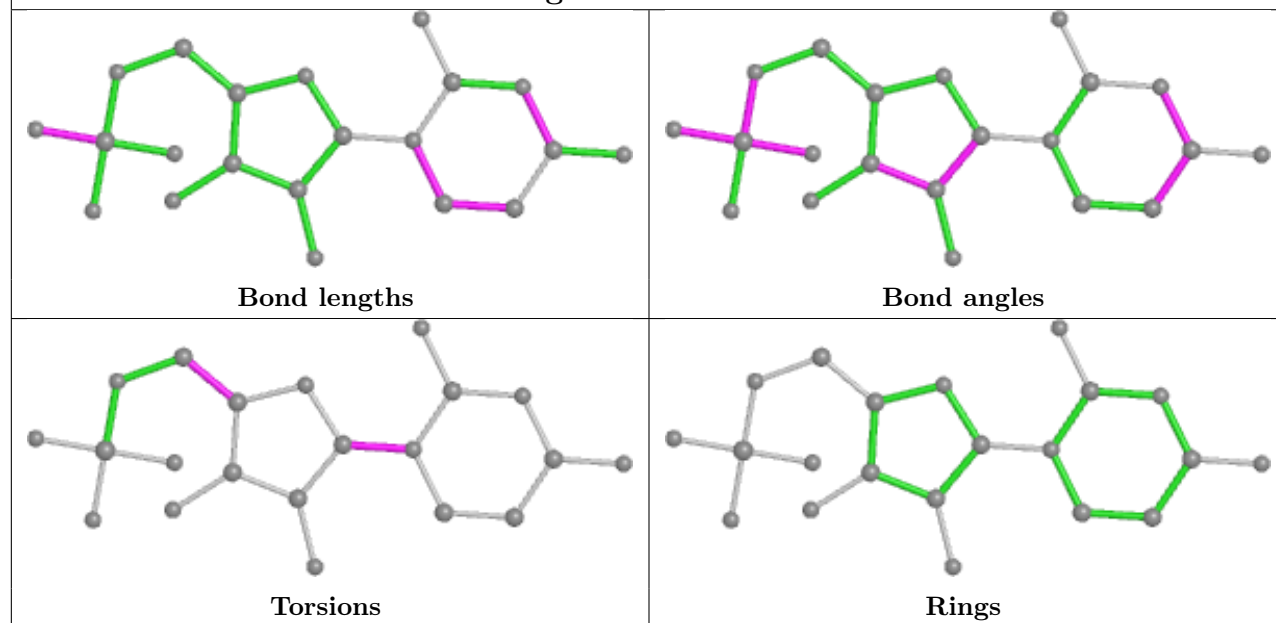
## Ligand U E 1093



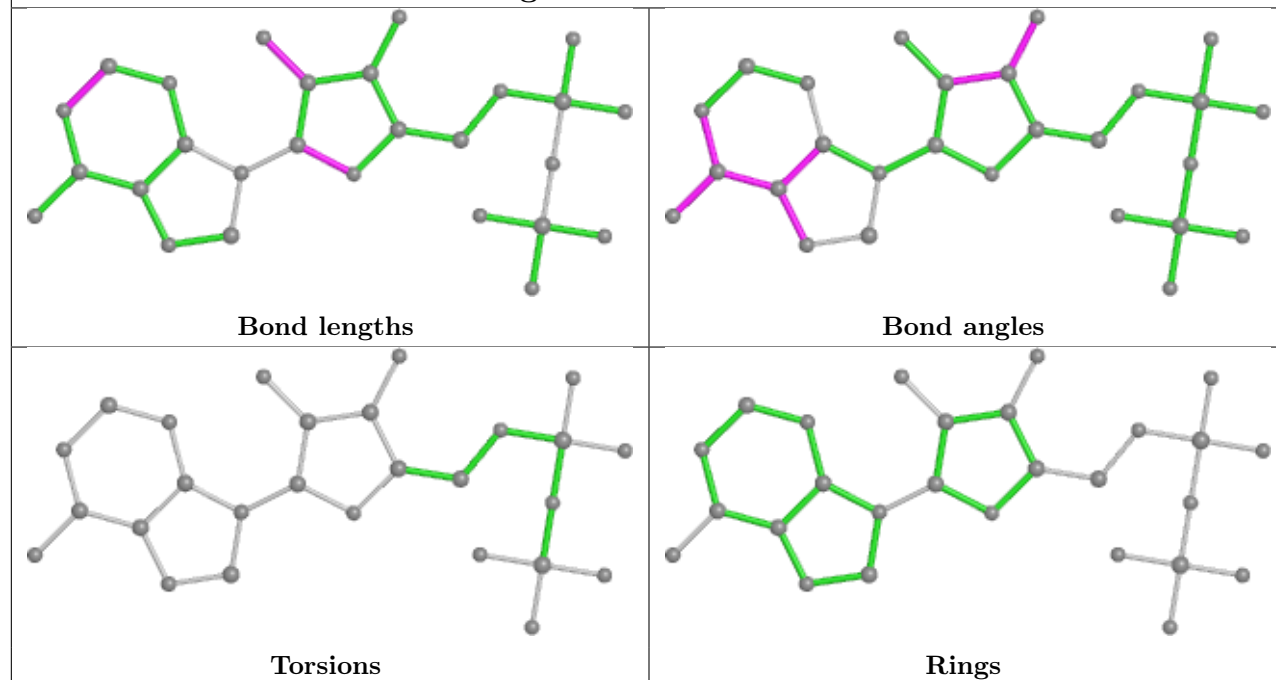
## Ligand ADP E 1089



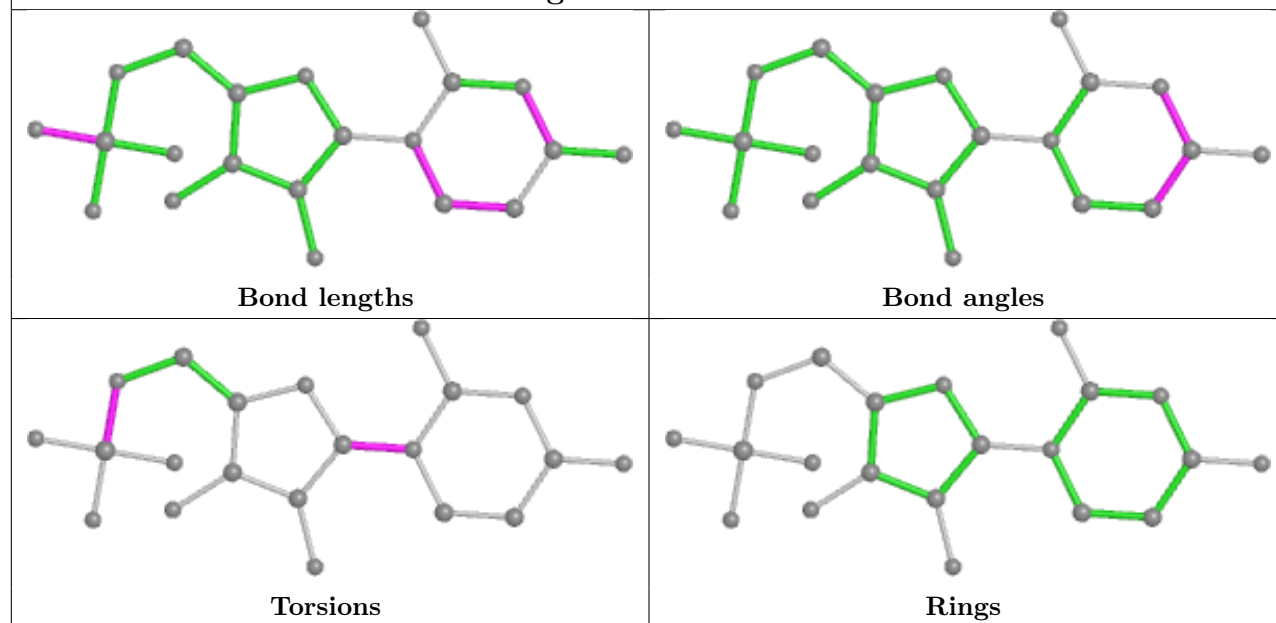
## Ligand U G 1093



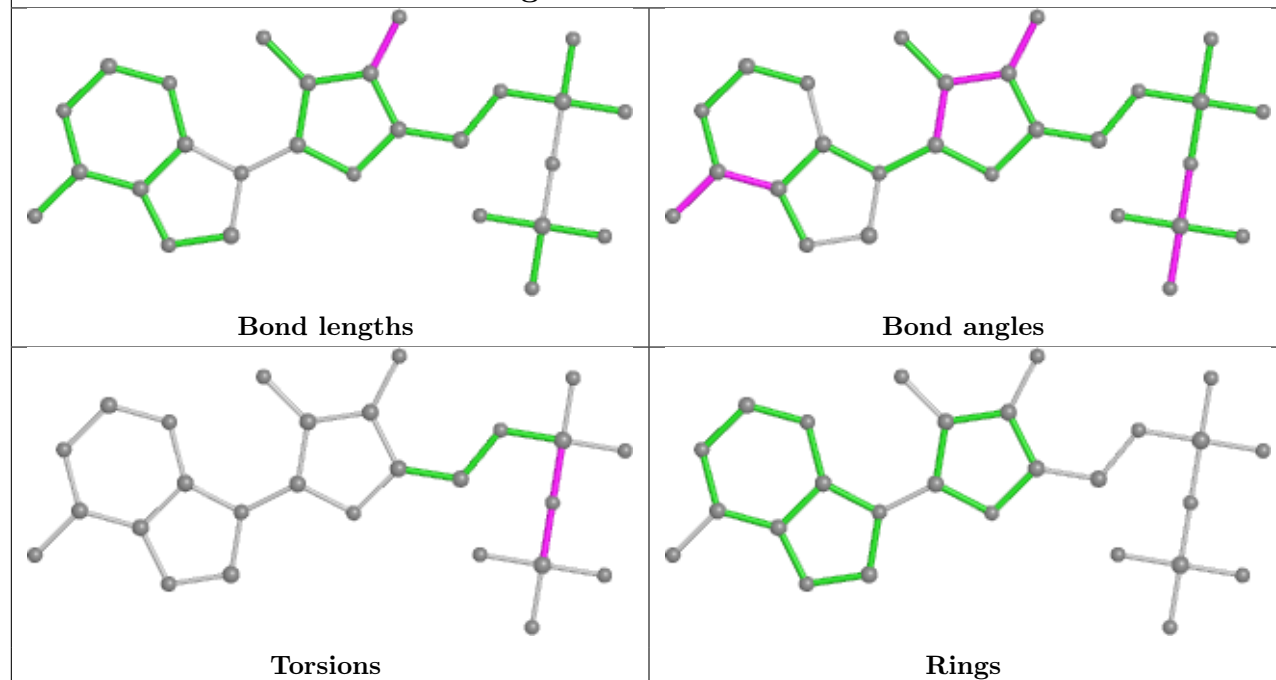
## Ligand ADP G 1089



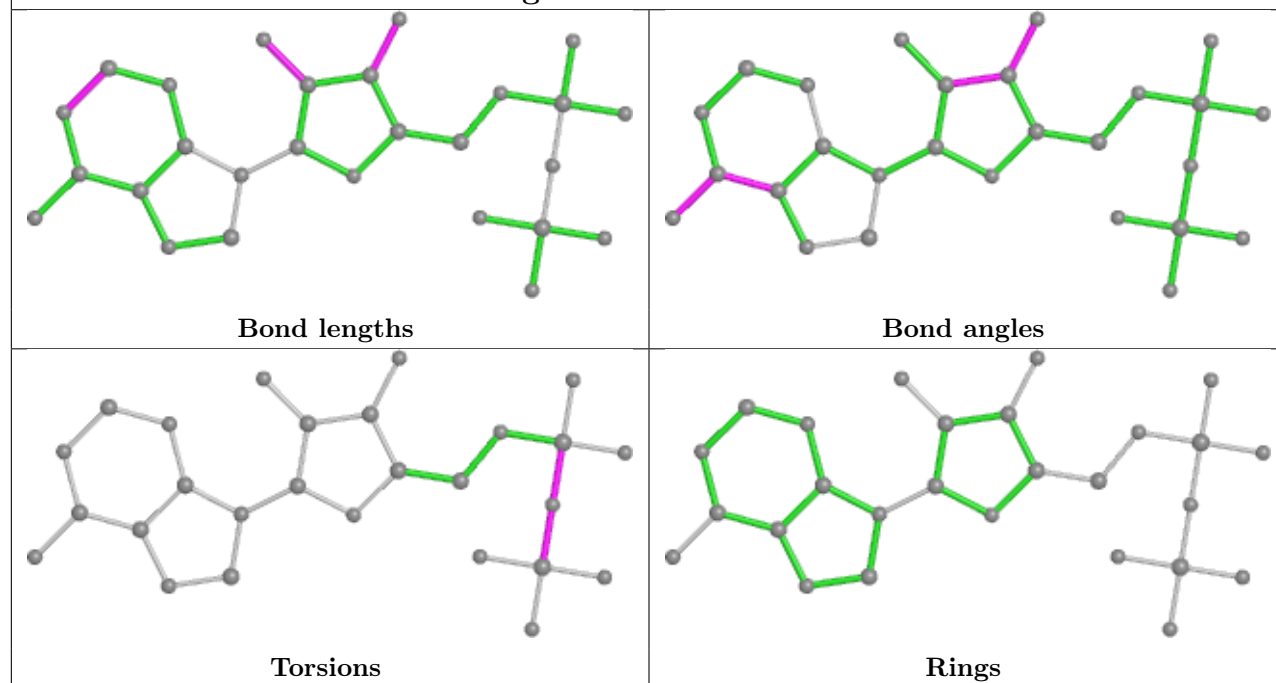
## Ligand U C 1093

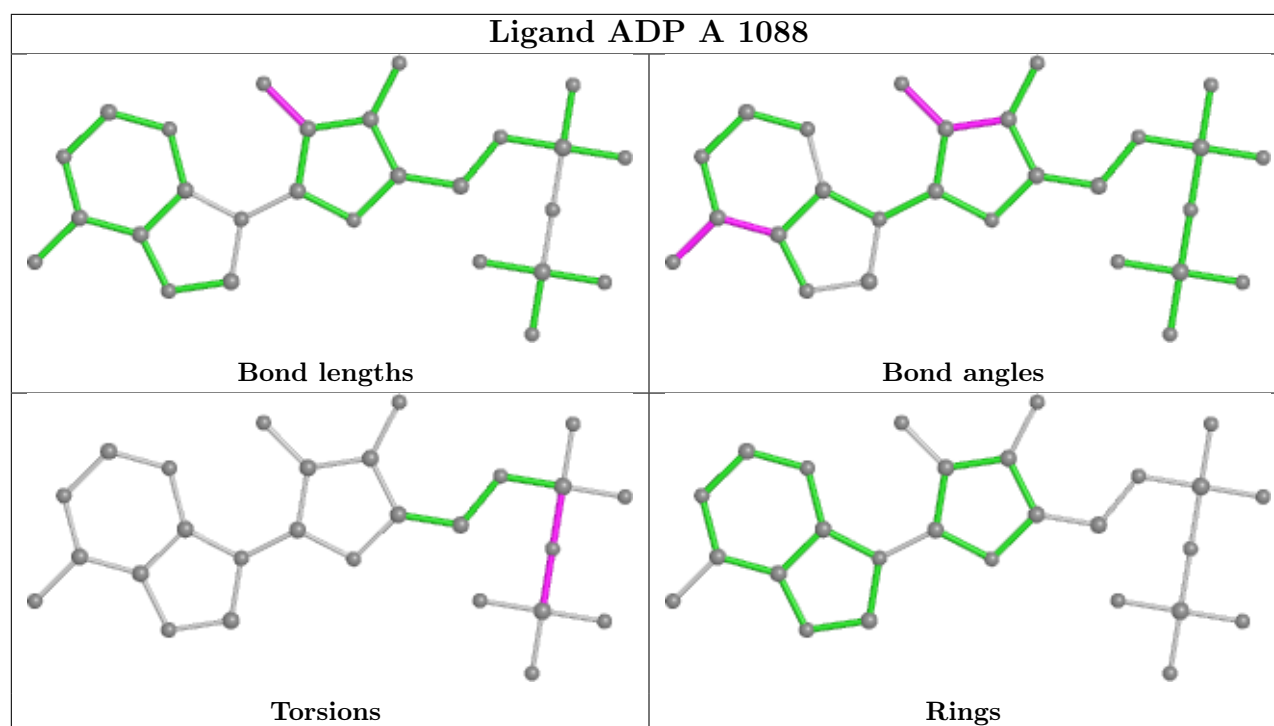


## Ligand ADP C 1090



## Ligand ADP E 1090





## 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     | 1058/1073 (98%) | -0.41  | 23 (2%) 62 66  | 17, 33, 73, 100       | 0     |
| 1   | C     | 1058/1073 (98%) | -0.28  | 25 (2%) 59 64  | 18, 35, 81, 100       | 0     |
| 1   | E     | 1058/1073 (98%) | -0.35  | 20 (1%) 66 71  | 17, 31, 75, 100       | 0     |
| 1   | G     | 1058/1073 (98%) | -0.11  | 40 (3%) 40 46  | 20, 42, 84, 100       | 0     |
| 2   | B     | 379/382 (99%)   | 0.02   | 16 (4%) 36 42  | 21, 48, 87, 100       | 0     |
| 2   | D     | 379/382 (99%)   | -0.04  | 11 (2%) 51 57  | 21, 40, 78, 100       | 0     |
| 2   | F     | 379/382 (99%)   | 0.17   | 24 (6%) 20 24  | 20, 47, 92, 100       | 0     |
| 2   | H     | 379/382 (99%)   | 0.47   | 36 (9%) 8 10   | 33, 63, 97, 100       | 0     |
| All | All   | 5748/5820 (98%) | -0.17  | 195 (3%) 45 51 | 17, 38, 84, 100       | 0     |

