



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:40 am BST

PDB ID : 5ZLP  
Title : Crystal structure of glutamine synthetase from helicobacter pylori  
Authors : Joo, H.K.; Lee, J.Y.  
Deposited on : 2018-03-29  
Resolution : 2.93 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 : 2.11  
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) : 2.11

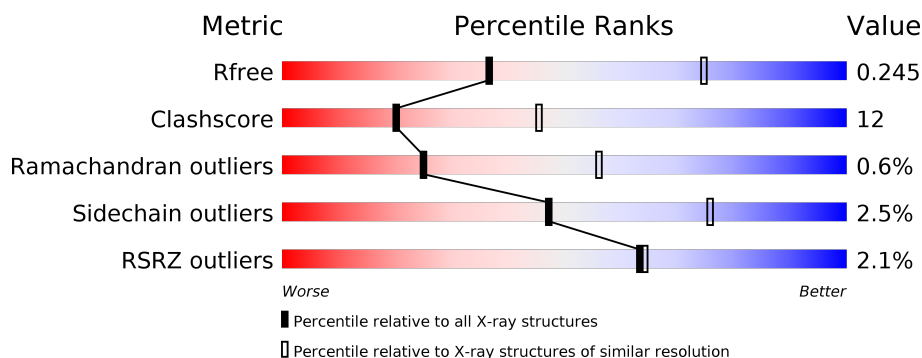
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2969 (2.98-2.90)                                      |
| Clashscore            | 141614                      | 3218 (2.98-2.90)                                      |
| Ramachandran outliers | 138981                      | 3122 (2.98-2.90)                                      |
| Sidechain outliers    | 138945                      | 3124 (2.98-2.90)                                      |
| RSRZ outliers         | 127900                      | 2902 (2.98-2.90)                                      |

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 on 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     | 481    | <div> <div>3%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div> </div> |
| 1   | B     | 481    | <div> <div>3%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div>..</div> </div> </div> |
| 1   | C     | 481    | <div> <div>3%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>..</div> </div> </div> |
| 1   | D     | 481    | <div> <div>2%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div>..</div> </div> </div> |
| 1   | E     | 481    | <div> <div>3%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>..</div> </div> </div> |
| 1   | F     | 481    | <div> <div>2%</div> <div> <div></div> <div>64%</div> <div>33%</div> <div>..</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 481    |                  |
| 1   | H     | 481    |                  |
| 1   | I     | 481    |                  |
| 1   | J     | 481    |                  |
| 1   | K     | 481    |                  |
| 1   | L     | 481    |                  |

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   | MG   | J     | 503 | -         | -        | -       | X                |

## 2 Entry composition

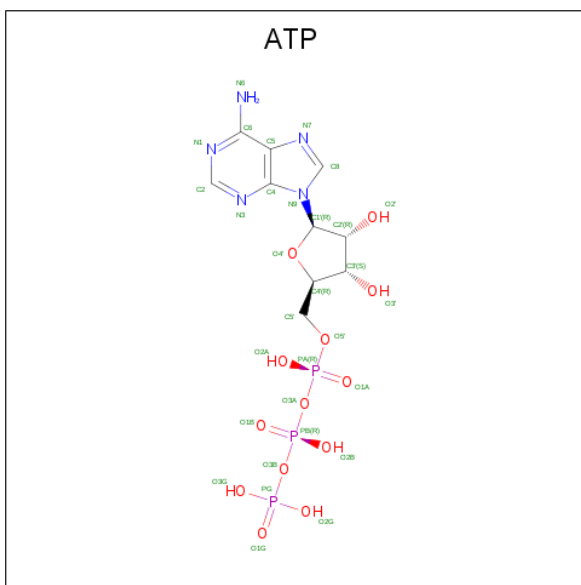
There are 7 unique types of molecules in this entry. The entry contains 46003 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

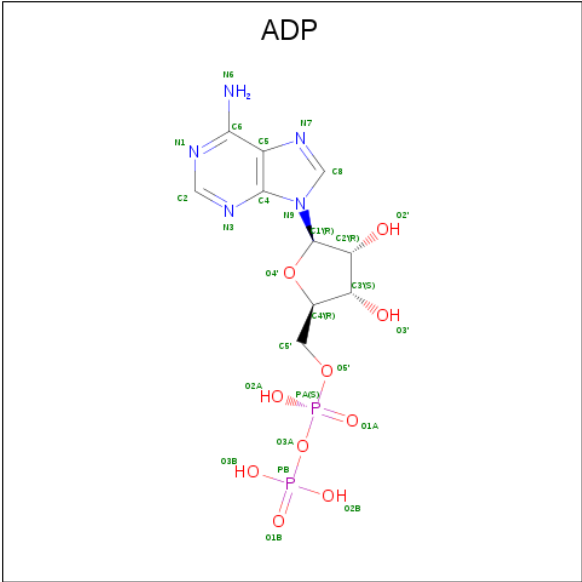
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3782  | 2422 | 629 | 713 | 18 |         |         |       |
| 1   | B     | 475      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3769  | 2414 | 627 | 710 | 18 |         |         |       |
| 1   | C     | 474      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3768  | 2414 | 626 | 710 | 18 |         |         |       |
| 1   | D     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3782  | 2422 | 630 | 712 | 18 |         |         |       |
| 1   | E     | 473      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3753  | 2407 | 625 | 703 | 18 |         |         |       |
| 1   | F     | 475      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3763  | 2411 | 627 | 707 | 18 |         |         |       |
| 1   | H     | 475      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3763  | 2411 | 627 | 707 | 18 |         |         |       |
| 1   | J     | 478      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3789  | 2424 | 634 | 713 | 18 |         |         |       |
| 1   | K     | 475      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3769  | 2415 | 628 | 708 | 18 |         |         |       |
| 1   | L     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3774  | 2417 | 629 | 710 | 18 |         |         |       |
| 1   | G     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3777  | 2418 | 630 | 711 | 18 |         |         |       |
| 1   | I     | 475      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3766  | 2412 | 627 | 709 | 18 |         |         |       |

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



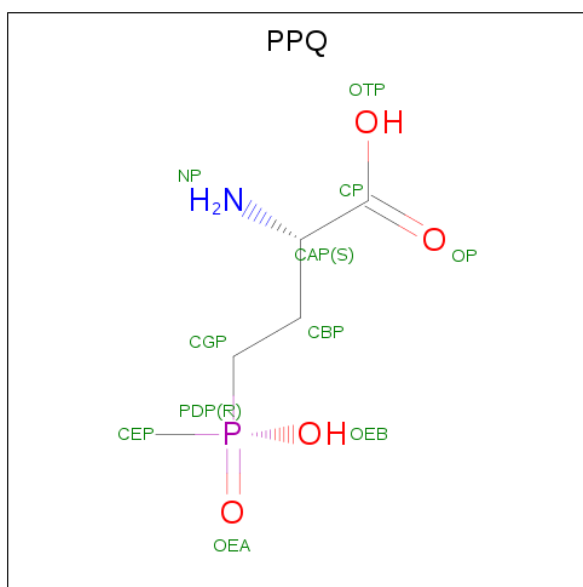
| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 2   | A     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 2   | B     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 2   | C     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 2   | K     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 2   | G     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



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

- Molecule 4 is PHOSPHINOTHRICIN (three-letter code: PPQ) (formula: C<sub>5</sub>H<sub>12</sub>NO<sub>4</sub>P).

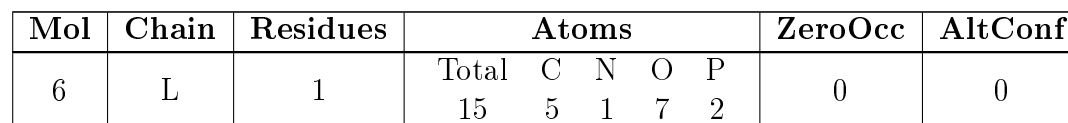


| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 4   | J     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 11    | 5 | 1 | 4 | 1 |         |         |
| 4   | K     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 11    | 5 | 1 | 4 | 1 |         |         |
| 4   | I     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 11    | 5 | 1 | 4 | 1 |         |         |

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | I     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | L     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 6 is (2S)-2-AMINO-4-[METHYL(PHOSPHONOOXY)PHOSPHORYL]BUTANOIC ACID (three-letter code: P3P) (formula: C<sub>5</sub>H<sub>13</sub>NO<sub>7</sub>P<sub>2</sub>).



- | Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 7   | A     | 25       | Total O<br>25 25 | 0       | 0       |
| 7   | B     | 20       | Total O<br>20 20 | 0       | 0       |
| 7   | C     | 17       | Total O<br>17 17 | 0       | 0       |
| 7   | D     | 26       | Total O<br>26 26 | 0       | 0       |
| 7   | E     | 26       | Total O<br>26 26 | 0       | 0       |
| 7   | F     | 19       | Total O<br>19 19 | 0       | 0       |
| 7   | H     | 27       | Total O<br>27 27 | 0       | 0       |
| 7   | J     | 40       | Total O<br>40 40 | 0       | 0       |
| 7   | K     | 36       | Total O<br>36 36 | 0       | 0       |
| 7   | L     | 42       | Total O<br>42 42 | 0       | 0       |
| 7   | G     | 42       | Total O<br>42 42 | 0       | 0       |

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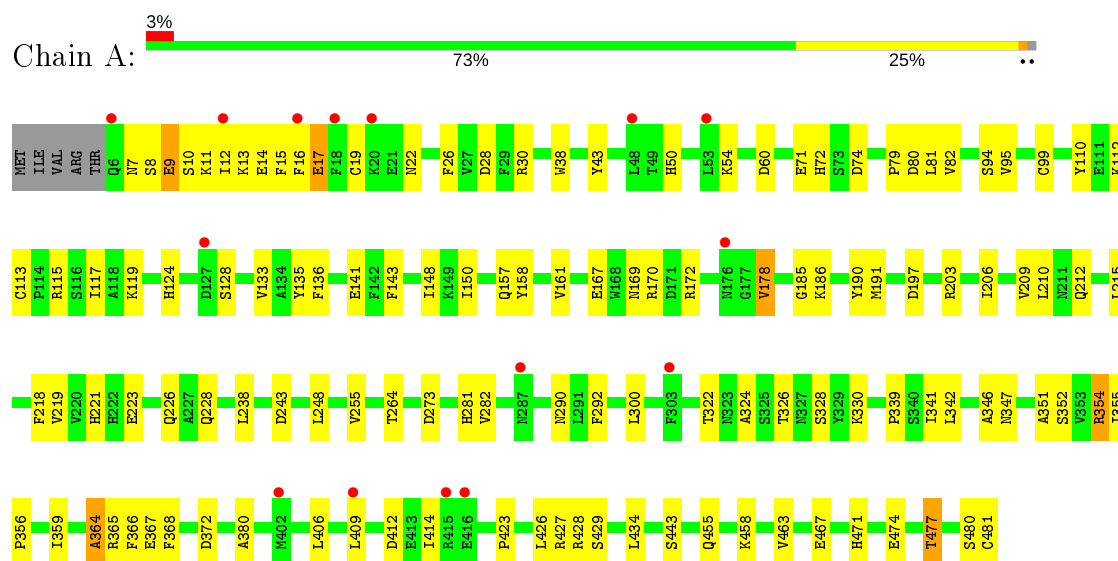
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | I     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |

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

These plots are drawn for all protein, RNA and DNA 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: Glutamine synthetase



#### • Molecule 1: Glutamine synthetase



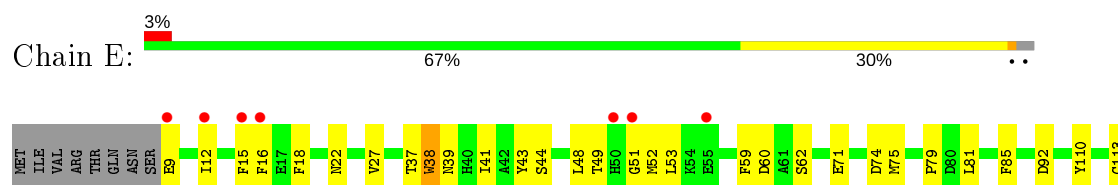
- Molecule 1: Glutamine synthetase

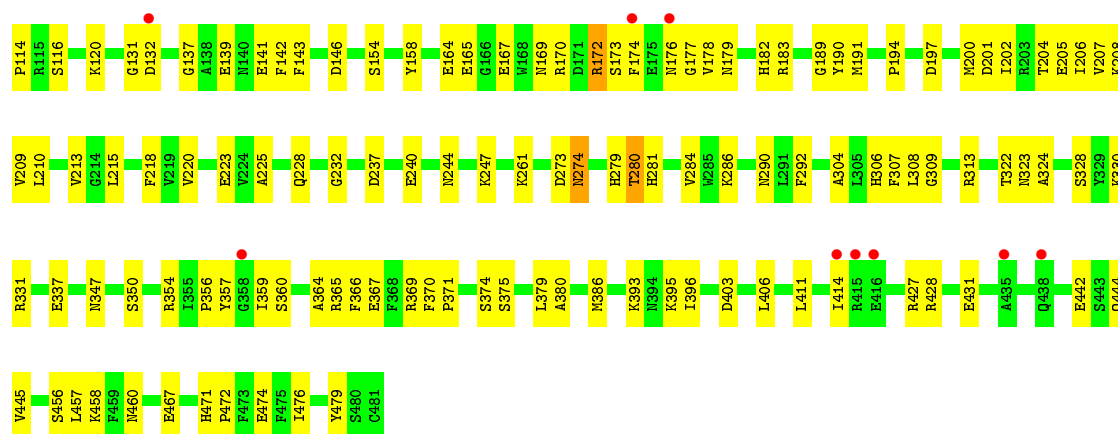


- Molecule 1: Glutamine synthetase

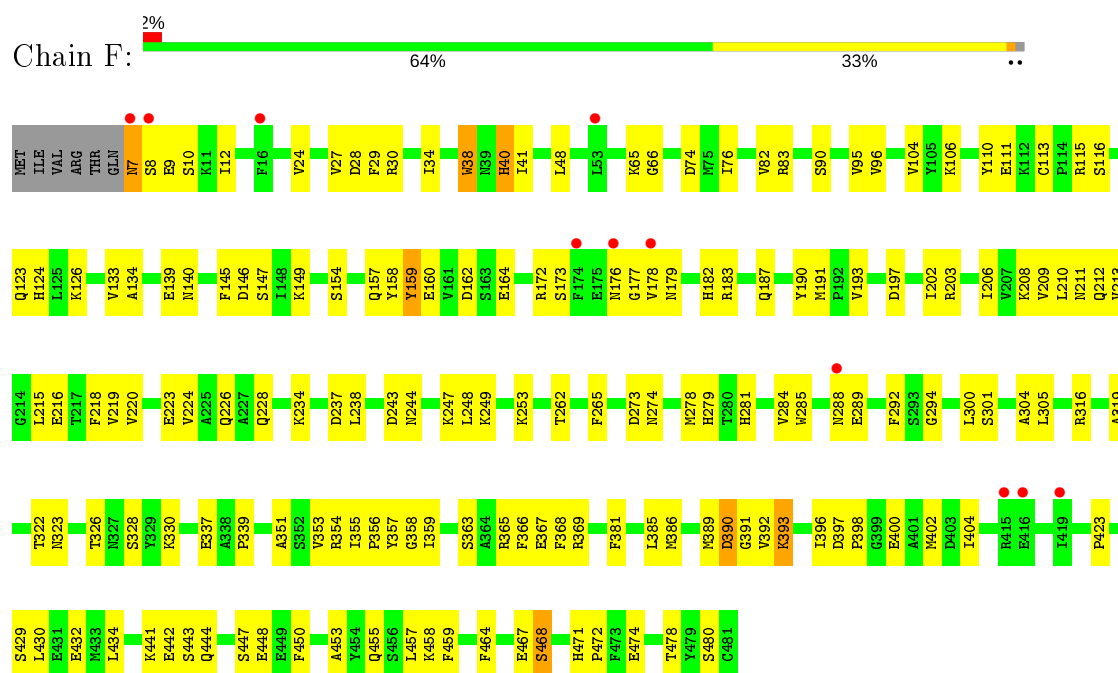


- Molecule 1: Glutamine synthetase

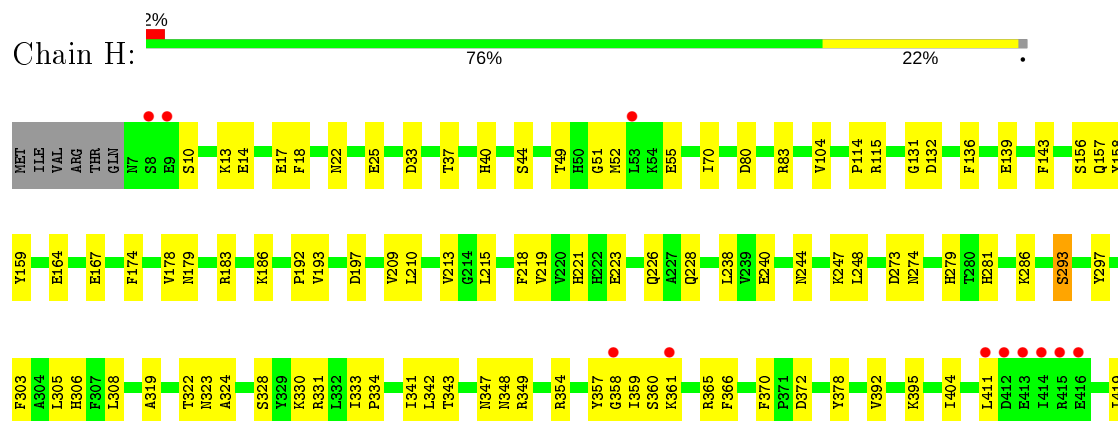




● Molecule 1: Glutamine synthetase

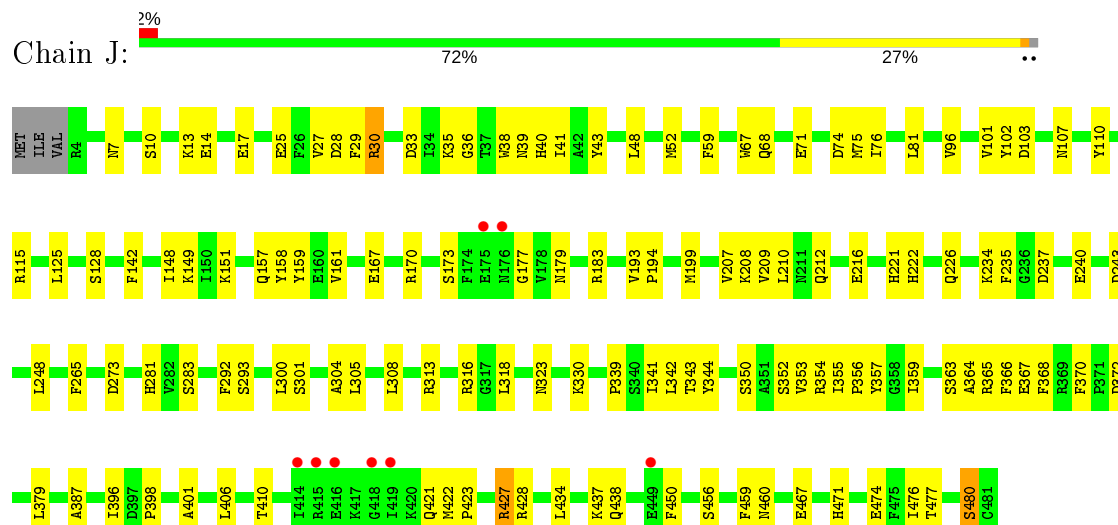


● Molecule 1: Glutamine synthetase

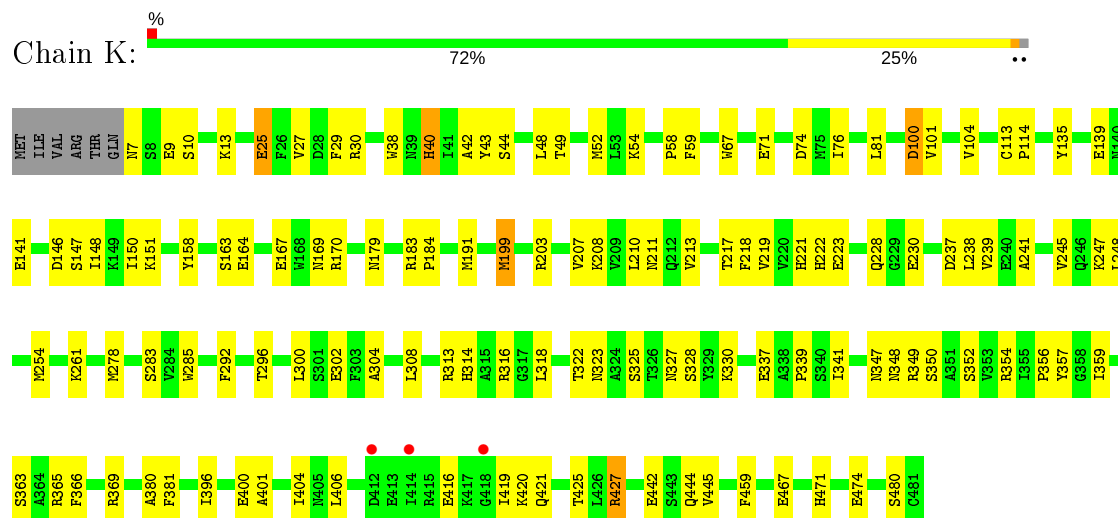




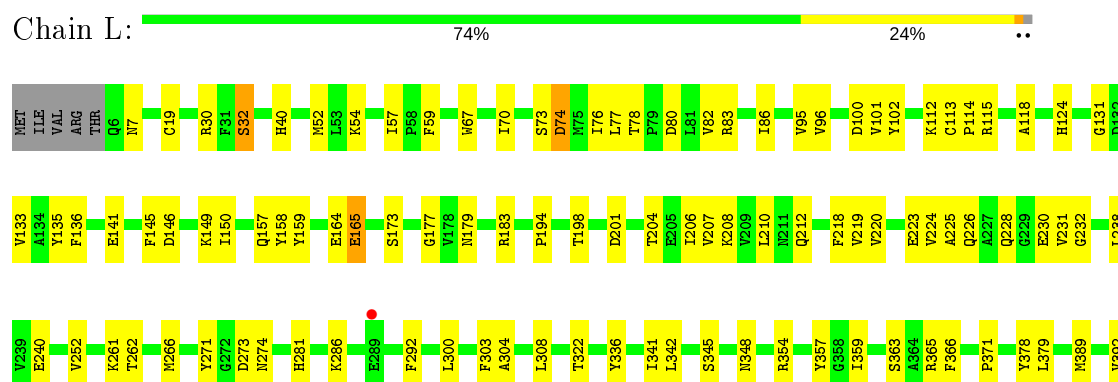
• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase

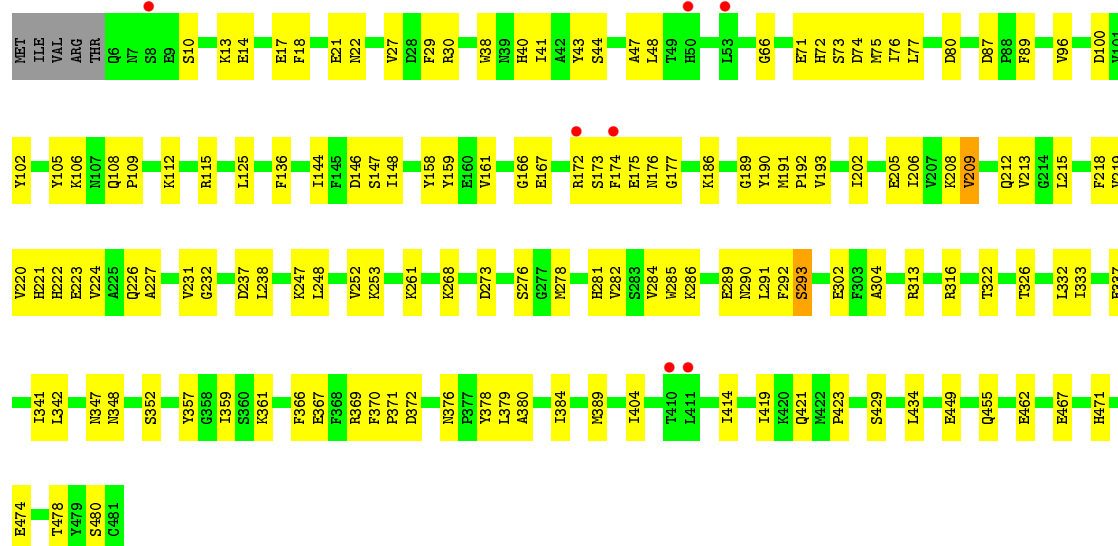


• Molecule 1: Glutamine synthetase

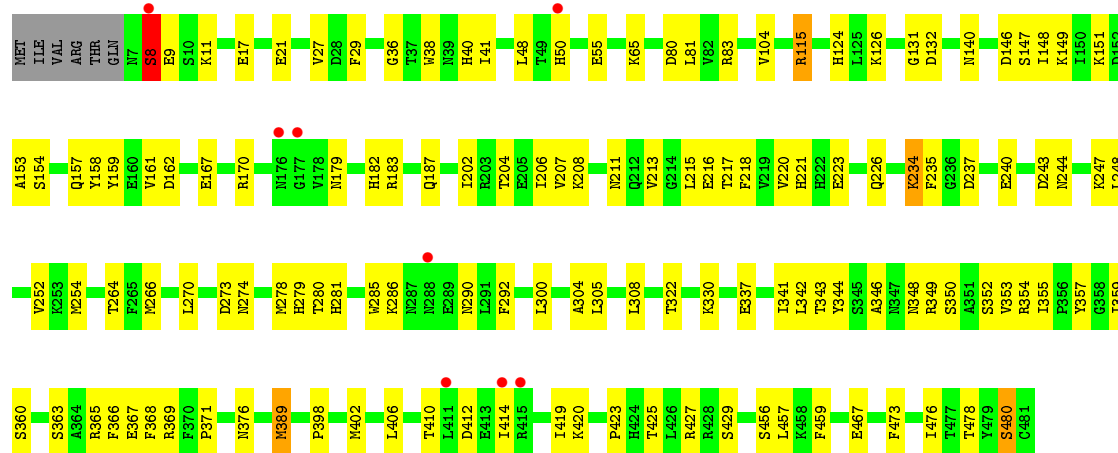




• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 234.41Å 135.17Å 203.08Å<br>90.00° 91.61° 90.00°   | Depositor        |
| Resolution (Å)  | 47.26 – 2.93<br>48.43 – 2.93  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (47.26-2.93)<br>100.0 (48.43-2.93)   | Depositor<br>EDS |
| $R_{merge}$   | 0.15  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 29.52 (at 2.91Å)  | Xtriage          |
| Refinement program  | PHENIX 1.10.1_2155  | Depositor        |
| R, $R_{free}$   | 0.168 , 0.246<br>0.168 , 0.245  | Depositor<br>DCC |
| $R_{free}$ test set   | 6740 reflections (4.96%)  | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 40.9  | Xtriage          |
| Anisotropy  | 0.158   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 46.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$   | Xtriage          |
| Estimated twinning fraction   | 0.058 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l<br>0.067 for -1/2*h+3/2*k,1/2*h+1/2*k,-l<br>0.018 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l<br>0.038 for 1/2*h+3/2*k,1/2*h-1/2*k,-l<br>0.019 for -h,-k,l | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 46003   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 29.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: ATP, MG, P3P, PPQ, ADP

