



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:05 PM UTC

PDB ID : 6U8N / pdb\_00006u8n  
EMDB ID : EMD-20688  
Title : Human IMPDH2 treated with ATP, IMP, and NAD<sup>+</sup>. Fully extended filament segment reconstruction.  
Authors : Johnson, M.C.; Kollman, J.M.  
Deposited on : 2019-09-05  
Resolution : 3.29 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:

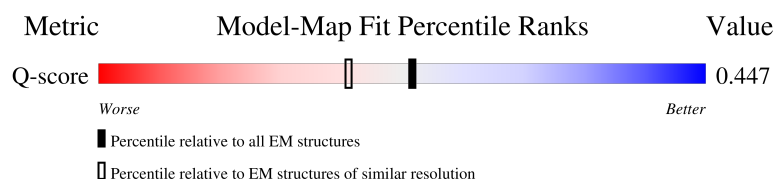
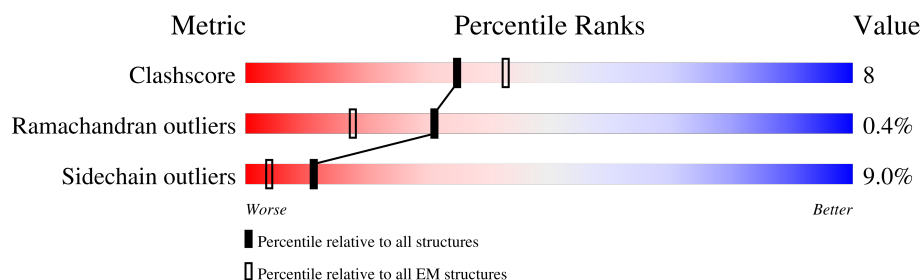
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.29 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.



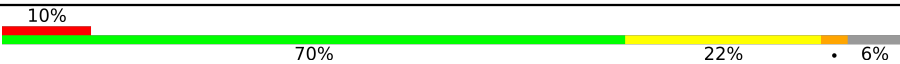
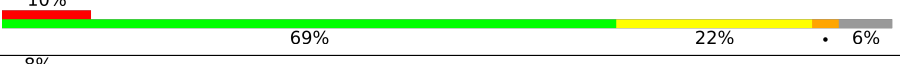
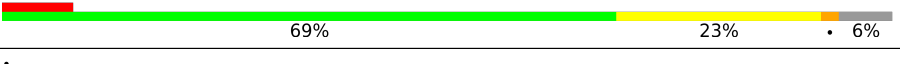
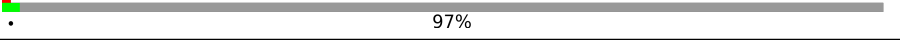
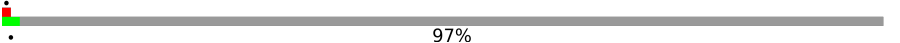
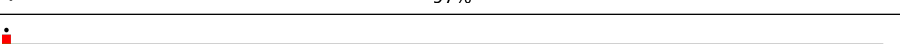
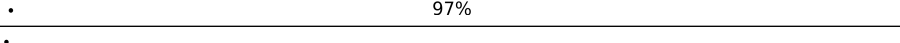
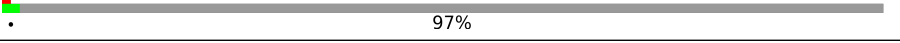
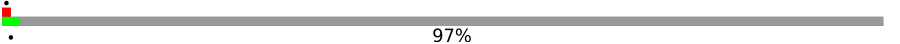
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14466 ( 2.79 - 3.79 )                                    |

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     | 519    |                  |
| 1   | B     | 519    |                  |
| 1   | C     | 519    |                  |
| 1   | D     | 519    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | E     | 519    |  |
| 1   | F     | 519    |  |
| 1   | G     | 519    |  |
| 1   | H     | 519    |  |
| 1   | I     | 519    |  |
| 1   | J     | 519    |  |
| 1   | K     | 519    |  |
| 1   | L     | 519    |  |
| 1   | M     | 519    |  |
| 1   | N     | 519    |  |
| 1   | O     | 519    |  |
| 1   | P     | 519    |  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 31528 atoms, of which 0 are hydrogens and 0 are deuteriums.

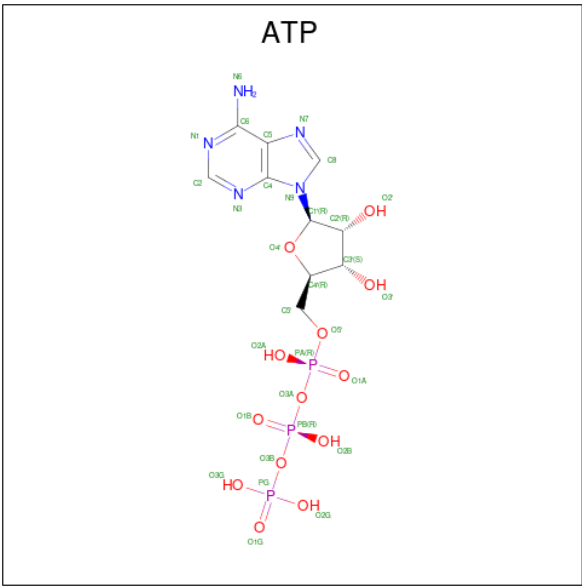
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | I     | 14       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 102   | 66   | 14  | 21  | 1  |         |       |
| 1   | A     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3710  | 2340 | 640 | 709 | 21 |         |       |
| 1   | J     | 14       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 102   | 66   | 14  | 21  | 1  |         |       |
| 1   | B     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3710  | 2340 | 640 | 709 | 21 |         |       |
| 1   | K     | 14       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 102   | 66   | 14  | 21  | 1  |         |       |
| 1   | C     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3710  | 2340 | 640 | 709 | 21 |         |       |
| 1   | L     | 14       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 102   | 66   | 14  | 21  | 1  |         |       |
| 1   | D     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3710  | 2340 | 640 | 709 | 21 |         |       |
| 1   | M     | 14       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 102   | 66   | 14  | 21  | 1  |         |       |
| 1   | E     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3710  | 2340 | 640 | 709 | 21 |         |       |
| 1   | N     | 14       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 102   | 66   | 14  | 21  | 1  |         |       |
| 1   | F     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3710  | 2340 | 640 | 709 | 21 |         |       |
| 1   | O     | 14       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 102   | 66   | 14  | 21  | 1  |         |       |
| 1   | G     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3710  | 2340 | 640 | 709 | 21 |         |       |
| 1   | P     | 14       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 102   | 66   | 14  | 21  | 1  |         |       |
| 1   | H     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3710  | 2340 | 640 | 709 | 21 |         |       |

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

(labeled as "Ligand of Interest" by depositor).



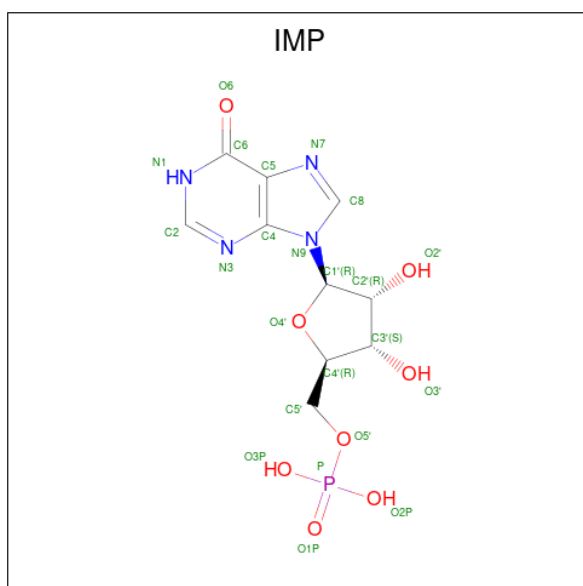
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | A     | 1        | Total | C  | N | O  | 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 |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 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:  $C_{10}H_{13}N_4O_8P$ ) (labeled as "Ligand of Interest" by depositor).