All (195) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 1   | MET  | 8.3  |
| 1   | E     | 1   | MET  | 8.0  |
| 1   | A     | 1   | MET  | 7.4  |
| 1   | G     | 1   | MET  | 6.9  |
| 1   | C     | 697 | ALA  | 5.4  |
| 1   | A     | 738 | PHE  | 5.4  |
| 1   | G     | 697 | ALA  | 5.2  |
| 2   | H     | 2   | ILE  | 5.1  |
| 1   | E     | 696 | THR  | 4.8  |
| 1   | A     | 698 | ILE  | 4.7  |
| 2   | H     | 380 | THR  | 4.6  |
| 1   | G     | 710 | TYR  | 4.4  |
| 1   | C     | 695 | VAL  | 4.4  |
| 2   | F     | 238 | LEU  | 4.2  |
| 1   | C     | 698 | ILE  | 4.2  |
| 1   | C     | 737 | TYR  | 4.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 738 | PHE  | 4.2  |
| 2   | F     | 237 | PHE  | 4.2  |
| 2   | H     | 153 | LEU  | 4.2  |
| 2   | D     | 2   | ILE  | 4.2  |
| 1   | A     | 740 | THR  | 4.1  |
| 1   | G     | 700 | MET  | 4.1  |
| 2   | H     | 152 | GLY  | 4.1  |
| 2   | F     | 268 | ILE  | 4.0  |
| 2   | F     | 2   | ILE  | 4.0  |
| 1   | G     | 740 | THR  | 4.0  |
| 1   | A     | 697 | ALA  | 4.0  |
| 1   | G     | 739 | GLN  | 4.0  |
| 1   | A     | 696 | THR  | 3.9  |
| 2   | B     | 2   | ILE  | 3.9  |
| 2   | F     | 250 | TYR  | 3.9  |
| 1   | E     | 701 | ALA  | 3.8  |
| 1   | A     | 737 | TYR  | 3.8  |
| 1   | G     | 737 | TYR  | 3.8  |
| 2   | H     | 157 | ASP  | 3.8  |
| 1   | G     | 741 | ALA  | 3.8  |
| 1   | C     | 696 | THR  | 3.8  |
| 2   | B     | 250 | TYR  | 3.8  |
| 1   | E     | 739 | GLN  | 3.7  |
| 1   | G     | 724 | ALA  | 3.7  |
| 1   | G     | 557 | THR  | 3.7  |
| 1   | C     | 738 | PHE  | 3.6  |
| 1   | G     | 705 | ALA  | 3.6  |
| 1   | G     | 680 | HIS  | 3.6  |
| 2   | F     | 380 | THR  | 3.5  |
| 1   | A     | 716 | PRO  | 3.5  |
| 2   | H     | 150 | PHE  | 3.5  |
| 1   | E     | 697 | ALA  | 3.5  |
| 1   | E     | 741 | ALA  | 3.5  |
| 1   | A     | 750 | VAL  | 3.5  |
| 2   | D     | 269 | CYS  | 3.4  |
| 2   | F     | 201 | ALA  | 3.4  |
| 1   | G     | 698 | ILE  | 3.4  |
| 2   | D     | 268 | ILE  | 3.4  |
| 2   | H     | 160 | LYS  | 3.4  |
| 1   | G     | 702 | VAL  | 3.3  |
| 2   | F     | 246 | ALA  | 3.3  |
| 2   | H     | 31  | VAL  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 738 | PHE  | 3.3  |
| 1   | A     | 739 | GLN  | 3.2  |
| 1   | A     | 341 | GLY  | 3.2  |
| 1   | C     | 701 | ALA  | 3.2  |
| 2   | B     | 156 | MET  | 3.2  |
| 2   | F     | 379 | LYS  | 3.2  |
| 1   | G     | 734 | LEU  | 3.2  |
| 1   | A     | 732 | ALA  | 3.2  |
| 2   | H     | 165 | ALA  | 3.2  |
| 2   | H     | 156 | MET  | 3.2  |
| 1   | E     | 2   | PRO  | 3.2  |
| 1   | A     | 701 | ALA  | 3.1  |
| 2   | D     | 238 | LEU  | 3.1  |
| 1   | C     | 703 | GLU  | 3.1  |
| 2   | B     | 152 | GLY  | 3.1  |
| 1   | G     | 732 | ALA  | 3.1  |
| 1   | A     | 342 | GLY  | 3.0  |
| 1   | C     | 741 | ALA  | 3.0  |
| 2   | H     | 151 | PRO  | 3.0  |
| 1   | E     | 700 | MET  | 3.0  |
| 1   | C     | 740 | THR  | 3.0  |
| 2   | B     | 155 | GLY  | 2.9  |
| 2   | B     | 248 | ASP  | 2.9  |
| 2   | H     | 138 | PRO  | 2.9  |
| 1   | C     | 739 | GLN  | 2.9  |
| 1   | G     | 559 | ARG  | 2.9  |
| 1   | C     | 700 | MET  | 2.9  |
| 1   | G     | 701 | ALA  | 2.9  |
| 2   | B     | 147 | ALA  | 2.9  |
| 1   | C     | 805 | ILE  | 2.9  |
| 2   | H     | 246 | ALA  | 2.9  |
| 2   | H     | 320 | THR  | 2.9  |
| 1   | E     | 750 | VAL  | 2.8  |
| 2   | B     | 246 | ALA  | 2.8  |
| 1   | G     | 703 | GLU  | 2.8  |
| 1   | G     | 696 | THR  | 2.8  |
| 2   | F     | 248 | ASP  | 2.8  |
| 2   | B     | 380 | THR  | 2.8  |
| 1   | G     | 735 | ARG  | 2.8  |
| 2   | H     | 142 | LEU  | 2.8  |
| 1   | A     | 702 | VAL  | 2.8  |
| 2   | D     | 250 | TYR  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 724  | ALA  | 2.7  |
| 2   | H     | 136  | ASP  | 2.7  |
| 2   | D     | 155  | GLY  | 2.7  |
| 1   | G     | 558  | ASP  | 2.7  |
| 1   | A     | 703  | GLU  | 2.7  |
| 1   | E     | 675  | ARG  | 2.7  |
| 2   | F     | 228  | VAL  | 2.7  |
| 1   | G     | 805  | ILE  | 2.7  |
| 2   | F     | 231  | MET  | 2.7  |
| 1   | G     | 1073 | LYS  | 2.7  |
| 2   | B     | 150  | PHE  | 2.7  |
| 1   | G     | 683  | GLU  | 2.7  |
| 2   | B     | 154  | ASN  | 2.7  |
| 1   | G     | 731  | GLU  | 2.6  |
| 2   | F     | 233  | PRO  | 2.6  |
| 2   | F     | 166  | GLU  | 2.6  |
| 2   | H     | 159  | ALA  | 2.6  |
| 1   | A     | 700  | MET  | 2.6  |
| 2   | B     | 153  | LEU  | 2.6  |
| 1   | G     | 675  | ARG  | 2.6  |
| 1   | G     | 695  | VAL  | 2.6  |
| 2   | F     | 377  | TYR  | 2.6  |
| 2   | H     | 53   | VAL  | 2.6  |
| 2   | H     | 268  | ILE  | 2.6  |
| 1   | C     | 733  | ASP  | 2.6  |
| 1   | E     | 737  | TYR  | 2.5  |
| 2   | D     | 154  | ASN  | 2.5  |
| 1   | G     | 676  | GLU  | 2.5  |
| 2   | D     | 248  | ASP  | 2.5  |
| 2   | H     | 248  | ASP  | 2.5  |
| 2   | H     | 250  | TYR  | 2.5  |
| 2   | F     | 266  | PHE  | 2.5  |
| 1   | G     | 479  | VAL  | 2.5  |
| 1   | G     | 750  | VAL  | 2.5  |
| 1   | C     | 693  | ALA  | 2.5  |
| 1   | C     | 736  | ARG  | 2.5  |
| 2   | H     | 154  | ASN  | 2.5  |
| 2   | H     | 377  | TYR  | 2.5  |
| 2   | D     | 156  | MET  | 2.4  |
| 1   | E     | 680  | HIS  | 2.4  |
| 1   | A     | 735  | ARG  | 2.4  |
| 2   | F     | 378  | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 699  | GLU  | 2.4  |
| 1   | C     | 1073 | LYS  | 2.4  |
| 1   | E     | 751  | LEU  | 2.3  |
| 2   | H     | 166  | GLU  | 2.3  |
| 2   | H     | 189  | GLU  | 2.3  |
| 1   | C     | 702  | VAL  | 2.3  |
| 1   | G     | 733  | ASP  | 2.3  |
| 2   | H     | 188  | ASP  | 2.3  |
| 1   | C     | 750  | VAL  | 2.3  |
| 2   | F     | 165  | ALA  | 2.3  |
| 1   | G     | 840  | ILE  | 2.3  |
| 2   | F     | 55   | LEU  | 2.3  |
| 1   | A     | 368  | ALA  | 2.3  |
| 1   | E     | 705  | ALA  | 2.3  |
| 2   | H     | 269  | CYS  | 2.3  |
| 2   | B     | 148  | ARG  | 2.3  |
| 2   | H     | 319  | ALA  | 2.2  |
| 2   | H     | 164  | THR  | 2.2  |
| 2   | H     | 266  | PHE  | 2.2  |
| 1   | E     | 343  | ARG  | 2.2  |
| 1   | E     | 707  | GLU  | 2.2  |