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 0.58         | 4/3882 (0.1%)  | 0.66        | 1/5247 (0.0%)  |
| 1   | B     | 0.51         | 0/3869         | 0.65        | 0/5230         |
| 1   | C     | 0.49         | 0/3868         | 0.63        | 0/5227         |
| 1   | D     | 0.56         | 2/3882 (0.1%)  | 0.66        | 1/5246 (0.0%)  |
| 1   | E     | 0.51         | 0/3853         | 0.64        | 0/5207         |
| 1   | F     | 0.52         | 0/3863         | 0.64        | 1/5222 (0.0%)  |
| 1   | G     | 0.57         | 0/3877         | 0.66        | 0/5239         |
| 1   | H     | 0.57         | 0/3863         | 0.67        | 0/5222         |
| 1   | I     | 0.58         | 0/3866         | 0.68        | 0/5226         |
| 1   | J     | 0.57         | 0/3889         | 0.68        | 2/5257 (0.0%)  |
| 1   | K     | 0.58         | 0/3869         | 0.68        | 0/5229         |
| 1   | L     | 0.55         | 0/3874         | 0.70        | 1/5237 (0.0%)  |
| All | All   | 0.55         | 6/46455 (0.0%) | 0.66        | 6/62789 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | H     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 17  | GLU  | CD-OE2 | -7.78 | 1.17        | 1.25     |
| 1   | A     | 17  | GLU  | CD-OE1 | -7.21 | 1.17        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 17  | GLU  | CG-CD   | -7.07 | 1.41        | 1.51     |
| 1   | A     | 9   | GLU  | CD-OE1  | -5.16 | 1.20        | 1.25     |
| 1   | D     | 38  | TRP  | NE1-CE2 | -5.15 | 1.30        | 1.37     |
| 1   | D     | 337 | GLU  | C-N     | 5.01  | 1.45        | 1.34     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | L     | 457 | LEU  | CB-CG-CD2 | -10.37 | 93.38       | 111.00   |
| 1   | J     | 248 | LEU  | CA-CB-CG  | 7.38   | 132.26      | 115.30   |
| 1   | D     | 258 | LEU  | CA-CB-CG  | 7.05   | 131.51      | 115.30   |
| 1   | J     | 30  | ARG  | NE-CZ-NH1 | -5.47  | 117.56      | 120.30   |
| 1   | A     | 354 | ARG  | NE-CZ-NH2 | 5.06   | 122.83      | 120.30   |
| 1   | F     | 393 | LYS  | CD-CE-NZ  | -5.01  | 100.17      | 111.70   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 185 | GLY  | Peptide |
| 1   | B     | 225 | ALA  | Peptide |
| 1   | H     | 55  | GLU  | Peptide |
| 1   | I     | 55  | GLU  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3782  | 0        | 3618     | 99      | 0            |
| 1   | B     | 3769  | 0        | 3604     | 108     | 0            |
| 1   | C     | 3768  | 0        | 3611     | 116     | 0            |
| 1   | D     | 3782  | 0        | 3623     | 109     | 0            |
| 1   | E     | 3753  | 0        | 3595     | 106     | 0            |
| 1   | F     | 3763  | 0        | 3595     | 131     | 0            |
| 1   | G     | 3777  | 0        | 3609     | 104     | 0            |
| 1   | H     | 3763  | 0        | 3595     | 79      | 0            |
| 1   | I     | 3766  | 0        | 3597     | 103     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | J     | 3789  | 0        | 3619     | 91      | 0            |
| 1   | K     | 3769  | 0        | 3611     | 97      | 0            |
| 1   | L     | 3774  | 0        | 3608     | 99      | 0            |
| 2   | A     | 31    | 0        | 12       | 0       | 0            |
| 2   | B     | 31    | 0        | 12       | 1       | 0            |
| 2   | C     | 31    | 0        | 12       | 0       | 0            |
| 2   | F     | 31    | 0        | 12       | 2       | 0            |
| 2   | G     | 31    | 0        | 12       | 0       | 0            |
| 2   | K     | 31    | 0        | 12       | 3       | 0            |
| 3   | D     | 27    | 0        | 12       | 0       | 0            |
| 3   | E     | 27    | 0        | 12       | 0       | 0            |
| 3   | H     | 27    | 0        | 12       | 0       | 0            |
| 3   | I     | 27    | 0        | 12       | 2       | 0            |
| 3   | J     | 27    | 0        | 12       | 2       | 0            |
| 3   | L     | 27    | 0        | 12       | 2       | 0            |
| 4   | I     | 11    | 0        | 10       | 3       | 0            |
| 4   | J     | 11    | 0        | 10       | 0       | 0            |
| 4   | K     | 11    | 0        | 10       | 3       | 0            |
| 5   | I     | 1     | 0        | 0        | 0       | 0            |
| 5   | J     | 1     | 0        | 0        | 0       | 0            |
| 5   | L     | 2     | 0        | 0        | 0       | 0            |
| 6   | L     | 15    | 0        | 10       | 0       | 0            |
| 7   | A     | 25    | 0        | 0        | 0       | 0            |
| 7   | B     | 20    | 0        | 0        | 1       | 0            |
| 7   | C     | 17    | 0        | 0        | 0       | 0            |
| 7   | D     | 26    | 0        | 0        | 2       | 0            |
| 7   | E     | 26    | 0        | 0        | 0       | 0            |
| 7   | F     | 19    | 0        | 0        | 0       | 0            |
| 7   | G     | 42    | 0        | 0        | 0       | 0            |
| 7   | H     | 27    | 0        | 0        | 2       | 0            |
| 7   | I     | 28    | 0        | 0        | 1       | 0            |
| 7   | J     | 40    | 0        | 0        | 0       | 0            |
| 7   | K     | 36    | 0        | 0        | 2       | 0            |
| 7   | L     | 42    | 0        | 0        | 3       | 0            |
| All | All   | 46003 | 0        | 43469    | 1110    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1110) 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:281:HIS:ND1  | 1:F:365:ARG:NH1  | 1.97                     | 1.10              |
| 1:C:39:ASN:HD22  | 1:D:191:MET:H    | 1.14                     | 0.96              |
| 1:F:480:SER:HG   | 1:I:182:HIS:HD1  | 1.15                     | 0.95              |
| 1:J:179:ASN:OD1  | 1:J:183:ARG:NH2  | 2.02                     | 0.93              |
| 1:G:376:ASN:HD22 | 1:G:379:LEU:H    | 1.17                     | 0.92              |
| 1:G:286:LYS:O    | 1:G:289:GLU:HG2  | 1.70                     | 0.91              |
| 1:L:179:ASN:OD1  | 1:L:183:ARG:NH2  | 2.04                     | 0.89              |
| 1:K:48:LEU:HD12  | 1:K:52:MET:HE2   | 1.57                     | 0.87              |
| 1:F:389:MET:HB3  | 1:F:393:LYS:NZ   | 1.89                     | 0.87              |
| 1:C:216:GLU:HB2  | 1:C:234:LYS:HG2  | 1.56                     | 0.86              |
| 1:A:28:ASP:OD2   | 1:A:30:ARG:NE    | 2.08                     | 0.86              |
| 1:A:300:LEU:HD21 | 1:A:355:ILE:HD12 | 1.58                     | 0.85              |
| 1:L:434:LEU:HD11 | 1:L:455:GLN:HG3  | 1.57                     | 0.85              |
| 1:A:339:PRO:HB3  | 1:A:352:SER:HA   | 1.59                     | 0.85              |
| 1:F:389:MET:C    | 1:F:393:LYS:HZ2  | 1.81                     | 0.84              |
| 1:I:346:ALA:HA   | 1:I:355:ILE:HG23 | 1.59                     | 0.84              |
| 1:D:189:GLY:O    | 1:D:191:MET:HA   | 1.80                     | 0.82              |
| 1:F:434:LEU:HD11 | 1:F:455:GLN:HG3  | 1.61                     | 0.82              |
| 1:D:179:ASN:OD1  | 1:D:183:ARG:NH2  | 2.13                     | 0.81              |
| 1:F:164:GLU:O    | 1:F:183:ARG:NH1  | 2.14                     | 0.81              |
| 1:L:416:GLU:O    | 1:L:418:GLY:N    | 2.14                     | 0.81              |
| 1:F:281:HIS:CE1  | 1:F:365:ARG:NH1  | 2.49                     | 0.80              |
| 1:I:337:GLU:O    | 1:I:369:ARG:NH1  | 2.15                     | 0.80              |
| 1:I:213:VAL:O    | 1:I:247:LYS:NZ   | 2.12                     | 0.79              |
| 1:L:226:GLN:HG3  | 1:L:273:ASP:OD2  | 1.81                     | 0.79              |
| 1:G:226:GLN:HG3  | 1:G:273:ASP:OD2  | 1.82                     | 0.79              |
| 1:E:179:ASN:OD1  | 1:E:183:ARG:NH2  | 2.16                     | 0.79              |
| 1:F:281:HIS:CE1  | 1:F:365:ARG:HH12 | 1.99                     | 0.79              |
| 1:C:223:GLU:HG3  | 1:C:224:VAL:H    | 1.47                     | 0.78              |
| 1:F:389:MET:HB3  | 1:F:393:LYS:HZ3  | 1.46                     | 0.78              |
| 1:A:43:TYR:CZ    | 1:B:219:VAL:HG22 | 2.18                     | 0.78              |
| 1:D:330:LYS:HE2  | 1:J:474:GLU:OE2  | 1.83                     | 0.78              |
| 1:J:434:LEU:O    | 1:J:437:LYS:NZ   | 2.16                     | 0.77              |
| 1:D:215:LEU:HD21 | 1:D:247:LYS:HD2  | 1.67                     | 0.77              |
| 1:C:74:ASP:OD2   | 1:D:347:ASN:HA   | 1.84                     | 0.77              |
| 1:D:18:PHE:O     | 1:D:22:ASN:ND2   | 2.18                     | 0.77              |
| 1:A:427:ARG:NH1  | 1:A:467:GLU:OE2  | 2.16                     | 0.77              |
| 1:B:179:ASN:OD1  | 1:B:183:ARG:NH2  | 2.16                     | 0.77              |
| 1:H:13:LYS:HG3   | 1:H:14:GLU:N     | 2.00                     | 0.77              |
| 1:F:389:MET:C    | 1:F:393:LYS:NZ   | 2.37                     | 0.76              |
| 1:J:25:GLU:OE1   | 1:K:208:LYS:NZ   | 2.17                     | 0.76              |
| 1:A:434:LEU:HD11 | 1:A:455:GLN:HG3  | 1.68                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:179:ASN:OD1  | 1:F:183:ARG:NH2  | 2.19                     | 0.76              |
| 1:B:158:TYR:HB2  | 1:L:158:TYR:HD1  | 1.49                     | 0.76              |
| 1:F:284:VAL:HG22 | 1:F:292:PHE:HE1  | 1.50                     | 0.76              |
| 1:D:354:ARG:NH2  | 1:D:367:GLU:OE1  | 2.19                     | 0.75              |
| 1:F:65:LYS:HB3   | 1:F:457:LEU:HD13 | 1.67                     | 0.75              |
| 1:G:27:VAL:HG21  | 1:G:48:LEU:HD22  | 1.68                     | 0.75              |
| 1:F:182:HIS:ND1  | 1:I:480:SER:OG   | 2.19                     | 0.75              |
| 1:C:27:VAL:HG21  | 1:C:48:LEU:HD22  | 1.68                     | 0.75              |
| 1:D:404:ILE:HD12 | 1:D:409:LEU:HD21 | 1.67                     | 0.75              |
| 1:L:342:LEU:HD21 | 1:L:422:MET:HE2  | 1.70                     | 0.74              |
| 1:F:182:HIS:HD1  | 1:I:480:SER:HG   | 1.30                     | 0.74              |
| 1:B:49:THR:HB    | 1:B:52:MET:HG3   | 1.70                     | 0.74              |
| 1:E:337:GLU:O    | 1:E:369:ARG:NH1  | 2.21                     | 0.74              |
| 1:E:158:TYR:HB2  | 1:I:158:TYR:HD1  | 1.53                     | 0.74              |
| 1:E:167:GLU:OE2  | 1:E:170:ARG:NH1  | 2.21                     | 0.73              |
| 1:B:190:TYR:HA   | 1:B:191:MET:HG3  | 1.69                     | 0.73              |
| 1:F:162:ASP:OD2  | 1:F:172:ARG:NH1  | 2.21                     | 0.73              |
| 1:A:7:ASN:OD1    | 1:A:12:ILE:HD11  | 1.89                     | 0.72              |
| 1:B:300:LEU:HD11 | 1:B:355:ILE:HD12 | 1.72                     | 0.72              |
| 1:C:218:PHE:HD2  | 1:C:219:VAL:HG23 | 1.54                     | 0.72              |
| 1:K:164:GLU:O    | 1:K:183:ARG:NH1  | 2.23                     | 0.72              |
| 1:F:223:GLU:HB3  | 1:F:228:GLN:HB3  | 1.70                     | 0.71              |
| 1:E:71:GLU:N     | 1:E:71:GLU:OE2   | 2.21                     | 0.71              |
| 1:I:281:HIS:HB3  | 1:I:365:ARG:HD2  | 1.73                     | 0.71              |
| 1:D:218:PHE:CD1  | 1:D:219:VAL:HG23 | 2.25                     | 0.71              |
| 1:B:471:HIS:O    | 1:B:474:GLU:HG2  | 1.90                     | 0.71              |
| 1:I:179:ASN:OD1  | 1:I:183:ARG:NH2  | 2.23                     | 0.71              |
| 1:F:393:LYS:HD2  | 1:F:393:LYS:H    | 1.54                     | 0.71              |
| 1:F:326:THR:OG1  | 1:H:474:GLU:OE2  | 2.06                     | 0.71              |
| 1:A:13:LYS:O     | 1:A:16:PHE:N     | 2.23                     | 0.71              |
| 1:L:300:LEU:HD21 | 1:L:359:ILE:HD11 | 1.71                     | 0.71              |
| 1:F:472:PRO:HG2  | 1:H:157:GLN:HB3  | 1.73                     | 0.71              |
| 1:A:191:MET:CE   | 1:A:221:HIS:HB2  | 2.20                     | 0.70              |
| 1:D:467:GLU:O    | 1:J:330:LYS:HD3  | 1.91                     | 0.70              |
| 1:H:341:ILE:HG23 | 1:H:419:ILE:HG21 | 1.73                     | 0.70              |
| 1:B:207:VAL:O    | 1:B:211:ASN:ND2  | 2.24                     | 0.70              |
| 1:A:8:SER:HB3    | 1:A:11:LYS:HE3   | 1.74                     | 0.70              |
| 1:B:349:ARG:NH2  | 2:B:501:ATP:O1G  | 2.24                     | 0.70              |
| 1:A:13:LYS:O     | 1:A:15:PHE:N     | 2.25                     | 0.70              |
| 1:D:477:THR:O    | 1:J:35:LYS:NZ    | 2.20                     | 0.70              |
| 1:B:321:PHE:O    | 1:B:375:SER:HB2  | 1.92                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:14:GLU:HA    | 1:A:17:GLU:OE1   | 1.92                     | 0.69              |
| 1:L:206:ILE:HD13 | 1:L:252:VAL:HG22 | 1.73                     | 0.69              |
| 1:A:167:GLU:OE2  | 1:A:186:LYS:HG3  | 1.92                     | 0.69              |
| 1:C:226:GLN:HG3  | 1:C:273:ASP:OD2  | 1.93                     | 0.69              |
| 1:D:148:ILE:HD13 | 1:D:161:VAL:HG12 | 1.75                     | 0.68              |
| 1:E:139:GLU:HB2  | 1:E:279:HIS:HB2  | 1.75                     | 0.68              |
| 1:I:355:ILE:HD11 | 1:I:359:ILE:HD12 | 1.75                     | 0.68              |
| 1:D:7:ASN:HB2    | 1:D:12:ILE:HD11  | 1.76                     | 0.68              |
| 1:G:302:GLU:H    | 1:G:302:GLU:CD   | 1.96                     | 0.68              |
| 1:I:423:PRO:HG2  | 1:I:429:SER:HB3  | 1.76                     | 0.68              |
| 1:A:351:ALA:HA   | 1:A:406:LEU:HD12 | 1.75                     | 0.68              |
| 1:L:198:THR:HG22 | 7:L:609:HOH:O    | 1.94                     | 0.68              |
| 1:C:132:ASP:OD2  | 1:C:287:ASN:N    | 2.22                     | 0.68              |
| 1:K:104:VAL:HB   | 1:L:357:TYR:CZ   | 2.30                     | 0.67              |
| 1:I:115:ARG:NH2  | 1:I:243:ASP:OD2  | 2.25                     | 0.67              |
| 1:K:425:THR:HG22 | 1:K:427:ARG:H    | 1.59                     | 0.67              |
| 1:I:8:SER:HB3    | 1:I:11:LYS:HB2   | 1.77                     | 0.67              |
| 1:I:216:GLU:OE1  | 1:I:234:LYS:NZ   | 2.21                     | 0.67              |
| 1:C:467:GLU:O    | 1:K:330:LYS:HD3  | 1.95                     | 0.67              |
| 1:B:218:PHE:HD2  | 1:B:219:VAL:HG23 | 1.59                     | 0.67              |
| 1:B:341:ILE:O    | 1:B:352:SER:OG   | 2.12                     | 0.67              |
| 1:C:30:ARG:HG3   | 1:C:96:VAL:HG13  | 1.77                     | 0.67              |
| 1:E:182:HIS:HD1  | 1:J:480:SER:HG   | 1.40                     | 0.67              |
| 1:I:207:VAL:HG21 | 1:I:220:VAL:HG21 | 1.77                     | 0.67              |
| 1:D:12:ILE:HB    | 1:D:13:LYS:HZ2   | 1.59                     | 0.67              |
| 1:F:82:VAL:HG12  | 1:F:83:ARG:HG3   | 1.77                     | 0.67              |
| 1:D:53:LEU:HD22  | 1:D:81:LEU:HD21  | 1.77                     | 0.67              |
| 1:I:354:ARG:NH2  | 1:I:367:GLU:OE1  | 2.27                     | 0.67              |
| 1:F:389:MET:CB   | 1:F:393:LYS:HZ3  | 2.06                     | 0.66              |
| 1:I:419:ILE:HD12 | 1:I:419:ILE:O    | 1.96                     | 0.66              |
| 1:L:131:GLY:HA2  | 1:L:286:LYS:HB2  | 1.77                     | 0.66              |
| 1:B:141:GLU:HG2  | 1:B:223:GLU:HG3  | 1.77                     | 0.66              |
| 1:F:316:ARG:NH2  | 1:F:432:GLU:OE1  | 2.27                     | 0.66              |
| 1:H:357:TYR:O    | 1:H:359:ILE:N    | 2.27                     | 0.66              |
| 1:A:354:ARG:NH2  | 1:A:367:GLU:OE1  | 2.28                     | 0.66              |
| 1:G:434:LEU:HD11 | 1:G:455:GLN:HG3  | 1.77                     | 0.66              |
| 1:J:354:ARG:NH2  | 3:J:501:ADP:O3B  | 2.25                     | 0.66              |
| 1:B:49:THR:HG22  | 1:B:51:GLY:H     | 1.61                     | 0.66              |
| 1:K:313:ARG:HH11 | 1:K:396:ILE:HD13 | 1.59                     | 0.66              |
| 1:K:348:ASN:ND2  | 1:K:404:ILE:O    | 2.27                     | 0.66              |
| 1:C:322:THR:HB   | 1:C:371:PRO:HB3  | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:369:ARG:HH22 | 4:I:502:PPQ:HGP2 | 1.60                     | 0.65              |
| 1:C:130:LEU:HD12 | 1:C:389:MET:HE3  | 1.78                     | 0.65              |
| 1:B:268:LYS:NZ   | 1:B:273:ASP:O    | 2.27                     | 0.65              |
| 1:F:305:LEU:HG   | 1:F:398:PRO:HG3  | 1.79                     | 0.65              |
| 1:K:167:GLU:O    | 1:K:170:ARG:HG3  | 1.97                     | 0.65              |
| 1:K:354:ARG:NH1  | 2:K:501:ATP:O2B  | 2.30                     | 0.65              |
| 1:E:324:ALA:HB1  | 1:E:458:LYS:HE2  | 1.77                     | 0.65              |
| 1:K:141:GLU:HG2  | 1:K:230:GLU:OE1  | 1.97                     | 0.65              |
| 1:L:363:SER:O    | 1:L:365:ARG:HD3  | 1.96                     | 0.65              |
| 1:L:341:ILE:HG21 | 1:L:406:LEU:HD22 | 1.79                     | 0.65              |
| 1:G:115:ARG:HG3  | 1:G:378:TYR:CE1  | 2.32                     | 0.64              |
| 1:K:48:LEU:HD12  | 1:K:52:MET:CE    | 2.26                     | 0.64              |
| 1:A:324:ALA:HB1  | 1:A:458:LYS:HE3  | 1.79                     | 0.64              |
| 1:G:332:LEU:C    | 1:G:333:ILE:HD12 | 2.17                     | 0.64              |
| 1:J:48:LEU:HD12  | 1:J:52:MET:HE2   | 1.78                     | 0.64              |
| 1:B:73:SER:OG    | 1:C:349:ARG:HG3  | 1.96                     | 0.64              |
| 1:D:176:ASN:O    | 1:D:176:ASN:ND2  | 2.30                     | 0.64              |
| 1:B:425:THR:HG22 | 1:B:427:ARG:H    | 1.63                     | 0.64              |
| 1:J:173:SER:HB3  | 1:J:177:GLY:HA2  | 1.79                     | 0.64              |
| 1:A:17:GLU:CD    | 1:A:17:GLU:H     | 2.00                     | 0.64              |
| 1:D:132:ASP:HB2  | 1:D:286:LYS:HA   | 1.80                     | 0.64              |
| 1:D:372:ASP:OD1  | 1:D:374:SER:OG   | 2.13                     | 0.64              |
| 1:F:226:GLN:HG3  | 1:F:273:ASP:OD2  | 1.96                     | 0.64              |
| 1:F:216:GLU:HB2  | 1:F:234:LYS:HB3  | 1.80                     | 0.64              |
| 1:D:9:GLU:HA     | 1:D:13:LYS:NZ    | 2.13                     | 0.63              |
| 1:D:13:LYS:O     | 1:D:17:GLU:HG2   | 1.98                     | 0.63              |
| 1:L:30:ARG:HG3   | 1:L:96:VAL:HG13  | 1.79                     | 0.63              |
| 1:F:281:HIS:HA   | 1:F:366:PHE:O    | 1.98                     | 0.63              |
| 1:F:249:LYS:O    | 1:F:253:LYS:HE3  | 1.99                     | 0.63              |
| 1:F:471:HIS:O    | 1:F:474:GLU:HG2  | 1.98                     | 0.63              |
| 1:L:146:ASP:OD1  | 1:L:261:LYS:NZ   | 2.25                     | 0.63              |
| 1:C:297:TYR:CE1  | 1:C:298:LYS:HG2  | 2.34                     | 0.62              |
| 1:E:330:LYS:HD3  | 1:I:467:GLU:O    | 1.98                     | 0.62              |
| 1:I:322:THR:HB   | 1:I:371:PRO:HB3  | 1.80                     | 0.62              |
| 1:H:215:LEU:HD21 | 1:H:244:ASN:HB3  | 1.80                     | 0.62              |
| 1:H:49:THR:HG22  | 1:H:51:GLY:N     | 2.14                     | 0.62              |
| 1:J:305:LEU:HG   | 1:J:398:PRO:HG3  | 1.82                     | 0.62              |
| 1:J:27:VAL:HG21  | 1:J:48:LEU:HD22  | 1.81                     | 0.62              |
| 1:C:190:TYR:CG   | 1:C:191:MET:HG3  | 2.35                     | 0.62              |
| 1:D:74:ASP:OD2   | 1:E:347:ASN:HA   | 1.98                     | 0.62              |
| 1:F:464:PHE:O    | 1:F:468:SER:OG   | 2.17                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:191:MET:HE1  | 1:A:221:HIS:HB2  | 1.81                     | 0.62              |
| 1:C:28:ASP:OD2   | 1:C:40:HIS:HB2   | 1.98                     | 0.62              |
| 1:F:284:VAL:HG22 | 1:F:292:PHE:CE1  | 2.32                     | 0.62              |
| 1:B:354:ARG:NH2  | 1:B:367:GLU:OE1  | 2.25                     | 0.62              |
| 1:C:218:PHE:CD2  | 1:C:219:VAL:HG23 | 2.35                     | 0.62              |
| 1:I:292:PHE:HA   | 1:I:304:ALA:HB2  | 1.81                     | 0.62              |
| 1:K:427:ARG:NH1  | 1:K:467:GLU:OE1  | 2.33                     | 0.62              |
| 1:A:14:GLU:CA    | 1:A:17:GLU:OE1   | 2.47                     | 0.62              |
| 1:E:131:GLY:HA2  | 1:E:286:LYS:HD2  | 1.80                     | 0.62              |
| 1:L:223:GLU:HG3  | 1:L:224:VAL:H    | 1.64                     | 0.61              |
| 1:B:478:THR:HG22 | 1:L:266:MET:HB2  | 1.81                     | 0.61              |
| 1:A:197:ASP:OD2  | 1:A:203:ARG:NH2  | 2.33                     | 0.61              |
| 1:H:83:ARG:HD3   | 1:H:240:GLU:HG3  | 1.81                     | 0.61              |
| 1:L:220:VAL:HG12 | 1:L:231:VAL:HG22 | 1.81                     | 0.61              |
| 1:F:173:SER:HB3  | 1:F:177:GLY:HA2  | 1.81                     | 0.61              |
| 1:I:206:ILE:HD13 | 1:I:252:VAL:HG22 | 1.82                     | 0.61              |
| 1:L:118:ALA:HB1  | 1:L:238:LEU:HD21 | 1.83                     | 0.61              |
| 1:E:74:ASP:OD2   | 1:F:354:ARG:NH1  | 2.31                     | 0.61              |
| 1:H:167:GLU:OE2  | 1:H:186:LYS:HG3  | 2.01                     | 0.61              |
| 1:L:76:ILE:HB    | 1:L:102:TYR:HB3  | 1.82                     | 0.61              |
| 1:L:207:VAL:HG21 | 1:L:220:VAL:HG11 | 1.82                     | 0.61              |
| 1:E:176:ASN:H    | 1:E:178:VAL:HG12 | 1.64                     | 0.61              |
| 1:J:115:ARG:NH2  | 1:J:243:ASP:OD2  | 2.31                     | 0.61              |
| 1:J:292:PHE:HA   | 1:J:304:ALA:HB2  | 1.82                     | 0.61              |
| 1:K:322:THR:HG22 | 1:K:380:ALA:HB1  | 1.83                     | 0.61              |
| 1:K:363:SER:OG   | 1:K:365:ARG:NH1  | 2.34                     | 0.61              |
| 1:A:14:GLU:HA    | 1:A:17:GLU:CD    | 2.20                     | 0.61              |
| 1:D:117:ILE:HD12 | 1:D:379:LEU:HD21 | 1.83                     | 0.61              |
| 1:F:30:ARG:HG3   | 1:F:96:VAL:HG13  | 1.83                     | 0.61              |
| 1:G:173:SER:HB3  | 1:G:177:GLY:HA2  | 1.83                     | 0.61              |
| 1:E:273:ASP:OD2  | 1:E:274:ASN:N    | 2.32                     | 0.60              |
| 1:F:8:SER:O      | 1:F:10:SER:N     | 2.34                     | 0.60              |
| 1:H:341:ILE:HG22 | 1:H:343:THR:HG22 | 1.83                     | 0.60              |
| 1:D:237:ASP:O    | 1:D:240:GLU:N    | 2.33                     | 0.60              |
| 1:H:354:ARG:NH2  | 1:G:74:ASP:OD2   | 2.34                     | 0.60              |
| 1:H:471:HIS:HB3  | 1:H:474:GLU:HG3  | 1.82                     | 0.60              |
| 1:I:80:ASP:O     | 7:I:601:HOH:O    | 2.16                     | 0.60              |
| 1:A:110:TYR:CZ   | 1:A:112:LYS:HB2  | 2.37                     | 0.60              |
| 1:F:292:PHE:HA   | 1:F:304:ALA:HB2  | 1.81                     | 0.60              |
| 1:B:324:ALA:HB1  | 1:B:458:LYS:HE3  | 1.82                     | 0.60              |
| 1:A:191:MET:HE2  | 1:F:40:HIS:O     | 2.02                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:333:ILE:HG23 | 1:H:334:PRO:HD2  | 1.83                     | 0.60              |
| 1:E:48:LEU:HD12  | 1:E:52:MET:HE2   | 1.84                     | 0.60              |
| 1:H:349:ARG:HH11 | 1:G:73:SER:HB3   | 1.65                     | 0.60              |
| 1:C:330:LYS:HD3  | 1:K:467:GLU:O    | 2.02                     | 0.60              |
| 1:L:412:ASP:O    | 1:L:416:GLU:N    | 2.29                     | 0.60              |
| 1:G:376:ASN:HD21 | 1:G:378:TYR:HB2  | 1.67                     | 0.60              |
| 1:A:423:PRO:HG2  | 1:A:429:SER:HB3  | 1.84                     | 0.60              |
| 1:K:341:ILE:HB   | 1:K:406:LEU:HD13 | 1.84                     | 0.60              |
| 1:F:244:ASN:OD1  | 1:F:247:LYS:HE2  | 2.02                     | 0.59              |
| 1:D:158:TYR:HD1  | 1:J:158:TYR:HB2  | 1.66                     | 0.59              |
| 1:B:434:LEU:HD11 | 1:B:455:GLN:HG3  | 1.83                     | 0.59              |
| 1:D:300:LEU:HD11 | 1:D:355:ILE:HD13 | 1.84                     | 0.59              |
| 1:G:205:GLU:O    | 1:G:209:VAL:HG23 | 2.01                     | 0.59              |
| 1:H:49:THR:HG22  | 1:H:51:GLY:H     | 1.68                     | 0.59              |
| 1:K:49:THR:OG1   | 1:K:52:MET:HG3   | 2.02                     | 0.59              |
| 1:C:210:LEU:HD22 | 1:C:248:LEU:HD12 | 1.84                     | 0.59              |
| 1:G:337:GLU:O    | 1:G:369:ARG:NH1  | 2.34                     | 0.59              |
| 1:I:353:VAL:HG22 | 1:I:368:PHE:HD1  | 1.67                     | 0.59              |
| 1:E:313:ARG:CZ   | 1:E:396:ILE:HD11 | 2.33                     | 0.59              |
| 1:J:237:ASP:OD1  | 1:J:240:GLU:HB3  | 2.02                     | 0.59              |
| 1:E:158:TYR:HD1  | 1:I:158:TYR:HB2  | 1.68                     | 0.59              |
| 1:E:347:ASN:OD1  | 1:E:357:TYR:HB2  | 2.03                     | 0.59              |
| 1:G:166:GLY:HA2  | 1:G:226:GLN:OE1  | 2.03                     | 0.59              |
| 1:A:191:MET:HE3  | 1:A:221:HIS:HB2  | 1.85                     | 0.59              |
| 1:C:151:LYS:HB3  | 1:C:158:TYR:HB3  | 1.84                     | 0.59              |
| 1:D:12:ILE:HG22  | 1:D:13:LYS:HD3   | 1.83                     | 0.59              |
| 1:G:471:HIS:HB3  | 1:G:474:GLU:HG3  | 1.85                     | 0.59              |
| 1:J:471:HIS:HB3  | 1:J:474:GLU:HG3  | 1.84                     | 0.59              |
| 1:A:359:ILE:HG13 | 1:A:364:ALA:HA   | 1.84                     | 0.59              |
| 1:K:25:GLU:OE1   | 1:L:208:LYS:NZ   | 2.29                     | 0.59              |
| 1:C:293:SER:O    | 1:C:301:SER:HB3  | 2.03                     | 0.58              |
| 1:J:281:HIS:NE2  | 1:J:367:GLU:HG3  | 2.18                     | 0.58              |
| 1:C:296:THR:HG21 | 1:C:302:GLU:HG3  | 1.85                     | 0.58              |
| 1:I:126:LYS:HE2  | 1:I:132:ASP:O    | 2.03                     | 0.58              |
| 1:I:281:HIS:CE1  | 1:I:367:GLU:HB3  | 2.38                     | 0.58              |
| 1:B:428:ARG:HG3  | 7:B:616:HOH:O    | 2.03                     | 0.58              |
| 1:D:223:GLU:HB3  | 1:D:228:GLN:HB3  | 1.86                     | 0.58              |
| 1:E:37:THR:O     | 1:E:39:ASN:ND2   | 2.36                     | 0.58              |
| 1:K:341:ILE:CG2  | 1:K:419:ILE:HD11 | 2.33                     | 0.58              |
| 1:L:427:ARG:NE   | 1:L:467:GLU:OE2  | 2.30                     | 0.58              |
| 1:C:129:GLY:O    | 1:C:286:LYS:NZ   | 2.37                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:39:ASN:ND2   | 1:C:64:PHE:HE2   | 2.02                     | 0.58              |
| 1:G:333:ILE:N    | 1:G:333:ILE:HD12 | 2.18                     | 0.58              |
| 1:L:133:VAL:HG11 | 1:L:135:TYR:CE1  | 2.39                     | 0.58              |
| 1:F:223:GLU:HG3  | 1:F:224:VAL:H    | 1.69                     | 0.58              |
| 1:K:313:ARG:NH1  | 1:K:396:ILE:HD13 | 2.19                     | 0.58              |
| 1:F:160:GLU:HB2  | 1:H:156:SER:HB2  | 1.85                     | 0.57              |
| 1:H:297:TYR:HB3  | 1:H:305:LEU:HD11 | 1.86                     | 0.57              |
| 1:A:210:LEU:HD22 | 1:A:215:LEU:HD12 | 1.86                     | 0.57              |
| 1:F:216:GLU:HG2  | 1:F:234:LYS:HD3  | 1.85                     | 0.57              |
| 1:F:389:MET:CB   | 1:F:393:LYS:NZ   | 2.63                     | 0.57              |
| 1:H:281:HIS:ND1  | 1:H:365:ARG:HD2  | 2.19                     | 0.57              |
| 1:A:223:GLU:HB2  | 1:A:228:GLN:HB3  | 1.87                     | 0.57              |
| 1:G:72:HIS:HB3   | 1:G:105:TYR:CZ   | 2.39                     | 0.57              |
| 1:B:226:GLN:HG3  | 1:B:273:ASP:OD2  | 2.03                     | 0.57              |
| 1:K:218:PHE:CD1  | 1:K:219:VAL:HG23 | 2.40                     | 0.57              |
| 1:K:323:ASN:HB3  | 1:K:328:SER:HB3  | 1.87                     | 0.57              |
| 1:E:27:VAL:HG21  | 1:E:48:LEU:HD22  | 1.86                     | 0.57              |
| 1:F:480:SER:OG   | 1:I:182:HIS:ND1  | 2.23                     | 0.57              |
| 1:L:40:HIS:CD2   | 1:G:193:VAL:HA   | 2.39                     | 0.57              |
| 1:H:293:SER:OG   | 1:H:361:LYS:HA   | 2.05                     | 0.57              |
| 1:I:151:LYS:HE3  | 1:I:153:ALA:HB2  | 1.86                     | 0.57              |
| 1:D:437:LYS:O    | 1:D:440:LEU:N    | 2.38                     | 0.57              |
| 1:E:322:THR:HG22 | 1:E:323:ASN:OD1  | 2.03                     | 0.57              |
| 1:F:391:GLY:HA2  | 1:F:396:ILE:HD12 | 1.87                     | 0.57              |
| 1:I:355:ILE:HD11 | 1:I:359:ILE:CD1  | 2.34                     | 0.57              |
| 1:C:391:GLY:HA2  | 1:C:396:ILE:HD12 | 1.85                     | 0.57              |
| 1:F:389:MET:HB3  | 1:F:393:LYS:HZ1  | 1.68                     | 0.57              |
| 1:E:59:PHE:CE1   | 1:E:75:MET:HB2   | 2.40                     | 0.57              |
| 1:A:14:GLU:C     | 1:A:17:GLU:OE1   | 2.44                     | 0.57              |
| 1:A:74:ASP:OD2   | 1:B:347:ASN:HA   | 2.04                     | 0.56              |
| 1:F:300:LEU:HD11 | 1:F:355:ILE:HD13 | 1.86                     | 0.56              |
| 1:A:226:GLN:HG3  | 1:A:273:ASP:OD2  | 2.05                     | 0.56              |
| 1:C:324:ALA:HB1  | 1:C:458:LYS:HE3  | 1.87                     | 0.56              |
| 1:J:216:GLU:OE2  | 1:J:216:GLU:HA   | 2.05                     | 0.56              |
| 1:C:216:GLU:HB2  | 1:C:234:LYS:CG   | 2.34                     | 0.56              |
| 1:D:65:LYS:HB3   | 1:D:457:LEU:HD13 | 1.86                     | 0.56              |
| 1:E:322:THR:HG21 | 1:E:370:PHE:CD1  | 2.40                     | 0.56              |
| 1:G:223:GLU:HG3  | 1:G:224:VAL:H    | 1.69                     | 0.56              |
| 1:A:480:SER:O    | 1:G:253:LYS:NZ   | 2.38                     | 0.56              |
| 1:I:215:LEU:HD11 | 1:I:247:LYS:HD2  | 1.85                     | 0.56              |
| 1:J:142:PHE:HB3  | 1:J:265:PHE:CE2  | 2.39                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:369:ARG:NH1  | 4:K:502:PPQ:OEB  | 2.38                     | 0.56              |
| 1:G:30:ARG:HG3   | 1:G:96:VAL:HG13  | 1.87                     | 0.56              |
| 1:J:323:ASN:ND2  | 1:J:370:PHE:O    | 2.38                     | 0.56              |
| 1:B:70:ILE:HD11  | 1:C:349:ARG:HB2  | 1.86                     | 0.56              |
| 1:H:273:ASP:OD1  | 1:H:274:ASN:N    | 2.36                     | 0.56              |
| 1:F:467:GLU:O    | 1:H:330:LYS:HD3  | 2.05                     | 0.56              |
| 1:K:218:PHE:HZ   | 2:K:501:ATP:H3'  | 1.71                     | 0.56              |
| 1:H:10:SER:O     | 1:H:13:LYS:HG2   | 2.05                     | 0.56              |
| 1:B:360:SER:N    | 1:B:363:SER:OG   | 2.30                     | 0.55              |
| 1:C:57:ILE:HB    | 1:C:77:LEU:HB2   | 1.88                     | 0.55              |
| 1:F:139:GLU:O    | 1:F:278:MET:HA   | 2.06                     | 0.55              |
| 1:H:164:GLU:HG3  | 1:H:174:PHE:CE2  | 2.41                     | 0.55              |
| 1:I:350:SER:O    | 1:I:406:LEU:HD12 | 2.06                     | 0.55              |
| 1:D:472:PRO:HG2  | 1:J:157:GLN:HB3  | 1.87                     | 0.55              |
| 1:L:118:ALA:HB1  | 1:L:238:LEU:CD2  | 2.37                     | 0.55              |
| 1:B:374:SER:HA   | 1:L:481:CYS:SG   | 2.45                     | 0.55              |
| 1:K:184:PRO:O    | 7:K:601:HOH:O    | 2.18                     | 0.55              |
| 1:A:427:ARG:NH1  | 1:A:467:GLU:CD   | 2.60                     | 0.55              |
| 1:E:471:HIS:HB3  | 1:E:474:GLU:HG3  | 1.88                     | 0.55              |
| 1:G:333:ILE:N    | 1:G:333:ILE:CD1  | 2.69                     | 0.55              |
| 1:L:32:SER:OG    | 7:L:601:HOH:O    | 2.12                     | 0.55              |
| 1:C:441:LYS:NZ   | 1:C:448:GLU:HB2  | 2.21                     | 0.55              |
| 1:F:146:ASP:N    | 1:F:162:ASP:O    | 2.32                     | 0.55              |
| 1:F:28:ASP:HB3   | 1:F:96:VAL:HG22  | 1.89                     | 0.55              |
| 1:I:207:VAL:HG21 | 1:I:220:VAL:CG2  | 2.37                     | 0.55              |
| 1:K:325:SER:O    | 1:K:328:SER:HB2  | 2.06                     | 0.55              |
| 1:E:172:ARG:HG3  | 1:E:173:SER:N    | 2.21                     | 0.55              |
| 1:I:343:THR:OG1  | 1:I:402:MET:HG3  | 2.07                     | 0.55              |
| 1:A:300:LEU:CD2  | 1:A:355:ILE:HD12 | 2.35                     | 0.55              |
| 1:A:426:LEU:HD23 | 1:A:463:VAL:HG23 | 1.87                     | 0.55              |
| 1:L:357:TYR:O    | 1:L:359:ILE:HG22 | 2.07                     | 0.55              |
| 1:K:350:SER:O    | 1:K:406:LEU:HD12 | 2.07                     | 0.55              |
| 1:A:7:ASN:HB2    | 1:A:11:LYS:HD2   | 1.88                     | 0.54              |
| 1:B:426:LEU:HD23 | 1:B:463:VAL:HG23 | 1.89                     | 0.54              |
| 1:H:219:VAL:HG22 | 1:G:43:TYR:CZ    | 2.43                     | 0.54              |
| 1:I:234:LYS:HG2  | 1:I:235:PHE:N    | 2.21                     | 0.54              |
| 1:E:9:GLU:HA     | 1:E:12:ILE:HD12  | 1.88                     | 0.54              |
| 1:G:80:ASP:OD2   | 1:G:115:ARG:NH1  | 2.39                     | 0.54              |
| 1:J:293:SER:O    | 1:J:301:SER:HB3  | 2.08                     | 0.54              |
| 1:K:104:VAL:HB   | 1:L:357:TYR:CE1  | 2.42                     | 0.54              |
| 1:K:444:GLN:O    | 1:K:444:GLN:HG2  | 2.06                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:410:THR:O    | 1:B:414:ILE:HG12 | 2.08                     | 0.54              |
| 1:L:345:SER:HB3  | 1:L:348:ASN:HB3  | 1.89                     | 0.54              |
| 1:B:29:PHE:HB3   | 1:B:99:CYS:SG    | 2.48                     | 0.54              |
| 1:D:49:THR:H     | 1:D:52:MET:HG3   | 1.73                     | 0.54              |
| 1:G:148:ILE:HD13 | 1:G:161:VAL:HG12 | 1.88                     | 0.54              |
| 1:G:281:HIS:HA   | 1:G:366:PHE:O    | 2.08                     | 0.54              |
| 1:J:115:ARG:NH2  | 1:J:243:ASP:OD1  | 2.40                     | 0.54              |
| 1:B:347:ASN:ND2  | 1:B:357:TYR:HB2  | 2.22                     | 0.54              |
| 1:G:220:VAL:HG23 | 1:G:231:VAL:HG22 | 1.90                     | 0.54              |
| 1:J:281:HIS:CE1  | 3:J:501:ADP:H5'1 | 2.41                     | 0.54              |
| 1:K:316:ARG:NH1  | 1:K:421:GLN:O    | 2.41                     | 0.54              |
| 1:F:356:PRO:HG2  | 1:F:365:ARG:CZ   | 2.37                     | 0.54              |
| 1:G:106:LYS:NZ   | 1:G:449:GLU:OE1  | 2.40                     | 0.54              |
| 1:L:416:GLU:C    | 1:L:418:GLY:H    | 2.10                     | 0.54              |
| 1:A:11:LYS:O     | 1:A:15:PHE:N     | 2.41                     | 0.54              |
| 1:D:150:ILE:HG21 | 1:J:476:ILE:HG13 | 1.88                     | 0.54              |
| 1:F:190:TYR:CD1  | 1:F:191:MET:HG3  | 2.43                     | 0.54              |
| 1:K:241:ALA:O    | 1:K:245:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:356:PRO:HG2  | 1:A:365:ARG:HE   | 1.72                     | 0.54              |
| 1:G:376:ASN:ND2  | 1:G:379:LEU:H    | 1.98                     | 0.54              |
| 1:B:297:TYR:CE1  | 1:B:298:LYS:HG3  | 2.43                     | 0.53              |
| 1:D:141:GLU:OE1  | 1:D:277:GLY:N    | 2.27                     | 0.53              |
| 1:G:208:LYS:O    | 1:G:212:GLN:HG3  | 2.08                     | 0.53              |
| 1:J:234:LYS:HD3  | 1:J:235:PHE:N    | 2.23                     | 0.53              |
| 1:K:207:VAL:HA   | 1:K:210:LEU:HD12 | 1.89                     | 0.53              |
| 1:B:172:ARG:HD3  | 1:B:174:PHE:CZ   | 2.43                     | 0.53              |
| 1:D:7:ASN:ND2    | 1:D:81:LEU:HG    | 2.24                     | 0.53              |
| 1:F:197:ASP:OD2  | 1:F:203:ARG:NH2  | 2.41                     | 0.53              |
| 1:C:455:GLN:HG2  | 1:C:459:PHE:HD2  | 1.74                     | 0.53              |
| 1:D:413:GLU:HG3  | 1:D:417:LYS:NZ   | 2.22                     | 0.53              |
| 1:E:167:GLU:O    | 1:E:170:ARG:HG3  | 2.07                     | 0.53              |
| 1:E:43:TYR:CE2   | 1:F:219:VAL:HG22 | 2.43                     | 0.53              |
| 1:D:27:VAL:HG21  | 1:D:48:LEU:HD22  | 1.89                     | 0.53              |
| 1:E:114:PRO:HB3  | 1:E:379:LEU:HG   | 1.91                     | 0.53              |
| 1:A:209:VAL:HA   | 1:A:212:GLN:HG2  | 1.90                     | 0.53              |
| 1:A:409:LEU:HB3  | 1:A:414:ILE:HG12 | 1.89                     | 0.53              |
| 1:E:292:PHE:HA   | 1:E:304:ALA:HB2  | 1.89                     | 0.53              |
| 1:F:172:ARG:HG3  | 1:F:173:SER:N    | 2.23                     | 0.53              |
| 1:G:219:VAL:HG12 | 1:G:232:GLY:HA3  | 1.89                     | 0.53              |
| 1:H:330:LYS:O    | 1:H:333:ILE:HD12 | 2.09                     | 0.53              |
| 1:C:290:ASN:OD1  | 1:C:292:PHE:HB2  | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:218:PHE:HD1  | 1:D:219:VAL:HG23 | 1.72                     | 0.53              |
| 1:E:205:GLU:O    | 1:E:209:VAL:HG23 | 2.09                     | 0.53              |
| 1:F:8:SER:HB3    | 1:F:12:ILE:HG13  | 1.91                     | 0.53              |
| 1:C:150:ILE:O    | 1:D:171:ASP:HB3  | 2.09                     | 0.53              |
| 1:L:173:SER:HB3  | 1:L:177:GLY:HA2  | 1.90                     | 0.53              |
| 1:B:454:TYR:O    | 1:B:457:LEU:N    | 2.41                     | 0.53              |
| 1:H:49:THR:HB    | 1:H:52:MET:HG3   | 1.91                     | 0.53              |
| 1:K:283:SER:HG   | 1:K:285:TRP:HE1  | 1.55                     | 0.53              |
| 1:B:158:TYR:HD1  | 1:L:158:TYR:HB2  | 1.74                     | 0.53              |
| 1:A:10:SER:O     | 1:A:14:GLU:HB2   | 2.08                     | 0.53              |
| 1:D:207:VAL:HG21 | 1:D:220:VAL:CG2  | 2.39                     | 0.53              |
| 1:D:443:SER:O    | 1:D:444:GLN:HG2  | 2.08                     | 0.53              |
| 1:F:158:TYR:OH   | 1:F:160:GLU:OE1  | 2.27                     | 0.53              |
| 1:H:348:ASN:ND2  | 1:H:404:ILE:O    | 2.41                     | 0.53              |
| 1:C:210:LEU:CD2  | 1:C:248:LEU:HD12 | 2.38                     | 0.52              |
| 1:H:209:VAL:O    | 1:H:213:VAL:HG13 | 2.08                     | 0.52              |
| 1:I:221:HIS:HE1  | 1:I:223:GLU:OE2  | 1.91                     | 0.52              |
| 1:F:34:ILE:HD12  | 1:F:66:GLY:HA3   | 1.92                     | 0.52              |
| 1:G:167:GLU:OE1  | 1:G:186:LYS:HE3  | 2.09                     | 0.52              |
| 1:J:370:PHE:CD2  | 1:J:422:MET:HE3  | 2.44                     | 0.52              |
| 1:C:216:GLU:H    | 1:C:234:LYS:CE   | 2.22                     | 0.52              |
| 1:C:305:LEU:HB3  | 1:C:398:PRO:HG3  | 1.91                     | 0.52              |
| 1:D:226:GLN:HG3  | 1:D:273:ASP:OD2  | 2.09                     | 0.52              |
| 1:G:221:HIS:HD2  | 1:G:222:HIS:O    | 1.92                     | 0.52              |
| 1:H:218:PHE:CD2  | 1:H:219:VAL:HG23 | 2.43                     | 0.52              |
| 1:H:349:ARG:HH11 | 1:G:73:SER:CB    | 2.23                     | 0.52              |
| 1:H:420:LYS:NZ   | 7:H:601:HOH:O    | 2.16                     | 0.52              |
| 1:I:151:LYS:HB3  | 1:I:158:TYR:HB3  | 1.91                     | 0.52              |
| 1:J:68:GLN:OE1   | 1:J:110:TYR:OH   | 2.20                     | 0.52              |
| 1:K:213:VAL:O    | 1:K:247:LYS:NZ   | 2.23                     | 0.52              |
| 1:B:157:GLN:HG2  | 1:L:159:TYR:HE1  | 1.75                     | 0.52              |
| 1:L:281:HIS:CE1  | 3:L:503:ADP:H5'2 | 2.44                     | 0.52              |
| 1:A:158:TYR:HD1  | 1:G:158:TYR:HB2  | 1.75                     | 0.52              |
| 1:B:25:GLU:OE1   | 1:C:208:LYS:NZ   | 2.42                     | 0.52              |
| 1:F:423:PRO:HG2  | 1:F:429:SER:HB3  | 1.92                     | 0.52              |
| 1:L:70:ILE:HD11  | 1:G:337:GLU:HG2  | 1.92                     | 0.52              |
| 1:A:141:GLU:HG2  | 1:A:223:GLU:HG3  | 1.92                     | 0.52              |
| 1:C:382:ALA:O    | 1:C:386:MET:HG2  | 2.10                     | 0.52              |
| 1:L:115:ARG:HG3  | 1:L:378:TYR:CE1  | 2.45                     | 0.52              |
| 1:A:471:HIS:HB3  | 1:A:474:GLU:HG3  | 1.92                     | 0.52              |
| 1:B:165:GLU:OE2  | 1:B:226:GLN:O    | 2.28                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:210:LEU:HD13 | 1:C:248:LEU:CD1  | 2.39                     | 0.52              |
| 1:D:91:ALA:HB2   | 1:E:201:ASP:OD2  | 2.10                     | 0.52              |
| 1:E:306:HIS:O    | 1:E:309:GLY:N    | 2.43                     | 0.52              |
| 1:D:9:GLU:O      | 1:D:13:LYS:HG2   | 2.10                     | 0.52              |
| 1:E:173:SER:OG   | 1:E:177:GLY:HA2  | 2.10                     | 0.52              |
| 1:A:113:CYS:O    | 1:A:117:ILE:HG13 | 2.10                     | 0.52              |
| 1:B:345:SER:HB3  | 1:B:348:ASN:HB3  | 1.92                     | 0.52              |
| 1:F:158:TYR:HD1  | 1:H:158:TYR:HB2  | 1.75                     | 0.52              |
| 1:G:357:TYR:O    | 1:G:359:ILE:HG22 | 2.10                     | 0.52              |
| 1:G:414:ILE:O    | 1:G:419:ILE:HG22 | 2.09                     | 0.52              |
| 1:J:343:THR:CG2  | 1:J:406:LEU:HD11 | 2.40                     | 0.52              |
| 1:A:8:SER:H      | 1:A:11:LYS:HZ2   | 1.57                     | 0.52              |
| 1:H:33:ASP:OD2   | 1:H:37:THR:HB    | 2.10                     | 0.52              |
| 1:J:350:SER:O    | 1:J:406:LEU:HD12 | 2.09                     | 0.52              |
| 1:J:76:ILE:HB    | 1:J:102:TYR:HB3  | 1.92                     | 0.52              |
| 1:L:462:GLU:O    | 1:L:465:PRO:HD2  | 2.10                     | 0.52              |
| 1:B:218:PHE:CD2  | 1:B:219:VAL:HG23 | 2.43                     | 0.51              |
| 1:A:158:TYR:HB2  | 1:G:158:TYR:HD1  | 1.75                     | 0.51              |
| 1:G:206:ILE:HD13 | 1:G:252:VAL:HG22 | 1.91                     | 0.51              |
| 1:D:348:ASN:ND2  | 1:D:404:ILE:O    | 2.41                     | 0.51              |
| 1:E:38:TRP:O     | 1:F:193:VAL:HG13 | 2.10                     | 0.51              |
| 1:I:202:ILE:O    | 1:I:206:ILE:HG13 | 2.10                     | 0.51              |
| 1:J:151:LYS:HB3  | 1:J:158:TYR:HB3  | 1.91                     | 0.51              |
| 1:J:316:ARG:HD2  | 1:J:421:GLN:O    | 2.10                     | 0.51              |
| 1:B:343:THR:OG1  | 1:B:402:MET:HG3  | 2.10                     | 0.51              |
| 1:B:331:ARG:NH1  | 1:B:372:ASP:HB3  | 2.25                     | 0.51              |
| 1:E:350:SER:O    | 1:E:406:LEU:HD12 | 2.10                     | 0.51              |
| 1:F:397:ASP:OD1  | 1:F:398:PRO:HD2  | 2.10                     | 0.51              |
| 1:I:346:ALA:HA   | 1:I:355:ILE:CG2  | 2.37                     | 0.51              |
| 1:E:51:GLY:O     | 1:E:52:MET:HG2   | 2.11                     | 0.51              |
| 1:G:146:ASP:OD1  | 1:G:261:LYS:HE3  | 2.10                     | 0.51              |
| 1:H:80:ASP:OD2   | 1:H:115:ARG:NH1  | 2.44                     | 0.51              |
| 1:C:303:PHE:CE1  | 1:C:392:VAL:HG11 | 2.45                     | 0.51              |
| 1:C:441:LYS:HZ2  | 1:C:448:GLU:HB2  | 1.76                     | 0.51              |
| 1:H:215:LEU:HD11 | 1:H:247:LYS:HD2  | 1.92                     | 0.51              |
| 1:K:7:ASN:OD1    | 1:K:81:LEU:HG    | 2.10                     | 0.51              |
| 1:D:194:PRO:HA   | 1:D:197:ASP:H    | 1.75                     | 0.51              |
| 1:E:308:LEU:HB2  | 1:E:366:PHE:CE2  | 2.46                     | 0.51              |
| 1:L:281:HIS:HA   | 1:L:366:PHE:O    | 2.10                     | 0.51              |
| 1:L:292:PHE:O    | 1:L:300:LEU:HA   | 2.10                     | 0.51              |
| 1:D:254:MET:SD   | 1:E:194:PRO:HB2  | 2.51                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:434:LEU:HD11 | 1:H:455:GLN:HG3  | 1.93                     | 0.51              |
| 1:J:193:VAL:HA   | 1:I:40:HIS:CD2   | 2.46                     | 0.51              |
| 1:L:86:ILE:O     | 7:L:602:HOH:O    | 2.19                     | 0.51              |
| 1:E:141:GLU:HG2  | 1:E:223:GLU:HG3  | 1.93                     | 0.51              |
| 1:J:149:LYS:O    | 1:J:159:TYR:HA   | 2.11                     | 0.51              |
| 1:J:341:ILE:HB   | 1:J:406:LEU:HD13 | 1.93                     | 0.51              |
| 1:B:470:PRO:HD2  | 1:L:271:TYR:HB2  | 1.93                     | 0.51              |
| 1:E:110:TYR:HB3  | 1:E:113:CYS:HB2  | 1.92                     | 0.51              |
| 1:L:165:GLU:OE1  | 1:L:198:THR:OG1  | 2.28                     | 0.51              |
| 1:A:351:ALA:HA   | 1:A:406:LEU:CD1  | 2.40                     | 0.51              |
| 1:A:43:TYR:CE1   | 1:B:219:VAL:HG22 | 2.45                     | 0.51              |
| 1:F:29:PHE:O     | 1:F:40:HIS:HA    | 2.11                     | 0.51              |
| 1:F:389:MET:O    | 1:F:392:VAL:N    | 2.39                     | 0.51              |
| 1:F:390:ASP:HA   | 1:F:393:LYS:HD3  | 1.93                     | 0.51              |
| 1:L:207:VAL:CG2  | 1:L:220:VAL:HG11 | 2.41                     | 0.51              |
| 1:D:9:GLU:O      | 1:D:13:LYS:NZ    | 2.44                     | 0.50              |
| 1:E:442:GLU:O    | 1:E:445:VAL:HG23 | 2.11                     | 0.50              |
| 1:C:197:ASP:OD2  | 1:C:203:ARG:NH2  | 2.26                     | 0.50              |
| 1:D:9:GLU:HA     | 1:D:13:LYS:HZ1   | 1.76                     | 0.50              |
| 1:I:207:VAL:HG13 | 1:I:217:THR:HG21 | 1.93                     | 0.50              |
| 1:F:182:HIS:CE1  | 1:I:480:SER:HG   | 2.30                     | 0.50              |
| 1:B:28:ASP:CG    | 1:B:40:HIS:HD1   | 2.14                     | 0.50              |
| 1:C:209:VAL:O    | 1:C:213:VAL:HG22 | 2.11                     | 0.50              |
| 1:G:14:GLU:OE2   | 1:G:17:GLU:HG3   | 2.12                     | 0.50              |
| 1:L:225:ALA:HB3  | 1:L:228:GLN:HB2  | 1.93                     | 0.50              |
| 1:C:290:ASN:ND2  | 1:C:364:ALA:HB3  | 2.26                     | 0.50              |
| 1:D:210:LEU:HD22 | 1:D:215:LEU:HD12 | 1.93                     | 0.50              |
| 1:E:442:GLU:OE2  | 1:E:442:GLU:HA   | 2.11                     | 0.50              |
| 1:L:114:PRO:HB3  | 1:L:379:LEU:CD2  | 2.42                     | 0.50              |
| 1:E:189:GLY:O    | 1:E:191:MET:HA   | 2.12                     | 0.50              |
| 1:E:207:VAL:HA   | 1:E:210:LEU:HD12 | 1.92                     | 0.50              |
| 1:G:13:LYS:O     | 1:G:17:GLU:HG2   | 2.11                     | 0.50              |
| 1:J:13:LYS:O     | 1:J:17:GLU:HG2   | 2.12                     | 0.50              |
| 1:A:133:VAL:HG11 | 1:A:135:TYR:CZ   | 2.47                     | 0.50              |
| 1:D:185:GLY:HA3  | 7:D:615:HOH:O    | 2.11                     | 0.50              |
| 1:G:29:PHE:O     | 1:G:40:HIS:HA    | 2.11                     | 0.50              |
| 1:K:30:ARG:HG2   | 1:K:40:HIS:HB3   | 1.93                     | 0.50              |
| 1:B:157:GLN:HG2  | 1:L:159:TYR:CE1  | 2.46                     | 0.50              |
| 1:L:303:PHE:CE1  | 1:L:392:VAL:HG11 | 2.47                     | 0.50              |
| 1:E:479:TYR:CE2  | 1:I:148:ILE:HD13 | 2.46                     | 0.50              |
| 1:F:210:LEU:HD21 | 1:F:248:LEU:HD12 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:204:THR:O    | 1:I:208:LYS:HG3  | 2.11                     | 0.50              |
| 1:B:357:TYR:O    | 1:B:359:ILE:HG22 | 2.11                     | 0.50              |
| 1:E:164:GLU:HG3  | 1:E:174:PHE:CE1  | 2.46                     | 0.50              |
| 1:K:139:GLU:HB3  | 1:K:230:GLU:OE2  | 2.12                     | 0.50              |
| 1:K:337:GLU:HB2  | 4:K:502:PPQ:HBP1 | 1.94                     | 0.50              |
| 1:G:209:VAL:O    | 1:G:213:VAL:HG13 | 2.12                     | 0.50              |
| 1:K:425:THR:HG22 | 1:K:427:ARG:N    | 2.24                     | 0.50              |
| 1:A:115:ARG:O    | 1:A:119:LYS:HG3  | 2.11                     | 0.49              |
| 1:A:206:ILE:HG13 | 1:A:255:VAL:HG11 | 1.94                     | 0.49              |
| 1:D:198:THR:HB   | 1:D:199:MET:HG3  | 1.94                     | 0.49              |
| 1:E:137:GLY:N    | 1:E:281:HIS:O    | 2.42                     | 0.49              |
| 1:F:149:LYS:O    | 1:F:159:TYR:HA   | 2.12                     | 0.49              |
| 1:G:348:ASN:ND2  | 1:G:404:ILE:O    | 2.42                     | 0.49              |
| 1:K:420:LYS:HG3  | 7:K:623:HOH:O    | 2.12                     | 0.49              |
| 1:B:165:GLU:OE2  | 1:B:227:ALA:HA   | 2.12                     | 0.49              |
| 1:C:135:TYR:HA   | 1:C:237:ASP:HA   | 1.94                     | 0.49              |
| 1:E:60:ASP:OD1   | 1:E:60:ASP:C     | 2.50                     | 0.49              |
| 1:I:341:ILE:HB   | 1:I:406:LEU:HD13 | 1.93                     | 0.49              |
| 1:K:296:THR:HG21 | 1:K:302:GLU:HG2  | 1.94                     | 0.49              |
| 1:B:74:ASP:OD2   | 1:C:347:ASN:ND2  | 2.40                     | 0.49              |
| 1:B:70:ILE:HD11  | 1:C:337:GLU:HG2  | 1.95                     | 0.49              |
| 1:F:480:SER:HG   | 1:I:182:HIS:CE1  | 2.30                     | 0.49              |
| 1:H:372:ASP:HB2  | 7:H:606:HOH:O    | 2.12                     | 0.49              |
| 1:I:427:ARG:HG3  | 1:I:459:PHE:HE1  | 1.77                     | 0.49              |
| 1:J:10:SER:O     | 1:J:14:GLU:HG3   | 2.13                     | 0.49              |
| 1:K:442:GLU:O    | 1:K:445:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:80:ASP:OD1   | 1:A:82:VAL:HG23  | 2.13                     | 0.49              |
| 1:C:29:PHE:O     | 1:C:40:HIS:HA    | 2.12                     | 0.49              |
| 1:D:460:ASN:HA   | 1:D:464:PHE:HD2  | 1.76                     | 0.49              |
| 1:G:44:SER:O     | 1:G:47:ALA:HB3   | 2.13                     | 0.49              |
| 1:J:221:HIS:HD2  | 1:J:222:HIS:O    | 1.95                     | 0.49              |
| 1:J:41:ILE:HB    | 1:K:191:MET:SD   | 2.52                     | 0.49              |
| 1:B:15:PHE:HE2   | 1:B:53:LEU:HD21  | 1.78                     | 0.49              |
| 1:B:341:ILE:HB   | 1:B:406:LEU:HD13 | 1.94                     | 0.49              |
| 1:B:80:ASP:OD1   | 1:B:82:VAL:HG22  | 2.13                     | 0.49              |
| 1:C:43:TYR:CZ    | 1:D:219:VAL:HG22 | 2.48                     | 0.49              |
| 1:E:202:ILE:O    | 1:E:205:GLU:HB3  | 2.13                     | 0.49              |
| 1:H:192:PRO:O    | 1:H:197:ASP:HB2  | 2.12                     | 0.49              |
| 1:B:18:PHE:O     | 1:B:22:ASN:ND2   | 2.45                     | 0.49              |
| 1:A:60:ASP:OD2   | 1:B:337:GLU:OE2  | 2.31                     | 0.49              |
| 1:E:85:PHE:CE1   | 1:E:247:LYS:HD3  | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:133:VAL:HG12 | 1:F:285:TRP:H    | 1.78                     | 0.49              |
| 1:C:281:HIS:CE1  | 1:C:367:GLU:HB2  | 2.47                     | 0.49              |
| 1:C:476:ILE:HG13 | 1:K:150:ILE:HG21 | 1.93                     | 0.49              |
| 1:D:281:HIS:HA   | 1:D:366:PHE:O    | 2.12                     | 0.49              |
| 1:J:363:SER:O    | 1:J:365:ARG:HD3  | 2.13                     | 0.49              |
| 1:K:347:ASN:ND2  | 1:K:357:TYR:HB2  | 2.28                     | 0.49              |
| 1:L:207:VAL:HA   | 1:L:210:LEU:HD12 | 1.94                     | 0.49              |
| 1:K:42:ALA:HB3   | 1:L:220:VAL:HG23 | 1.95                     | 0.49              |
| 1:C:43:TYR:CE2   | 1:D:219:VAL:HG22 | 2.48                     | 0.49              |
| 1:E:41:ILE:HB    | 1:F:191:MET:SD   | 2.53                     | 0.49              |
| 1:G:74:ASP:O     | 1:G:75:MET:HG2   | 2.12                     | 0.49              |
| 1:J:344:TYR:CE2  | 1:J:401:ALA:HB2  | 2.47                     | 0.49              |
| 1:K:151:LYS:HB3  | 1:K:158:TYR:HB3  | 1.95                     | 0.49              |
| 1:B:24:VAL:HA    | 1:B:93:VAL:HG12  | 1.94                     | 0.49              |
| 1:E:357:TYR:O    | 1:E:359:ILE:HG22 | 2.13                     | 0.49              |
| 1:E:456:SER:O    | 1:E:460:ASN:ND2  | 2.42                     | 0.49              |
| 1:G:202:ILE:O    | 1:G:206:ILE:HG13 | 2.13                     | 0.49              |
| 1:G:322:THR:HG22 | 1:G:380:ALA:HB1  | 1.95                     | 0.49              |
| 1:H:218:PHE:CE2  | 1:H:219:VAL:HG23 | 2.48                     | 0.48              |
| 1:A:50:HIS:O     | 1:A:54:LYS:HG3   | 2.12                     | 0.48              |
| 1:I:161:VAL:HG21 | 1:I:270:LEU:HD21 | 1.94                     | 0.48              |
| 1:K:163:SER:O    | 1:K:169:ASN:ND2  | 2.46                     | 0.48              |
| 1:C:397:ASP:OD1  | 1:C:398:PRO:HD2  | 2.13                     | 0.48              |
| 1:D:103:ASP:HB2  | 1:D:110:TYR:HA   | 1.94                     | 0.48              |
| 1:E:165:GLU:O    | 1:E:183:ARG:HG2  | 2.12                     | 0.48              |
| 1:F:176:ASN:H    | 1:F:178:VAL:HG12 | 1.78                     | 0.48              |
| 1:H:324:ALA:O    | 1:H:458:LYS:HE3  | 2.14                     | 0.48              |
| 1:I:226:GLN:HG2  | 1:I:273:ASP:OD2  | 2.13                     | 0.48              |
| 1:H:70:ILE:HG12  | 1:I:349:ARG:HB2  | 1.95                     | 0.48              |
| 1:J:342:LEU:HD21 | 1:J:422:MET:CE   | 2.43                     | 0.48              |
| 1:L:218:PHE:HZ   | 3:L:503:ADP:H3'  | 1.78                     | 0.48              |
| 1:A:167:GLU:O    | 1:A:170:ARG:HG3  | 2.14                     | 0.48              |
| 1:E:209:VAL:O    | 1:E:213:VAL:HG22 | 2.13                     | 0.48              |
| 1:G:370:PHE:CG   | 1:G:371:PRO:HD3  | 2.48                     | 0.48              |
| 1:I:218:PHE:HZ   | 3:I:501:ADP:H3'  | 1.79                     | 0.48              |
| 1:I:281:HIS:HA   | 1:I:366:PHE:O    | 2.14                     | 0.48              |
| 1:B:330:LYS:NZ   | 1:L:474:GLU:OE2  | 2.26                     | 0.48              |
| 1:L:80:ASP:OD2   | 1:L:115:ARG:NH1  | 2.46                     | 0.48              |
| 1:D:207:VAL:HG21 | 1:D:220:VAL:HG22 | 1.95                     | 0.48              |
| 1:J:167:GLU:O    | 1:J:170:ARG:HG3  | 2.14                     | 0.48              |
| 1:J:41:ILE:HG13  | 1:K:221:HIS:HB3  | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:LEU:O    | 1:A:215:LEU:HB2  | 2.14                     | 0.48              |
| 1:A:219:VAL:HG11 | 1:F:41:ILE:HD11  | 1.95                     | 0.48              |
| 1:C:144:ILE:HD13 | 1:C:202:ILE:HD13 | 1.96                     | 0.48              |
| 1:E:142:PHE:O    | 1:E:228:GLN:HG2  | 2.13                     | 0.48              |
| 1:J:300:LEU:HD11 | 1:J:355:ILE:HG12 | 1.94                     | 0.48              |
| 1:K:400:GLU:HG3  | 1:K:401:ALA:H    | 1.78                     | 0.48              |
| 1:D:74:ASP:OD2   | 1:E:354:ARG:NH2  | 2.46                     | 0.48              |
| 1:E:375:SER:HB2  | 1:E:380:ALA:HB2  | 1.95                     | 0.48              |
| 1:E:427:ARG:O    | 1:E:431:GLU:HG3  | 2.14                     | 0.48              |
| 1:E:74:ASP:CG    | 1:F:354:ARG:HH11 | 2.15                     | 0.48              |
| 1:E:472:PRO:HG2  | 1:I:157:GLN:HB3  | 1.95                     | 0.48              |
| 1:I:215:LEU:HD21 | 1:I:244:ASN:HB3  | 1.96                     | 0.48              |
| 1:I:346:ALA:CA   | 1:I:355:ILE:HG23 | 2.38                     | 0.48              |
| 1:J:193:VAL:HG22 | 1:I:38:TRP:O     | 2.14                     | 0.48              |
| 1:K:218:PHE:CE1  | 1:K:219:VAL:HG23 | 2.49                     | 0.48              |
| 1:D:437:LYS:O    | 1:D:439:TYR:N    | 2.46                     | 0.48              |
| 1:F:190:TYR:CZ   | 1:F:191:MET:HE3  | 2.48                     | 0.48              |
| 1:G:213:VAL:HG23 | 1:G:247:LYS:HD3  | 1.95                     | 0.48              |
| 1:A:26:PHE:HB2   | 1:A:94:SER:HB3   | 1.96                     | 0.48              |
| 1:E:60:ASP:OD1   | 1:E:62:SER:N     | 2.45                     | 0.48              |
| 1:L:206:ILE:HG22 | 1:L:210:LEU:HD11 | 1.95                     | 0.48              |
| 1:L:83:ARG:HD3   | 1:L:240:GLU:HG3  | 1.96                     | 0.48              |
| 1:A:9:GLU:HA     | 1:A:12:ILE:HB    | 1.96                     | 0.47              |
| 1:B:464:PHE:O    | 1:B:468:SER:OG   | 2.17                     | 0.47              |
| 1:C:333:ILE:HG23 | 1:C:334:PRO:HD2  | 1.95                     | 0.47              |
| 1:G:172:ARG:HD2  | 1:G:174:PHE:CZ   | 2.49                     | 0.47              |
| 1:I:337:GLU:OE2  | 1:I:349:ARG:HD3  | 2.13                     | 0.47              |
| 1:I:279:HIS:NE2  | 4:I:502:PPQ:OP   | 2.40                     | 0.47              |
| 1:L:322:THR:HB   | 1:L:371:PRO:HB3  | 1.96                     | 0.47              |
| 1:B:425:THR:HG22 | 1:B:427:ARG:N    | 2.28                     | 0.47              |
| 1:D:151:LYS:HE3  | 1:D:153:ALA:HB2  | 1.95                     | 0.47              |
| 1:I:300:LEU:HD21 | 1:I:355:ILE:HD13 | 1.96                     | 0.47              |
| 1:K:67:TRP:HZ2   | 1:K:114:PRO:HD3  | 1.77                     | 0.47              |
| 1:H:193:VAL:HA   | 1:G:40:HIS:CD2   | 2.48                     | 0.47              |
| 1:G:71:GLU:OE1   | 1:G:71:GLU:N     | 2.41                     | 0.47              |
| 1:I:353:VAL:HG22 | 1:I:368:PHE:CD1  | 2.48                     | 0.47              |
| 1:J:7:ASN:ND2    | 1:J:81:LEU:HG    | 2.29                     | 0.47              |
| 1:A:9:GLU:HG3    | 1:A:12:ILE:HB    | 1.96                     | 0.47              |
| 1:C:223:GLU:HG3  | 1:C:224:VAL:N    | 2.24                     | 0.47              |
| 1:J:357:TYR:CE1  | 1:I:104:VAL:HB   | 2.50                     | 0.47              |
| 1:K:300:LEU:HD21 | 1:K:359:ILE:HD11 | 1.96                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:290:ASN:ND2 | 1:E:364:ALA:HB3  | 2.29                     | 0.47              |
| 1:F:294:GLY:HA3 | 1:F:301:SER:HB3  | 1.96                     | 0.47              |
| 1:G:189:GLY:O   | 1:G:192:PRO:HD2  | 2.14                     | 0.47              |
| 1:L:78:THR:OG1  | 1:L:100:ASP:HB2  | 2.14                     | 0.47              |
| 1:B:223:GLU:CB  | 1:B:228:GLN:HB3  | 2.44                     | 0.47              |
| 1:C:216:GLU:H   | 1:C:234:LYS:HE3  | 1.79                     | 0.47              |
| 1:G:293:SER:OG  | 1:G:361:LYS:HA   | 2.14                     | 0.47              |
| 1:C:171:ASP:N   | 1:C:171:ASP:OD1  | 2.47                     | 0.47              |
| 1:E:18:PHE:O    | 1:E:22:ASN:ND2   | 2.48                     | 0.47              |
| 1:H:179:ASN:OD1 | 1:H:183:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:191:MET:HE1 | 1:A:221:HIS:CB   | 2.44                     | 0.47              |
| 1:D:273:ASP:OD1 | 1:D:274:ASN:N    | 2.45                     | 0.47              |
| 1:F:202:ILE:O   | 1:F:206:ILE:HG13 | 2.15                     | 0.47              |
| 1:I:131:GLY:HA2 | 1:I:286:LYS:HB2  | 1.97                     | 0.47              |
| 1:A:115:ARG:NH2 | 1:A:243:ASP:OD1  | 2.33                     | 0.47              |
| 1:B:339:PRO:HB3 | 1:B:352:SER:HA   | 1.96                     | 0.47              |
| 1:B:74:ASP:OD2  | 1:C:347:ASN:HA   | 2.15                     | 0.47              |
| 1:G:221:HIS:NE2 | 1:G:223:GLU:OE2  | 2.47                     | 0.47              |
| 1:G:341:ILE:O   | 1:G:352:SER:OG   | 2.33                     | 0.47              |
| 1:J:313:ARG:HD2 | 1:J:396:ILE:HD13 | 1.97                     | 0.47              |
| 1:J:456:SER:O   | 1:J:460:ASN:ND2  | 2.48                     | 0.47              |
| 1:A:190:TYR:CD1 | 1:A:191:MET:HG3  | 2.49                     | 0.47              |
| 1:H:226:GLN:HG2 | 1:H:273:ASP:OD2  | 2.14                     | 0.47              |
| 1:D:37:THR:O    | 1:D:39:ASN:ND2   | 2.48                     | 0.46              |
| 1:F:28:ASP:OD2  | 1:F:40:HIS:HB2   | 2.15                     | 0.46              |
| 1:J:194:PRO:HB2 | 1:I:254:MET:SD   | 2.55                     | 0.46              |
| 1:I:305:LEU:O   | 1:I:308:LEU:HB3  | 2.15                     | 0.46              |
| 1:L:201:ASP:HA  | 1:L:204:THR:HG22 | 1.96                     | 0.46              |
| 1:B:15:PHE:CE2  | 1:B:53:LEU:HD21  | 2.50                     | 0.46              |
| 1:C:210:LEU:CD1 | 1:C:248:LEU:CD1  | 2.93                     | 0.46              |
| 1:E:280:THR:OG1 | 1:E:371:PRO:HG2  | 2.14                     | 0.46              |
| 1:F:24:VAL:HG11 | 1:F:95:VAL:HG12  | 1.96                     | 0.46              |
| 1:I:343:THR:O   | 1:I:352:SER:HB2  | 2.15                     | 0.46              |
| 1:C:330:LYS:HE2 | 1:K:474:GLU:OE1  | 2.16                     | 0.46              |
| 1:L:112:LYS:HE3 | 1:L:449:GLU:OE2  | 2.16                     | 0.46              |
| 1:A:13:LYS:O    | 1:A:17:GLU:OE1   | 2.33                     | 0.46              |
| 1:E:132:ASP:CG  | 1:E:286:LYS:HG3  | 2.36                     | 0.46              |
| 1:F:172:ARG:O   | 1:F:179:ASN:ND2  | 2.42                     | 0.46              |
| 1:G:268:LYS:NZ  | 1:G:273:ASP:O    | 2.37                     | 0.46              |
| 1:H:341:ILE:CG2 | 1:H:419:ILE:HG21 | 2.43                     | 0.46              |
| 1:K:218:PHE:CZ  | 2:K:501:ATP:H3'  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:124:HIS:CE1  | 1:A:443:SER:HG   | 2.34                     | 0.46              |
| 1:C:132:ASP:HB2  | 1:C:286:LYS:HA   | 1.97                     | 0.46              |
| 1:C:440:LEU:O    | 1:C:446:PHE:HB2  | 2.14                     | 0.46              |
| 1:D:16:PHE:O     | 1:D:20:LYS:HG3   | 2.16                     | 0.46              |
| 1:E:223:GLU:HB2  | 1:E:228:GLN:HB3  | 1.97                     | 0.46              |
| 1:F:441:LYS:NZ   | 1:F:448:GLU:HB2  | 2.29                     | 0.46              |
| 1:F:330:LYS:HE2  | 1:H:474:GLU:OE1  | 2.15                     | 0.46              |
| 1:L:136:PHE:CE1  | 1:L:238:LEU:HD12 | 2.50                     | 0.46              |
| 1:C:39:ASN:ND2   | 1:D:191:MET:H    | 1.97                     | 0.46              |
| 1:D:341:ILE:O    | 1:D:352:SER:OG   | 2.24                     | 0.46              |
| 1:F:216:GLU:HG2  | 1:F:234:LYS:CD   | 2.45                     | 0.46              |
| 1:G:175:GLU:HG3  | 1:G:176:ASN:H    | 1.79                     | 0.46              |
| 1:G:218:PHE:N    | 1:G:232:GLY:O    | 2.40                     | 0.46              |
| 1:G:66:GLY:O     | 1:G:112:LYS:HD3  | 2.15                     | 0.46              |
| 1:J:179:ASN:O    | 1:I:147:SER:HA   | 2.14                     | 0.46              |
| 1:K:237:ASP:OD1  | 1:K:239:VAL:N    | 2.48                     | 0.46              |
| 1:A:355:ILE:HD11 | 1:A:359:ILE:HD12 | 1.98                     | 0.46              |
| 1:B:70:ILE:CD1   | 1:C:349:ARG:HB2  | 2.46                     | 0.46              |
| 1:C:455:GLN:HG2  | 1:C:459:PHE:CD2  | 2.50                     | 0.46              |
| 1:F:367:GLU:HG2  | 1:F:369:ARG:HG2  | 1.97                     | 0.46              |
| 1:G:76:ILE:O     | 1:G:102:TYR:N    | 2.42                     | 0.46              |
| 1:H:303:PHE:CE2  | 1:H:392:VAL:HG11 | 2.50                     | 0.46              |
| 1:I:360:SER:N    | 1:I:363:SER:OG   | 2.46                     | 0.46              |
| 1:J:43:TYR:CZ    | 1:K:219:VAL:HG22 | 2.50                     | 0.46              |
| 1:D:8:SER:O      | 1:D:11:LYS:N     | 2.48                     | 0.46              |
| 1:G:292:PHE:HA   | 1:G:304:ALA:HB2  | 1.97                     | 0.46              |
| 1:I:124:HIS:ND1  | 1:I:389:MET:CE   | 2.79                     | 0.46              |
| 1:J:423:PRO:HB3  | 1:J:428:ARG:HG3  | 1.96                     | 0.46              |
| 1:D:126:LYS:HB3  | 1:D:126:LYS:HE2  | 1.70                     | 0.46              |
| 1:D:442:GLU:HG2  | 7:D:620:HOH:O    | 2.15                     | 0.46              |
| 1:F:363:SER:HA   | 2:F:501:ATP:HN61 | 1.80                     | 0.46              |
| 1:J:148:ILE:HD13 | 1:J:161:VAL:HG12 | 1.98                     | 0.46              |
| 1:D:35:LYS:NZ    | 1:J:477:THR:O    | 2.49                     | 0.46              |
| 1:L:223:GLU:HG3  | 1:L:224:VAL:N    | 2.31                     | 0.46              |
| 1:L:52:MET:HE3   | 1:L:57:ILE:HD11  | 1.96                     | 0.46              |
| 1:E:411:LEU:HA   | 1:E:414:ILE:HD13 | 1.97                     | 0.46              |
| 1:B:285:TRP:CZ2  | 1:B:290:ASN:HB2  | 2.50                     | 0.46              |
| 1:B:306:HIS:HB3  | 1:B:392:VAL:HA   | 1.97                     | 0.46              |
| 1:C:139:GLU:O    | 1:C:278:MET:HA   | 2.15                     | 0.46              |
| 1:B:60:ASP:OD2   | 1:C:349:ARG:HD2  | 2.16                     | 0.46              |
| 1:E:207:VAL:HG21 | 1:E:220:VAL:CG2  | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:238:LEU:HG   | 1:F:381:PHE:HB3  | 1.97                     | 0.46              |
| 1:I:65:LYS:O     | 1:I:457:LEU:HD12 | 2.15                     | 0.46              |
| 1:A:341:ILE:HD11 | 1:A:414:ILE:HD13 | 1.98                     | 0.45              |
| 1:C:133:VAL:HG11 | 1:C:135:TYR:CZ   | 2.52                     | 0.45              |
| 1:F:218:PHE:CZ   | 2:F:501:ATP:H3'  | 2.51                     | 0.45              |
| 1:A:342:LEU:HA   | 1:A:352:SER:OG   | 2.16                     | 0.45              |
| 1:G:278:MET:H    | 1:G:372:ASP:HA   | 1.80                     | 0.45              |
| 1:H:306:HIS:CE1  | 1:H:395:LYS:HG2  | 2.51                     | 0.45              |
| 1:L:78:THR:HG1   | 1:L:100:ASP:HB2  | 1.81                     | 0.45              |
| 1:L:165:GLU:HA   | 1:L:183:ARG:HG2  | 1.98                     | 0.45              |
| 1:L:145:PHE:HB2  | 1:L:262:THR:HG23 | 1.98                     | 0.45              |
| 1:A:178:VAL:HG22 | 1:F:147:SER:HB2  | 1.99                     | 0.45              |
| 1:I:208:LYS:O    | 1:I:211:ASN:HB2  | 2.16                     | 0.45              |
| 1:I:187:GLN:HG3  | 1:I:273:ASP:OD1  | 2.16                     | 0.45              |
| 1:I:36:GLY:HA2   | 1:I:376:ASN:ND2  | 2.31                     | 0.45              |
| 1:K:146:ASP:OD1  | 1:K:261:LYS:HE3  | 2.16                     | 0.45              |
| 1:B:148:ILE:O    | 1:C:179:ASN:HB3  | 2.17                     | 0.45              |
| 1:F:385:LEU:O    | 1:F:389:MET:HG3  | 2.17                     | 0.45              |
| 1:J:339:PRO:HB3  | 1:J:352:SER:HA   | 1.99                     | 0.45              |
| 1:C:85:PHE:CE1   | 1:C:247:LYS:HD2  | 2.52                     | 0.45              |
| 1:A:136:PHE:CE1  | 1:A:238:LEU:HD12 | 2.52                     | 0.45              |
| 1:A:355:ILE:HD11 | 1:A:359:ILE:CD1  | 2.47                     | 0.45              |
| 1:B:203:ARG:NH1  | 1:B:222:HIS:HB2  | 2.32                     | 0.45              |
| 1:D:139:GLU:O    | 1:D:278:MET:HA   | 2.17                     | 0.45              |
| 1:H:33:ASP:O     | 1:H:114:PRO:HG2  | 2.16                     | 0.45              |
| 1:K:207:VAL:HG13 | 1:K:217:THR:HG21 | 1.98                     | 0.45              |
| 1:A:143:PHE:HB2  | 1:A:264:THR:HG23 | 1.98                     | 0.45              |
| 1:B:111:GLU:OE2  | 1:B:449:GLU:HB2  | 2.17                     | 0.45              |
| 1:E:92:ASP:CG    | 1:F:208:LYS:HZ3  | 2.20                     | 0.45              |
| 1:I:285:TRP:CZ2  | 1:I:290:ASN:HB2  | 2.52                     | 0.45              |
| 1:J:283:SER:HA   | 1:J:292:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:281:HIS:HA   | 1:A:366:PHE:O    | 2.17                     | 0.45              |
| 1:B:106:LYS:HB2  | 1:B:108:GLN:HG2  | 1.98                     | 0.45              |
| 1:B:474:GLU:O    | 1:B:478:THR:HB   | 2.17                     | 0.45              |
| 1:C:234:LYS:O    | 1:C:234:LYS:HD2  | 2.17                     | 0.45              |
| 1:C:28:ASP:OD2   | 1:C:40:HIS:ND1   | 2.49                     | 0.45              |
| 1:F:113:CYS:HB3  | 1:F:116:SER:HB2  | 1.98                     | 0.45              |
| 1:G:370:PHE:CD2  | 1:G:371:PRO:HD3  | 2.52                     | 0.45              |
| 1:G:48:LEU:HD12  | 1:G:48:LEU:HA    | 1.78                     | 0.45              |
| 1:I:17:GLU:O     | 1:I:21:GLU:HG2   | 2.16                     | 0.45              |
| 1:J:226:GLN:HG2  | 1:J:273:ASP:OD2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:281:HIS:HA   | 1:J:366:PHE:O    | 2.17                     | 0.45              |
| 1:K:308:LEU:HD22 | 1:K:366:PHE:CE1  | 2.52                     | 0.45              |
| 1:C:281:HIS:HA   | 1:C:366:PHE:O    | 2.17                     | 0.45              |
| 1:H:370:PHE:CG   | 1:H:422:MET:HE3  | 2.52                     | 0.45              |
| 1:F:159:TYR:CE1  | 1:H:475:PHE:CZ   | 3.05                     | 0.45              |
| 1:J:353:VAL:HG22 | 1:J:368:PHE:HD1  | 1.82                     | 0.45              |
| 1:J:427:ARG:NE   | 1:J:459:PHE:HE1  | 2.14                     | 0.45              |
| 1:K:292:PHE:HA   | 1:K:304:ALA:HB2  | 1.98                     | 0.45              |
| 1:A:74:ASP:OD1   | 1:B:349:ARG:NH1  | 2.50                     | 0.44              |
| 1:B:281:HIS:HA   | 1:B:366:PHE:O    | 2.17                     | 0.44              |
| 1:H:18:PHE:O     | 1:H:22:ASN:ND2   | 2.43                     | 0.44              |
| 1:J:125:LEU:O    | 1:J:128:SER:OG   | 2.34                     | 0.44              |
| 1:J:281:HIS:CD2  | 1:J:367:GLU:HG3  | 2.51                     | 0.44              |
| 1:C:474:GLU:HG2  | 1:K:327:ASN:HB2  | 1.99                     | 0.44              |
| 1:K:341:ILE:HG22 | 1:K:419:ILE:HD11 | 1.99                     | 0.44              |
| 1:C:336:TYR:N    | 1:C:336:TYR:CD2  | 2.84                     | 0.44              |
| 1:C:370:PHE:N    | 1:C:371:PRO:HD3  | 2.32                     | 0.44              |
| 1:D:189:GLY:O    | 1:D:192:PRO:HD2  | 2.17                     | 0.44              |
| 1:D:92:ASP:OD1   | 1:E:208:LYS:NZ   | 2.48                     | 0.44              |
| 1:F:134:ALA:O    | 1:F:237:ASP:HA   | 2.16                     | 0.44              |
| 1:G:125:LEU:HA   | 1:G:389:MET:CE   | 2.48                     | 0.44              |
| 1:I:237:ASP:OD1  | 1:I:237:ASP:C    | 2.56                     | 0.44              |
| 1:I:341:ILE:HD12 | 1:I:419:ILE:HD13 | 1.98                     | 0.44              |
| 1:J:354:ARG:O    | 1:J:356:PRO:HD3  | 2.17                     | 0.44              |
| 1:A:19:CYS:SG    | 1:A:95:VAL:HG11  | 2.58                     | 0.44              |
| 1:B:78:THR:CG2   | 1:B:102:TYR:HB2  | 2.47                     | 0.44              |
| 1:E:313:ARG:NE   | 1:E:396:ILE:HD11 | 2.32                     | 0.44              |
| 1:F:211:ASN:O    | 1:F:213:VAL:N    | 2.50                     | 0.44              |
| 1:E:467:GLU:O    | 1:I:330:LYS:HD3  | 2.17                     | 0.44              |
| 1:C:133:VAL:HG12 | 1:C:285:TRP:HB2  | 1.98                     | 0.44              |
| 1:E:116:SER:O    | 1:E:120:LYS:HG3  | 2.18                     | 0.44              |
| 1:E:169:ASN:HB3  | 1:E:174:PHE:HZ   | 1.82                     | 0.44              |
| 1:G:18:PHE:O     | 1:G:22:ASN:ND2   | 2.50                     | 0.44              |
| 1:H:132:ASP:HB2  | 1:H:286:LYS:HA   | 1.99                     | 0.44              |
| 1:J:115:ARG:NH2  | 1:J:243:ASP:CG   | 2.70                     | 0.44              |
| 1:L:300:LEU:CD2  | 1:L:359:ILE:HD11 | 2.45                     | 0.44              |
| 1:L:419:ILE:HD12 | 1:L:419:ILE:H    | 1.82                     | 0.44              |
| 1:A:8:SER:H      | 1:A:11:LYS:NZ    | 2.15                     | 0.44              |
| 1:G:423:PRO:HG2  | 1:G:429:SER:HB3  | 1.98                     | 0.44              |
| 1:A:326:THR:OG1  | 1:G:474:GLU:OE1  | 2.20                     | 0.44              |
| 1:K:199:MET:O    | 1:K:203:ARG:HB2  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:ASN:HD21   | 1:A:81:LEU:HG    | 1.82                     | 0.44              |
| 1:C:357:TYR:O    | 1:C:359:ILE:HG22 | 2.17                     | 0.44              |
| 1:C:363:SER:O    | 1:C:365:ARG:HD3  | 2.18                     | 0.44              |
| 1:D:462:GLU:C    | 1:D:465:PRO:HD2  | 2.37                     | 0.44              |
| 1:H:319:ALA:HA   | 1:H:322:THR:OG1  | 2.17                     | 0.44              |
| 1:I:344:TYR:CE1  | 1:I:398:PRO:HB2  | 2.52                     | 0.44              |
| 1:K:207:VAL:O    | 1:K:211:ASN:OD1  | 2.35                     | 0.44              |
| 1:L:357:TYR:O    | 1:L:359:ILE:N    | 2.51                     | 0.44              |
| 1:B:264:THR:HB   | 1:L:479:TYR:CE1  | 2.53                     | 0.44              |
| 1:E:48:LEU:HD12  | 1:E:52:MET:CE    | 2.47                     | 0.44              |
| 1:G:87:ASP:C     | 1:G:87:ASP:OD1   | 2.56                     | 0.44              |
| 1:H:305:LEU:O    | 1:H:308:LEU:HB3  | 2.18                     | 0.44              |
| 1:J:341:ILE:O    | 1:J:352:SER:OG   | 2.34                     | 0.44              |
| 1:J:29:PHE:O     | 1:J:40:HIS:HA    | 2.17                     | 0.44              |
| 1:K:354:ARG:NH1  | 1:K:356:PRO:HB3  | 2.33                     | 0.44              |
| 1:K:43:TYR:HA    | 1:L:218:PHE:O    | 2.18                     | 0.44              |
| 1:K:9:GLU:O      | 1:K:13:LYS:HG2   | 2.18                     | 0.44              |
| 1:A:157:GLN:HG2  | 1:G:159:TYR:HE1  | 1.82                     | 0.44              |
| 1:E:200:MET:HE2  | 1:E:204:THR:HG23 | 1.99                     | 0.44              |
| 1:I:235:PHE:CD2  | 3:I:501:ADP:C4   | 3.05                     | 0.44              |
| 1:K:58:PRO:HA    | 1:K:76:ILE:HD13  | 2.00                     | 0.44              |
| 1:A:322:THR:HG22 | 1:A:380:ALA:HB1  | 2.00                     | 0.44              |
| 1:B:113:CYS:O    | 1:B:117:ILE:HG13 | 2.17                     | 0.44              |
| 1:C:216:GLU:OE2  | 1:C:234:LYS:HG2  | 2.17                     | 0.44              |
| 1:E:206:ILE:HG22 | 1:E:210:LEU:HD11 | 2.00                     | 0.44              |
| 1:E:356:PRO:HG2  | 1:E:365:ARG:CG   | 2.47                     | 0.44              |
| 1:J:368:PHE:HB3  | 1:J:370:PHE:CE1  | 2.53                     | 0.44              |
| 1:K:100:ASP:N    | 1:K:100:ASP:OD1  | 2.49                     | 0.44              |
| 1:K:135:TYR:HD2  | 1:K:285:TRP:CD1  | 2.35                     | 0.44              |
| 1:K:223:GLU:HB3  | 1:K:228:GLN:OE1  | 2.18                     | 0.44              |
| 1:B:115:ARG:HG3  | 1:B:378:TYR:CE1  | 2.53                     | 0.43              |
| 1:C:370:PHE:CG   | 1:C:422:MET:HE3  | 2.52                     | 0.43              |
| 1:F:281:HIS:CE1  | 1:F:367:GLU:HB2  | 2.52                     | 0.43              |
| 1:G:284:VAL:C    | 1:G:285:TRP:CD1  | 2.91                     | 0.43              |
| 1:G:376:ASN:HD22 | 1:G:379:LEU:N    | 1.99                     | 0.43              |
| 1:A:148:ILE:HD13 | 1:A:161:VAL:HG12 | 2.00                     | 0.43              |
| 1:B:103:ASP:HB2  | 1:B:110:TYR:HA   | 2.01                     | 0.43              |
| 1:E:53:LEU:HA    | 1:E:79:PRO:HG2   | 2.00                     | 0.43              |
| 1:B:194:PRO:HD3  | 1:B:197:ASP:HB3  | 1.99                     | 0.43              |
| 1:B:354:ARG:HD3  | 1:B:367:GLU:OE1  | 2.18                     | 0.43              |
| 1:C:19:CYS:HB3   | 1:C:24:VAL:HB    | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:341:ILE:HD12 | 1:C:406:LEU:HB3  | 1.99                     | 0.43              |
| 1:C:74:ASP:OD2   | 1:D:347:ASN:ND2  | 2.43                     | 0.43              |
| 1:D:268:LYS:N    | 1:D:327:ASN:OD1  | 2.38                     | 0.43              |
| 1:D:345:SER:HB3  | 1:D:348:ASN:HB3  | 2.00                     | 0.43              |
| 1:E:237:ASP:HB3  | 1:E:240:GLU:HB3  | 2.01                     | 0.43              |
| 1:E:306:HIS:O    | 1:E:307:PHE:C    | 2.57                     | 0.43              |
| 1:E:354:ARG:NH2  | 1:E:356:PRO:HA   | 2.33                     | 0.43              |
| 1:F:40:HIS:O     | 1:F:40:HIS:CD2   | 2.71                     | 0.43              |
| 1:F:7:ASN:ND2    | 1:F:7:ASN:O      | 2.46                     | 0.43              |
| 1:G:316:ARG:NH1  | 1:G:421:GLN:O    | 2.50                     | 0.43              |
| 1:H:341:ILE:HD13 | 1:H:421:GLN:HB3  | 2.01                     | 0.43              |
| 1:L:114:PRO:HB3  | 1:L:379:LEU:HD21 | 1.99                     | 0.43              |
| 1:A:427:ARG:HH12 | 1:A:467:GLU:CD   | 2.22                     | 0.43              |
| 1:B:308:LEU:HD22 | 1:B:366:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:60:ASP:OD2   | 1:C:337:GLU:OE1  | 2.35                     | 0.43              |
| 1:D:9:GLU:HA     | 1:D:13:LYS:HZ3   | 1.84                     | 0.43              |
| 1:F:140:ASN:HB3  | 1:F:265:PHE:CE2  | 2.53                     | 0.43              |
| 1:F:442:GLU:O    | 1:F:444:GLN:N    | 2.51                     | 0.43              |
| 1:J:71:GLU:OE2   | 1:J:71:GLU:N     | 2.39                     | 0.43              |
| 1:A:12:ILE:HD13  | 1:A:81:LEU:CD1   | 2.48                     | 0.43              |
| 1:B:459:PHE:HA   | 1:B:463:VAL:HB   | 2.00                     | 0.43              |
| 1:C:167:GLU:OE1  | 1:C:186:LYS:HG3  | 2.19                     | 0.43              |
| 1:C:324:ALA:HB1  | 1:C:458:LYS:CE   | 2.49                     | 0.43              |
| 1:C:33:ASP:OD2   | 1:C:37:THR:HB    | 2.19                     | 0.43              |
| 1:E:143:PHE:CZ   | 1:E:228:GLN:HG3  | 2.54                     | 0.43              |
| 1:G:136:PHE:CE1  | 1:G:238:LEU:HD12 | 2.53                     | 0.43              |
| 1:H:223:GLU:HB3  | 1:H:228:GLN:OE1  | 2.19                     | 0.43              |
| 1:I:473:PHE:CD1  | 1:I:476:ILE:HD12 | 2.54                     | 0.43              |
| 1:J:28:ASP:HB3   | 1:J:96:VAL:HG22  | 2.01                     | 0.43              |
| 1:K:471:HIS:HB3  | 1:K:474:GLU:HG3  | 2.00                     | 0.43              |
| 1:L:164:GLU:O    | 1:L:183:ARG:NH1  | 2.51                     | 0.43              |
| 1:B:159:TYR:HE1  | 1:L:157:GLN:HG2  | 1.84                     | 0.43              |
| 1:B:236:GLY:HA3  | 1:B:240:GLU:HG2  | 2.01                     | 0.43              |
| 1:E:190:TYR:CG   | 1:E:191:MET:HG2  | 2.54                     | 0.43              |
| 1:E:43:TYR:CZ    | 1:F:219:VAL:HG22 | 2.53                     | 0.43              |
| 1:I:360:SER:O    | 1:I:363:SER:N    | 2.48                     | 0.43              |
| 1:K:316:ARG:HG3  | 1:K:420:LYS:HZ2  | 1.84                     | 0.43              |
| 1:C:114:PRO:HB3  | 1:C:379:LEU:HG   | 2.01                     | 0.43              |
| 1:C:210:LEU:HD23 | 1:C:251:VAL:HG11 | 2.01                     | 0.43              |
| 1:C:434:LEU:HD11 | 1:C:455:GLN:HG3  | 2.01                     | 0.43              |
| 1:D:330:LYS:HD3  | 1:J:467:GLU:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:386:MET:HE1  | 1:F:442:GLU:HB2  | 2.00                     | 0.43              |
| 1:F:402:MET:HB3  | 1:F:404:ILE:HD12 | 2.00                     | 0.43              |
| 1:G:278:MET:O    | 1:G:371:PRO:HB2  | 2.19                     | 0.43              |
| 1:I:11:LYS:HE2   | 1:I:81:LEU:O     | 2.19                     | 0.43              |
| 1:I:167:GLU:O    | 1:I:170:ARG:HG3  | 2.19                     | 0.43              |
| 1:B:353:VAL:HA   | 1:B:367:GLU:O    | 2.18                     | 0.43              |
| 1:F:106:LYS:NZ   | 1:F:111:GLU:OE1  | 2.43                     | 0.43              |
| 1:A:347:ASN:ND2  | 1:F:74:ASP:OD2   | 2.40                     | 0.43              |
| 1:G:189:GLY:O    | 1:G:191:MET:HA   | 2.19                     | 0.43              |
| 1:G:190:TYR:CD1  | 1:G:191:MET:HG3  | 2.53                     | 0.43              |
| 1:J:209:VAL:HA   | 1:J:212:GLN:HG3  | 2.00                     | 0.43              |
| 1:J:74:ASP:OD1   | 1:K:349:ARG:NH1  | 2.46                     | 0.43              |
| 1:K:179:ASN:OD1  | 1:K:183:ARG:NH2  | 2.51                     | 0.43              |
| 1:K:254:MET:SD   | 1:L:194:PRO:HB2  | 2.57                     | 0.43              |
| 1:D:7:ASN:HB2    | 1:D:12:ILE:CD1   | 2.45                     | 0.43              |
| 1:F:357:TYR:O    | 1:F:359:ILE:HG22 | 2.19                     | 0.43              |
| 1:H:139:GLU:HB2  | 1:H:279:HIS:HB2  | 2.00                     | 0.43              |
| 1:I:140:ASN:HB2  | 1:I:248:LEU:CD2  | 2.49                     | 0.43              |
| 1:I:146:ASP:N    | 1:I:162:ASP:O    | 2.36                     | 0.43              |
| 1:I:354:ARG:HD3  | 1:I:367:GLU:OE1  | 2.19                     | 0.43              |
| 1:K:59:PHE:HE1   | 1:K:101:VAL:HG13 | 1.83                     | 0.43              |
| 1:B:342:LEU:HA   | 1:B:352:SER:OG   | 2.18                     | 0.43              |
| 1:C:51:GLY:O     | 1:C:54:LYS:N     | 2.45                     | 0.43              |
| 1:F:8:SER:HB3    | 1:F:12:ILE:CG1   | 2.49                     | 0.43              |
| 1:A:7:ASN:HB2    | 1:A:11:LYS:CD    | 2.48                     | 0.42              |
| 1:C:359:ILE:HG13 | 1:C:364:ALA:HA   | 2.01                     | 0.42              |
| 1:C:66:GLY:O     | 1:C:67:TRP:HD1   | 2.02                     | 0.42              |
| 1:D:124:HIS:CE1  | 1:D:443:SER:HG   | 2.37                     | 0.42              |
| 1:D:148:ILE:CD1  | 1:D:161:VAL:HG12 | 2.46                     | 0.42              |
| 1:G:286:LYS:HB3  | 1:G:291:LEU:HD11 | 2.01                     | 0.42              |
| 1:J:318:LEU:HD13 | 1:J:387:ALA:HB2  | 2.00                     | 0.42              |
| 1:K:316:ARG:HG3  | 1:K:420:LYS:NZ   | 2.34                     | 0.42              |
| 1:K:7:ASN:HD21   | 1:K:81:LEU:H     | 1.67                     | 0.42              |
| 1:L:308:LEU:HD22 | 1:L:366:PHE:CE1  | 2.54                     | 0.42              |
| 1:L:59:PHE:CD1   | 1:L:77:LEU:HG    | 2.53                     | 0.42              |
| 1:L:70:ILE:O     | 1:L:73:SER:OG    | 2.37                     | 0.42              |
| 1:L:77:LEU:HA    | 1:L:100:ASP:O    | 2.19                     | 0.42              |
| 1:A:290:ASN:OD1  | 1:A:292:PHE:HB2  | 2.19                     | 0.42              |
| 1:A:330:LYS:HD3  | 1:G:467:GLU:O    | 2.18                     | 0.42              |
| 1:C:297:TYR:CD1  | 1:C:298:LYS:HG2  | 2.54                     | 0.42              |
| 1:C:34:ILE:HD12  | 1:C:66:GLY:HA3   | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:25:GLU:N     | 1:D:93:VAL:O     | 2.51                     | 0.42              |
| 1:E:225:ALA:HA   | 1:E:273:ASP:OD1  | 2.19                     | 0.42              |
| 1:E:215:LEU:HD21 | 1:E:244:ASN:HB3  | 2.01                     | 0.42              |
| 1:F:123:GLN:O    | 1:F:126:LYS:N    | 2.52                     | 0.42              |
| 1:F:187:GLN:HG2  | 1:F:274:ASN:OD1  | 2.19                     | 0.42              |
| 1:F:281:HIS:HB3  | 1:F:365:ARG:HD2  | 2.00                     | 0.42              |
| 1:F:450:PHE:O    | 1:F:453:ALA:N    | 2.51                     | 0.42              |
| 1:G:125:LEU:HA   | 1:G:389:MET:HE1  | 2.01                     | 0.42              |
| 1:H:136:PHE:CE1  | 1:H:238:LEU:HD12 | 2.54                     | 0.42              |
| 1:J:359:ILE:HG13 | 1:J:364:ALA:HA   | 2.01                     | 0.42              |
| 1:K:238:LEU:HG   | 1:K:381:PHE:HB3  | 1.99                     | 0.42              |
| 1:L:141:GLU:HG2  | 1:L:230:GLU:OE1  | 2.19                     | 0.42              |
| 1:L:149:LYS:O    | 1:L:159:TYR:HA   | 2.19                     | 0.42              |
| 1:L:292:PHE:HA   | 1:L:304:ALA:HB2  | 2.00                     | 0.42              |
| 1:A:328:SER:HB3  | 1:A:372:ASP:OD2  | 2.19                     | 0.42              |
| 1:B:165:GLU:O    | 1:B:183:ARG:HG2  | 2.19                     | 0.42              |
| 1:B:43:TYR:CZ    | 1:C:219:VAL:HG22 | 2.54                     | 0.42              |
| 1:E:322:THR:HG21 | 1:E:370:PHE:HD1  | 1.82                     | 0.42              |
| 1:F:139:GLU:OE2  | 1:F:279:HIS:HB2  | 2.19                     | 0.42              |
| 1:F:30:ARG:HB3   | 1:F:38:TRP:CE2   | 2.54                     | 0.42              |
| 1:F:442:GLU:O    | 1:F:443:SER:C    | 2.57                     | 0.42              |
| 1:G:175:GLU:CG   | 1:G:176:ASN:H    | 2.33                     | 0.42              |
| 1:G:281:HIS:CE1  | 1:G:367:GLU:HB2  | 2.54                     | 0.42              |
| 1:G:285:TRP:CD1  | 1:G:285:TRP:N    | 2.86                     | 0.42              |
| 1:H:143:PHE:CZ   | 1:H:228:GLN:HG3  | 2.54                     | 0.42              |
| 1:I:342:LEU:HB2  | 1:I:420:LYS:O    | 2.19                     | 0.42              |
| 1:J:67:TRP:CH2   | 1:J:101:VAL:HG21 | 2.53                     | 0.42              |
| 1:A:169:ASN:OD1  | 1:A:172:ARG:HD3  | 2.19                     | 0.42              |
| 1:B:219:VAL:CG1  | 1:B:221:HIS:HD2  | 2.32                     | 0.42              |
| 1:F:145:PHE:O    | 1:F:262:THR:HG22 | 2.20                     | 0.42              |
| 1:F:27:VAL:HG21  | 1:F:48:LEU:HD22  | 2.02                     | 0.42              |
| 1:H:342:LEU:HB2  | 1:H:420:LYS:O    | 2.20                     | 0.42              |
| 1:K:347:ASN:HD21 | 1:K:357:TYR:HB2  | 1.84                     | 0.42              |
| 1:D:348:ASN:OD1  | 1:D:350:SER:N    | 2.52                     | 0.42              |
| 1:D:404:ILE:HG13 | 1:D:406:LEU:HG   | 2.02                     | 0.42              |
| 1:H:210:LEU:HA   | 1:H:213:VAL:HG22 | 2.00                     | 0.42              |
| 1:H:430:LEU:HD13 | 1:H:459:PHE:CD2  | 2.54                     | 0.42              |
| 1:L:7:ASN:O      | 1:L:54:LYS:NZ    | 2.52                     | 0.42              |
| 1:C:166:GLY:HA2  | 1:C:226:GLN:OE1  | 2.20                     | 0.42              |
| 1:C:343:THR:HG21 | 1:C:406:LEU:HD21 | 2.02                     | 0.42              |
| 1:C:442:GLU:HA   | 1:C:442:GLU:OE1  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:114:PRO:HB3  | 1:D:379:LEU:HG   | 2.01                     | 0.42              |
| 1:D:133:VAL:HG11 | 1:D:135:TYR:CZ   | 2.55                     | 0.42              |
| 1:D:225:ALA:HB3  | 1:D:228:GLN:HB2  | 2.02                     | 0.42              |
| 1:D:61:ALA:CB    | 1:D:75:MET:HG3   | 2.49                     | 0.42              |
| 1:E:146:ASP:OD1  | 1:E:261:LYS:NZ   | 2.43                     | 0.42              |
| 1:G:100:ASP:OD1  | 1:G:115:ARG:HB3  | 2.19                     | 0.42              |
| 1:H:244:ASN:HA   | 1:H:247:LYS:HB2  | 2.01                     | 0.42              |
| 1:I:215:LEU:CD1  | 1:I:247:LYS:HD2  | 2.49                     | 0.42              |
| 1:I:290:ASN:OD1  | 1:I:292:PHE:HB2  | 2.19                     | 0.42              |
| 1:K:139:GLU:O    | 1:K:278:MET:HA   | 2.19                     | 0.42              |
| 1:B:13:LYS:HD2   | 1:B:50:HIS:NE2   | 2.34                     | 0.42              |
| 1:B:359:ILE:HG13 | 1:B:364:ALA:HA   | 2.02                     | 0.42              |
| 1:B:437:LYS:HE3  | 1:B:441:LYS:NZ   | 2.34                     | 0.42              |
| 1:E:428:ARG:HA   | 1:E:428:ARG:HD2  | 1.79                     | 0.42              |
| 1:F:430:LEU:HD11 | 1:F:458:LYS:HB2  | 2.02                     | 0.42              |
| 1:G:108:GLN:O    | 1:G:109:PRO:C    | 2.57                     | 0.42              |
| 1:A:477:THR:HG21 | 1:G:462:GLU:OE2  | 2.20                     | 0.42              |
| 1:H:323:ASN:HB3  | 1:H:328:SER:HB3  | 2.00                     | 0.42              |
| 1:I:278:MET:O    | 1:I:371:PRO:HG2  | 2.19                     | 0.42              |
| 1:J:342:LEU:HD21 | 1:J:422:MET:HE2  | 2.00                     | 0.42              |
| 1:L:74:ASP:OD1   | 1:G:347:ASN:HB3  | 2.19                     | 0.42              |
| 1:A:346:ALA:HA   | 1:A:355:ILE:HG23 | 2.02                     | 0.42              |
| 1:B:333:ILE:HG22 | 1:B:334:PRO:HD2  | 2.02                     | 0.42              |
| 1:C:243:ASP:O    | 1:C:247:LYS:HG3  | 2.20                     | 0.42              |
| 1:C:349:ARG:HD3  | 1:C:369:ARG:NH1  | 2.34                     | 0.42              |
| 1:E:322:THR:HG21 | 1:E:370:PHE:CE1  | 2.54                     | 0.42              |
| 1:E:15:PHE:HB2   | 1:E:81:LEU:HD13  | 2.00                     | 0.42              |
| 1:G:326:THR:HG23 | 1:G:462:GLU:HB3  | 2.01                     | 0.42              |
| 1:H:131:GLY:HA2  | 1:H:286:LYS:HB2  | 2.01                     | 0.42              |
| 1:H:471:HIS:HB3  | 1:H:474:GLU:CG   | 2.47                     | 0.42              |
| 1:I:348:ASN:OD1  | 1:I:350:SER:HB3  | 2.20                     | 0.42              |
| 1:I:369:ARG:NH2  | 4:I:502:PPQ:HGP2 | 2.32                     | 0.42              |
| 1:B:40:HIS:HB3   | 1:C:193:VAL:HG12 | 2.01                     | 0.42              |
| 1:D:300:LEU:CD1  | 1:D:355:ILE:HD13 | 2.48                     | 0.42              |
| 1:G:284:VAL:C    | 1:G:285:TRP:HD1  | 2.24                     | 0.42              |
| 1:I:149:LYS:O    | 1:I:159:TYR:HA   | 2.20                     | 0.42              |
| 1:J:43:TYR:HA    | 1:K:218:PHE:O    | 2.20                     | 0.42              |
| 1:L:428:ARG:HD2  | 1:L:428:ARG:HA   | 1.84                     | 0.42              |
| 1:D:113:CYS:HB3  | 1:D:116:SER:HB2  | 2.01                     | 0.42              |
| 1:E:281:HIS:NE2  | 1:E:367:GLU:HB2  | 2.34                     | 0.42              |
| 1:E:457:LEU:HA   | 1:E:457:LEU:HD12 | 1.65                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:207:VAL:HA   | 1:J:210:LEU:HD12 | 2.02                     | 0.42              |
| 1:J:344:TYR:CZ   | 1:J:401:ALA:HB2  | 2.54                     | 0.42              |
| 1:L:19:CYS:SG    | 1:L:95:VAL:HG11  | 2.59                     | 0.42              |
| 1:B:360:SER:H    | 1:B:363:SER:HG   | 1.60                     | 0.41              |
| 1:C:423:PRO:CG   | 1:C:429:SER:HB3  | 2.50                     | 0.41              |
| 1:D:199:MET:HB3  | 1:D:202:ILE:HG22 | 2.02                     | 0.41              |
| 1:E:190:TYR:CD2  | 1:E:191:MET:HG2  | 2.54                     | 0.41              |
| 1:E:218:PHE:CE1  | 1:E:232:GLY:HA3  | 2.55                     | 0.41              |
| 1:E:328:SER:O    | 1:E:331:ARG:HB3  | 2.20                     | 0.41              |
| 1:H:221:HIS:HB3  | 1:G:41:ILE:HG13  | 2.01                     | 0.41              |
| 1:H:331:ARG:HG3  | 1:H:331:ARG:O    | 2.20                     | 0.41              |
| 1:I:27:VAL:HG21  | 1:I:48:LEU:HD22  | 2.02                     | 0.41              |
| 1:I:29:PHE:O     | 1:I:40:HIS:HA    | 2.20                     | 0.41              |
| 1:I:83:ARG:NH1   | 1:I:240:GLU:HG3  | 2.35                     | 0.41              |
| 1:K:148:ILE:O    | 1:L:179:ASN:HB3  | 2.20                     | 0.41              |
| 1:A:423:PRO:HB3  | 1:A:428:ARG:HG3  | 2.02                     | 0.41              |
| 1:B:337:GLU:O    | 1:B:369:ARG:NH1  | 2.45                     | 0.41              |
| 1:G:342:LEU:HA   | 1:G:352:SER:OG   | 2.20                     | 0.41              |
| 1:G:77:LEU:HA    | 1:G:100:ASP:O    | 2.20                     | 0.41              |
| 1:F:157:GLN:HG2  | 1:H:159:TYR:HE2  | 1.86                     | 0.41              |
| 1:H:347:ASN:HA   | 1:G:74:ASP:OD2   | 2.20                     | 0.41              |
| 1:H:281:HIS:HA   | 1:H:366:PHE:O    | 2.19                     | 0.41              |
| 1:H:342:LEU:HD21 | 1:H:422:MET:CE   | 2.50                     | 0.41              |
| 1:K:146:ASP:OD2  | 1:K:164:GLU:OE1  | 2.38                     | 0.41              |
| 1:L:208:LYS:O    | 1:L:212:GLN:HG3  | 2.21                     | 0.41              |
| 1:A:215:LEU:HA   | 1:A:215:LEU:HD23 | 1.76                     | 0.41              |
| 1:D:285:TRP:N    | 1:D:285:TRP:CD1  | 2.88                     | 0.41              |
| 1:E:476:ILE:HD13 | 1:E:476:ILE:HG21 | 1.89                     | 0.41              |
| 1:F:209:VAL:O    | 1:F:213:VAL:HG22 | 2.20                     | 0.41              |
| 1:F:339:PRO:HB3  | 1:F:351:ALA:O    | 2.20                     | 0.41              |
| 1:G:290:ASN:H    | 1:G:361:LYS:NZ   | 2.18                     | 0.41              |
| 1:J:33:ASP:O     | 1:J:36:GLY:N     | 2.52                     | 0.41              |
| 1:K:74:ASP:CG    | 1:L:354:ARG:HH11 | 2.23                     | 0.41              |
| 1:L:80:ASP:OD1   | 1:L:82:VAL:HG22  | 2.20                     | 0.41              |
| 1:B:223:GLU:HB2  | 1:B:228:GLN:HB3  | 2.02                     | 0.41              |
| 1:D:117:ILE:HD12 | 1:D:379:LEU:CD2  | 2.50                     | 0.41              |
| 1:I:264:THR:OG1  | 1:I:266:MET:HG2  | 2.20                     | 0.41              |
| 1:L:219:VAL:HG12 | 1:L:232:GLY:HA3  | 2.02                     | 0.41              |
| 1:L:67:TRP:CH2   | 1:L:101:VAL:HG21 | 2.56                     | 0.41              |
| 1:A:43:TYR:HA    | 1:B:218:PHE:O    | 2.20                     | 0.41              |
| 1:B:111:GLU:OE2  | 1:B:447:SER:OG   | 2.25                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:211:ASN:C    | 1:C:213:VAL:H    | 2.24                     | 0.41              |
| 1:D:62:SER:OG    | 1:D:70:ILE:HD12  | 2.21                     | 0.41              |
| 1:F:215:LEU:HD21 | 1:F:244:ASN:HB3  | 2.03                     | 0.41              |
| 1:G:380:ALA:O    | 1:G:384:ILE:HD12 | 2.20                     | 0.41              |
| 1:J:221:HIS:HB3  | 1:I:41:ILE:HG13  | 2.02                     | 0.41              |
| 1:L:101:VAL:HB   | 1:L:113:CYS:HB2  | 2.02                     | 0.41              |
| 1:A:71:GLU:HG2   | 1:A:72:HIS:ND1   | 2.35                     | 0.41              |
| 1:D:313:ARG:HE   | 1:D:396:ILE:HG21 | 1.84                     | 0.41              |
| 1:D:59:PHE:CE1   | 1:D:75:MET:HB2   | 2.56                     | 0.41              |
| 1:F:223:GLU:CG   | 1:F:224:VAL:H    | 2.33                     | 0.41              |
| 1:F:83:ARG:HB3   | 1:F:247:LYS:NZ   | 2.35                     | 0.41              |
| 1:G:136:PHE:CE2  | 1:G:282:VAL:HG22 | 2.55                     | 0.41              |
| 1:H:115:ARG:HG3  | 1:H:378:TYR:CE1  | 2.56                     | 0.41              |
| 1:K:147:SER:OG   | 1:L:179:ASN:N    | 2.44                     | 0.41              |
| 1:C:141:GLU:HB2  | 1:C:277:GLY:H    | 1.86                     | 0.41              |
| 1:C:73:SER:HB2   | 1:D:349:ARG:HH11 | 1.86                     | 0.41              |
| 1:F:430:LEU:HD23 | 1:F:430:LEU:HA   | 1.94                     | 0.41              |
| 1:F:455:GLN:O    | 1:F:459:PHE:HD2  | 2.02                     | 0.41              |
| 1:G:215:LEU:N    | 1:G:215:LEU:HD23 | 2.35                     | 0.41              |
| 1:H:25:GLU:OE2   | 1:I:208:LYS:HE3  | 2.21                     | 0.41              |
| 1:H:104:VAL:HB   | 1:I:357:TYR:CZ   | 2.54                     | 0.41              |
| 1:C:427:ARG:O    | 1:C:431:GLU:HG3  | 2.20                     | 0.41              |
| 1:C:8:SER:HB3    | 1:C:11:LYS:HB2   | 2.03                     | 0.41              |
| 1:H:357:TYR:O    | 1:H:359:ILE:HG22 | 2.20                     | 0.41              |
| 1:H:476:ILE:HG12 | 1:H:476:ILE:H    | 1.71                     | 0.41              |
| 1:K:314:HIS:O    | 1:K:318:LEU:N    | 2.39                     | 0.41              |
| 1:L:83:ARG:NH1   | 1:L:240:GLU:HG3  | 2.36                     | 0.41              |
| 1:C:8:SER:O      | 1:C:12:ILE:HG13  | 2.21                     | 0.41              |
| 1:B:41:ILE:HG13  | 1:C:221:HIS:HB3  | 2.01                     | 0.41              |
| 1:D:48:LEU:HD12  | 1:D:48:LEU:HA    | 1.72                     | 0.41              |
| 1:I:367:GLU:HG3  | 1:I:367:GLU:O    | 2.21                     | 0.41              |
| 1:K:29:PHE:O     | 1:K:40:HIS:HA    | 2.21                     | 0.41              |
| 1:A:79:PRO:HA    | 1:A:99:CYS:SG    | 2.60                     | 0.41              |
| 1:B:347:ASN:HD21 | 1:B:357:TYR:HB2  | 1.85                     | 0.41              |
| 1:C:220:VAL:HG13 | 1:C:231:VAL:HG22 | 2.02                     | 0.41              |
| 1:D:213:VAL:HG23 | 1:D:215:LEU:HG   | 2.03                     | 0.41              |
| 1:F:244:ASN:OD1  | 1:F:247:LYS:CE   | 2.68                     | 0.41              |
| 1:F:323:ASN:HB3  | 1:F:328:SER:HB3  | 2.03                     | 0.41              |
| 1:F:353:VAL:HG22 | 1:F:368:PHE:HD1  | 1.85                     | 0.41              |
| 1:B:476:ILE:HG13 | 1:L:150:ILE:HG21 | 2.03                     | 0.41              |
| 1:D:128:SER:O    | 1:D:130:LEU:N    | 2.52                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:339:PRO:HG3  | 1:D:369:ARG:HB2  | 2.02                     | 0.41              |
| 1:E:207:VAL:HG21 | 1:E:220:VAL:HG21 | 2.02                     | 0.41              |
| 1:F:288:ASN:O    | 1:F:289:GLU:OE2  | 2.39                     | 0.41              |
| 1:F:319:ALA:HA   | 1:F:322:THR:OG1  | 2.21                     | 0.41              |
| 1:F:76:ILE:HG12  | 1:F:104:VAL:HG11 | 2.02                     | 0.41              |
| 1:H:178:VAL:HG22 | 1:G:147:SER:HB2  | 2.03                     | 0.41              |
| 1:J:308:LEU:HD11 | 1:J:353:VAL:HG21 | 2.02                     | 0.41              |
| 1:J:30:ARG:HA    | 1:J:39:ASN:O     | 2.21                     | 0.41              |
| 1:A:150:ILE:HA   | 1:A:158:TYR:O    | 2.21                     | 0.40              |
| 1:B:148:ILE:HG22 | 1:C:179:ASN:O    | 2.19                     | 0.40              |
| 1:C:87:ASP:HB3   | 1:C:90:SER:OG    | 2.21                     | 0.40              |
| 1:D:182:HIS:HA   | 1:K:480:SER:OG   | 2.21                     | 0.40              |
| 1:E:210:LEU:HA   | 1:E:213:VAL:HG22 | 2.03                     | 0.40              |
| 1:G:144:ILE:O    | 1:G:227:ALA:HB1  | 2.21                     | 0.40              |
| 1:J:208:LYS:O    | 1:J:212:GLN:HG3  | 2.21                     | 0.40              |
| 1:E:284:VAL:HB   | 1:E:292:PHE:HE1  | 1.85                     | 0.40              |
| 1:I:8:SER:OG     | 1:I:9:GLU:N      | 2.53                     | 0.40              |
| 1:K:369:ARG:HH12 | 4:K:502:PPQ:HBP2 | 1.85                     | 0.40              |
| 1:B:238:LEU:HD11 | 1:B:382:ALA:HA   | 2.03                     | 0.40              |
| 1:B:339:PRO:CB   | 1:B:352:SER:HA   | 2.51                     | 0.40              |
| 1:D:291:LEU:HD23 | 1:D:291:LEU:HA   | 1.83                     | 0.40              |
| 1:D:245:VAL:CG1  | 1:D:377:PRO:HG3  | 2.52                     | 0.40              |
| 1:F:224:VAL:HG21 | 1:F:337:GLU:OE1  | 2.20                     | 0.40              |
| 1:J:59:PHE:CE1   | 1:J:75:MET:HB2   | 2.56                     | 0.40              |
| 1:A:282:VAL:HB   | 1:A:368:PHE:HE2  | 1.86                     | 0.40              |
| 1:B:204:THR:O    | 1:B:208:LYS:HG2  | 2.21                     | 0.40              |
| 1:C:339:PRO:HB3  | 1:C:351:ALA:O    | 2.21                     | 0.40              |
| 1:D:83:ARG:HG3   | 1:D:83:ARG:HH11  | 1.87                     | 0.40              |
| 1:E:172:ARG:HG3  | 1:E:173:SER:H    | 1.87                     | 0.40              |
| 1:E:386:MET:CE   | 1:E:442:GLU:HB2  | 2.52                     | 0.40              |
| 1:E:49:THR:OG1   | 1:E:52:MET:HG3   | 2.21                     | 0.40              |
| 1:I:410:THR:O    | 1:I:414:ILE:N    | 2.49                     | 0.40              |
| 1:J:379:LEU:HD11 | 1:J:450:PHE:HZ   | 1.85                     | 0.40              |
| 1:K:27:VAL:HG21  | 1:K:48:LEU:HD22  | 2.03                     | 0.40              |
| 1:L:124:HIS:CD2  | 1:L:389:MET:SD   | 3.15                     | 0.40              |
| 1:D:12:ILE:N     | 1:D:12:ILE:HD12  | 2.36                     | 0.40              |
| 1:D:385:LEU:O    | 1:D:388:GLY:N    | 2.54                     | 0.40              |
| 1:D:439:TYR:CZ   | 1:D:440:LEU:HG   | 2.57                     | 0.40              |
| 1:J:103:ASP:O    | 1:J:107:ASN:N    | 2.49                     | 0.40              |
| 1:K:207:VAL:O    | 1:K:210:LEU:HB2  | 2.21                     | 0.40              |
| 1:K:221:HIS:ND1  | 1:K:222:HIS:O    | 2.30                     | 0.40              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:K:339:PRO:CB | 1:K:352:SER:HA  | 2.52                     | 0.40              |
| 1:L:274:ASN:HA | 1:L:336:TYR:HB3 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 474/481 (98%)   | 427 (90%)  | 44 (9%)  | 3 (1%)   | 25          | 56  |
| 1   | B     | 473/481 (98%)   | 431 (91%)  | 33 (7%)  | 9 (2%)   | 8           | 26  |
| 1   | C     | 472/481 (98%)   | 428 (91%)  | 38 (8%)  | 6 (1%)   | 12          | 35  |
| 1   | D     | 474/481 (98%)   | 427 (90%)  | 44 (9%)  | 3 (1%)   | 25          | 56  |
| 1   | E     | 471/481 (98%)   | 423 (90%)  | 46 (10%) | 2 (0%)   | 34          | 64  |
| 1   | F     | 473/481 (98%)   | 428 (90%)  | 40 (8%)  | 5 (1%)   | 14          | 40  |
| 1   | G     | 474/481 (98%)   | 438 (92%)  | 36 (8%)  | 0        | 100         | 100 |
| 1   | H     | 473/481 (98%)   | 445 (94%)  | 26 (6%)  | 2 (0%)   | 34          | 64  |
| 1   | I     | 473/481 (98%)   | 437 (92%)  | 35 (7%)  | 1 (0%)   | 47          | 76  |
| 1   | J     | 476/481 (99%)   | 449 (94%)  | 27 (6%)  | 0        | 100         | 100 |
| 1   | K     | 473/481 (98%)   | 438 (93%)  | 34 (7%)  | 1 (0%)   | 47          | 76  |
| 1   | L     | 474/481 (98%)   | 435 (92%)  | 37 (8%)  | 2 (0%)   | 34          | 64  |
| All | All   | 5680/5772 (98%) | 5206 (92%) | 440 (8%) | 34 (1%)  | 25          | 56  |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 298 | LYS  |
| 1   | F     | 9   | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 417 | LYS  |
| 1   | I     | 8   | SER  |
| 1   | A     | 218 | PHE  |
| 1   | A     | 364 | ALA  |
| 1   | B     | 70  | ILE  |
| 1   | C     | 175 | GLU  |
| 1   | C     | 409 | LEU  |
| 1   | F     | 212 | GLN  |
| 1   | L     | 416 | GLU  |
| 1   | B     | 170 | ARG  |
| 1   | B     | 395 | LYS  |
| 1   | B     | 445 | VAL  |
| 1   | E     | 395 | LYS  |
| 1   | F     | 124 | HIS  |
| 1   | F     | 390 | ASP  |
| 1   | H     | 358 | GLY  |
| 1   | C     | 167 | GLU  |
| 1   | C     | 212 | GLN  |
| 1   | D     | 238 | LEU  |
| 1   | D     | 247 | LYS  |
| 1   | E     | 444 | GLN  |
| 1   | F     | 358 | GLY  |
| 1   | H     | 411 | LEU  |
| 1   | A     | 128 | SER  |
| 1   | B     | 415 | ARG  |
| 1   | B     | 454 | TYR  |
| 1   | D     | 413 | GLU  |
| 1   | B     | 174 | PHE  |
| 1   | K     | 416 | GLU  |
| 1   | C     | 445 | VAL  |
| 1   | B     | 206 | ILE  |
| 1   | B     | 358 | 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     | 404/415 (97%)   | 397 (98%)  | 7 (2%)   | 60          | 83 |
| 1   | B     | 402/415 (97%)   | 394 (98%)  | 8 (2%)   | 55          | 80 |
| 1   | C     | 403/415 (97%)   | 391 (97%)  | 12 (3%)  | 41          | 72 |
| 1   | D     | 404/415 (97%)   | 394 (98%)  | 10 (2%)  | 47          | 76 |
| 1   | E     | 399/415 (96%)   | 387 (97%)  | 12 (3%)  | 41          | 72 |
| 1   | F     | 400/415 (96%)   | 386 (96%)  | 14 (4%)  | 36          | 67 |
| 1   | G     | 402/415 (97%)   | 390 (97%)  | 12 (3%)  | 41          | 72 |
| 1   | H     | 400/415 (96%)   | 394 (98%)  | 6 (2%)   | 65          | 85 |
| 1   | I     | 401/415 (97%)   | 388 (97%)  | 13 (3%)  | 39          | 70 |
| 1   | J     | 403/415 (97%)   | 396 (98%)  | 7 (2%)   | 60          | 83 |
| 1   | K     | 402/415 (97%)   | 389 (97%)  | 13 (3%)  | 39          | 70 |
| 1   | L     | 402/415 (97%)   | 397 (99%)  | 5 (1%)   | 71          | 89 |
| All | All   | 4822/4980 (97%) | 4703 (98%) | 119 (2%) | 47          | 76 |