| 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 |         |

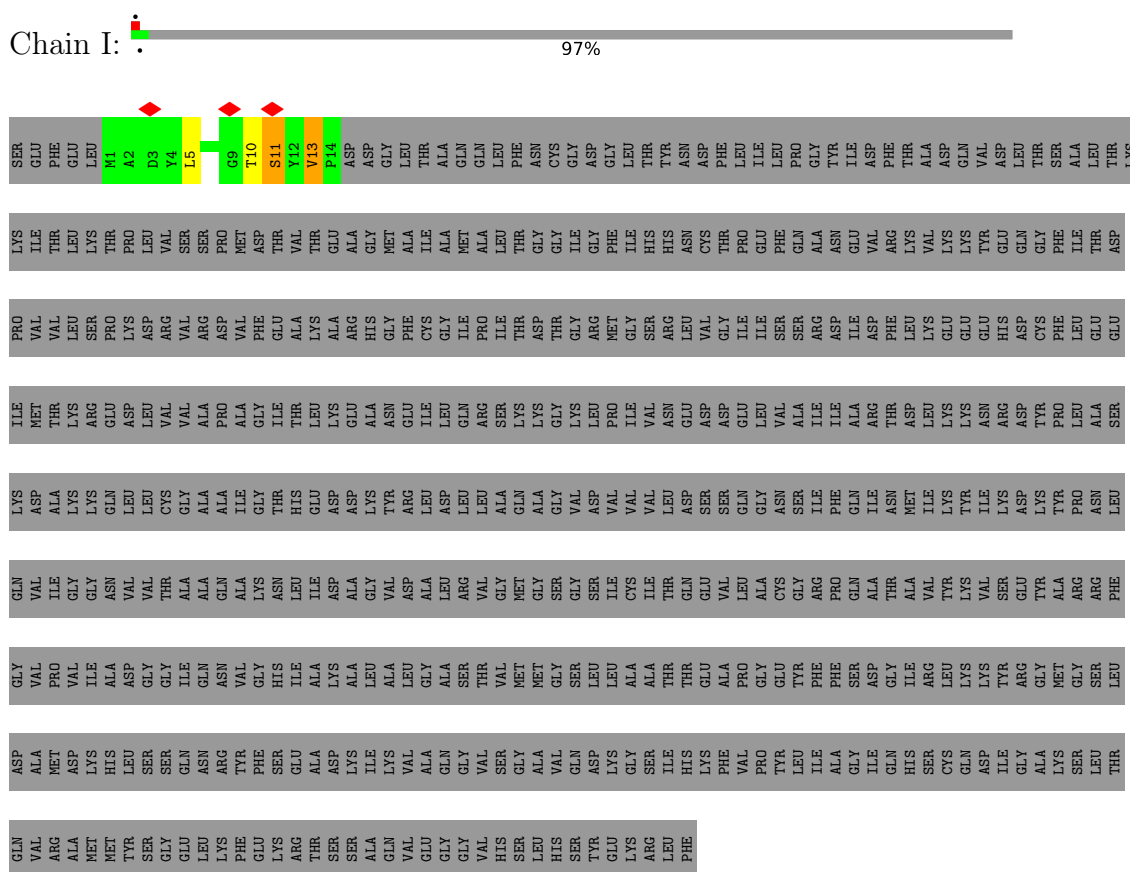
- # NAD
- 
- The image displays the chemical structure of Nicotinamide Adenine Dinucleotide (NAD). The molecule is composed of two nucleotides linked by a pyrophosphate bridge. The top nucleotide consists of a nicotinamide ring (labeled N1A, N3A, C3A, C4A, C5A, C6A) attached to a ribose sugar (labeled C12R, C13R, C14R, C15R, C16R). The bottom nucleotide consists of an adenine ring (labeled N1N, N3N, C3N, C4N, C5N, C6N) attached to a ribose sugar (labeled C12N, C13N, C14N, C15N, C16N). The two ribose sugars are linked by a pyrophosphate bridge (labeled C12R, C13R, C14R, C15R, C16R). The structure is color-coded: the nicotinamide ring is blue, the adenine ring is green, and the ribose sugars are red. The pyrophosphate bridge is yellow. The labels N1A, N3A, C3A, C4A, C5A, C6A, N1N, N3N, C3N, C4N, C5N, C6N, C12R, C13R, C14R, C15R, C16R, C12N, C13N, C14N, C15N, C16R are placed around the structure to identify specific atoms.



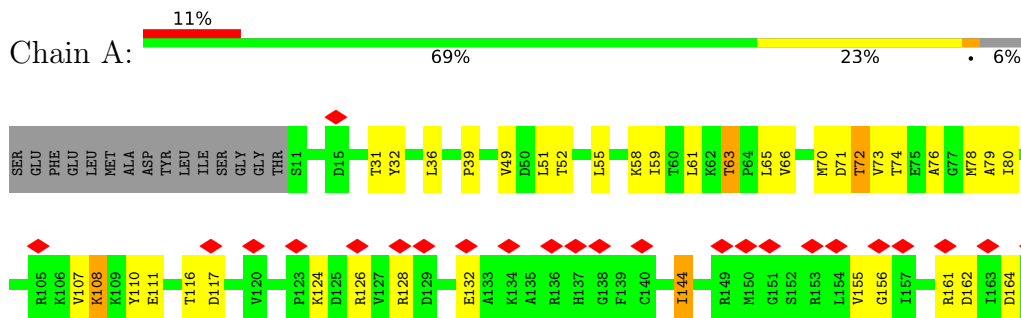
### 3 Residue-property plots

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.

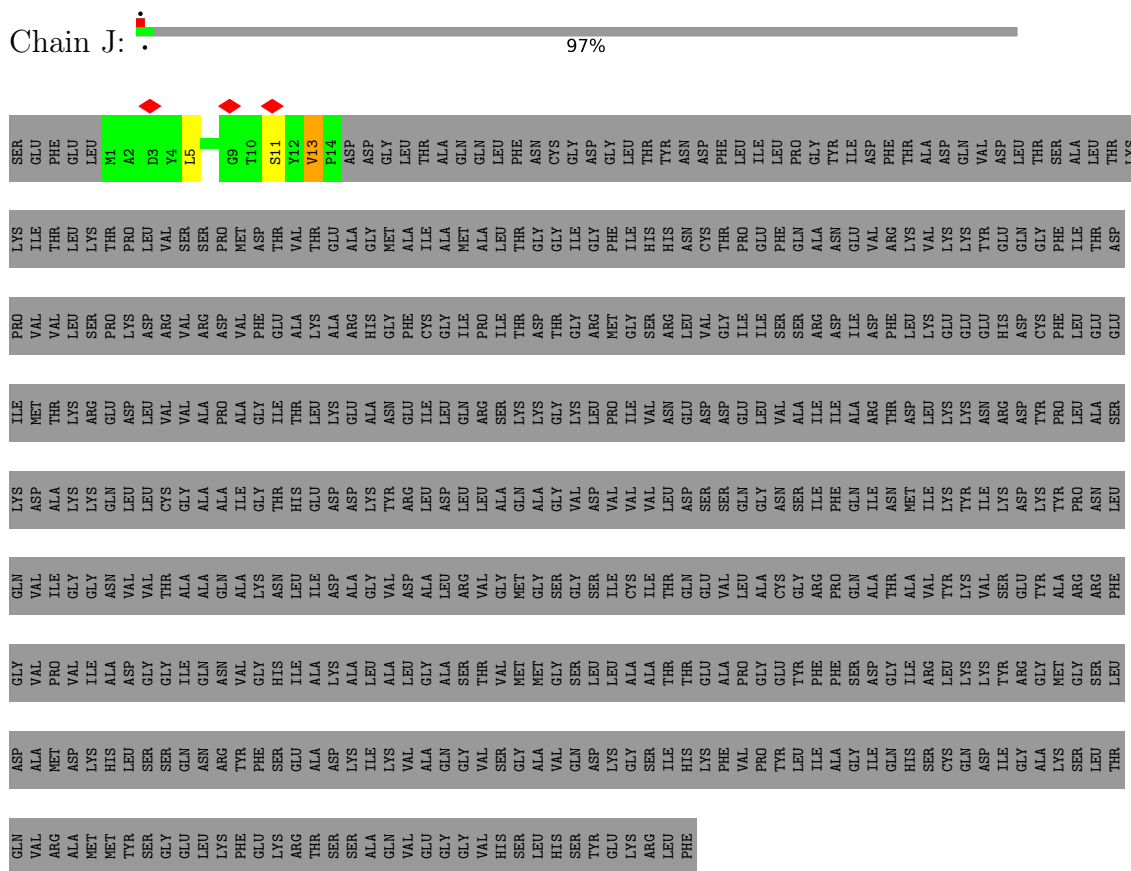
#### • Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



#### • Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

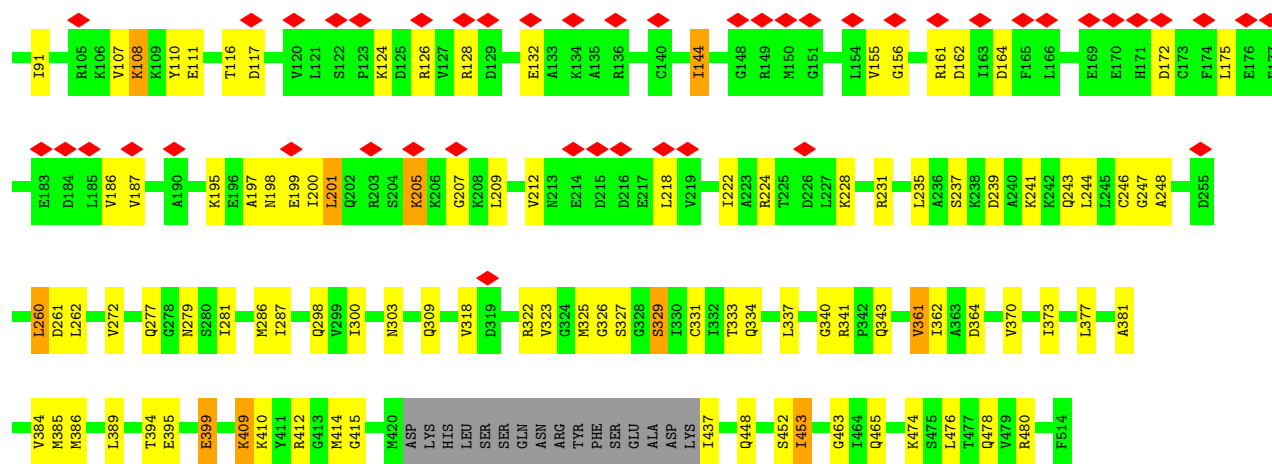


- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

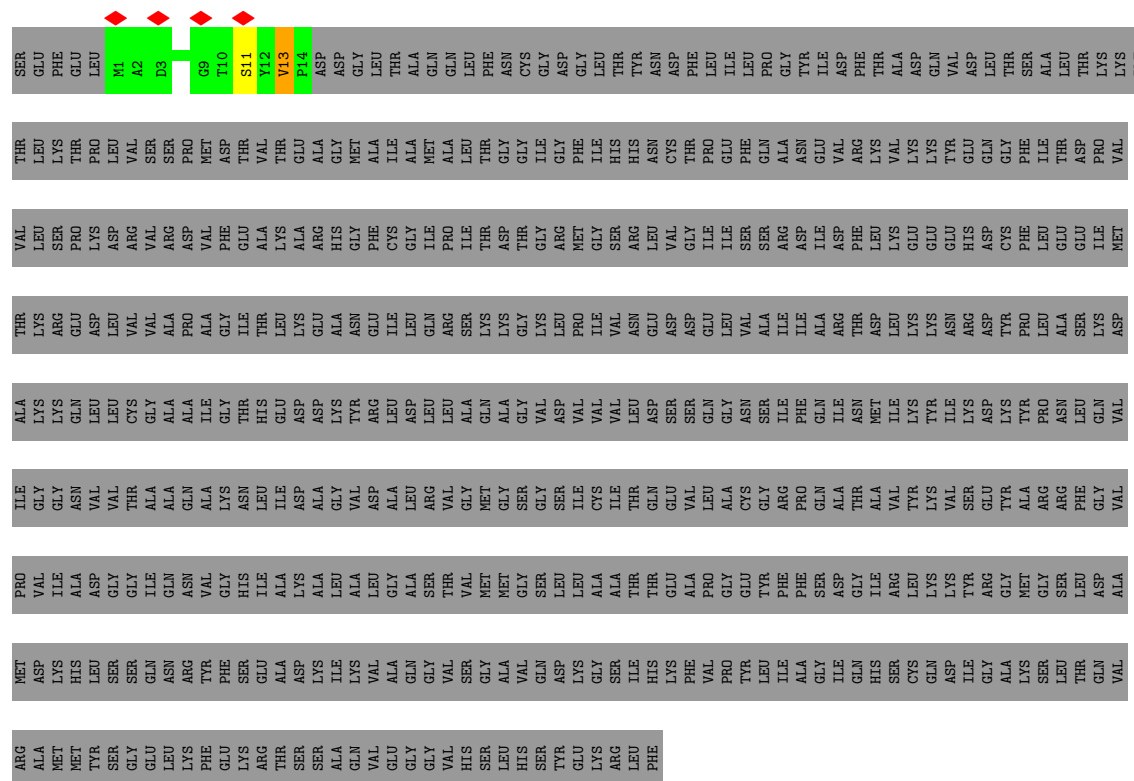


- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2





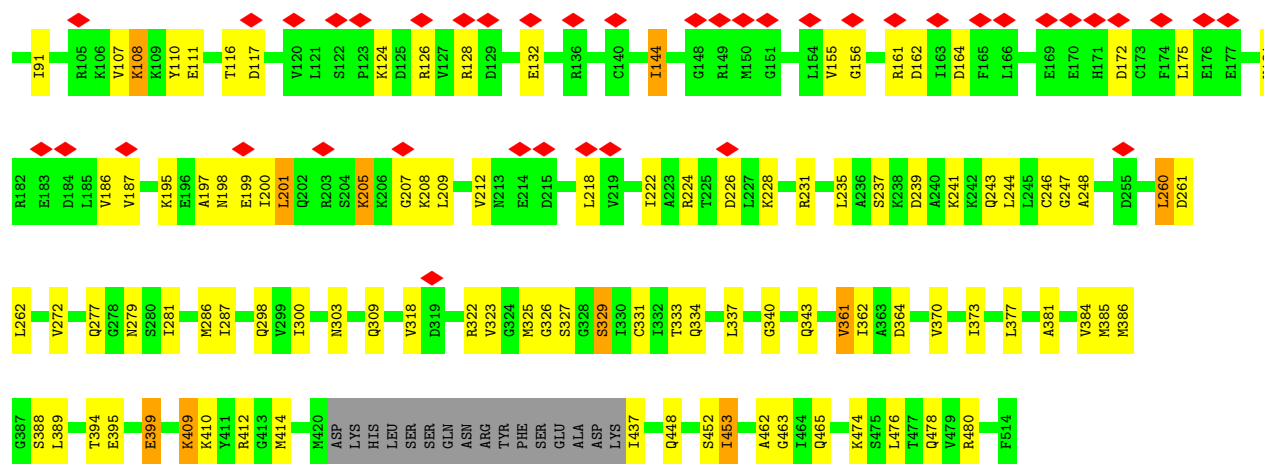
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