| 1   | E     | 695  | VAL  | 2.2  |
| 2   | F     | 230  | LYS  | 2.2  |
| 1   | G     | 699  | GLU  | 2.2  |
| 2   | D     | 320  | THR  | 2.2  |
| 1   | G     | 2    | PRO  | 2.2  |
| 1   | A     | 741  | ALA  | 2.2  |
| 2   | H     | 52   | ILE  | 2.1  |
| 1   | A     | 695  | VAL  | 2.1  |
| 1   | G     | 682  | VAL  | 2.1  |
| 1   | E     | 740  | THR  | 2.1  |
| 2   | D     | 246  | ALA  | 2.1  |
| 2   | B     | 255  | ILE  | 2.1  |
| 1   | G     | 678  | PHE  | 2.1  |
| 1   | C     | 683  | GLU  | 2.1  |
| 1   | C     | 751  | LEU  | 2.1  |
| 2   | H     | 376  | GLN  | 2.1  |
| 1   | E     | 1073 | LYS  | 2.1  |
| 2   | B     | 268  | ILE  | 2.1  |
| 2   | F     | 205  | ILE  | 2.1  |
| 1   | C     | 734  | LEU  | 2.1  |
| 1   | A     | 736  | ARG  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 151 | PRO  | 2.1  |
| 1   | G     | 343 | ARG  | 2.1  |
| 2   | H     | 162 | VAL  | 2.1  |
| 1   | G     | 686 | LYS  | 2.1  |
| 2   | F     | 271 | GLY  | 2.1  |
| 2   | H     | 238 | LEU  | 2.0  |
| 2   | H     | 261 | THR  | 2.0  |
| 2   | F     | 192 | PHE  | 2.0  |
| 2   | F     | 247 | PRO  | 2.0  |
| 2   | H     | 30  | VAL  | 2.0  |
| 1   | C     | 111 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 6   | CL   | E     | 1084 | 1/1   | 0.82 | 0.15 | 74,74,74,74                 | 0     |
| 6   | CL   | G     | 1084 | 1/1   | 0.83 | 0.22 | 72,72,72,72                 | 0     |
| 6   | CL   | H     | 385  | 1/1   | 0.84 | 0.07 | 82,82,82,82                 | 0     |
| 6   | CL   | C     | 1083 | 1/1   | 0.91 | 0.16 | 77,77,77,77                 | 0     |
| 6   | CL   | A     | 1083 | 1/1   | 0.91 | 0.10 | 66,66,66,66                 | 0     |
| 6   | CL   | G     | 1086 | 1/1   | 0.92 | 0.07 | 54,54,54,54                 | 0     |
| 5   | PO4  | C     | 1088 | 5/5   | 0.92 | 0.21 | 80,80,80,80                 | 0     |
| 6   | CL   | E     | 1087 | 1/1   | 0.94 | 0.06 | 54,54,54,54                 | 0     |
| 10  | U    | G     | 1093 | 21/21 | 0.94 | 0.12 | 31,57,80,85                 | 0     |
| 6   | CL   | H     | 384  | 1/1   | 0.95 | 0.13 | 67,67,67,67                 | 0     |
| 4   | K    | E     | 1081 | 1/1   | 0.95 | 0.06 | 42,42,42,42                 | 0     |
| 8   | ORN  | A     | 1089 | 9/9   | 0.95 | 0.18 | 24,29,36,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 10  | U    | C     | 1093 | 21/21 | 0.95 | 0.12 | 33,51,83,89                 | 0     |
| 6   | CL   | C     | 1086 | 1/1   | 0.95 | 0.11 | 67,67,67,67                 | 0     |
| 4   | K    | C     | 1082 | 1/1   | 0.96 | 0.06 | 44,44,44,44                 | 0     |
| 8   | ORN  | G     | 1091 | 9/9   | 0.96 | 0.17 | 28,33,36,63                 | 0     |
| 10  | U    | A     | 1091 | 21/21 | 0.96 | 0.10 | 28,58,80,81                 | 0     |
| 6   | CL   | C     | 1084 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 10  | U    | E     | 1093 | 21/21 | 0.96 | 0.10 | 37,54,80,89                 | 0     |
| 6   | CL   | A     | 1086 | 1/1   | 0.96 | 0.06 | 56,56,56,56                 | 0     |
| 4   | K    | G     | 1081 | 1/1   | 0.97 | 0.06 | 46,46,46,46                 | 0     |
| 4   | K    | H     | 383  | 1/1   | 0.97 | 0.11 | 64,64,64,64                 | 0     |
| 6   | CL   | G     | 1088 | 1/1   | 0.97 | 0.17 | 67,67,67,67                 | 0     |
| 8   | ORN  | C     | 1091 | 9/9   | 0.97 | 0.19 | 20,29,35,39                 | 0     |
| 8   | ORN  | E     | 1091 | 9/9   | 0.97 | 0.13 | 16,25,37,40                 | 0     |
| 6   | CL   | G     | 1085 | 1/1   | 0.98 | 0.06 | 46,46,46,46                 | 0     |
| 4   | K    | E     | 1083 | 1/1   | 0.98 | 0.05 | 58,58,58,58                 | 0     |
| 6   | CL   | G     | 1087 | 1/1   | 0.98 | 0.09 | 81,81,81,81                 | 0     |
| 6   | CL   | E     | 1085 | 1/1   | 0.98 | 0.05 | 49,49,49,49                 | 0     |
| 9   | NET  | A     | 1090 | 9/9   | 0.98 | 0.10 | 18,23,28,38                 | 0     |
| 9   | NET  | E     | 1092 | 9/9   | 0.98 | 0.18 | 15,23,27,28                 | 0     |
| 4   | K    | A     | 1082 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 4   | K    | B     | 383  | 1/1   | 0.98 | 0.06 | 45,45,45,45                 | 0     |
| 7   | ADP  | C     | 1090 | 27/27 | 0.98 | 0.08 | 26,42,61,77                 | 0     |
| 7   | ADP  | G     | 1090 | 27/27 | 0.98 | 0.09 | 29,47,80,89                 | 0     |
| 4   | K    | E     | 1077 | 1/1   | 0.99 | 0.12 | 30,30,30,30                 | 0     |
| 6   | CL   | C     | 1087 | 1/1   | 0.99 | 0.15 | 63,63,63,63                 | 0     |
| 6   | CL   | D     | 384  | 1/1   | 0.99 | 0.07 | 34,34,34,34                 | 0     |
| 4   | K    | E     | 1080 | 1/1   | 0.99 | 0.06 | 27,27,27,27                 | 0     |
| 4   | K    | A     | 1077 | 1/1   | 0.99 | 0.08 | 27,27,27,27                 | 0     |
| 6   | CL   | E     | 1086 | 1/1   | 0.99 | 0.07 | 41,41,41,41                 | 0     |
| 4   | K    | A     | 1080 | 1/1   | 0.99 | 0.08 | 29,29,29,29                 | 0     |
| 6   | CL   | E     | 1088 | 1/1   | 0.99 | 0.10 | 44,44,44,44                 | 0     |
| 6   | CL   | G     | 1082 | 1/1   | 0.99 | 0.10 | 29,29,29,29                 | 0     |
| 4   | K    | F     | 383  | 1/1   | 0.99 | 0.07 | 36,36,36,36                 | 0     |
| 4   | K    | G     | 1077 | 1/1   | 0.99 | 0.10 | 38,38,38,38                 | 0     |
| 4   | K    | G     | 1080 | 1/1   | 0.99 | 0.07 | 38,38,38,38                 | 0     |
| 3   | MN   | C     | 1075 | 1/1   | 0.99 | 0.07 | 25,25,25,25                 | 0     |
| 4   | K    | G     | 1083 | 1/1   | 0.99 | 0.05 | 52,52,52,52                 | 0     |
| 3   | MN   | C     | 1079 | 1/1   | 0.99 | 0.05 | 46,46,46,46                 | 0     |
| 5   | PO4  | A     | 1078 | 5/5   | 0.99 | 0.08 | 17,21,24,29                 | 0     |
| 7   | ADP  | A     | 1087 | 27/27 | 0.99 | 0.09 | 16,22,31,38                 | 0     |
| 7   | ADP  | A     | 1088 | 27/27 | 0.99 | 0.07 | 20,33,47,60                 | 0     |
| 7   | ADP  | C     | 1089 | 27/27 | 0.99 | 0.10 | 16,23,31,44                 | 0     |