All (119) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | ASN  |
| 1   | A     | 38  | TRP  |
| 1   | A     | 178 | VAL  |
| 1   | A     | 248 | LEU  |
| 1   | A     | 412 | ASP  |
| 1   | A     | 477 | THR  |
| 1   | A     | 481 | CYS  |
| 1   | B     | 32  | SER  |
| 1   | B     | 38  | TRP  |
| 1   | B     | 104 | VAL  |
| 1   | B     | 147 | SER  |
| 1   | B     | 293 | SER  |
| 1   | B     | 374 | SER  |
| 1   | B     | 428 | ARG  |
| 1   | B     | 443 | SER  |
| 1   | C     | 28  | ASP  |
| 1   | C     | 38  | TRP  |
| 1   | C     | 50  | HIS  |
| 1   | C     | 73  | SER  |
| 1   | C     | 159 | TYR  |
| 1   | C     | 220 | VAL  |
| 1   | C     | 234 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 280 | THR  |
| 1   | C     | 393 | LYS  |
| 1   | C     | 420 | LYS  |
| 1   | C     | 427 | ARG  |
| 1   | C     | 456 | SER  |
| 1   | D     | 38  | TRP  |
| 1   | D     | 44  | SER  |
| 1   | D     | 59  | PHE  |
| 1   | D     | 89  | PHE  |
| 1   | D     | 146 | ASP  |
| 1   | D     | 248 | LEU  |
| 1   | D     | 262 | THR  |
| 1   | D     | 289 | GLU  |
| 1   | D     | 427 | ARG  |
| 1   | D     | 481 | CYS  |
| 1   | E     | 16  | PHE  |
| 1   | E     | 38  | TRP  |
| 1   | E     | 44  | SER  |
| 1   | E     | 154 | SER  |
| 1   | E     | 172 | ARG  |
| 1   | E     | 197 | ASP  |
| 1   | E     | 274 | ASN  |
| 1   | E     | 280 | THR  |
| 1   | E     | 360 | SER  |
| 1   | E     | 374 | SER  |
| 1   | E     | 393 | LYS  |
| 1   | E     | 403 | ASP  |
| 1   | F     | 7   | ASN  |
| 1   | F     | 38  | TRP  |
| 1   | F     | 40  | HIS  |
| 1   | F     | 90  | SER  |
| 1   | F     | 110 | TYR  |
| 1   | F     | 115 | ARG  |
| 1   | F     | 154 | SER  |
| 1   | F     | 159 | TYR  |
| 1   | F     | 220 | VAL  |
| 1   | F     | 243 | ASP  |
| 1   | F     | 400 | GLU  |
| 1   | F     | 447 | SER  |
| 1   | F     | 468 | SER  |
| 1   | F     | 478 | THR  |
| 1   | H     | 17  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 40  | HIS  |
| 1   | H     | 44  | SER  |
| 1   | H     | 248 | LEU  |
| 1   | H     | 293 | SER  |
| 1   | H     | 360 | SER  |
| 1   | J     | 38  | TRP  |
| 1   | J     | 199 | MET  |
| 1   | J     | 372 | ASP  |
| 1   | J     | 410 | THR  |
| 1   | J     | 427 | ARG  |
| 1   | J     | 438 | GLN  |
| 1   | J     | 480 | SER  |
| 1   | K     | 10  | SER  |
| 1   | K     | 25  | GLU  |
| 1   | K     | 38  | TRP  |
| 1   | K     | 40  | HIS  |
| 1   | K     | 44  | SER  |
| 1   | K     | 54  | LYS  |
| 1   | K     | 71  | GLU  |
| 1   | K     | 100 | ASP  |
| 1   | K     | 113 | CYS  |
| 1   | K     | 199 | MET  |
| 1   | K     | 248 | LEU  |
| 1   | K     | 427 | ARG  |
| 1   | K     | 459 | PHE  |
| 1   | L     | 32  | SER  |
| 1   | L     | 74  | ASP  |
| 1   | L     | 165 | GLU  |
| 1   | L     | 455 | GLN  |
| 1   | L     | 481 | CYS  |
| 1   | G     | 10  | SER  |
| 1   | G     | 21  | GLU  |
| 1   | G     | 38  | TRP  |
| 1   | G     | 89  | PHE  |
| 1   | G     | 209 | VAL  |
| 1   | G     | 237 | ASP  |
| 1   | G     | 248 | LEU  |
| 1   | G     | 276 | SER  |
| 1   | G     | 293 | SER  |
| 1   | G     | 313 | ARG  |
| 1   | G     | 478 | THR  |
| 1   | G     | 480 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 8   | SER  |
| 1   | I     | 50  | HIS  |
| 1   | I     | 115 | ARG  |
| 1   | I     | 154 | SER  |
| 1   | I     | 234 | LYS  |
| 1   | I     | 274 | ASN  |
| 1   | I     | 280 | THR  |
| 1   | I     | 389 | MET  |
| 1   | I     | 412 | ASP  |
| 1   | I     | 425 | THR  |
| 1   | I     | 456 | SER  |
| 1   | I     | 478 | THR  |
| 1   | I     | 480 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 279 | HIS  |
| 1   | C     | 39  | ASN  |
| 1   | D     | 50  | HIS  |
| 1   | K     | 7   | ASN  |
| 1   | K     | 444 | GLN  |
| 1   | G     | 376 | ASN  |
| 1   | I     | 50  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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 |
| 4   | PPQ  | J     | 502 | 5    | 4,10,10      | 3.31 | 1 (25%)  | 2,14,14     | 1.39 | 0        |
| 3   | ADP  | J     | 501 | -    | 24,29,29     | 1.25 | 2 (8%)   | 29,45,45    | 2.31 | 8 (27%)  |
| 4   | PPQ  | K     | 502 | -    | 4,10,10      | 3.35 | 1 (25%)  | 2,14,14     | 0.81 | 0        |
| 2   | ATP  | A     | 501 | -    | 26,33,33     | 1.22 | 3 (11%)  | 31,52,52    | 1.64 | 7 (22%)  |
| 6   | P3P  | L     | 501 | 5    | 6,14,14      | 2.50 | 1 (16%)  | 8,21,21     | 0.93 | 0        |
| 3   | ADP  | E     | 501 | -    | 24,29,29     | 1.34 | 4 (16%)  | 29,45,45    | 2.06 | 7 (24%)  |
| 2   | ATP  | B     | 501 | -    | 26,33,33     | 1.20 | 3 (11%)  | 31,52,52    | 1.58 | 8 (25%)  |
| 2   | ATP  | F     | 501 | -    | 26,33,33     | 1.17 | 3 (11%)  | 31,52,52    | 1.52 | 9 (29%)  |
| 3   | ADP  | L     | 503 | 5    | 24,29,29     | 1.42 | 5 (20%)  | 29,45,45    | 2.36 | 10 (34%) |
| 2   | ATP  | C     | 501 | -    | 26,33,33     | 1.24 | 2 (7%)   | 31,52,52    | 1.68 | 6 (19%)  |
| 2   | ATP  | G     | 501 | -    | 26,33,33     | 1.08 | 2 (7%)   | 31,52,52    | 1.66 | 8 (25%)  |
| 3   | ADP  | D     | 501 | -    | 24,29,29     | 1.49 | 5 (20%)  | 29,45,45    | 2.27 | 10 (34%) |
| 3   | ADP  | I     | 501 | -    | 24,29,29     | 1.23 | 3 (12%)  | 29,45,45    | 2.18 | 9 (31%)  |
| 4   | PPQ  | I     | 502 | 5    | 4,10,10      | 4.34 | 2 (50%)  | 2,14,14     | 0.87 | 0        |
| 2   | ATP  | K     | 501 | -    | 26,33,33     | 1.08 | 2 (7%)   | 31,52,52    | 1.47 | 6 (19%)  |
| 3   | ADP  | H     | 501 | -    | 24,29,29     | 1.34 | 4 (16%)  | 29,45,45    | 2.08 | 9 (31%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | PPQ  | J     | 502 | 5    | -       | 3/6/10/10  | -       |
| 3   | ADP  | J     | 501 | -    | -       | 2/12/32/32 | 0/3/3/3 |
| 4   | PPQ  | K     | 502 | -    | -       | 5/6/10/10  | -       |
| 2   | ATP  | A     | 501 | -    | -       | 4/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 6   | P3P  | L     | 501 | 5    | -       | 7/8/16/16  | -       |
| 3   | ADP  | E     | 501 | -    | -       | 0/12/32/32 | 0/3/3/3 |
| 2   | ATP  | B     | 501 | -    | -       | 5/18/38/38 | 0/3/3/3 |
| 2   | ATP  | F     | 501 | -    | -       | 2/18/38/38 | 0/3/3/3 |
| 3   | ADP  | L     | 503 | 5    | -       | 3/12/32/32 | 0/3/3/3 |
| 2   | ATP  | C     | 501 | -    | -       | 6/18/38/38 | 0/3/3/3 |
| 2   | ATP  | G     | 501 | -    | -       | 4/18/38/38 | 0/3/3/3 |
| 3   | ADP  | D     | 501 | -    | -       | 2/12/32/32 | 0/3/3/3 |
| 3   | ADP  | I     | 501 | -    | -       | 6/12/32/32 | 0/3/3/3 |
| 4   | PPQ  | I     | 502 | 5    | -       | 5/6/10/10  | -       |
| 2   | ATP  | K     | 501 | -    | -       | 1/18/38/38 | 0/3/3/3 |
| 3   | ADP  | H     | 501 | -    | -       | 1/12/32/32 | 0/3/3/3 |