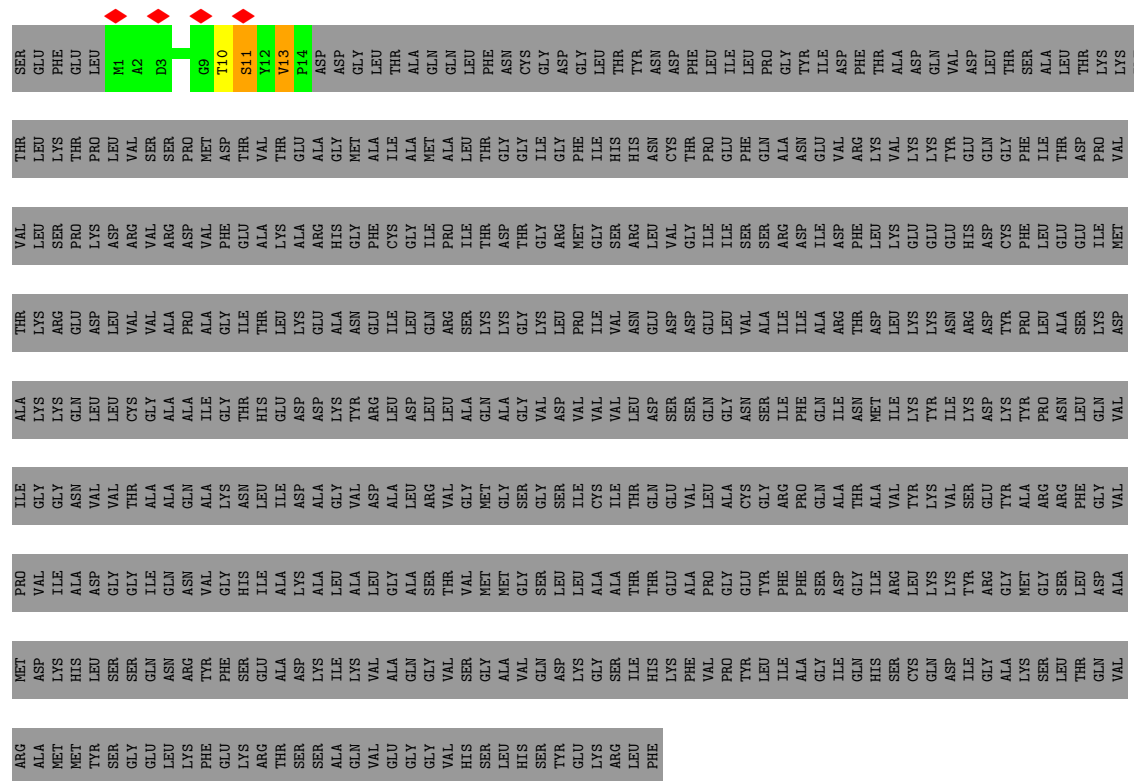






• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

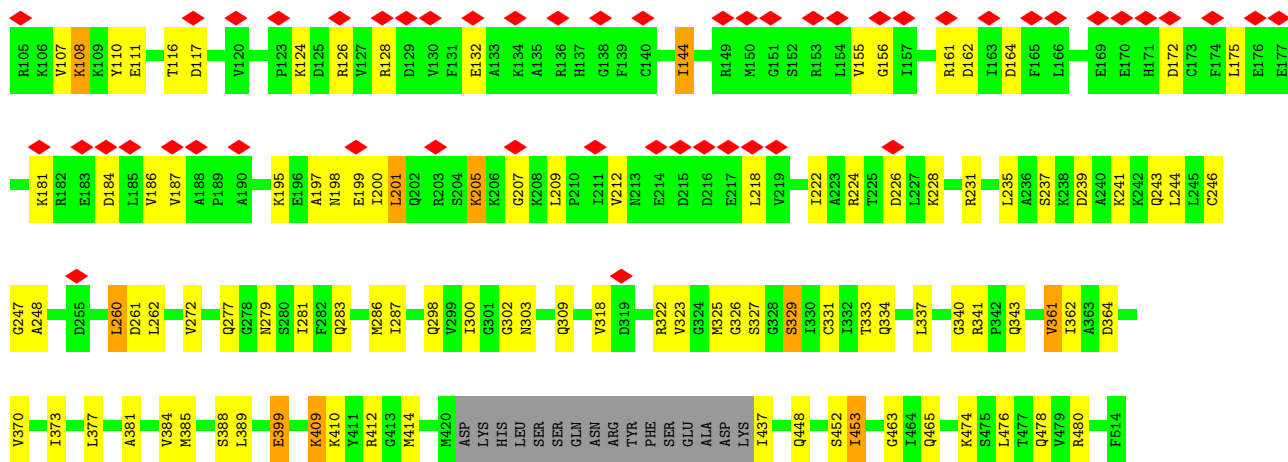
Chain M: 97%



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

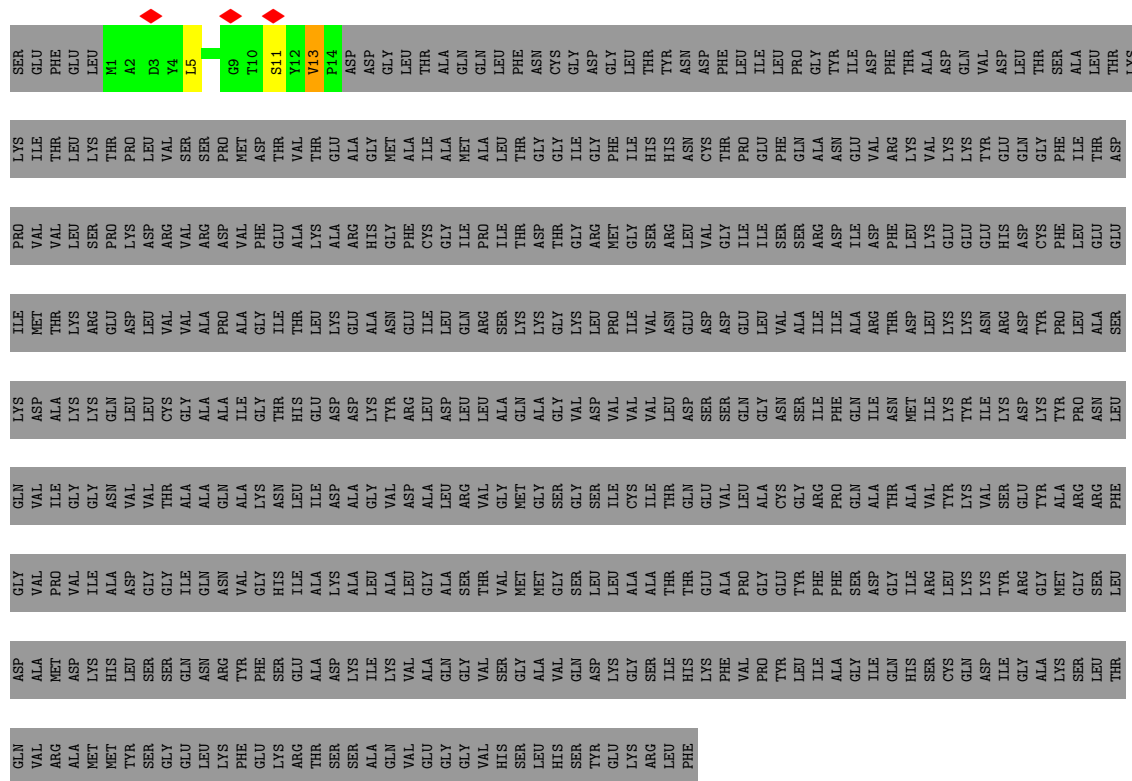