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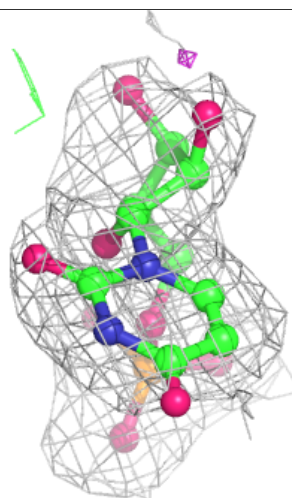
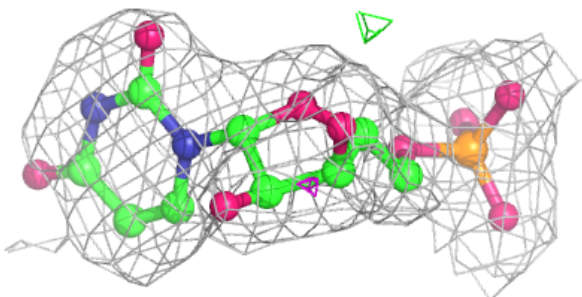
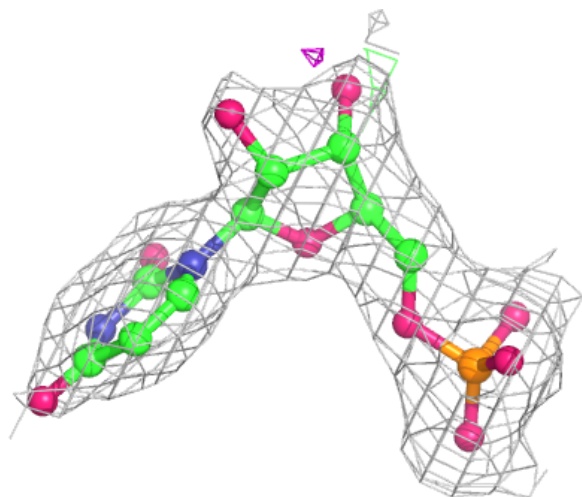
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 5   | PO4  | C     | 1078 | 5/5   | 0.99 | 0.09 | 16,22,24,25                 | 0     |
| 7   | ADP  | E     | 1089 | 27/27 | 0.99 | 0.12 | 15,26,34,36                 | 0     |
| 7   | ADP  | E     | 1090 | 27/27 | 0.99 | 0.06 | 23,35,48,56                 | 0     |
| 7   | ADP  | G     | 1089 | 27/27 | 0.99 | 0.11 | 17,27,35,41                 | 0     |
| 4   | K    | C     | 1077 | 1/1   | 0.99 | 0.11 | 27,27,27,27                 | 0     |
| 5   | PO4  | E     | 1078 | 5/5   | 0.99 | 0.08 | 19,22,26,27                 | 0     |
| 5   | PO4  | G     | 1078 | 5/5   | 0.99 | 0.07 | 17,24,31,35                 | 0     |
| 6   | CL   | A     | 1081 | 1/1   | 0.99 | 0.08 | 28,28,28,28                 | 0     |
| 4   | K    | C     | 1080 | 1/1   | 0.99 | 0.08 | 36,36,36,36                 | 0     |
| 6   | CL   | A     | 1084 | 1/1   | 0.99 | 0.05 | 40,40,40,40                 | 0     |
| 9   | NET  | C     | 1092 | 9/9   | 0.99 | 0.13 | 16,21,23,29                 | 0     |
| 6   | CL   | A     | 1085 | 1/1   | 0.99 | 0.06 | 39,39,39,39                 | 0     |
| 9   | NET  | G     | 1092 | 9/9   | 0.99 | 0.13 | 18,28,29,37                 | 0     |
| 3   | MN   | G     | 1079 | 1/1   | 0.99 | 0.05 | 47,47,47,47                 | 0     |
| 6   | CL   | C     | 1081 | 1/1   | 0.99 | 0.10 | 29,29,29,29                 | 0     |
| 4   | K    | D     | 383  | 1/1   | 0.99 | 0.03 | 34,34,34,34                 | 0     |
| 4   | K    | E     | 1076 | 1/1   | 0.99 | 0.09 | 25,25,25,25                 | 0     |
| 3   | MN   | E     | 1075 | 1/1   | 1.00 | 0.08 | 27,27,27,27                 | 0     |
| 6   | CL   | F     | 384  | 1/1   | 1.00 | 0.06 | 32,32,32,32                 | 0     |
| 3   | MN   | E     | 1079 | 1/1   | 1.00 | 0.05 | 41,41,41,41                 | 0     |
| 3   | MN   | G     | 1074 | 1/1   | 1.00 | 0.07 | 31,31,31,31                 | 0     |
| 3   | MN   | G     | 1075 | 1/1   | 1.00 | 0.08 | 28,28,28,28                 | 0     |
| 3   | MN   | A     | 1079 | 1/1   | 1.00 | 0.05 | 37,37,37,37                 | 0     |
| 6   | CL   | C     | 1085 | 1/1   | 1.00 | 0.07 | 39,39,39,39                 | 0     |
| 4   | K    | A     | 1076 | 1/1   | 1.00 | 0.07 | 21,21,21,21                 | 0     |
| 3   | MN   | C     | 1074 | 1/1   | 1.00 | 0.08 | 27,27,27,27                 | 0     |
| 3   | MN   | A     | 1074 | 1/1   | 1.00 | 0.07 | 25,25,25,25                 | 0     |
| 6   | CL   | E     | 1082 | 1/1   | 1.00 | 0.14 | 24,24,24,24                 | 0     |
| 3   | MN   | A     | 1075 | 1/1   | 1.00 | 0.06 | 23,23,23,23                 | 0     |
| 3   | MN   | E     | 1074 | 1/1   | 1.00 | 0.09 | 27,27,27,27                 | 0     |
| 4   | K    | G     | 1076 | 1/1   | 1.00 | 0.09 | 28,28,28,28                 | 0     |
| 4   | K    | C     | 1076 | 1/1   | 1.00 | 0.07 | 22,22,22,22                 | 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 U G 1093:**