All (43) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4   | I     | 502 | PPQ  | PDP-CGP | 8.20 | 1.87        | 1.79     |
| 4   | K     | 502 | PPQ  | PDP-CGP | 6.53 | 1.85        | 1.79     |
| 4   | J     | 502 | PPQ  | PDP-CGP | 6.43 | 1.85        | 1.79     |
| 6   | L     | 501 | P3P  | PDP-CGP | 5.45 | 1.84        | 1.79     |
| 2   | C     | 501 | ATP  | O4'-C1' | 3.27 | 1.45        | 1.41     |
| 3   | D     | 501 | ADP  | C2-N3   | 3.22 | 1.37        | 1.32     |
| 2   | B     | 501 | ATP  | O4'-C1' | 3.12 | 1.45        | 1.41     |
| 2   | B     | 501 | ATP  | C5-C4   | 3.08 | 1.49        | 1.40     |
| 2   | A     | 501 | ATP  | C5-C4   | 3.08 | 1.49        | 1.40     |
| 3   | E     | 501 | ADP  | C2-N3   | 3.04 | 1.37        | 1.32     |
| 2   | C     | 501 | ATP  | C5-C4   | 2.93 | 1.48        | 1.40     |
| 3   | H     | 501 | ADP  | C2-N3   | 2.90 | 1.36        | 1.32     |
| 3   | L     | 503 | ADP  | O4'-C1' | 2.79 | 1.45        | 1.41     |
| 2   | A     | 501 | ATP  | O4'-C1' | 2.77 | 1.44        | 1.41     |
| 2   | F     | 501 | ATP  | C5-C4   | 2.77 | 1.48        | 1.40     |
| 3   | I     | 501 | ADP  | C2-N3   | 2.66 | 1.36        | 1.32     |
| 2   | K     | 501 | ATP  | C5-C4   | 2.65 | 1.47        | 1.40     |
| 4   | I     | 502 | PPQ  | CBP-CGP | 2.64 | 1.55        | 1.53     |
| 2   | F     | 501 | ATP  | O4'-C1' | 2.59 | 1.44        | 1.41     |
| 3   | L     | 503 | ADP  | C5-C4   | 2.59 | 1.47        | 1.40     |
| 2   | G     | 501 | ATP  | C5-C4   | 2.58 | 1.47        | 1.40     |
| 3   | J     | 501 | ADP  | C2-N3   | 2.51 | 1.36        | 1.32     |
| 3   | L     | 503 | ADP  | C2-N3   | 2.47 | 1.36        | 1.32     |
| 3   | E     | 501 | ADP  | O4'-C1' | 2.46 | 1.44        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | I     | 501 | ADP  | O4'-C1' | 2.46 | 1.44        | 1.41     |
| 3   | E     | 501 | ADP  | C5-C4   | 2.45 | 1.47        | 1.40     |
| 3   | D     | 501 | ADP  | C6-C5   | 2.43 | 1.52        | 1.43     |
| 2   | K     | 501 | ATP  | O4'-C1' | 2.41 | 1.44        | 1.41     |
| 2   | F     | 501 | ATP  | C2-N3   | 2.41 | 1.36        | 1.32     |
| 3   | H     | 501 | ADP  | O4'-C1' | 2.40 | 1.44        | 1.41     |
| 3   | E     | 501 | ADP  | C6-C5   | 2.39 | 1.52        | 1.43     |
| 3   | D     | 501 | ADP  | C5-C4   | 2.38 | 1.47        | 1.40     |
| 3   | H     | 501 | ADP  | C5-C4   | 2.34 | 1.47        | 1.40     |
| 3   | D     | 501 | ADP  | O4'-C1' | 2.27 | 1.44        | 1.41     |
| 3   | L     | 503 | ADP  | C4-N3   | 2.26 | 1.38        | 1.35     |
| 3   | D     | 501 | ADP  | O3'-C3' | 2.25 | 1.48        | 1.43     |
| 3   | J     | 501 | ADP  | O4'-C1' | 2.24 | 1.44        | 1.41     |
| 2   | B     | 501 | ATP  | C2-N3   | 2.14 | 1.35        | 1.32     |
| 2   | A     | 501 | ATP  | C2-N3   | 2.10 | 1.35        | 1.32     |
| 2   | G     | 501 | ATP  | O4'-C1' | 2.07 | 1.44        | 1.41     |
| 3   | H     | 501 | ADP  | C6-C5   | 2.06 | 1.50        | 1.43     |
| 3   | I     | 501 | ADP  | C6-C5   | 2.05 | 1.50        | 1.43     |
| 3   | L     | 503 | ADP  | C6-C5   | 2.03 | 1.50        | 1.43     |