Chain E: 10% 70% 22% 6%





• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

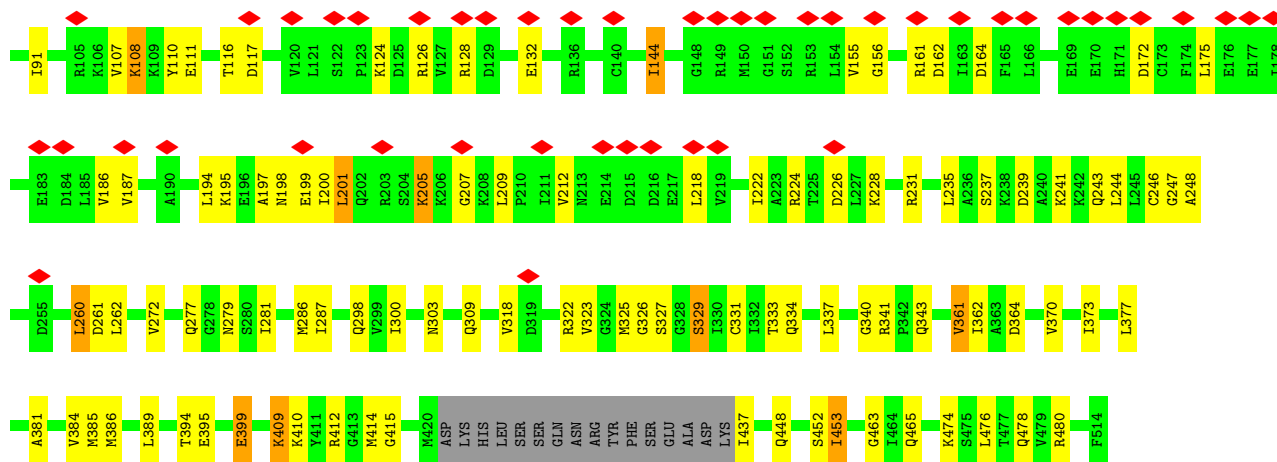
Chain N: 97%



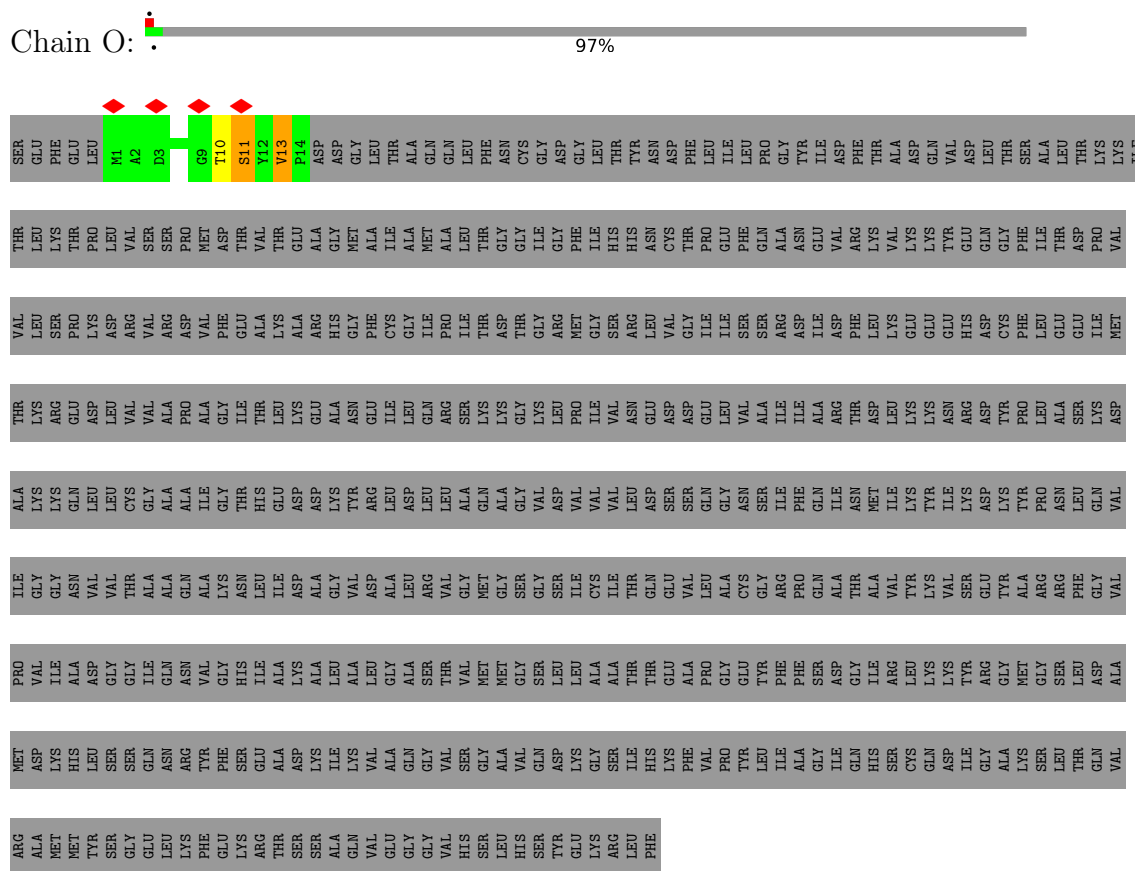
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain F: 9% 69% 22% 6%