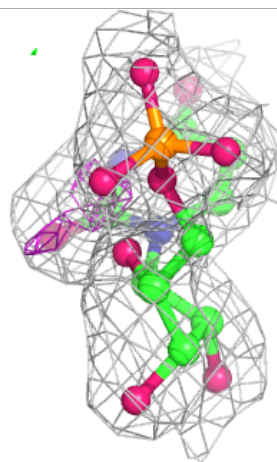
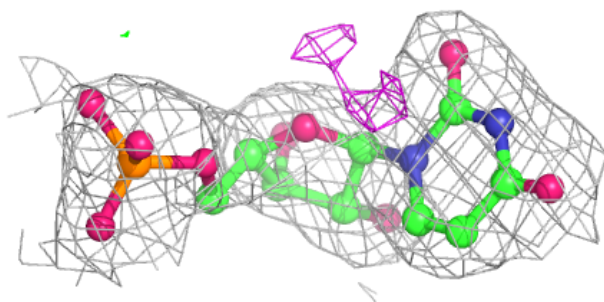
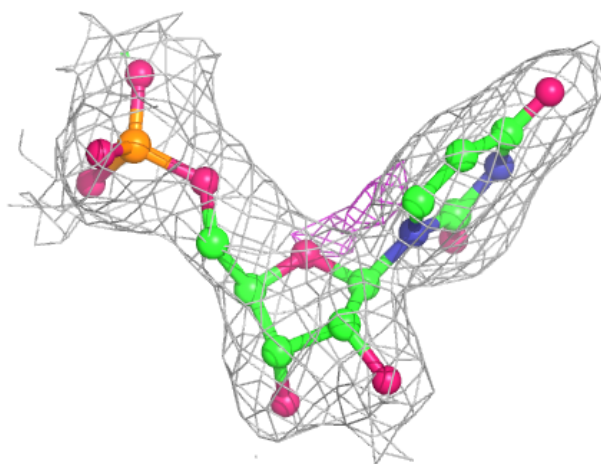
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





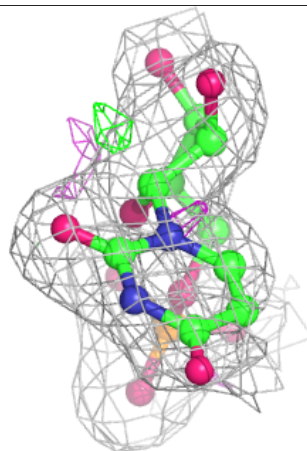
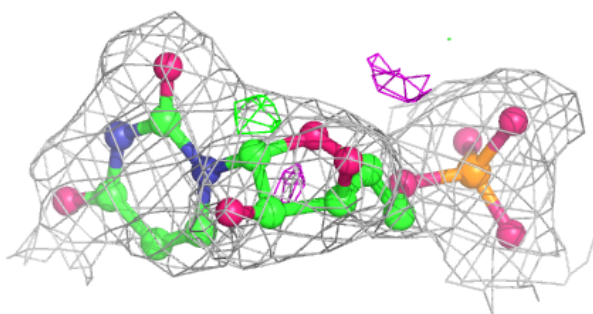
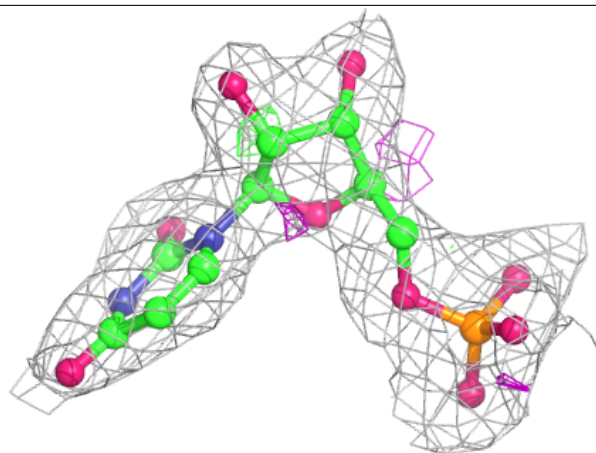
**Electron density around U C 1093:**

