



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:55 AM UTC

PDB ID : 7RES / pdb\_00007res  
EMDB ID : EMD-24438  
Title : HUMAN IMPDH1 TREATED WITH ATP, IMP, AND NAD<sup>+</sup>, OCTAMER-CENTERED  
Authors : Burrell, A.L.; Kollman, J.M.  
Deposited on : 2021-07-13  
Resolution : 3.05 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

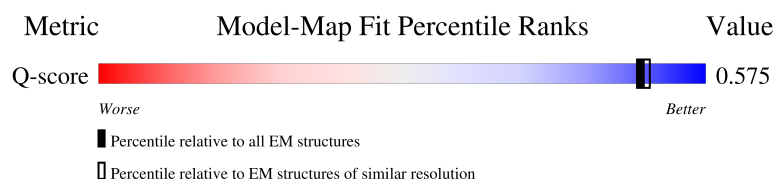
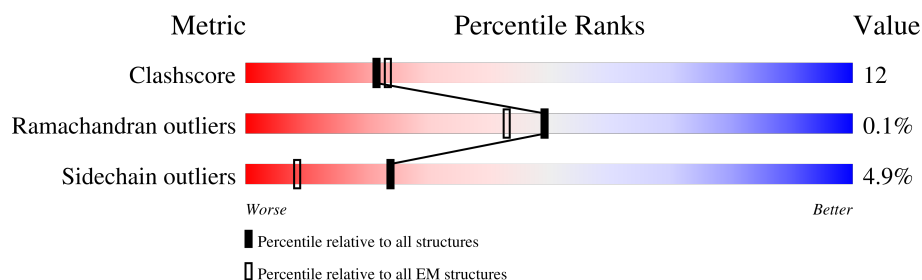
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.05 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.



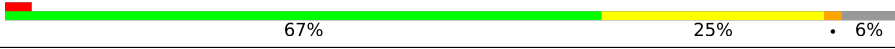
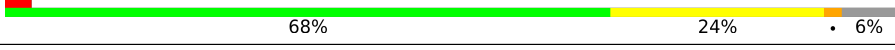
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13971 ( 2.55 - 3.55 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 514    |                  |
| 1   | B     | 514    |                  |
| 1   | C     | 514    |                  |
| 1   | D     | 514    |                  |

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| Mol | Chain | Length | Quality of chain                                                                            |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 1   | E     | 514    |  66%26%6% |
| 1   | F     | 514    |  68%25%6% |
| 1   | G     | 514    |  67%25%6% |
| 1   | H     | 514    |  68%24%6% |

## 2 Entry composition [i](#)

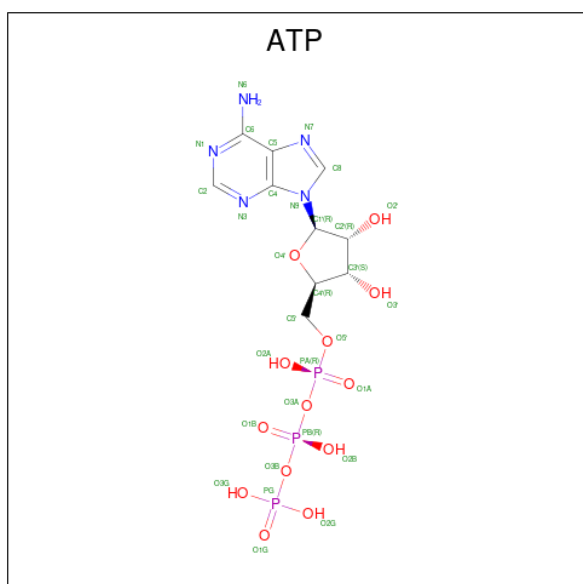
There are 4 unique types of molecules in this entry. The entry contains 30088 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1.

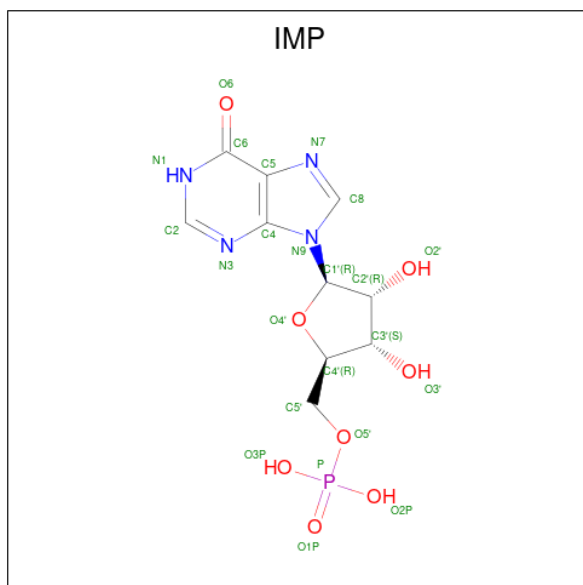
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2295 | 623 | 691 | 23 |         |       |
| 1   | B     | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2295 | 623 | 691 | 23 |         |       |
| 1   | C     | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2295 | 623 | 691 | 23 |         |       |
| 1   | D     | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2295 | 623 | 691 | 23 |         |       |
| 1   | E     | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2295 | 623 | 691 | 23 |         |       |
| 1   | F     | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2295 | 623 | 691 | 23 |         |       |
| 1   | G     | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2295 | 623 | 691 | 23 |         |       |
| 1   | H     | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2295 | 623 | 691 | 23 |         |       |

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



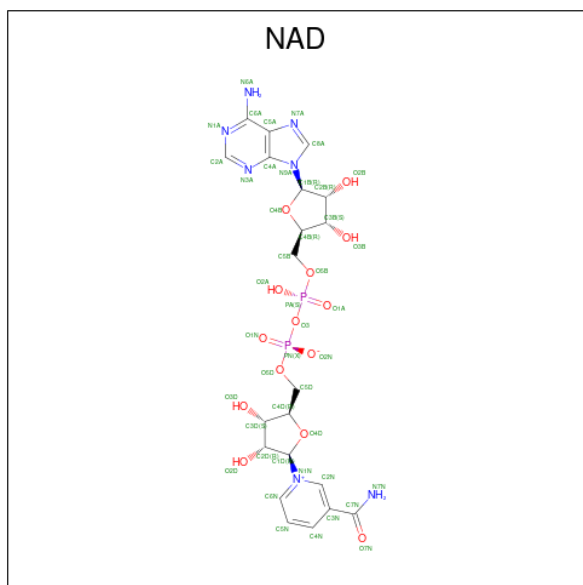
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 3 is INOSINIC ACID (CCD ID: IMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 10 | 4 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 10 | 4 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 10 | 4 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 10 | 4 | 8 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 10 | 4 | 8 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 10 | 4 | 8 | 1 |         |
| 3   | G     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 10 | 4 | 8 | 1 |         |
| 3   | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 10 | 4 | 8 | 1 |         |

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).

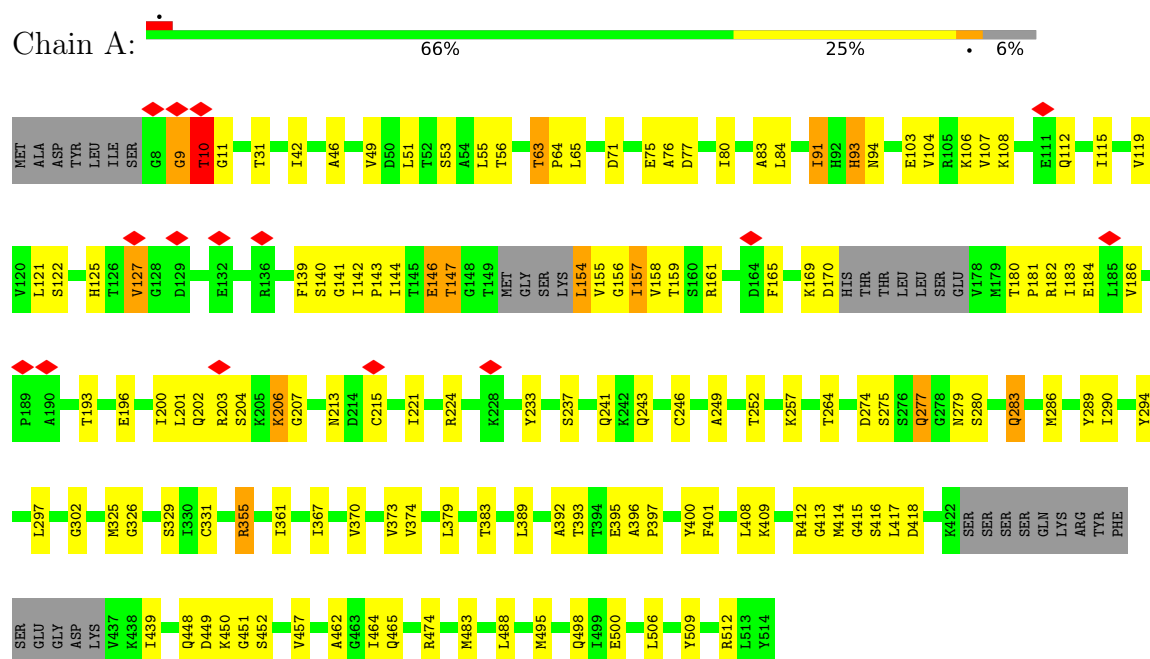


| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 4   | A     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |
| 4   | B     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |
| 4   | C     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |
| 4   | D     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |
| 4   | E     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |
| 4   | F     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |
| 4   | G     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |
| 4   | H     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |

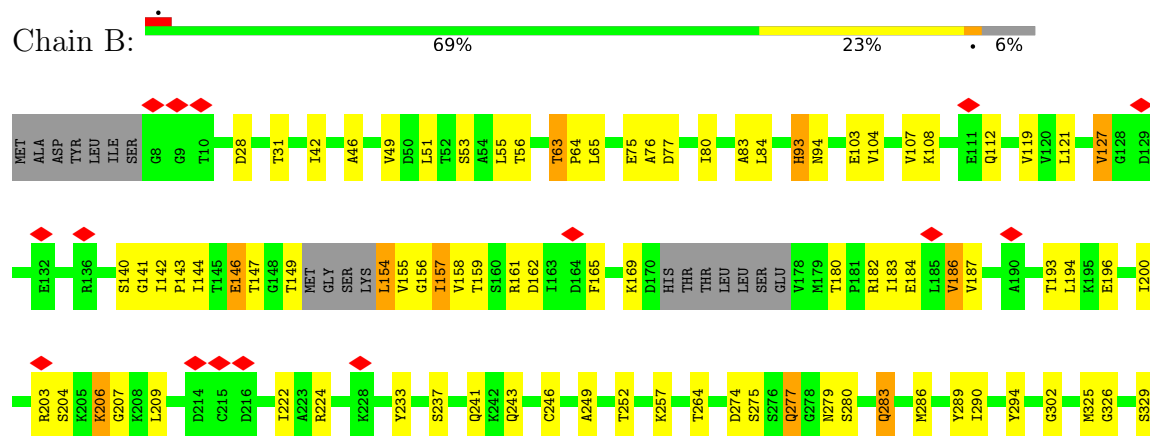
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

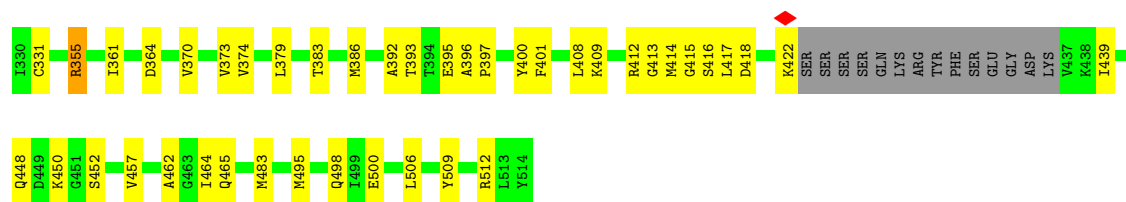
- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



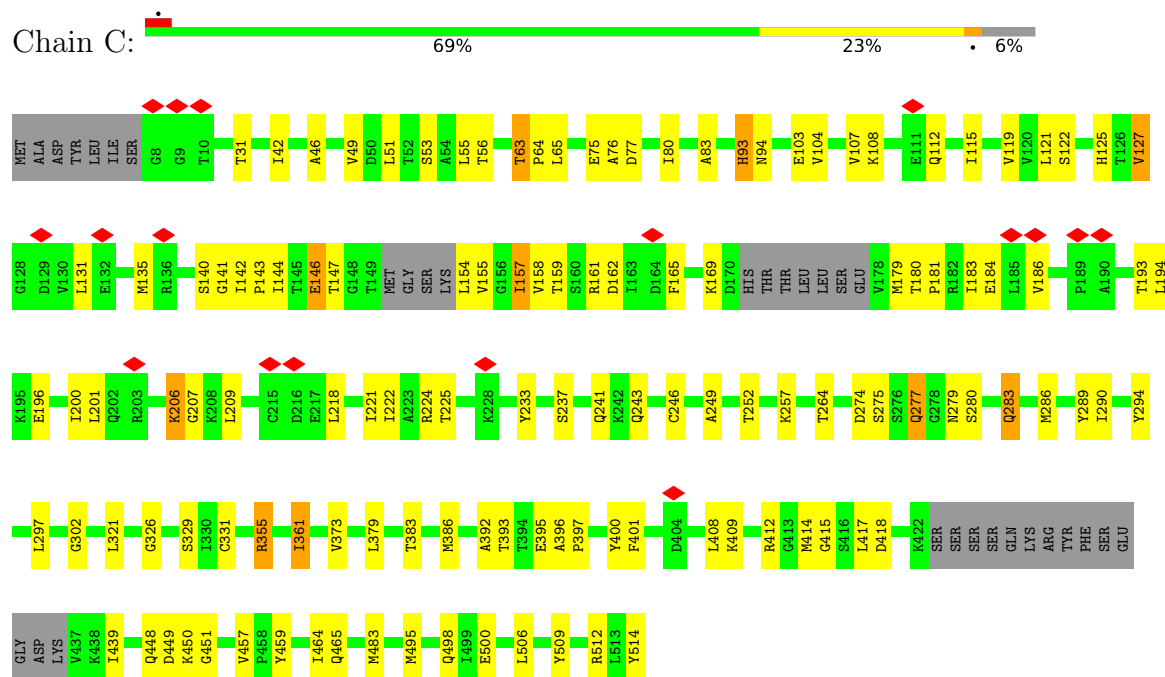
- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



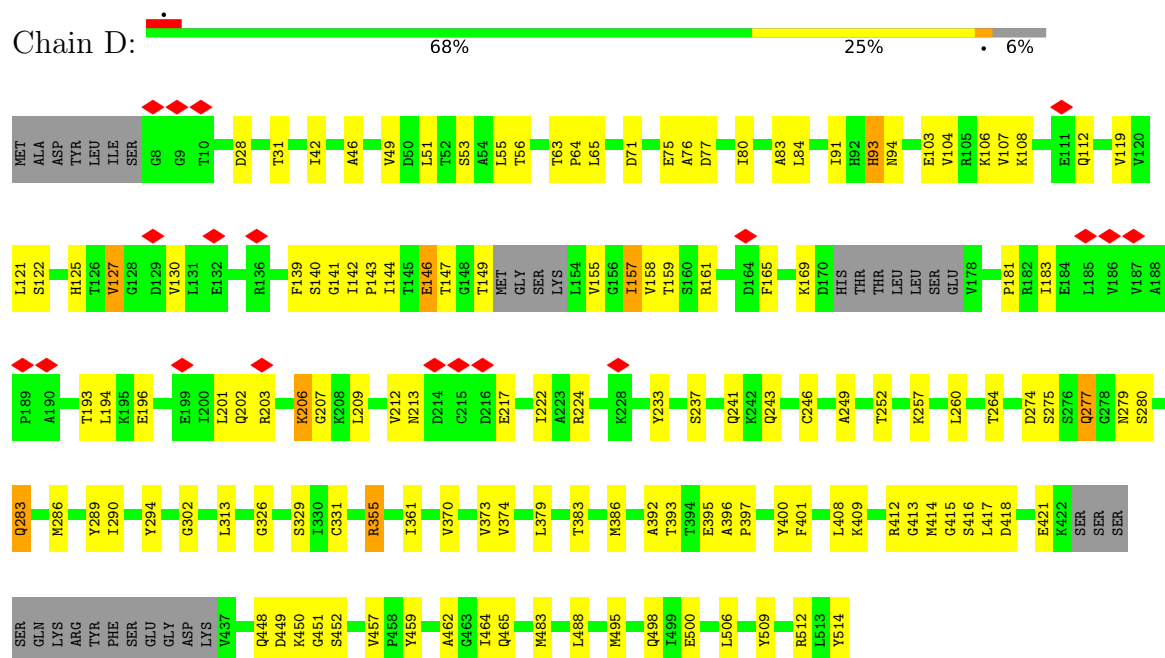




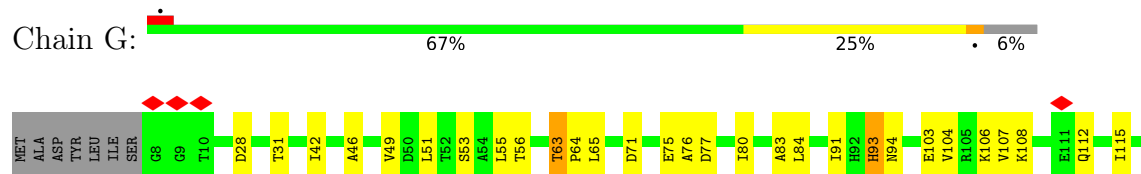
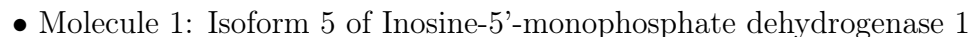
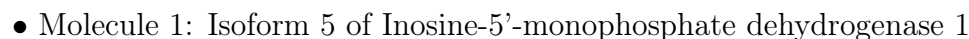
- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1

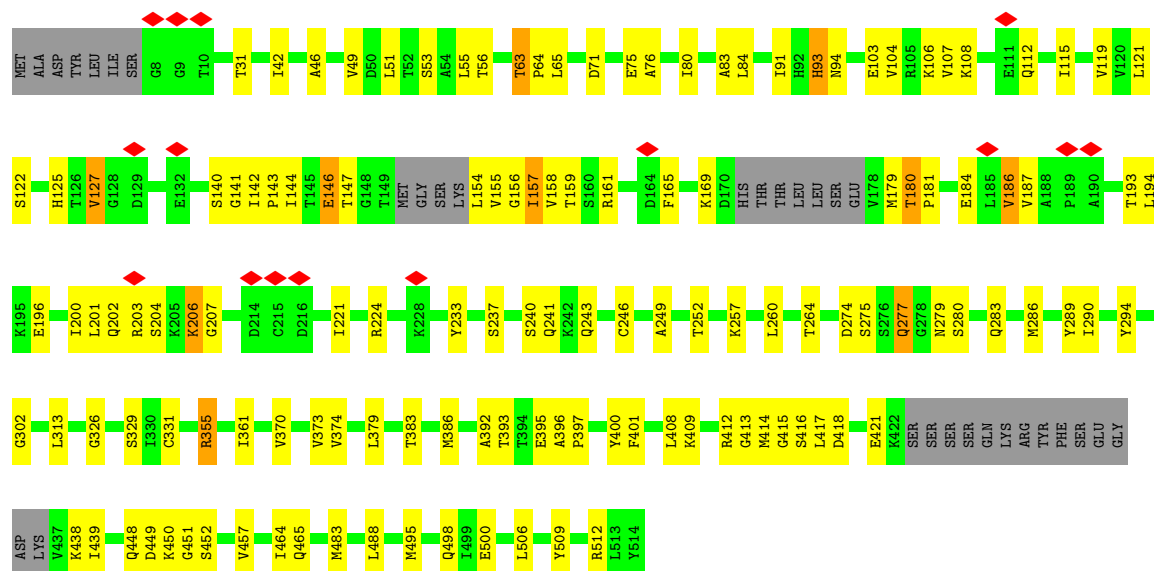


- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 58000                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 10.743                                  | Depositor |
| Minimum map value                    | -6.672                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.256                                   | Depositor |
| Recommended contour level            | 0.804                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 336.0, 336.0, 336.0                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.05, 1.05, 1.05                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, IMP, ATP

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     | 0.46         | 0/3685         | 0.46        | 2/4972 (0.0%)  |
| 1   | B     | 0.44         | 0/3685         | 0.42        | 0/4972         |
| 1   | C     | 0.44         | 0/3685         | 0.42        | 0/4972         |
| 1   | D     | 0.44         | 0/3685         | 0.42        | 0/4972         |
| 1   | E     | 0.67         | 9/3685 (0.2%)  | 0.46        | 1/4972 (0.0%)  |
| 1   | F     | 0.44         | 0/3685         | 0.42        | 0/4972         |
| 1   | G     | 0.44         | 0/3685         | 0.43        | 0/4972         |
| 1   | H     | 0.44         | 0/3685         | 0.43        | 0/4972         |
| All | All   | 0.48         | 9/29480 (0.0%) | 0.43        | 3/39776 (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   | E     | 0                   | 1                   |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | E     | 12  | TYR  | CA-CB  | -13.85 | 1.34        | 1.53     |
| 1   | E     | 12  | TYR  | N-CA   | -11.79 | 1.31        | 1.46     |
| 1   | E     | 12  | TYR  | CA-C   | -10.48 | 1.39        | 1.52     |
| 1   | E     | 12  | TYR  | C-O    | -9.76  | 1.12        | 1.24     |
| 1   | E     | 12  | TYR  | CG-CD2 | -8.57  | 1.21        | 1.39     |
| 1   | E     | 12  | TYR  | CB-CG  | -7.95  | 1.34        | 1.51     |
| 1   | E     | 12  | TYR  | CE1-CZ | -6.81  | 1.22        | 1.38     |
| 1   | E     | 12  | TYR  | CZ-OH  | -5.79  | 1.25        | 1.38     |
| 1   | E     | 11  | GLY  | CA-C   | -5.76  | 1.45        | 1.51     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 11  | GLY  | CA-C-O | -5.80 | 117.19      | 122.24   |
| 1   | A     | 9   | GLY  | CA-C-O | -5.23 | 117.69      | 122.24   |
| 1   | A     | 10  | THR  | N-CA-C | 5.10  | 121.67      | 110.80   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | E     | 12  | TYR  | Mainchain |