All (97) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | L     | 503 | ADP  | N3-C2-N1    | -6.80 | 118.05      | 128.68   |
| 3   | J     | 501 | ADP  | N3-C2-N1    | -6.62 | 118.33      | 128.68   |
| 3   | D     | 501 | ADP  | N3-C2-N1    | -6.46 | 118.58      | 128.68   |
| 3   | E     | 501 | ADP  | C4-C5-N7    | -6.12 | 103.02      | 109.40   |
| 3   | I     | 501 | ADP  | N3-C2-N1    | -6.02 | 119.27      | 128.68   |
| 3   | D     | 501 | ADP  | C4-C5-N7    | -6.02 | 103.13      | 109.40   |
| 3   | H     | 501 | ADP  | N3-C2-N1    | -5.64 | 119.86      | 128.68   |
| 3   | E     | 501 | ADP  | N3-C2-N1    | -5.12 | 120.68      | 128.68   |
| 3   | H     | 501 | ADP  | C4-C5-N7    | -5.04 | 104.15      | 109.40   |
| 3   | L     | 503 | ADP  | C4-C5-N7    | -5.02 | 104.16      | 109.40   |
| 3   | J     | 501 | ADP  | C4-C5-N7    | -4.85 | 104.35      | 109.40   |
| 3   | I     | 501 | ADP  | C4-C5-N7    | -4.71 | 104.49      | 109.40   |
| 3   | L     | 503 | ADP  | C2-N1-C6    | 4.52  | 126.49      | 118.75   |
| 3   | J     | 501 | ADP  | C3'-C2'-C1' | -4.47 | 94.25       | 100.98   |
| 3   | J     | 501 | ADP  | C2-N1-C6    | 4.13  | 125.82      | 118.75   |
| 3   | D     | 501 | ADP  | C2-N1-C6    | 3.82  | 125.28      | 118.75   |
| 2   | C     | 501 | ATP  | C4-C5-N7    | -3.80 | 105.44      | 109.40   |
| 3   | I     | 501 | ADP  | C2-N1-C6    | 3.69  | 125.06      | 118.75   |
| 3   | H     | 501 | ADP  | C2-N1-C6    | 3.67  | 125.03      | 118.75   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 501 | ATP  | C5-C6-N6    | 3.61  | 125.83      | 120.35   |
| 2   | G     | 501 | ATP  | C1'-N9-C4   | -3.60 | 120.31      | 126.64   |
| 3   | L     | 503 | ADP  | C3'-C2'-C1' | -3.46 | 95.76       | 100.98   |
| 2   | A     | 501 | ATP  | PA-O3A-PB   | 3.40  | 144.50      | 132.83   |
| 3   | H     | 501 | ADP  | O3'-C3'-C4' | 3.38  | 120.81      | 111.05   |
| 3   | E     | 501 | ADP  | C5-C6-N6    | 3.37  | 125.47      | 120.35   |
| 2   | C     | 501 | ATP  | O4'-C1'-C2' | -3.30 | 102.11      | 106.93   |
| 2   | F     | 501 | ATP  | C4-C5-N7    | -3.28 | 105.98      | 109.40   |
| 3   | I     | 501 | ADP  | C3'-C2'-C1' | -3.26 | 96.08       | 100.98   |
| 2   | B     | 501 | ATP  | C1'-N9-C4   | -3.15 | 121.10      | 126.64   |
| 2   | G     | 501 | ATP  | C4-C5-N7    | -3.15 | 106.12      | 109.40   |
| 2   | A     | 501 | ATP  | C2'-C3'-C4' | -3.11 | 96.59       | 102.64   |
| 3   | J     | 501 | ADP  | O5'-C5'-C4' | 3.07  | 119.54      | 108.99   |
| 3   | D     | 501 | ADP  | O5'-PA-O1A  | -3.05 | 97.15       | 109.07   |
| 2   | G     | 501 | ATP  | C5-C6-N6    | 3.00  | 124.92      | 120.35   |
| 3   | E     | 501 | ADP  | C2-N1-C6    | 2.99  | 123.88      | 118.75   |
| 2   | K     | 501 | ATP  | N3-C2-N1    | -2.93 | 124.09      | 128.68   |
| 3   | I     | 501 | ADP  | O4'-C1'-C2' | -2.91 | 102.68      | 106.93   |
| 3   | H     | 501 | ADP  | O4'-C4'-C5' | -2.90 | 99.82       | 109.37   |
| 2   | G     | 501 | ATP  | O4'-C1'-C2' | -2.80 | 102.84      | 106.93   |
| 3   | D     | 501 | ADP  | C5-C6-N6    | 2.75  | 124.53      | 120.35   |
| 3   | L     | 503 | ADP  | C1'-N9-C4   | -2.73 | 121.84      | 126.64   |
| 3   | I     | 501 | ADP  | O5'-C5'-C4' | 2.69  | 118.23      | 108.99   |
| 2   | A     | 501 | ATP  | C4-C5-N7    | -2.64 | 106.65      | 109.40   |
| 2   | G     | 501 | ATP  | N3-C2-N1    | -2.63 | 124.57      | 128.68   |
| 3   | H     | 501 | ADP  | C1'-N9-C4   | -2.62 | 122.04      | 126.64   |
| 2   | G     | 501 | ATP  | C2-N1-C6    | 2.59  | 123.18      | 118.75   |
| 2   | K     | 501 | ATP  | C1'-N9-C4   | -2.58 | 122.10      | 126.64   |
| 2   | B     | 501 | ATP  | C3'-C2'-C1' | -2.57 | 97.11       | 100.98   |
| 2   | K     | 501 | ATP  | O4'-C1'-C2' | -2.57 | 103.17      | 106.93   |
| 3   | D     | 501 | ADP  | O4'-C4'-C5' | -2.56 | 100.94      | 109.37   |
| 2   | F     | 501 | ATP  | N3-C2-N1    | -2.47 | 124.82      | 128.68   |
| 2   | C     | 501 | ATP  | C1'-N9-C4   | -2.46 | 122.31      | 126.64   |
| 3   | I     | 501 | ADP  | O3B-PB-O3A  | 2.44  | 112.83      | 104.64   |
| 2   | G     | 501 | ATP  | O3G-PG-O2G  | 2.41  | 116.83      | 107.64   |
| 2   | B     | 501 | ATP  | O2'-C2'-C1' | 2.34  | 119.48      | 110.85   |
| 3   | H     | 501 | ADP  | C5-C6-N1    | -2.33 | 115.08      | 120.35   |
| 2   | F     | 501 | ATP  | C1'-N9-C4   | -2.33 | 122.56      | 126.64   |
| 2   | K     | 501 | ATP  | O2'-C2'-C1' | 2.31  | 119.38      | 110.85   |
| 2   | F     | 501 | ATP  | C5-C6-N6    | 2.30  | 123.85      | 120.35   |
| 3   | L     | 503 | ADP  | C2'-C3'-C4' | -2.30 | 98.17       | 102.64   |
| 3   | D     | 501 | ADP  | O3'-C3'-C4' | 2.30  | 117.70      | 111.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | L     | 503 | ADP  | O3B-PB-O3A  | 2.30  | 112.33      | 104.64   |
| 2   | B     | 501 | ATP  | O4'-C1'-C2' | -2.28 | 103.59      | 106.93   |
| 3   | H     | 501 | ADP  | C5-C6-N6    | 2.28  | 123.81      | 120.35   |
| 3   | J     | 501 | ADP  | C1'-N9-C4   | -2.27 | 122.65      | 126.64   |
| 2   | A     | 501 | ATP  | C5-C6-N1    | -2.27 | 115.21      | 120.35   |
| 2   | A     | 501 | ATP  | C5-C6-N6    | 2.26  | 123.79      | 120.35   |
| 3   | J     | 501 | ADP  | O4'-C1'-C2' | -2.26 | 103.62      | 106.93   |
| 3   | J     | 501 | ADP  | C5-C6-N1    | -2.25 | 115.24      | 120.35   |
| 3   | L     | 503 | ADP  | C5-C6-N1    | -2.25 | 115.26      | 120.35   |
| 2   | F     | 501 | ATP  | C2'-C3'-C4' | -2.24 | 98.29       | 102.64   |
| 2   | B     | 501 | ATP  | C2-N1-C6    | 2.23  | 122.58      | 118.75   |
| 2   | G     | 501 | ATP  | C5-C6-N1    | -2.23 | 115.29      | 120.35   |
| 3   | L     | 503 | ADP  | C5-C6-N6    | 2.23  | 123.74      | 120.35   |
| 3   | E     | 501 | ADP  | O2'-C2'-C3' | 2.23  | 119.04      | 111.82   |
| 3   | D     | 501 | ADP  | C3'-C2'-C1' | 2.21  | 104.31      | 100.98   |
| 2   | B     | 501 | ATP  | C4-C5-N7    | -2.19 | 107.11      | 109.40   |
| 3   | E     | 501 | ADP  | C5-C6-N1    | -2.19 | 115.39      | 120.35   |
| 3   | D     | 501 | ADP  | C5-C6-N1    | -2.19 | 115.40      | 120.35   |
| 2   | B     | 501 | ATP  | C2'-C3'-C4' | -2.18 | 98.41       | 102.64   |
| 3   | I     | 501 | ADP  | C5-C6-N1    | -2.17 | 115.42      | 120.35   |
| 2   | C     | 501 | ATP  | C2-N1-C6    | 2.16  | 122.45      | 118.75   |
| 2   | C     | 501 | ATP  | C5-C6-N1    | -2.16 | 115.46      | 120.35   |
| 2   | F     | 501 | ATP  | C2-N1-C6    | 2.11  | 122.37      | 118.75   |
| 2   | K     | 501 | ATP  | O4'-C4'-C5' | -2.10 | 102.47      | 109.37   |
| 2   | K     | 501 | ATP  | C2-N1-C6    | 2.08  | 122.31      | 118.75   |
| 3   | D     | 501 | ADP  | O2A-PA-O1A  | 2.07  | 122.49      | 112.24   |
| 3   | H     | 501 | ADP  | O5'-PA-O1A  | -2.07 | 100.97      | 109.07   |
| 2   | F     | 501 | ATP  | PA-O3A-PB   | 2.07  | 139.93      | 132.83   |
| 3   | L     | 503 | ADP  | O4'-C4'-C5' | -2.07 | 102.56      | 109.37   |
| 3   | I     | 501 | ADP  | O5'-PA-O1A  | -2.05 | 101.05      | 109.07   |
| 2   | A     | 501 | ATP  | C2-N1-C6    | 2.04  | 122.25      | 118.75   |
| 2   | F     | 501 | ATP  | O2'-C2'-C3' | 2.04  | 118.42      | 111.82   |
| 3   | E     | 501 | ADP  | O2A-PA-O1A  | 2.02  | 122.22      | 112.24   |
| 2   | F     | 501 | ATP  | O3G-PG-O1G  | 2.01  | 118.55      | 110.68   |
| 2   | A     | 501 | ATP  | C5'-C4'-C3' | -2.01 | 107.66      | 115.18   |
| 2   | B     | 501 | ATP  | C5-C6-N1    | -2.01 | 115.80      | 120.35   |