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



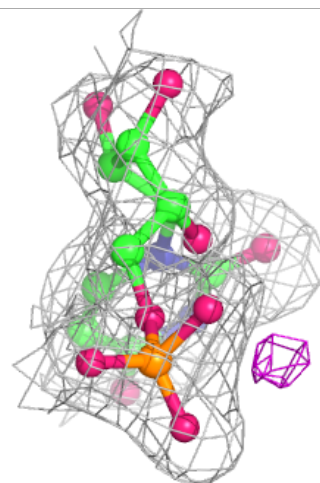
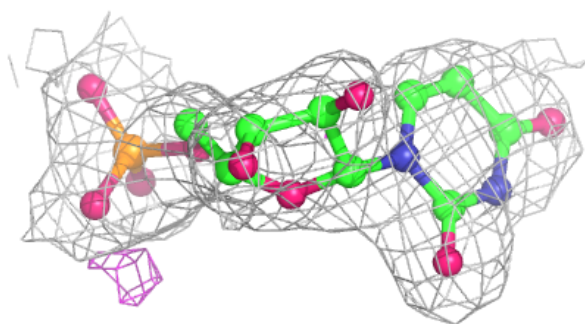
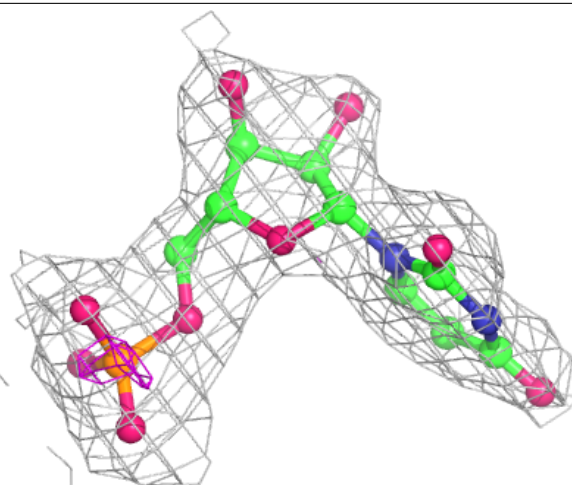
**Electron density around U A 1091:**

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



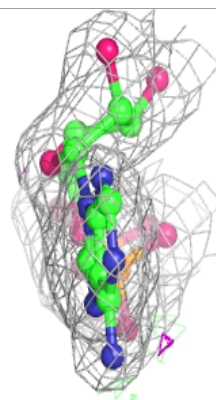
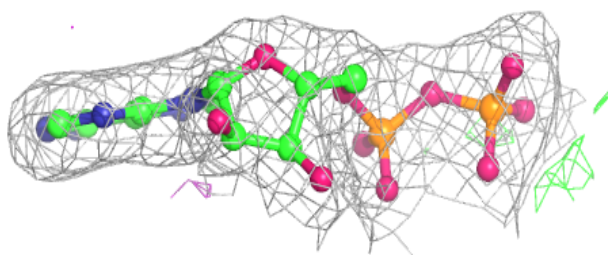
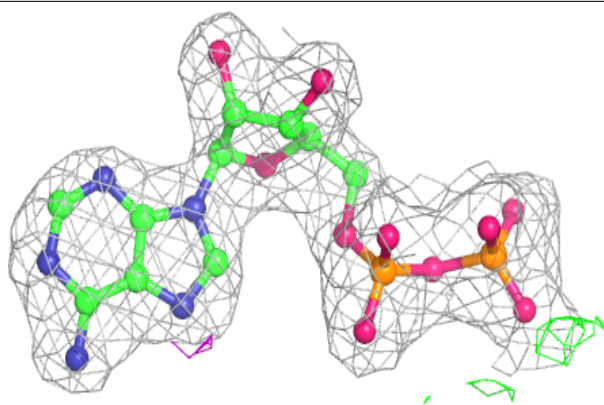
**Electron density around U E 1093:**

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

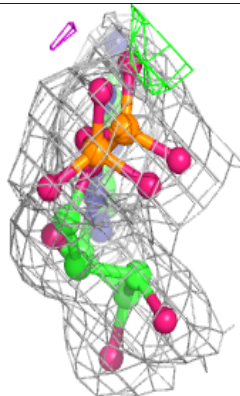
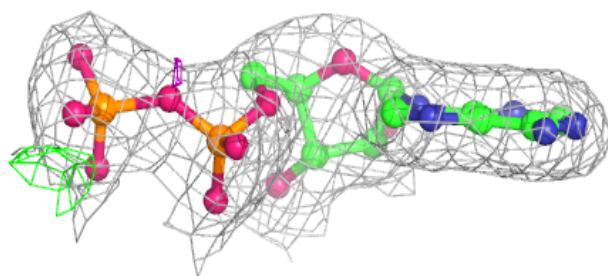
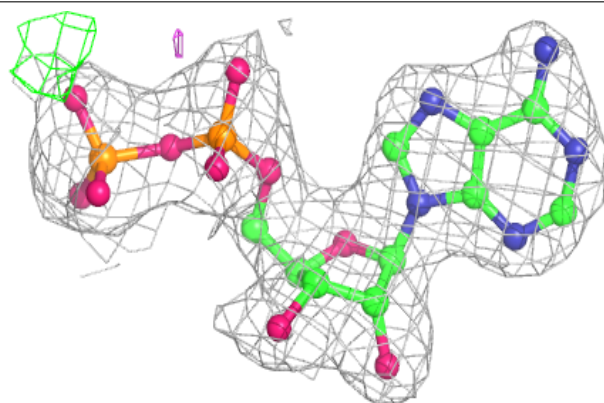


**Electron density around ADP C 1090:**

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

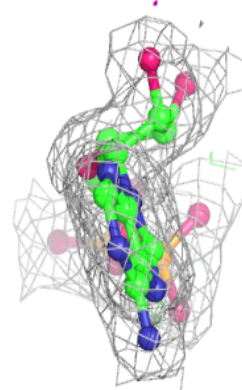
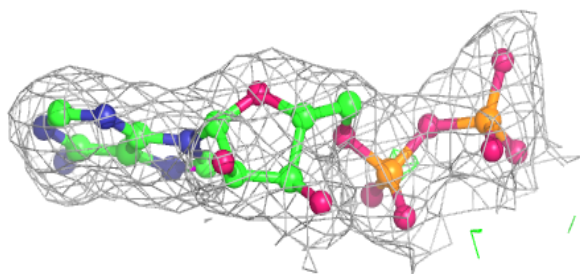
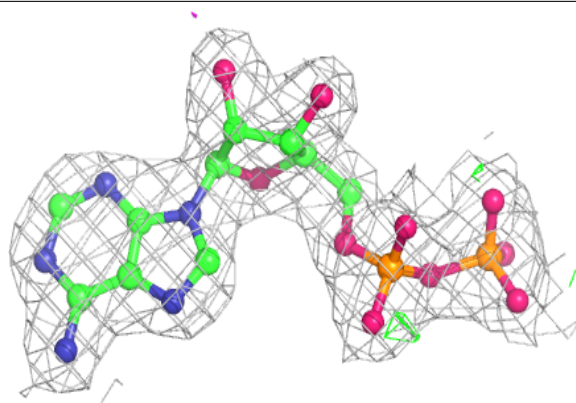
**Electron density around ADP G 1090:**

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

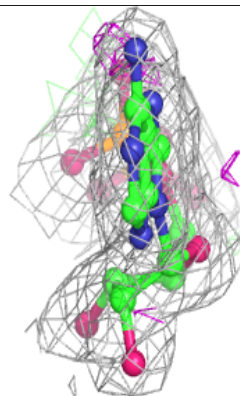
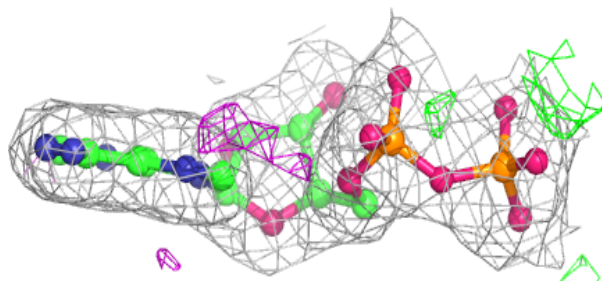
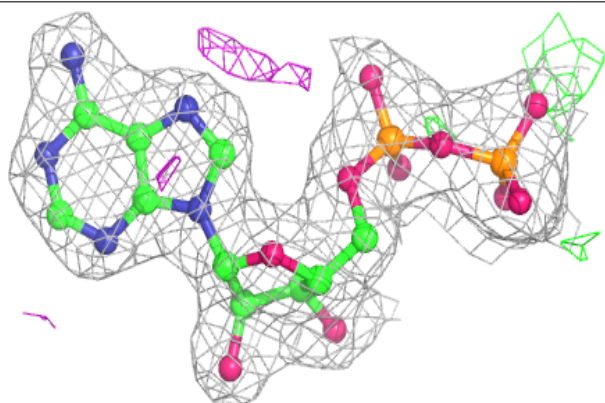