## 5.2 Too-close contacts [i](#)

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     | 3632  | 0        | 3700     | 99      | 0            |
| 1   | B     | 3632  | 0        | 3700     | 87      | 0            |
| 1   | C     | 3632  | 0        | 3700     | 87      | 0            |
| 1   | D     | 3632  | 0        | 3700     | 89      | 0            |
| 1   | E     | 3632  | 0        | 3700     | 94      | 0            |
| 1   | F     | 3632  | 0        | 3700     | 92      | 0            |
| 1   | G     | 3632  | 0        | 3700     | 96      | 0            |
| 1   | H     | 3632  | 0        | 3700     | 98      | 0            |
| 2   | A     | 62    | 0        | 23       | 3       | 0            |
| 2   | B     | 62    | 0        | 23       | 5       | 0            |
| 2   | C     | 62    | 0        | 24       | 7       | 0            |
| 2   | D     | 62    | 0        | 23       | 6       | 0            |
| 2   | E     | 62    | 0        | 23       | 5       | 0            |
| 2   | F     | 62    | 0        | 24       | 5       | 0            |
| 2   | G     | 62    | 0        | 24       | 4       | 0            |
| 2   | H     | 62    | 0        | 23       | 4       | 0            |
| 3   | A     | 23    | 0        | 11       | 3       | 0            |
| 3   | B     | 23    | 0        | 11       | 4       | 0            |
| 3   | C     | 23    | 0        | 11       | 3       | 0            |
| 3   | D     | 23    | 0        | 11       | 3       | 0            |
| 3   | E     | 23    | 0        | 11       | 3       | 0            |
| 3   | F     | 23    | 0        | 11       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | G     | 23    | 0        | 11       | 3       | 0            |
| 3   | H     | 23    | 0        | 11       | 3       | 0            |
| 4   | A     | 44    | 0        | 24       | 3       | 0            |
| 4   | B     | 44    | 0        | 24       | 1       | 0            |
| 4   | C     | 44    | 0        | 24       | 0       | 0            |
| 4   | D     | 44    | 0        | 24       | 1       | 0            |
| 4   | E     | 44    | 0        | 24       | 1       | 0            |
| 4   | F     | 44    | 0        | 24       | 3       | 0            |
| 4   | G     | 44    | 0        | 24       | 1       | 0            |
| 4   | H     | 44    | 0        | 24       | 0       | 0            |
| All | All   | 30088 | 0        | 30067    | 701     | 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 (701) 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:D:252:THR:HG21 | 1:D:283:GLN:HG2  | 1.62                     | 0.81              |
| 1:F:252:THR:HG21 | 1:F:283:GLN:HG2  | 1.62                     | 0.81              |
| 1:H:252:THR:HG21 | 1:H:283:GLN:HG2  | 1.62                     | 0.81              |
| 1:B:252:THR:HG21 | 1:B:283:GLN:HG2  | 1.63                     | 0.81              |
| 1:E:252:THR:HG21 | 1:E:283:GLN:HG2  | 1.62                     | 0.79              |
| 1:A:252:THR:HG21 | 1:A:283:GLN:HG2  | 1.63                     | 0.79              |
| 1:C:252:THR:HG21 | 1:C:283:GLN:HG2  | 1.63                     | 0.78              |
| 1:G:396:ALA:O    | 1:G:409:LYS:NZ   | 2.19                     | 0.75              |
| 1:C:396:ALA:O    | 1:C:409:LYS:NZ   | 2.20                     | 0.75              |
| 1:B:396:ALA:O    | 1:B:409:LYS:NZ   | 2.20                     | 0.74              |
| 1:F:396:ALA:O    | 1:F:409:LYS:NZ   | 2.20                     | 0.74              |
| 2:B:601:ATP:O2A  | 1:G:161:ARG:NH1  | 2.20                     | 0.73              |
| 1:D:396:ALA:O    | 1:D:409:LYS:NZ   | 2.19                     | 0.73              |
| 1:E:396:ALA:O    | 1:E:409:LYS:NZ   | 2.20                     | 0.72              |
| 1:A:396:ALA:O    | 1:A:409:LYS:NZ   | 2.19                     | 0.71              |
| 1:B:121:LEU:HB2  | 1:B:144:ILE:HG22 | 1.73                     | 0.71              |
| 1:C:331:CYS:SG   | 3:C:603:IMP:H2   | 2.31                     | 0.70              |
| 1:G:331:CYS:SG   | 3:G:603:IMP:H2   | 2.32                     | 0.70              |
| 1:H:94:ASN:HB2   | 1:H:414:MET:HE1  | 1.74                     | 0.70              |
| 1:C:141:GLY:HA2  | 1:C:159:THR:HA   | 1.74                     | 0.70              |
| 1:F:331:CYS:SG   | 3:F:603:IMP:H2   | 2.32                     | 0.69              |
| 1:H:331:CYS:SG   | 3:H:603:IMP:H2   | 2.32                     | 0.69              |
| 1:A:141:GLY:HA2  | 1:A:159:THR:HA   | 1.73                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:331:CYS:SG   | 3:B:603:IMP:H2   | 2.32                     | 0.69              |
| 1:G:252:THR:HG21 | 1:G:283:GLN:HG2  | 1.74                     | 0.69              |
| 1:E:141:GLY:HA2  | 1:E:159:THR:HA   | 1.73                     | 0.69              |
| 1:E:331:CYS:SG   | 3:E:603:IMP:H2   | 2.32                     | 0.69              |
| 1:A:331:CYS:SG   | 3:A:603:IMP:H2   | 2.32                     | 0.69              |
| 1:C:283:GLN:NE2  | 1:C:302:GLY:O    | 2.26                     | 0.69              |
| 1:H:141:GLY:HA2  | 1:H:159:THR:HA   | 1.73                     | 0.69              |
| 1:D:331:CYS:SG   | 3:D:603:IMP:H2   | 2.32                     | 0.69              |
| 1:H:283:GLN:NE2  | 1:H:302:GLY:O    | 2.25                     | 0.68              |
| 1:A:94:ASN:HB2   | 1:A:414:MET:HE1  | 1.76                     | 0.68              |
| 1:H:396:ALA:O    | 1:H:409:LYS:NZ   | 2.20                     | 0.68              |
| 1:D:94:ASN:HB2   | 1:D:414:MET:HE1  | 1.76                     | 0.68              |
| 1:E:94:ASN:HB2   | 1:E:414:MET:HE1  | 1.76                     | 0.68              |
| 1:G:141:GLY:HA2  | 1:G:159:THR:HA   | 1.76                     | 0.68              |
| 1:F:283:GLN:NE2  | 1:F:302:GLY:O    | 2.27                     | 0.67              |
| 1:B:141:GLY:HA2  | 1:B:159:THR:HA   | 1.74                     | 0.67              |
| 1:F:121:LEU:HB2  | 1:F:144:ILE:HG22 | 1.76                     | 0.67              |
| 1:B:94:ASN:HB2   | 1:B:414:MET:HE1  | 1.75                     | 0.67              |
| 1:C:94:ASN:HB2   | 1:C:414:MET:HE1  | 1.76                     | 0.67              |
| 1:A:325:MET:HA   | 4:A:604:NAD:H72N | 1.60                     | 0.66              |
| 1:E:193:THR:HG23 | 1:E:196:GLU:H    | 1.61                     | 0.66              |
| 1:F:141:GLY:HA2  | 1:F:159:THR:HA   | 1.74                     | 0.66              |
| 1:F:94:ASN:HB2   | 1:F:414:MET:HE1  | 1.76                     | 0.66              |
| 1:H:121:LEU:HB2  | 1:H:144:ILE:HG22 | 1.76                     | 0.66              |
| 1:D:121:LEU:HB2  | 1:D:144:ILE:HG22 | 1.78                     | 0.65              |
| 1:E:121:LEU:HB2  | 1:E:144:ILE:HG22 | 1.76                     | 0.65              |
| 1:F:193:THR:HG23 | 1:F:196:GLU:H    | 1.62                     | 0.65              |
| 1:D:141:GLY:HA2  | 1:D:159:THR:HA   | 1.77                     | 0.65              |
| 1:E:283:GLN:NE2  | 1:E:302:GLY:O    | 2.30                     | 0.65              |
| 1:C:121:LEU:HB2  | 1:C:144:ILE:HG22 | 1.77                     | 0.65              |
| 1:D:283:GLN:NE2  | 1:D:302:GLY:O    | 2.30                     | 0.65              |
| 1:A:283:GLN:NE2  | 1:A:302:GLY:O    | 2.30                     | 0.64              |
| 1:B:283:GLN:NE2  | 1:B:302:GLY:O    | 2.30                     | 0.64              |
| 1:F:143:PRO:HA   | 1:F:157:ILE:HG22 | 1.79                     | 0.64              |
| 1:G:94:ASN:HB2   | 1:G:414:MET:HE1  | 1.78                     | 0.64              |
| 1:B:193:THR:HG23 | 1:B:196:GLU:H    | 1.63                     | 0.64              |
| 1:A:193:THR:HG23 | 1:A:196:GLU:H    | 1.63                     | 0.64              |
| 1:H:193:THR:HG23 | 1:H:196:GLU:H    | 1.62                     | 0.64              |
| 1:E:112:GLN:HE22 | 1:E:233:TYR:HD1  | 1.46                     | 0.63              |
| 1:D:161:ARG:NH1  | 2:E:601:ATP:O2A  | 2.29                     | 0.63              |
| 1:F:512:ARG:HB3  | 1:G:417:LEU:HD12 | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:512:ARG:HB3  | 1:H:417:LEU:HD12 | 1.81                     | 0.62              |
| 1:G:121:LEU:HB2  | 1:G:144:ILE:HG22 | 1.80                     | 0.62              |
| 1:G:146:GLU:OE2  | 1:G:147:THR:N    | 2.31                     | 0.62              |
| 1:A:512:ARG:HB3  | 1:B:417:LEU:HD12 | 1.82                     | 0.61              |
| 1:E:512:ARG:HB3  | 1:F:417:LEU:HD12 | 1.82                     | 0.61              |
| 1:A:417:LEU:HD12 | 1:D:512:ARG:HB3  | 1.83                     | 0.61              |
| 1:H:415:GLY:N    | 3:H:603:IMP:O6   | 2.24                     | 0.61              |
| 1:B:42:ILE:HB    | 1:C:280:SER:HB3  | 1.82                     | 0.61              |
| 1:E:280:SER:HB3  | 1:H:42:ILE:HB    | 1.82                     | 0.61              |
| 1:E:417:LEU:HD12 | 1:H:512:ARG:HB3  | 1.83                     | 0.61              |
| 1:A:280:SER:HB3  | 1:D:42:ILE:HB    | 1.82                     | 0.61              |
| 1:F:42:ILE:HB    | 1:G:280:SER:HB3  | 1.82                     | 0.61              |
| 1:A:121:LEU:HB2  | 1:A:144:ILE:HG22 | 1.82                     | 0.61              |
| 1:C:112:GLN:HE22 | 1:C:233:TYR:HD1  | 1.47                     | 0.60              |
| 1:C:512:ARG:HB3  | 1:D:417:LEU:HD12 | 1.83                     | 0.60              |
| 1:D:143:PRO:HA   | 1:D:157:ILE:HG22 | 1.83                     | 0.60              |
| 1:A:42:ILE:HB    | 1:B:280:SER:HB3  | 1.82                     | 0.60              |
| 1:B:143:PRO:HA   | 1:B:157:ILE:HG22 | 1.84                     | 0.60              |
| 1:G:193:THR:HG23 | 1:G:196:GLU:H    | 1.66                     | 0.60              |
| 1:H:275:SER:HB3  | 1:H:283:GLN:HE21 | 1.66                     | 0.60              |
| 1:B:512:ARG:HB3  | 1:C:417:LEU:HD12 | 1.84                     | 0.60              |
| 1:G:415:GLY:N    | 3:G:603:IMP:O6   | 2.25                     | 0.60              |
| 1:A:512:ARG:NH1  | 1:B:418:ASP:OD1  | 2.32                     | 0.60              |
| 1:C:412:ARG:NH2  | 1:C:418:ASP:O    | 2.35                     | 0.60              |
| 1:E:42:ILE:HB    | 1:F:280:SER:HB3  | 1.82                     | 0.60              |
| 1:F:506:LEU:HD23 | 1:F:509:TYR:HB3  | 1.84                     | 0.60              |
| 1:C:193:THR:HG23 | 1:C:196:GLU:H    | 1.66                     | 0.60              |
| 1:E:143:PRO:HA   | 1:E:157:ILE:HG22 | 1.84                     | 0.60              |
| 1:G:112:GLN:HE22 | 1:G:233:TYR:HD1  | 1.48                     | 0.60              |
| 1:C:143:PRO:HA   | 1:C:157:ILE:HG22 | 1.84                     | 0.60              |
| 1:D:412:ARG:NH2  | 1:D:418:ASP:O    | 2.35                     | 0.59              |
| 1:F:412:ARG:NH2  | 1:F:418:ASP:O    | 2.35                     | 0.59              |
| 1:H:412:ARG:NH2  | 1:H:418:ASP:O    | 2.35                     | 0.59              |
| 1:A:412:ARG:NH2  | 1:A:418:ASP:O    | 2.34                     | 0.59              |
| 1:B:112:GLN:HE22 | 1:B:233:TYR:HD1  | 1.49                     | 0.59              |
| 1:D:415:GLY:N    | 3:D:603:IMP:O6   | 2.26                     | 0.59              |
| 1:F:188:ALA:HB3  | 1:F:211:ILE:HG23 | 1.84                     | 0.59              |
| 1:G:42:ILE:HB    | 1:H:280:SER:HB3  | 1.83                     | 0.59              |
| 1:G:127:VAL:HG12 | 1:G:169:LYS:HA   | 1.84                     | 0.59              |
| 1:G:412:ARG:NH2  | 1:G:418:ASP:O    | 2.35                     | 0.59              |
| 1:B:412:ARG:NH2  | 1:B:418:ASP:O    | 2.36                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:42:ILE:HB    | 1:D:280:SER:HB3  | 1.82                     | 0.59              |
| 1:D:506:LEU:HD23 | 1:D:509:TYR:HB3  | 1.84                     | 0.59              |
| 1:G:512:ARG:NH1  | 1:H:418:ASP:OD1  | 2.35                     | 0.59              |
| 1:A:213:ASN:HD21 | 1:A:215:CYS:HB3  | 1.67                     | 0.59              |
| 1:E:412:ARG:NH2  | 1:E:418:ASP:O    | 2.35                     | 0.59              |
| 1:B:506:LEU:HD23 | 1:B:509:TYR:HB3  | 1.85                     | 0.59              |
| 1:D:206:LYS:HD3  | 2:D:601:ATP:C2   | 2.37                     | 0.59              |
| 1:A:112:GLN:HE22 | 1:A:233:TYR:HD1  | 1.50                     | 0.59              |
| 1:C:512:ARG:NH1  | 1:D:418:ASP:OD1  | 2.34                     | 0.59              |
| 1:C:131:LEU:HB3  | 1:C:135:MET:HE3  | 1.85                     | 0.58              |
| 1:A:395:GLU:N    | 1:A:395:GLU:OE2  | 2.37                     | 0.58              |
| 1:H:506:LEU:HD23 | 1:H:509:TYR:HB3  | 1.84                     | 0.58              |
| 1:A:206:LYS:HD3  | 2:A:601:ATP:C2   | 2.39                     | 0.58              |
| 1:E:241:GLN:O    | 1:E:243:GLN:NE2  | 2.37                     | 0.58              |
| 1:F:76:ALA:HB2   | 1:F:103:GLU:HG3  | 1.85                     | 0.58              |
| 1:A:415:GLY:N    | 3:A:603:IMP:O6   | 2.26                     | 0.58              |
| 1:E:506:LEU:HD23 | 1:E:509:TYR:HB3  | 1.84                     | 0.58              |
| 1:F:275:SER:HB3  | 1:F:283:GLN:HE21 | 1.69                     | 0.58              |
| 1:H:395:GLU:N    | 1:H:395:GLU:OE2  | 2.37                     | 0.58              |
| 1:A:76:ALA:HB2   | 1:A:103:GLU:HG3  | 1.86                     | 0.58              |
| 1:C:506:LEU:HD23 | 1:C:509:TYR:HB3  | 1.84                     | 0.58              |
| 1:E:144:ILE:HD11 | 1:E:179:MET:HB3  | 1.84                     | 0.58              |
| 1:H:76:ALA:HB2   | 1:H:103:GLU:HG3  | 1.86                     | 0.58              |
| 1:D:275:SER:HB3  | 1:D:283:GLN:HE21 | 1.69                     | 0.57              |
| 2:D:601:ATP:PA   | 1:E:161:ARG:HH12 | 2.27                     | 0.57              |
| 1:E:206:LYS:HD3  | 2:E:601:ATP:C2   | 2.39                     | 0.57              |
| 1:E:395:GLU:OE2  | 1:E:395:GLU:N    | 2.37                     | 0.57              |
| 1:E:76:ALA:HB2   | 1:E:103:GLU:HG3  | 1.87                     | 0.57              |
| 1:H:241:GLN:O    | 1:H:243:GLN:NE2  | 2.37                     | 0.57              |
| 1:A:275:SER:HB3  | 1:A:283:GLN:HE21 | 1.70                     | 0.57              |
| 1:E:415:GLY:N    | 3:E:603:IMP:O6   | 2.26                     | 0.57              |
| 1:A:506:LEU:HD23 | 1:A:509:TYR:HB3  | 1.85                     | 0.57              |
| 1:D:76:ALA:HB2   | 1:D:103:GLU:HG3  | 1.86                     | 0.57              |
| 1:E:275:SER:HB3  | 1:E:283:GLN:HE21 | 1.70                     | 0.57              |
| 1:C:241:GLN:O    | 1:C:243:GLN:NE2  | 2.37                     | 0.57              |
| 1:E:188:ALA:HB3  | 1:E:211:ILE:HG23 | 1.86                     | 0.57              |
| 1:G:506:LEU:HD23 | 1:G:509:TYR:HB3  | 1.84                     | 0.57              |
| 1:B:76:ALA:HB2   | 1:B:103:GLU:HG3  | 1.86                     | 0.57              |
| 1:F:395:GLU:N    | 1:F:395:GLU:OE2  | 2.38                     | 0.57              |
| 1:C:76:ALA:HB2   | 1:C:103:GLU:HG3  | 1.86                     | 0.57              |
| 1:C:275:SER:HB3  | 1:C:283:GLN:HE21 | 1.68                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:415:GLY:N    | 3:C:603:IMP:O6   | 2.28                     | 0.56              |
| 1:E:512:ARG:NH1  | 1:F:418:ASP:OD1  | 2.37                     | 0.56              |
| 1:F:241:GLN:O    | 1:F:243:GLN:NE2  | 2.38                     | 0.56              |
| 1:A:241:GLN:O    | 1:A:243:GLN:NE2  | 2.38                     | 0.56              |
| 1:C:395:GLU:N    | 1:C:395:GLU:OE2  | 2.38                     | 0.56              |
| 1:D:241:GLN:O    | 1:D:243:GLN:NE2  | 2.38                     | 0.56              |
| 1:G:76:ALA:HB2   | 1:G:103:GLU:HG3  | 1.86                     | 0.56              |
| 2:C:601:ATP:O2A  | 1:F:161:ARG:NH1  | 2.36                     | 0.56              |
| 1:D:193:THR:HG23 | 1:D:196:GLU:H    | 1.69                     | 0.56              |
| 1:H:201:LEU:HD12 | 1:H:224:ARG:HG3  | 1.88                     | 0.56              |
| 1:B:395:GLU:OE2  | 1:B:395:GLU:N    | 2.39                     | 0.56              |
| 1:B:512:ARG:NH1  | 1:C:418:ASP:OD1  | 2.34                     | 0.56              |
| 1:D:395:GLU:N    | 1:D:395:GLU:OE2  | 2.39                     | 0.56              |
| 1:E:277:GLN:NE2  | 1:E:279:ASN:H    | 2.04                     | 0.56              |
| 1:B:241:GLN:O    | 1:B:243:GLN:NE2  | 2.39                     | 0.56              |
| 1:B:275:SER:HB3  | 1:B:283:GLN:HE21 | 1.70                     | 0.56              |
| 1:F:277:GLN:NE2  | 1:F:279:ASN:H    | 2.04                     | 0.56              |
| 1:G:241:GLN:O    | 1:G:243:GLN:NE2  | 2.39                     | 0.56              |
| 1:A:201:LEU:HD12 | 1:A:224:ARG:HG3  | 1.87                     | 0.56              |
| 1:A:161:ARG:NH1  | 2:H:601:ATP:O2A  | 2.37                     | 0.56              |
| 1:B:206:LYS:HD3  | 2:B:601:ATP:C2   | 2.41                     | 0.56              |
| 1:H:55:LEU:HG    | 1:H:56:THR:HG23  | 1.88                     | 0.55              |
| 1:D:112:GLN:HE22 | 1:D:233:TYR:HD1  | 1.52                     | 0.55              |
| 1:G:395:GLU:OE2  | 1:G:395:GLU:N    | 2.39                     | 0.55              |
| 1:B:277:GLN:NE2  | 1:B:279:ASN:H    | 2.05                     | 0.55              |
| 1:D:329:SER:OG   | 3:D:603:IMP:O1P  | 2.24                     | 0.55              |
| 1:E:329:SER:OG   | 3:E:603:IMP:O3P  | 2.24                     | 0.55              |
| 1:G:206:LYS:HD3  | 2:G:601:ATP:C2   | 2.42                     | 0.55              |
| 1:A:143:PRO:HA   | 1:A:157:ILE:HG22 | 1.89                     | 0.55              |
| 1:A:277:GLN:NE2  | 1:A:279:ASN:H    | 2.05                     | 0.55              |
| 1:C:146:GLU:OE2  | 1:C:147:THR:N    | 2.31                     | 0.55              |
| 1:H:206:LYS:HD3  | 2:H:601:ATP:C2   | 2.41                     | 0.55              |
| 2:A:601:ATP:O2A  | 1:H:161:ARG:NH1  | 2.37                     | 0.55              |
| 1:C:326:GLY:HA2  | 1:C:331:CYS:SG   | 2.46                     | 0.55              |
| 1:C:277:GLN:NE2  | 1:C:279:ASN:H    | 2.05                     | 0.55              |
| 1:D:201:LEU:HD12 | 1:D:224:ARG:HG3  | 1.89                     | 0.55              |
| 1:D:277:GLN:NE2  | 1:D:279:ASN:H    | 2.04                     | 0.55              |
| 1:C:249:ALA:HB1  | 1:C:274:ASP:HB2  | 1.89                     | 0.54              |
| 1:F:326:GLY:HA2  | 1:F:331:CYS:SG   | 2.47                     | 0.54              |
| 1:A:329:SER:OG   | 3:A:603:IMP:O1P  | 2.24                     | 0.54              |
| 1:B:329:SER:OG   | 3:B:603:IMP:O1P  | 2.25                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:512:ARG:NH1  | 1:G:418:ASP:OD1  | 2.36                     | 0.54              |
| 1:G:277:GLN:NE2  | 1:G:279:ASN:H    | 2.05                     | 0.54              |
| 1:H:143:PRO:HA   | 1:H:157:ILE:HG22 | 1.90                     | 0.54              |
| 1:H:277:GLN:NE2  | 1:H:279:ASN:H    | 2.04                     | 0.54              |
| 1:H:326:GLY:HA2  | 1:H:331:CYS:SG   | 2.47                     | 0.54              |
| 1:F:112:GLN:HE22 | 1:F:233:TYR:HD1  | 1.54                     | 0.54              |
| 1:F:146:GLU:OE2  | 1:F:147:THR:N    | 2.37                     | 0.54              |
| 1:G:143:PRO:HA   | 1:G:157:ILE:HG22 | 1.88                     | 0.54              |
| 1:D:326:GLY:HA2  | 1:D:331:CYS:SG   | 2.48                     | 0.54              |
| 1:D:55:LEU:HG    | 1:D:56:THR:HG23  | 1.90                     | 0.54              |
| 1:E:326:GLY:HA2  | 1:E:331:CYS:SG   | 2.47                     | 0.54              |
| 1:F:329:SER:OG   | 3:F:603:IMP:O3P  | 2.26                     | 0.54              |
| 1:F:415:GLY:N    | 3:F:603:IMP:O6   | 2.26                     | 0.54              |
| 1:G:326:GLY:HA2  | 1:G:331:CYS:SG   | 2.47                     | 0.54              |
| 1:B:326:GLY:HA2  | 1:B:331:CYS:SG   | 2.48                     | 0.53              |
| 1:A:93:HIS:HB3   | 1:A:249:ALA:O    | 2.09                     | 0.53              |
| 1:B:55:LEU:HG    | 1:B:56:THR:HG23  | 1.89                     | 0.53              |
| 1:F:201:LEU:HD12 | 1:F:224:ARG:HG3  | 1.90                     | 0.53              |
| 1:H:93:HIS:HB3   | 1:H:249:ALA:O    | 2.08                     | 0.53              |
| 1:A:55:LEU:HG    | 1:A:56:THR:HG23  | 1.89                     | 0.53              |
| 1:A:274:ASP:OD1  | 4:A:604:NAD:O2D  | 2.26                     | 0.53              |
| 1:A:326:GLY:HA2  | 1:A:331:CYS:SG   | 2.48                     | 0.53              |
| 1:D:181:PRO:HD2  | 1:D:183:ILE:HD11 | 1.91                     | 0.53              |
| 1:B:93:HIS:HB3   | 1:B:249:ALA:O    | 2.09                     | 0.53              |
| 1:B:415:GLY:N    | 3:B:603:IMP:O6   | 2.26                     | 0.53              |
| 1:H:413:GLY:O    | 1:H:416:SER:OG   | 2.24                     | 0.53              |
| 1:G:283:GLN:NE2  | 1:G:302:GLY:O    | 2.41                     | 0.53              |
| 1:D:146:GLU:OE2  | 1:D:147:THR:N    | 2.35                     | 0.53              |
| 1:C:55:LEU:HG    | 1:C:56:THR:HG23  | 1.90                     | 0.52              |
| 1:G:329:SER:OG   | 3:G:603:IMP:O3P  | 2.26                     | 0.52              |
| 1:C:206:LYS:HD3  | 2:C:601:ATP:C2   | 2.43                     | 0.52              |
| 1:E:93:HIS:HB3   | 1:E:249:ALA:O    | 2.10                     | 0.52              |
| 1:G:55:LEU:HG    | 1:G:56:THR:HG23  | 1.89                     | 0.52              |
| 1:F:93:HIS:HB3   | 1:F:249:ALA:O    | 2.10                     | 0.52              |
| 1:F:213:ASN:OD1  | 1:F:217:GLU:N    | 2.40                     | 0.52              |
| 1:G:93:HIS:HB3   | 1:G:249:ALA:O    | 2.09                     | 0.52              |
| 1:C:201:LEU:HD12 | 1:C:224:ARG:HG3  | 1.92                     | 0.52              |
| 1:D:93:HIS:HB3   | 1:D:249:ALA:O    | 2.10                     | 0.52              |
| 1:H:355:ARG:HH11 | 1:H:355:ARG:HG2  | 1.75                     | 0.52              |
| 1:B:393:THR:HG22 | 1:B:450:LYS:HB2  | 1.92                     | 0.52              |
| 1:A:249:ALA:HB1  | 1:A:274:ASP:HB2  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:80:ILE:HG13  | 1:C:107:VAL:HG22 | 1.92                     | 0.51              |
| 1:H:329:SER:OG   | 3:H:603:IMP:O2P  | 2.26                     | 0.51              |
| 1:A:49:VAL:HB    | 1:A:465:GLN:HG2  | 1.91                     | 0.51              |
| 1:B:80:ILE:HG13  | 1:B:107:VAL:HG22 | 1.91                     | 0.51              |
| 1:E:55:LEU:HG    | 1:E:56:THR:HG23  | 1.90                     | 0.51              |
| 1:H:112:GLN:HE22 | 1:H:233:TYR:HD1  | 1.57                     | 0.51              |
| 1:E:213:ASN:HD21 | 1:E:215:CYS:HB3  | 1.75                     | 0.51              |
| 1:E:393:THR:HG22 | 1:E:450:LYS:HB2  | 1.92                     | 0.51              |
| 1:F:55:LEU:HG    | 1:F:56:THR:HG23  | 1.91                     | 0.51              |
| 1:H:49:VAL:HB    | 1:H:465:GLN:HG2  | 1.92                     | 0.51              |
| 1:D:249:ALA:HB1  | 1:D:274:ASP:HB2  | 1.92                     | 0.51              |
| 1:G:80:ILE:HG13  | 1:G:107:VAL:HG22 | 1.92                     | 0.51              |
| 1:F:80:ILE:HG13  | 1:F:107:VAL:HG22 | 1.91                     | 0.51              |
| 1:F:206:LYS:HD3  | 2:F:601:ATP:C2   | 2.46                     | 0.51              |
| 1:D:274:ASP:OD2  | 4:D:604:NAD:O2D  | 2.28                     | 0.51              |
| 2:D:601:ATP:O2A  | 1:E:161:ARG:NH1  | 2.41                     | 0.51              |
| 1:G:46:ALA:O     | 1:G:465:GLN:HB3  | 2.10                     | 0.51              |
| 1:H:449:ASP:OD1  | 1:H:451:GLY:N    | 2.43                     | 0.51              |
| 1:D:157:ILE:HD11 | 2:D:601:ATP:C5   | 2.45                     | 0.51              |
| 1:G:449:ASP:OD1  | 1:G:451:GLY:N    | 2.42                     | 0.51              |
| 1:B:355:ARG:HG2  | 1:B:355:ARG:HH11 | 1.76                     | 0.50              |
| 1:E:201:LEU:HD12 | 1:E:224:ARG:HG3  | 1.92                     | 0.50              |
| 1:F:393:THR:HG22 | 1:F:450:LYS:HB2  | 1.93                     | 0.50              |
| 1:G:49:VAL:HB    | 1:G:465:GLN:HG2  | 1.94                     | 0.50              |
| 1:C:355:ARG:HH11 | 1:C:355:ARG:HG2  | 1.76                     | 0.50              |
| 1:E:80:ILE:HG13  | 1:E:107:VAL:HG22 | 1.92                     | 0.50              |
| 1:H:249:ALA:HB1  | 1:H:274:ASP:HB2  | 1.92                     | 0.50              |
| 1:A:127:VAL:HG12 | 1:A:169:LYS:HA   | 1.94                     | 0.50              |
| 1:A:418:ASP:OD1  | 1:D:512:ARG:NH1  | 2.37                     | 0.50              |
| 1:B:162:ASP:OD1  | 2:B:601:ATP:O3'  | 2.30                     | 0.50              |
| 1:F:157:ILE:HD11 | 2:F:601:ATP:C5   | 2.46                     | 0.50              |
| 1:B:161:ARG:NH1  | 2:G:601:ATP:O2A  | 2.40                     | 0.50              |
| 1:D:49:VAL:HB    | 1:D:465:GLN:HG2  | 1.93                     | 0.50              |
| 1:H:80:ILE:HG13  | 1:H:107:VAL:HG22 | 1.92                     | 0.50              |
| 1:E:274:ASP:OD1  | 4:E:604:NAD:O2D  | 2.29                     | 0.50              |
| 1:H:46:ALA:O     | 1:H:465:GLN:HB3  | 2.12                     | 0.50              |
| 1:C:162:ASP:OD1  | 2:C:601:ATP:O3'  | 2.25                     | 0.50              |
| 1:D:393:THR:HG22 | 1:D:450:LYS:HB2  | 1.93                     | 0.50              |
| 1:G:126:THR:HG23 | 1:G:128:GLY:H    | 1.76                     | 0.50              |
| 1:G:274:ASP:OD2  | 4:G:604:NAD:O3D  | 2.27                     | 0.50              |
| 1:B:165:PHE:HB2  | 1:G:202:GLN:HE21 | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:241:GLN:HB3  | 1:F:243:GLN:HE22 | 1.75                     | 0.50              |
| 1:C:393:THR:HG22 | 1:C:450:LYS:HB2  | 1.93                     | 0.49              |
| 1:G:275:SER:HB3  | 1:G:283:GLN:HE21 | 1.77                     | 0.49              |
| 1:A:241:GLN:HB3  | 1:A:243:GLN:HE22 | 1.77                     | 0.49              |
| 1:C:161:ARG:NH1  | 2:F:601:ATP:O2A  | 2.43                     | 0.49              |
| 1:H:115:ILE:HG12 | 1:H:221:ILE:O    | 2.11                     | 0.49              |
| 1:A:80:ILE:HG13  | 1:A:107:VAL:HG22 | 1.92                     | 0.49              |
| 1:F:355:ARG:HG2  | 1:F:355:ARG:HH11 | 1.78                     | 0.49              |
| 1:A:393:THR:HG22 | 1:A:450:LYS:HB2  | 1.94                     | 0.49              |
| 1:D:71:ASP:OD2   | 1:D:412:ARG:NH1  | 2.29                     | 0.49              |
| 1:E:156:GLY:HA2  | 1:E:184:GLU:OE2  | 2.12                     | 0.49              |
| 1:G:241:GLN:HB3  | 1:G:243:GLN:HE22 | 1.78                     | 0.49              |
| 1:H:144:ILE:HD11 | 1:H:179:MET:HB3  | 1.94                     | 0.49              |
| 1:C:46:ALA:O     | 1:C:465:GLN:HB3  | 2.12                     | 0.49              |
| 1:E:241:GLN:HB3  | 1:E:243:GLN:HE22 | 1.77                     | 0.49              |
| 4:F:604:NAD:H51N | 4:F:604:NAD:O1A  | 2.13                     | 0.49              |
| 1:D:80:ILE:HG13  | 1:D:107:VAL:HG22 | 1.93                     | 0.49              |
| 1:F:46:ALA:O     | 1:F:465:GLN:HB3  | 2.12                     | 0.49              |
| 1:C:93:HIS:HB3   | 1:C:249:ALA:O    | 2.12                     | 0.49              |
| 1:E:49:VAL:HB    | 1:E:465:GLN:HG2  | 1.94                     | 0.49              |
| 1:B:200:ILE:O    | 1:B:204:SER:HB3  | 2.12                     | 0.49              |
| 1:C:225:THR:OG1  | 2:C:602:ATP:O2A  | 2.30                     | 0.49              |
| 1:E:46:ALA:O     | 1:E:465:GLN:HB3  | 2.13                     | 0.49              |
| 1:G:393:THR:HG22 | 1:G:450:LYS:HB2  | 1.94                     | 0.49              |
| 1:D:46:ALA:O     | 1:D:465:GLN:HB3  | 2.13                     | 0.49              |
| 1:E:157:ILE:HD11 | 2:E:601:ATP:C5   | 2.47                     | 0.49              |
| 1:E:257:LYS:HD3  | 1:E:289:TYR:CZ   | 2.48                     | 0.49              |
| 1:A:355:ARG:HG2  | 1:A:355:ARG:HH11 | 1.78                     | 0.48              |
| 1:C:49:VAL:HB    | 1:C:465:GLN:HG2  | 1.95                     | 0.48              |
| 1:F:115:ILE:HG12 | 1:F:221:ILE:O    | 2.12                     | 0.48              |
| 1:H:200:ILE:O    | 1:H:204:SER:HB3  | 2.13                     | 0.48              |
| 1:A:83:ALA:O     | 1:A:237:SER:HB3  | 2.13                     | 0.48              |
| 1:B:249:ALA:HB1  | 1:B:274:ASP:HB2  | 1.94                     | 0.48              |
| 1:D:241:GLN:HB3  | 1:D:243:GLN:HE22 | 1.77                     | 0.48              |
| 1:F:71:ASP:OD2   | 1:F:412:ARG:NH1  | 2.29                     | 0.48              |
| 1:G:249:ALA:HB1  | 1:G:274:ASP:HB2  | 1.95                     | 0.48              |
| 1:H:71:ASP:OD2   | 1:H:412:ARG:NH1  | 2.30                     | 0.48              |
| 1:A:202:GLN:HE21 | 1:H:165:PHE:HB2  | 1.78                     | 0.48              |
| 1:B:49:VAL:HB    | 1:B:465:GLN:HG2  | 1.95                     | 0.48              |
| 1:E:392:ALA:HA   | 1:E:409:LYS:HD2  | 1.96                     | 0.48              |
| 1:F:49:VAL:HB    | 1:F:465:GLN:HG2  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:203:ARG:HG2  | 1:F:203:ARG:HH21 | 1.79                     | 0.48              |
| 1:G:156:GLY:HA2  | 1:G:184:GLU:OE2  | 2.13                     | 0.48              |
| 1:A:46:ALA:O     | 1:A:465:GLN:HB3  | 2.14                     | 0.48              |
| 1:H:393:THR:HG22 | 1:H:450:LYS:HB2  | 1.95                     | 0.48              |
| 1:C:241:GLN:HB3  | 1:C:243:GLN:HE22 | 1.78                     | 0.48              |
| 1:E:249:ALA:HB1  | 1:E:274:ASP:HB2  | 1.94                     | 0.48              |
| 1:E:355:ARG:HG2  | 1:E:355:ARG:HH11 | 1.79                     | 0.48              |
| 1:F:257:LYS:HD3  | 1:F:289:TYR:CZ   | 2.49                     | 0.48              |
| 4:F:604:NAD:O2A  | 4:F:604:NAD:H8A  | 2.14                     | 0.48              |
| 1:G:157:ILE:HD11 | 2:G:601:ATP:C5   | 2.49                     | 0.48              |
| 1:H:156:GLY:HA3  | 1:H:180:THR:O    | 2.14                     | 0.48              |
| 1:B:46:ALA:O     | 1:B:465:GLN:HB3  | 2.14                     | 0.48              |
| 1:C:449:ASP:OD1  | 1:C:450:LYS:N    | 2.47                     | 0.48              |
| 1:E:140:SER:O    | 1:E:140:SER:OG   | 2.32                     | 0.48              |
| 1:F:249:ALA:HB1  | 1:F:274:ASP:HB2  | 1.95                     | 0.48              |
| 1:G:83:ALA:O     | 1:G:237:SER:HB3  | 2.13                     | 0.48              |
| 1:G:355:ARG:HG2  | 1:G:355:ARG:HH11 | 1.79                     | 0.48              |
| 1:B:83:ALA:O     | 1:B:237:SER:HB3  | 2.13                     | 0.48              |
| 1:B:157:ILE:HD13 | 1:B:184:GLU:OE1  | 2.14                     | 0.48              |
| 1:B:156:GLY:HA2  | 1:B:184:GLU:CD   | 2.39                     | 0.48              |
| 1:D:83:ALA:O     | 1:D:237:SER:HB3  | 2.13                     | 0.48              |
| 1:E:107:VAL:HG11 | 1:E:246:CYS:HB2  | 1.96                     | 0.48              |
| 1:H:83:ALA:O     | 1:H:237:SER:HB3  | 2.13                     | 0.48              |
| 1:C:392:ALA:HA   | 1:C:409:LYS:HD2  | 1.96                     | 0.48              |
| 1:E:83:ALA:O     | 1:E:237:SER:HB3  | 2.14                     | 0.48              |
| 1:F:134:LYS:NZ   | 1:F:138:GLY:O    | 2.41                     | 0.48              |
| 1:F:392:ALA:HA   | 1:F:409:LYS:HD2  | 1.96                     | 0.48              |
| 1:A:107:VAL:HG11 | 1:A:246:CYS:HB2  | 1.96                     | 0.47              |
| 1:B:127:VAL:HG12 | 1:B:169:LYS:HA   | 1.95                     | 0.47              |
| 1:H:241:GLN:HB3  | 1:H:243:GLN:HE22 | 1.79                     | 0.47              |
| 1:A:156:GLY:HA2  | 1:A:184:GLU:OE2  | 2.13                     | 0.47              |
| 1:C:83:ALA:O     | 1:C:237:SER:HB3  | 2.14                     | 0.47              |
| 1:F:449:ASP:OD1  | 1:F:450:LYS:N    | 2.48                     | 0.47              |
| 1:A:392:ALA:HA   | 1:A:409:LYS:HD2  | 1.96                     | 0.47              |
| 1:C:264:THR:HG21 | 1:C:294:TYR:CE1  | 2.50                     | 0.47              |
| 1:F:364:ASP:OD2  | 3:F:603:IMP:O3'  | 2.23                     | 0.47              |
| 1:H:386:MET:HE3  | 1:H:386:MET:HB2  | 1.80                     | 0.47              |
| 1:B:392:ALA:HA   | 1:B:409:LYS:HD2  | 1.96                     | 0.47              |
| 1:C:122:SER:HB2  | 1:C:125:HIS:CE1  | 2.49                     | 0.47              |
| 1:E:156:GLY:HA3  | 1:E:180:THR:O    | 2.13                     | 0.47              |
| 1:F:264:THR:HG21 | 1:F:294:TYR:CE1  | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:75:GLU:HB2   | 1:G:397:PRO:HG3  | 1.96                     | 0.47              |
| 1:H:107:VAL:HG11 | 1:H:246:CYS:HB2  | 1.96                     | 0.47              |
| 1:F:277:GLN:HE21 | 1:F:279:ASN:H    | 1.62                     | 0.47              |
| 1:G:188:ALA:HB3  | 1:G:211:ILE:HG23 | 1.95                     | 0.47              |
| 1:H:146:GLU:OE2  | 1:H:147:THR:N    | 2.33                     | 0.47              |
| 1:A:140:SER:O    | 1:A:140:SER:OG   | 2.33                     | 0.47              |
| 1:A:146:GLU:OE2  | 1:A:147:THR:N    | 2.33                     | 0.47              |
| 1:C:329:SER:N    | 3:C:603:IMP:O2P  | 2.40                     | 0.47              |
| 1:G:264:THR:HG21 | 1:G:294:TYR:CE1  | 2.50                     | 0.47              |
| 1:G:413:GLY:O    | 1:G:416:SER:OG   | 2.29                     | 0.47              |
| 1:D:107:VAL:HG11 | 1:D:246:CYS:HB2  | 1.97                     | 0.47              |
| 1:D:386:MET:HB2  | 1:D:386:MET:HE3  | 1.80                     | 0.47              |
| 1:F:107:VAL:HG11 | 1:F:246:CYS:HB2  | 1.95                     | 0.47              |
| 1:D:355:ARG:HG2  | 1:D:355:ARG:HH11 | 1.80                     | 0.47              |
| 1:A:207:GLY:HA2  | 1:A:224:ARG:HB2  | 1.97                     | 0.47              |
| 1:E:119:VAL:O    | 1:E:142:ILE:HG23 | 2.15                     | 0.47              |
| 1:H:203:ARG:HG2  | 1:H:203:ARG:HH21 | 1.79                     | 0.47              |
| 1:C:107:VAL:HG11 | 1:C:246:CYS:HB2  | 1.97                     | 0.46              |
| 1:C:157:ILE:HD11 | 2:C:601:ATP:C5   | 2.50                     | 0.46              |
| 1:D:392:ALA:HA   | 1:D:409:LYS:HD2  | 1.96                     | 0.46              |
| 1:A:400:TYR:CD1  | 1:A:409:LYS:HG3  | 2.51                     | 0.46              |
| 1:C:119:VAL:O    | 1:C:142:ILE:HG23 | 2.16                     | 0.46              |
| 1:D:203:ARG:HH21 | 1:D:203:ARG:HG2  | 1.80                     | 0.46              |
| 1:H:400:TYR:CD1  | 1:H:409:LYS:HG3  | 2.50                     | 0.46              |
| 1:C:115:ILE:HG12 | 1:C:221:ILE:O    | 2.15                     | 0.46              |
| 1:E:413:GLY:O    | 1:E:416:SER:OG   | 2.26                     | 0.46              |
| 1:H:75:GLU:HB2   | 1:H:397:PRO:HG3  | 1.97                     | 0.46              |
| 1:B:119:VAL:O    | 1:B:142:ILE:HG23 | 2.15                     | 0.46              |
| 1:B:241:GLN:HB3  | 1:B:243:GLN:HE22 | 1.79                     | 0.46              |
| 1:F:140:SER:O    | 1:F:140:SER:OG   | 2.32                     | 0.46              |
| 1:G:386:MET:HE3  | 1:G:386:MET:HB2  | 1.80                     | 0.46              |
| 1:H:122:SER:HB2  | 1:H:125:HIS:CE1  | 2.51                     | 0.46              |
| 1:B:264:THR:HG21 | 1:B:294:TYR:CE1  | 2.51                     | 0.46              |
| 1:F:83:ALA:O     | 1:F:237:SER:HB3  | 2.15                     | 0.46              |
| 1:G:140:SER:O    | 1:G:140:SER:OG   | 2.31                     | 0.46              |
| 1:H:392:ALA:HA   | 1:H:409:LYS:HD2  | 1.97                     | 0.46              |
| 1:A:115:ILE:HG12 | 1:A:221:ILE:O    | 2.15                     | 0.46              |
| 1:A:274:ASP:CG   | 4:A:604:NAD:HO3N | 2.24                     | 0.46              |
| 1:B:107:VAL:HG11 | 1:B:246:CYS:HB2  | 1.96                     | 0.46              |
| 1:D:264:THR:HG21 | 1:D:294:TYR:CE1  | 2.50                     | 0.46              |
| 1:E:418:ASP:OD1  | 1:H:512:ARG:NH1  | 2.42                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:392:ALA:HA   | 1:G:409:LYS:HD2  | 1.98                     | 0.46              |
| 1:A:277:GLN:HE21 | 1:A:279:ASN:H    | 1.63                     | 0.46              |
| 1:B:165:PHE:HB2  | 1:G:202:GLN:NE2  | 2.31                     | 0.46              |
| 1:G:107:VAL:HG11 | 1:G:246:CYS:HB2  | 1.97                     | 0.46              |
| 1:H:264:THR:HG21 | 1:H:294:TYR:CE1  | 2.51                     | 0.46              |
| 1:B:257:LYS:HD3  | 1:B:289:TYR:CZ   | 2.51                     | 0.46              |
| 1:B:277:GLN:HE21 | 1:B:279:ASN:H    | 1.64                     | 0.46              |
| 1:B:325:MET:HA   | 4:B:604:NAD:O7N  | 2.16                     | 0.46              |
| 1:C:75:GLU:HB2   | 1:C:397:PRO:HG3  | 1.98                     | 0.46              |
| 1:C:165:PHE:HB2  | 1:F:202:GLN:OE1  | 2.16                     | 0.46              |
| 2:D:602:ATP:H5'1 | 2:D:602:ATP:C8   | 2.50                     | 0.46              |
| 1:E:400:TYR:CD1  | 1:E:409:LYS:HG3  | 2.51                     | 0.46              |
| 1:F:184:GLU:HB3  | 2:F:601:ATP:N1   | 2.30                     | 0.46              |
| 1:G:71:ASP:OD2   | 1:G:412:ARG:NH1  | 2.30                     | 0.46              |
| 1:B:140:SER:O    | 1:B:140:SER:OG   | 2.32                     | 0.45              |
| 1:C:144:ILE:HD11 | 1:C:179:MET:HB3  | 1.98                     | 0.45              |
| 1:C:209:LEU:HD23 | 1:C:222:ILE:HD12 | 1.98                     | 0.45              |
| 1:D:277:GLN:HE21 | 1:D:279:ASN:H    | 1.63                     | 0.45              |
| 1:H:194:LEU:HD23 | 1:H:194:LEU:HA   | 1.83                     | 0.45              |
| 1:H:277:GLN:HE21 | 1:H:279:ASN:H    | 1.63                     | 0.45              |
| 1:B:207:GLY:HA2  | 1:B:224:ARG:HB2  | 1.98                     | 0.45              |
| 1:B:400:TYR:CD1  | 1:B:409:LYS:HG3  | 2.51                     | 0.45              |
| 1:B:401:PHE:CE2  | 1:B:408:LEU:HB2  | 2.51                     | 0.45              |
| 1:D:400:TYR:CD1  | 1:D:409:LYS:HG3  | 2.51                     | 0.45              |
| 1:E:184:GLU:C    | 1:E:186:VAL:H    | 2.23                     | 0.45              |
| 1:E:203:ARG:HG2  | 1:E:203:ARG:HH21 | 1.80                     | 0.45              |
| 1:G:257:LYS:HD3  | 1:G:289:TYR:CZ   | 2.50                     | 0.45              |
| 1:A:157:ILE:HD11 | 2:A:601:ATP:C5   | 2.51                     | 0.45              |
| 1:A:264:THR:HG21 | 1:A:294:TYR:CE1  | 2.51                     | 0.45              |
| 1:C:257:LYS:HD3  | 1:C:289:TYR:CZ   | 2.51                     | 0.45              |
| 1:E:277:GLN:HE21 | 1:E:279:ASN:H    | 1.63                     | 0.45              |
| 1:D:75:GLU:HB2   | 1:D:397:PRO:HG3  | 1.98                     | 0.45              |
| 1:D:119:VAL:O    | 1:D:142:ILE:HG23 | 2.16                     | 0.45              |
| 1:E:194:LEU:HD23 | 1:E:194:LEU:HA   | 1.85                     | 0.45              |
| 1:F:408:LEU:HD23 | 1:F:448:GLN:HA   | 1.99                     | 0.45              |
| 1:G:119:VAL:O    | 1:G:142:ILE:HG23 | 2.16                     | 0.45              |
| 1:A:257:LYS:HD3  | 1:A:289:TYR:CZ   | 2.52                     | 0.45              |
| 1:E:65:LEU:HD12  | 1:E:457:VAL:HG13 | 1.99                     | 0.45              |
| 1:E:401:PHE:CE2  | 1:E:408:LEU:HB2  | 2.51                     | 0.45              |
| 1:F:226:ASP:OD1  | 2:F:602:ATP:O3'  | 2.19                     | 0.45              |
| 1:E:264:THR:HG21 | 1:E:294:TYR:CE1  | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:65:LEU:HD12  | 1:F:457:VAL:HG13 | 1.99                     | 0.45              |
| 1:G:194:LEU:HD23 | 1:G:194:LEU:HA   | 1.83                     | 0.45              |
| 1:G:207:GLY:HA2  | 1:G:224:ARG:HB2  | 1.99                     | 0.45              |
| 1:B:157:ILE:HD11 | 2:B:601:ATP:C4   | 2.52                     | 0.45              |
| 1:D:207:GLY:HA2  | 1:D:224:ARG:HB2  | 1.99                     | 0.45              |
| 1:D:413:GLY:O    | 1:D:416:SER:OG   | 2.25                     | 0.45              |
| 1:G:277:GLN:HE21 | 1:G:279:ASN:H    | 1.63                     | 0.45              |
| 1:E:207:GLY:HA2  | 1:E:224:ARG:HB2  | 1.99                     | 0.45              |
| 1:G:65:LEU:HD12  | 1:G:457:VAL:HG13 | 1.98                     | 0.45              |
| 1:A:71:ASP:OD2   | 1:A:412:ARG:NH1  | 2.30                     | 0.45              |
| 1:C:386:MET:HE3  | 1:C:386:MET:HB2  | 1.81                     | 0.45              |
| 1:D:495:MET:SD   | 1:D:498:GLN:NE2  | 2.90                     | 0.45              |
| 1:H:127:VAL:HG12 | 1:H:169:LYS:HA   | 1.98                     | 0.45              |
| 1:B:75:GLU:HB2   | 1:B:397:PRO:HG3  | 1.98                     | 0.45              |
| 1:B:146:GLU:OE2  | 1:B:147:THR:N    | 2.43                     | 0.45              |
| 1:B:364:ASP:OD2  | 3:B:603:IMP:O3'  | 2.24                     | 0.45              |
| 1:C:401:PHE:CE2  | 1:C:408:LEU:HB2  | 2.52                     | 0.45              |
| 1:D:65:LEU:HD12  | 1:D:457:VAL:HG13 | 1.99                     | 0.45              |
| 1:D:140:SER:O    | 1:D:140:SER:OG   | 2.31                     | 0.45              |
| 1:D:257:LYS:HD3  | 1:D:289:TYR:CZ   | 2.51                     | 0.45              |
| 1:H:157:ILE:HD13 | 1:H:184:GLU:OE1  | 2.17                     | 0.45              |
| 1:H:257:LYS:HD3  | 1:H:289:TYR:CZ   | 2.52                     | 0.45              |
| 1:E:146:GLU:OE2  | 1:E:147:THR:N    | 2.35                     | 0.44              |
| 1:C:459:TYR:CD1  | 1:C:514:TYR:HB3  | 2.52                     | 0.44              |
| 1:A:119:VAL:O    | 1:A:142:ILE:HG23 | 2.17                     | 0.44              |
| 1:C:140:SER:O    | 1:C:140:SER:OG   | 2.32                     | 0.44              |
| 1:E:438:LYS:HA   | 1:E:438:LYS:HD2  | 1.79                     | 0.44              |
| 1:H:119:VAL:O    | 1:H:142:ILE:HG23 | 2.17                     | 0.44              |
| 1:C:277:GLN:HE21 | 1:C:279:ASN:H    | 1.64                     | 0.44              |
| 1:E:160:SER:HB3  | 2:E:601:ATP:O1B  | 2.17                     | 0.44              |
| 1:G:438:LYS:HA   | 1:G:438:LYS:HD2  | 1.73                     | 0.44              |
| 1:B:495:MET:SD   | 1:B:498:GLN:NE2  | 2.90                     | 0.44              |
| 1:D:127:VAL:HG12 | 1:D:169:LYS:HA   | 1.99                     | 0.44              |
| 1:F:75:GLU:HB2   | 1:F:397:PRO:HG3  | 1.99                     | 0.44              |
| 1:A:65:LEU:HD12  | 1:A:457:VAL:HG13 | 2.00                     | 0.44              |
| 1:A:127:VAL:N    | 1:A:170:ASP:OD1  | 2.47                     | 0.44              |
| 1:A:401:PHE:CE2  | 1:A:408:LEU:HB2  | 2.52                     | 0.44              |
| 1:B:65:LEU:HD12  | 1:B:457:VAL:HG13 | 2.00                     | 0.44              |
| 1:E:106:LYS:HB2  | 1:E:106:LYS:HE3  | 1.70                     | 0.44              |
| 1:E:495:MET:SD   | 1:E:498:GLN:NE2  | 2.91                     | 0.44              |
| 1:G:127:VAL:N    | 1:G:170:ASP:OD1  | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:400:TYR:CD1  | 1:G:409:LYS:HG3  | 2.53                     | 0.44              |
| 1:A:184:GLU:C    | 1:A:186:VAL:H    | 2.26                     | 0.44              |
| 1:A:297:LEU:HD12 | 1:A:297:LEU:HA   | 1.70                     | 0.44              |
| 1:C:65:LEU:HD12  | 1:C:457:VAL:HG13 | 1.99                     | 0.44              |
| 1:F:122:SER:HB2  | 1:F:125:HIS:CE1  | 2.53                     | 0.44              |
| 1:G:184:GLU:C    | 1:G:186:VAL:N    | 2.76                     | 0.44              |
| 1:G:495:MET:SD   | 1:G:498:GLN:NE2  | 2.90                     | 0.44              |
| 1:C:207:GLY:HA2  | 1:C:224:ARG:HB2  | 2.00                     | 0.44              |
| 1:F:286:MET:O    | 1:F:290:ILE:HG13 | 2.18                     | 0.44              |
| 1:H:156:GLY:HA2  | 1:H:184:GLU:OE2  | 2.17                     | 0.44              |
| 1:H:157:ILE:HD11 | 2:H:601:ATP:C5   | 2.53                     | 0.44              |
| 1:H:313:LEU:HD23 | 1:H:313:LEU:HA   | 1.75                     | 0.44              |
| 1:C:400:TYR:CD1  | 1:C:409:LYS:HG3  | 2.53                     | 0.43              |
| 1:C:408:LEU:HD23 | 1:C:448:GLN:HA   | 2.00                     | 0.43              |
| 1:E:184:GLU:C    | 1:E:186:VAL:N    | 2.76                     | 0.43              |
| 1:F:207:GLY:HA2  | 1:F:224:ARG:HB2  | 1.99                     | 0.43              |
| 1:H:156:GLY:HA2  | 1:H:184:GLU:CD   | 2.43                     | 0.43              |
| 1:C:194:LEU:HD23 | 1:C:194:LEU:HA   | 1.86                     | 0.43              |
| 1:C:286:MET:O    | 1:C:290:ILE:HG13 | 2.18                     | 0.43              |
| 1:G:286:MET:O    | 1:G:290:ILE:HG13 | 2.18                     | 0.43              |
| 1:H:495:MET:SD   | 1:H:498:GLN:NE2  | 2.91                     | 0.43              |
| 1:A:91:ILE:H     | 1:A:91:ILE:HG12  | 1.70                     | 0.43              |
| 1:A:213:ASN:ND2  | 1:A:215:CYS:HB3  | 2.33                     | 0.43              |
| 1:A:413:GLY:O    | 1:A:416:SER:OG   | 2.29                     | 0.43              |
| 1:C:321:LEU:HB2  | 1:C:361:ILE:HG22 | 1.99                     | 0.43              |
| 1:E:286:MET:O    | 1:E:290:ILE:HG13 | 2.18                     | 0.43              |
| 1:E:408:LEU:HD23 | 1:E:448:GLN:HA   | 2.01                     | 0.43              |
| 1:F:178:VAL:O    | 1:F:180:THR:N    | 2.52                     | 0.43              |
| 1:G:186:VAL:HG11 | 1:G:204:SER:HB2  | 2.00                     | 0.43              |
| 1:A:462:ALA:HB1  | 1:B:439:ILE:HD11 | 2.00                     | 0.43              |
| 1:B:286:MET:O    | 1:B:290:ILE:HG13 | 2.19                     | 0.43              |
| 1:G:459:TYR:CD1  | 1:G:514:TYR:HB3  | 2.52                     | 0.43              |
| 1:A:104:VAL:O    | 1:A:108:LYS:HG2  | 2.19                     | 0.43              |
| 1:A:122:SER:HB2  | 1:A:125:HIS:CE1  | 2.53                     | 0.43              |
| 1:B:408:LEU:HD23 | 1:B:448:GLN:HA   | 2.01                     | 0.43              |
| 1:A:286:MET:O    | 1:A:290:ILE:HG13 | 2.19                     | 0.43              |
| 1:A:495:MET:SD   | 1:A:498:GLN:NE2  | 2.92                     | 0.43              |
| 1:B:104:VAL:O    | 1:B:108:LYS:HG2  | 2.19                     | 0.43              |
| 1:E:379:LEU:C    | 1:E:483:MET:HE2  | 2.44                     | 0.43              |
| 1:G:206:LYS:H    | 1:G:206:LYS:HG2  | 1.70                     | 0.43              |
| 1:H:65:LEU:HD12  | 1:H:457:VAL:HG13 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:104:VAL:O    | 1:H:108:LYS:HG2  | 2.19                     | 0.43              |
| 1:C:379:LEU:C    | 1:C:483:MET:HE2  | 2.44                     | 0.43              |
| 1:D:379:LEU:C    | 1:D:483:MET:HE2  | 2.44                     | 0.43              |
| 1:E:75:GLU:HB2   | 1:E:397:PRO:HG3  | 1.99                     | 0.43              |
| 1:F:104:VAL:O    | 1:F:108:LYS:HG2  | 2.19                     | 0.43              |
| 1:F:200:ILE:O    | 1:F:204:SER:HB3  | 2.18                     | 0.43              |
| 1:A:106:LYS:HB2  | 1:A:106:LYS:HE3  | 1.71                     | 0.43              |
| 1:A:379:LEU:C    | 1:A:483:MET:HE2  | 2.44                     | 0.43              |
| 1:E:71:ASP:OD2   | 1:E:412:ARG:NH1  | 2.31                     | 0.43              |
| 1:E:115:ILE:HG12 | 1:E:221:ILE:O    | 2.19                     | 0.43              |
| 1:E:386:MET:HB2  | 1:E:386:MET:HE3  | 1.80                     | 0.43              |
| 1:G:200:ILE:O    | 1:G:204:SER:HB3  | 2.19                     | 0.43              |
| 1:A:75:GLU:HB2   | 1:A:397:PRO:HG3  | 2.00                     | 0.43              |
| 1:A:157:ILE:HD13 | 1:A:184:GLU:OE1  | 2.19                     | 0.43              |
| 1:B:157:ILE:HD11 | 2:B:601:ATP:C5   | 2.54                     | 0.43              |
| 1:E:297:LEU:HD12 | 1:E:297:LEU:HA   | 1.71                     | 0.43              |
| 1:F:379:LEU:C    | 1:F:483:MET:HE2  | 2.44                     | 0.43              |
| 1:F:401:PHE:CE2  | 1:F:408:LEU:HB2  | 2.53                     | 0.43              |
| 1:H:207:GLY:HA2  | 1:H:224:ARG:HB2  | 2.01                     | 0.43              |
| 1:A:165:PHE:HB2  | 1:H:202:GLN:NE2  | 2.34                     | 0.43              |
| 1:A:373:VAL:HG11 | 1:A:464:ILE:HD11 | 2.01                     | 0.43              |
| 1:B:373:VAL:HG11 | 1:B:464:ILE:HD11 | 2.01                     | 0.43              |
| 1:B:379:LEU:C    | 1:B:483:MET:HE2  | 2.44                     | 0.43              |
| 1:C:297:LEU:HD12 | 1:C:297:LEU:HA   | 1.69                     | 0.43              |
| 1:D:106:LYS:HB2  | 1:D:106:LYS:HE3  | 1.70                     | 0.43              |
| 1:D:401:PHE:CE2  | 1:D:408:LEU:HB2  | 2.53                     | 0.43              |
| 1:D:408:LEU:HD23 | 1:D:448:GLN:HA   | 2.01                     | 0.43              |
| 1:G:104:VAL:O    | 1:G:108:LYS:HG2  | 2.18                     | 0.43              |
| 1:G:297:LEU:HA   | 1:G:297:LEU:HD12 | 1.69                     | 0.43              |
| 1:G:379:LEU:C    | 1:G:483:MET:HE2  | 2.44                     | 0.43              |
| 1:G:408:LEU:HD23 | 1:G:448:GLN:HA   | 2.01                     | 0.43              |
| 1:H:373:VAL:HG11 | 1:H:464:ILE:HD11 | 2.01                     | 0.43              |
| 1:H:379:LEU:C    | 1:H:483:MET:HE2  | 2.44                     | 0.43              |
| 1:H:417:LEU:O    | 1:H:421:GLU:HG2  | 2.19                     | 0.43              |
| 1:B:146:GLU:OE2  | 1:B:147:THR:HG22 | 2.19                     | 0.42              |
| 1:C:184:GLU:HB3  | 2:C:601:ATP:C2   | 2.54                     | 0.42              |
| 1:D:193:THR:OG1  | 1:D:194:LEU:N    | 2.52                     | 0.42              |
| 1:D:373:VAL:HG11 | 1:D:464:ILE:HD11 | 2.01                     | 0.42              |
| 1:F:417:LEU:O    | 1:F:421:GLU:HG2  | 2.20                     | 0.42              |
| 1:H:146:GLU:H    | 1:H:146:GLU:HG3  | 1.57                     | 0.42              |
| 1:A:154:LEU:O    | 1:A:182:ARG:HD3  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:413:GLY:O    | 1:B:416:SER:OG   | 2.26                     | 0.42              |
| 1:C:186:VAL:HG23 | 1:C:186:VAL:O    | 2.19                     | 0.42              |
| 1:D:104:VAL:O    | 1:D:108:LYS:HG2  | 2.19                     | 0.42              |
| 1:D:286:MET:O    | 1:D:290:ILE:HG13 | 2.19                     | 0.42              |
| 1:E:134:LYS:NZ   | 1:E:138:GLY:O    | 2.45                     | 0.42              |
| 1:G:373:VAL:HG11 | 1:G:464:ILE:HD11 | 2.01                     | 0.42              |
| 1:H:286:MET:O    | 1:H:290:ILE:HG13 | 2.19                     | 0.42              |
| 1:H:438:LYS:HA   | 1:H:438:LYS:HD3  | 1.85                     | 0.42              |
| 1:B:500:GLU:OE1  | 1:C:31:THR:OG1   | 2.37                     | 0.42              |
| 1:D:127:VAL:O    | 1:D:130:VAL:HG22 | 2.20                     | 0.42              |
| 1:E:373:VAL:HG11 | 1:E:464:ILE:HD11 | 2.01                     | 0.42              |
| 1:F:373:VAL:HG11 | 1:F:464:ILE:HD11 | 2.02                     | 0.42              |
| 1:G:106:LYS:HE3  | 1:G:106:LYS:HB2  | 1.70                     | 0.42              |
| 1:G:115:ILE:HG12 | 1:G:221:ILE:O    | 2.20                     | 0.42              |
| 1:G:122:SER:HB2  | 1:G:125:HIS:CE1  | 2.55                     | 0.42              |
| 1:A:184:GLU:C    | 1:A:186:VAL:N    | 2.76                     | 0.42              |
| 1:B:156:GLY:HA3  | 1:B:180:THR:O    | 2.19                     | 0.42              |
| 1:F:180:THR:HA   | 1:F:181:PRO:HD3  | 1.89                     | 0.42              |
| 1:H:84:LEU:HD22  | 1:H:233:TYR:CD1  | 2.55                     | 0.42              |
| 1:A:449:ASP:OD1  | 1:A:451:GLY:N    | 2.52                     | 0.42              |
| 1:C:373:VAL:HG11 | 1:C:464:ILE:HD11 | 2.01                     | 0.42              |
| 1:C:449:ASP:OD1  | 1:C:451:GLY:N    | 2.41                     | 0.42              |
| 1:C:495:MET:SD   | 1:C:498:GLN:NE2  | 2.92                     | 0.42              |
| 1:D:212:VAL:HA   | 1:D:217:GLU:O    | 2.20                     | 0.42              |
| 1:D:313:LEU:HD23 | 1:D:313:LEU:HA   | 1.75                     | 0.42              |
| 1:E:157:ILE:HD13 | 1:E:184:GLU:OE1  | 2.19                     | 0.42              |
| 1:E:200:ILE:O    | 1:E:204:SER:HB3  | 2.19                     | 0.42              |
| 1:F:274:ASP:OD1  | 4:F:604:NAD:O2D  | 2.37                     | 0.42              |
| 1:F:500:GLU:OE1  | 1:G:31:THR:OG1   | 2.38                     | 0.42              |
| 1:A:156:GLY:HA3  | 1:A:180:THR:O    | 2.20                     | 0.42              |
| 1:E:500:GLU:OE1  | 1:F:31:THR:OG1   | 2.38                     | 0.42              |
| 1:G:184:GLU:C    | 1:G:186:VAL:H    | 2.26                     | 0.42              |
| 1:H:401:PHE:CE2  | 1:H:408:LEU:HB2  | 2.54                     | 0.42              |
| 1:A:180:THR:HA   | 1:A:181:PRO:HD3  | 1.93                     | 0.42              |
| 1:A:200:ILE:O    | 1:A:204:SER:HB3  | 2.20                     | 0.42              |
| 1:B:84:LEU:HD22  | 1:B:233:TYR:CD1  | 2.55                     | 0.42              |
| 1:C:180:THR:HA   | 1:C:181:PRO:HD3  | 1.91                     | 0.42              |
| 1:D:417:LEU:O    | 1:D:421:GLU:HG2  | 2.19                     | 0.42              |
| 1:D:483:MET:HA   | 1:D:488:LEU:HB3  | 2.02                     | 0.42              |
| 1:E:180:THR:HA   | 1:E:181:PRO:HD3  | 1.95                     | 0.42              |
| 1:F:194:LEU:HD23 | 1:F:194:LEU:HA   | 1.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:157:ILE:HD11 | 2:G:601:ATP:C4   | 2.54                     | 0.42              |
| 1:H:184:GLU:C    | 1:H:186:VAL:N    | 2.77                     | 0.42              |
| 1:B:194:LEU:HD23 | 1:B:194:LEU:HA   | 1.83                     | 0.41              |
| 1:B:209:LEU:HD12 | 1:B:222:ILE:HD12 | 2.01                     | 0.41              |
| 1:D:260:LEU:HD21 | 1:D:290:ILE:HG12 | 2.02                     | 0.41              |
| 1:F:495:MET:SD   | 1:F:498:GLN:NE2  | 2.93                     | 0.41              |
| 1:H:184:GLU:C    | 1:H:186:VAL:H    | 2.27                     | 0.41              |
| 1:H:240:SER:OG   | 1:H:241:GLN:OE1  | 2.38                     | 0.41              |
| 1:A:9:GLY:O      | 1:A:11:GLY:N     | 2.52                     | 0.41              |
| 1:D:209:LEU:HD12 | 1:D:222:ILE:HD12 | 2.01                     | 0.41              |
| 1:F:400:TYR:CD1  | 1:F:409:LYS:HG3  | 2.55                     | 0.41              |
| 1:G:401:PHE:CE2  | 1:G:408:LEU:HB2  | 2.54                     | 0.41              |
| 1:A:49:VAL:HA    | 1:A:474:ARG:O    | 2.21                     | 0.41              |
| 1:B:193:THR:OG1  | 1:B:194:LEU:N    | 2.53                     | 0.41              |
| 1:E:226:ASP:OD1  | 2:E:602:ATP:O3'  | 2.19                     | 0.41              |
| 1:F:63:THR:HG22  | 1:F:65:LEU:H     | 1.85                     | 0.41              |
| 1:F:386:MET:HE3  | 1:F:386:MET:HB2  | 1.80                     | 0.41              |
| 1:H:106:LYS:HB2  | 1:H:106:LYS:HE3  | 1.71                     | 0.41              |
| 1:A:31:THR:OG1   | 1:D:500:GLU:OE1  | 2.37                     | 0.41              |
| 1:A:483:MET:HA   | 1:A:488:LEU:HB3  | 2.02                     | 0.41              |
| 1:B:386:MET:HE3  | 1:B:386:MET:HB2  | 1.80                     | 0.41              |
| 1:D:84:LEU:HD22  | 1:D:233:TYR:CD1  | 2.56                     | 0.41              |
| 1:E:122:SER:HB2  | 1:E:125:HIS:CE1  | 2.55                     | 0.41              |
| 1:E:367:ILE:HG22 | 1:E:389:LEU:HD22 | 2.02                     | 0.41              |
| 1:H:483:MET:HA   | 1:H:488:LEU:HB3  | 2.02                     | 0.41              |
| 1:A:500:GLU:OE1  | 1:B:31:THR:OG1   | 2.39                     | 0.41              |
| 1:B:63:THR:HG22  | 1:B:65:LEU:H     | 1.85                     | 0.41              |
| 1:B:462:ALA:HB1  | 1:C:439:ILE:HD11 | 2.03                     | 0.41              |
| 1:F:209:LEU:HD12 | 1:F:222:ILE:HD12 | 2.02                     | 0.41              |
| 1:F:370:VAL:O    | 1:F:374:VAL:HG23 | 2.21                     | 0.41              |
| 1:H:51:LEU:HB3   | 1:H:64:PRO:HD3   | 2.02                     | 0.41              |
| 1:A:156:GLY:HA2  | 1:A:184:GLU:CD   | 2.46                     | 0.41              |
| 1:C:127:VAL:HG12 | 1:C:169:LYS:HA   | 2.02                     | 0.41              |
| 1:H:260:LEU:HD21 | 1:H:290:ILE:HG12 | 2.03                     | 0.41              |
| 1:H:408:LEU:HD23 | 1:H:448:GLN:HA   | 2.03                     | 0.41              |
| 1:B:370:VAL:O    | 1:B:374:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:104:VAL:O    | 1:C:108:LYS:HG2  | 2.20                     | 0.41              |
| 1:C:218:LEU:HD12 | 1:C:218:LEU:HA   | 1.91                     | 0.41              |
| 1:D:51:LEU:HB3   | 1:D:64:PRO:HD3   | 2.03                     | 0.41              |
| 1:D:459:TYR:CD1  | 1:D:514:TYR:HB3  | 2.55                     | 0.41              |
| 1:F:106:LYS:HE3  | 1:F:106:LYS:HB2  | 1.70                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:127:VAL:O    | 1:F:130:VAL:HG22 | 2.21                     | 0.41              |
| 1:G:157:ILE:HD13 | 1:G:184:GLU:OE1  | 2.20                     | 0.41              |
| 1:G:182:ARG:HD2  | 1:G:182:ARG:HA   | 1.84                     | 0.41              |
| 1:H:63:THR:HG22  | 1:H:65:LEU:H     | 1.85                     | 0.41              |
| 1:H:140:SER:O    | 1:H:140:SER:OG   | 2.34                     | 0.41              |
| 1:H:186:VAL:HG11 | 1:H:204:SER:HB2  | 2.02                     | 0.41              |
| 1:H:370:VAL:O    | 1:H:374:VAL:HG23 | 2.21                     | 0.41              |
| 1:E:51:LEU:HB3   | 1:E:64:PRO:HD3   | 2.03                     | 0.41              |
| 1:E:483:MET:HA   | 1:E:488:LEU:HB3  | 2.02                     | 0.41              |
| 1:F:51:LEU:HB3   | 1:F:64:PRO:HD3   | 2.02                     | 0.41              |
| 1:F:184:GLU:H    | 1:F:184:GLU:HG2  | 1.50                     | 0.41              |
| 1:A:51:LEU:HB3   | 1:A:64:PRO:HD3   | 2.03                     | 0.41              |
| 1:A:408:LEU:HD23 | 1:A:448:GLN:HA   | 2.03                     | 0.41              |
| 1:B:51:LEU:HB3   | 1:B:64:PRO:HD3   | 2.02                     | 0.41              |
| 1:B:154:LEU:O    | 1:B:182:ARG:HD3  | 2.21                     | 0.41              |
| 1:B:203:ARG:HG2  | 1:B:203:ARG:HH21 | 1.86                     | 0.41              |
| 1:B:422:LYS:HD3  | 1:B:422:LYS:HA   | 1.91                     | 0.41              |
| 1:C:63:THR:HG22  | 1:C:65:LEU:H     | 1.85                     | 0.41              |
| 1:C:157:ILE:HD11 | 2:C:601:ATP:C4   | 2.56                     | 0.41              |
| 1:C:196:GLU:O    | 1:C:200:ILE:HG13 | 2.20                     | 0.41              |
| 1:D:122:SER:HB2  | 1:D:125:HIS:CE1  | 2.56                     | 0.41              |
| 1:D:202:GLN:NE2  | 1:E:165:PHE:HB2  | 2.36                     | 0.41              |
| 1:D:370:VAL:O    | 1:D:374:VAL:HG23 | 2.21                     | 0.41              |
| 1:E:84:LEU:HD22  | 1:E:233:TYR:CD1  | 2.56                     | 0.41              |
| 1:E:449:ASP:OD1  | 1:E:451:GLY:N    | 2.53                     | 0.41              |
| 1:H:206:LYS:NZ   | 1:H:206:LYS:HB3  | 2.36                     | 0.41              |
| 1:A:439:ILE:HD11 | 1:D:462:ALA:HB1  | 2.02                     | 0.41              |
| 1:D:157:ILE:HD11 | 2:D:601:ATP:C4   | 2.55                     | 0.41              |
| 1:D:165:PHE:HB2  | 1:E:202:GLN:NE2  | 2.35                     | 0.41              |
| 1:D:213:ASN:OD1  | 1:D:217:GLU:N    | 2.48                     | 0.41              |
| 1:F:49:VAL:HA    | 1:F:474:ARG:O    | 2.21                     | 0.41              |
| 1:F:297:LEU:HD12 | 1:F:297:LEU:HA   | 1.71                     | 0.41              |
| 1:F:462:ALA:HB1  | 1:G:439:ILE:HD11 | 2.03                     | 0.41              |
| 1:A:370:VAL:O    | 1:A:374:VAL:HG23 | 2.21                     | 0.40              |
| 1:F:206:LYS:NZ   | 1:F:206:LYS:HB3  | 2.35                     | 0.40              |
| 1:F:213:ASN:HD21 | 1:F:217:GLU:HB2  | 1.86                     | 0.40              |
| 1:G:84:LEU:HD22  | 1:G:233:TYR:CD1  | 2.56                     | 0.40              |
| 1:G:203:ARG:HH21 | 1:G:203:ARG:HG2  | 1.86                     | 0.40              |
| 1:C:500:GLU:OE1  | 1:D:31:THR:OG1   | 2.38                     | 0.40              |
| 1:E:104:VAL:O    | 1:E:108:LYS:HG2  | 2.22                     | 0.40              |
| 1:F:84:LEU:HD22  | 1:F:233:TYR:CD1  | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:51:LEU:HB3   | 1:G:64:PRO:HD3   | 2.02                     | 0.40              |
| 1:G:483:MET:HA   | 1:G:488:LEU:HB3  | 2.02                     | 0.40              |
| 1:G:500:GLU:OE1  | 1:H:31:THR:OG1   | 2.38                     | 0.40              |
| 1:A:84:LEU:HD22  | 1:A:233:TYR:CD1  | 2.57                     | 0.40              |
| 1:A:367:ILE:HG22 | 1:A:389:LEU:HD22 | 2.04                     | 0.40              |
| 1:H:186:VAL:HG23 | 2:H:601:ATP:HN62 | 1.86                     | 0.40              |
| 1:A:63:THR:HG22  | 1:A:65:LEU:H     | 1.86                     | 0.40              |
| 1:A:203:ARG:HH21 | 1:A:203:ARG:HG2  | 1.86                     | 0.40              |
| 1:B:186:VAL:HG11 | 1:B:204:SER:HB2  | 2.04                     | 0.40              |
| 1:D:119:VAL:HB   | 1:D:139:PHE:HE1  | 1.85                     | 0.40              |
| 1:G:63:THR:HG22  | 1:G:65:LEU:H     | 1.86                     | 0.40              |
| 1:G:196:GLU:O    | 1:G:200:ILE:HG13 | 2.21                     | 0.40              |
| 1:G:462:ALA:HB1  | 1:H:439:ILE:HD11 | 2.02                     | 0.40              |
| 1:H:180:THR:HA   | 1:H:181:PRO:HD3  | 1.92                     | 0.40              |
| 1:H:203:ARG:HG2  | 1:H:203:ARG:NH2  | 2.36                     | 0.40              |
| 1:A:119:VAL:HB   | 1:A:139:PHE:HE1  | 1.87                     | 0.40              |
| 1:C:51:LEU:HB3   | 1:C:64:PRO:HD3   | 2.03                     | 0.40              |
| 1:C:206:LYS:H    | 1:C:206:LYS:HG2  | 1.71                     | 0.40              |
| 1:D:449:ASP:OD1  | 1:D:451:GLY:N    | 2.54                     | 0.40              |
| 1:E:31:THR:OG1   | 1:H:500:GLU:OE1  | 2.38                     | 0.40              |
| 1:E:370:VAL:O    | 1:E:374:VAL:HG23 | 2.21                     | 0.40              |
| 1:G:370:VAL:O    | 1:G:374:VAL:HG23 | 2.21                     | 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 PDB entries followed by that with respect to all EM entries.