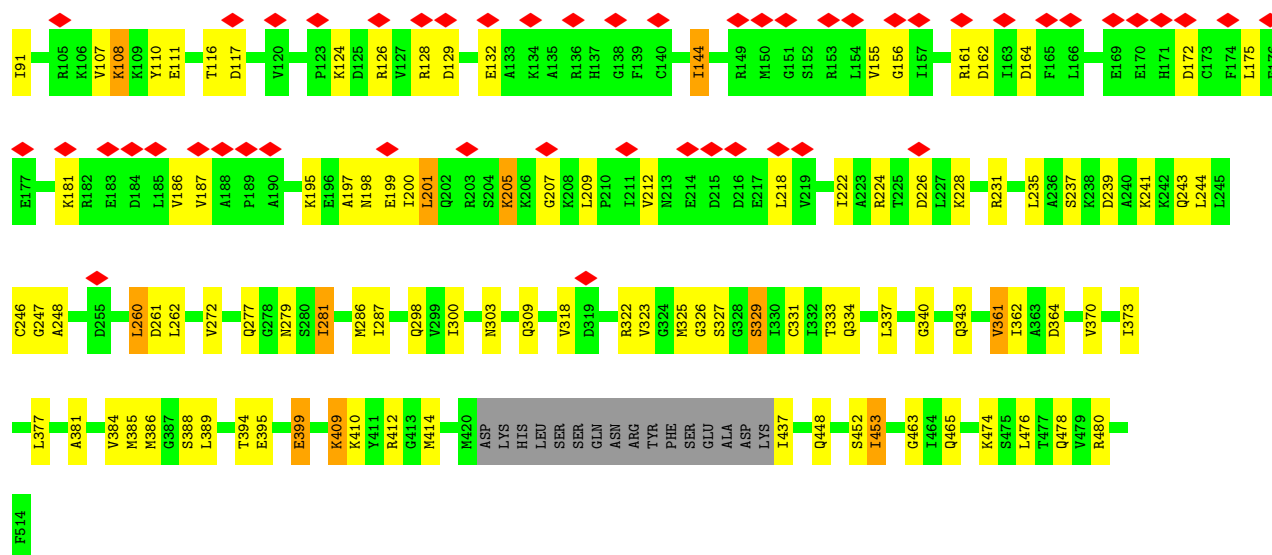


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

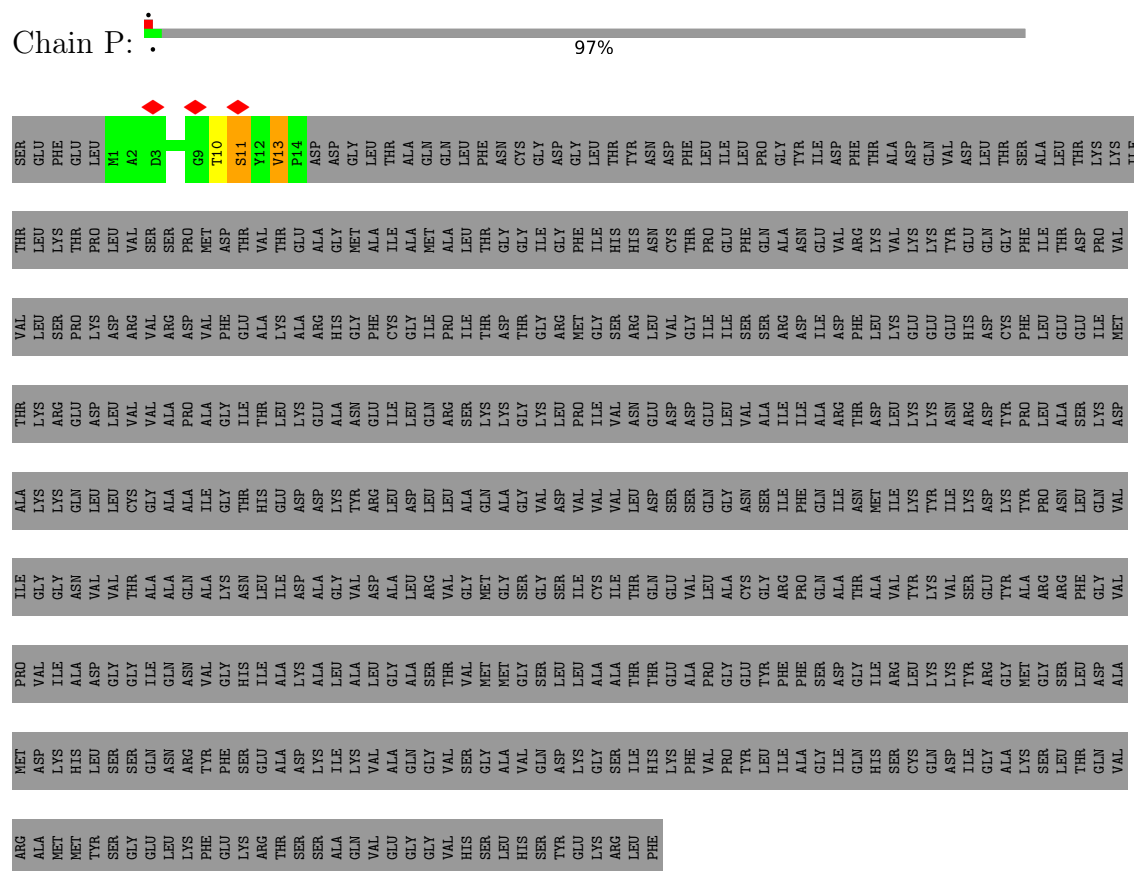


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



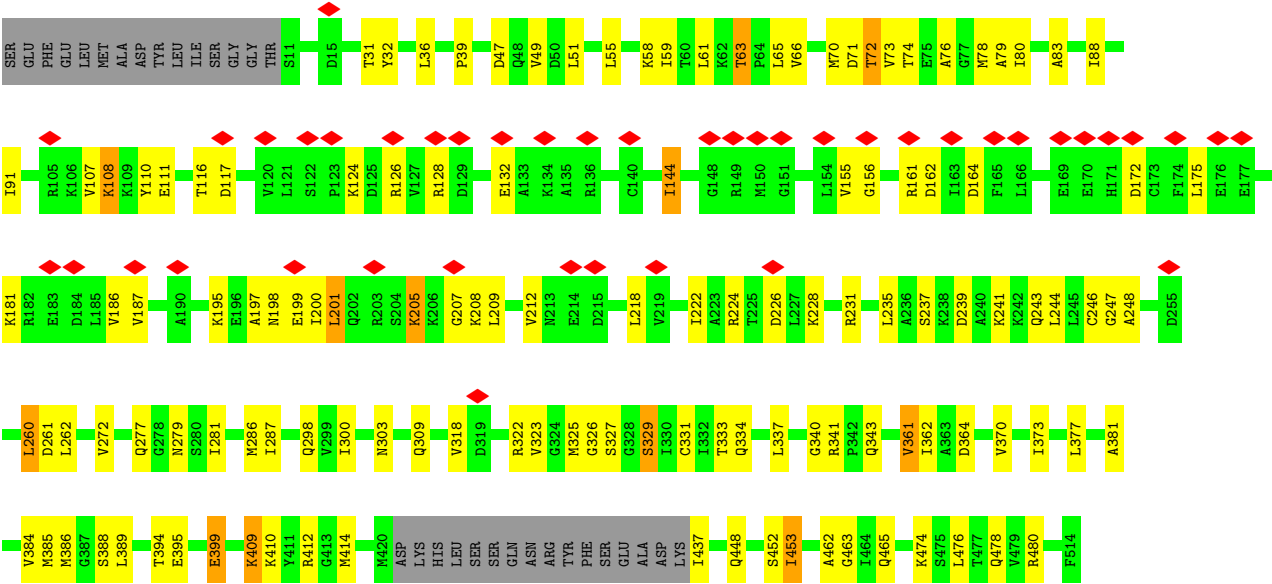


- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, D4                               | Depositor |
| Number of particles used             | 9124                                    | 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 ( $e^-/\text{\AA}^2$ ) | 100                                     | 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                    | 84.532                                  | Depositor |
| Minimum map value                    | -64.696                                 | Depositor |
| Average map value                    | 0.073                                   | Depositor |
| Map value standard deviation         | 2.647                                   | Depositor |
| Recommended contour level            | 17                                      | Depositor |
| Map size (Å)                         | 336.0, 336.0, 336.0                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 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: IMP, NAD, 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     | 0.60         | 1/3766 (0.0%)  | 0.87        | 8/5078 (0.2%)   |
| 1   | B     | 0.60         | 1/3766 (0.0%)  | 0.87        | 8/5078 (0.2%)   |
| 1   | C     | 0.60         | 1/3766 (0.0%)  | 0.87        | 8/5078 (0.2%)   |
| 1   | D     | 0.60         | 1/3766 (0.0%)  | 0.87        | 8/5078 (0.2%)   |
| 1   | E     | 0.60         | 1/3766 (0.0%)  | 0.87        | 8/5078 (0.2%)   |
| 1   | F     | 0.60         | 1/3766 (0.0%)  | 0.87        | 8/5078 (0.2%)   |
| 1   | G     | 0.60         | 1/3766 (0.0%)  | 0.87        | 8/5078 (0.2%)   |
| 1   | H     | 0.60         | 1/3766 (0.0%)  | 0.87        | 8/5078 (0.2%)   |
| 1   | I     | 0.47         | 0/104          | 1.01        | 1/141 (0.7%)    |
| 1   | J     | 0.47         | 0/104          | 1.01        | 1/141 (0.7%)    |
| 1   | K     | 0.47         | 0/104          | 1.01        | 1/141 (0.7%)    |
| 1   | L     | 0.47         | 0/104          | 1.01        | 1/141 (0.7%)    |
| 1   | M     | 0.47         | 0/104          | 1.00        | 1/141 (0.7%)    |
| 1   | N     | 0.47         | 0/104          | 1.01        | 1/141 (0.7%)    |
| 1   | O     | 0.47         | 0/104          | 1.01        | 1/141 (0.7%)    |
| 1   | P     | 0.47         | 0/104          | 1.01        | 1/141 (0.7%)    |
| All | All   | 0.59         | 8/30960 (0.0%) | 0.87        | 72/41752 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | H     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 329 | SER  | CA-C  | -5.33 | 1.45        | 1.52     |
| 1   | E     | 329 | SER  | CA-C  | -5.29 | 1.45        | 1.52     |
| 1   | A     | 329 | SER  | CA-C  | -5.28 | 1.45        | 1.52     |
| 1   | D     | 329 | SER  | CA-C  | -5.28 | 1.45        | 1.52     |
| 1   | G     | 329 | SER  | CA-C  | -5.28 | 1.45        | 1.52     |
| 1   | C     | 329 | SER  | CA-C  | -5.24 | 1.45        | 1.52     |
| 1   | F     | 329 | SER  | CA-C  | -5.24 | 1.45        | 1.52     |
| 1   | H     | 329 | SER  | CA-C  | -5.24 | 1.45        | 1.52     |