**Electron density around ADP A 1087:**

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

**Electron density around ADP A 1088:**

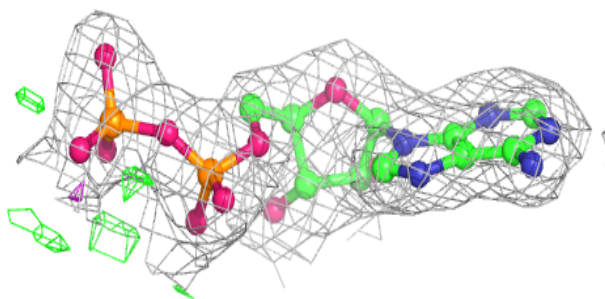
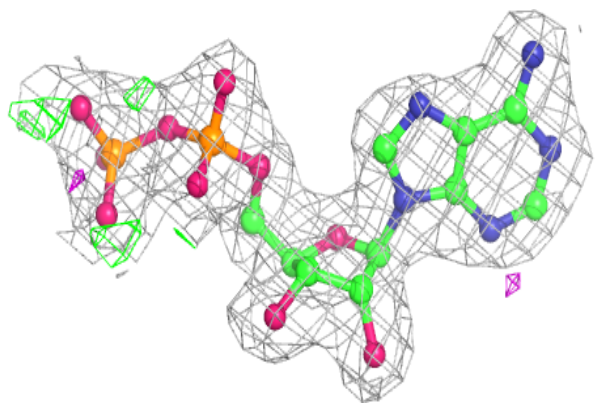
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



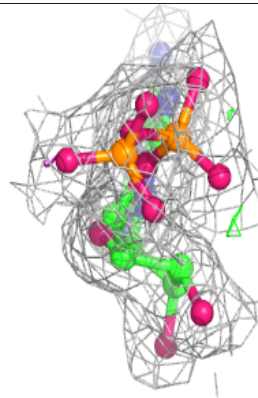
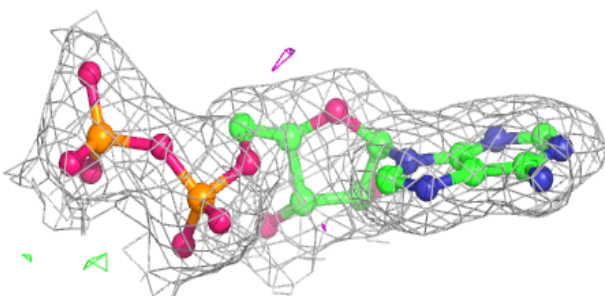
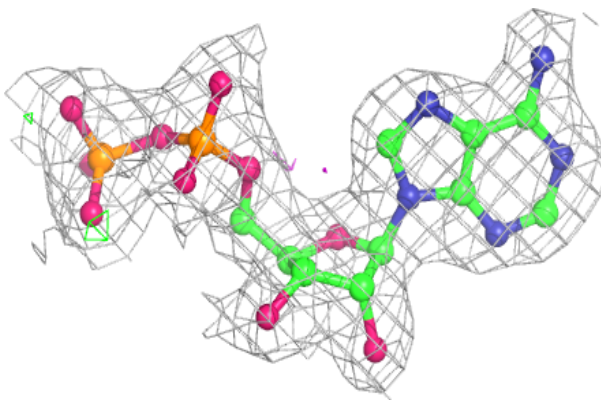


**Electron density around ADP C 1089:**

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

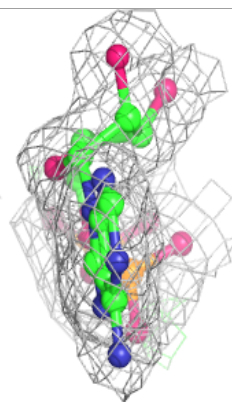
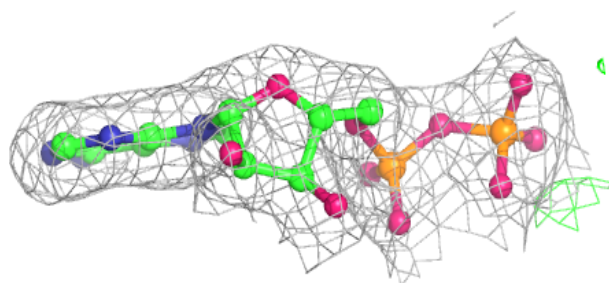
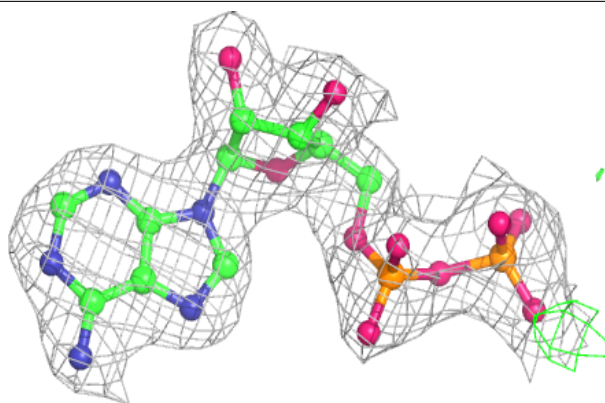
**Electron density around ADP E 1089:**

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

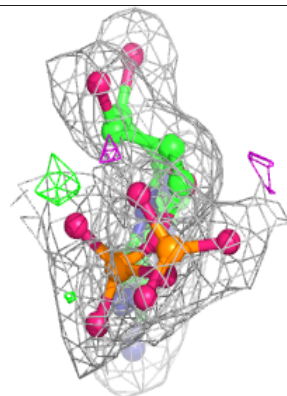
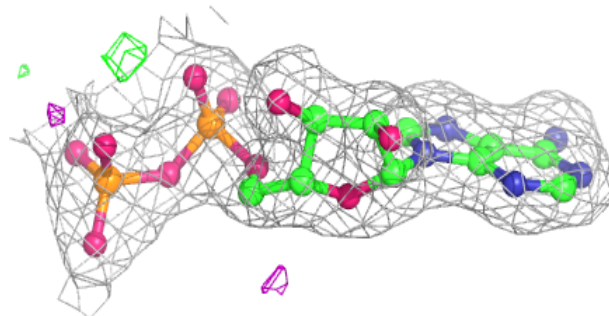
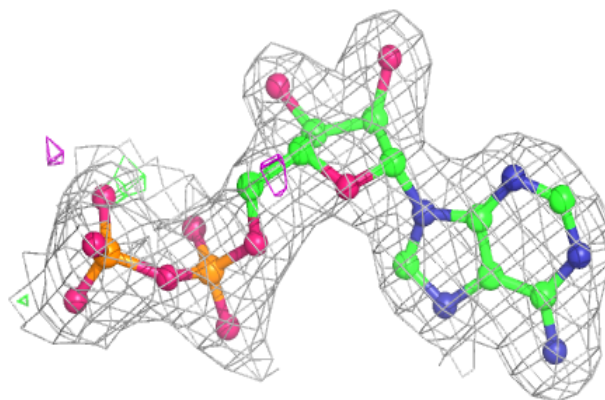


**Electron density around ADP E 1090:**

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

**Electron density around ADP G 1089:**

$2mF_o-DF_c$  (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.