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     | 474/514 (92%) | 436 (92%) | 37 (8%) | 1 (0%)   | 43          | 70  |
| 1   | B     | 474/514 (92%) | 441 (93%) | 33 (7%) | 0        | 100         | 100 |
| 1   | C     | 474/514 (92%) | 441 (93%) | 33 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | D     | 474/514 (92%)   | 446 (94%)  | 28 (6%)  | 0        | 100         | 100 |
| 1   | E     | 474/514 (92%)   | 434 (92%)  | 39 (8%)  | 1 (0%)   | 43          | 70  |
| 1   | F     | 474/514 (92%)   | 443 (94%)  | 31 (6%)  | 0        | 100         | 100 |
| 1   | G     | 474/514 (92%)   | 443 (94%)  | 31 (6%)  | 0        | 100         | 100 |
| 1   | H     | 474/514 (92%)   | 441 (93%)  | 33 (7%)  | 0        | 100         | 100 |
| All | All   | 3792/4112 (92%) | 3525 (93%) | 265 (7%) | 2 (0%)   | 49          | 75  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | THR  |
| 1   | E     | 10  | THR  |

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 390/419 (93%)   | 369 (95%)  | 21 (5%)  | 20          | 46 |
| 1   | B     | 390/419 (93%)   | 368 (94%)  | 22 (6%)  | 19          | 45 |
| 1   | C     | 390/419 (93%)   | 373 (96%)  | 17 (4%)  | 25          | 53 |
| 1   | D     | 390/419 (93%)   | 371 (95%)  | 19 (5%)  | 22          | 50 |
| 1   | E     | 390/419 (93%)   | 373 (96%)  | 17 (4%)  | 25          | 53 |
| 1   | F     | 390/419 (93%)   | 373 (96%)  | 17 (4%)  | 25          | 53 |
| 1   | G     | 390/419 (93%)   | 370 (95%)  | 20 (5%)  | 21          | 48 |
| 1   | H     | 390/419 (93%)   | 371 (95%)  | 19 (5%)  | 22          | 50 |
| All | All   | 3120/3352 (93%) | 2968 (95%) | 152 (5%) | 24          | 50 |

All (152) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 53  | SER  |
| 1   | A     | 63  | THR  |
| 1   | A     | 77  | ASP  |
| 1   | A     | 91  | ILE  |
| 1   | A     | 93  | HIS  |
| 1   | A     | 127 | VAL  |
| 1   | A     | 146 | GLU  |
| 1   | A     | 147 | THR  |
| 1   | A     | 154 | LEU  |
| 1   | A     | 155 | VAL  |
| 1   | A     | 157 | ILE  |
| 1   | A     | 158 | VAL  |
| 1   | A     | 183 | ILE  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 277 | GLN  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 355 | ARG  |
| 1   | A     | 361 | ILE  |
| 1   | A     | 383 | THR  |
| 1   | A     | 452 | SER  |
| 1   | B     | 28  | ASP  |
| 1   | B     | 53  | SER  |
| 1   | B     | 63  | THR  |
| 1   | B     | 77  | ASP  |
| 1   | B     | 93  | HIS  |
| 1   | B     | 127 | VAL  |
| 1   | B     | 146 | GLU  |
| 1   | B     | 149 | THR  |
| 1   | B     | 154 | LEU  |
| 1   | B     | 155 | VAL  |
| 1   | B     | 157 | ILE  |
| 1   | B     | 158 | VAL  |
| 1   | B     | 183 | ILE  |
| 1   | B     | 186 | VAL  |
| 1   | B     | 187 | VAL  |
| 1   | B     | 206 | LYS  |
| 1   | B     | 277 | GLN  |
| 1   | B     | 283 | GLN  |
| 1   | B     | 355 | ARG  |
| 1   | B     | 361 | ILE  |
| 1   | B     | 383 | THR  |
| 1   | B     | 452 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 53  | SER  |
| 1   | C     | 63  | THR  |
| 1   | C     | 77  | ASP  |
| 1   | C     | 93  | HIS  |
| 1   | C     | 127 | VAL  |
| 1   | C     | 146 | GLU  |
| 1   | C     | 154 | LEU  |
| 1   | C     | 155 | VAL  |
| 1   | C     | 157 | ILE  |
| 1   | C     | 158 | VAL  |
| 1   | C     | 183 | ILE  |
| 1   | C     | 206 | LYS  |
| 1   | C     | 277 | GLN  |
| 1   | C     | 283 | GLN  |
| 1   | C     | 355 | ARG  |
| 1   | C     | 361 | ILE  |
| 1   | C     | 383 | THR  |
| 1   | D     | 28  | ASP  |
| 1   | D     | 53  | SER  |
| 1   | D     | 63  | THR  |
| 1   | D     | 77  | ASP  |
| 1   | D     | 91  | ILE  |
| 1   | D     | 93  | HIS  |
| 1   | D     | 127 | VAL  |
| 1   | D     | 146 | GLU  |
| 1   | D     | 149 | THR  |
| 1   | D     | 155 | VAL  |
| 1   | D     | 157 | ILE  |
| 1   | D     | 158 | VAL  |
| 1   | D     | 206 | LYS  |
| 1   | D     | 277 | GLN  |
| 1   | D     | 283 | GLN  |
| 1   | D     | 355 | ARG  |
| 1   | D     | 361 | ILE  |
| 1   | D     | 383 | THR  |
| 1   | D     | 452 | SER  |
| 1   | E     | 28  | ASP  |
| 1   | E     | 53  | SER  |
| 1   | E     | 63  | THR  |
| 1   | E     | 93  | HIS  |
| 1   | E     | 146 | GLU  |
| 1   | E     | 155 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 157 | ILE  |
| 1   | E     | 158 | VAL  |
| 1   | E     | 183 | ILE  |
| 1   | E     | 187 | VAL  |
| 1   | E     | 206 | LYS  |
| 1   | E     | 277 | GLN  |
| 1   | E     | 283 | GLN  |
| 1   | E     | 355 | ARG  |
| 1   | E     | 361 | ILE  |
| 1   | E     | 383 | THR  |
| 1   | E     | 452 | SER  |
| 1   | F     | 53  | SER  |
| 1   | F     | 63  | THR  |
| 1   | F     | 77  | ASP  |
| 1   | F     | 91  | ILE  |
| 1   | F     | 93  | HIS  |
| 1   | F     | 146 | GLU  |
| 1   | F     | 149 | THR  |
| 1   | F     | 155 | VAL  |
| 1   | F     | 157 | ILE  |
| 1   | F     | 158 | VAL  |
| 1   | F     | 187 | VAL  |
| 1   | F     | 206 | LYS  |
| 1   | F     | 277 | GLN  |
| 1   | F     | 283 | GLN  |
| 1   | F     | 355 | ARG  |
| 1   | F     | 361 | ILE  |
| 1   | F     | 383 | THR  |
| 1   | G     | 28  | ASP  |
| 1   | G     | 53  | SER  |
| 1   | G     | 63  | THR  |
| 1   | G     | 77  | ASP  |
| 1   | G     | 91  | ILE  |
| 1   | G     | 93  | HIS  |
| 1   | G     | 127 | VAL  |
| 1   | G     | 146 | GLU  |
| 1   | G     | 154 | LEU  |
| 1   | G     | 157 | ILE  |
| 1   | G     | 158 | VAL  |
| 1   | G     | 183 | ILE  |
| 1   | G     | 187 | VAL  |
| 1   | G     | 206 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 277 | GLN  |
| 1   | G     | 283 | GLN  |
| 1   | G     | 355 | ARG  |
| 1   | G     | 361 | ILE  |
| 1   | G     | 383 | THR  |
| 1   | G     | 452 | SER  |
| 1   | H     | 53  | SER  |
| 1   | H     | 63  | THR  |
| 1   | H     | 91  | ILE  |
| 1   | H     | 93  | HIS  |
| 1   | H     | 127 | VAL  |
| 1   | H     | 146 | GLU  |
| 1   | H     | 154 | LEU  |
| 1   | H     | 155 | VAL  |
| 1   | H     | 157 | ILE  |
| 1   | H     | 158 | VAL  |
| 1   | H     | 180 | THR  |
| 1   | H     | 186 | VAL  |
| 1   | H     | 187 | VAL  |
| 1   | H     | 206 | LYS  |
| 1   | H     | 277 | GLN  |
| 1   | H     | 355 | ARG  |
| 1   | H     | 361 | ILE  |
| 1   | H     | 383 | THR  |
| 1   | H     | 452 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 202 | GLN  |
| 1   | A     | 277 | GLN  |
| 1   | A     | 296 | HIS  |
| 1   | A     | 303 | ASN  |
| 1   | A     | 454 | GLN  |
| 1   | A     | 498 | GLN  |
| 1   | A     | 507 | HIS  |
| 1   | B     | 112 | GLN  |
| 1   | B     | 277 | GLN  |
| 1   | B     | 454 | GLN  |
| 1   | B     | 498 | GLN  |
| 1   | B     | 507 | HIS  |
| 1   | C     | 112 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 277 | GLN  |
| 1   | C     | 296 | HIS  |
| 1   | C     | 498 | GLN  |
| 1   | C     | 507 | HIS  |
| 1   | D     | 277 | GLN  |
| 1   | D     | 296 | HIS  |
| 1   | D     | 498 | GLN  |
| 1   | D     | 507 | HIS  |
| 1   | E     | 277 | GLN  |
| 1   | E     | 296 | HIS  |
| 1   | E     | 303 | ASN  |
| 1   | E     | 454 | GLN  |
| 1   | E     | 498 | GLN  |
| 1   | E     | 507 | HIS  |
| 1   | F     | 277 | GLN  |
| 1   | F     | 296 | HIS  |
| 1   | F     | 303 | ASN  |
| 1   | F     | 498 | GLN  |
| 1   | F     | 507 | HIS  |
| 1   | G     | 202 | GLN  |
| 1   | G     | 277 | GLN  |
| 1   | G     | 498 | GLN  |
| 1   | G     | 507 | HIS  |
| 1   | H     | 277 | GLN  |
| 1   | H     | 296 | HIS  |
| 1   | H     | 454 | GLN  |
| 1   | H     | 498 | GLN  |
| 1   | H     | 507 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

32 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAD  | A     | 604 | -    | 46,48,48     | 3.57 | 21 (45%) | 64,73,73    | 2.37 | 15 (23%) |
| 2   | ATP  | F     | 602 | -    | 32,33,33     | 3.16 | 16 (50%) | 48,52,52    | 2.90 | 12 (25%) |
| 4   | NAD  | E     | 604 | -    | 46,48,48     | 3.59 | 21 (45%) | 64,73,73    | 2.25 | 12 (18%) |
| 2   | ATP  | C     | 602 | -    | 32,33,33     | 3.16 | 16 (50%) | 48,52,52    | 2.88 | 12 (25%) |
| 2   | ATP  | E     | 602 | -    | 32,33,33     | 3.17 | 16 (50%) | 48,52,52    | 2.91 | 13 (27%) |
| 3   | IMP  | B     | 603 | -    | 25,25,25     | 2.66 | 7 (28%)  | 37,38,38    | 2.25 | 10 (27%) |
| 2   | ATP  | E     | 601 | -    | 32,33,33     | 3.21 | 17 (53%) | 48,52,52    | 2.83 | 13 (27%) |
| 3   | IMP  | H     | 603 | -    | 25,25,25     | 2.66 | 7 (28%)  | 37,38,38    | 2.25 | 10 (27%) |
| 4   | NAD  | C     | 604 | -    | 46,48,48     | 3.58 | 21 (45%) | 64,73,73    | 2.31 | 12 (18%) |
| 2   | ATP  | C     | 601 | -    | 32,33,33     | 3.17 | 17 (53%) | 48,52,52    | 2.91 | 13 (27%) |
| 3   | IMP  | A     | 603 | -    | 25,25,25     | 2.65 | 7 (28%)  | 37,38,38    | 2.25 | 11 (29%) |
| 2   | ATP  | H     | 601 | -    | 32,33,33     | 3.16 | 17 (53%) | 48,52,52    | 2.92 | 12 (25%) |
| 4   | NAD  | G     | 604 | -    | 46,48,48     | 3.54 | 21 (45%) | 64,73,73    | 2.36 | 15 (23%) |
| 2   | ATP  | G     | 602 | -    | 32,33,33     | 3.19 | 16 (50%) | 48,52,52    | 2.87 | 12 (25%) |
| 4   | NAD  | H     | 604 | -    | 46,48,48     | 3.55 | 21 (45%) | 64,73,73    | 2.45 | 18 (28%) |
| 2   | ATP  | A     | 602 | -    | 32,33,33     | 3.19 | 16 (50%) | 48,52,52    | 2.88 | 13 (27%) |
| 2   | ATP  | F     | 601 | -    | 32,33,33     | 3.16 | 17 (53%) | 48,52,52    | 2.85 | 13 (27%) |
| 2   | ATP  | G     | 601 | -    | 32,33,33     | 3.16 | 17 (53%) | 48,52,52    | 2.92 | 12 (25%) |
| 3   | IMP  | G     | 603 | -    | 25,25,25     | 2.65 | 7 (28%)  | 37,38,38    | 2.30 | 11 (29%) |
| 4   | NAD  | F     | 604 | -    | 46,48,48     | 3.58 | 21 (45%) | 64,73,73    | 2.28 | 13 (20%) |
| 2   | ATP  | A     | 601 | -    | 32,33,33     | 3.17 | 16 (50%) | 48,52,52    | 2.86 | 13 (27%) |
| 3   | IMP  | E     | 603 | -    | 25,25,25     | 2.65 | 7 (28%)  | 37,38,38    | 2.25 | 10 (27%) |
| 2   | ATP  | D     | 601 | -    | 32,33,33     | 3.17 | 17 (53%) | 48,52,52    | 2.90 | 14 (29%) |
| 3   | IMP  | F     | 603 | -    | 25,25,25     | 2.65 | 7 (28%)  | 37,38,38    | 2.29 | 11 (29%) |
| 2   | ATP  | B     | 601 | -    | 32,33,33     | 3.15 | 18 (56%) | 48,52,52    | 2.96 | 13 (27%) |
| 3   | IMP  | C     | 603 | -    | 25,25,25     | 2.65 | 7 (28%)  | 37,38,38    | 2.28 | 11 (29%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | ATP  | D     | 602 | -    | 32,33,33     | 3.18 | 16 (50%) | 48,52,52    | 2.90 | 13 (27%) |
| 3   | IMP  | D     | 603 | -    | 25,25,25     | 2.66 | 7 (28%)  | 37,38,38    | 2.25 | 11 (29%) |
| 2   | ATP  | B     | 602 | -    | 32,33,33     | 3.16 | 16 (50%) | 48,52,52    | 2.88 | 12 (25%) |
| 4   | NAD  | B     | 604 | -    | 46,48,48     | 3.57 | 21 (45%) | 64,73,73    | 2.33 | 15 (23%) |
| 4   | NAD  | D     | 604 | -    | 46,48,48     | 3.58 | 21 (45%) | 64,73,73    | 2.31 | 14 (21%) |
| 2   | ATP  | H     | 602 | -    | 32,33,33     | 3.18 | 16 (50%) | 48,52,52    | 2.91 | 13 (27%) |

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   | NAD  | A     | 604 | -    | -       | 10/30/62/62 | 0/5/5/5 |
| 2   | ATP  | F     | 602 | -    | -       | 3/22/38/38  | 0/3/3/3 |
| 4   | NAD  | E     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 2   | ATP  | C     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 2   | ATP  | E     | 602 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 3   | IMP  | B     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 2   | ATP  | E     | 601 | -    | -       | 5/22/38/38  | 0/3/3/3 |
| 3   | IMP  | H     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 4   | NAD  | C     | 604 | -    | -       | 14/30/62/62 | 0/5/5/5 |
| 2   | ATP  | C     | 601 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 3   | IMP  | A     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 2   | ATP  | H     | 601 | -    | -       | 8/22/38/38  | 0/3/3/3 |
| 4   | NAD  | G     | 604 | -    | -       | 11/30/62/62 | 0/5/5/5 |
| 2   | ATP  | G     | 602 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 4   | NAD  | H     | 604 | -    | -       | 15/30/62/62 | 0/5/5/5 |
| 2   | ATP  | A     | 602 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 2   | ATP  | F     | 601 | -    | -       | 0/22/38/38  | 0/3/3/3 |
| 2   | ATP  | G     | 601 | -    | -       | 7/22/38/38  | 0/3/3/3 |
| 3   | IMP  | G     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 4   | NAD  | F     | 604 | -    | -       | 15/30/62/62 | 0/5/5/5 |
| 2   | ATP  | A     | 601 | -    | -       | 0/22/38/38  | 0/3/3/3 |
| 3   | IMP  | E     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 2   | ATP  | D     | 601 | -    | -       | 6/22/38/38  | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | IMP  | F     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 2   | ATP  | B     | 601 | -    | -       | 5/22/38/38  | 0/3/3/3 |
| 3   | IMP  | C     | 603 | -    | -       | 3/10/26/26  | 0/3/3/3 |
| 2   | ATP  | D     | 602 | -    | -       | 8/22/38/38  | 0/3/3/3 |
| 3   | IMP  | D     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 2   | ATP  | B     | 602 | -    | -       | 3/22/38/38  | 0/3/3/3 |
| 4   | NAD  | B     | 604 | -    | -       | 9/30/62/62  | 0/5/5/5 |
| 4   | NAD  | D     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 2   | ATP  | H     | 602 | -    | -       | 3/22/38/38  | 0/3/3/3 |