There are no chirality outliers.

All (56) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | J     | 502 | PPQ  | CBP-CGP-PDP-CEP |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | J     | 502 | PPQ  | CBP-CGP-PDP-OEA |
| 4   | J     | 502 | PPQ  | CBP-CGP-PDP-OEB |
| 4   | K     | 502 | PPQ  | NP-CAP-CBP-CGP  |
| 4   | K     | 502 | PPQ  | CP-CAP-CBP-CGP  |
| 4   | K     | 502 | PPQ  | CBP-CGP-PDP-CEP |
| 4   | K     | 502 | PPQ  | CBP-CGP-PDP-OEA |
| 4   | K     | 502 | PPQ  | CBP-CGP-PDP-OEB |
| 2   | A     | 501 | ATP  | C5'-O5'-PA-O1A  |
| 2   | A     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 6   | L     | 501 | P3P  | CP-CAP-CBP-CGP  |
| 6   | L     | 501 | P3P  | NP-CAP-CBP-CGP  |
| 6   | L     | 501 | P3P  | CBP-CGP-PDP-OEA |
| 6   | L     | 501 | P3P  | CBP-CGP-PDP-CEP |
| 6   | L     | 501 | P3P  | CBP-CGP-PDP-OEB |
| 6   | L     | 501 | P3P  | PDP-OEB-P12-O13 |
| 2   | B     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 2   | C     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 2   | C     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 3   | I     | 501 | ADP  | C5'-O5'-PA-O1A  |
| 3   | I     | 501 | ADP  | C5'-O5'-PA-O2A  |
| 3   | I     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 4   | I     | 502 | PPQ  | NP-CAP-CBP-CGP  |
| 4   | I     | 502 | PPQ  | CP-CAP-CBP-CGP  |
| 4   | I     | 502 | PPQ  | CBP-CGP-PDP-CEP |
| 4   | I     | 502 | PPQ  | CBP-CGP-PDP-OEA |
| 4   | I     | 502 | PPQ  | CBP-CGP-PDP-OEB |
| 3   | D     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 3   | I     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 3   | D     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 2   | G     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 2   | G     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 2   | B     | 501 | ATP  | PB-O3A-PA-O5'   |
| 2   | C     | 501 | ATP  | PB-O3A-PA-O5'   |
| 2   | F     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 3   | L     | 503 | ADP  | O4'-C4'-C5'-O5' |
| 2   | C     | 501 | ATP  | PB-O3B-PG-O1G   |
| 2   | A     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 3   | I     | 501 | ADP  | C5'-O5'-PA-O3A  |
| 2   | B     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 2   | B     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 2   | F     | 501 | ATP  | PA-O3A-PB-O2B   |
| 2   | A     | 501 | ATP  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | K     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 2   | G     | 501 | ATP  | PG-O3B-PB-O1B   |
| 3   | J     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 3   | J     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 6   | L     | 501 | P3P  | PDP-OEB-P12-O14 |
| 2   | C     | 501 | ATP  | PB-O3B-PG-O2G   |
| 2   | C     | 501 | ATP  | PB-O3B-PG-O3G   |
| 3   | I     | 501 | ADP  | PA-O3A-PB-O3B   |
| 3   | H     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 2   | B     | 501 | ATP  | PB-O3A-PA-O1A   |
| 3   | L     | 503 | ADP  | PB-O3A-PA-O1A   |
| 2   | G     | 501 | ATP  | PA-O3A-PB-O2B   |
| 3   | L     | 503 | ADP  | C5'-O5'-PA-O1A  |

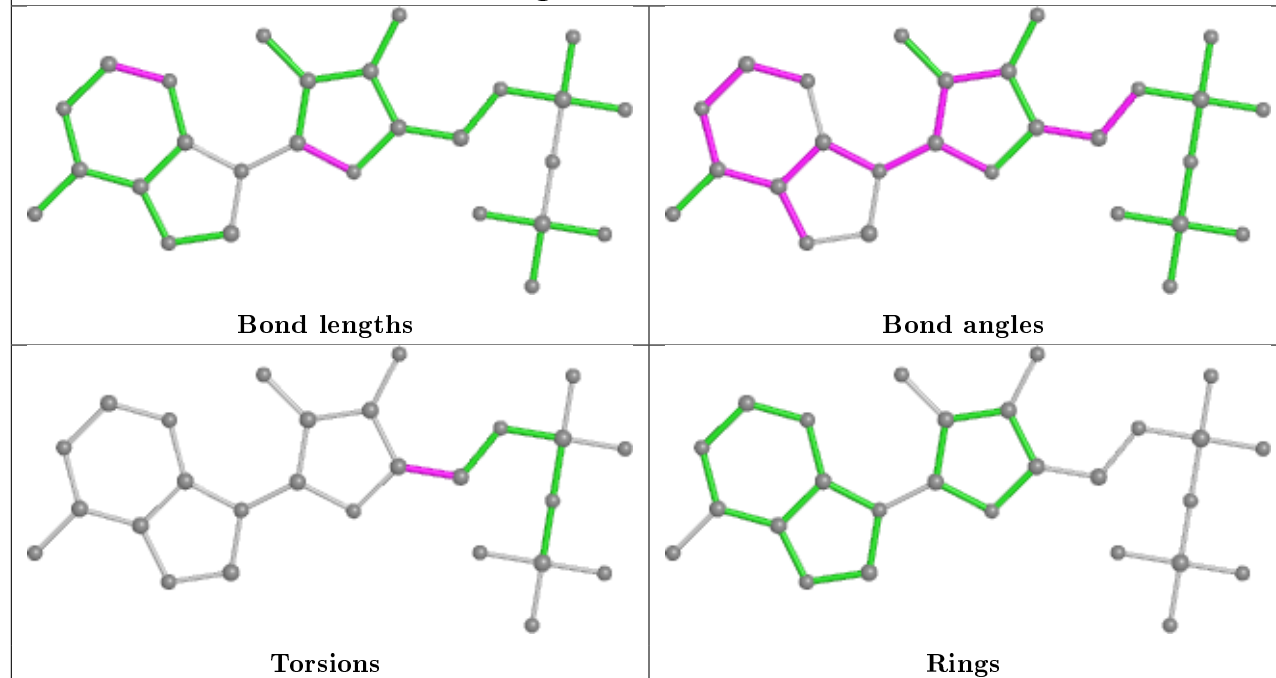
There are no ring outliers.

8 monomers are involved in 18 short contacts:

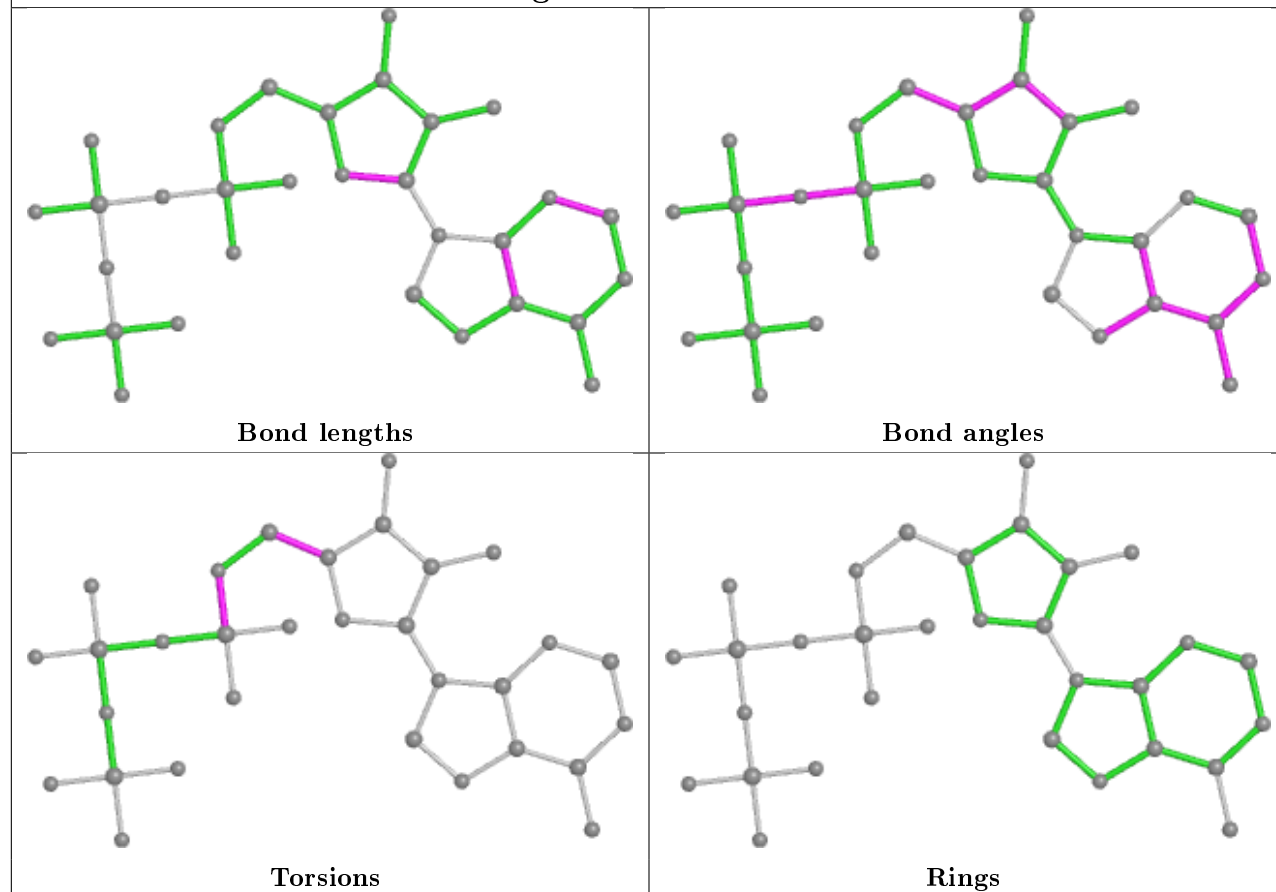
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | J     | 501 | ADP  | 2       | 0            |
| 4   | K     | 502 | PPQ  | 3       | 0            |
| 2   | B     | 501 | ATP  | 1       | 0            |
| 2   | F     | 501 | ATP  | 2       | 0            |
| 3   | L     | 503 | ADP  | 2       | 0            |
| 3   | I     | 501 | ADP  | 2       | 0            |
| 4   | I     | 502 | PPQ  | 3       | 0            |
| 2   | K     | 501 | ATP  | 3       | 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.