All (72) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | H     | 108 | LYS  | CA-CB-CG  | 5.94  | 125.98      | 114.10   |
| 1   | D     | 108 | LYS  | CA-CB-CG  | 5.93  | 125.97      | 114.10   |
| 1   | G     | 108 | LYS  | CA-CB-CG  | 5.93  | 125.97      | 114.10   |
| 1   | C     | 108 | LYS  | CA-CB-CG  | 5.92  | 125.95      | 114.10   |
| 1   | F     | 108 | LYS  | CA-CB-CG  | 5.92  | 125.94      | 114.10   |
| 1   | B     | 108 | LYS  | CA-CB-CG  | 5.91  | 125.92      | 114.10   |
| 1   | E     | 108 | LYS  | CA-CB-CG  | 5.91  | 125.92      | 114.10   |
| 1   | A     | 108 | LYS  | CA-CB-CG  | 5.90  | 125.89      | 114.10   |
| 1   | E     | 261 | ASP  | CA-C-O    | -5.83 | 111.65      | 119.11   |
| 1   | C     | 261 | ASP  | CA-C-O    | -5.81 | 111.67      | 119.11   |
| 1   | F     | 261 | ASP  | CA-C-O    | -5.81 | 111.67      | 119.11   |
| 1   | D     | 261 | ASP  | CA-C-O    | -5.79 | 111.69      | 119.11   |
| 1   | A     | 261 | ASP  | CA-C-O    | -5.79 | 111.70      | 119.11   |
| 1   | G     | 261 | ASP  | CA-C-O    | -5.79 | 111.70      | 119.11   |
| 1   | H     | 261 | ASP  | CA-C-O    | -5.79 | 111.70      | 119.11   |
| 1   | B     | 261 | ASP  | CA-C-O    | -5.79 | 111.70      | 119.11   |
| 1   | I     | 13  | VAL  | CA-CB-CG2 | 5.43  | 119.64      | 110.40   |
| 1   | N     | 13  | VAL  | CA-CB-CG2 | 5.43  | 119.64      | 110.40   |
| 1   | K     | 13  | VAL  | CA-CB-CG2 | 5.42  | 119.62      | 110.40   |
| 1   | O     | 13  | VAL  | CA-CB-CG2 | 5.42  | 119.61      | 110.40   |
| 1   | L     | 13  | VAL  | CA-CB-CG2 | 5.41  | 119.60      | 110.40   |
| 1   | J     | 13  | VAL  | CA-CB-CG2 | 5.41  | 119.59      | 110.40   |
| 1   | M     | 13  | VAL  | CA-CB-CG2 | 5.41  | 119.59      | 110.40   |
| 1   | P     | 13  | VAL  | CA-CB-CG2 | 5.40  | 119.58      | 110.40   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 260 | LEU  | CA-C-N   | -5.21 | 111.42      | 121.58   |
| 1   | D     | 260 | LEU  | C-N-CA   | -5.21 | 111.42      | 121.58   |
| 1   | G     | 260 | LEU  | CA-C-N   | -5.21 | 111.43      | 121.58   |
| 1   | G     | 260 | LEU  | C-N-CA   | -5.21 | 111.43      | 121.58   |
| 1   | C     | 72  | THR  | CA-C-N   | -5.20 | 117.31      | 122.77   |
| 1   | C     | 72  | THR  | C-N-CA   | -5.20 | 117.31      | 122.77   |
| 1   | H     | 260 | LEU  | CA-C-N   | -5.20 | 111.44      | 121.58   |
| 1   | H     | 260 | LEU  | C-N-CA   | -5.20 | 111.44      | 121.58   |
| 1   | E     | 72  | THR  | CA-C-N   | -5.20 | 117.31      | 122.77   |
| 1   | E     | 72  | THR  | C-N-CA   | -5.20 | 117.31      | 122.77   |
| 1   | F     | 72  | THR  | CA-C-N   | -5.20 | 117.31      | 122.77   |
| 1   | F     | 72  | THR  | C-N-CA   | -5.20 | 117.31      | 122.77   |
| 1   | A     | 260 | LEU  | CA-C-N   | -5.19 | 111.46      | 121.58   |
| 1   | A     | 260 | LEU  | C-N-CA   | -5.19 | 111.46      | 121.58   |
| 1   | B     | 72  | THR  | CA-C-N   | -5.19 | 117.32      | 122.77   |
| 1   | B     | 72  | THR  | C-N-CA   | -5.19 | 117.32      | 122.77   |
| 1   | D     | 72  | THR  | CA-C-N   | -5.19 | 117.33      | 122.77   |
| 1   | D     | 72  | THR  | C-N-CA   | -5.19 | 117.33      | 122.77   |
| 1   | F     | 260 | LEU  | CA-C-N   | -5.18 | 111.47      | 121.58   |
| 1   | F     | 260 | LEU  | C-N-CA   | -5.18 | 111.47      | 121.58   |
| 1   | B     | 260 | LEU  | CA-C-N   | -5.18 | 111.48      | 121.58   |
| 1   | B     | 260 | LEU  | C-N-CA   | -5.18 | 111.48      | 121.58   |
| 1   | E     | 260 | LEU  | CA-C-N   | -5.18 | 111.48      | 121.58   |
| 1   | E     | 260 | LEU  | C-N-CA   | -5.18 | 111.48      | 121.58   |
| 1   | G     | 72  | THR  | CA-C-N   | -5.18 | 117.33      | 122.77   |
| 1   | G     | 72  | THR  | C-N-CA   | -5.18 | 117.33      | 122.77   |
| 1   | A     | 72  | THR  | CA-C-N   | -5.17 | 117.34      | 122.77   |
| 1   | A     | 72  | THR  | C-N-CA   | -5.17 | 117.34      | 122.77   |
| 1   | C     | 260 | LEU  | CA-C-N   | -5.16 | 111.51      | 121.58   |
| 1   | C     | 260 | LEU  | C-N-CA   | -5.16 | 111.51      | 121.58   |
| 1   | H     | 72  | THR  | CA-C-N   | -5.15 | 117.37      | 122.77   |
| 1   | H     | 72  | THR  | C-N-CA   | -5.15 | 117.37      | 122.77   |
| 1   | A     | 108 | LYS  | CB-CG-CD | 5.13  | 123.11      | 111.30   |
| 1   | F     | 108 | LYS  | CB-CG-CD | 5.13  | 123.10      | 111.30   |
| 1   | C     | 108 | LYS  | CB-CG-CD | 5.13  | 123.09      | 111.30   |
| 1   | G     | 108 | LYS  | CB-CG-CD | 5.13  | 123.09      | 111.30   |
| 1   | B     | 108 | LYS  | CB-CG-CD | 5.13  | 123.09      | 111.30   |
| 1   | D     | 108 | LYS  | CB-CG-CD | 5.11  | 123.06      | 111.30   |
| 1   | H     | 108 | LYS  | CB-CG-CD | 5.11  | 123.06      | 111.30   |
| 1   | E     | 108 | LYS  | CB-CG-CD | 5.11  | 123.06      | 111.30   |
| 1   | H     | 399 | GLU  | CA-CB-CG | 5.03  | 124.16      | 114.10   |
| 1   | A     | 399 | GLU  | CA-CB-CG | 5.03  | 124.15      | 114.10   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | B     | 399 | GLU  | CA-CB-CG | 5.02 | 124.14      | 114.10   |
| 1   | E     | 399 | GLU  | CA-CB-CG | 5.02 | 124.14      | 114.10   |
| 1   | F     | 399 | GLU  | CA-CB-CG | 5.01 | 124.12      | 114.10   |
| 1   | C     | 399 | GLU  | CA-CB-CG | 5.01 | 124.12      | 114.10   |
| 1   | D     | 399 | GLU  | CA-CB-CG | 5.01 | 124.11      | 114.10   |
| 1   | G     | 399 | GLU  | CA-CB-CG | 5.01 | 124.11      | 114.10   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 437 | ILE  | Peptide |
| 1   | B     | 437 | ILE  | Peptide |
| 1   | C     | 437 | ILE  | Peptide |
| 1   | D     | 437 | ILE  | Peptide |
| 1   | E     | 437 | ILE  | Peptide |
| 1   | F     | 437 | ILE  | Peptide |
| 1   | G     | 437 | ILE  | Peptide |
| 1   | H     | 437 | ILE  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3710  | 0        | 3764     | 66      | 0            |
| 1   | B     | 3710  | 0        | 3764     | 64      | 0            |
| 1   | C     | 3710  | 0        | 3764     | 64      | 0            |
| 1   | D     | 3710  | 0        | 3764     | 66      | 0            |
| 1   | E     | 3710  | 0        | 3764     | 66      | 0            |
| 1   | F     | 3710  | 0        | 3764     | 67      | 0            |
| 1   | G     | 3710  | 0        | 3764     | 67      | 0            |
| 1   | H     | 3710  | 0        | 3764     | 66      | 0            |
| 1   | I     | 102   | 0        | 99       | 2       | 0            |
| 1   | J     | 102   | 0        | 99       | 1       | 0            |
| 1   | K     | 102   | 0        | 99       | 0       | 0            |
| 1   | L     | 102   | 0        | 99       | 2       | 0            |
| 1   | M     | 102   | 0        | 99       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | N     | 102   | 0        | 99       | 1       | 0            |
| 1   | O     | 102   | 0        | 99       | 1       | 0            |
| 1   | P     | 102   | 0        | 99       | 1       | 0            |
| 2   | A     | 62    | 0        | 24       | 1       | 0            |
| 2   | B     | 62    | 0        | 24       | 1       | 0            |
| 2   | C     | 62    | 0        | 24       | 1       | 0            |
| 2   | D     | 62    | 0        | 24       | 1       | 0            |
| 2   | E     | 62    | 0        | 24       | 1       | 0            |
| 2   | F     | 62    | 0        | 24       | 1       | 0            |
| 2   | G     | 62    | 0        | 24       | 1       | 0            |
| 2   | H     | 62    | 0        | 24       | 1       | 0            |
| 3   | A     | 23    | 0        | 10       | 4       | 0            |
| 3   | B     | 23    | 0        | 10       | 3       | 0            |
| 3   | C     | 23    | 0        | 10       | 2       | 0            |
| 3   | D     | 23    | 0        | 10       | 3       | 0            |
| 3   | E     | 23    | 0        | 10       | 4       | 0            |
| 3   | F     | 23    | 0        | 10       | 4       | 0            |
| 3   | G     | 23    | 0        | 10       | 4       | 0            |
| 3   | H     | 23    | 0        | 10       | 3       | 0            |
| 4   | A     | 44    | 0        | 22       | 1       | 0            |
| 4   | B     | 44    | 0        | 22       | 1       | 0            |
| 4   | C     | 44    | 0        | 22       | 1       | 0            |
| 4   | D     | 44    | 0        | 22       | 1       | 0            |
| 4   | E     | 44    | 0        | 22       | 1       | 0            |
| 4   | F     | 44    | 0        | 22       | 1       | 0            |
| 4   | G     | 44    | 0        | 22       | 2       | 0            |
| 4   | H     | 44    | 0        | 22       | 1       | 0            |
| All | All   | 31528 | 0        | 31352    | 500     | 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 8.