All (488) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | B     | 601 | ATP  | C2'-C3' | -10.64 | 1.24        | 1.53     |
| 2   | E     | 601 | ATP  | C2'-C3' | -10.63 | 1.24        | 1.53     |
| 2   | G     | 601 | ATP  | C2'-C3' | -10.61 | 1.24        | 1.53     |
| 2   | H     | 601 | ATP  | C2'-C3' | -10.59 | 1.24        | 1.53     |
| 2   | F     | 601 | ATP  | C2'-C3' | -10.59 | 1.24        | 1.53     |
| 2   | A     | 601 | ATP  | C2'-C3' | -10.58 | 1.24        | 1.53     |
| 2   | C     | 601 | ATP  | C2'-C3' | -10.55 | 1.24        | 1.53     |
| 2   | D     | 601 | ATP  | C2'-C3' | -10.51 | 1.24        | 1.53     |
| 2   | E     | 602 | ATP  | C2'-C3' | -10.44 | 1.25        | 1.53     |
| 2   | F     | 602 | ATP  | C2'-C3' | -10.39 | 1.25        | 1.53     |
| 2   | B     | 602 | ATP  | C2'-C3' | -10.34 | 1.25        | 1.53     |
| 2   | C     | 602 | ATP  | C2'-C3' | -10.33 | 1.25        | 1.53     |
| 2   | G     | 602 | ATP  | C2'-C3' | -10.31 | 1.25        | 1.53     |
| 2   | A     | 602 | ATP  | C2'-C3' | -10.27 | 1.25        | 1.53     |
| 2   | H     | 602 | ATP  | C2'-C3' | -10.27 | 1.25        | 1.53     |
| 2   | D     | 602 | ATP  | C2'-C3' | -10.24 | 1.25        | 1.53     |
| 4   | C     | 604 | NAD  | C3D-C4D | -9.38  | 1.29        | 1.53     |
| 4   | D     | 604 | NAD  | C3B-C4B | -9.21  | 1.29        | 1.53     |
| 4   | F     | 604 | NAD  | C3B-C4B | -9.18  | 1.29        | 1.53     |
| 4   | A     | 604 | NAD  | C3D-C4D | -9.16  | 1.29        | 1.53     |
| 4   | H     | 604 | NAD  | C3D-C4D | -9.14  | 1.29        | 1.53     |
| 4   | B     | 604 | NAD  | C3B-C4B | -9.14  | 1.29        | 1.53     |
| 4   | A     | 604 | NAD  | C3B-C4B | -9.14  | 1.29        | 1.53     |
| 4   | E     | 604 | NAD  | C3B-C4B | -9.09  | 1.29        | 1.53     |
| 4   | G     | 604 | NAD  | C3B-C4B | -9.04  | 1.30        | 1.53     |
| 4   | E     | 604 | NAD  | C3D-C4D | -9.03  | 1.30        | 1.53     |
| 4   | B     | 604 | NAD  | C3D-C4D | -9.00  | 1.30        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 604 | NAD  | C3D-C4D | -8.98 | 1.30        | 1.53     |
| 4   | C     | 604 | NAD  | C3B-C4B | -8.97 | 1.30        | 1.53     |
| 4   | F     | 604 | NAD  | C3D-C4D | -8.95 | 1.30        | 1.53     |
| 4   | G     | 604 | NAD  | C3D-C4D | -8.84 | 1.30        | 1.53     |
| 4   | H     | 604 | NAD  | C3B-C4B | -8.80 | 1.30        | 1.53     |
| 4   | D     | 604 | NAD  | O4D-C1D | -8.71 | 1.29        | 1.40     |
| 4   | G     | 604 | NAD  | O4D-C1D | -8.66 | 1.29        | 1.40     |
| 3   | A     | 603 | IMP  | C2-N3   | 8.59  | 1.45        | 1.30     |
| 3   | H     | 603 | IMP  | C2-N3   | 8.57  | 1.45        | 1.30     |
| 3   | F     | 603 | IMP  | C2-N3   | 8.57  | 1.45        | 1.30     |
| 3   | D     | 603 | IMP  | C2-N3   | 8.56  | 1.45        | 1.30     |
| 3   | B     | 603 | IMP  | C2-N3   | 8.53  | 1.45        | 1.30     |
| 3   | E     | 603 | IMP  | C2-N3   | 8.53  | 1.45        | 1.30     |
| 3   | C     | 603 | IMP  | C2-N3   | 8.51  | 1.45        | 1.30     |
| 3   | G     | 603 | IMP  | C2-N3   | 8.50  | 1.45        | 1.30     |
| 4   | A     | 604 | NAD  | O4D-C1D | -8.21 | 1.30        | 1.40     |
| 4   | F     | 604 | NAD  | O4D-C1D | -8.13 | 1.30        | 1.40     |
| 4   | B     | 604 | NAD  | O4D-C1D | -8.07 | 1.30        | 1.40     |
| 4   | E     | 604 | NAD  | O4D-C1D | -8.02 | 1.30        | 1.40     |
| 4   | H     | 604 | NAD  | O4D-C4D | 7.74  | 1.62        | 1.45     |
| 4   | E     | 604 | NAD  | O4B-C4B | 7.74  | 1.62        | 1.45     |
| 4   | H     | 604 | NAD  | O4B-C4B | 7.66  | 1.62        | 1.45     |
| 4   | H     | 604 | NAD  | O4D-C1D | -7.66 | 1.30        | 1.40     |
| 4   | C     | 604 | NAD  | O4B-C4B | 7.62  | 1.61        | 1.45     |
| 4   | C     | 604 | NAD  | O4D-C4D | 7.62  | 1.61        | 1.45     |
| 4   | B     | 604 | NAD  | O4D-C4D | 7.59  | 1.61        | 1.45     |
| 4   | E     | 604 | NAD  | O4D-C4D | 7.59  | 1.61        | 1.45     |
| 4   | G     | 604 | NAD  | O4B-C4B | 7.57  | 1.61        | 1.45     |
| 4   | C     | 604 | NAD  | O4D-C1D | -7.56 | 1.31        | 1.40     |
| 4   | D     | 604 | NAD  | O4B-C4B | 7.53  | 1.61        | 1.45     |
| 4   | A     | 604 | NAD  | O4B-C4B | 7.48  | 1.61        | 1.45     |
| 4   | F     | 604 | NAD  | O4D-C4D | 7.40  | 1.61        | 1.45     |
| 4   | B     | 604 | NAD  | O4B-C4B | 7.36  | 1.61        | 1.45     |
| 4   | D     | 604 | NAD  | O4D-C4D | 7.31  | 1.61        | 1.45     |
| 4   | A     | 604 | NAD  | O4D-C4D | 7.29  | 1.61        | 1.45     |
| 4   | F     | 604 | NAD  | O4B-C4B | 7.25  | 1.61        | 1.45     |
| 4   | G     | 604 | NAD  | O4D-C4D | 7.24  | 1.61        | 1.45     |
| 4   | D     | 604 | NAD  | C7N-N7N | 6.80  | 1.45        | 1.33     |
| 4   | E     | 604 | NAD  | C7N-N7N | 6.80  | 1.45        | 1.33     |
| 4   | F     | 604 | NAD  | C7N-N7N | 6.78  | 1.45        | 1.33     |
| 4   | C     | 604 | NAD  | C7N-N7N | 6.66  | 1.45        | 1.33     |
| 4   | B     | 604 | NAD  | C7N-N7N | 6.66  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | H     | 604 | NAD  | C7N-N7N | 6.63  | 1.45        | 1.33     |
| 4   | A     | 604 | NAD  | C7N-N7N | 6.49  | 1.44        | 1.33     |
| 4   | G     | 604 | NAD  | C7N-N7N | 6.48  | 1.44        | 1.33     |
| 3   | B     | 603 | IMP  | C4-N3   | 6.19  | 1.48        | 1.35     |
| 3   | E     | 603 | IMP  | C4-N3   | 6.17  | 1.48        | 1.35     |
| 3   | C     | 603 | IMP  | C4-N3   | 6.16  | 1.48        | 1.35     |
| 3   | G     | 603 | IMP  | C4-N3   | 6.16  | 1.48        | 1.35     |
| 3   | A     | 603 | IMP  | C4-N3   | 6.15  | 1.48        | 1.35     |
| 3   | H     | 603 | IMP  | C4-N3   | 6.15  | 1.48        | 1.35     |
| 3   | D     | 603 | IMP  | C4-N3   | 6.15  | 1.48        | 1.35     |
| 3   | F     | 603 | IMP  | C4-N3   | 6.13  | 1.48        | 1.35     |
| 2   | G     | 602 | ATP  | PA-O3A  | 6.00  | 1.66        | 1.59     |
| 2   | E     | 602 | ATP  | PA-O3A  | 5.87  | 1.65        | 1.59     |
| 2   | C     | 602 | ATP  | PA-O3A  | 5.83  | 1.65        | 1.59     |
| 2   | D     | 602 | ATP  | PB-O3A  | 5.80  | 1.65        | 1.59     |
| 2   | H     | 602 | ATP  | PB-O3A  | 5.80  | 1.65        | 1.59     |
| 2   | F     | 602 | ATP  | PA-O3A  | 5.75  | 1.65        | 1.59     |
| 2   | E     | 601 | ATP  | PA-O3A  | 5.74  | 1.65        | 1.59     |
| 2   | H     | 602 | ATP  | PA-O3A  | 5.73  | 1.65        | 1.59     |
| 2   | A     | 602 | ATP  | PA-O3A  | 5.73  | 1.65        | 1.59     |
| 2   | D     | 602 | ATP  | PA-O3A  | 5.72  | 1.65        | 1.59     |
| 2   | A     | 602 | ATP  | PB-O3A  | 5.67  | 1.65        | 1.59     |
| 2   | B     | 602 | ATP  | PA-O3A  | 5.64  | 1.65        | 1.59     |
| 4   | F     | 604 | NAD  | PN-O3   | 5.62  | 1.65        | 1.59     |
| 2   | A     | 601 | ATP  | PA-O3A  | 5.60  | 1.65        | 1.59     |
| 2   | G     | 602 | ATP  | PB-O3A  | 5.57  | 1.65        | 1.59     |
| 2   | E     | 601 | ATP  | PB-O3A  | 5.53  | 1.65        | 1.59     |
| 2   | C     | 601 | ATP  | PA-O3A  | 5.44  | 1.65        | 1.59     |
| 2   | C     | 602 | ATP  | PB-O3A  | 5.42  | 1.65        | 1.59     |
| 2   | B     | 602 | ATP  | PB-O3A  | 5.41  | 1.65        | 1.59     |
| 2   | G     | 601 | ATP  | PA-O3A  | 5.39  | 1.65        | 1.59     |
| 2   | E     | 602 | ATP  | PB-O3A  | 5.38  | 1.65        | 1.59     |
| 4   | E     | 604 | NAD  | PN-O3   | 5.37  | 1.65        | 1.59     |
| 2   | H     | 601 | ATP  | PA-O3A  | 5.37  | 1.65        | 1.59     |
| 4   | B     | 604 | NAD  | O4B-C1B | -5.36 | 1.29        | 1.42     |
| 4   | C     | 604 | NAD  | O4B-C1B | -5.31 | 1.29        | 1.42     |
| 2   | F     | 602 | ATP  | PB-O3A  | 5.29  | 1.65        | 1.59     |
| 4   | A     | 604 | NAD  | PN-O3   | 5.28  | 1.65        | 1.59     |
| 4   | C     | 604 | NAD  | PN-O3   | 5.28  | 1.65        | 1.59     |
| 4   | A     | 604 | NAD  | PA-O3   | 5.25  | 1.65        | 1.59     |
| 2   | F     | 601 | ATP  | PA-O3A  | 5.23  | 1.65        | 1.59     |
| 4   | F     | 604 | NAD  | O4B-C1B | -5.22 | 1.29        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | H     | 604 | NAD  | O4B-C1B | -5.20 | 1.30        | 1.42     |
| 4   | E     | 604 | NAD  | O4B-C1B | -5.20 | 1.30        | 1.42     |
| 2   | C     | 601 | ATP  | PB-O3A  | 5.19  | 1.65        | 1.59     |
| 4   | C     | 604 | NAD  | PA-O3   | 5.17  | 1.65        | 1.59     |
| 2   | H     | 601 | ATP  | PB-O3A  | 5.12  | 1.65        | 1.59     |
| 4   | D     | 604 | NAD  | O4B-C1B | -5.10 | 1.30        | 1.42     |
| 2   | G     | 601 | ATP  | PB-O3A  | 5.09  | 1.65        | 1.59     |
| 4   | A     | 604 | NAD  | O4B-C1B | -5.08 | 1.30        | 1.42     |
| 4   | G     | 604 | NAD  | O4B-C1B | -5.07 | 1.30        | 1.42     |
| 2   | A     | 601 | ATP  | PB-O3A  | 5.07  | 1.65        | 1.59     |
| 4   | H     | 604 | NAD  | PA-O3   | 5.07  | 1.65        | 1.59     |
| 4   | B     | 604 | NAD  | PA-O3   | 5.05  | 1.64        | 1.59     |
| 2   | F     | 601 | ATP  | PB-O3A  | 5.04  | 1.64        | 1.59     |
| 2   | B     | 601 | ATP  | PA-O3A  | 5.02  | 1.64        | 1.59     |
| 4   | E     | 604 | NAD  | PA-O3   | 4.96  | 1.64        | 1.59     |
| 2   | D     | 601 | ATP  | PA-O3A  | 4.91  | 1.64        | 1.59     |
| 4   | D     | 604 | NAD  | PN-O3   | 4.89  | 1.64        | 1.59     |
| 2   | B     | 601 | ATP  | PB-O3A  | 4.82  | 1.64        | 1.59     |
| 4   | G     | 604 | NAD  | PN-O3   | 4.81  | 1.64        | 1.59     |
| 4   | B     | 604 | NAD  | PN-O3   | 4.78  | 1.64        | 1.59     |
| 4   | F     | 604 | NAD  | PA-O3   | 4.77  | 1.64        | 1.59     |
| 2   | D     | 601 | ATP  | PB-O3A  | 4.76  | 1.64        | 1.59     |
| 4   | G     | 604 | NAD  | PA-O3   | 4.58  | 1.64        | 1.59     |
| 2   | D     | 601 | ATP  | O4'-C1' | -4.56 | 1.31        | 1.42     |
| 4   | D     | 604 | NAD  | PA-O3   | 4.54  | 1.64        | 1.59     |
| 2   | B     | 601 | ATP  | O4'-C1' | -4.47 | 1.31        | 1.42     |
| 2   | H     | 601 | ATP  | O4'-C1' | -4.46 | 1.31        | 1.42     |
| 2   | A     | 601 | ATP  | O4'-C1' | -4.44 | 1.31        | 1.42     |
| 2   | G     | 601 | ATP  | O4'-C1' | -4.42 | 1.31        | 1.42     |
| 2   | F     | 601 | ATP  | O4'-C1' | -4.42 | 1.31        | 1.42     |
| 2   | C     | 601 | ATP  | O4'-C1' | -4.41 | 1.31        | 1.42     |
| 4   | H     | 604 | NAD  | C6A-N6A | 4.37  | 1.45        | 1.34     |
| 2   | E     | 601 | ATP  | O4'-C1' | -4.34 | 1.32        | 1.42     |
| 2   | G     | 602 | ATP  | O4'-C1' | -4.33 | 1.32        | 1.42     |
| 2   | A     | 602 | ATP  | O4'-C1' | -4.32 | 1.32        | 1.42     |
| 4   | H     | 604 | NAD  | PN-O3   | 4.31  | 1.64        | 1.59     |
| 2   | H     | 602 | ATP  | O4'-C1' | -4.30 | 1.32        | 1.42     |
| 2   | D     | 602 | ATP  | O4'-C1' | -4.28 | 1.32        | 1.42     |
| 2   | C     | 602 | ATP  | O4'-C1' | -4.28 | 1.32        | 1.42     |
| 2   | E     | 602 | ATP  | O4'-C1' | -4.28 | 1.32        | 1.42     |
| 2   | B     | 602 | ATP  | O4'-C1' | -4.26 | 1.32        | 1.42     |
| 2   | F     | 602 | ATP  | O4'-C1' | -4.23 | 1.32        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | F     | 604 | NAD  | C6A-N6A | 4.22  | 1.45        | 1.34     |
| 4   | E     | 604 | NAD  | C6A-N6A | 4.18  | 1.44        | 1.34     |
| 4   | C     | 604 | NAD  | C6A-N6A | 4.17  | 1.44        | 1.34     |
| 4   | D     | 604 | NAD  | C6A-N6A | 4.16  | 1.44        | 1.34     |
| 4   | A     | 604 | NAD  | C6A-N6A | 4.16  | 1.44        | 1.34     |
| 4   | B     | 604 | NAD  | C6A-N6A | 4.16  | 1.44        | 1.34     |
| 4   | G     | 604 | NAD  | C6A-N6A | 4.15  | 1.44        | 1.34     |
| 3   | C     | 603 | IMP  | C2-N1   | 4.14  | 1.42        | 1.35     |
| 3   | E     | 603 | IMP  | C2-N1   | 4.14  | 1.42        | 1.35     |
| 3   | H     | 603 | IMP  | C2-N1   | 4.13  | 1.42        | 1.35     |
| 3   | F     | 603 | IMP  | C2-N1   | 4.12  | 1.42        | 1.35     |
| 3   | G     | 603 | IMP  | C2-N1   | 4.11  | 1.42        | 1.35     |
| 3   | D     | 603 | IMP  | C2-N1   | 4.07  | 1.42        | 1.35     |
| 3   | B     | 603 | IMP  | C2-N1   | 4.06  | 1.42        | 1.35     |
| 3   | A     | 603 | IMP  | C2-N1   | 3.96  | 1.42        | 1.35     |
| 2   | D     | 601 | ATP  | PB-O3B  | 3.92  | 1.63        | 1.59     |
| 2   | B     | 601 | ATP  | C5'-C4' | -3.88 | 1.39        | 1.51     |
| 2   | E     | 602 | ATP  | C2'-C1' | 3.87  | 1.65        | 1.53     |
| 2   | F     | 602 | ATP  | C2'-C1' | 3.86  | 1.65        | 1.53     |
| 2   | B     | 602 | ATP  | C2'-C1' | 3.82  | 1.65        | 1.53     |
| 2   | H     | 602 | ATP  | C2'-C1' | 3.82  | 1.65        | 1.53     |
| 2   | E     | 601 | ATP  | C2'-C1' | 3.81  | 1.65        | 1.53     |
| 2   | A     | 602 | ATP  | C2'-C1' | 3.81  | 1.65        | 1.53     |
| 2   | C     | 602 | ATP  | C2'-C1' | 3.80  | 1.65        | 1.53     |
| 2   | B     | 601 | ATP  | C2'-C1' | 3.79  | 1.65        | 1.53     |
| 2   | H     | 601 | ATP  | C2'-C1' | 3.79  | 1.65        | 1.53     |
| 2   | D     | 601 | ATP  | C2'-C1' | 3.79  | 1.65        | 1.53     |
| 2   | C     | 601 | ATP  | C2'-C1' | 3.78  | 1.65        | 1.53     |
| 2   | D     | 602 | ATP  | C2'-C1' | 3.78  | 1.65        | 1.53     |
| 2   | G     | 602 | ATP  | C2'-C1' | 3.78  | 1.65        | 1.53     |
| 2   | A     | 601 | ATP  | C2'-C1' | 3.77  | 1.65        | 1.53     |
| 2   | F     | 601 | ATP  | C2'-C1' | 3.77  | 1.65        | 1.53     |
| 2   | G     | 601 | ATP  | C2'-C1' | 3.77  | 1.65        | 1.53     |
| 2   | E     | 602 | ATP  | C5'-C4' | -3.74 | 1.40        | 1.51     |
| 2   | F     | 602 | ATP  | C5'-C4' | -3.73 | 1.40        | 1.51     |
| 2   | A     | 601 | ATP  | C6-N6   | 3.70  | 1.43        | 1.34     |
| 2   | F     | 601 | ATP  | C6-N6   | 3.69  | 1.43        | 1.34     |
| 2   | A     | 602 | ATP  | C6-N6   | 3.69  | 1.43        | 1.34     |
| 4   | C     | 604 | NAD  | C5A-C4A | -3.69 | 1.32        | 1.39     |
| 2   | C     | 602 | ATP  | C6-N6   | 3.68  | 1.43        | 1.34     |
| 2   | H     | 602 | ATP  | C5'-C4' | -3.68 | 1.40        | 1.51     |
| 2   | B     | 601 | ATP  | C5-C4   | -3.68 | 1.32        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | F     | 602 | ATP  | C6-N6   | 3.68  | 1.43        | 1.34     |
| 2   | B     | 601 | ATP  | C6-N6   | 3.68  | 1.43        | 1.34     |
| 2   | B     | 602 | ATP  | C5'-C4' | -3.67 | 1.40        | 1.51     |
| 2   | C     | 601 | ATP  | C6-N6   | 3.67  | 1.43        | 1.34     |
| 2   | E     | 602 | ATP  | C6-N6   | 3.66  | 1.43        | 1.34     |
| 4   | B     | 604 | NAD  | C5A-C4A | -3.66 | 1.32        | 1.39     |
| 2   | D     | 601 | ATP  | C5'-C4' | -3.66 | 1.40        | 1.51     |
| 2   | B     | 602 | ATP  | C6-N6   | 3.65  | 1.43        | 1.34     |
| 2   | D     | 602 | ATP  | C6-N6   | 3.65  | 1.43        | 1.34     |
| 2   | A     | 602 | ATP  | C5'-C4' | -3.65 | 1.40        | 1.51     |
| 2   | E     | 601 | ATP  | C6-N6   | 3.65  | 1.43        | 1.34     |
| 2   | D     | 601 | ATP  | C6-N6   | 3.65  | 1.43        | 1.34     |
| 2   | G     | 602 | ATP  | C6-N6   | 3.65  | 1.43        | 1.34     |
| 2   | G     | 601 | ATP  | C6-N6   | 3.65  | 1.43        | 1.34     |
| 2   | H     | 602 | ATP  | C6-N6   | 3.65  | 1.43        | 1.34     |
| 2   | H     | 601 | ATP  | C6-N6   | 3.65  | 1.43        | 1.34     |
| 4   | D     | 604 | NAD  | C5A-C4A | -3.63 | 1.32        | 1.39     |
| 2   | G     | 601 | ATP  | C5-C4   | -3.62 | 1.32        | 1.39     |
| 4   | F     | 604 | NAD  | C5A-C4A | -3.62 | 1.32        | 1.39     |
| 2   | D     | 602 | ATP  | C5'-C4' | -3.61 | 1.40        | 1.51     |
| 2   | H     | 601 | ATP  | C5-C4   | -3.61 | 1.32        | 1.39     |
| 4   | G     | 604 | NAD  | C5A-C4A | -3.61 | 1.32        | 1.39     |
| 2   | E     | 601 | ATP  | C5'-C4' | -3.60 | 1.40        | 1.51     |
| 2   | F     | 602 | ATP  | C5-C4   | -3.59 | 1.32        | 1.39     |
| 2   | D     | 601 | ATP  | C5-C4   | -3.59 | 1.32        | 1.39     |
| 2   | A     | 601 | ATP  | C5-C4   | -3.59 | 1.32        | 1.39     |
| 2   | E     | 601 | ATP  | C5-C4   | -3.58 | 1.32        | 1.39     |
| 4   | A     | 604 | NAD  | C5A-C4A | -3.58 | 1.32        | 1.39     |
| 4   | E     | 604 | NAD  | C5A-C4A | -3.57 | 1.32        | 1.39     |
| 2   | F     | 601 | ATP  | C5-C4   | -3.57 | 1.32        | 1.39     |
| 2   | G     | 602 | ATP  | C5-C4   | -3.56 | 1.32        | 1.39     |
| 2   | C     | 601 | ATP  | C5-C4   | -3.56 | 1.32        | 1.39     |
| 2   | C     | 602 | ATP  | C5-C4   | -3.56 | 1.32        | 1.39     |
| 2   | H     | 602 | ATP  | C5-C4   | -3.56 | 1.32        | 1.39     |
| 2   | B     | 602 | ATP  | C5-C4   | -3.56 | 1.32        | 1.39     |
| 2   | A     | 602 | ATP  | C5-C4   | -3.55 | 1.32        | 1.39     |
| 2   | E     | 602 | ATP  | C5-C4   | -3.55 | 1.32        | 1.39     |
| 2   | C     | 602 | ATP  | C5'-C4' | -3.54 | 1.40        | 1.51     |
| 2   | D     | 602 | ATP  | C5-C4   | -3.53 | 1.32        | 1.39     |
| 2   | C     | 601 | ATP  | C5'-C4' | -3.50 | 1.41        | 1.51     |
| 2   | H     | 601 | ATP  | C5'-C4' | -3.50 | 1.41        | 1.51     |
| 3   | C     | 603 | IMP  | C5-N7   | -3.49 | 1.32        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | H     | 604 | NAD  | C5A-C4A | -3.49 | 1.32        | 1.39     |
| 3   | B     | 603 | IMP  | C5-N7   | -3.47 | 1.32        | 1.39     |
| 3   | G     | 603 | IMP  | C5-N7   | -3.47 | 1.32        | 1.39     |
| 4   | B     | 604 | NAD  | O7N-C7N | -3.47 | 1.17        | 1.24     |
| 3   | H     | 603 | IMP  | C5-N7   | -3.46 | 1.32        | 1.39     |
| 3   | D     | 603 | IMP  | C5-N7   | -3.46 | 1.32        | 1.39     |
| 3   | A     | 603 | IMP  | O6-C6   | -3.45 | 1.17        | 1.23     |
| 2   | G     | 601 | ATP  | C5'-C4' | -3.45 | 1.41        | 1.51     |
| 2   | F     | 601 | ATP  | C5'-C4' | -3.45 | 1.41        | 1.51     |
| 3   | E     | 603 | IMP  | C5-N7   | -3.45 | 1.32        | 1.39     |
| 3   | F     | 603 | IMP  | C5-N7   | -3.43 | 1.32        | 1.39     |
| 2   | G     | 602 | ATP  | C5'-C4' | -3.42 | 1.41        | 1.51     |
| 2   | A     | 601 | ATP  | C5'-C4' | -3.40 | 1.41        | 1.51     |
| 3   | A     | 603 | IMP  | C5-N7   | -3.39 | 1.32        | 1.39     |
| 3   | F     | 603 | IMP  | O6-C6   | -3.39 | 1.17        | 1.23     |
| 3   | B     | 603 | IMP  | O6-C6   | -3.38 | 1.17        | 1.23     |
| 3   | E     | 603 | IMP  | O6-C6   | -3.38 | 1.17        | 1.23     |
| 3   | G     | 603 | IMP  | O6-C6   | -3.37 | 1.17        | 1.23     |
| 3   | D     | 603 | IMP  | O6-C6   | -3.37 | 1.17        | 1.23     |
| 3   | H     | 603 | IMP  | O6-C6   | -3.36 | 1.17        | 1.23     |
| 4   | C     | 604 | NAD  | O7N-C7N | -3.36 | 1.17        | 1.24     |
| 3   | C     | 603 | IMP  | O6-C6   | -3.35 | 1.17        | 1.23     |
| 4   | G     | 604 | NAD  | O7N-C7N | -3.31 | 1.18        | 1.24     |
| 4   | F     | 604 | NAD  | O7N-C7N | -3.30 | 1.18        | 1.24     |
| 4   | A     | 604 | NAD  | O7N-C7N | -3.29 | 1.18        | 1.24     |
| 4   | D     | 604 | NAD  | O7N-C7N | -3.29 | 1.18        | 1.24     |
| 4   | E     | 604 | NAD  | O7N-C7N | -3.28 | 1.18        | 1.24     |
| 4   | H     | 604 | NAD  | O7N-C7N | -3.24 | 1.18        | 1.24     |
| 2   | A     | 601 | ATP  | C8-N9   | -3.19 | 1.32        | 1.37     |
| 2   | B     | 601 | ATP  | C8-N9   | -3.19 | 1.32        | 1.37     |
| 2   | D     | 601 | ATP  | C8-N9   | -3.18 | 1.32        | 1.37     |
| 2   | H     | 601 | ATP  | C8-N9   | -3.18 | 1.32        | 1.37     |
| 2   | C     | 601 | ATP  | C8-N9   | -3.17 | 1.32        | 1.37     |
| 2   | E     | 601 | ATP  | C8-N9   | -3.16 | 1.32        | 1.37     |
| 2   | F     | 601 | ATP  | C8-N9   | -3.16 | 1.32        | 1.37     |
| 2   | D     | 602 | ATP  | O3'-C3' | 3.15  | 1.50        | 1.43     |
| 2   | H     | 602 | ATP  | O3'-C3' | 3.14  | 1.50        | 1.43     |
| 2   | B     | 602 | ATP  | O3'-C3' | 3.12  | 1.50        | 1.43     |
| 2   | F     | 602 | ATP  | O3'-C3' | 3.12  | 1.50        | 1.43     |
| 2   | G     | 601 | ATP  | C8-N9   | -3.11 | 1.32        | 1.37     |
| 2   | E     | 602 | ATP  | O3'-C3' | 3.09  | 1.50        | 1.43     |
| 2   | A     | 602 | ATP  | O3'-C3' | 3.09  | 1.50        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | B     | 604 | NAD  | O2D-C2D | -3.08 | 1.35        | 1.43     |
| 4   | C     | 604 | NAD  | O2D-C2D | -3.08 | 1.35        | 1.43     |
| 2   | G     | 602 | ATP  | O3'-C3' | 3.07  | 1.50        | 1.43     |
| 4   | H     | 604 | NAD  | O2D-C2D | -3.07 | 1.35        | 1.43     |
| 2   | C     | 602 | ATP  | O3'-C3' | 3.07  | 1.50        | 1.43     |
| 4   | F     | 604 | NAD  | O2D-C2D | -3.07 | 1.35        | 1.43     |
| 2   | G     | 602 | ATP  | C8-N9   | -3.04 | 1.32        | 1.37     |
| 2   | A     | 601 | ATP  | O3'-C3' | 3.03  | 1.50        | 1.43     |
| 4   | G     | 604 | NAD  | O2D-C2D | -3.03 | 1.35        | 1.43     |
| 2   | D     | 601 | ATP  | O3'-C3' | 3.02  | 1.50        | 1.43     |
| 2   | E     | 602 | ATP  | C8-N9   | -3.01 | 1.32        | 1.37     |
| 4   | H     | 604 | NAD  | C8A-N9A | -3.01 | 1.32        | 1.37     |
| 2   | D     | 602 | ATP  | C3'-C4' | 3.01  | 1.60        | 1.53     |
| 4   | D     | 604 | NAD  | O2D-C2D | -3.01 | 1.35        | 1.43     |
| 2   | D     | 602 | ATP  | PA-O5'  | 3.01  | 1.71        | 1.59     |
| 2   | G     | 601 | ATP  | O3'-C3' | 3.00  | 1.50        | 1.43     |
| 4   | E     | 604 | NAD  | O2D-C2D | -3.00 | 1.35        | 1.43     |
| 2   | F     | 602 | ATP  | C8-N9   | -3.00 | 1.32        | 1.37     |
| 2   | C     | 601 | ATP  | O3'-C3' | 3.00  | 1.50        | 1.43     |
| 2   | F     | 601 | ATP  | O3'-C3' | 3.00  | 1.50        | 1.43     |
| 2   | A     | 602 | ATP  | C8-N9   | -3.00 | 1.32        | 1.37     |
| 2   | E     | 601 | ATP  | O3'-C3' | 2.99  | 1.50        | 1.43     |
| 4   | A     | 604 | NAD  | O2D-C2D | -2.99 | 1.35        | 1.43     |
| 2   | E     | 601 | ATP  | C5-N7   | -2.99 | 1.33        | 1.39     |
| 2   | H     | 601 | ATP  | O3'-C3' | 2.99  | 1.50        | 1.43     |
| 2   | H     | 602 | ATP  | PA-O5'  | 2.99  | 1.71        | 1.59     |
| 2   | A     | 601 | ATP  | C3'-C4' | 2.98  | 1.60        | 1.53     |
| 2   | C     | 602 | ATP  | C8-N9   | -2.98 | 1.32        | 1.37     |
| 2   | H     | 602 | ATP  | C3'-C4' | 2.98  | 1.60        | 1.53     |
| 2   | G     | 602 | ATP  | C3'-C4' | 2.98  | 1.60        | 1.53     |
| 2   | F     | 602 | ATP  | PA-O5'  | 2.97  | 1.71        | 1.59     |
| 2   | D     | 602 | ATP  | C8-N9   | -2.96 | 1.32        | 1.37     |
| 2   | A     | 602 | ATP  | C3'-C4' | 2.96  | 1.60        | 1.53     |
| 2   | E     | 602 | ATP  | PA-O5'  | 2.96  | 1.71        | 1.59     |
| 2   | C     | 602 | ATP  | C3'-C4' | 2.96  | 1.60        | 1.53     |
| 2   | B     | 602 | ATP  | PA-O5'  | 2.94  | 1.70        | 1.59     |
| 2   | B     | 602 | ATP  | C8-N9   | -2.94 | 1.32        | 1.37     |
| 2   | H     | 602 | ATP  | C8-N9   | -2.94 | 1.32        | 1.37     |
| 2   | D     | 601 | ATP  | C5-N7   | -2.92 | 1.33        | 1.39     |
| 2   | F     | 601 | ATP  | C3'-C4' | 2.91  | 1.60        | 1.53     |
| 4   | A     | 604 | NAD  | O2B-C2B | -2.91 | 1.35        | 1.43     |
| 2   | B     | 601 | ATP  | O3'-C3' | 2.91  | 1.50        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 601 | ATP  | PA-O5'  | 2.90  | 1.70        | 1.59     |
| 4   | H     | 604 | NAD  | O2B-C2B | -2.90 | 1.35        | 1.43     |
| 2   | F     | 601 | ATP  | C5-N7   | -2.90 | 1.33        | 1.39     |
| 2   | G     | 602 | ATP  | PB-O3B  | 2.90  | 1.62        | 1.59     |
| 2   | G     | 601 | ATP  | C3'-C4' | 2.89  | 1.60        | 1.53     |
| 2   | H     | 601 | ATP  | C3'-C4' | 2.89  | 1.60        | 1.53     |
| 2   | A     | 602 | ATP  | PA-O5'  | 2.89  | 1.70        | 1.59     |
| 4   | E     | 604 | NAD  | O2B-C2B | -2.89 | 1.35        | 1.43     |
| 2   | C     | 601 | ATP  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 2   | C     | 601 | ATP  | C3'-C4' | 2.88  | 1.60        | 1.53     |
| 4   | D     | 604 | NAD  | O2B-C2B | -2.88 | 1.35        | 1.43     |
| 4   | G     | 604 | NAD  | O2B-C2B | -2.86 | 1.35        | 1.43     |
| 2   | C     | 602 | ATP  | PA-O5'  | 2.86  | 1.70        | 1.59     |
| 4   | E     | 604 | NAD  | C5A-N7A | -2.86 | 1.33        | 1.39     |
| 2   | B     | 602 | ATP  | C3'-C4' | 2.85  | 1.60        | 1.53     |
| 2   | D     | 601 | ATP  | C3'-C4' | 2.85  | 1.60        | 1.53     |
| 2   | C     | 601 | ATP  | PA-O5'  | 2.85  | 1.70        | 1.59     |
| 4   | B     | 604 | NAD  | O2B-C2B | -2.84 | 1.35        | 1.43     |
| 2   | G     | 602 | ATP  | PA-O5'  | 2.84  | 1.70        | 1.59     |
| 2   | E     | 602 | ATP  | C3'-C4' | 2.84  | 1.60        | 1.53     |
| 4   | F     | 604 | NAD  | C5A-N7A | -2.84 | 1.33        | 1.39     |
| 4   | G     | 604 | NAD  | C4N-C3N | -2.84 | 1.35        | 1.39     |
| 2   | C     | 602 | ATP  | C5-N7   | -2.83 | 1.33        | 1.39     |
| 2   | H     | 601 | ATP  | C5-N7   | -2.83 | 1.33        | 1.39     |
| 4   | C     | 604 | NAD  | O2B-C2B | -2.83 | 1.35        | 1.43     |
| 4   | H     | 604 | NAD  | C5A-N7A | -2.82 | 1.33        | 1.39     |
| 2   | H     | 601 | ATP  | PA-O5'  | 2.82  | 1.70        | 1.59     |
| 2   | F     | 602 | ATP  | C3'-C4' | 2.82  | 1.60        | 1.53     |
| 2   | A     | 602 | ATP  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 2   | A     | 601 | ATP  | PA-O5'  | 2.81  | 1.70        | 1.59     |
| 4   | F     | 604 | NAD  | O2B-C2B | -2.81 | 1.36        | 1.43     |
| 4   | D     | 604 | NAD  | C5A-N7A | -2.81 | 1.33        | 1.39     |
| 4   | B     | 604 | NAD  | C4N-C3N | -2.81 | 1.35        | 1.39     |
| 2   | A     | 601 | ATP  | C5-N7   | -2.80 | 1.34        | 1.39     |
| 2   | G     | 601 | ATP  | C5-N7   | -2.80 | 1.34        | 1.39     |
| 4   | A     | 604 | NAD  | C5A-N7A | -2.80 | 1.34        | 1.39     |
| 2   | G     | 601 | ATP  | PA-O5'  | 2.80  | 1.70        | 1.59     |
| 2   | B     | 601 | ATP  | C5-N7   | -2.79 | 1.34        | 1.39     |
| 4   | G     | 604 | NAD  | C5A-N7A | -2.79 | 1.34        | 1.39     |
| 2   | B     | 602 | ATP  | C5-N7   | -2.79 | 1.34        | 1.39     |
| 2   | E     | 601 | ATP  | C3'-C4' | 2.78  | 1.60        | 1.53     |
| 2   | D     | 602 | ATP  | PB-O3B  | 2.78  | 1.62        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | G     | 602 | ATP  | C5-N7   | -2.78 | 1.34        | 1.39     |
| 2   | D     | 602 | ATP  | C5-N7   | -2.77 | 1.34        | 1.39     |
| 3   | D     | 603 | IMP  | C4-N9   | -2.76 | 1.31        | 1.38     |
| 2   | F     | 601 | ATP  | PA-O5'  | 2.75  | 1.70        | 1.59     |
| 2   | E     | 602 | ATP  | C5-N7   | -2.75 | 1.34        | 1.39     |
| 4   | C     | 604 | NAD  | C5A-N7A | -2.75 | 1.34        | 1.39     |
| 4   | F     | 604 | NAD  | C8A-N9A | -2.75 | 1.32        | 1.37     |
| 4   | A     | 604 | NAD  | C4N-C3N | -2.75 | 1.35        | 1.39     |
| 2   | H     | 602 | ATP  | C5-N7   | -2.74 | 1.34        | 1.39     |
| 4   | B     | 604 | NAD  | C5A-N7A | -2.74 | 1.34        | 1.39     |
| 2   | F     | 602 | ATP  | C5-N7   | -2.72 | 1.34        | 1.39     |
| 4   | H     | 604 | NAD  | C4N-C3N | -2.72 | 1.35        | 1.39     |
| 4   | D     | 604 | NAD  | C8A-N9A | -2.72 | 1.32        | 1.37     |
| 2   | E     | 601 | ATP  | O4'-C4' | 2.71  | 1.51        | 1.45     |
| 4   | D     | 604 | NAD  | C4N-C3N | -2.70 | 1.35        | 1.39     |
| 4   | B     | 604 | NAD  | C8A-N9A | -2.70 | 1.33        | 1.37     |
| 2   | B     | 601 | ATP  | PA-O5'  | 2.69  | 1.69        | 1.59     |
| 2   | E     | 601 | ATP  | PA-O5'  | 2.69  | 1.69        | 1.59     |
| 2   | B     | 601 | ATP  | C3'-C4' | 2.69  | 1.59        | 1.53     |
| 2   | A     | 602 | ATP  | PB-O3B  | 2.69  | 1.62        | 1.59     |
| 4   | E     | 604 | NAD  | C8A-N9A | -2.69 | 1.33        | 1.37     |
| 4   | C     | 604 | NAD  | C4N-C3N | -2.68 | 1.35        | 1.39     |
| 3   | G     | 603 | IMP  | C4-N9   | -2.68 | 1.31        | 1.38     |
| 2   | A     | 601 | ATP  | O4'-C4' | 2.68  | 1.51        | 1.45     |
| 4   | H     | 604 | NAD  | O3B-C3B | 2.68  | 1.49        | 1.43     |
| 4   | C     | 604 | NAD  | C8A-N9A | -2.68 | 1.33        | 1.37     |
| 4   | A     | 604 | NAD  | C8A-N9A | -2.68 | 1.33        | 1.37     |
| 3   | B     | 603 | IMP  | C4-N9   | -2.68 | 1.31        | 1.38     |
| 4   | E     | 604 | NAD  | C4N-C3N | -2.67 | 1.35        | 1.39     |
| 2   | C     | 602 | ATP  | O4'-C4' | 2.67  | 1.50        | 1.45     |
| 3   | H     | 603 | IMP  | C4-N9   | -2.67 | 1.31        | 1.38     |
| 4   | G     | 604 | NAD  | C8A-N9A | -2.67 | 1.33        | 1.37     |
| 3   | A     | 603 | IMP  | C4-N9   | -2.67 | 1.31        | 1.38     |
| 3   | F     | 603 | IMP  | C4-N9   | -2.67 | 1.31        | 1.38     |
| 3   | E     | 603 | IMP  | C4-N9   | -2.66 | 1.31        | 1.38     |
| 4   | F     | 604 | NAD  | O3B-C3B | 2.65  | 1.49        | 1.43     |
| 2   | A     | 602 | ATP  | O4'-C4' | 2.65  | 1.50        | 1.45     |
| 4   | F     | 604 | NAD  | C4N-C3N | -2.65 | 1.35        | 1.39     |
| 2   | G     | 602 | ATP  | O4'-C4' | 2.64  | 1.50        | 1.45     |
| 4   | C     | 604 | NAD  | O3B-C3B | 2.64  | 1.49        | 1.43     |
| 2   | G     | 601 | ATP  | O4'-C4' | 2.64  | 1.50        | 1.45     |
| 2   | F     | 601 | ATP  | O4'-C4' | 2.63  | 1.50        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 602 | ATP  | O4'-C4' | 2.63  | 1.50        | 1.45     |
| 2   | F     | 601 | ATP  | PB-O3B  | 2.63  | 1.62        | 1.59     |
| 3   | C     | 603 | IMP  | C4-N9   | -2.61 | 1.31        | 1.38     |
| 4   | E     | 604 | NAD  | O3B-C3B | 2.60  | 1.49        | 1.43     |
| 2   | H     | 601 | ATP  | O4'-C4' | 2.60  | 1.50        | 1.45     |
| 2   | D     | 602 | ATP  | O4'-C4' | 2.59  | 1.50        | 1.45     |
| 2   | C     | 601 | ATP  | O4'-C4' | 2.59  | 1.50        | 1.45     |
| 4   | B     | 604 | NAD  | O3B-C3B | 2.56  | 1.49        | 1.43     |
| 4   | A     | 604 | NAD  | O3B-C3B | 2.56  | 1.49        | 1.43     |
| 4   | F     | 604 | NAD  | O3D-C3D | 2.55  | 1.49        | 1.43     |
| 4   | G     | 604 | NAD  | O3B-C3B | 2.55  | 1.49        | 1.43     |
| 2   | E     | 601 | ATP  | PB-O3B  | 2.54  | 1.62        | 1.59     |
| 2   | D     | 601 | ATP  | O4'-C4' | 2.53  | 1.50        | 1.45     |
| 2   | F     | 602 | ATP  | O4'-C4' | 2.52  | 1.50        | 1.45     |
| 4   | E     | 604 | NAD  | O3D-C3D | 2.52  | 1.49        | 1.43     |
| 4   | G     | 604 | NAD  | O3D-C3D | 2.52  | 1.49        | 1.43     |
| 4   | D     | 604 | NAD  | O3B-C3B | 2.52  | 1.49        | 1.43     |
| 2   | B     | 602 | ATP  | O4'-C4' | 2.51  | 1.50        | 1.45     |
| 4   | B     | 604 | NAD  | O3D-C3D | 2.51  | 1.49        | 1.43     |
| 4   | H     | 604 | NAD  | O3D-C3D | 2.51  | 1.49        | 1.43     |
| 4   | C     | 604 | NAD  | O3D-C3D | 2.50  | 1.49        | 1.43     |
| 2   | E     | 602 | ATP  | O4'-C4' | 2.49  | 1.50        | 1.45     |
| 4   | H     | 604 | NAD  | C4A-N9A | -2.46 | 1.32        | 1.37     |
| 4   | D     | 604 | NAD  | O3D-C3D | 2.44  | 1.49        | 1.43     |
| 2   | B     | 601 | ATP  | O4'-C4' | 2.42  | 1.50        | 1.45     |
| 2   | B     | 601 | ATP  | PB-O3B  | 2.41  | 1.62        | 1.59     |
| 2   | B     | 602 | ATP  | PB-O3B  | 2.40  | 1.62        | 1.59     |
| 4   | C     | 604 | NAD  | C4A-N9A | -2.38 | 1.32        | 1.37     |
| 4   | A     | 604 | NAD  | O3D-C3D | 2.38  | 1.48        | 1.43     |
| 2   | H     | 602 | ATP  | PB-O3B  | 2.35  | 1.62        | 1.59     |
| 4   | B     | 604 | NAD  | C4A-N9A | -2.33 | 1.32        | 1.37     |
| 2   | F     | 602 | ATP  | PB-O3B  | 2.32  | 1.62        | 1.59     |
| 2   | A     | 602 | ATP  | O2'-C2' | 2.32  | 1.48        | 1.43     |
| 2   | B     | 602 | ATP  | O2'-C2' | 2.31  | 1.48        | 1.43     |
| 2   | E     | 602 | ATP  | O2'-C2' | 2.30  | 1.48        | 1.43     |
| 2   | F     | 602 | ATP  | O2'-C2' | 2.30  | 1.48        | 1.43     |
| 2   | C     | 602 | ATP  | O2'-C2' | 2.29  | 1.48        | 1.43     |
| 2   | D     | 602 | ATP  | O2'-C2' | 2.28  | 1.48        | 1.43     |
| 2   | G     | 602 | ATP  | O2'-C2' | 2.27  | 1.48        | 1.43     |
| 4   | G     | 604 | NAD  | C4A-N9A | -2.27 | 1.33        | 1.37     |
| 4   | A     | 604 | NAD  | C5N-C4N | -2.26 | 1.35        | 1.38     |
| 2   | G     | 601 | ATP  | C1'-N9  | -2.26 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 602 | ATP  | O2'-C2' | 2.26  | 1.48        | 1.43     |
| 2   | C     | 601 | ATP  | C1'-N9  | -2.26 | 1.40        | 1.46     |
| 2   | A     | 601 | ATP  | C1'-N9  | -2.25 | 1.40        | 1.46     |
| 2   | D     | 601 | ATP  | O2'-C2' | 2.25  | 1.48        | 1.43     |
| 2   | D     | 601 | ATP  | C1'-N9  | -2.24 | 1.40        | 1.46     |
| 2   | C     | 602 | ATP  | PB-O3B  | 2.24  | 1.61        | 1.59     |
| 2   | C     | 601 | ATP  | O2'-C2' | 2.24  | 1.48        | 1.43     |
| 2   | F     | 601 | ATP  | C1'-N9  | -2.24 | 1.40        | 1.46     |
| 4   | A     | 604 | NAD  | C4A-N9A | -2.23 | 1.33        | 1.37     |
| 2   | H     | 601 | ATP  | C1'-N9  | -2.23 | 1.40        | 1.46     |
| 4   | C     | 604 | NAD  | C5N-C4N | -2.23 | 1.35        | 1.38     |
| 2   | E     | 601 | ATP  | O2'-C2' | 2.23  | 1.48        | 1.43     |
| 2   | B     | 601 | ATP  | O2'-C2' | 2.23  | 1.48        | 1.43     |
| 4   | F     | 604 | NAD  | C4A-N9A | -2.22 | 1.33        | 1.37     |
| 2   | A     | 601 | ATP  | O2'-C2' | 2.22  | 1.48        | 1.43     |
| 4   | G     | 604 | NAD  | C5N-C4N | -2.21 | 1.35        | 1.38     |
| 4   | E     | 604 | NAD  | C4A-N9A | -2.21 | 1.33        | 1.37     |
| 4   | D     | 604 | NAD  | C4A-N9A | -2.21 | 1.33        | 1.37     |
| 2   | F     | 601 | ATP  | O2'-C2' | 2.20  | 1.48        | 1.43     |
| 2   | G     | 601 | ATP  | O2'-C2' | 2.20  | 1.48        | 1.43     |
| 2   | E     | 601 | ATP  | C1'-N9  | -2.20 | 1.40        | 1.46     |
| 2   | H     | 601 | ATP  | O2'-C2' | 2.19  | 1.48        | 1.43     |
| 2   | C     | 601 | ATP  | PB-O3B  | 2.19  | 1.61        | 1.59     |
| 2   | B     | 601 | ATP  | C1'-N9  | -2.18 | 1.40        | 1.46     |
| 4   | H     | 604 | NAD  | C5N-C4N | -2.17 | 1.35        | 1.38     |
| 4   | B     | 604 | NAD  | C5N-C4N | -2.17 | 1.35        | 1.38     |
| 4   | F     | 604 | NAD  | C5N-C4N | -2.15 | 1.35        | 1.38     |
| 2   | E     | 602 | ATP  | PB-O3B  | 2.14  | 1.61        | 1.59     |
| 4   | D     | 604 | NAD  | C5N-C4N | -2.13 | 1.35        | 1.38     |
| 4   | E     | 604 | NAD  | C5N-C4N | -2.12 | 1.35        | 1.38     |
| 2   | G     | 601 | ATP  | PB-O3B  | 2.06  | 1.61        | 1.59     |
| 3   | B     | 603 | IMP  | C5-C6   | 2.06  | 1.52        | 1.44     |
| 3   | G     | 603 | IMP  | C5-C6   | 2.05  | 1.52        | 1.44     |
| 3   | H     | 603 | IMP  | C5-C6   | 2.05  | 1.52        | 1.44     |
| 3   | C     | 603 | IMP  | C5-C6   | 2.05  | 1.52        | 1.44     |
| 3   | D     | 603 | IMP  | C5-C6   | 2.04  | 1.52        | 1.44     |
| 3   | F     | 603 | IMP  | C5-C6   | 2.04  | 1.52        | 1.44     |
| 3   | E     | 603 | IMP  | C5-C6   | 2.04  | 1.52        | 1.44     |
| 2   | H     | 601 | ATP  | PB-O3B  | 2.03  | 1.61        | 1.59     |
| 2   | B     | 601 | ATP  | C4-N9   | -2.02 | 1.33        | 1.37     |
| 3   | A     | 603 | IMP  | C5-C6   | 2.02  | 1.52        | 1.44     |