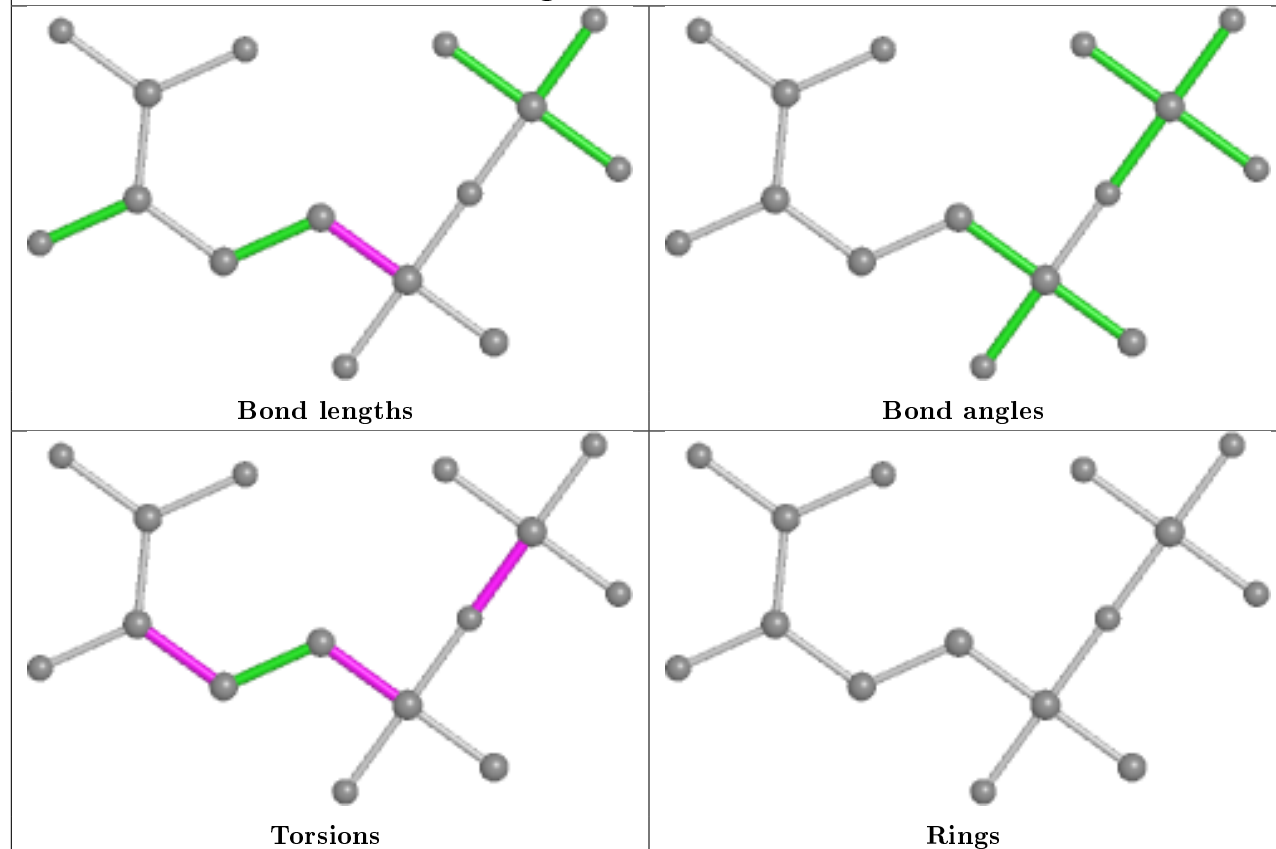
## Ligand ADP J 501



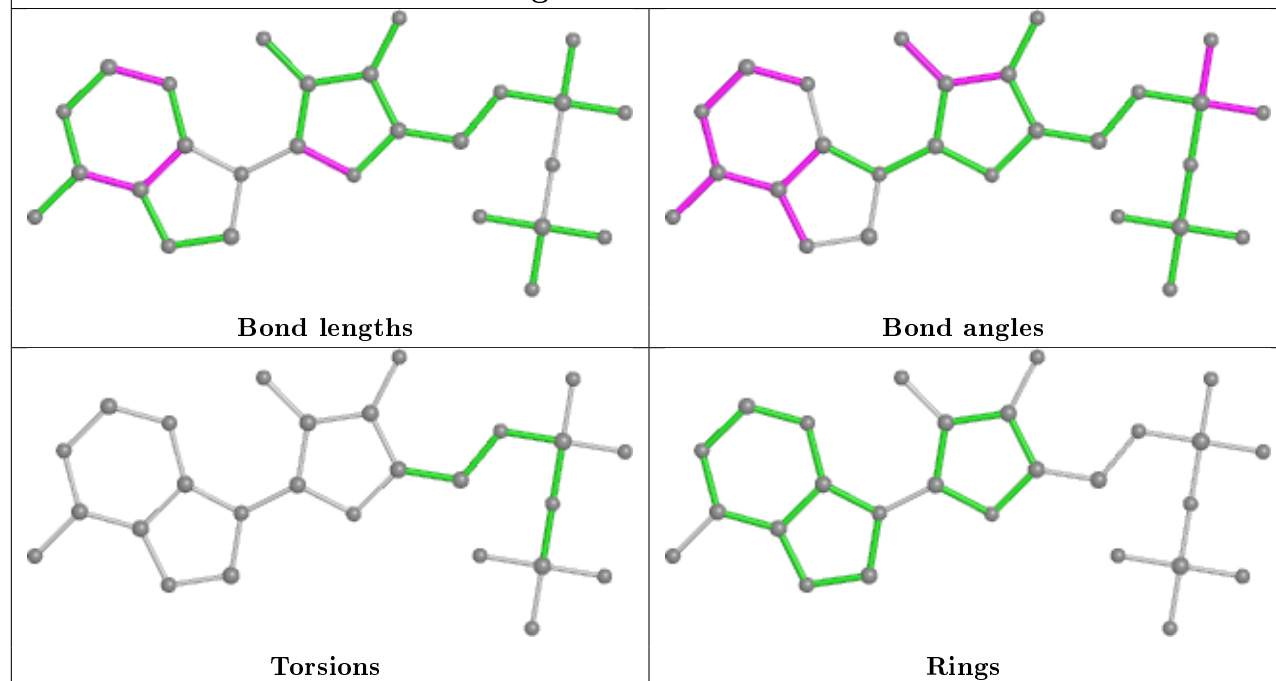
## Ligand ATP A 501

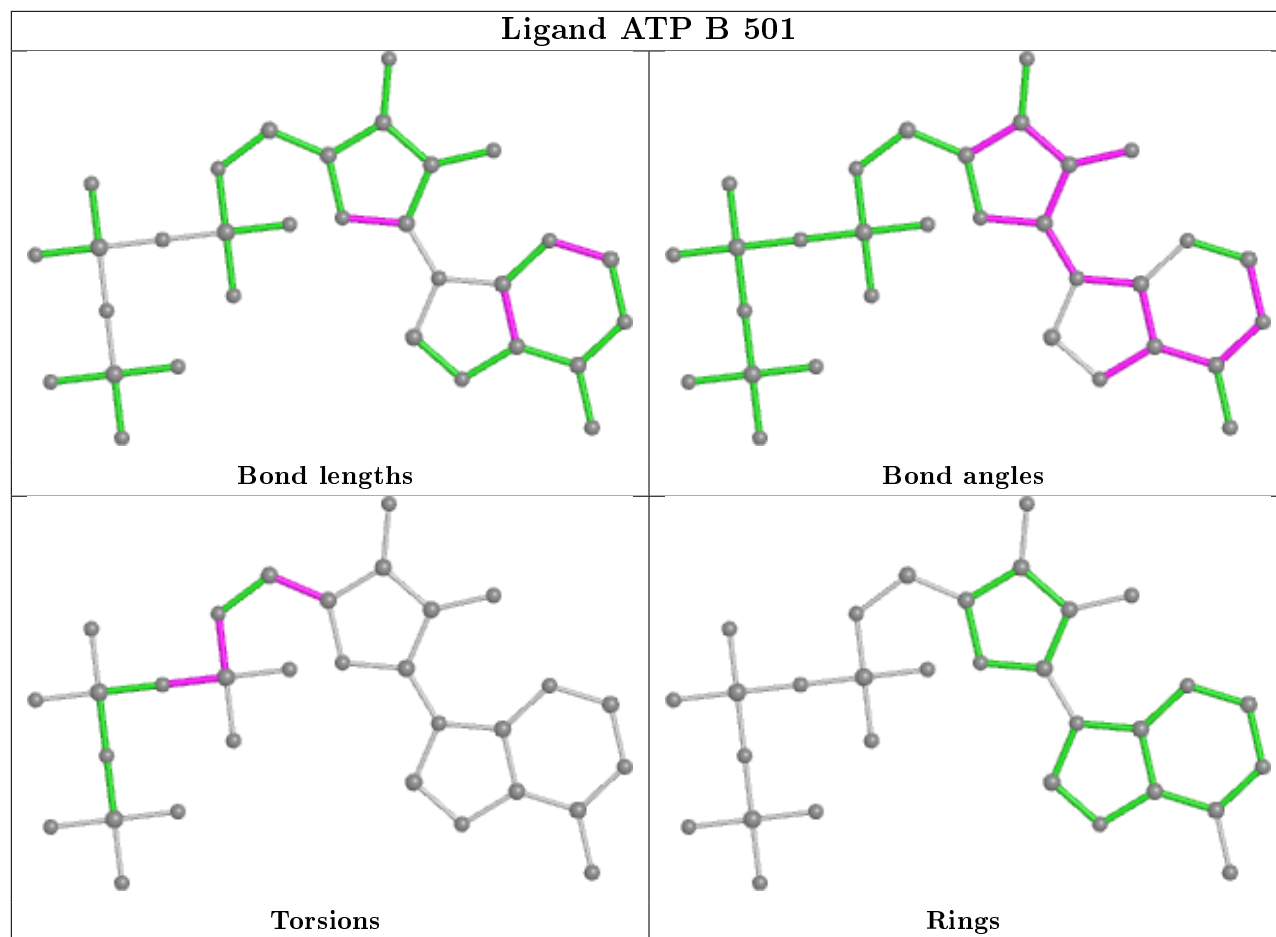


## Ligand P3P L 501

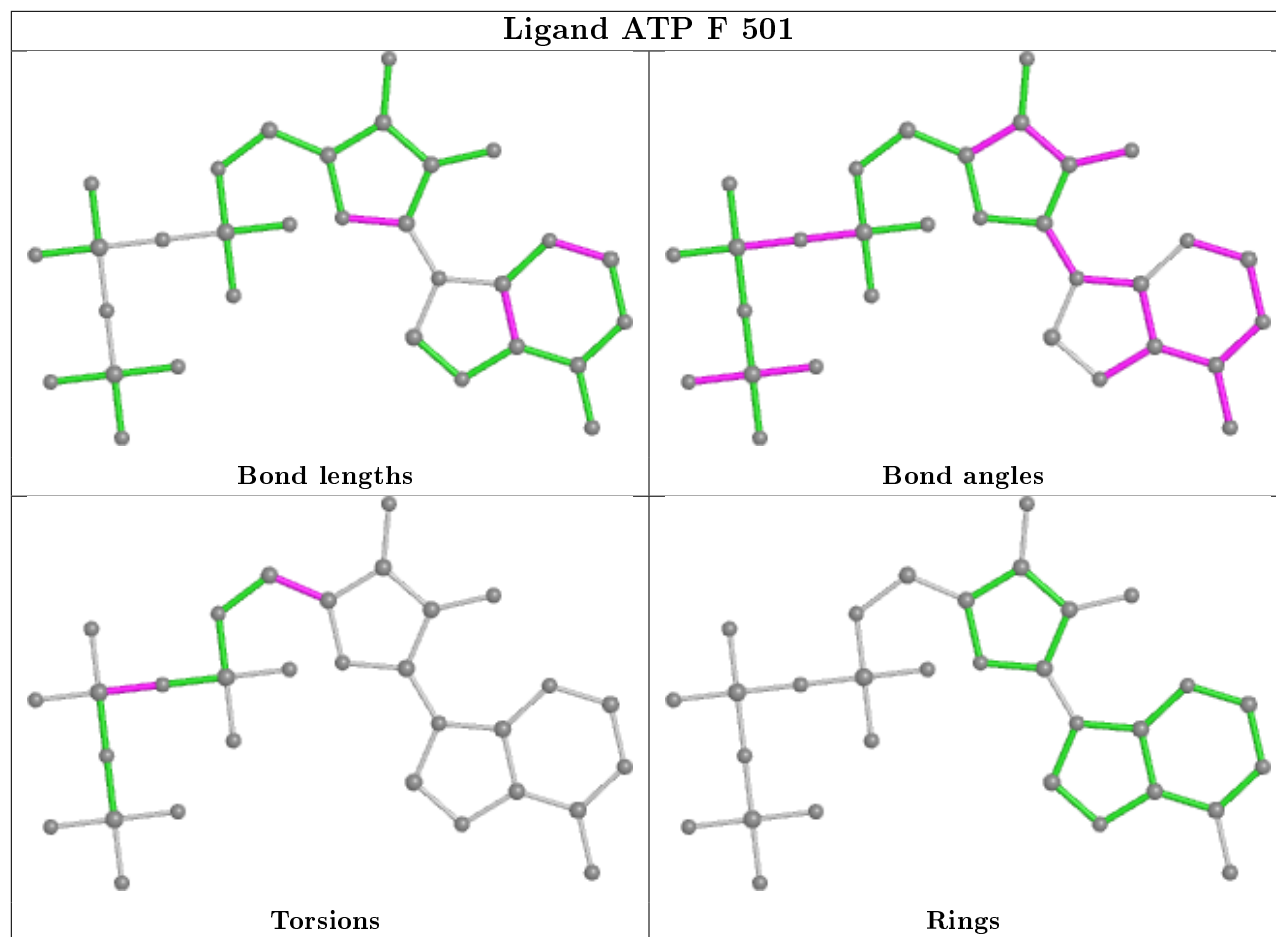


## Ligand ADP E 501

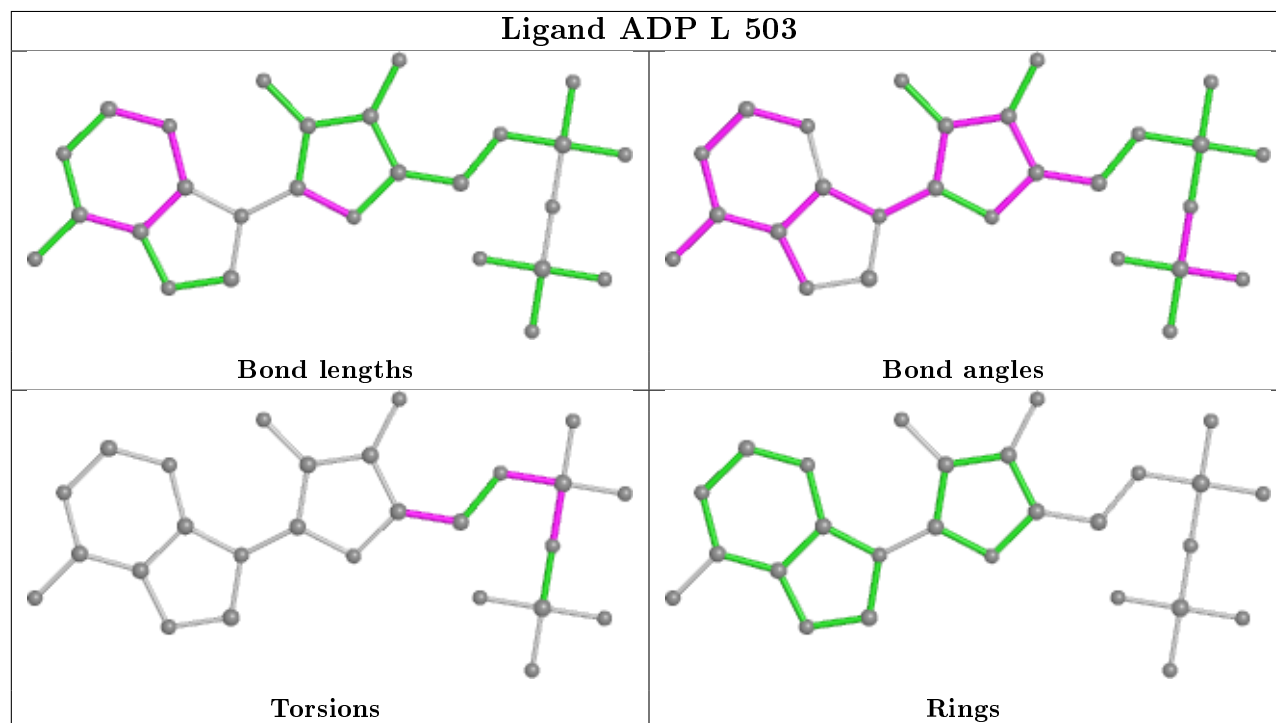


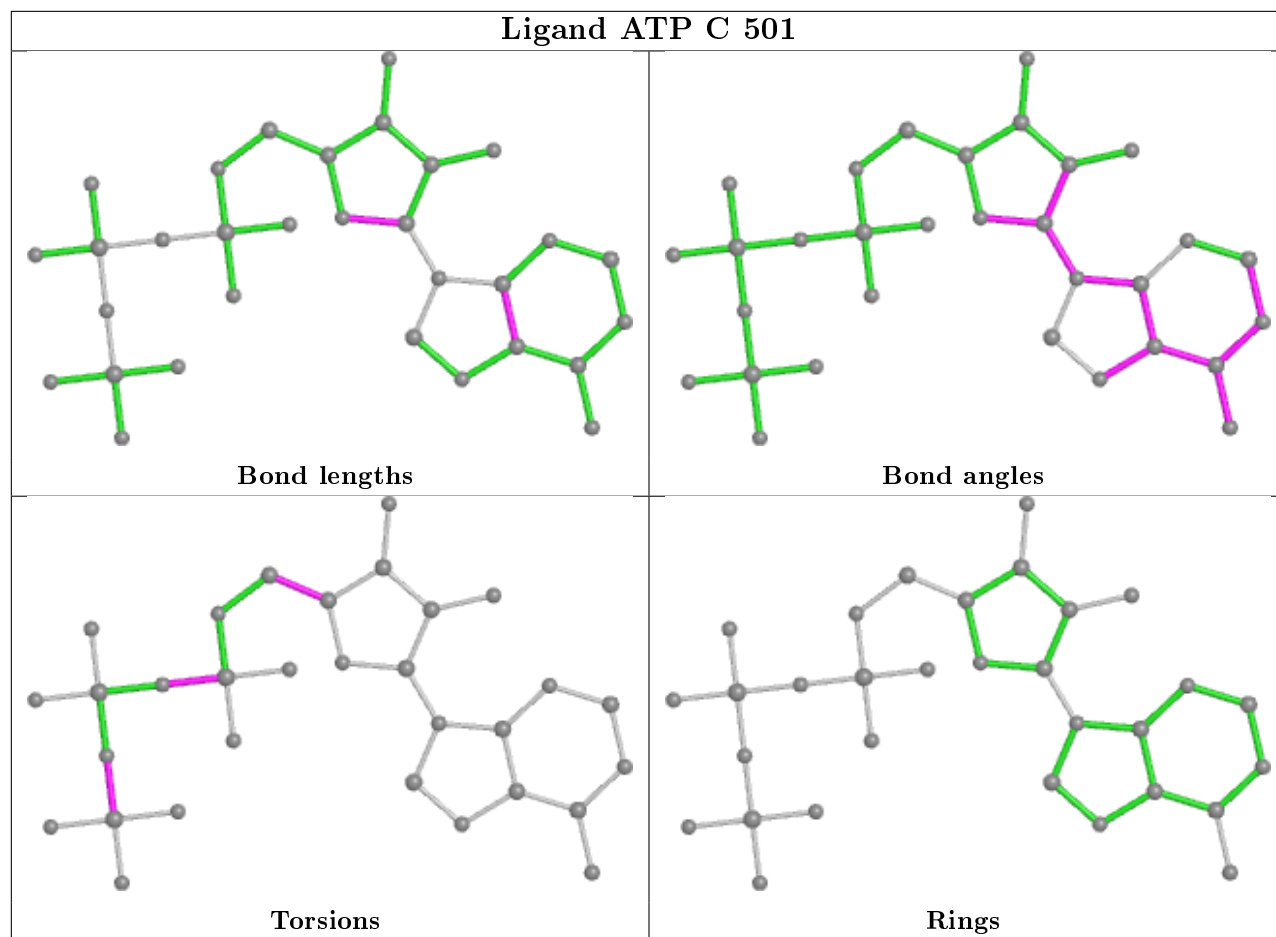


## Ligand ATP F 501

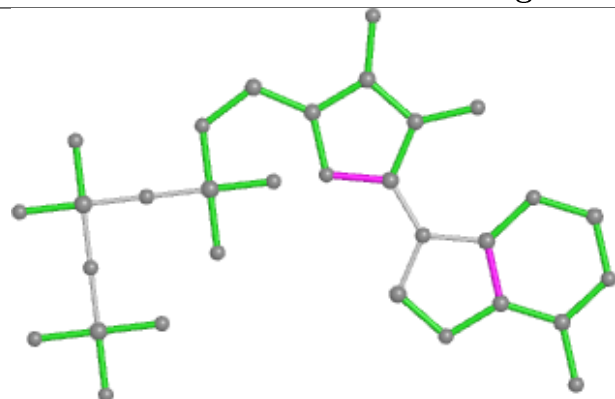


## Ligand ADP L 503

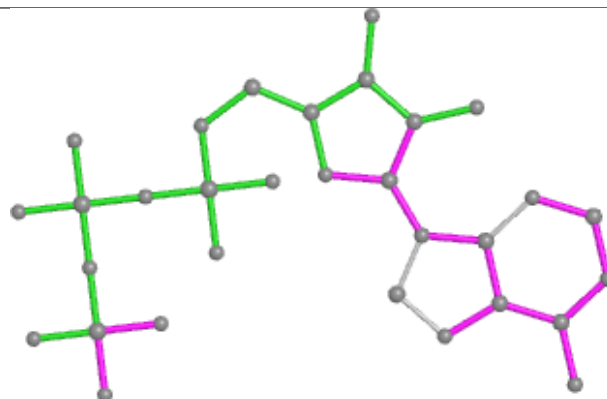




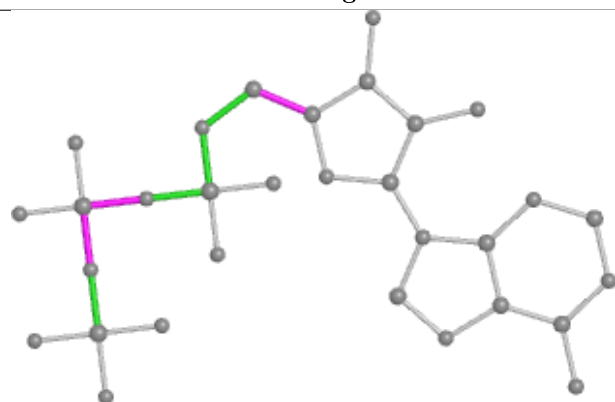
## Ligand ATP G 501



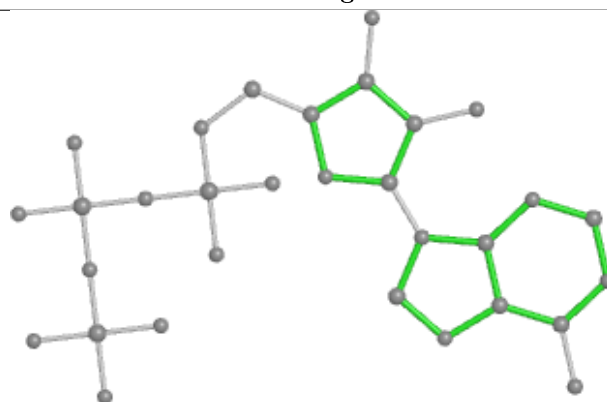
Bond lengths



Bond angles

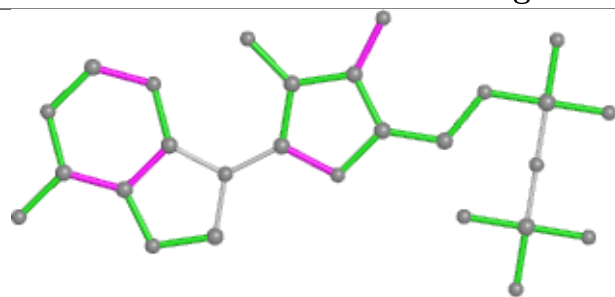


Torsions

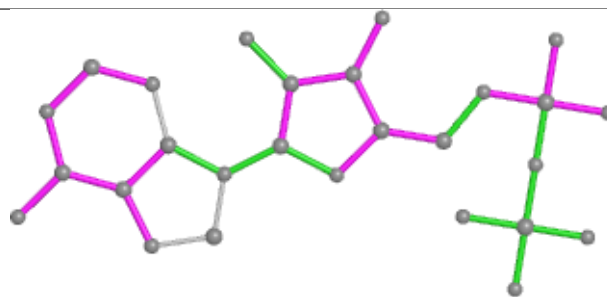


Rings

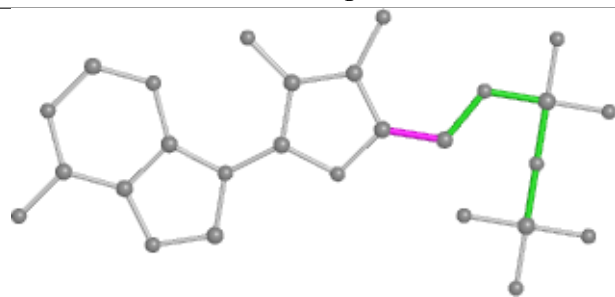
## Ligand ADP D 501



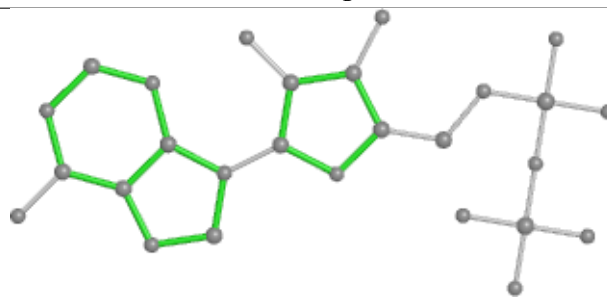
Bond lengths



Bond angles



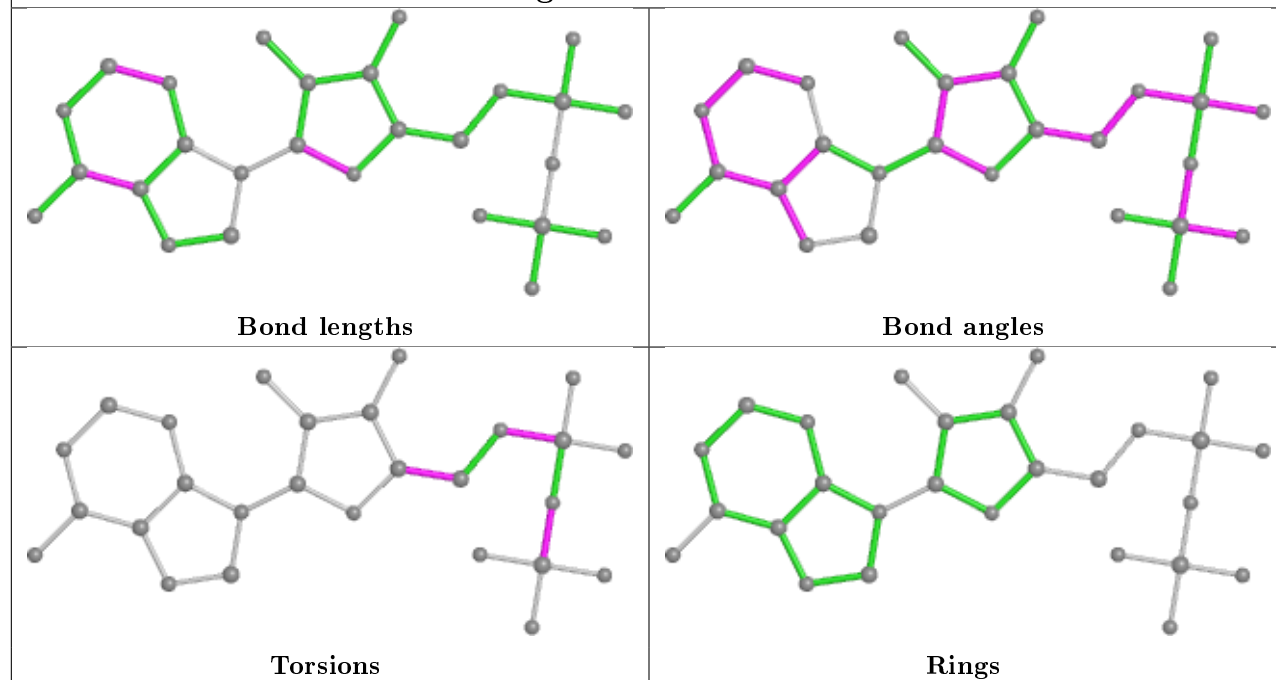
Torsions



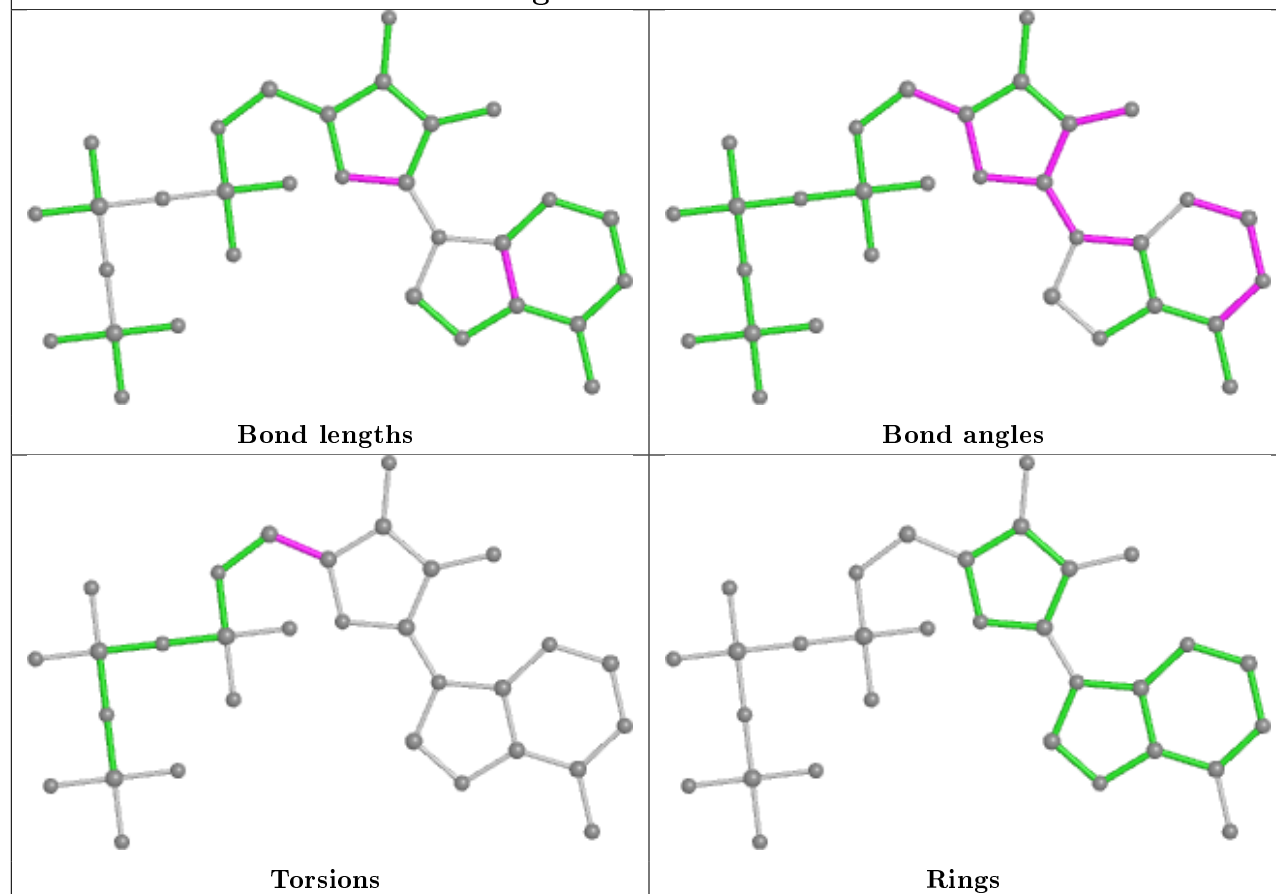
Rings

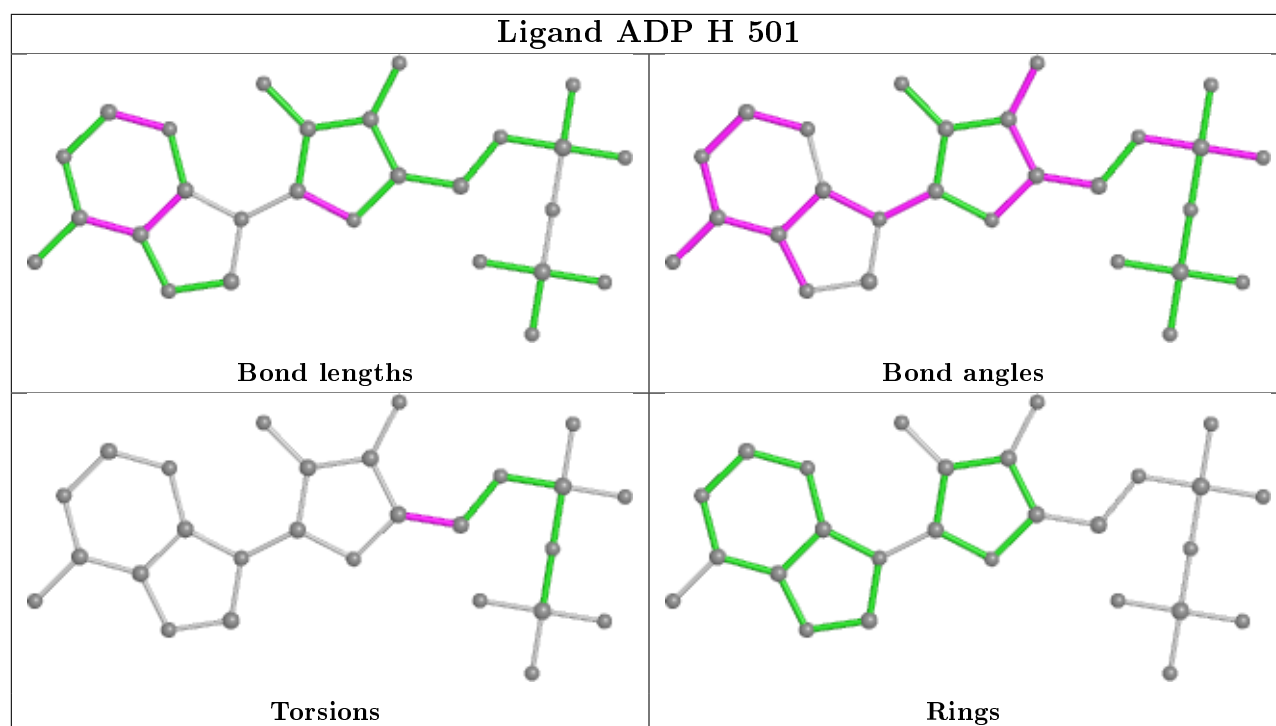


## Ligand ADP I 501



## Ligand ATP K 501





## 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     | 476/481 (98%)   | -0.01  | 15 (3%) 47 46  | 14, 33, 61, 89        | 0     |
| 1   | B     | 475/481 (98%)   | -0.07  | 16 (3%) 45 43  | 17, 34, 55, 76        | 0     |
| 1   | C     | 474/481 (98%)   | -0.03  | 14 (2%) 50 49  | 15, 32, 59, 90        | 0     |
| 1   | D     | 476/481 (98%)   | -0.09  | 10 (2%) 63 64  | 14, 32, 55, 71        | 0     |
| 1   | E     | 473/481 (98%)   | -0.06  | 16 (3%) 45 43  | 16, 33, 56, 76        | 0     |
| 1   | F     | 475/481 (98%)   | -0.07  | 11 (2%) 60 61  | 12, 33, 56, 79        | 0     |
| 1   | G     | 476/481 (98%)   | -0.26  | 7 (1%) 73 75   | 10, 22, 43, 85        | 0     |
| 1   | H     | 475/481 (98%)   | -0.28  | 11 (2%) 60 61  | 10, 22, 44, 79        | 0     |
| 1   | I     | 475/481 (98%)   | -0.29  | 8 (1%) 70 71   | 9, 20, 39, 73         | 0     |
| 1   | J     | 478/481 (99%)   | -0.23  | 8 (1%) 70 71   | 10, 21, 42, 88        | 0     |
| 1   | K     | 475/481 (98%)   | -0.26  | 3 (0%) 89 90   | 10, 21, 43, 75        | 0     |
| 1   | L     | 476/481 (98%)   | -0.31  | 1 (0%) 95 95   | 10, 22, 38, 60        | 0     |
| All | All   | 5704/5772 (98%) | -0.16  | 120 (2%) 63 64 | 9, 27, 52, 90         | 0     |