All (402) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | E     | 602 | ATP  | N6-C6-N1  | -9.18 | 97.92       | 118.38   |
| 2   | F     | 602 | ATP  | N6-C6-N1  | -9.14 | 98.01       | 118.38   |
| 2   | H     | 602 | ATP  | N6-C6-N1  | -9.14 | 98.03       | 118.38   |
| 2   | D     | 602 | ATP  | N6-C6-N1  | -9.13 | 98.04       | 118.38   |
| 2   | C     | 602 | ATP  | N6-C6-N1  | -9.12 | 98.05       | 118.38   |
| 2   | A     | 602 | ATP  | N6-C6-N1  | -9.12 | 98.07       | 118.38   |
| 2   | B     | 602 | ATP  | N6-C6-N1  | -9.10 | 98.11       | 118.38   |
| 2   | G     | 602 | ATP  | N6-C6-N1  | -9.05 | 98.22       | 118.38   |
| 2   | D     | 601 | ATP  | N6-C6-N1  | -9.04 | 98.25       | 118.38   |
| 2   | B     | 601 | ATP  | N6-C6-N1  | -9.03 | 98.27       | 118.38   |
| 2   | G     | 601 | ATP  | N6-C6-N1  | -8.98 | 98.37       | 118.38   |
| 2   | H     | 601 | ATP  | N6-C6-N1  | -8.98 | 98.38       | 118.38   |
| 2   | C     | 601 | ATP  | N6-C6-N1  | -8.97 | 98.41       | 118.38   |
| 2   | A     | 601 | ATP  | N6-C6-N1  | -8.93 | 98.48       | 118.38   |
| 2   | F     | 601 | ATP  | N6-C6-N1  | -8.88 | 98.60       | 118.38   |
| 2   | E     | 601 | ATP  | N6-C6-N1  | -8.77 | 98.85       | 118.38   |
| 2   | B     | 601 | ATP  | C4-N9-C1' | -7.86 | 108.26      | 126.63   |
| 2   | B     | 601 | ATP  | C5-C6-N6  | 7.67  | 142.28      | 123.29   |
| 2   | C     | 602 | ATP  | C5-C6-N6  | 7.62  | 142.14      | 123.29   |
| 2   | D     | 601 | ATP  | C5-C6-N6  | 7.62  | 142.14      | 123.29   |
| 2   | E     | 602 | ATP  | C5-C6-N6  | 7.60  | 142.11      | 123.29   |
| 2   | F     | 602 | ATP  | C5-C6-N6  | 7.59  | 142.08      | 123.29   |
| 2   | G     | 601 | ATP  | C5-C6-N6  | 7.56  | 142.00      | 123.29   |
| 2   | H     | 602 | ATP  | C5-C6-N6  | 7.56  | 142.00      | 123.29   |
| 2   | D     | 602 | ATP  | C5-C6-N6  | 7.55  | 141.97      | 123.29   |
| 2   | A     | 602 | ATP  | C5-C6-N6  | 7.54  | 141.96      | 123.29   |
| 2   | G     | 602 | ATP  | C5-C6-N6  | 7.54  | 141.96      | 123.29   |
| 2   | H     | 602 | ATP  | C4-N9-C1' | -7.54 | 108.99      | 126.63   |
| 2   | B     | 602 | ATP  | C5-C6-N6  | 7.54  | 141.96      | 123.29   |
| 2   | H     | 601 | ATP  | C5-C6-N6  | 7.54  | 141.95      | 123.29   |
| 2   | H     | 601 | ATP  | C4-N9-C1' | -7.54 | 109.00      | 126.63   |
| 2   | A     | 601 | ATP  | C5-C6-N6  | 7.51  | 141.88      | 123.29   |
| 2   | C     | 601 | ATP  | C5-C6-N6  | 7.51  | 141.88      | 123.29   |
| 2   | B     | 602 | ATP  | C4-N9-C1' | -7.49 | 109.12      | 126.63   |
| 2   | A     | 602 | ATP  | C4-N9-C1' | -7.48 | 109.15      | 126.63   |
| 2   | F     | 601 | ATP  | C5-C6-N6  | 7.45  | 141.73      | 123.29   |
| 2   | D     | 602 | ATP  | C4-N9-C1' | -7.44 | 109.22      | 126.63   |
| 2   | F     | 602 | ATP  | C4-N9-C1' | -7.43 | 109.25      | 126.63   |
| 3   | E     | 603 | IMP  | C5-C6-N1  | 7.42  | 121.44      | 110.78   |
| 2   | G     | 601 | ATP  | C4-N9-C1' | -7.41 | 109.31      | 126.63   |
| 3   | H     | 603 | IMP  | C5-C6-N1  | 7.39  | 121.41      | 110.78   |
| 2   | G     | 602 | ATP  | C4-N9-C1' | -7.39 | 109.35      | 126.63   |
| 2   | C     | 602 | ATP  | C4-N9-C1' | -7.39 | 109.35      | 126.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 601 | ATP  | C5-C6-N6    | 7.38  | 141.56      | 123.29   |
| 3   | G     | 603 | IMP  | C5-C6-N1    | 7.37  | 121.38      | 110.78   |
| 3   | D     | 603 | IMP  | C5-C6-N1    | 7.36  | 121.36      | 110.78   |
| 3   | B     | 603 | IMP  | C5-C6-N1    | 7.36  | 121.36      | 110.78   |
| 3   | F     | 603 | IMP  | C5-C6-N1    | 7.34  | 121.34      | 110.78   |
| 3   | A     | 603 | IMP  | C5-C6-N1    | 7.32  | 121.30      | 110.78   |
| 2   | E     | 602 | ATP  | C4-N9-C1'   | -7.29 | 109.57      | 126.63   |
| 3   | C     | 603 | IMP  | C5-C6-N1    | 7.28  | 121.24      | 110.78   |
| 2   | A     | 601 | ATP  | C4-N9-C1'   | -7.17 | 109.86      | 126.63   |
| 4   | H     | 604 | NAD  | N6A-C6A-N1A | -7.16 | 102.44      | 118.38   |
| 4   | A     | 604 | NAD  | N6A-C6A-N1A | -7.14 | 102.47      | 118.38   |
| 2   | C     | 601 | ATP  | C4-N9-C1'   | -7.09 | 110.04      | 126.63   |
| 2   | D     | 601 | ATP  | C4-N9-C1'   | -7.06 | 110.12      | 126.63   |
| 4   | H     | 604 | NAD  | C4A-N9A-C1B | -7.06 | 110.13      | 126.63   |
| 2   | E     | 601 | ATP  | C4-N9-C1'   | -7.05 | 110.15      | 126.63   |
| 2   | F     | 601 | ATP  | C4-N9-C1'   | -7.02 | 110.22      | 126.63   |
| 4   | G     | 604 | NAD  | N6A-C6A-N1A | -7.01 | 102.77      | 118.38   |
| 4   | C     | 604 | NAD  | N6A-C6A-N1A | -6.91 | 102.98      | 118.38   |
| 4   | D     | 604 | NAD  | N6A-C6A-N1A | -6.91 | 102.99      | 118.38   |
| 4   | C     | 604 | NAD  | C4A-N9A-C1B | -6.90 | 110.49      | 126.63   |
| 4   | B     | 604 | NAD  | N6A-C6A-N1A | -6.89 | 103.02      | 118.38   |
| 4   | E     | 604 | NAD  | N6A-C6A-N1A | -6.86 | 103.09      | 118.38   |
| 4   | F     | 604 | NAD  | N6A-C6A-N1A | -6.85 | 103.11      | 118.38   |
| 4   | A     | 604 | NAD  | C4A-N9A-C1B | -6.71 | 110.93      | 126.63   |
| 4   | B     | 604 | NAD  | C4A-N9A-C1B | -6.71 | 110.93      | 126.63   |
| 4   | G     | 604 | NAD  | C4A-N9A-C1B | -6.69 | 110.98      | 126.63   |
| 4   | D     | 604 | NAD  | C4A-N9A-C1B | -6.65 | 111.07      | 126.63   |
| 4   | E     | 604 | NAD  | C4A-N9A-C1B | -6.47 | 111.49      | 126.63   |
| 4   | F     | 604 | NAD  | C4A-N9A-C1B | -6.46 | 111.51      | 126.63   |
| 2   | B     | 601 | ATP  | C1'-N9-C8   | 6.29  | 141.05      | 127.09   |
| 2   | H     | 602 | ATP  | C1'-N9-C8   | 6.04  | 140.50      | 127.09   |
| 2   | A     | 602 | ATP  | C1'-N9-C8   | 6.02  | 140.45      | 127.09   |
| 2   | D     | 602 | ATP  | C1'-N9-C8   | 6.01  | 140.42      | 127.09   |
| 2   | B     | 602 | ATP  | C1'-N9-C8   | 5.96  | 140.33      | 127.09   |
| 2   | C     | 602 | ATP  | C1'-N9-C8   | 5.96  | 140.32      | 127.09   |
| 2   | H     | 601 | ATP  | C1'-N9-C8   | 5.91  | 140.21      | 127.09   |
| 2   | F     | 602 | ATP  | C1'-N9-C8   | 5.91  | 140.21      | 127.09   |
| 2   | G     | 602 | ATP  | C1'-N9-C8   | 5.89  | 140.16      | 127.09   |
| 2   | B     | 601 | ATP  | N3-C2-N1    | -5.83 | 119.75      | 128.58   |
| 2   | G     | 601 | ATP  | N3-C2-N1    | -5.83 | 119.76      | 128.58   |
| 2   | H     | 601 | ATP  | N3-C2-N1    | -5.82 | 119.78      | 128.58   |
| 4   | C     | 604 | NAD  | N3A-C2A-N1A | -5.80 | 119.81      | 128.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | G     | 601 | ATP  | C1'-N9-C8   | 5.79  | 139.95      | 127.09   |
| 4   | H     | 604 | NAD  | C5A-C6A-N6A | 5.78  | 137.60      | 123.29   |
| 4   | G     | 604 | NAD  | N3A-C2A-N1A | -5.77 | 119.85      | 128.58   |
| 4   | A     | 604 | NAD  | N3A-C2A-N1A | -5.77 | 119.85      | 128.58   |
| 2   | C     | 601 | ATP  | N3-C2-N1    | -5.76 | 119.86      | 128.58   |
| 4   | B     | 604 | NAD  | N3A-C2A-N1A | -5.75 | 119.88      | 128.58   |
| 4   | D     | 604 | NAD  | N3A-C2A-N1A | -5.75 | 119.88      | 128.58   |
| 2   | E     | 602 | ATP  | C1'-N9-C8   | 5.71  | 139.78      | 127.09   |
| 4   | F     | 604 | NAD  | N3A-C2A-N1A | -5.70 | 119.95      | 128.58   |
| 2   | D     | 601 | ATP  | N3-C2-N1    | -5.70 | 119.95      | 128.58   |
| 2   | F     | 601 | ATP  | N3-C2-N1    | -5.70 | 119.96      | 128.58   |
| 2   | G     | 601 | ATP  | N9-C8-N7    | -5.69 | 105.86      | 113.94   |
| 2   | E     | 601 | ATP  | N3-C2-N1    | -5.69 | 119.97      | 128.58   |
| 4   | A     | 604 | NAD  | C5A-C6A-N6A | 5.69  | 137.37      | 123.29   |
| 2   | A     | 601 | ATP  | N3-C2-N1    | -5.68 | 119.98      | 128.58   |
| 2   | H     | 601 | ATP  | N9-C8-N7    | -5.66 | 105.90      | 113.94   |
| 2   | E     | 602 | ATP  | N3-C2-N1    | -5.66 | 120.01      | 128.58   |
| 2   | E     | 602 | ATP  | N9-C8-N7    | -5.64 | 105.94      | 113.94   |
| 4   | E     | 604 | NAD  | N3A-C2A-N1A | -5.64 | 120.05      | 128.58   |
| 2   | H     | 602 | ATP  | N3-C2-N1    | -5.63 | 120.05      | 128.58   |
| 2   | C     | 601 | ATP  | N9-C8-N7    | -5.62 | 105.96      | 113.94   |
| 2   | B     | 601 | ATP  | N9-C8-N7    | -5.62 | 105.97      | 113.94   |
| 4   | H     | 604 | NAD  | N9A-C8A-N7A | -5.61 | 105.97      | 113.94   |
| 2   | F     | 602 | ATP  | N3-C2-N1    | -5.60 | 120.11      | 128.58   |
| 2   | B     | 602 | ATP  | N3-C2-N1    | -5.60 | 120.11      | 128.58   |
| 2   | D     | 602 | ATP  | N3-C2-N1    | -5.60 | 120.11      | 128.58   |
| 2   | H     | 602 | ATP  | N9-C8-N7    | -5.60 | 106.00      | 113.94   |
| 2   | A     | 601 | ATP  | C1'-N9-C8   | 5.59  | 139.51      | 127.09   |
| 4   | G     | 604 | NAD  | C5A-C6A-N6A | 5.58  | 137.11      | 123.29   |
| 2   | F     | 602 | ATP  | N9-C8-N7    | -5.58 | 106.02      | 113.94   |
| 2   | E     | 601 | ATP  | C1'-N9-C8   | 5.57  | 139.45      | 127.09   |
| 2   | B     | 602 | ATP  | N9-C8-N7    | -5.56 | 106.05      | 113.94   |
| 2   | C     | 602 | ATP  | N3-C2-N1    | -5.55 | 120.17      | 128.58   |
| 2   | D     | 601 | ATP  | C1'-N9-C8   | 5.55  | 139.41      | 127.09   |
| 2   | A     | 602 | ATP  | N3-C2-N1    | -5.55 | 120.18      | 128.58   |
| 2   | G     | 602 | ATP  | N3-C2-N1    | -5.54 | 120.20      | 128.58   |
| 4   | H     | 604 | NAD  | C1B-N9A-C8A | 5.53  | 139.37      | 127.09   |
| 4   | B     | 604 | NAD  | C5A-C6A-N6A | 5.52  | 136.95      | 123.29   |
| 2   | A     | 601 | ATP  | N9-C8-N7    | -5.52 | 106.11      | 113.94   |
| 4   | C     | 604 | NAD  | N9A-C8A-N7A | -5.51 | 106.12      | 113.94   |
| 4   | D     | 604 | NAD  | C5A-C6A-N6A | 5.51  | 136.92      | 123.29   |
| 2   | F     | 601 | ATP  | N9-C8-N7    | -5.50 | 106.13      | 113.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | C     | 604 | NAD  | C5A-C6A-N6A | 5.50  | 136.91      | 123.29   |
| 2   | D     | 602 | ATP  | N9-C8-N7    | -5.47 | 106.17      | 113.94   |
| 4   | E     | 604 | NAD  | C5A-C6A-N6A | 5.47  | 136.83      | 123.29   |
| 4   | B     | 604 | NAD  | N9A-C8A-N7A | -5.47 | 106.18      | 113.94   |
| 2   | D     | 601 | ATP  | N9-C8-N7    | -5.46 | 106.18      | 113.94   |
| 2   | C     | 601 | ATP  | C1'-N9-C8   | 5.46  | 139.22      | 127.09   |
| 2   | F     | 601 | ATP  | C1'-N9-C8   | 5.46  | 139.21      | 127.09   |
| 2   | G     | 602 | ATP  | N9-C8-N7    | -5.46 | 106.19      | 113.94   |
| 2   | C     | 602 | ATP  | N9-C8-N7    | -5.45 | 106.20      | 113.94   |
| 2   | A     | 602 | ATP  | N9-C8-N7    | -5.45 | 106.21      | 113.94   |
| 4   | F     | 604 | NAD  | C5A-C6A-N6A | 5.44  | 136.76      | 123.29   |
| 4   | H     | 604 | NAD  | N3A-C2A-N1A | -5.40 | 120.41      | 128.58   |
| 4   | A     | 604 | NAD  | C1B-N9A-C8A | 5.40  | 139.07      | 127.09   |
| 2   | E     | 601 | ATP  | N9-C8-N7    | -5.39 | 106.28      | 113.94   |
| 4   | C     | 604 | NAD  | C1B-N9A-C8A | 5.39  | 139.05      | 127.09   |
| 4   | G     | 604 | NAD  | N9A-C8A-N7A | -5.38 | 106.31      | 113.94   |
| 4   | D     | 604 | NAD  | N9A-C8A-N7A | -5.32 | 106.39      | 113.94   |
| 4   | G     | 604 | NAD  | C1B-N9A-C8A | 5.29  | 138.83      | 127.09   |
| 4   | E     | 604 | NAD  | N9A-C8A-N7A | -5.28 | 106.44      | 113.94   |
| 4   | D     | 604 | NAD  | C1B-N9A-C8A | 5.26  | 138.77      | 127.09   |
| 4   | A     | 604 | NAD  | N9A-C8A-N7A | -5.25 | 106.49      | 113.94   |
| 4   | B     | 604 | NAD  | C1B-N9A-C8A | 5.22  | 138.67      | 127.09   |
| 4   | F     | 604 | NAD  | N9A-C8A-N7A | -5.20 | 106.56      | 113.94   |
| 3   | C     | 603 | IMP  | C2-N1-C6    | -5.12 | 118.07      | 125.09   |
| 4   | E     | 604 | NAD  | C1B-N9A-C8A | 5.12  | 138.46      | 127.09   |
| 4   | F     | 604 | NAD  | C1B-N9A-C8A | 5.11  | 138.44      | 127.09   |
| 3   | F     | 603 | IMP  | C2-N1-C6    | -5.09 | 118.12      | 125.09   |
| 3   | G     | 603 | IMP  | C2-N1-C6    | -5.07 | 118.14      | 125.09   |
| 3   | E     | 603 | IMP  | C2-N1-C6    | -5.06 | 118.15      | 125.09   |
| 3   | H     | 603 | IMP  | C2-N1-C6    | -5.06 | 118.16      | 125.09   |
| 3   | A     | 603 | IMP  | C2-N1-C6    | -5.04 | 118.19      | 125.09   |
| 3   | B     | 603 | IMP  | C2-N1-C6    | -5.01 | 118.22      | 125.09   |
| 3   | D     | 603 | IMP  | C2-N1-C6    | -4.97 | 118.28      | 125.09   |
| 2   | H     | 601 | ATP  | C4-N9-C8    | 4.80  | 110.77      | 105.74   |
| 3   | C     | 603 | IMP  | C5-C4-N3    | -4.79 | 120.21      | 127.27   |
| 2   | C     | 601 | ATP  | C4-N9-C8    | 4.74  | 110.72      | 105.74   |
| 2   | G     | 601 | ATP  | C4-N9-C8    | 4.74  | 110.72      | 105.74   |
| 2   | B     | 601 | ATP  | C4-N9-C8    | 4.71  | 110.69      | 105.74   |
| 2   | E     | 602 | ATP  | C4-N9-C8    | 4.67  | 110.64      | 105.74   |
| 3   | A     | 603 | IMP  | C5-C4-N3    | -4.67 | 120.39      | 127.27   |
| 3   | B     | 603 | IMP  | C5-C4-N3    | -4.65 | 120.42      | 127.27   |
| 3   | F     | 603 | IMP  | C5-C4-N3    | -4.65 | 120.43      | 127.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | G     | 603 | IMP  | C5-C4-N3    | -4.64 | 120.44      | 127.27   |
| 3   | E     | 603 | IMP  | C5-C4-N3    | -4.64 | 120.45      | 127.27   |
| 3   | H     | 603 | IMP  | C5-C4-N3    | -4.63 | 120.45      | 127.27   |
| 2   | A     | 601 | ATP  | C4-N9-C8    | 4.63  | 110.60      | 105.74   |
| 4   | E     | 604 | NAD  | C5A-C4A-N3A | -4.61 | 120.37      | 126.72   |
| 2   | F     | 601 | ATP  | C4-N9-C8    | 4.57  | 110.54      | 105.74   |
| 4   | D     | 604 | NAD  | C5A-C4A-N3A | -4.57 | 120.42      | 126.72   |
| 2   | B     | 602 | ATP  | C4-N9-C8    | 4.57  | 110.54      | 105.74   |
| 3   | D     | 603 | IMP  | C5-C4-N3    | -4.57 | 120.54      | 127.27   |
| 2   | F     | 602 | ATP  | C4-N9-C8    | 4.57  | 110.53      | 105.74   |
| 2   | H     | 602 | ATP  | C4-N9-C8    | 4.53  | 110.50      | 105.74   |
| 4   | F     | 604 | NAD  | C5A-C4A-N3A | -4.52 | 120.49      | 126.72   |
| 4   | H     | 604 | NAD  | C4A-N9A-C8A | 4.52  | 110.48      | 105.74   |
| 2   | G     | 602 | ATP  | C4-N9-C8    | 4.51  | 110.47      | 105.74   |
| 3   | B     | 603 | IMP  | C2-N3-C4    | 4.51  | 119.46      | 111.53   |
| 3   | A     | 603 | IMP  | C2-N3-C4    | 4.50  | 119.45      | 111.53   |
| 3   | E     | 603 | IMP  | C2-N3-C4    | 4.50  | 119.44      | 111.53   |
| 2   | D     | 601 | ATP  | C5-C4-N3    | -4.50 | 120.53      | 126.72   |
| 4   | G     | 604 | NAD  | C4D-O4D-C1D | -4.50 | 105.81      | 109.92   |
| 4   | A     | 604 | NAD  | C5A-C4A-N3A | -4.49 | 120.53      | 126.72   |
| 4   | C     | 604 | NAD  | C4A-N9A-C8A | 4.49  | 110.45      | 105.74   |
| 4   | G     | 604 | NAD  | C5A-C4A-N3A | -4.48 | 120.55      | 126.72   |
| 2   | D     | 602 | ATP  | C5-C4-N3    | -4.48 | 120.55      | 126.72   |
| 2   | D     | 601 | ATP  | C4-N9-C8    | 4.48  | 110.44      | 105.74   |
| 2   | E     | 601 | ATP  | C5-C4-N3    | -4.48 | 120.55      | 126.72   |
| 3   | H     | 603 | IMP  | C2-N3-C4    | 4.47  | 119.40      | 111.53   |
| 3   | C     | 603 | IMP  | C2-N3-C4    | 4.46  | 119.38      | 111.53   |
| 2   | G     | 602 | ATP  | C5-C4-N3    | -4.46 | 120.58      | 126.72   |
| 3   | D     | 603 | IMP  | C2-N3-C4    | 4.46  | 119.37      | 111.53   |
| 3   | G     | 603 | IMP  | C2-N3-C4    | 4.45  | 119.36      | 111.53   |
| 3   | F     | 603 | IMP  | C2-N3-C4    | 4.44  | 119.34      | 111.53   |
| 2   | F     | 601 | ATP  | C5-C4-N3    | -4.44 | 120.61      | 126.72   |
| 4   | B     | 604 | NAD  | C4A-N9A-C8A | 4.44  | 110.39      | 105.74   |
| 2   | A     | 602 | ATP  | C4-N9-C8    | 4.43  | 110.39      | 105.74   |
| 2   | H     | 602 | ATP  | C5-C4-N3    | -4.42 | 120.62      | 126.72   |
| 2   | C     | 601 | ATP  | C5-C4-N3    | -4.42 | 120.63      | 126.72   |
| 4   | B     | 604 | NAD  | C5A-C4A-N3A | -4.42 | 120.63      | 126.72   |
| 2   | E     | 601 | ATP  | C4-N9-C8    | 4.42  | 110.38      | 105.74   |
| 2   | C     | 602 | ATP  | C5-C4-N3    | -4.41 | 120.65      | 126.72   |
| 2   | F     | 602 | ATP  | C5-C4-N3    | -4.39 | 120.67      | 126.72   |
| 4   | H     | 604 | NAD  | C5A-C4A-N3A | -4.39 | 120.67      | 126.72   |
| 4   | C     | 604 | NAD  | C5A-C4A-N3A | -4.39 | 120.67      | 126.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 602 | ATP  | C5-C4-N3    | -4.39 | 120.67      | 126.72   |
| 2   | A     | 602 | ATP  | C5-C4-N3    | -4.38 | 120.68      | 126.72   |
| 2   | D     | 602 | ATP  | C4-N9-C8    | 4.38  | 110.34      | 105.74   |
| 2   | A     | 601 | ATP  | C5-C4-N3    | -4.36 | 120.71      | 126.72   |
| 2   | C     | 602 | ATP  | C4-N9-C8    | 4.35  | 110.31      | 105.74   |
| 2   | G     | 601 | ATP  | C5-C4-N3    | -4.30 | 120.80      | 126.72   |
| 2   | B     | 602 | ATP  | C5-C4-N3    | -4.27 | 120.84      | 126.72   |
| 2   | H     | 601 | ATP  | C5-C4-N3    | -4.25 | 120.86      | 126.72   |
| 4   | G     | 604 | NAD  | C4A-N9A-C8A | 4.24  | 110.19      | 105.74   |
| 4   | D     | 604 | NAD  | C4A-N9A-C8A | 4.20  | 110.15      | 105.74   |
| 4   | E     | 604 | NAD  | C4A-N9A-C8A | 4.11  | 110.05      | 105.74   |
| 4   | F     | 604 | NAD  | C4A-N9A-C8A | 4.10  | 110.04      | 105.74   |
| 4   | A     | 604 | NAD  | C4A-N9A-C8A | 4.06  | 110.00      | 105.74   |
| 2   | B     | 601 | ATP  | C5-C4-N3    | -3.97 | 121.24      | 126.72   |
| 4   | A     | 604 | NAD  | C4D-O4D-C1D | -3.95 | 106.31      | 109.92   |
| 2   | C     | 601 | ATP  | C3'-C2'-C1' | 3.87  | 108.79      | 101.46   |
| 3   | E     | 603 | IMP  | N1-C2-N3    | -3.87 | 121.05      | 125.50   |
| 3   | D     | 603 | IMP  | N1-C2-N3    | -3.86 | 121.05      | 125.50   |
| 3   | B     | 603 | IMP  | N1-C2-N3    | -3.85 | 121.07      | 125.50   |
| 3   | H     | 603 | IMP  | N1-C2-N3    | -3.83 | 121.09      | 125.50   |
| 3   | A     | 603 | IMP  | N1-C2-N3    | -3.83 | 121.09      | 125.50   |
| 3   | B     | 603 | IMP  | N9-C8-N7    | -3.76 | 106.43      | 113.40   |
| 3   | F     | 603 | IMP  | N1-C2-N3    | -3.75 | 121.18      | 125.50   |
| 3   | D     | 603 | IMP  | N9-C8-N7    | -3.75 | 106.45      | 113.40   |
| 3   | G     | 603 | IMP  | N1-C2-N3    | -3.74 | 121.19      | 125.50   |
| 3   | F     | 603 | IMP  | N9-C8-N7    | -3.73 | 106.48      | 113.40   |
| 3   | G     | 603 | IMP  | N9-C8-N7    | -3.71 | 106.53      | 113.40   |
| 3   | H     | 603 | IMP  | N9-C8-N7    | -3.68 | 106.58      | 113.40   |
| 3   | E     | 603 | IMP  | N9-C8-N7    | -3.68 | 106.58      | 113.40   |
| 3   | A     | 603 | IMP  | N9-C8-N7    | -3.65 | 106.63      | 113.40   |
| 3   | C     | 603 | IMP  | N1-C2-N3    | -3.64 | 121.31      | 125.50   |
| 3   | C     | 603 | IMP  | N9-C8-N7    | -3.61 | 106.70      | 113.40   |
| 2   | C     | 601 | ATP  | N3-C4-N9    | 3.57  | 133.25      | 127.17   |
| 2   | E     | 601 | ATP  | N3-C4-N9    | 3.57  | 133.24      | 127.17   |
| 2   | F     | 601 | ATP  | N3-C4-N9    | 3.54  | 133.19      | 127.17   |
| 2   | B     | 601 | ATP  | C3'-C2'-C1' | 3.52  | 108.13      | 101.46   |
| 2   | G     | 602 | ATP  | N3-C4-N9    | 3.51  | 133.14      | 127.17   |
| 2   | D     | 601 | ATP  | N3-C4-N9    | 3.51  | 133.13      | 127.17   |
| 2   | E     | 602 | ATP  | N3-C4-N9    | 3.49  | 133.11      | 127.17   |
| 2   | D     | 602 | ATP  | N3-C4-N9    | 3.45  | 133.04      | 127.17   |
| 4   | H     | 604 | NAD  | C4B-O4B-C1B | -3.45 | 101.84      | 109.47   |
| 4   | E     | 604 | NAD  | N3A-C4A-N9A | 3.45  | 133.03      | 127.17   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4   | D     | 604 | NAD  | N3A-C4A-N9A | 3.45 | 133.03      | 127.17   |
| 2   | A     | 601 | ATP  | N3-C4-N9    | 3.44 | 133.02      | 127.17   |
| 2   | A     | 602 | ATP  | N3-C4-N9    | 3.44 | 133.02      | 127.17   |
| 2   | F     | 602 | ATP  | N3-C4-N9    | 3.43 | 133.01      | 127.17   |
| 2   | H     | 602 | ATP  | N3-C4-N9    | 3.43 | 132.99      | 127.17   |
| 2   | G     | 601 | ATP  | C3'-C2'-C1' | 3.42 | 107.93      | 101.46   |
| 4   | F     | 604 | NAD  | N3A-C4A-N9A | 3.40 | 132.95      | 127.17   |
| 2   | D     | 602 | ATP  | C3'-C2'-C1' | 3.39 | 107.88      | 101.46   |
| 2   | C     | 602 | ATP  | N3-C4-N9    | 3.39 | 132.93      | 127.17   |
| 3   | G     | 603 | IMP  | O3P-P-O2P   | 3.37 | 120.45      | 107.80   |
| 2   | B     | 602 | ATP  | N3-C4-N9    | 3.37 | 132.90      | 127.17   |
| 4   | H     | 604 | NAD  | O4B-C1B-N9A | 3.36 | 114.54      | 108.09   |
| 4   | B     | 604 | NAD  | N3A-C4A-N9A | 3.36 | 132.88      | 127.17   |
| 2   | H     | 601 | ATP  | N3-C4-N9    | 3.35 | 132.87      | 127.17   |
| 2   | H     | 601 | ATP  | C3'-C2'-C1' | 3.35 | 107.81      | 101.46   |
| 4   | H     | 604 | NAD  | C5A-N7A-C8A | 3.34 | 108.70      | 103.45   |
| 4   | C     | 604 | NAD  | N3A-C4A-N9A | 3.34 | 132.85      | 127.17   |
| 4   | G     | 604 | NAD  | N3A-C4A-N9A | 3.34 | 132.84      | 127.17   |
| 2   | G     | 601 | ATP  | N3-C4-N9    | 3.34 | 132.84      | 127.17   |
| 3   | F     | 603 | IMP  | O3P-P-O2P   | 3.33 | 120.29      | 107.80   |
| 2   | E     | 602 | ATP  | C5-N7-C8    | 3.30 | 108.63      | 103.45   |
| 2   | E     | 602 | ATP  | C3'-C2'-C1' | 3.29 | 107.69      | 101.46   |
| 4   | A     | 604 | NAD  | N3A-C4A-N9A | 3.28 | 132.75      | 127.17   |
| 2   | C     | 601 | ATP  | C5-N7-C8    | 3.28 | 108.60      | 103.45   |
| 2   | H     | 602 | ATP  | C5-N7-C8    | 3.28 | 108.60      | 103.45   |
| 2   | G     | 601 | ATP  | C5-N7-C8    | 3.27 | 108.59      | 103.45   |
| 2   | F     | 602 | ATP  | C5-N7-C8    | 3.26 | 108.57      | 103.45   |
| 2   | H     | 602 | ATP  | C3'-C2'-C1' | 3.26 | 107.62      | 101.46   |
| 2   | D     | 602 | ATP  | C5-N7-C8    | 3.25 | 108.56      | 103.45   |
| 2   | A     | 602 | ATP  | C3'-C2'-C1' | 3.23 | 107.58      | 101.46   |
| 2   | H     | 601 | ATP  | C5-N7-C8    | 3.23 | 108.53      | 103.45   |
| 4   | A     | 604 | NAD  | C2A-N3A-C4A | 3.23 | 119.72      | 111.83   |
| 4   | D     | 604 | NAD  | C2A-N3A-C4A | 3.23 | 119.72      | 111.83   |
| 4   | G     | 604 | NAD  | C2A-N3A-C4A | 3.22 | 119.70      | 111.83   |
| 2   | B     | 602 | ATP  | C5-N7-C8    | 3.21 | 108.50      | 103.45   |
| 2   | F     | 601 | ATP  | C5-N7-C8    | 3.21 | 108.49      | 103.45   |
| 2   | B     | 602 | ATP  | C3'-C2'-C1' | 3.21 | 107.53      | 101.46   |
| 2   | C     | 602 | ATP  | C5-N7-C8    | 3.20 | 108.48      | 103.45   |
| 4   | C     | 604 | NAD  | C2A-N3A-C4A | 3.19 | 119.63      | 111.83   |
| 4   | E     | 604 | NAD  | C5A-N7A-C8A | 3.19 | 108.46      | 103.45   |
| 4   | G     | 604 | NAD  | C5A-N7A-C8A | 3.18 | 108.45      | 103.45   |
| 4   | E     | 604 | NAD  | C2A-N3A-C4A | 3.18 | 119.60      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 601 | ATP  | C5-N7-C8    | 3.18  | 108.45      | 103.45   |
| 4   | F     | 604 | NAD  | C2A-N3A-C4A | 3.18  | 119.60      | 111.83   |
| 2   | A     | 602 | ATP  | C5-N7-C8    | 3.18  | 108.45      | 103.45   |
| 2   | A     | 601 | ATP  | C5-N7-C8    | 3.18  | 108.45      | 103.45   |
| 2   | D     | 601 | ATP  | C3'-C2'-C1' | 3.18  | 107.47      | 101.46   |
| 4   | H     | 604 | NAD  | C2A-N3A-C4A | 3.18  | 119.59      | 111.83   |
| 2   | B     | 601 | ATP  | C5-N7-C8    | 3.17  | 108.44      | 103.45   |
| 4   | B     | 604 | NAD  | C5A-N7A-C8A | 3.17  | 108.44      | 103.45   |
| 4   | B     | 604 | NAD  | C2A-N3A-C4A | 3.17  | 119.56      | 111.83   |
| 4   | C     | 604 | NAD  | C5A-N7A-C8A | 3.16  | 108.42      | 103.45   |
| 2   | E     | 601 | ATP  | C5-N7-C8    | 3.16  | 108.42      | 103.45   |
| 2   | E     | 602 | ATP  | C2-N3-C4    | 3.14  | 119.51      | 111.83   |
| 2   | G     | 601 | ATP  | C2-N3-C4    | 3.14  | 119.50      | 111.83   |
| 2   | G     | 602 | ATP  | C5-N7-C8    | 3.14  | 108.38      | 103.45   |
| 2   | D     | 602 | ATP  | C2-N3-C4    | 3.13  | 119.49      | 111.83   |
| 2   | D     | 601 | ATP  | C2-N3-C4    | 3.13  | 119.48      | 111.83   |
| 2   | C     | 601 | ATP  | C2-N3-C4    | 3.13  | 119.48      | 111.83   |
| 4   | D     | 604 | NAD  | C5A-N7A-C8A | 3.13  | 108.37      | 103.45   |
| 2   | H     | 602 | ATP  | C2-N3-C4    | 3.13  | 119.47      | 111.83   |
| 2   | F     | 601 | ATP  | C2-N3-C4    | 3.12  | 119.45      | 111.83   |
| 2   | H     | 601 | ATP  | C2-N3-C4    | 3.12  | 119.45      | 111.83   |
| 4   | A     | 604 | NAD  | C5A-N7A-C8A | 3.12  | 108.35      | 103.45   |
| 2   | F     | 602 | ATP  | C2-N3-C4    | 3.11  | 119.42      | 111.83   |
| 2   | F     | 602 | ATP  | C3'-C2'-C1' | 3.11  | 107.34      | 101.46   |
| 2   | E     | 601 | ATP  | C2-N3-C4    | 3.10  | 119.40      | 111.83   |
| 4   | D     | 604 | NAD  | C4D-O4D-C1D | -3.09 | 107.09      | 109.92   |
| 2   | A     | 601 | ATP  | C2-N3-C4    | 3.08  | 119.34      | 111.83   |
| 4   | H     | 604 | NAD  | N3A-C4A-N9A | 3.07  | 132.39      | 127.17   |
| 2   | A     | 602 | ATP  | C2-N3-C4    | 3.06  | 119.31      | 111.83   |
| 2   | B     | 602 | ATP  | C2-N3-C4    | 3.06  | 119.29      | 111.83   |
| 2   | C     | 602 | ATP  | C2-N3-C4    | 3.05  | 119.28      | 111.83   |
| 4   | F     | 604 | NAD  | C5A-N7A-C8A | 3.05  | 108.25      | 103.45   |
| 2   | G     | 602 | ATP  | C2-N3-C4    | 3.05  | 119.28      | 111.83   |
| 2   | C     | 602 | ATP  | C3'-C2'-C1' | 3.05  | 107.23      | 101.46   |
| 2   | B     | 601 | ATP  | C2-N3-C4    | 3.04  | 119.25      | 111.83   |
| 2   | B     | 601 | ATP  | N3-C4-N9    | 3.04  | 132.33      | 127.17   |
| 2   | F     | 601 | ATP  | C3'-C2'-C1' | 3.03  | 107.20      | 101.46   |
| 2   | G     | 602 | ATP  | C3'-C2'-C1' | 2.97  | 107.08      | 101.46   |
| 2   | A     | 601 | ATP  | C3'-C2'-C1' | 2.93  | 107.01      | 101.46   |
| 3   | C     | 603 | IMP  | O3P-P-O2P   | 2.90  | 118.66      | 107.80   |
| 4   | H     | 604 | NAD  | O4B-C1B-C2B | -2.84 | 100.54      | 106.62   |
| 4   | H     | 604 | NAD  | C4D-O4D-C1D | -2.67 | 107.48      | 109.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | H     | 603 | IMP  | O6-C6-C5    | -2.67 | 119.48      | 126.53   |
| 2   | E     | 601 | ATP  | C3'-C2'-C1' | 2.66  | 106.50      | 101.46   |
| 3   | D     | 603 | IMP  | O6-C6-C5    | -2.65 | 119.53      | 126.53   |
| 3   | C     | 603 | IMP  | O6-C6-C5    | -2.65 | 119.53      | 126.53   |
| 4   | B     | 604 | NAD  | C4B-O4B-C1B | -2.65 | 103.62      | 109.47   |
| 3   | B     | 603 | IMP  | O6-C6-C5    | -2.64 | 119.57      | 126.53   |
| 3   | G     | 603 | IMP  | O6-C6-C5    | -2.64 | 119.57      | 126.53   |
| 3   | F     | 603 | IMP  | O6-C6-C5    | -2.64 | 119.57      | 126.53   |
| 3   | E     | 603 | IMP  | O6-C6-C5    | -2.64 | 119.57      | 126.53   |
| 3   | C     | 603 | IMP  | N9-C4-N3    | 2.63  | 132.88      | 126.90   |
| 3   | A     | 603 | IMP  | O6-C6-C5    | -2.61 | 119.64      | 126.53   |
| 2   | C     | 601 | ATP  | C2'-C3'-C4' | 2.61  | 107.65      | 102.61   |
| 3   | B     | 603 | IMP  | N9-C4-N3    | 2.55  | 132.70      | 126.90   |
| 3   | F     | 603 | IMP  | N9-C4-N3    | 2.53  | 132.65      | 126.90   |
| 3   | A     | 603 | IMP  | N9-C4-N3    | 2.52  | 132.64      | 126.90   |
| 3   | H     | 603 | IMP  | N9-C4-N3    | 2.51  | 132.62      | 126.90   |
| 2   | B     | 601 | ATP  | C2'-C3'-C4' | 2.51  | 107.46      | 102.61   |
| 3   | G     | 603 | IMP  | N9-C4-N3    | 2.51  | 132.61      | 126.90   |
| 3   | E     | 603 | IMP  | N9-C4-N3    | 2.49  | 132.56      | 126.90   |
| 3   | D     | 603 | IMP  | N9-C4-N3    | 2.48  | 132.54      | 126.90   |
| 3   | A     | 603 | IMP  | O3P-P-O2P   | 2.41  | 116.85      | 107.80   |
| 4   | B     | 604 | NAD  | C4D-O4D-C1D | -2.41 | 107.72      | 109.92   |
| 3   | D     | 603 | IMP  | O3P-P-O2P   | 2.39  | 116.77      | 107.80   |
| 4   | F     | 604 | NAD  | C2D-C3D-C4D | 2.38  | 107.21      | 102.61   |
| 4   | G     | 604 | NAD  | C2D-C3D-C4D | 2.37  | 107.20      | 102.61   |
| 4   | A     | 604 | NAD  | C3B-C2B-C1B | 2.36  | 105.92      | 101.46   |
| 4   | H     | 604 | NAD  | C4A-C5A-N7A | -2.35 | 107.89      | 110.58   |
| 4   | A     | 604 | NAD  | C2N-C3N-C4N | 2.35  | 120.99      | 118.26   |
| 4   | G     | 604 | NAD  | C2N-C3N-C4N | 2.34  | 120.98      | 118.26   |
| 2   | D     | 602 | ATP  | C2'-C3'-C4' | 2.33  | 107.12      | 102.61   |
| 4   | D     | 604 | NAD  | C2D-C3D-C4D | 2.33  | 107.10      | 102.61   |
| 3   | B     | 603 | IMP  | C8-N7-C5    | 2.31  | 108.37      | 104.26   |
| 3   | F     | 603 | IMP  | C8-N7-C5    | 2.30  | 108.36      | 104.26   |
| 3   | D     | 603 | IMP  | C8-N7-C5    | 2.30  | 108.35      | 104.26   |
| 3   | G     | 603 | IMP  | C8-N7-C5    | 2.30  | 108.35      | 104.26   |
| 4   | H     | 604 | NAD  | C5B-C4B-C3B | -2.28 | 106.99      | 115.21   |
| 4   | F     | 604 | NAD  | C3B-C2B-C1B | 2.28  | 105.77      | 101.46   |
| 3   | H     | 603 | IMP  | C8-N7-C5    | 2.27  | 108.30      | 104.26   |
| 3   | E     | 603 | IMP  | C8-N7-C5    | 2.27  | 108.30      | 104.26   |
| 4   | H     | 604 | NAD  | C3N-C7N-N7N | 2.27  | 120.53      | 117.74   |
| 3   | C     | 603 | IMP  | C8-N7-C5    | 2.26  | 108.28      | 104.26   |
| 3   | A     | 603 | IMP  | C8-N7-C5    | 2.25  | 108.27      | 104.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 604 | NAD  | C3N-C7N-N7N | 2.24  | 120.49      | 117.74   |
| 4   | G     | 604 | NAD  | C3N-C7N-N7N | 2.23  | 120.49      | 117.74   |
| 2   | H     | 602 | ATP  | C2'-C3'-C4' | 2.22  | 106.90      | 102.61   |
| 4   | A     | 604 | NAD  | C2D-C3D-C4D | 2.21  | 106.88      | 102.61   |
| 4   | E     | 604 | NAD  | C4D-O4D-C1D | -2.20 | 107.91      | 109.92   |
| 4   | C     | 604 | NAD  | C4D-O4D-C1D | -2.19 | 107.92      | 109.92   |
| 2   | E     | 601 | ATP  | C6-C5-C4    | 2.17  | 120.14      | 117.18   |
| 3   | D     | 603 | IMP  | C8-N9-C4    | 2.13  | 110.03      | 106.03   |
| 3   | B     | 603 | IMP  | C8-N9-C4    | 2.12  | 110.00      | 106.03   |
| 3   | F     | 603 | IMP  | C8-N9-C4    | 2.10  | 109.96      | 106.03   |
| 2   | D     | 601 | ATP  | C6-C5-C4    | 2.08  | 120.02      | 117.18   |
| 3   | G     | 603 | IMP  | C8-N9-C4    | 2.07  | 109.90      | 106.03   |
| 3   | H     | 603 | IMP  | C8-N9-C4    | 2.07  | 109.90      | 106.03   |
| 3   | A     | 603 | IMP  | C8-N9-C4    | 2.06  | 109.88      | 106.03   |
| 2   | F     | 601 | ATP  | C6-C5-C4    | 2.05  | 119.97      | 117.18   |
| 4   | B     | 604 | NAD  | C2N-C3N-C4N | 2.05  | 120.64      | 118.26   |
| 3   | E     | 603 | IMP  | C8-N9-C4    | 2.04  | 109.86      | 106.03   |
| 2   | A     | 601 | ATP  | C6-C5-C4    | 2.03  | 119.95      | 117.18   |
| 2   | E     | 602 | ATP  | C2'-C3'-C4' | 2.02  | 106.50      | 102.61   |
| 4   | D     | 604 | NAD  | C2N-C3N-C4N | 2.01  | 120.60      | 118.26   |
| 3   | C     | 603 | IMP  | C8-N9-C4    | 2.00  | 109.78      | 106.03   |
| 2   | A     | 602 | ATP  | C2'-C3'-C4' | 2.00  | 106.48      | 102.61   |
| 2   | D     | 601 | ATP  | O3A-PB-O1B  | -2.00 | 104.69      | 110.70   |

There are no chirality outliers.

All (219) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | A     | 602 | ATP  | C5'-O5'-PA-O1A |
| 2   | A     | 602 | ATP  | C5'-O5'-PA-O2A |
| 2   | A     | 602 | ATP  | C5'-O5'-PA-O3A |
| 2   | B     | 601 | ATP  | PB-O3B-PG-O3G  |
| 2   | B     | 602 | ATP  | PB-O3B-PG-O3G  |
| 2   | C     | 601 | ATP  | PB-O3A-PA-O5'  |
| 2   | C     | 601 | ATP  | C5'-O5'-PA-O1A |
| 2   | C     | 601 | ATP  | C5'-O5'-PA-O2A |
| 2   | C     | 601 | ATP  | C5'-O5'-PA-O3A |
| 2   | C     | 602 | ATP  | C5'-O5'-PA-O1A |
| 2   | C     | 602 | ATP  | C5'-O5'-PA-O2A |
| 2   | C     | 602 | ATP  | C5'-O5'-PA-O3A |
| 2   | D     | 601 | ATP  | C5'-O5'-PA-O3A |
| 2   | D     | 602 | ATP  | PB-O3B-PG-O3G  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | D     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | E     | 601 | ATP  | C5'-O5'-PA-O2A  |
| 2   | E     | 601 | ATP  | C5'-O5'-PA-O3A  |
| 2   | G     | 601 | ATP  | C5'-O5'-PA-O1A  |
| 2   | G     | 601 | ATP  | C5'-O5'-PA-O2A  |
| 2   | G     | 601 | ATP  | C5'-O5'-PA-O3A  |
| 2   | G     | 602 | ATP  | C5'-O5'-PA-O1A  |
| 2   | G     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | G     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 2   | H     | 601 | ATP  | PB-O3A-PA-O5'   |
| 2   | H     | 601 | ATP  | C5'-O5'-PA-O1A  |
| 2   | H     | 601 | ATP  | C5'-O5'-PA-O2A  |
| 2   | H     | 601 | ATP  | C5'-O5'-PA-O3A  |
| 2   | H     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | H     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 3   | A     | 603 | IMP  | C5'-O5'-P-O1P   |
| 3   | A     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | A     | 603 | IMP  | C5'-O5'-P-O3P   |
| 3   | B     | 603 | IMP  | C5'-O5'-P-O1P   |
| 3   | B     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | B     | 603 | IMP  | C5'-O5'-P-O3P   |
| 3   | C     | 603 | IMP  | C5'-O5'-P-O1P   |
| 3   | D     | 603 | IMP  | C5'-O5'-P-O1P   |
| 3   | D     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | D     | 603 | IMP  | C5'-O5'-P-O3P   |
| 3   | E     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | E     | 603 | IMP  | C5'-O5'-P-O3P   |
| 3   | F     | 603 | IMP  | C5'-O5'-P-O1P   |
| 3   | F     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | F     | 603 | IMP  | C5'-O5'-P-O3P   |
| 3   | F     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | G     | 603 | IMP  | C5'-O5'-P-O1P   |
| 3   | G     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | G     | 603 | IMP  | C5'-O5'-P-O3P   |
| 3   | G     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | G     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | H     | 603 | IMP  | C5'-O5'-P-O1P   |
| 3   | H     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | H     | 603 | IMP  | C5'-O5'-P-O3P   |
| 4   | A     | 604 | NAD  | C5D-O5D-PN-O3   |
| 4   | A     | 604 | NAD  | C5D-O5D-PN-O1N  |
| 4   | A     | 604 | NAD  | C5D-O5D-PN-O2N  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | A     | 604 | NAD  | O4D-C4D-C5D-O5D |
| 4   | B     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | B     | 604 | NAD  | PN-O3-PA-O5B    |
| 4   | B     | 604 | NAD  | C5D-O5D-PN-O1N  |
| 4   | B     | 604 | NAD  | C5D-O5D-PN-O2N  |
| 4   | B     | 604 | NAD  | O4D-C4D-C5D-O5D |
| 4   | C     | 604 | NAD  | C5D-O5D-PN-O3   |
| 4   | C     | 604 | NAD  | C5D-O5D-PN-O2N  |
| 4   | D     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | E     | 604 | NAD  | C5B-O5B-PA-O1A  |
| 4   | E     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | E     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | F     | 604 | NAD  | C5B-O5B-PA-O2A  |
| 4   | F     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | F     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | F     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | F     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | F     | 604 | NAD  | O4D-C4D-C5D-O5D |
| 4   | F     | 604 | NAD  | C3D-C4D-C5D-O5D |
| 4   | G     | 604 | NAD  | C5B-O5B-PA-O1A  |
| 4   | G     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | G     | 604 | NAD  | PN-O3-PA-O5B    |
| 4   | G     | 604 | NAD  | O4D-C1D-N1N-C2N |
| 4   | H     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | H     | 604 | NAD  | C5D-O5D-PN-O3   |
| 4   | H     | 604 | NAD  | C5D-O5D-PN-O1N  |
| 4   | H     | 604 | NAD  | C5D-O5D-PN-O2N  |
| 4   | H     | 604 | NAD  | O4D-C4D-C5D-O5D |
| 4   | H     | 604 | NAD  | C3D-C4D-C5D-O5D |
| 4   | H     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | H     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | D     | 604 | NAD  | C2N-C3N-C7N-O7N |
| 4   | D     | 604 | NAD  | C2N-C3N-C7N-N7N |
| 4   | F     | 604 | NAD  | C2N-C3N-C7N-O7N |
| 2   | E     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | E     | 602 | ATP  | O4'-C4'-C5'-O5' |
| 3   | A     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | A     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | B     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | B     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | D     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | D     | 603 | IMP  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | E     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | E     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | F     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | H     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | H     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 4   | A     | 604 | NAD  | C3D-C4D-C5D-O5D |
| 4   | G     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | E     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | H     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | E     | 604 | NAD  | C2N-C3N-C7N-O7N |
| 4   | E     | 604 | NAD  | C2N-C3N-C7N-N7N |
| 4   | F     | 604 | NAD  | C2N-C3N-C7N-N7N |
| 2   | H     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | H     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 4   | B     | 604 | NAD  | C3D-C4D-C5D-O5D |
| 4   | D     | 604 | NAD  | O4D-C4D-C5D-O5D |
| 4   | E     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | E     | 604 | NAD  | C3D-C4D-C5D-O5D |
| 4   | G     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | G     | 604 | NAD  | O4D-C4D-C5D-O5D |
| 4   | G     | 604 | NAD  | C3D-C4D-C5D-O5D |
| 4   | H     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | C     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | H     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | D     | 604 | NAD  | C4N-C3N-C7N-N7N |
| 2   | A     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 4   | F     | 604 | NAD  | C4N-C3N-C7N-N7N |
| 4   | E     | 604 | NAD  | C4N-C3N-C7N-N7N |
| 4   | D     | 604 | NAD  | C4N-C3N-C7N-O7N |
| 4   | F     | 604 | NAD  | C4N-C3N-C7N-O7N |
| 4   | E     | 604 | NAD  | C4N-C3N-C7N-O7N |
| 2   | E     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | G     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | H     | 602 | ATP  | O4'-C4'-C5'-O5' |
| 2   | A     | 602 | ATP  | O4'-C4'-C5'-O5' |
| 2   | C     | 602 | ATP  | O4'-C4'-C5'-O5' |
| 2   | D     | 602 | ATP  | O4'-C4'-C5'-O5' |
| 2   | G     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 4   | C     | 604 | NAD  | C3D-C4D-C5D-O5D |
| 4   | E     | 604 | NAD  | O4D-C4D-C5D-O5D |
| 2   | C     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 4   | C     | 604 | NAD  | O4B-C4B-C5B-O5B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | C     | 604 | NAD  | C2N-C3N-C7N-O7N |
| 3   | E     | 603 | IMP  | C5'-O5'-P-O1P   |
| 4   | C     | 604 | NAD  | C2N-C3N-C7N-N7N |
| 2   | C     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | E     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 4   | H     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 2   | A     | 602 | ATP  | PG-O3B-PB-O1B   |
| 4   | A     | 604 | NAD  | PA-O3-PN-O1N    |
| 2   | C     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | G     | 602 | ATP  | O4'-C4'-C5'-O5' |
| 4   | C     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | D     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | H     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 2   | D     | 601 | ATP  | PB-O3A-PA-O5'   |
| 2   | G     | 601 | ATP  | PB-O3A-PA-O5'   |
| 2   | G     | 602 | ATP  | PB-O3A-PA-O5'   |
| 4   | A     | 604 | NAD  | PN-O3-PA-O5B    |
| 4   | C     | 604 | NAD  | PN-O3-PA-O5B    |
| 4   | D     | 604 | NAD  | PN-O3-PA-O5B    |
| 4   | E     | 604 | NAD  | PN-O3-PA-O5B    |
| 4   | F     | 604 | NAD  | PA-O3-PN-O5D    |
| 2   | F     | 602 | ATP  | O4'-C4'-C5'-O5' |
| 4   | D     | 604 | NAD  | C3D-C4D-C5D-O5D |
| 4   | C     | 604 | NAD  | C4N-C3N-C7N-N7N |
| 4   | C     | 604 | NAD  | C4N-C3N-C7N-O7N |
| 2   | G     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | B     | 601 | ATP  | C2'-C1'-N9-C8   |
| 4   | A     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | D     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | G     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 2   | C     | 602 | ATP  | PG-O3B-PB-O1B   |
| 2   | C     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | F     | 602 | ATP  | PG-O3B-PB-O1B   |
| 2   | F     | 602 | ATP  | PA-O3A-PB-O2B   |
| 4   | G     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 2   | G     | 601 | ATP  | C2'-C1'-N9-C8   |
| 2   | H     | 601 | ATP  | C2'-C1'-N9-C8   |
| 2   | D     | 601 | ATP  | C5'-O5'-PA-O1A  |
| 2   | D     | 602 | ATP  | C5'-O5'-PA-O1A  |
| 2   | D     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 4   | B     | 604 | NAD  | C5B-O5B-PA-O1A  |
| 4   | B     | 604 | NAD  | C5D-O5D-PN-O3   |

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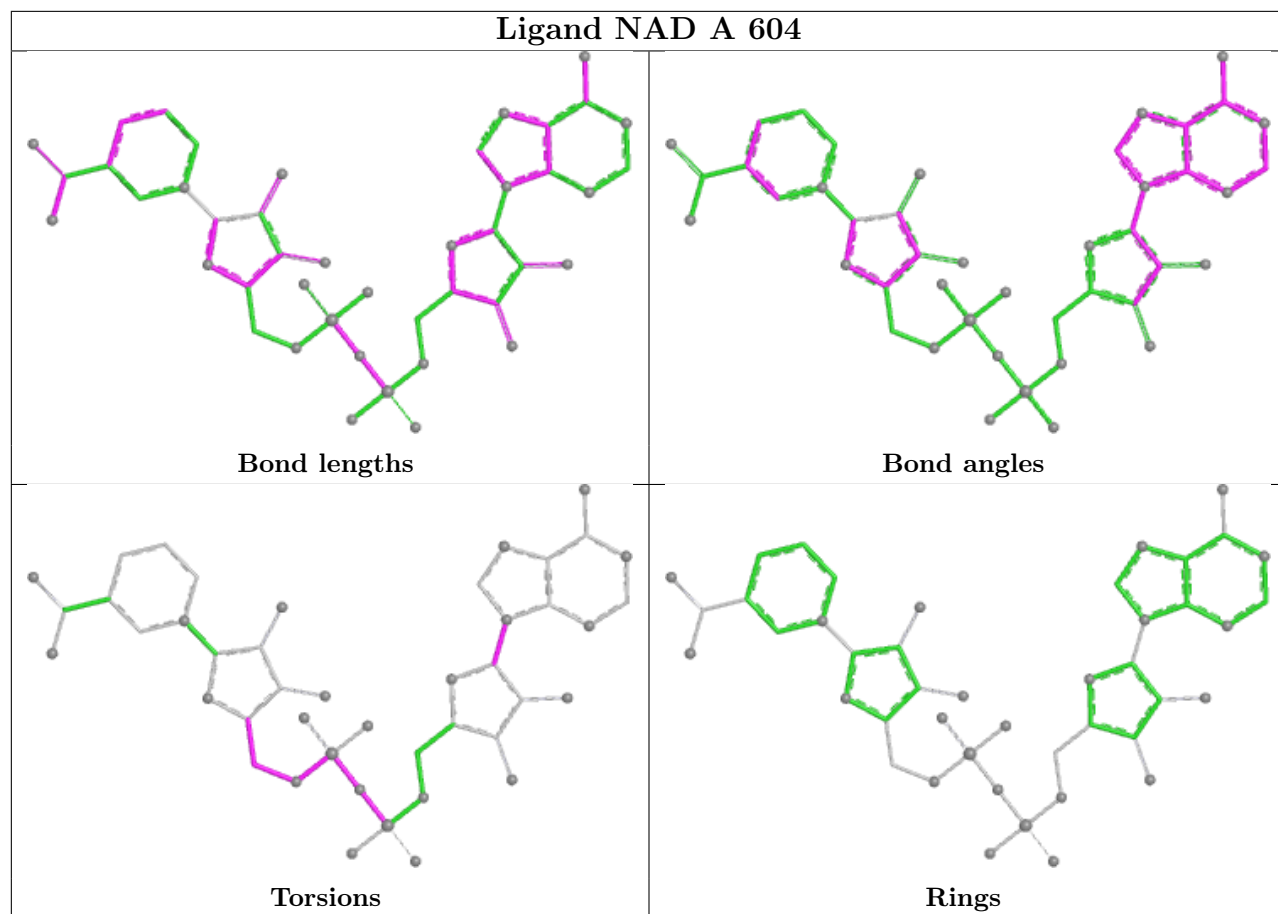
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | D     | 604 | NAD  | C5B-O5B-PA-O1A  |
| 4   | E     | 604 | NAD  | C5B-O5B-PA-O2A  |
| 4   | H     | 604 | NAD  | C5B-O5B-PA-O1A  |
| 2   | E     | 602 | ATP  | PG-O3B-PB-O2B   |
| 2   | E     | 602 | ATP  | PA-O3A-PB-O2B   |
| 4   | A     | 604 | NAD  | PN-O3-PA-O1A    |
| 4   | C     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | C     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | A     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 2   | D     | 601 | ATP  | C4'-C5'-O5'-PA  |
| 4   | F     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 3   | C     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | C     | 603 | IMP  | C5'-O5'-P-O3P   |
| 2   | D     | 602 | ATP  | PB-O3B-PG-O1G   |
| 2   | B     | 601 | ATP  | PB-O3B-PG-O2G   |
| 2   | B     | 602 | ATP  | PB-O3B-PG-O2G   |
| 2   | D     | 602 | ATP  | PB-O3B-PG-O2G   |
| 2   | B     | 601 | ATP  | O4'-C1'-N9-C8   |
| 2   | H     | 601 | ATP  | O4'-C1'-N9-C8   |
| 4   | G     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 2   | B     | 602 | ATP  | PB-O3A-PA-O2A   |
| 2   | D     | 601 | ATP  | PB-O3A-PA-O2A   |
| 2   | D     | 602 | ATP  | PB-O3A-PA-O1A   |
| 2   | E     | 602 | ATP  | PG-O3B-PB-O1B   |
| 2   | E     | 602 | ATP  | PA-O3A-PB-O1B   |
| 4   | D     | 604 | NAD  | PN-O3-PA-O2A    |
| 4   | F     | 604 | NAD  | PA-O3-PN-O1N    |
| 4   | D     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 4   | H     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 2   | D     | 601 | ATP  | C2'-C1'-N9-C8   |
| 2   | B     | 601 | ATP  | PB-O3B-PG-O1G   |
| 2   | E     | 601 | ATP  | C2'-C1'-N9-C8   |
| 4   | B     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 2   | C     | 602 | ATP  | PG-O3B-PB-O2B   |
| 2   | C     | 602 | ATP  | PA-O3A-PB-O2B   |
| 4   | F     | 604 | NAD  | PA-O3-PN-O2N    |
| 4   | C     | 604 | NAD  | O4D-C4D-C5D-O5D |

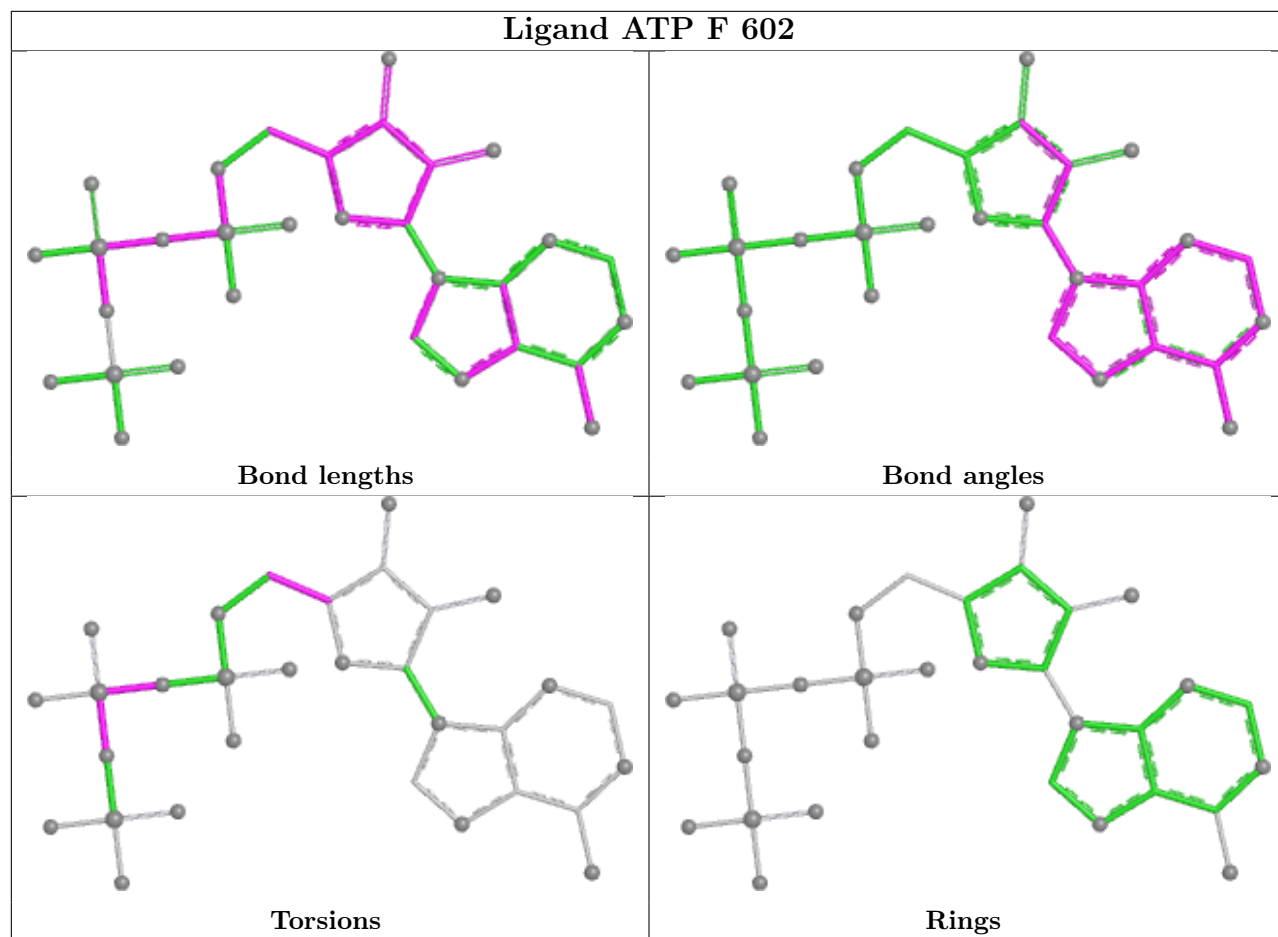
There are no ring outliers.

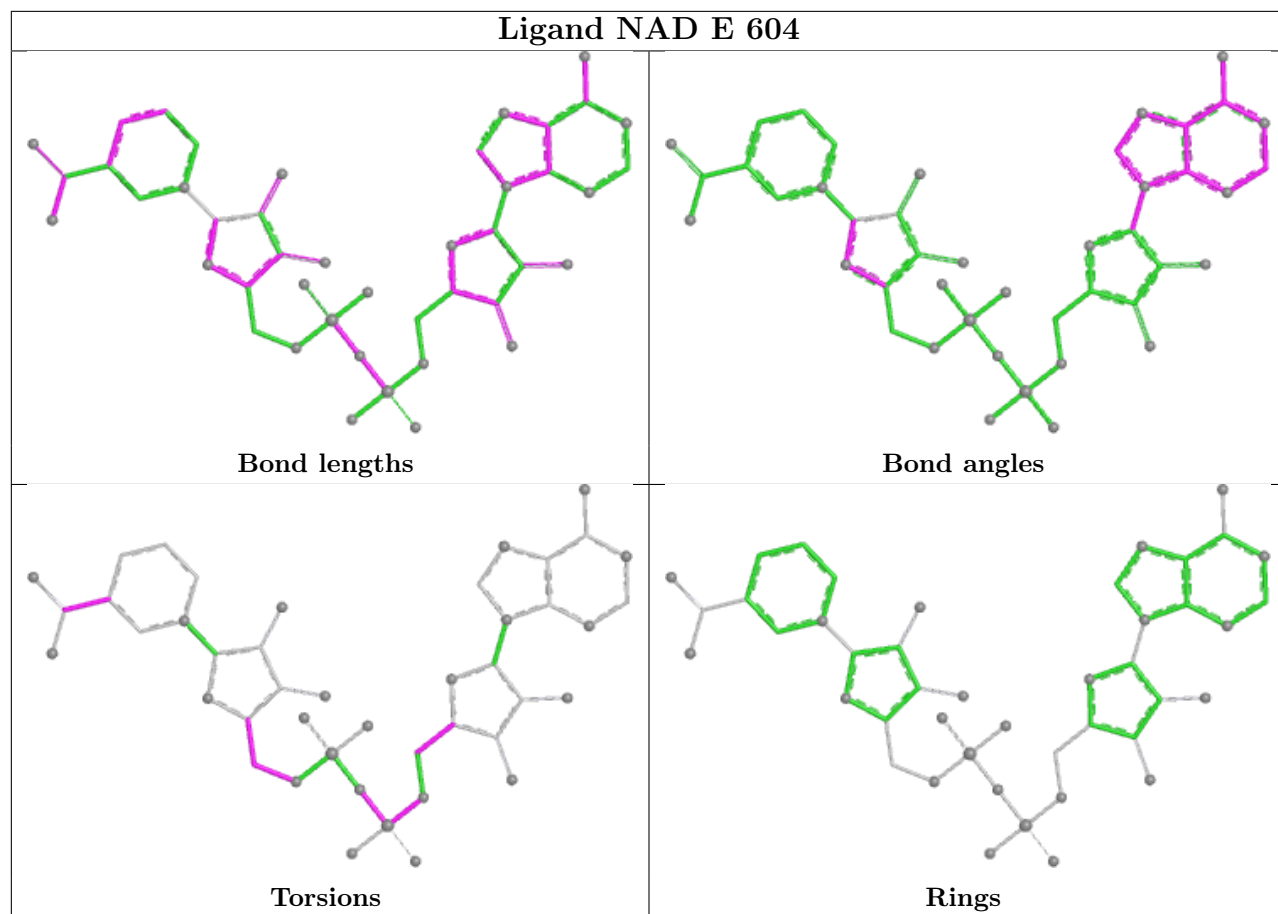
26 monomers are involved in 75 short contacts:

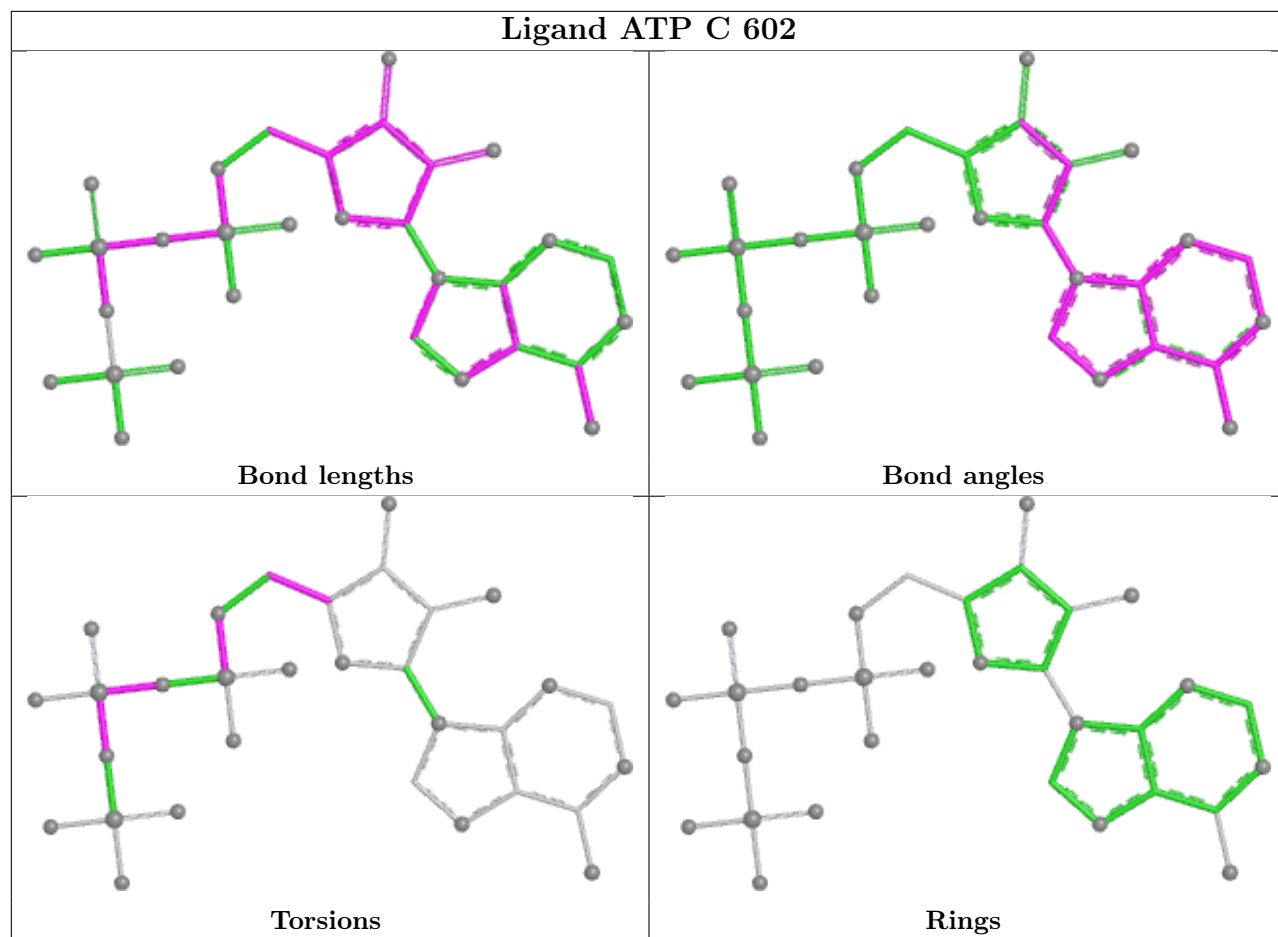
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 604 | NAD  | 3       | 0            |
| 2   | F     | 602 | ATP  | 1       | 0            |
| 4   | E     | 604 | NAD  | 1       | 0            |
| 2   | C     | 602 | ATP  | 1       | 0            |
| 2   | E     | 602 | ATP  | 1       | 0            |
| 3   | B     | 603 | IMP  | 4       | 0            |
| 2   | E     | 601 | ATP  | 4       | 0            |
| 3   | H     | 603 | IMP  | 3       | 0            |
| 2   | C     | 601 | ATP  | 6       | 0            |
| 3   | A     | 603 | IMP  | 3       | 0            |
| 2   | H     | 601 | ATP  | 4       | 0            |
| 4   | G     | 604 | NAD  | 1       | 0            |
| 2   | F     | 601 | ATP  | 4       | 0            |
| 2   | G     | 601 | ATP  | 4       | 0            |
| 3   | G     | 603 | IMP  | 3       | 0            |
| 4   | F     | 604 | NAD  | 3       | 0            |
| 2   | A     | 601 | ATP  | 3       | 0            |
| 3   | E     | 603 | IMP  | 3       | 0            |
| 2   | D     | 601 | ATP  | 5       | 0            |
| 3   | F     | 603 | IMP  | 4       | 0            |
| 2   | B     | 601 | ATP  | 5       | 0            |
| 3   | C     | 603 | IMP  | 3       | 0            |
| 2   | D     | 602 | ATP  | 1       | 0            |
| 3   | D     | 603 | IMP  | 3       | 0            |
| 4   | B     | 604 | NAD  | 1       | 0            |
| 4   | D     | 604 | NAD  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