All (120) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 412 | ASP  | 4.2  |
| 1   | E     | 414 | ILE  | 4.0  |
| 1   | D     | 16  | PHE  | 3.8  |
| 1   | B     | 414 | ILE  | 3.6  |
| 1   | H     | 411 | LEU  | 3.4  |
| 1   | B     | 288 | ASN  | 3.4  |
| 1   | D     | 10  | SER  | 3.4  |
| 1   | D     | 53  | LEU  | 3.3  |
| 1   | F     | 176 | ASN  | 3.2  |
| 1   | H     | 415 | ARG  | 3.2  |
| 1   | F     | 416 | GLU  | 3.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | E            | 176        | ASN         | 3.2         |
| 1          | B            | 410        | THR         | 3.1         |
| 1          | G            | 53         | LEU         | 3.1         |
| 1          | J            | 415        | ARG         | 3.1         |
| 1          | I            | 414        | ILE         | 3.0         |
| 1          | E            | 16         | PHE         | 3.0         |
| 1          | J            | 414        | ILE         | 3.0         |
| 1          | I            | 177        | GLY         | 3.0         |
| 1          | C            | 416        | GLU         | 2.9         |
| 1          | E            | 9          | GLU         | 2.9         |
| 1          | E            | 416        | GLU         | 2.9         |
| 1          | F            | 16         | PHE         | 2.9         |
| 1          | F            | 174        | PHE         | 2.9         |
| 1          | A            | 415        | ARG         | 2.9         |
| 1          | C            | 53         | LEU         | 2.9         |
| 1          | J            | 418        | GLY         | 2.9         |
| 1          | H            | 416        | GLU         | 2.8         |
| 1          | C            | 50         | HIS         | 2.8         |
| 1          | F            | 7          | ASN         | 2.8         |
| 1          | A            | 127        | ASP         | 2.8         |
| 1          | K            | 412        | ASP         | 2.8         |
| 1          | H            | 413        | GLU         | 2.8         |
| 1          | A            | 20         | LYS         | 2.8         |
| 1          | B            | 132        | ASP         | 2.7         |
| 1          | K            | 414        | ILE         | 2.7         |
| 1          | F            | 53         | LEU         | 2.7         |
| 1          | B            | 7          | ASN         | 2.7         |
| 1          | I            | 288        | ASN         | 2.7         |
| 1          | H            | 8          | SER         | 2.7         |
| 1          | J            | 419        | ILE         | 2.7         |
| 1          | F            | 419        | ILE         | 2.6         |
| 1          | B            | 15         | PHE         | 2.6         |
| 1          | B            | 12         | ILE         | 2.6         |
| 1          | E            | 358        | GLY         | 2.6         |
| 1          | B            | 133        | VAL         | 2.6         |
| 1          | H            | 9          | GLU         | 2.6         |
| 1          | C            | 8          | SER         | 2.6         |
| 1          | E            | 132        | ASP         | 2.6         |
| 1          | E            | 174        | PHE         | 2.6         |
| 1          | H            | 414        | ILE         | 2.6         |
| 1          | B            | 50         | HIS         | 2.6         |
| 1          | C            | 10         | SER         | 2.5         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 176 | ASN  | 2.5  |
| 1   | E     | 438 | GLN  | 2.5  |
| 1   | I     | 50  | HIS  | 2.5  |
| 1   | E     | 15  | PHE  | 2.5  |
| 1   | B     | 419 | ILE  | 2.5  |
| 1   | C     | 178 | VAL  | 2.5  |
| 1   | D     | 84  | TYR  | 2.5  |
| 1   | C     | 417 | LYS  | 2.5  |
| 1   | G     | 172 | ARG  | 2.5  |
| 1   | A     | 18  | PHE  | 2.4  |
| 1   | A     | 303 | PHE  | 2.4  |
| 1   | C     | 15  | PHE  | 2.4  |
| 1   | A     | 416 | GLU  | 2.4  |
| 1   | G     | 410 | THR  | 2.4  |
| 1   | B     | 175 | GLU  | 2.4  |
| 1   | L     | 289 | GLU  | 2.4  |
| 1   | E     | 51  | GLY  | 2.4  |
| 1   | C     | 174 | PHE  | 2.3  |
| 1   | E     | 435 | ALA  | 2.3  |
| 1   | I     | 411 | LEU  | 2.3  |
| 1   | I     | 415 | ARG  | 2.3  |
| 1   | A     | 12  | ILE  | 2.3  |
| 1   | I     | 8   | SER  | 2.3  |
| 1   | D     | 9   | GLU  | 2.3  |
| 1   | B     | 415 | ARG  | 2.3  |
| 1   | D     | 174 | PHE  | 2.3  |
| 1   | A     | 287 | ASN  | 2.3  |
| 1   | F     | 415 | ARG  | 2.3  |
| 1   | A     | 6   | GLN  | 2.3  |
| 1   | B     | 9   | GLU  | 2.3  |
| 1   | E     | 55  | GLU  | 2.3  |
| 1   | J     | 449 | GLU  | 2.3  |
| 1   | C     | 177 | GLY  | 2.2  |
| 1   | E     | 12  | ILE  | 2.2  |
| 1   | D     | 175 | GLU  | 2.2  |
| 1   | G     | 174 | PHE  | 2.2  |
| 1   | F     | 178 | VAL  | 2.2  |
| 1   | A     | 176 | ASN  | 2.2  |
| 1   | A     | 48  | LEU  | 2.2  |
| 1   | C     | 419 | ILE  | 2.2  |
| 1   | H     | 358 | GLY  | 2.2  |
| 1   | C     | 16  | PHE  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 55  | GLU  | 2.2  |
| 1   | A     | 409 | LEU  | 2.2  |
| 1   | G     | 411 | LEU  | 2.2  |
| 1   | E     | 50  | HIS  | 2.2  |
| 1   | I     | 176 | ASN  | 2.2  |
| 1   | H     | 53  | LEU  | 2.2  |
| 1   | G     | 8   | SER  | 2.2  |
| 1   | K     | 418 | GLY  | 2.1  |
| 1   | E     | 415 | ARG  | 2.1  |
| 1   | J     | 176 | ASN  | 2.1  |
| 1   | G     | 50  | HIS  | 2.1  |
| 1   | B     | 286 | LYS  | 2.1  |
| 1   | H     | 361 | LYS  | 2.1  |
| 1   | A     | 16  | PHE  | 2.1  |
| 1   | J     | 416 | GLU  | 2.1  |
| 1   | A     | 402 | MET  | 2.1  |
| 1   | C     | 13  | LYS  | 2.1  |
| 1   | J     | 175 | GLU  | 2.0  |
| 1   | B     | 10  | SER  | 2.0  |
| 1   | A     | 53  | LEU  | 2.0  |
| 1   | F     | 288 | ASN  | 2.0  |
| 1   | C     | 173 | SER  | 2.0  |
| 1   | D     | 358 | GLY  | 2.0  |
| 1   | D     | 410 | THR  | 2.0  |
| 1   | F     | 8   | SER  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

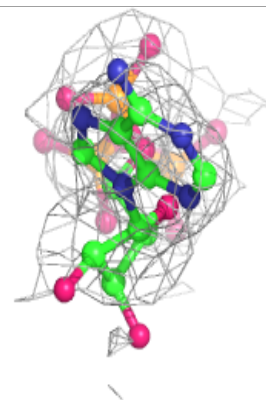
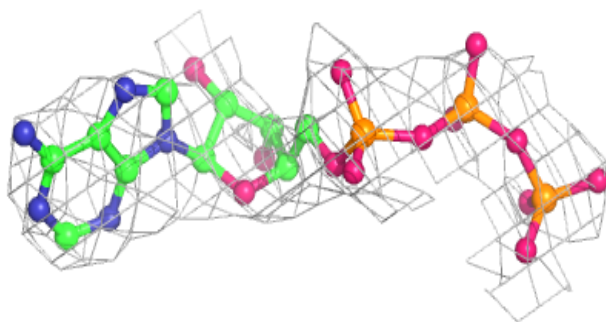
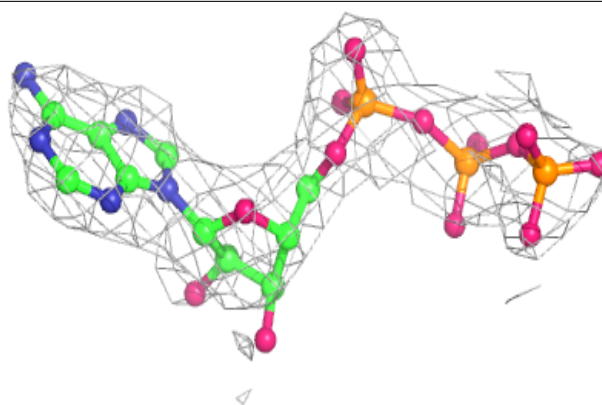
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | MG   | J     | 503 | 1/1   | 0.79 | 0.46 | 41,41,41,41                 | 0     |
| 5   | MG   | L     | 504 | 1/1   | 0.81 | 0.31 | 53,53,53,53                 | 0     |
| 2   | ATP  | A     | 501 | 31/31 | 0.85 | 0.24 | 42,63,115,116               | 0     |
| 3   | ADP  | E     | 501 | 27/27 | 0.85 | 0.25 | 40,56,78,102                | 0     |
| 4   | PPQ  | I     | 502 | 11/11 | 0.85 | 0.25 | 28,36,51,58                 | 0     |
| 2   | ATP  | B     | 501 | 31/31 | 0.87 | 0.20 | 38,55,90,96                 | 0     |
| 2   | ATP  | C     | 501 | 31/31 | 0.87 | 0.21 | 48,60,91,94                 | 0     |
| 5   | MG   | I     | 503 | 1/1   | 0.88 | 0.25 | 44,44,44,44                 | 0     |
| 3   | ADP  | D     | 501 | 27/27 | 0.88 | 0.24 | 46,53,95,113                | 0     |
| 2   | ATP  | F     | 501 | 31/31 | 0.88 | 0.20 | 45,57,95,104                | 0     |
| 3   | ADP  | L     | 503 | 27/27 | 0.89 | 0.18 | 24,38,77,85                 | 0     |
| 3   | ADP  | H     | 501 | 27/27 | 0.89 | 0.23 | 29,39,81,100                | 0     |
| 2   | ATP  | K     | 501 | 31/31 | 0.90 | 0.22 | 23,40,96,99                 | 0     |
| 6   | P3P  | L     | 501 | 15/15 | 0.90 | 0.21 | 24,41,68,78                 | 0     |
| 3   | ADP  | I     | 501 | 27/27 | 0.91 | 0.20 | 25,34,79,106                | 0     |
| 2   | ATP  | G     | 501 | 31/31 | 0.92 | 0.18 | 22,35,83,98                 | 0     |
| 4   | PPQ  | J     | 502 | 11/11 | 0.92 | 0.20 | 25,29,37,45                 | 11    |
| 3   | ADP  | J     | 501 | 27/27 | 0.93 | 0.18 | 26,35,83,102                | 0     |
| 4   | PPQ  | K     | 502 | 11/11 | 0.95 | 0.19 | 22,28,41,43                 | 11    |
| 5   | MG   | L     | 502 | 1/1   | 0.95 | 0.11 | 48,48,48,48                 | 0     |

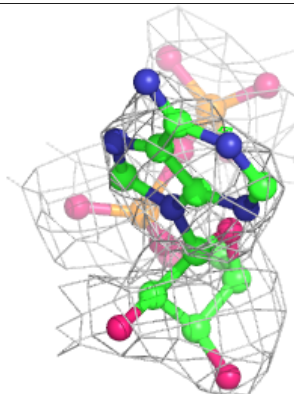
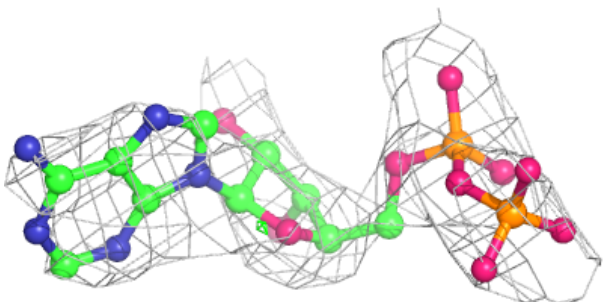
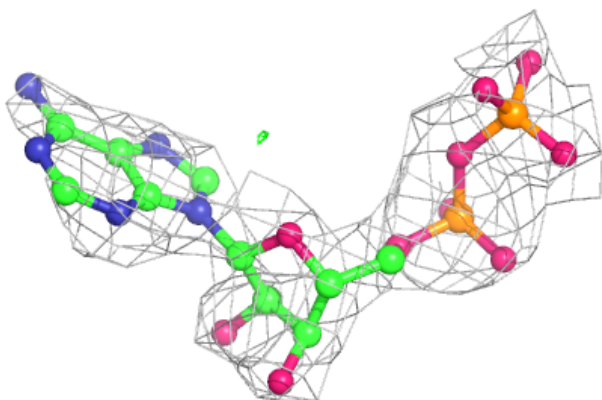
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP A 501:**

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

**Electron density around ADP E 501:**

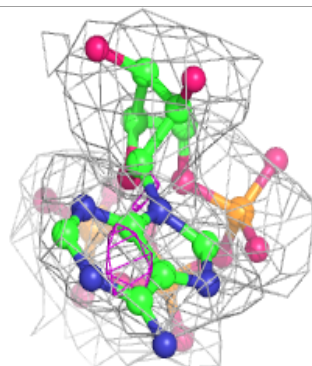
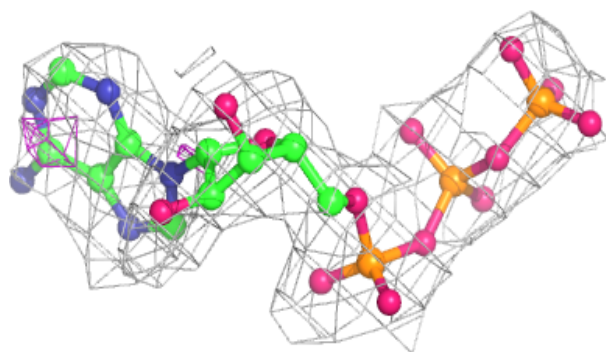
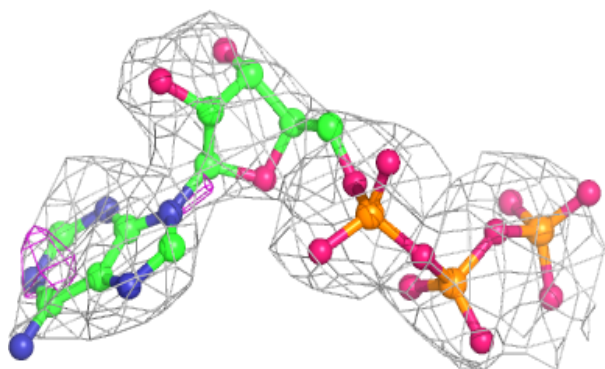
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



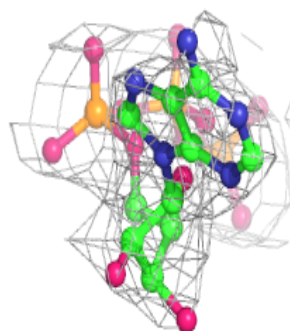
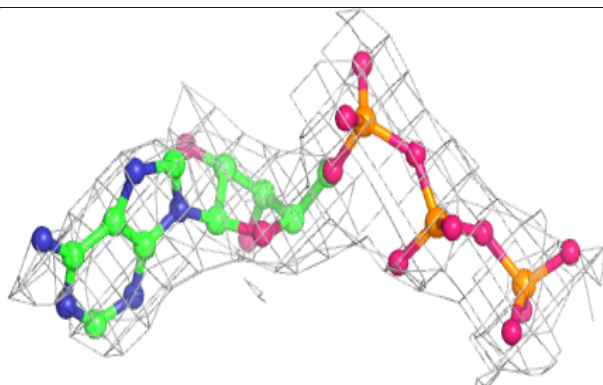
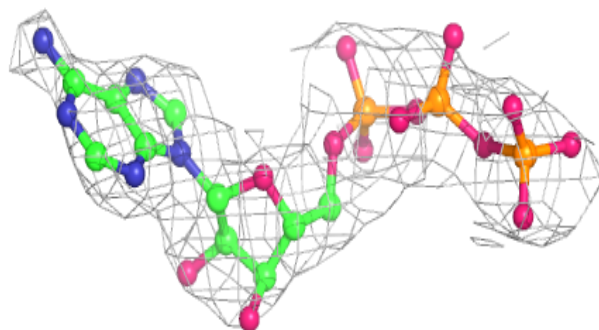


**Electron density around ATP B 501:**

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

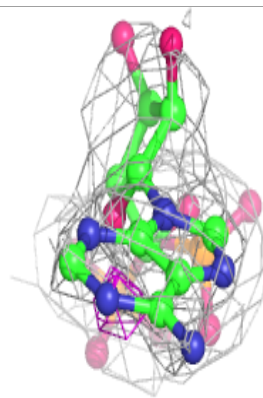
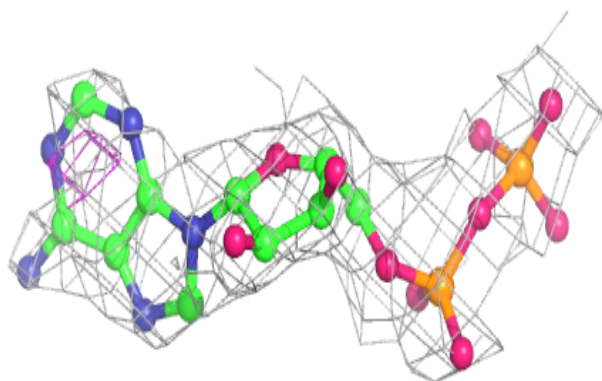
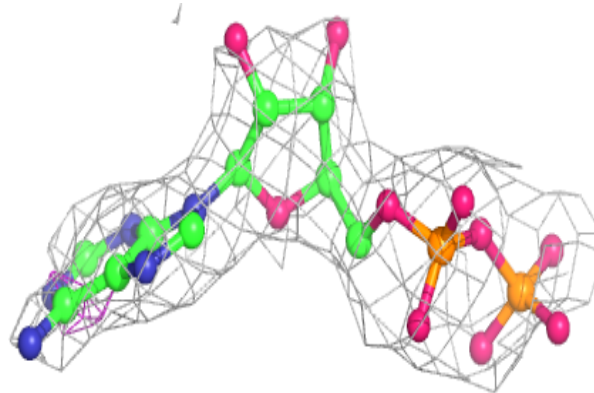
**Electron density around ATP C 501:**

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

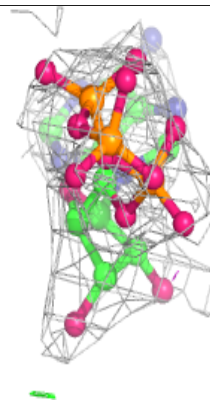
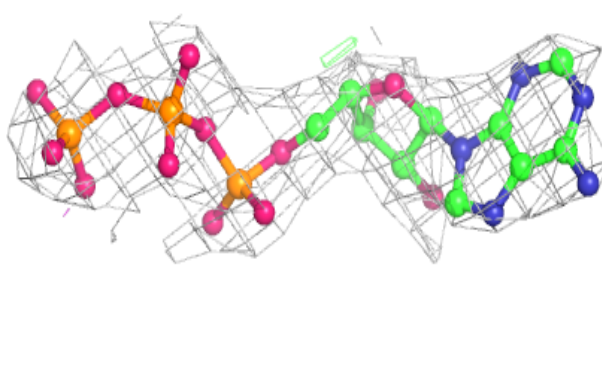
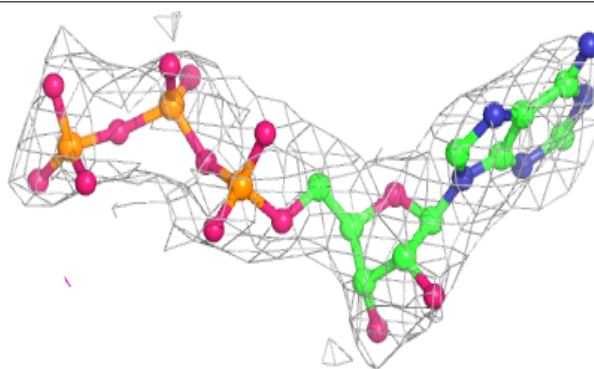


**Electron density around ADP D 501:**

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

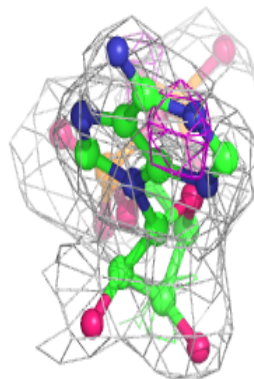
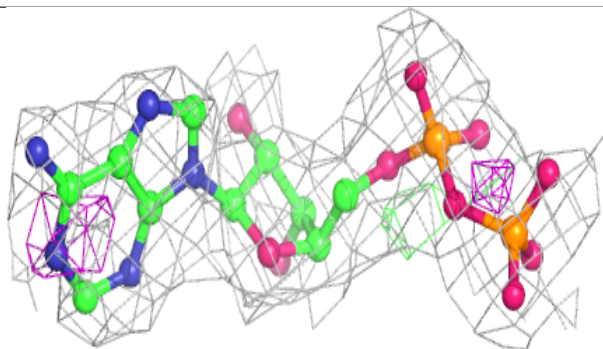
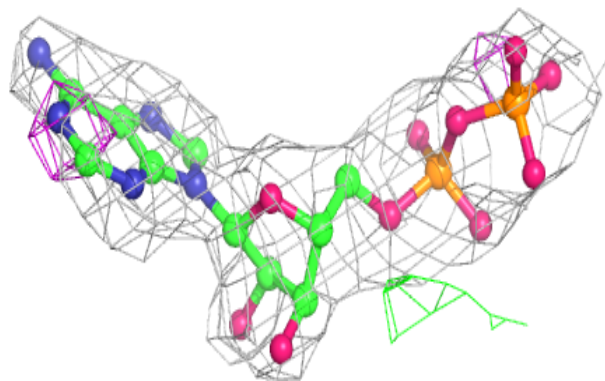
**Electron density around ATP F 501:**

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

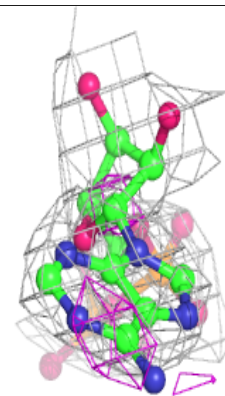
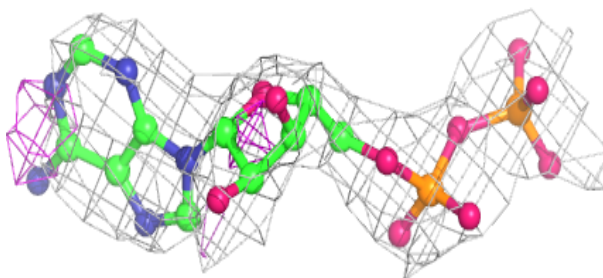
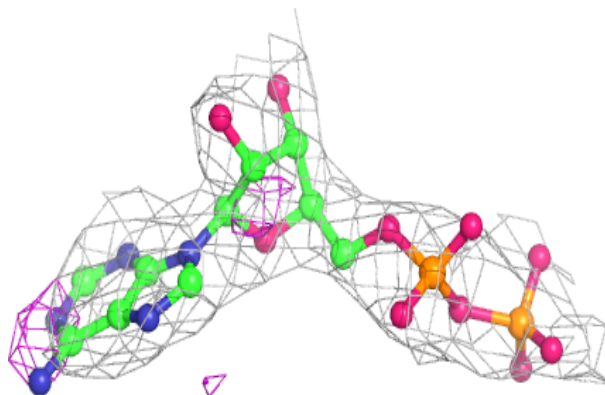


**Electron density around ADP L 503:**

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

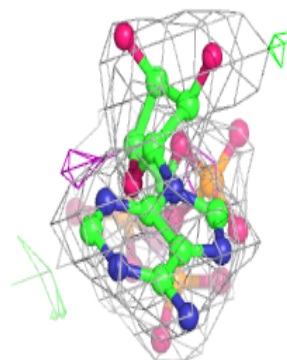
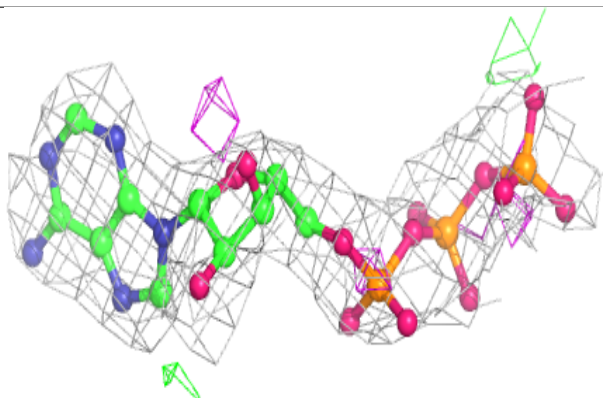
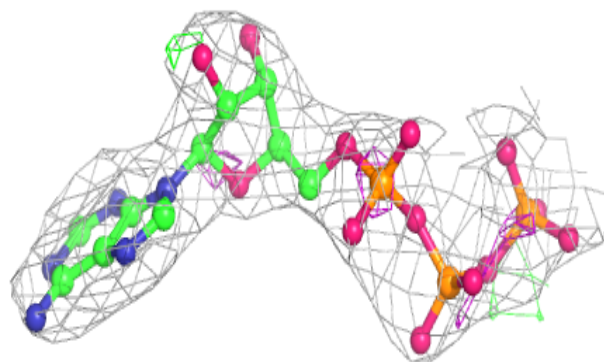
**Electron density around ADP H 501:**

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

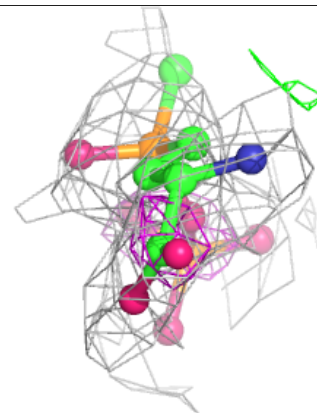
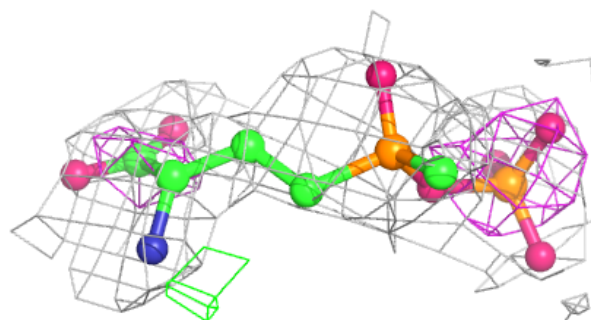
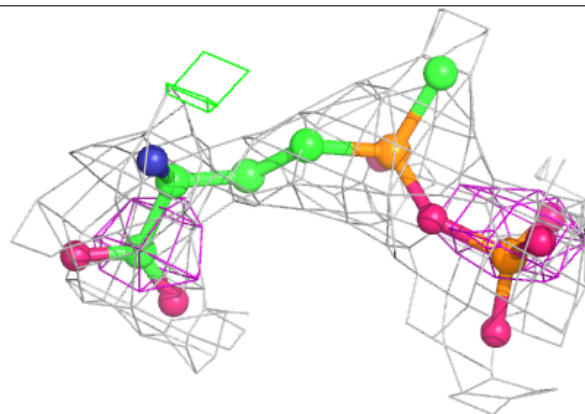


**Electron density around ATP K 501:**

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

**Electron density around P3P L 501:**

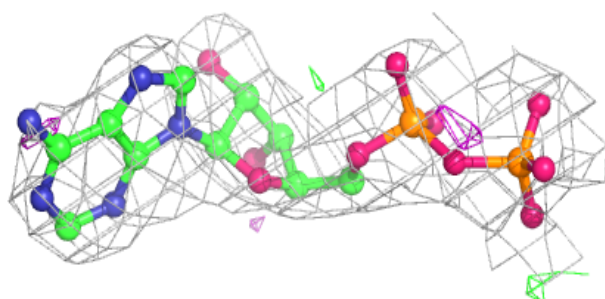
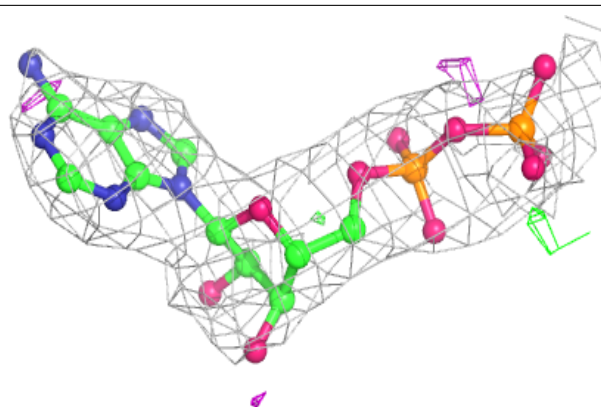
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



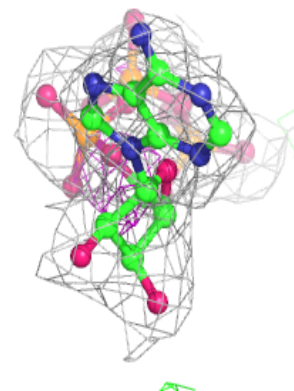
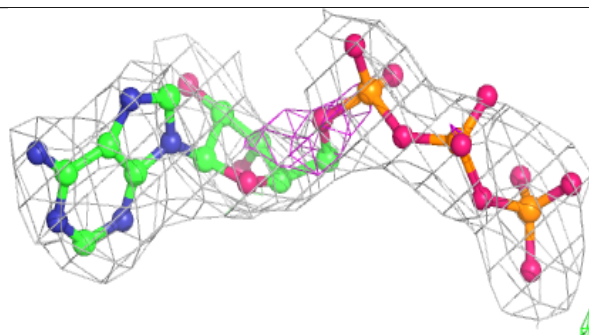
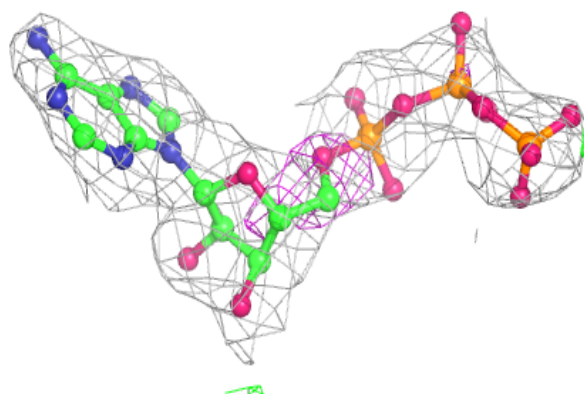


**Electron density around ADP I 501:**

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

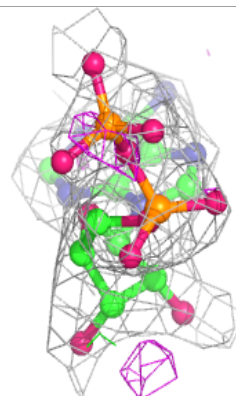
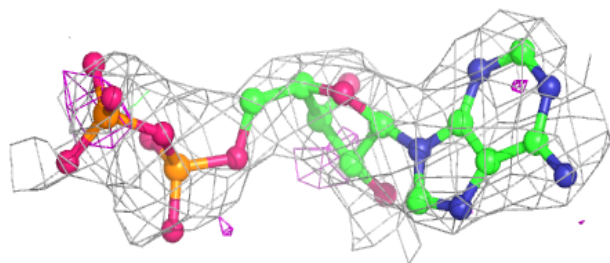
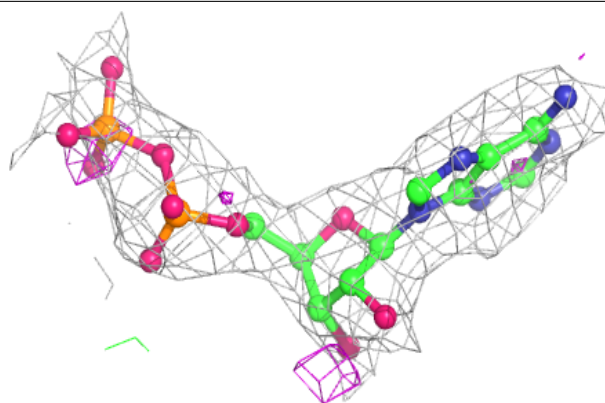
**Electron density around ATP G 501:**

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



**Electron density around ADP J 501:**

$2mF_o-DF_c$  (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.