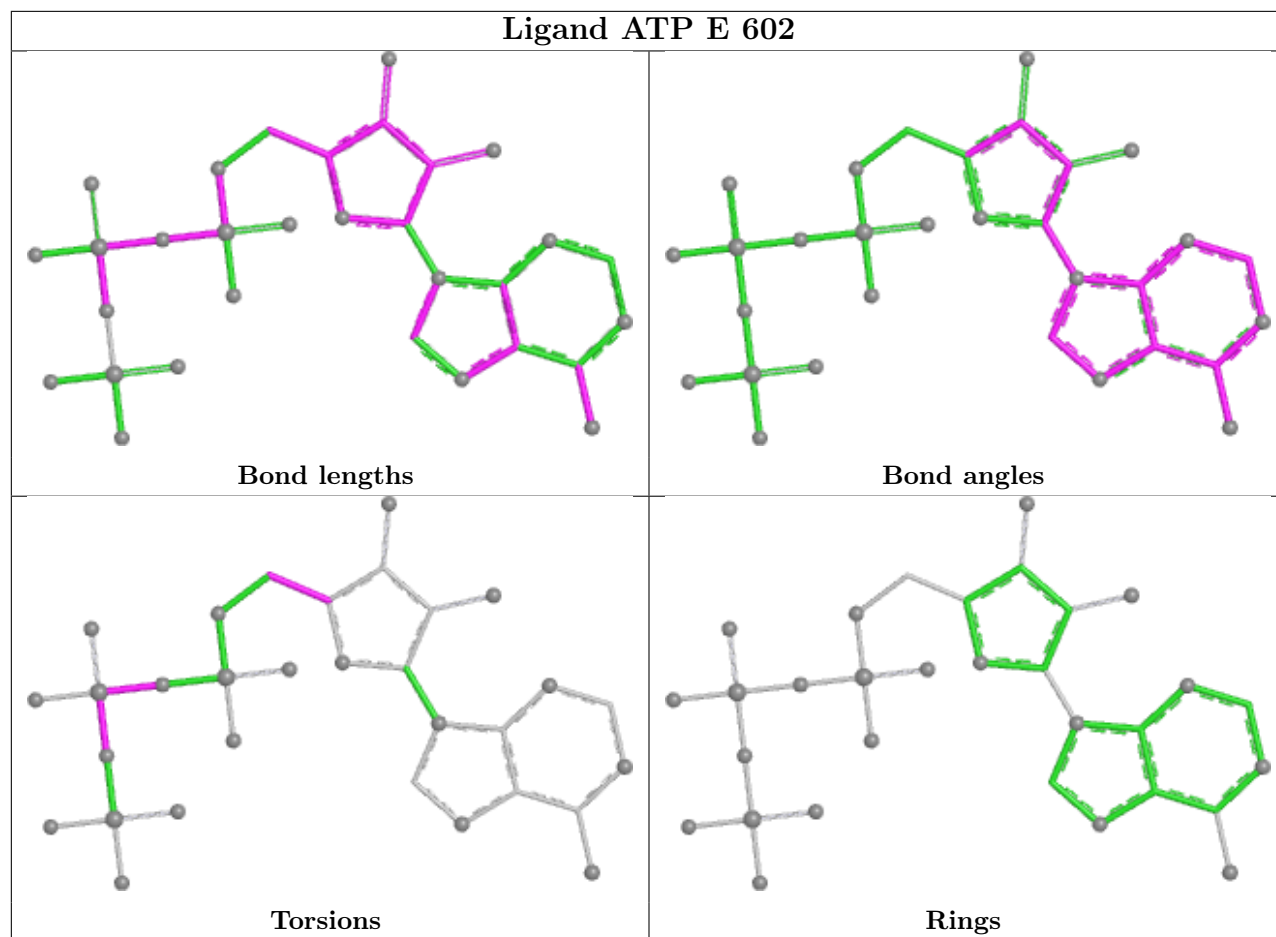




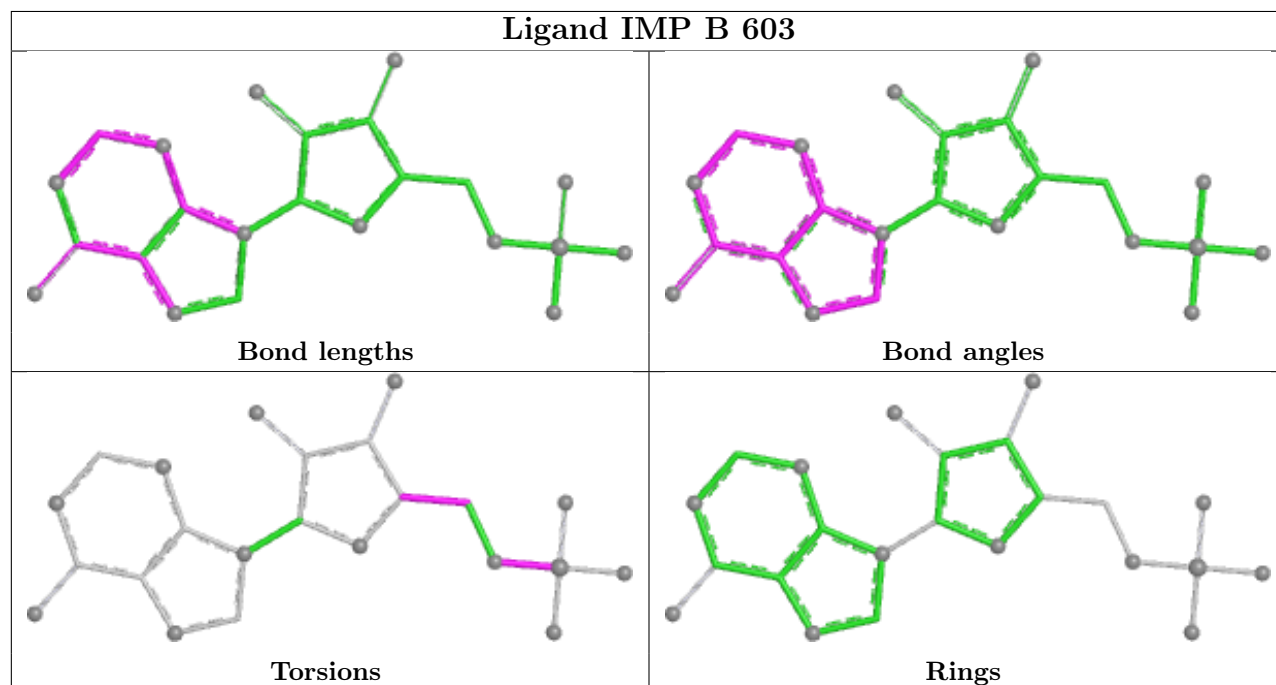




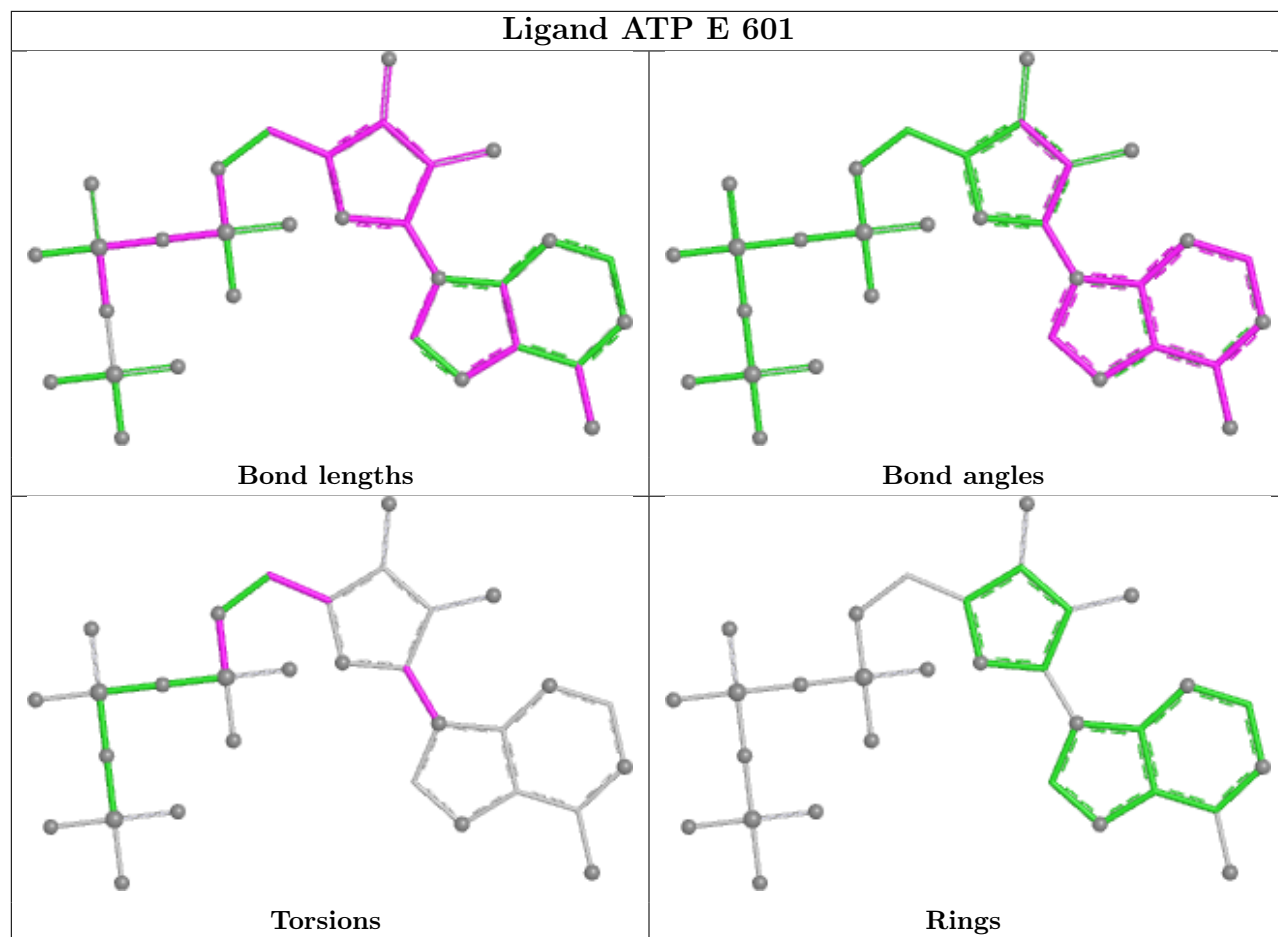
## Ligand ATP E 602



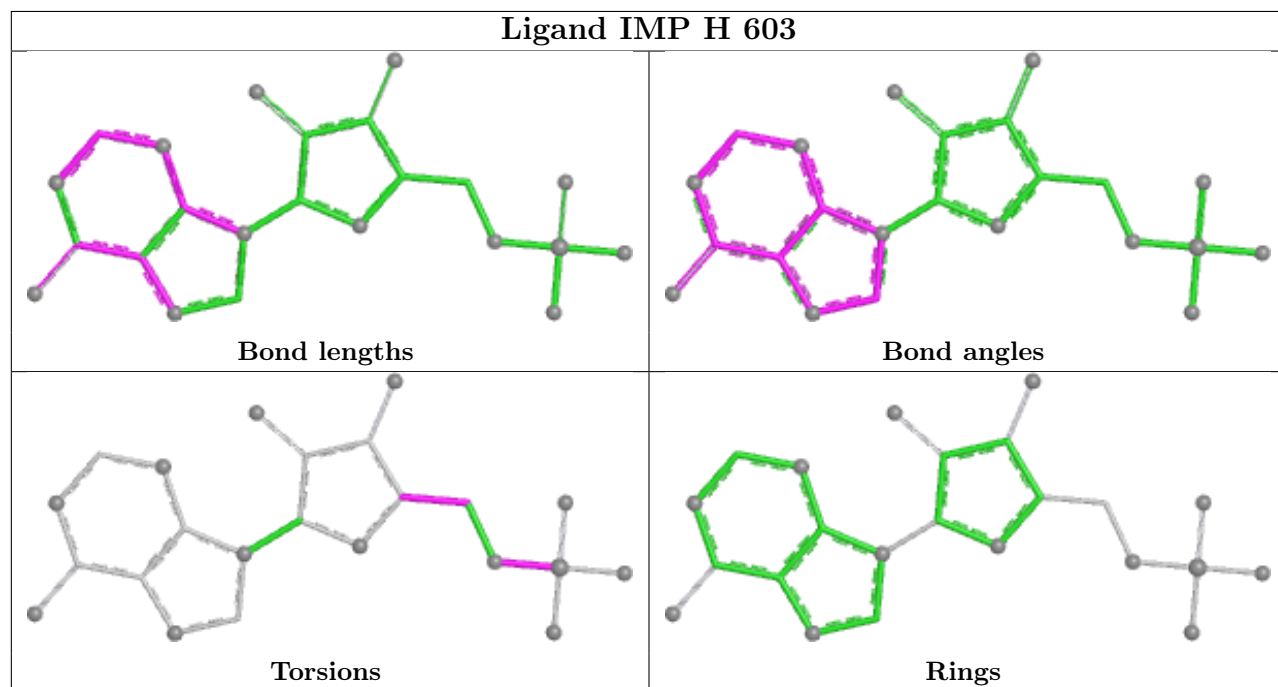
## Ligand IMP B 603

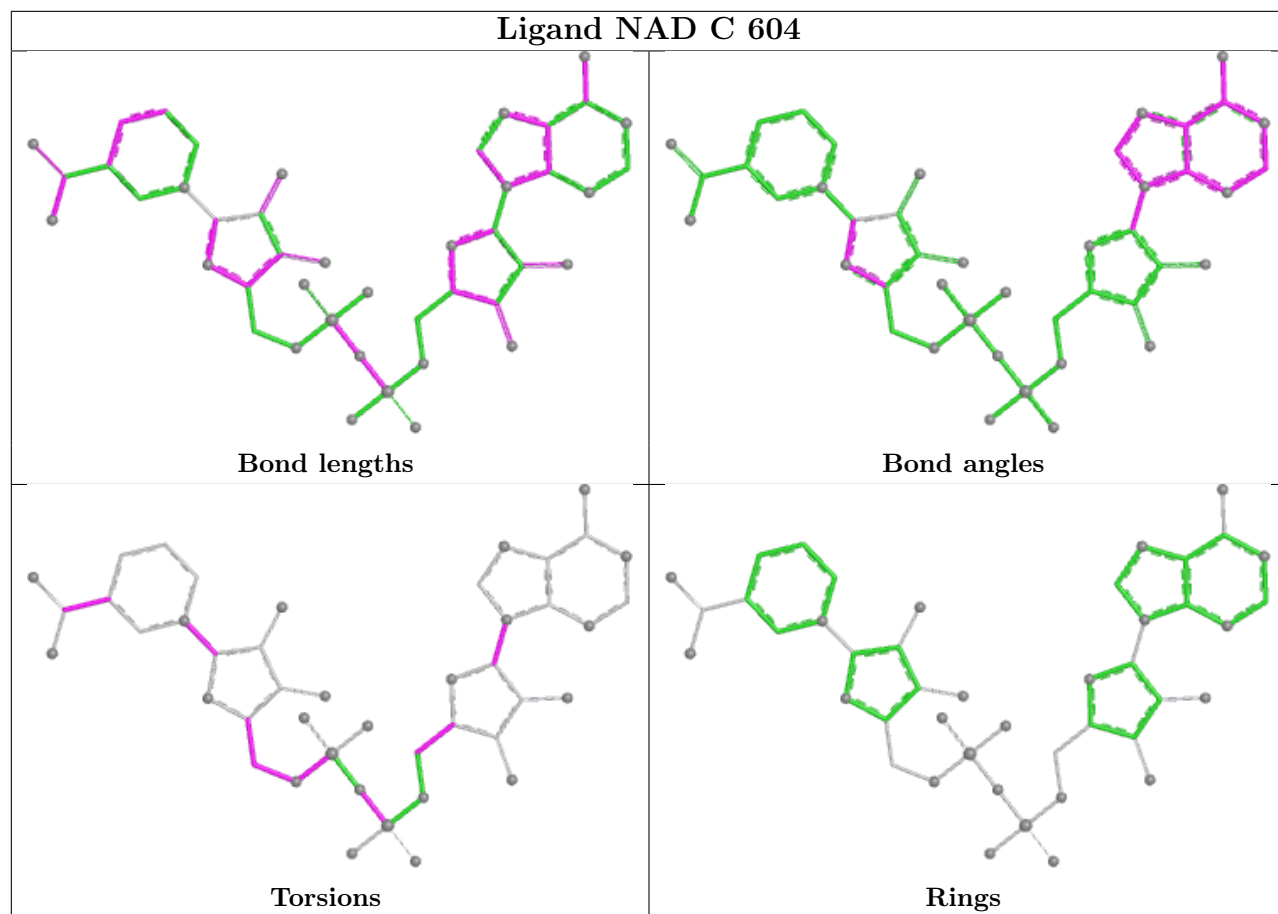


## Ligand ATP E 601

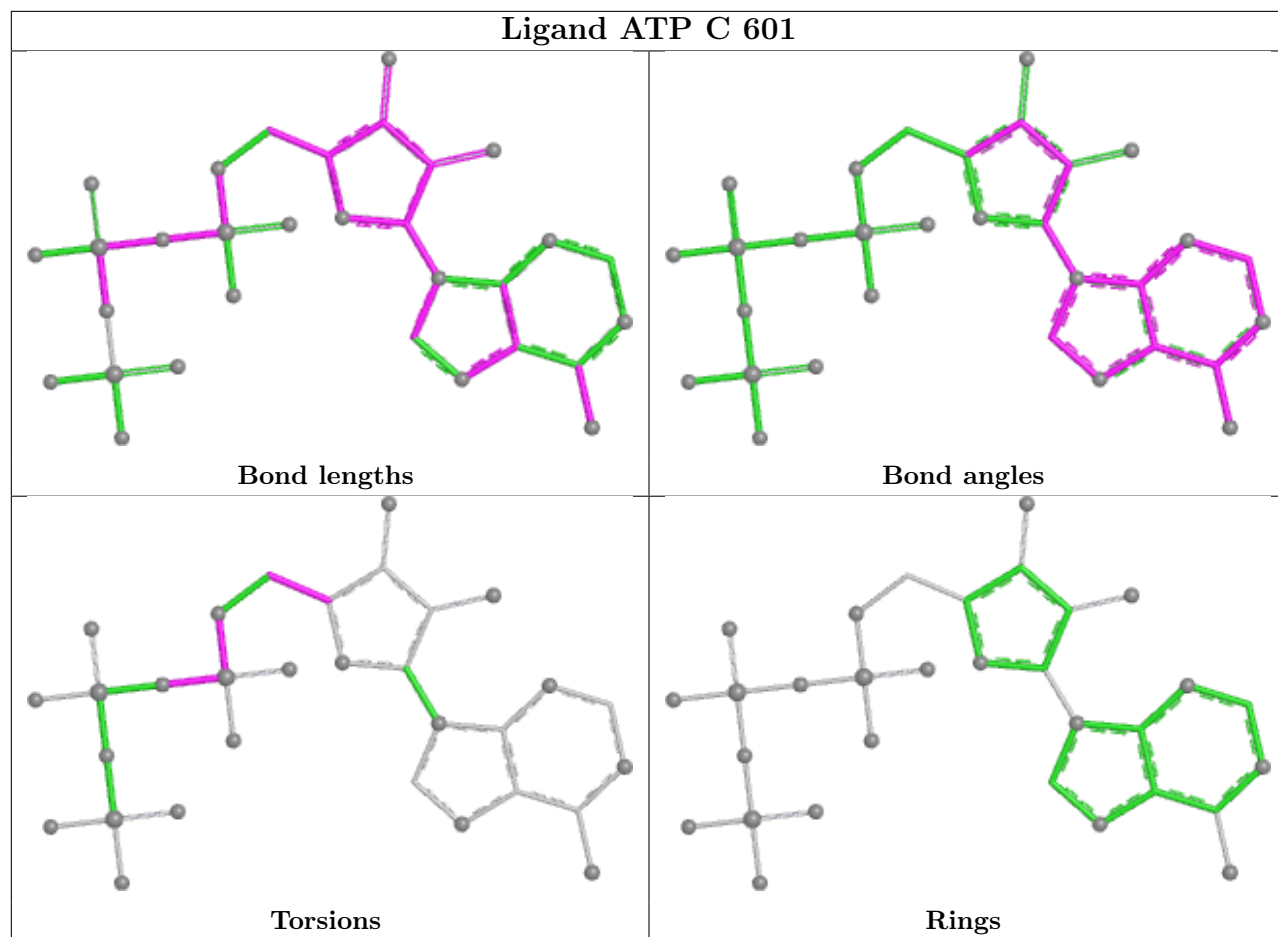


## Ligand IMP H 603

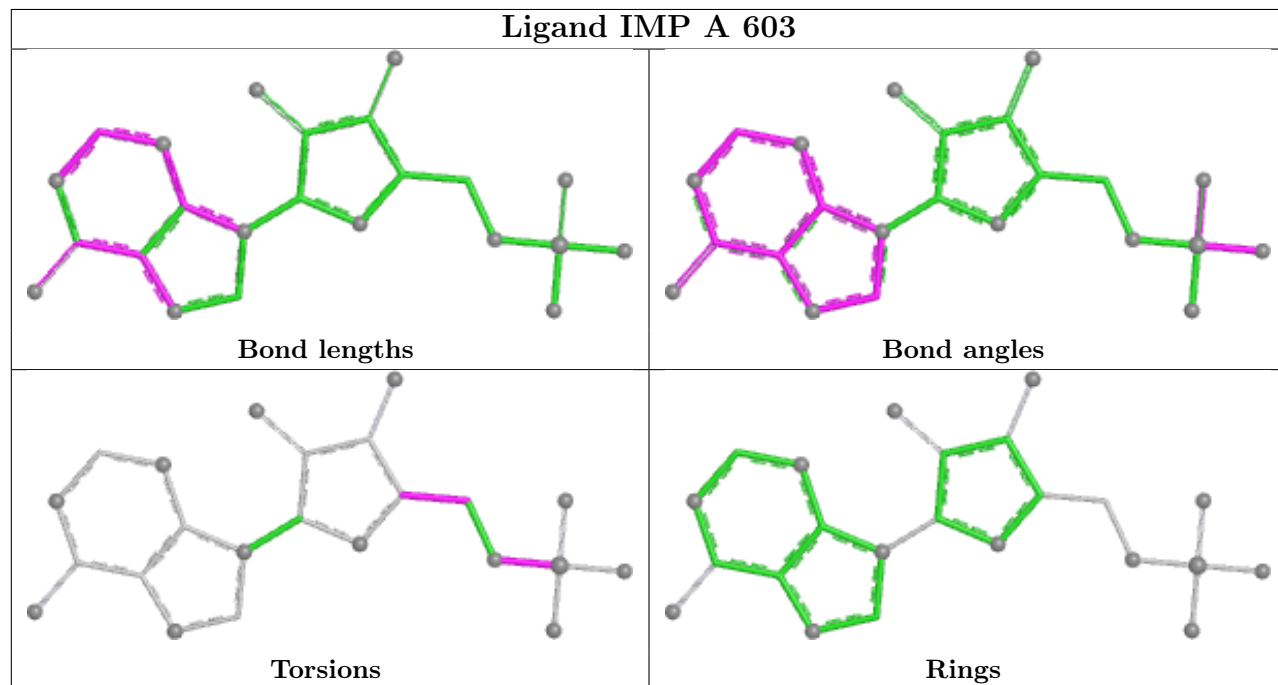


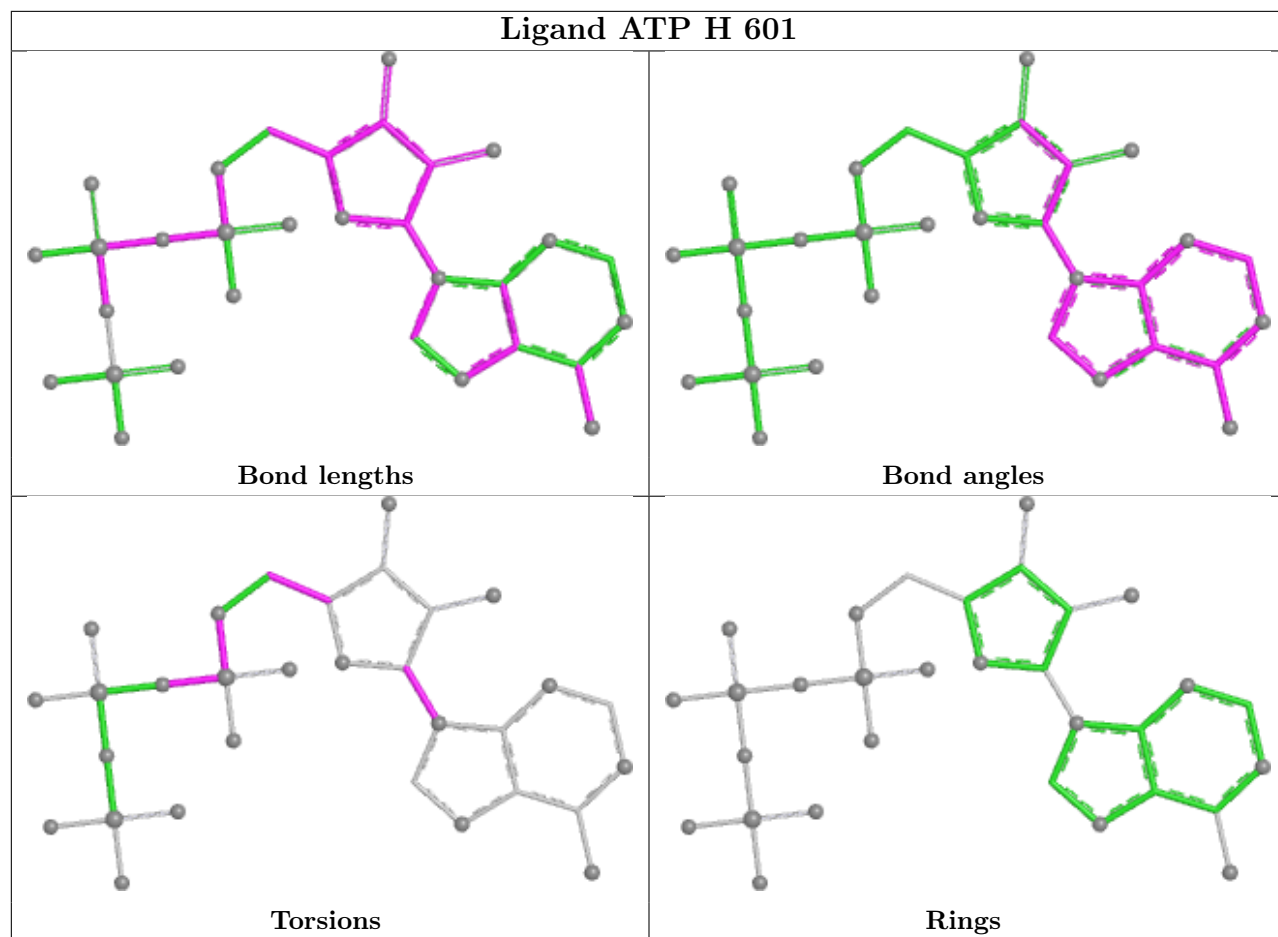


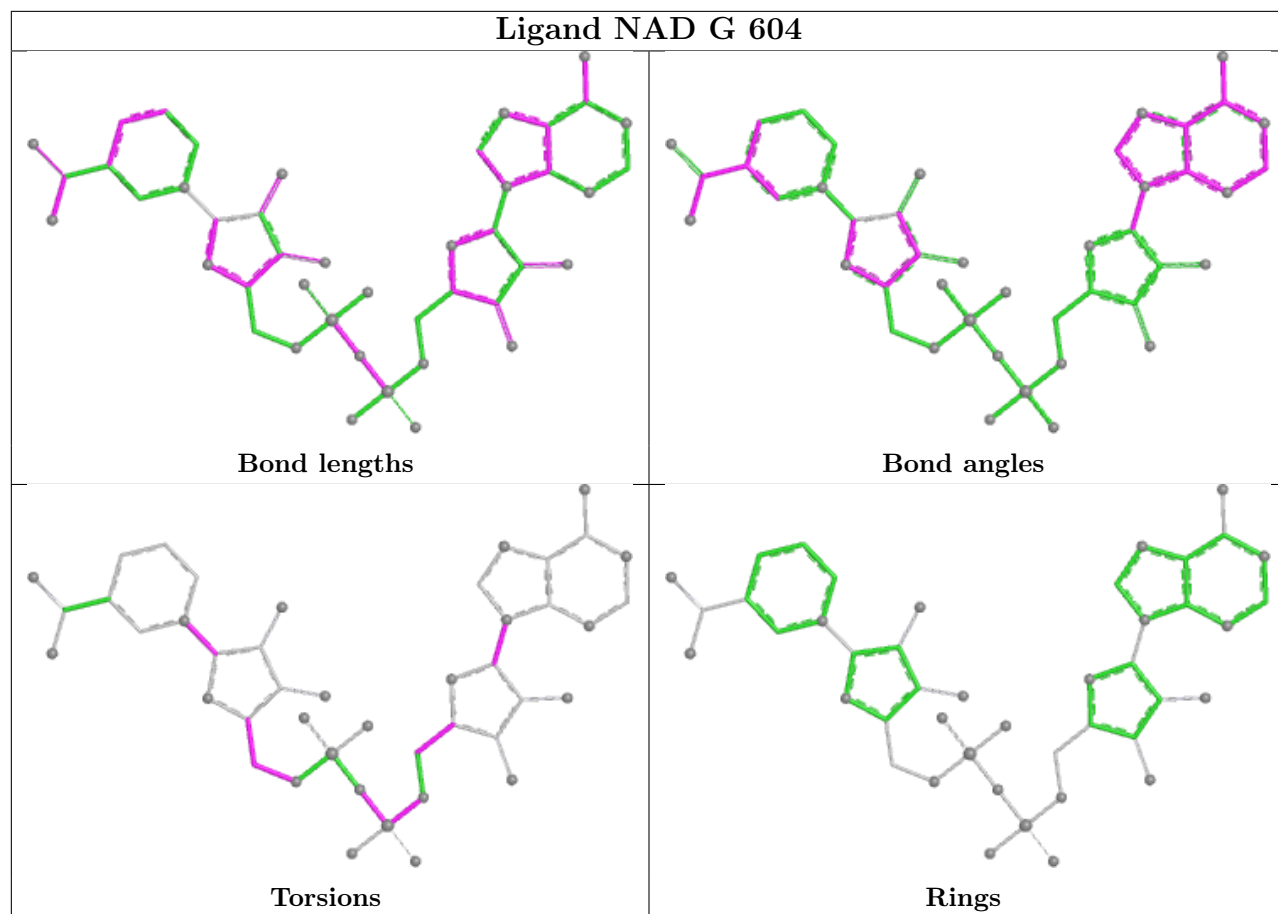
## Ligand ATP C 601

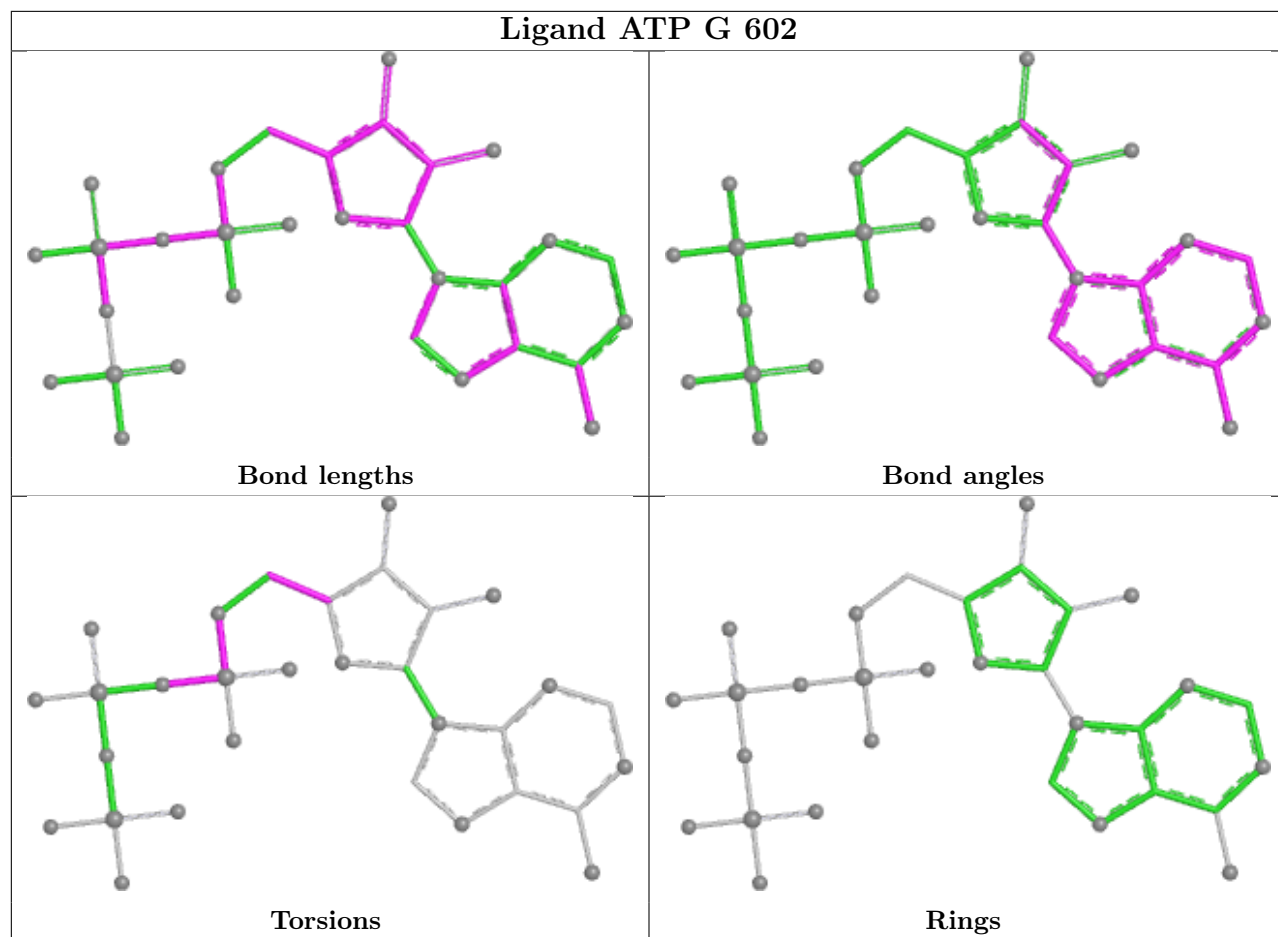


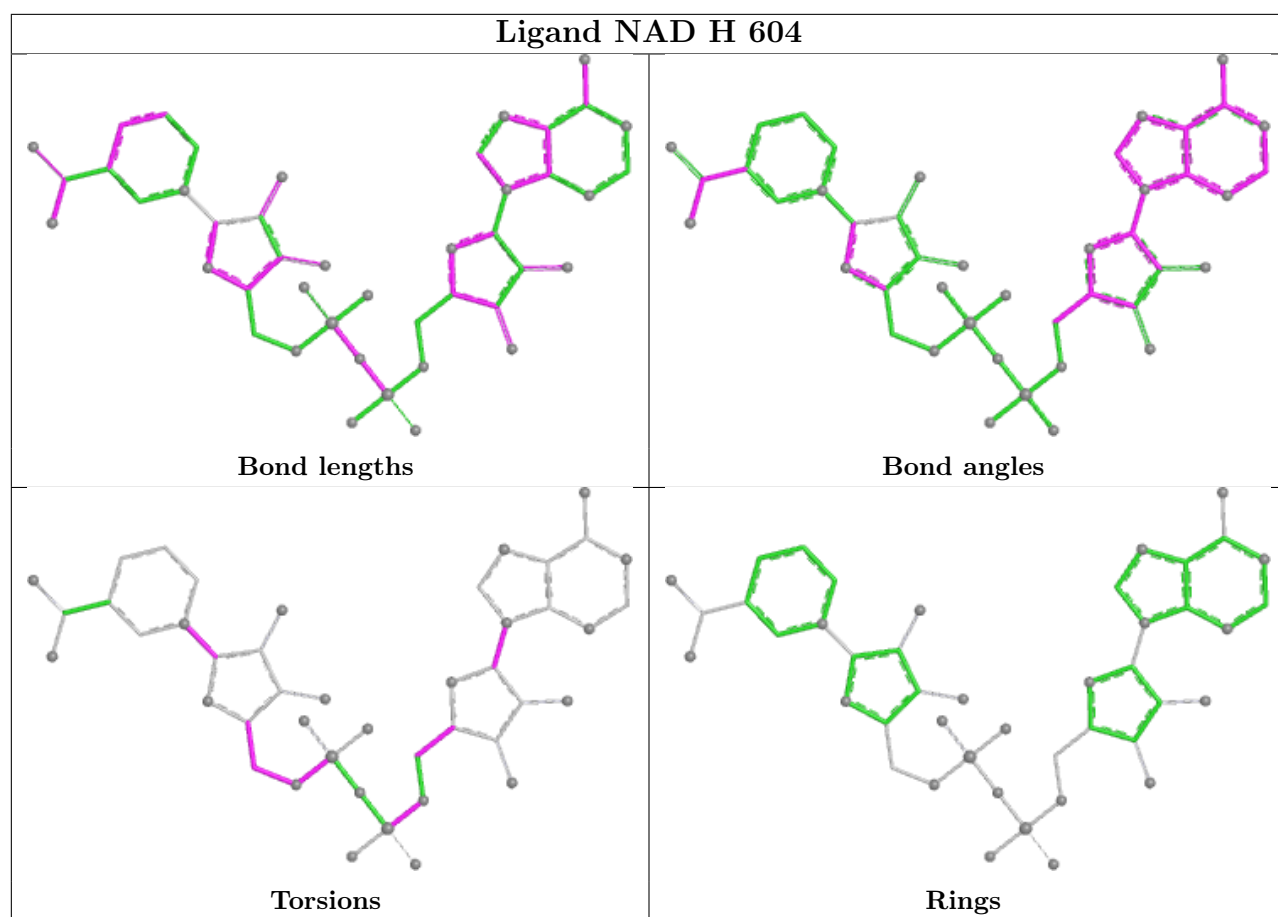
## Ligand IMP A 603



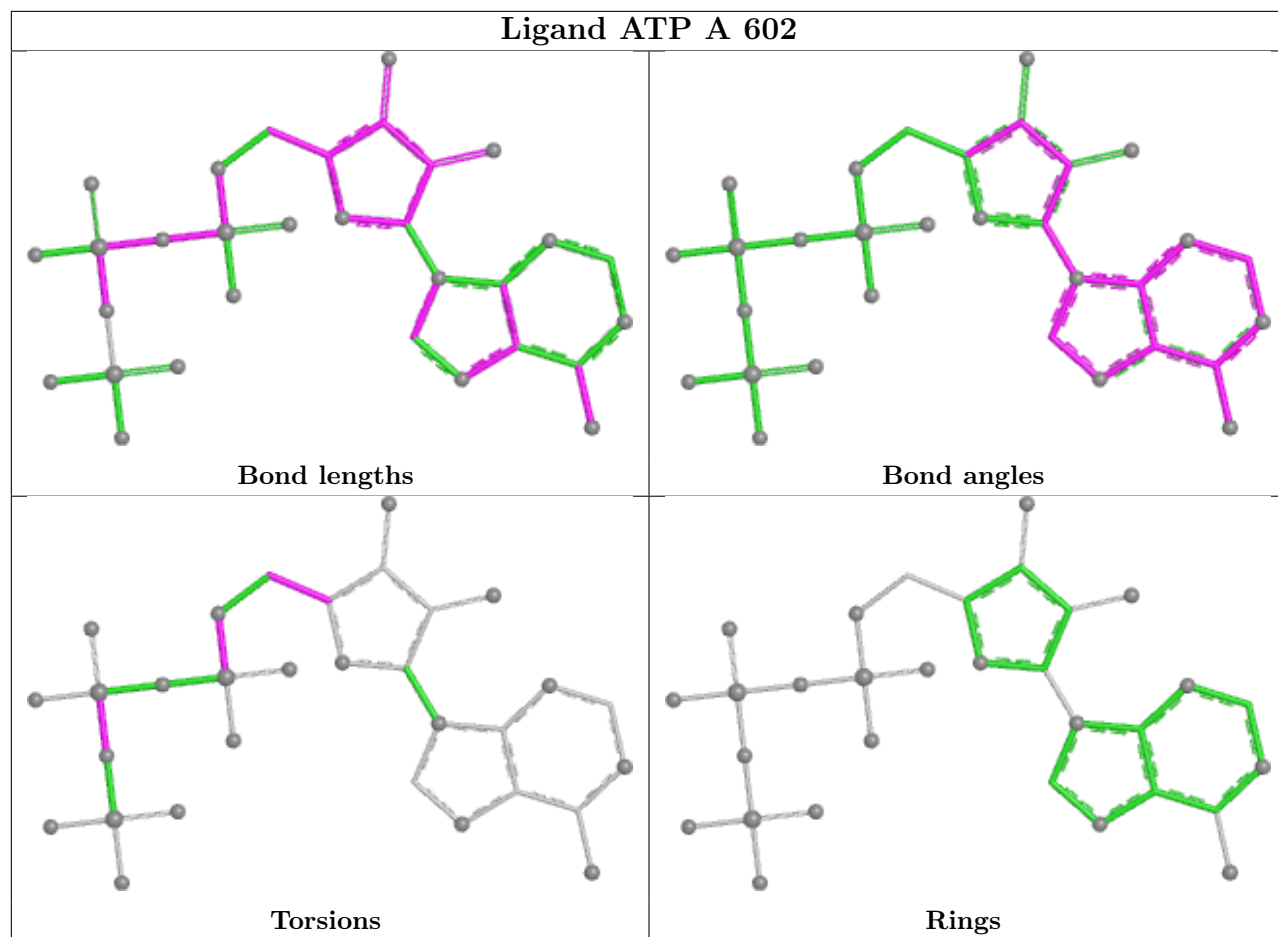


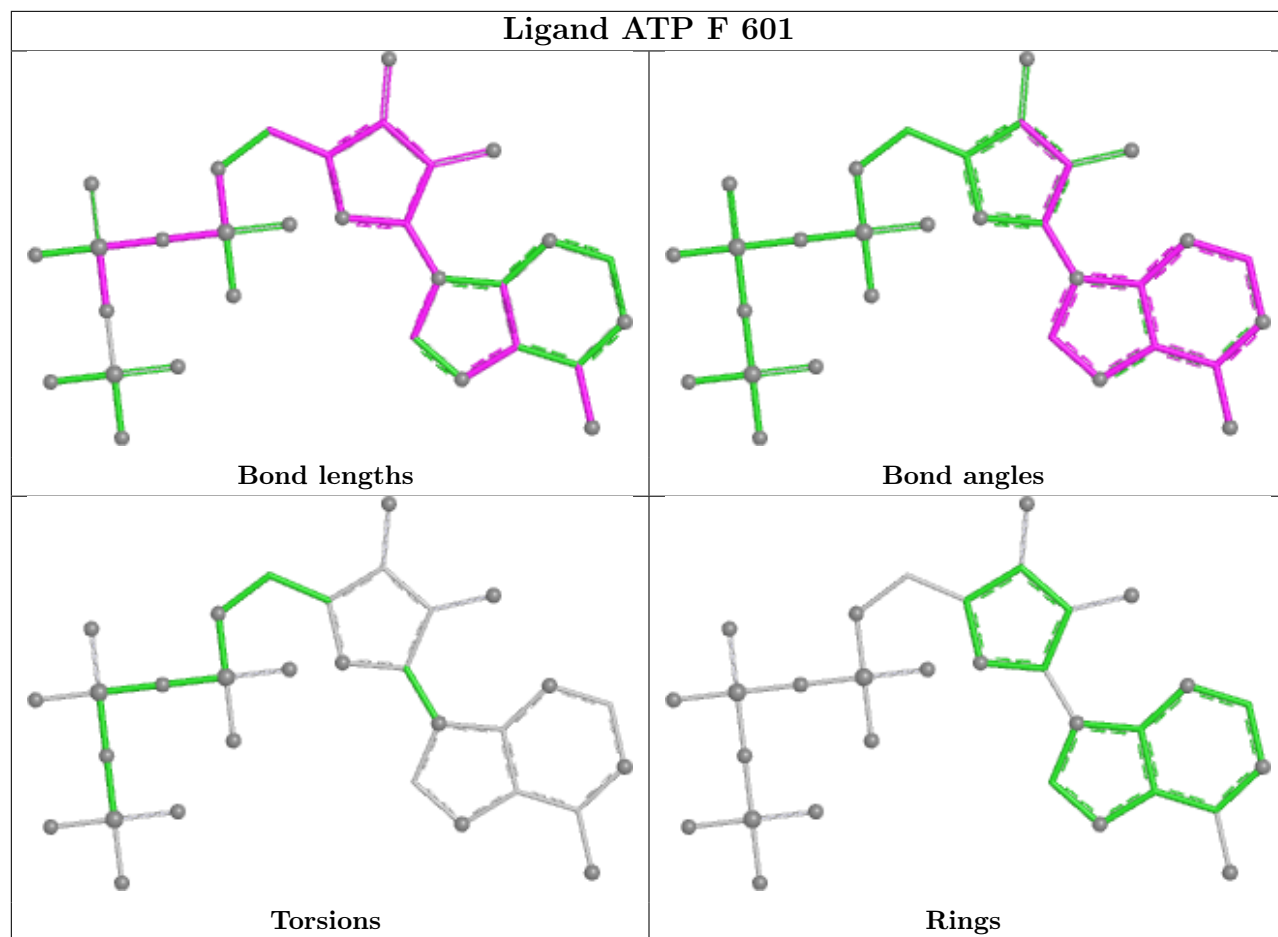




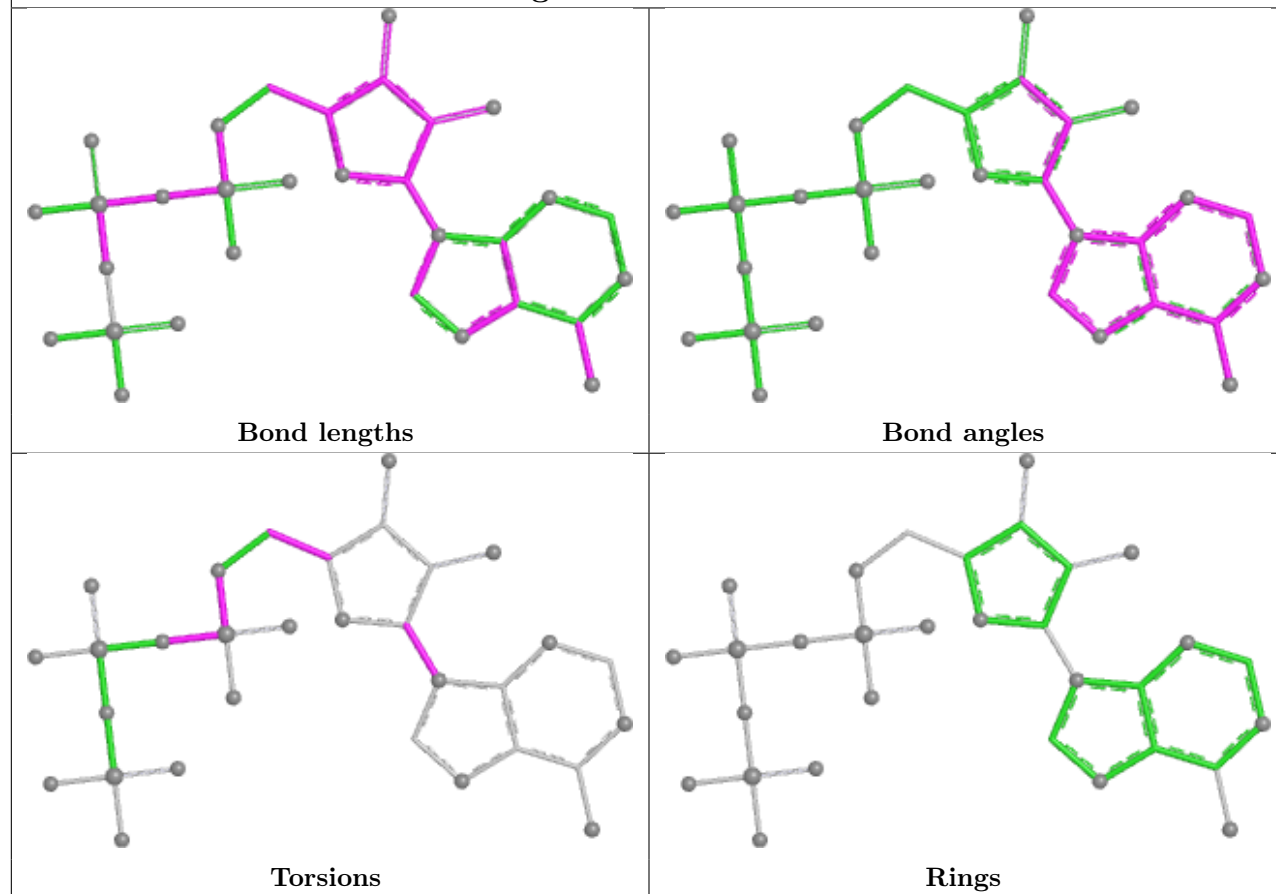




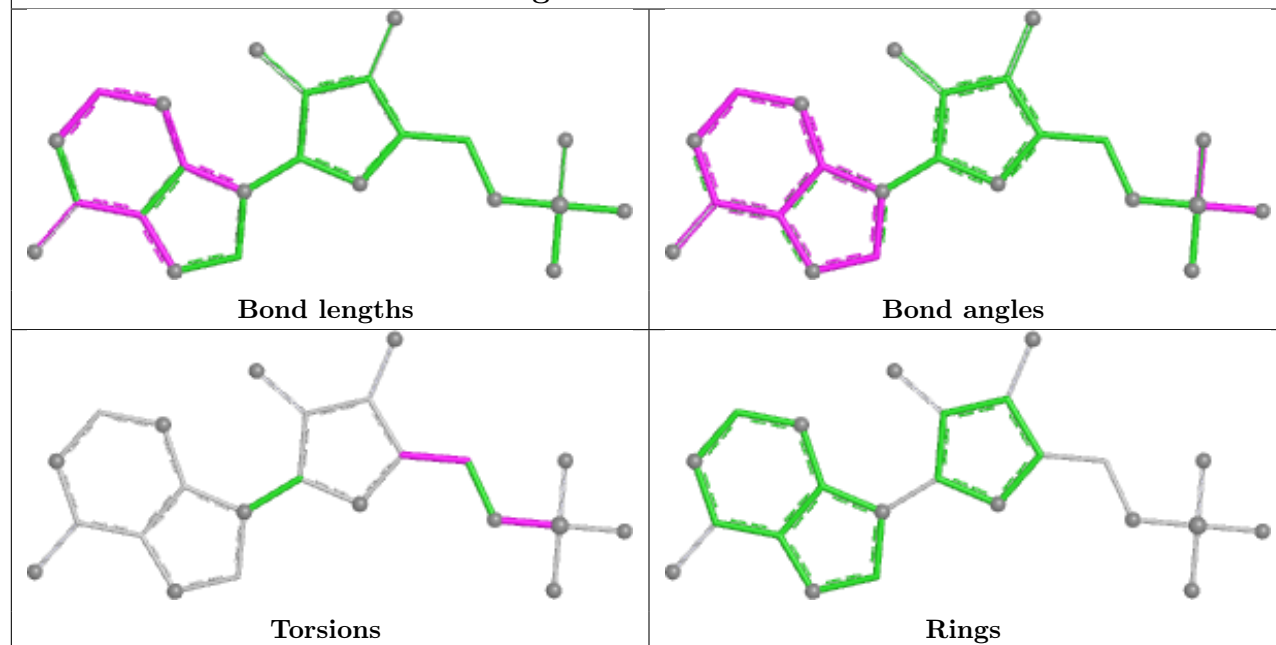


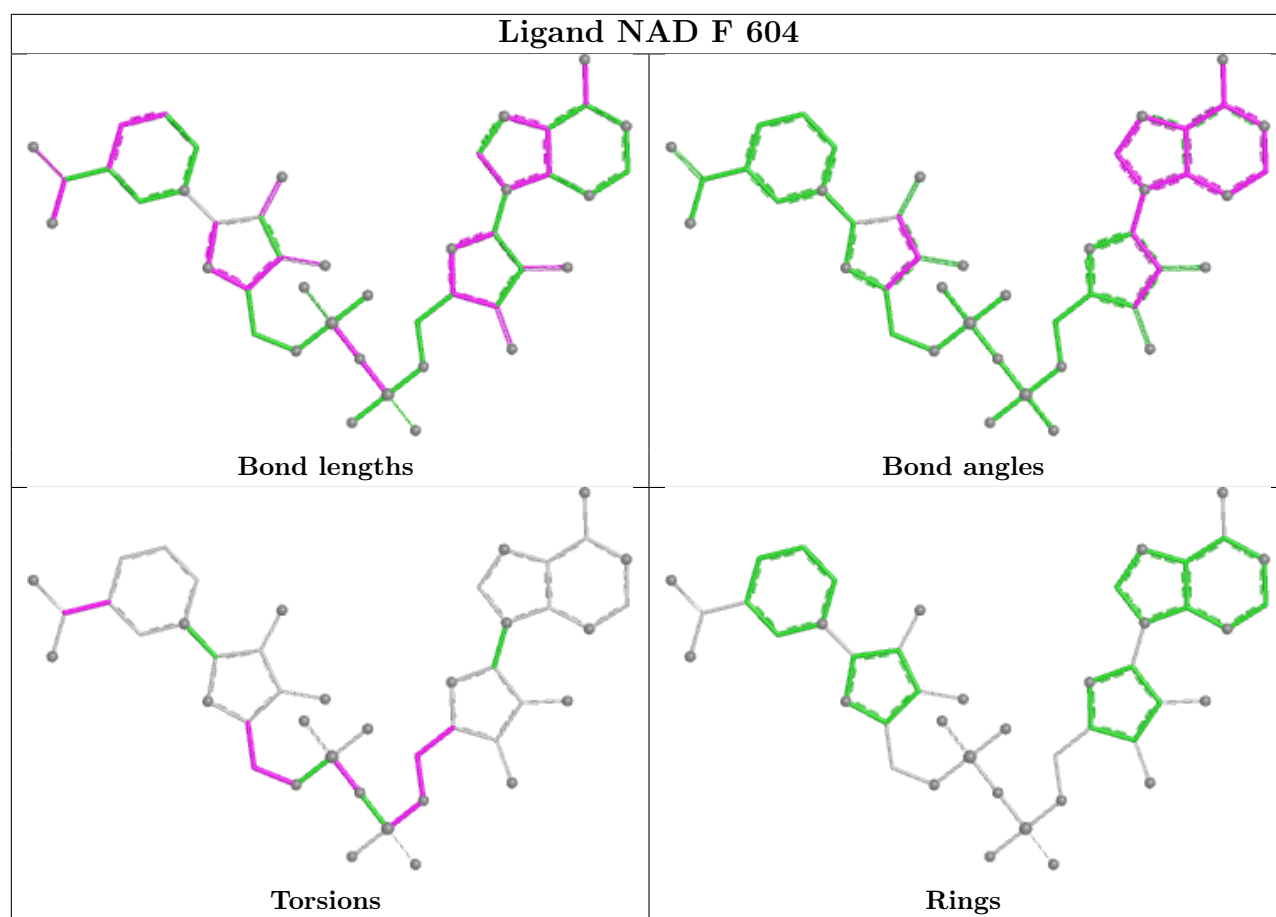


## Ligand ATP G 601

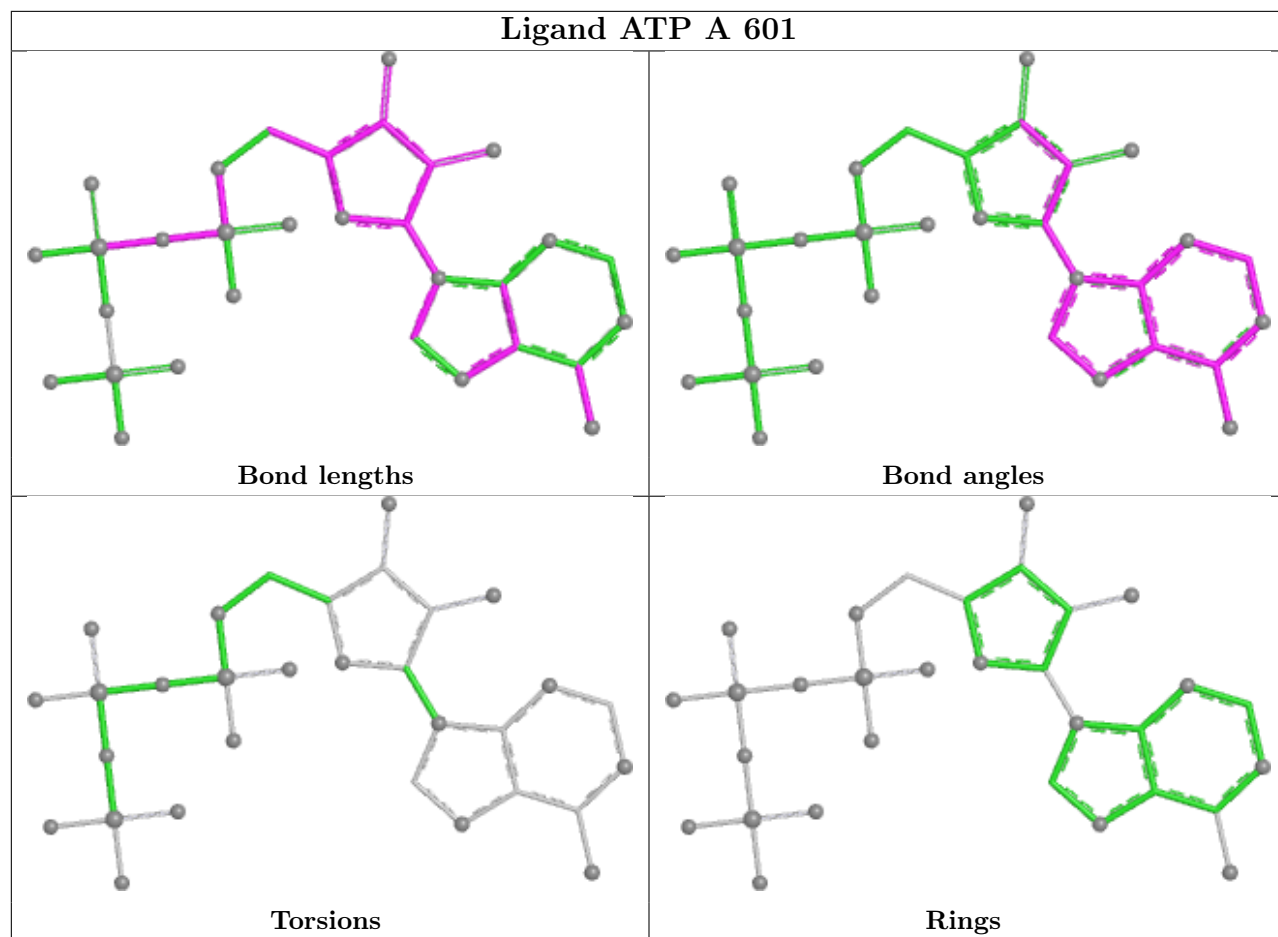


## Ligand IMP G 603

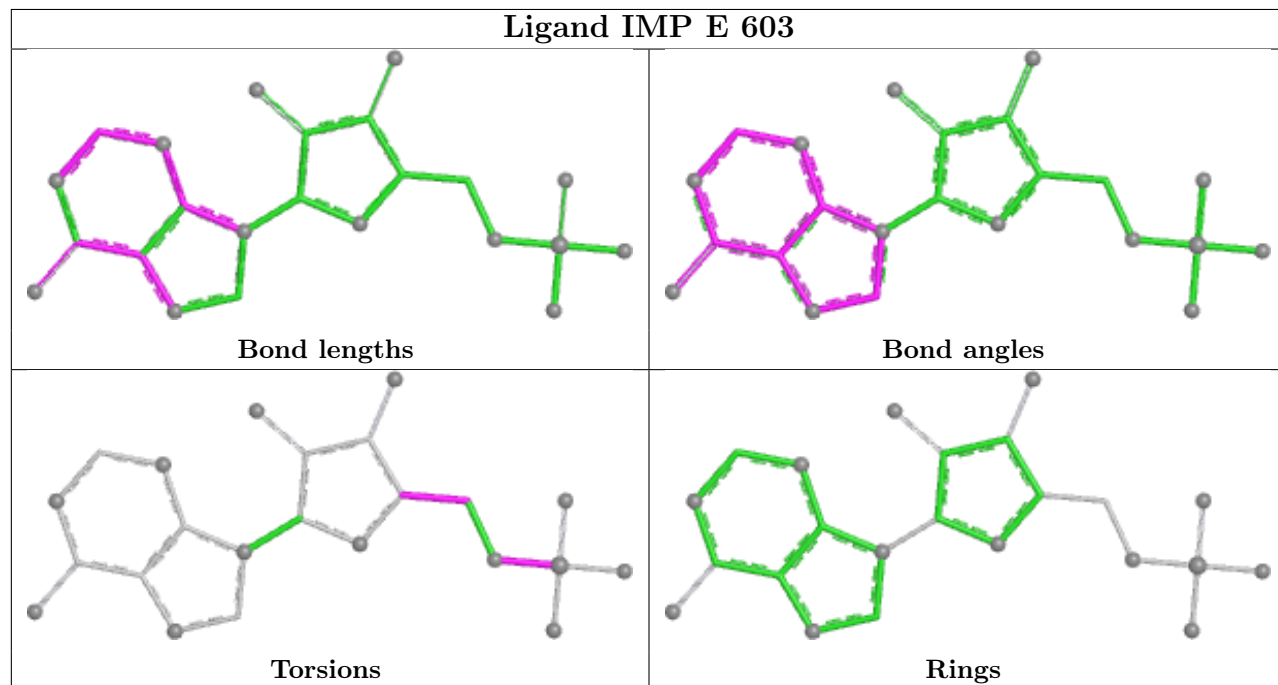




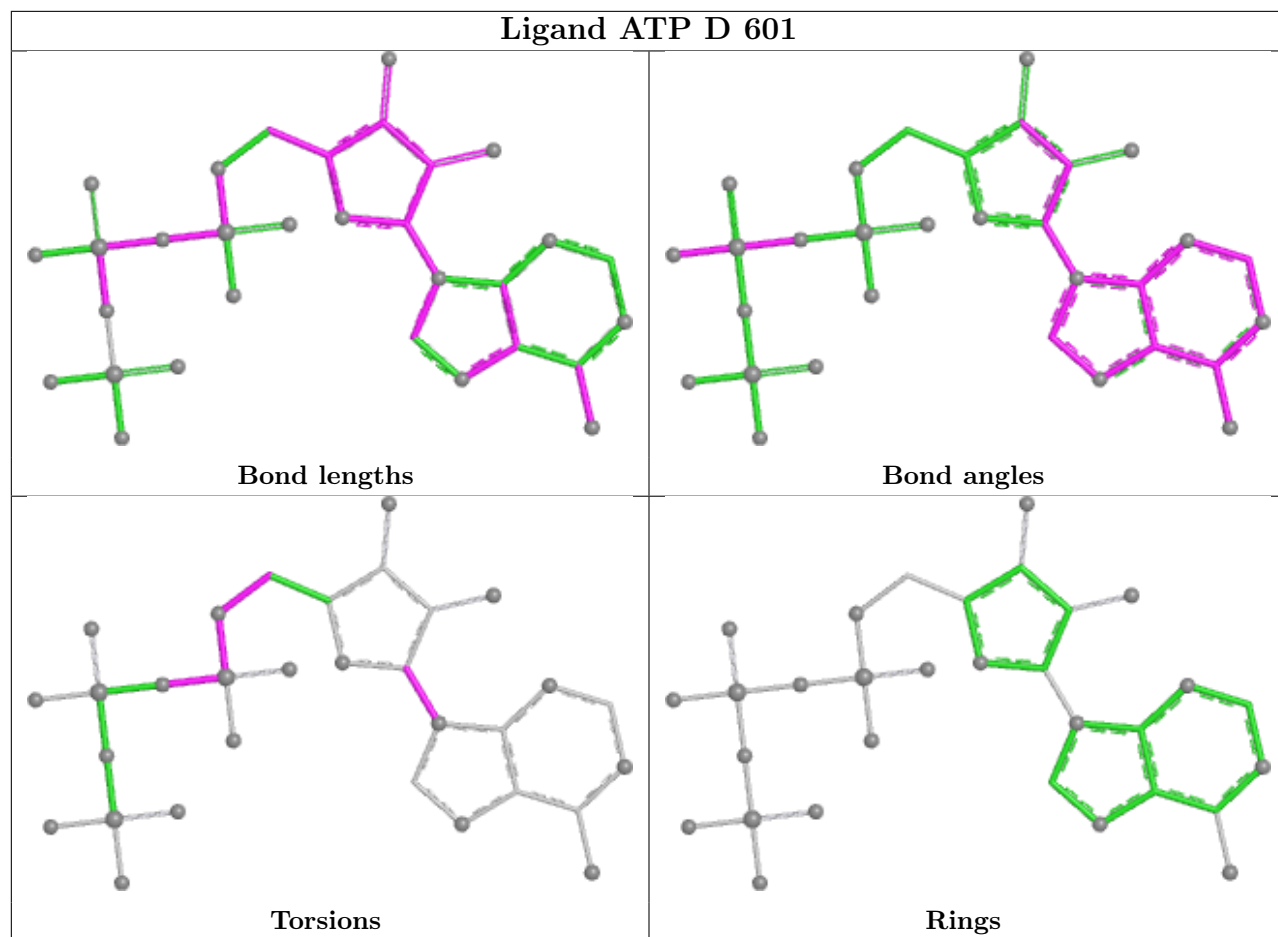
## Ligand ATP A 601



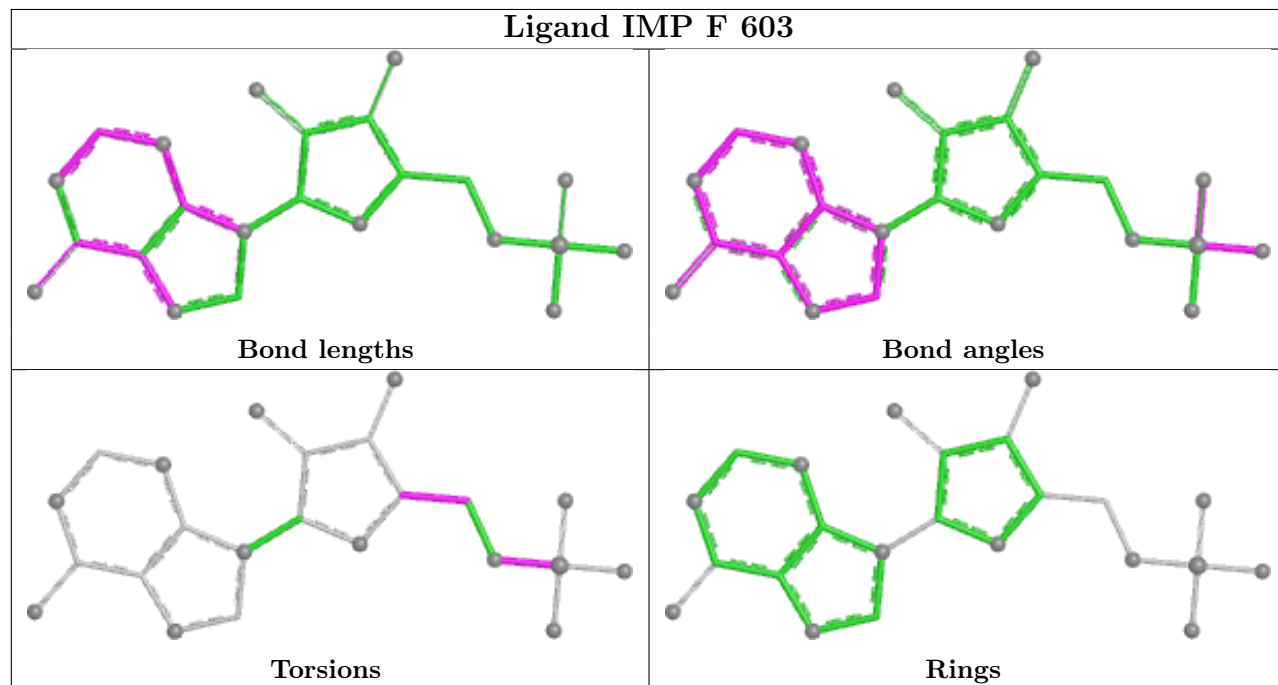
## Ligand IMP E 603



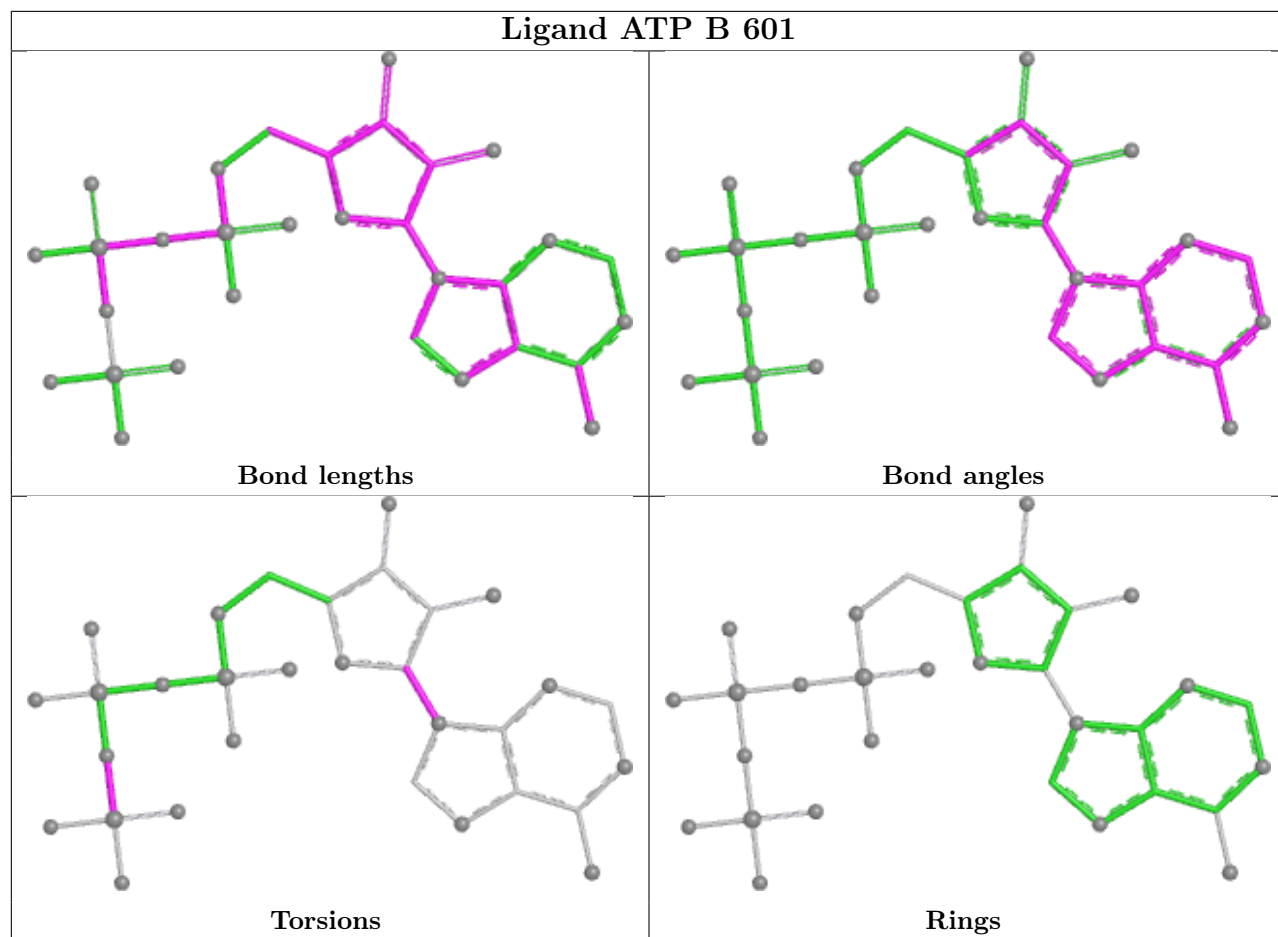
## Ligand ATP D 601



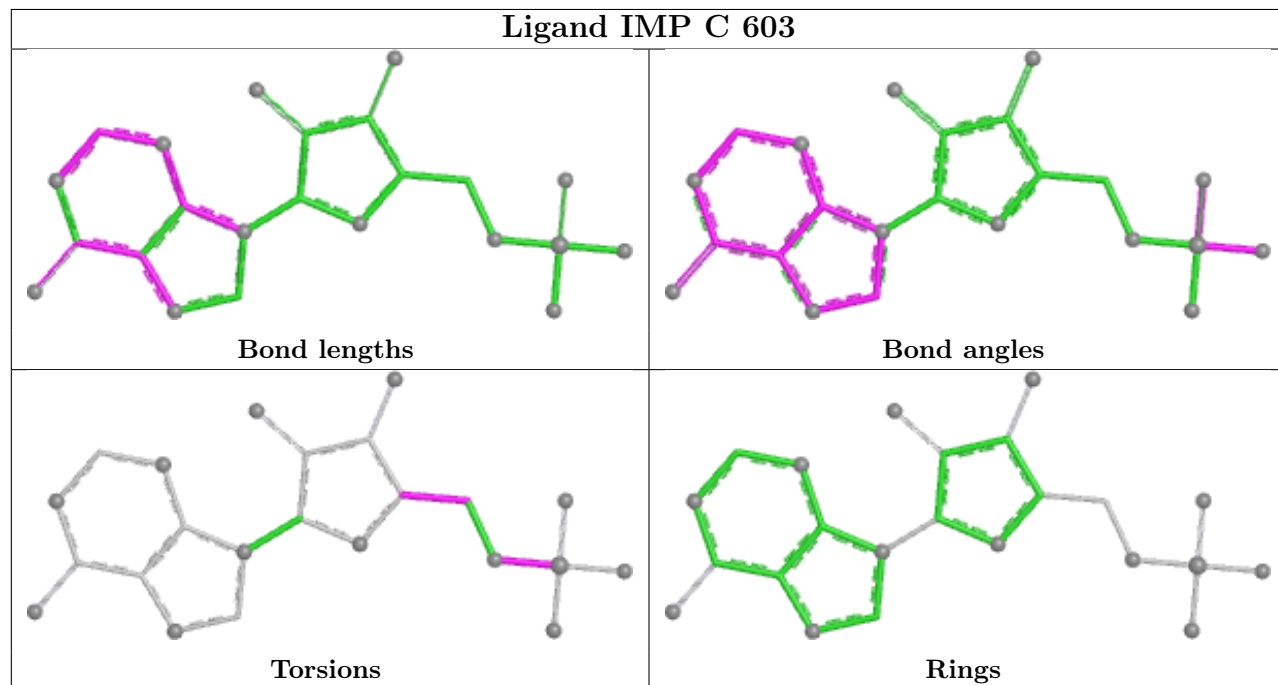
## Ligand IMP F 603



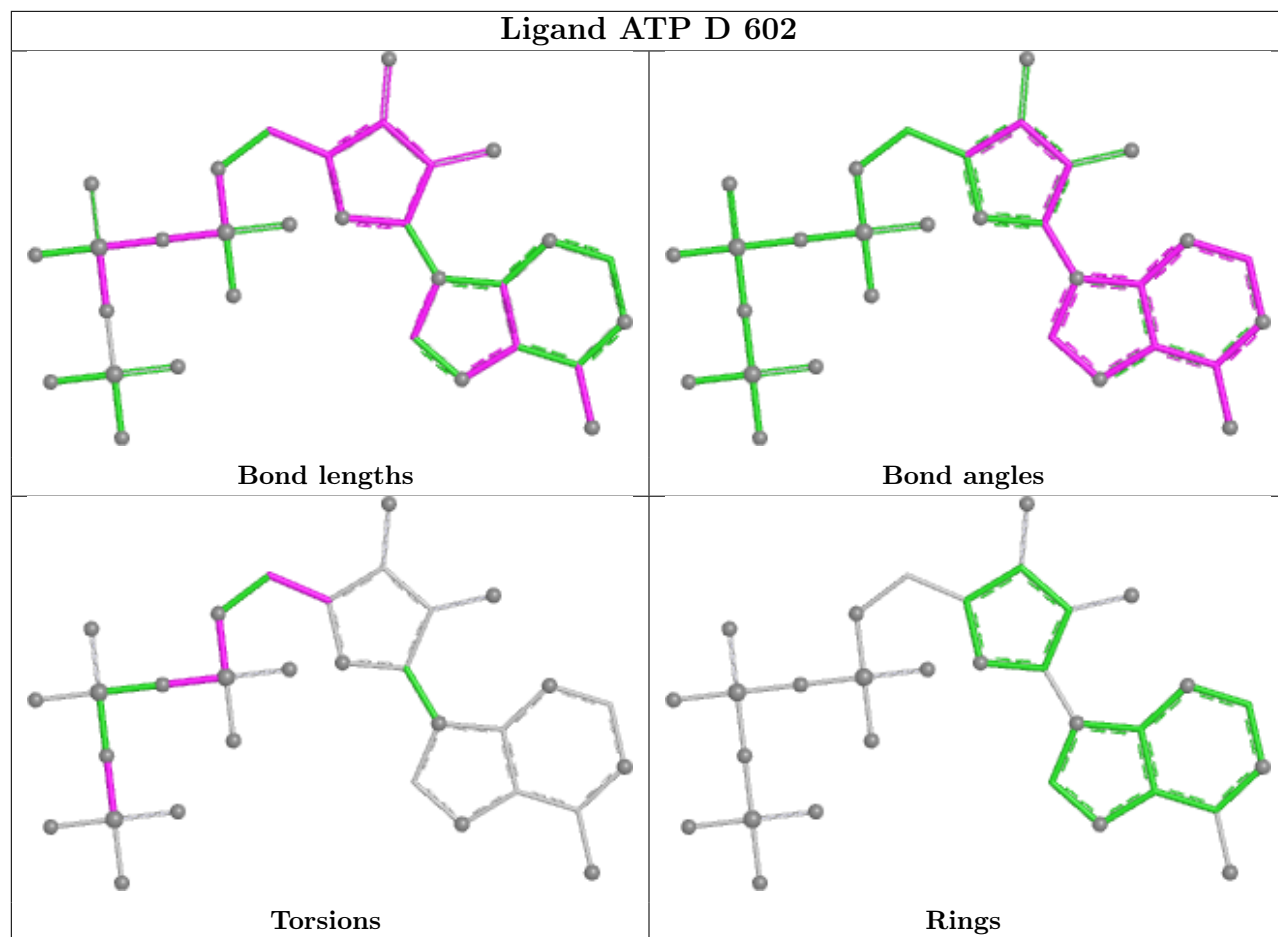
## Ligand ATP B 601



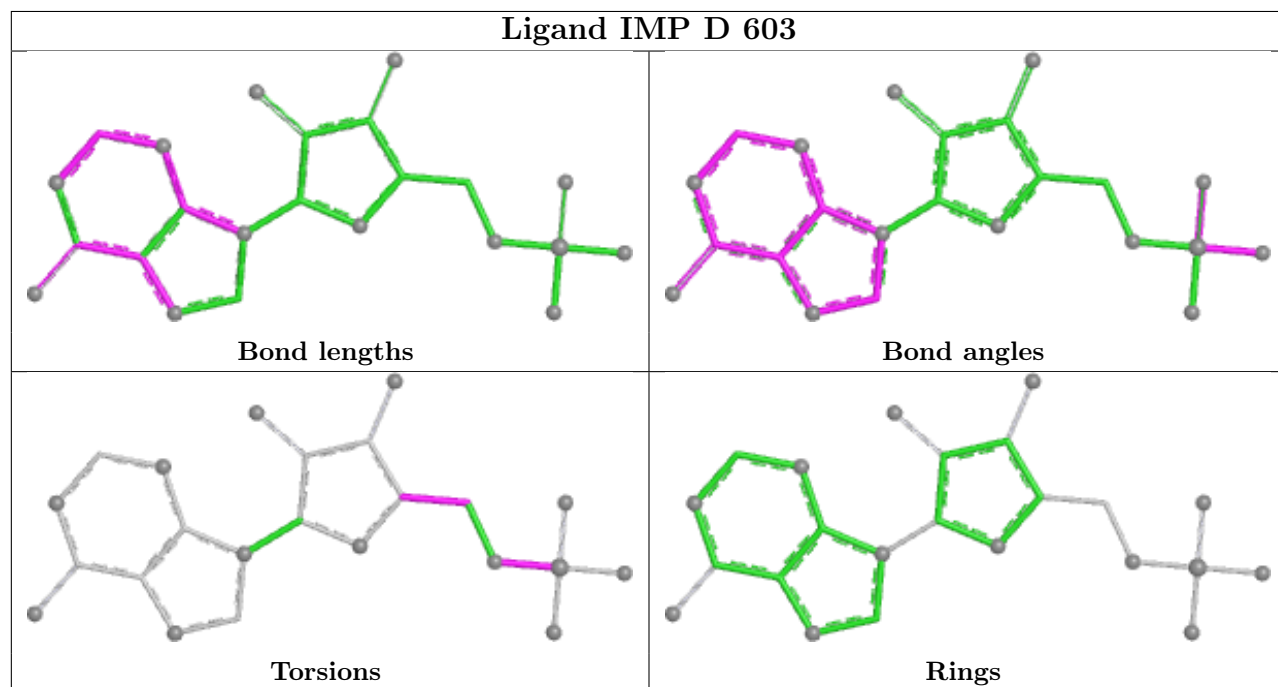
## Ligand IMP C 603



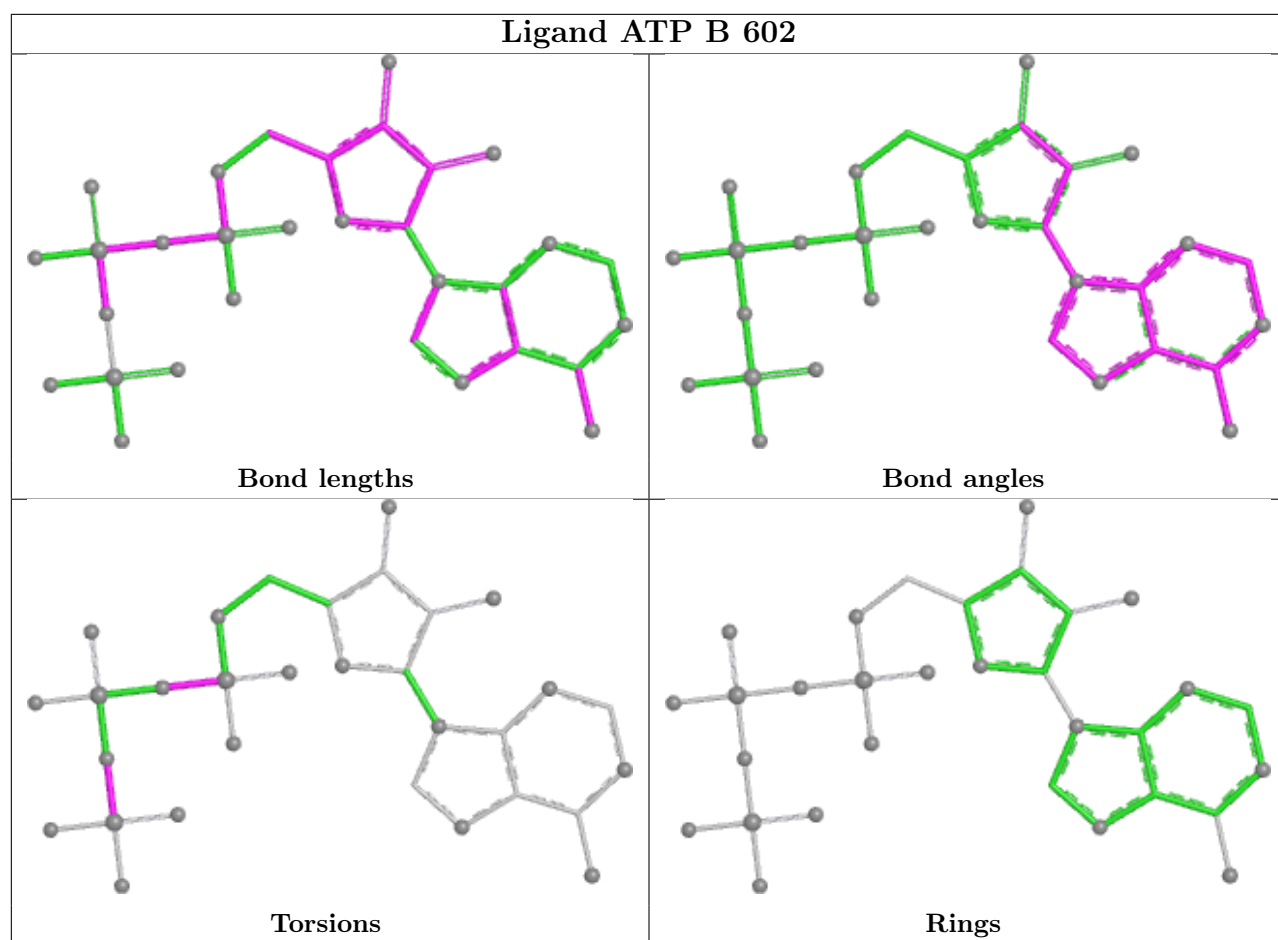
## Ligand ATP D 602

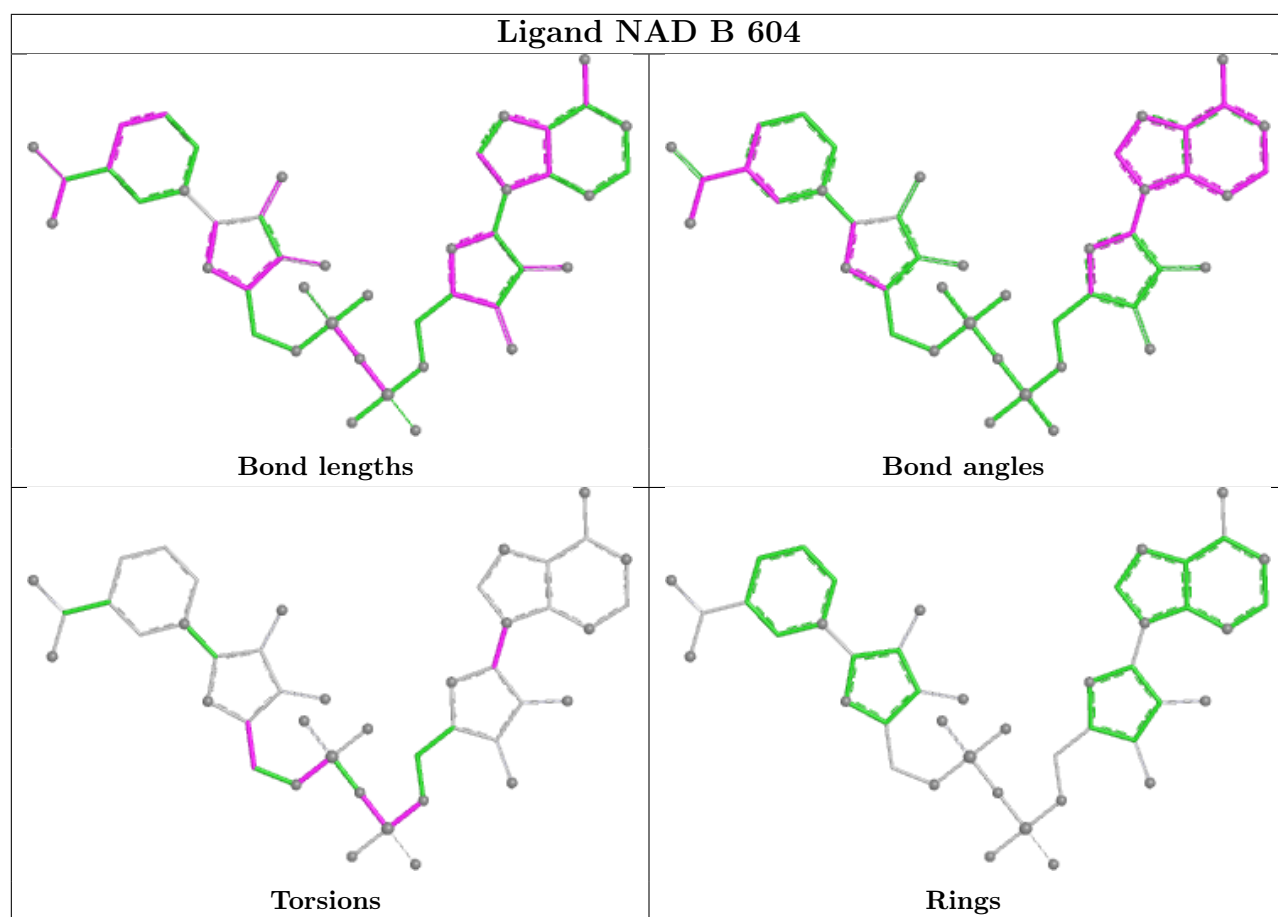


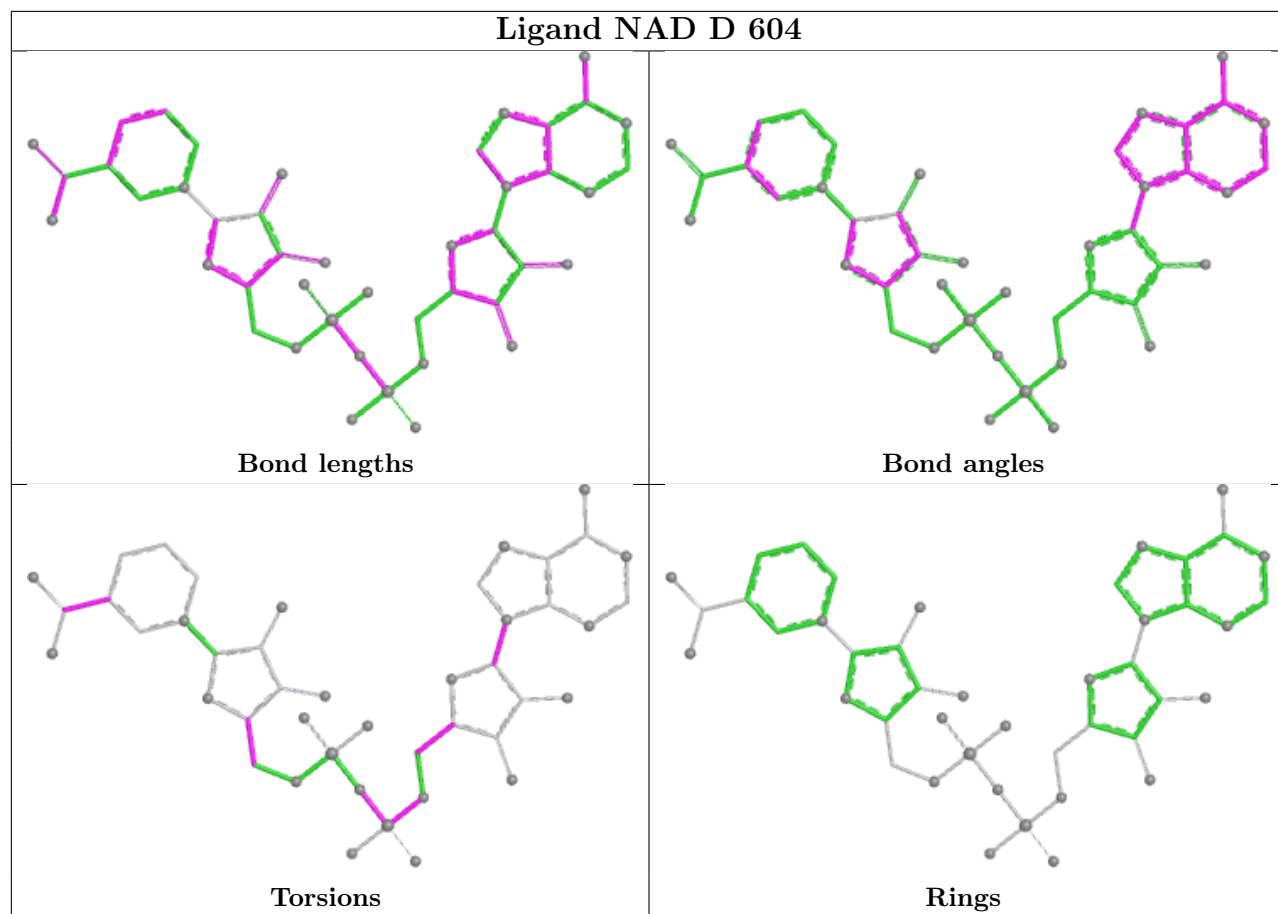
## Ligand IMP D 603

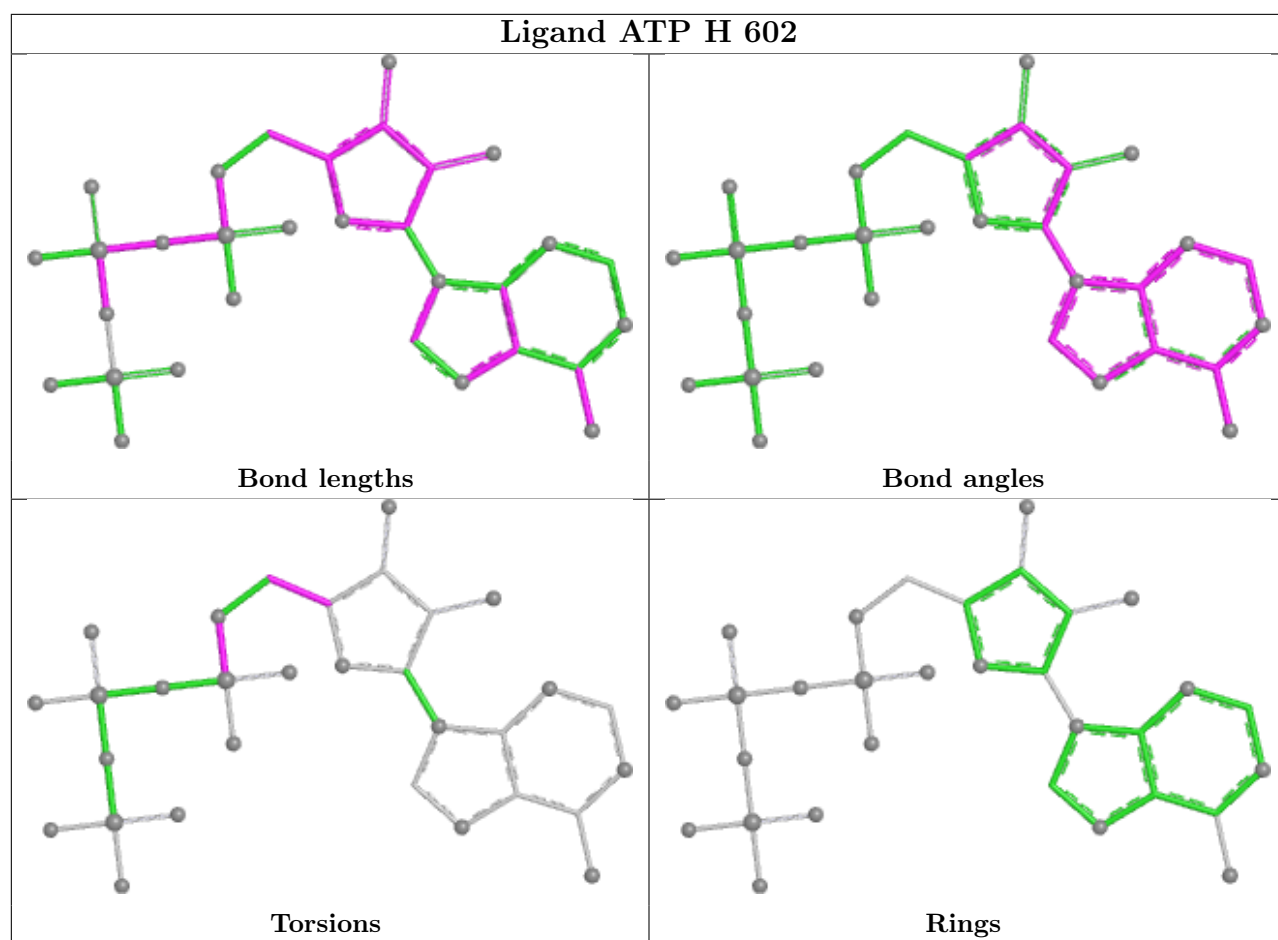












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

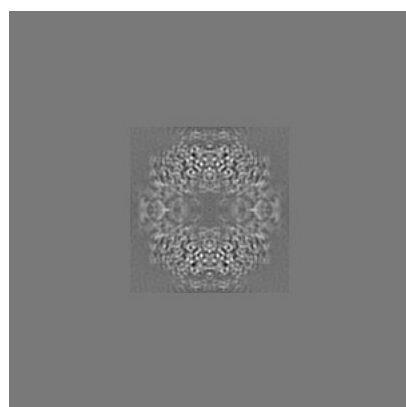
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24438. These allow visual inspection of the internal detail of the map and identification of artifacts.

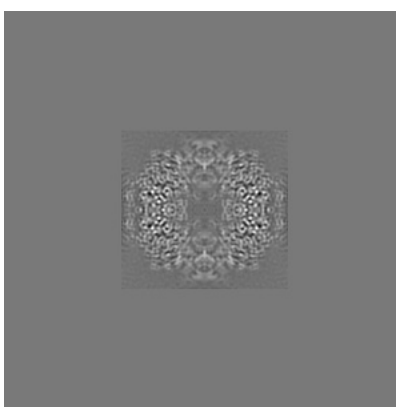
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

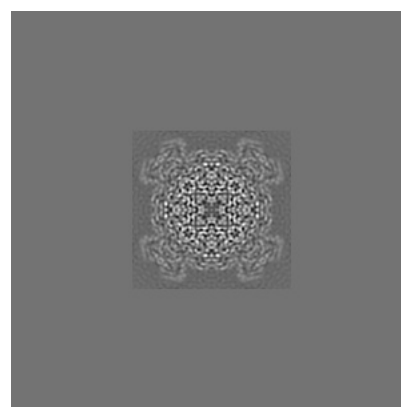
#### 6.1.1 Primary map



X



Y

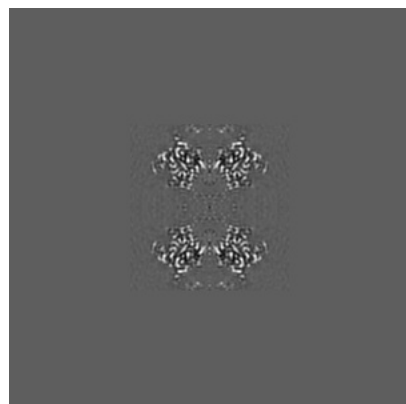


Z

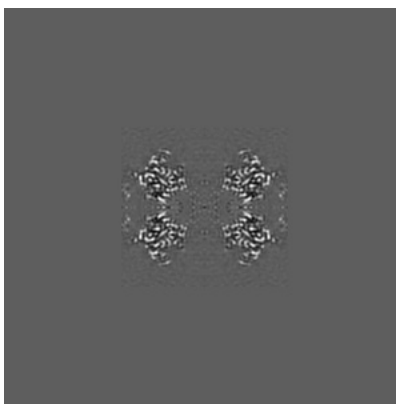
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

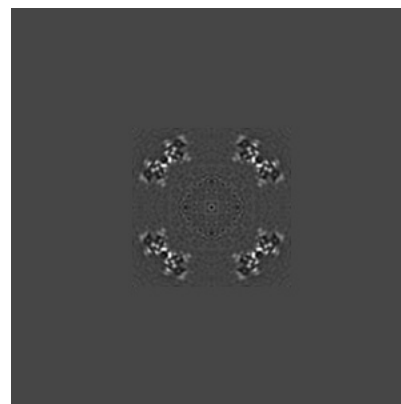
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

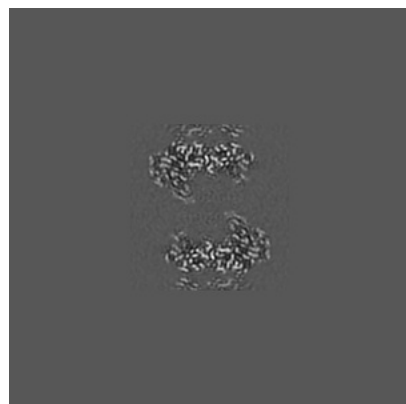


Z Index: 160

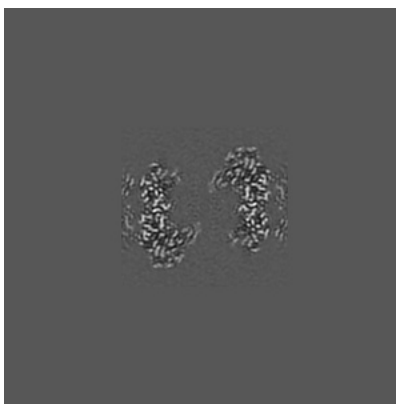
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

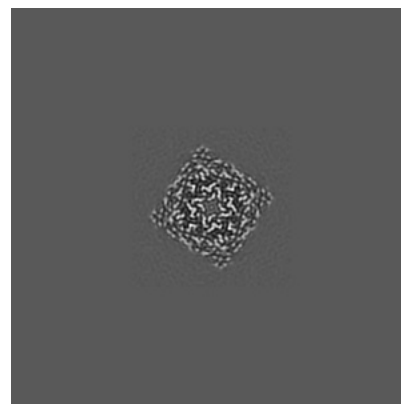
### 6.3.1 Primary map



X Index: 170



Y Index: 170

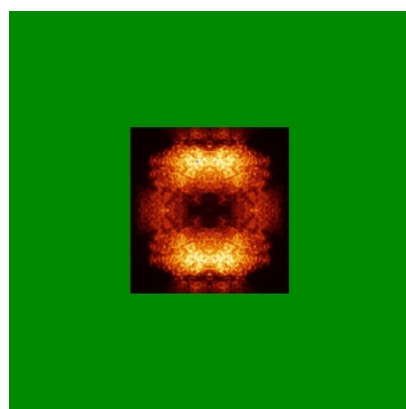


Z Index: 197

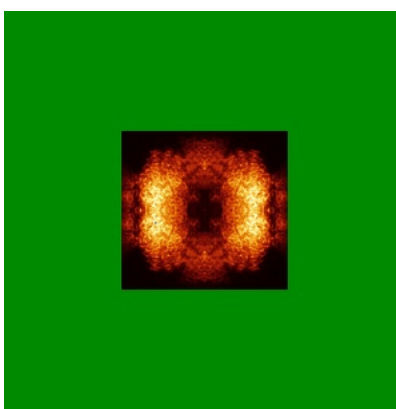
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

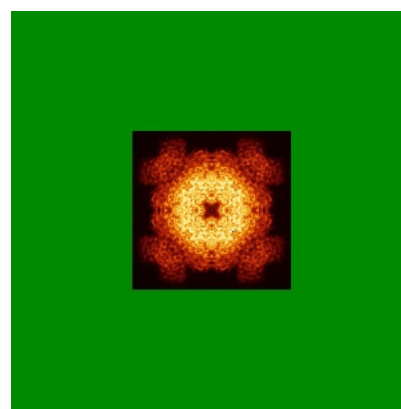
### 6.4.1 Primary map



X



Y

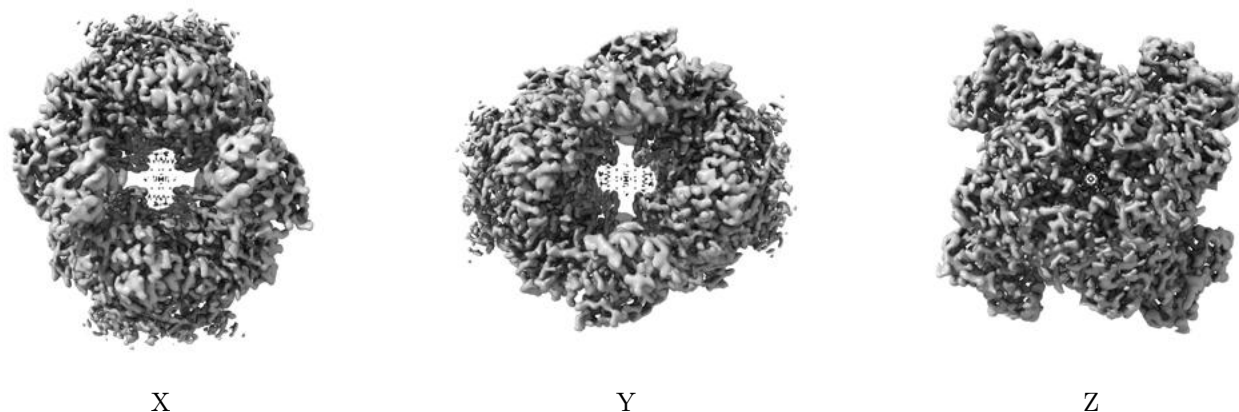


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.804. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

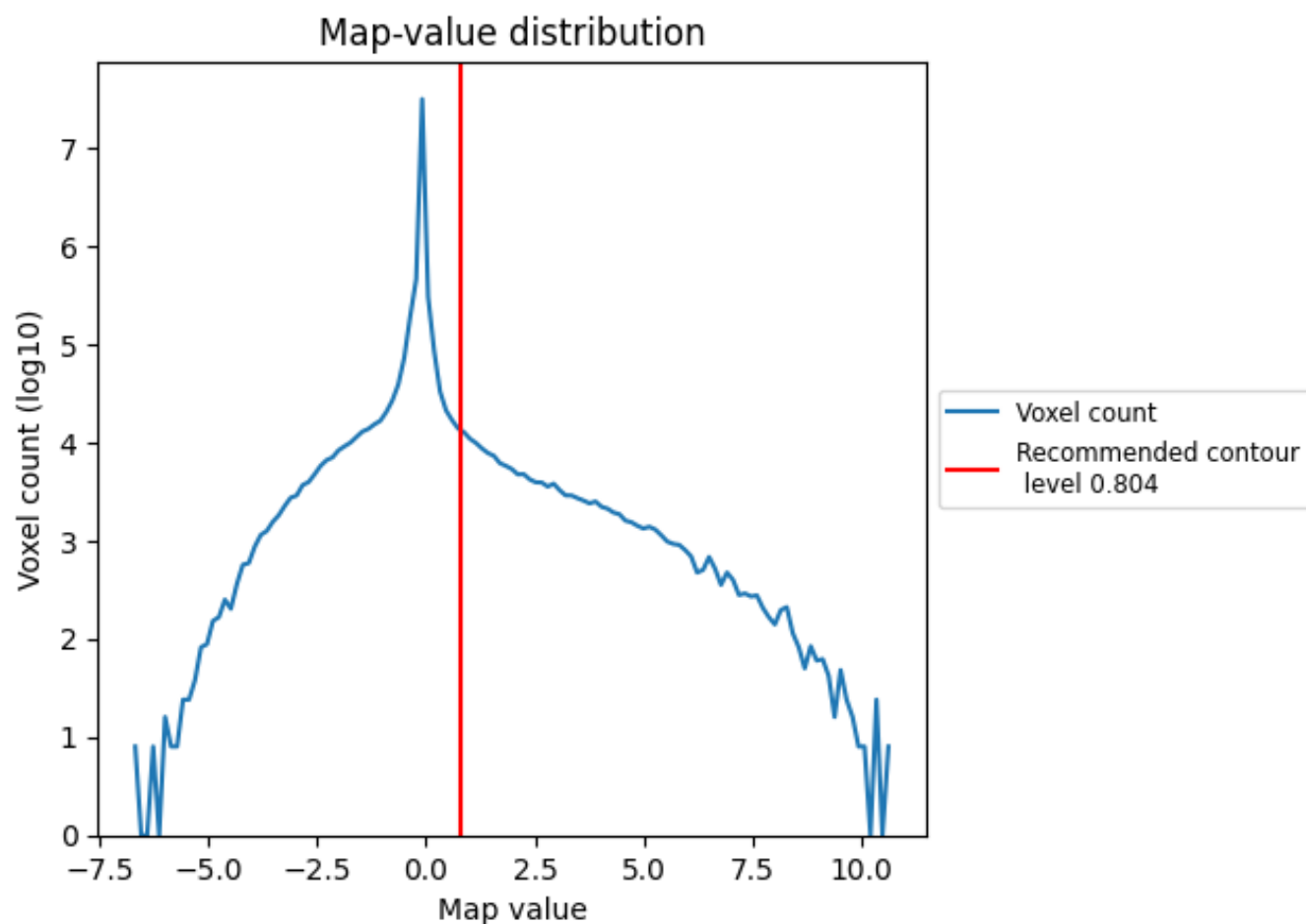
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

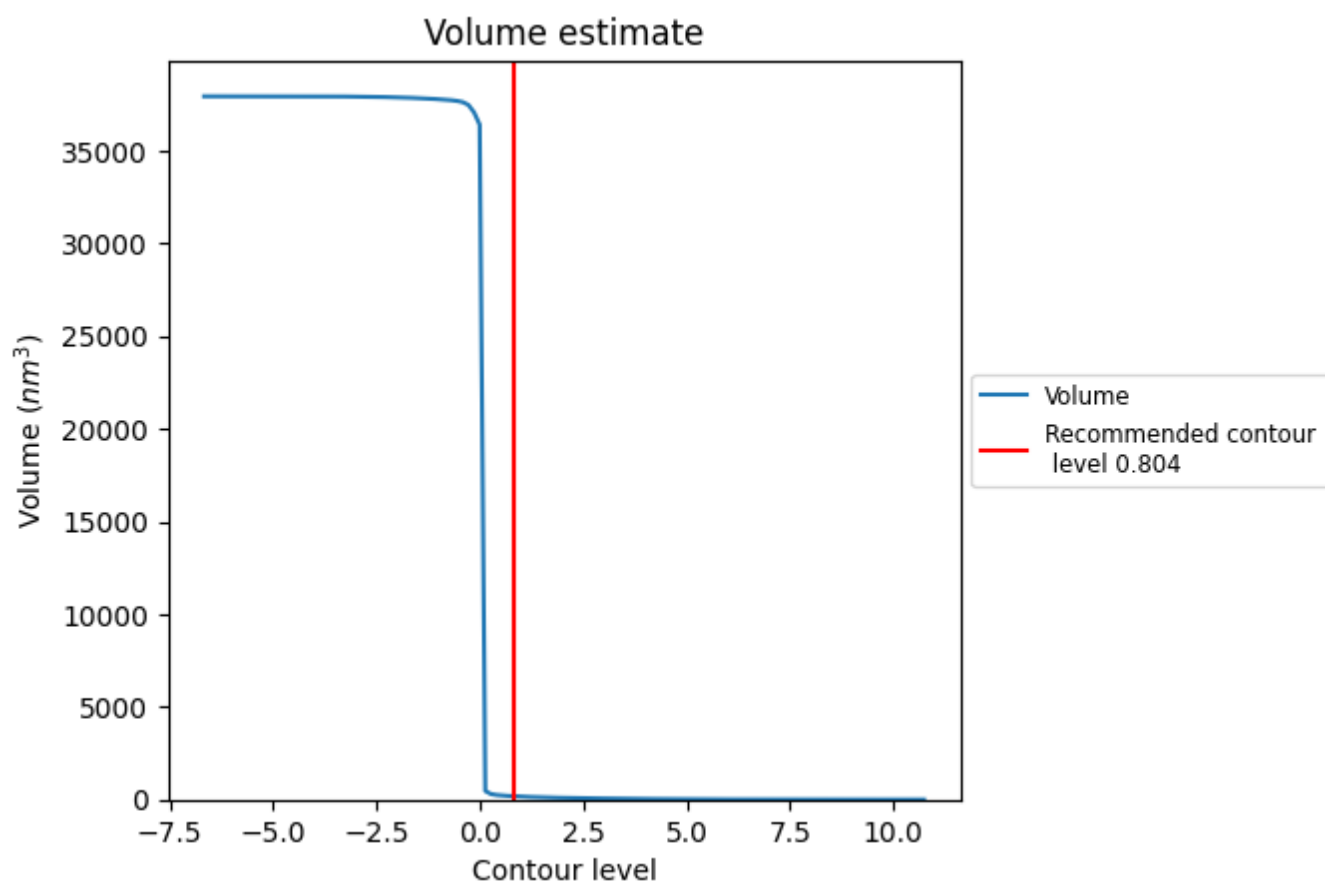
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



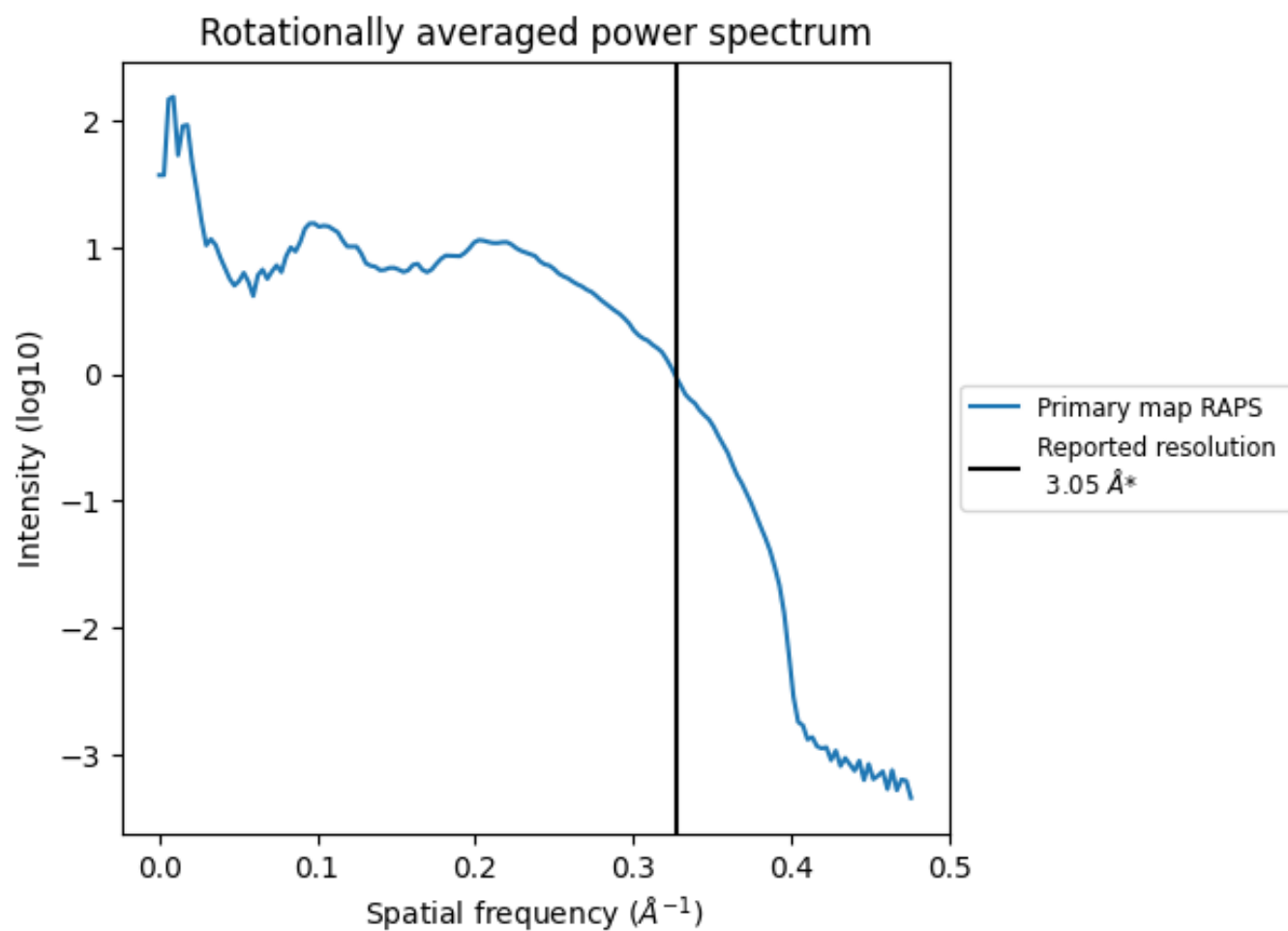
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182  $\text{nm}^3$ ; this corresponds to an approximate mass of 164 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.328 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

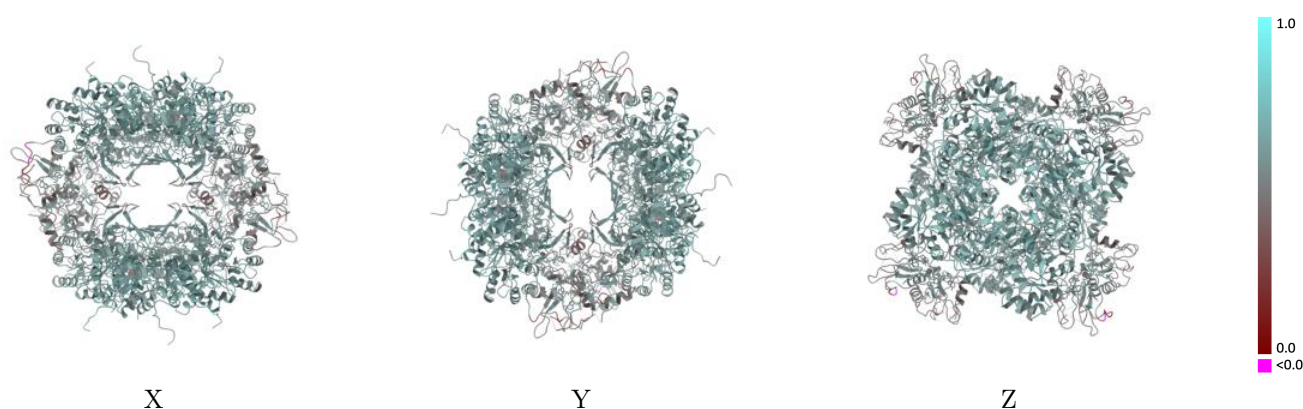
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24438 and PDB model 7RES. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)

This section was not generated.

### 9.2 Q-score mapped to coordinate model [i](#)

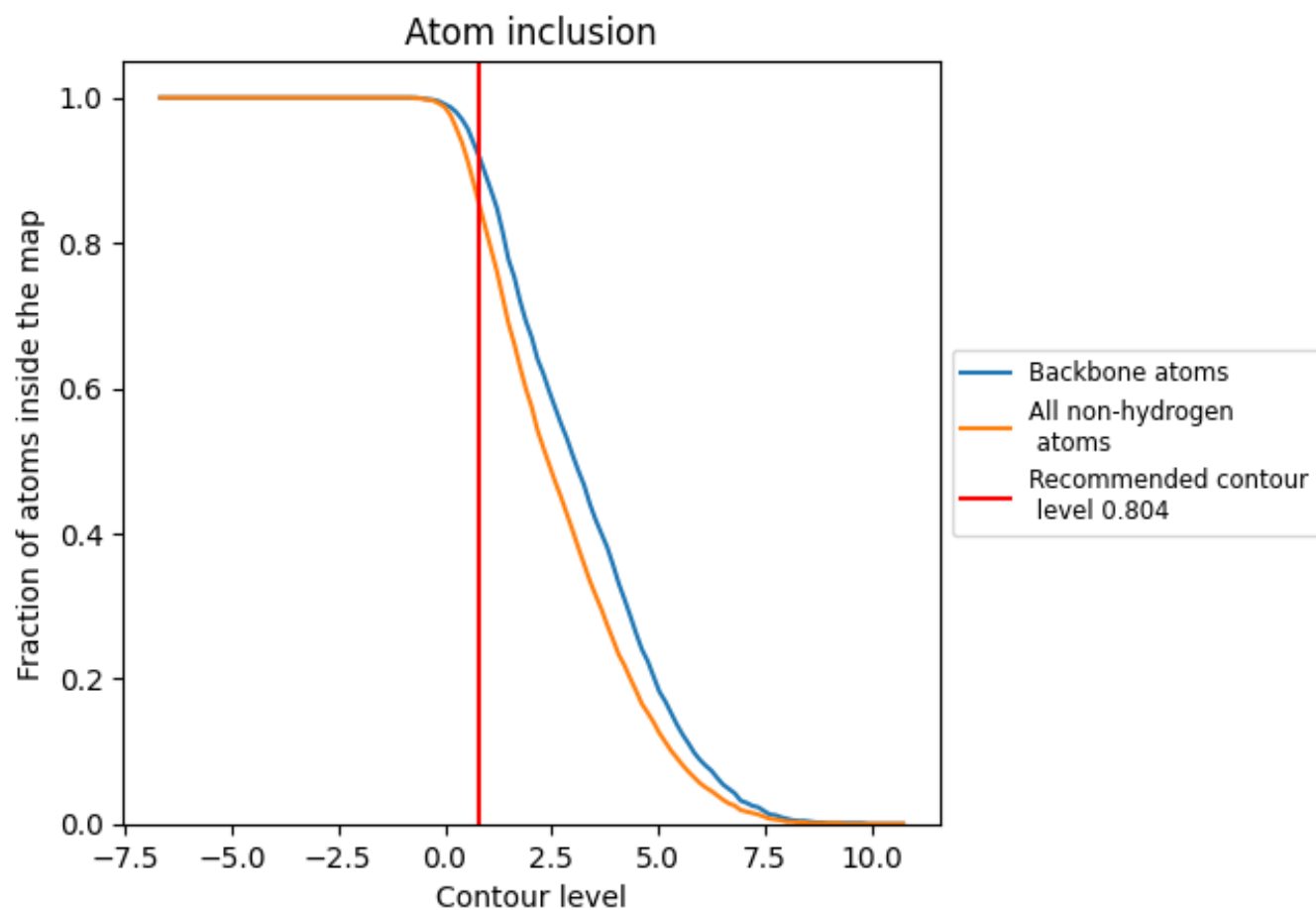


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.804) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.8530 | <div><div></div></div> 0.5750 |
| A     | <div><div></div></div> 0.8540 | <div><div></div></div> 0.5750 |
| B     | <div><div></div></div> 0.8520 | <div><div></div></div> 0.5750 |
| C     | <div><div></div></div> 0.8520 | <div><div></div></div> 0.5760 |
| D     | <div><div></div></div> 0.8480 | <div><div></div></div> 0.5720 |
| E     | <div><div></div></div> 0.8540 | <div><div></div></div> 0.5760 |
| F     | <div><div></div></div> 0.8510 | <div><div></div></div> 0.5730 |
| G     | <div><div></div></div> 0.8550 | <div><div></div></div> 0.5750 |
| H     | <div><div></div></div> 0.8540 | <div><div></div></div> 0.5770 |

1.0

0.0

<0.0