All (500) 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:197:ALA:O | 1:D:201:LEU:HB2 | 1.86                     | 0.76              |
| 1:H:197:ALA:O | 1:H:201:LEU:HB2 | 1.86                     | 0.76              |
| 1:E:197:ALA:O | 1:E:201:LEU:HB2 | 1.86                     | 0.76              |
| 1:A:197:ALA:O | 1:A:201:LEU:HB2 | 1.86                     | 0.76              |
| 1:G:197:ALA:O | 1:G:201:LEU:HB2 | 1.85                     | 0.76              |
| 1:C:197:ALA:O | 1:C:201:LEU:HB2 | 1.86                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:197:ALA:O    | 1:F:201:LEU:HB2  | 1.86                     | 0.74              |
| 1:B:197:ALA:O    | 1:B:201:LEU:HB2  | 1.86                     | 0.74              |
| 1:C:58:LYS:HB2   | 1:C:298:GLN:HE22 | 1.53                     | 0.73              |
| 1:G:58:LYS:HB2   | 1:G:298:GLN:HE22 | 1.53                     | 0.73              |
| 1:F:58:LYS:HB2   | 1:F:298:GLN:HE22 | 1.53                     | 0.73              |
| 1:E:58:LYS:HB2   | 1:E:298:GLN:HE22 | 1.53                     | 0.72              |
| 1:H:58:LYS:HB2   | 1:H:298:GLN:HE22 | 1.52                     | 0.72              |
| 1:A:58:LYS:HB2   | 1:A:298:GLN:HE22 | 1.53                     | 0.72              |
| 1:B:58:LYS:HB2   | 1:B:298:GLN:HE22 | 1.53                     | 0.72              |
| 1:D:58:LYS:HB2   | 1:D:298:GLN:HE22 | 1.53                     | 0.72              |
| 1:A:474:LYS:H    | 1:A:478:GLN:HE21 | 1.41                     | 0.69              |
| 1:E:474:LYS:H    | 1:E:478:GLN:HE21 | 1.41                     | 0.69              |
| 1:H:474:LYS:H    | 1:H:478:GLN:HE21 | 1.41                     | 0.69              |
| 1:D:474:LYS:H    | 1:D:478:GLN:HE21 | 1.41                     | 0.69              |
| 1:B:474:LYS:H    | 1:B:478:GLN:HE21 | 1.40                     | 0.68              |
| 1:C:474:LYS:H    | 1:C:478:GLN:HE21 | 1.40                     | 0.68              |
| 1:G:474:LYS:H    | 1:G:478:GLN:HE21 | 1.40                     | 0.68              |
| 1:F:474:LYS:H    | 1:F:478:GLN:HE21 | 1.41                     | 0.68              |
| 1:D:327:SER:OG   | 1:D:343:GLN:NE2  | 2.32                     | 0.63              |
| 1:H:327:SER:OG   | 1:H:343:GLN:NE2  | 2.32                     | 0.63              |
| 1:C:327:SER:OG   | 1:C:343:GLN:NE2  | 2.32                     | 0.63              |
| 1:G:327:SER:OG   | 1:G:343:GLN:NE2  | 2.32                     | 0.63              |
| 1:B:327:SER:OG   | 1:B:343:GLN:NE2  | 2.32                     | 0.63              |
| 1:F:327:SER:OG   | 1:F:343:GLN:NE2  | 2.32                     | 0.62              |
| 1:E:327:SER:OG   | 1:E:343:GLN:NE2  | 2.32                     | 0.62              |
| 1:A:327:SER:OG   | 1:A:343:GLN:NE2  | 2.32                     | 0.62              |
| 1:H:91:ILE:H     | 1:H:248:ALA:HA   | 1.65                     | 0.62              |
| 1:D:91:ILE:H     | 1:D:248:ALA:HA   | 1.65                     | 0.61              |
| 1:C:91:ILE:H     | 1:C:248:ALA:HA   | 1.65                     | 0.61              |
| 1:F:91:ILE:H     | 1:F:248:ALA:HA   | 1.65                     | 0.61              |
| 1:A:91:ILE:H     | 1:A:248:ALA:HA   | 1.65                     | 0.61              |
| 1:B:91:ILE:H     | 1:B:248:ALA:HA   | 1.65                     | 0.61              |
| 1:G:91:ILE:H     | 1:G:248:ALA:HA   | 1.65                     | 0.61              |
| 1:E:91:ILE:H     | 1:E:248:ALA:HA   | 1.65                     | 0.61              |
| 1:D:72:THR:HG21  | 1:D:412:ARG:H    | 1.66                     | 0.61              |
| 1:H:72:THR:HG21  | 1:H:412:ARG:H    | 1.66                     | 0.61              |
| 1:G:72:THR:HG21  | 1:G:412:ARG:H    | 1.66                     | 0.60              |
| 1:C:72:THR:HG21  | 1:C:412:ARG:H    | 1.66                     | 0.60              |
| 1:G:309:GLN:HE22 | 1:H:39:PRO:HG2   | 1.66                     | 0.60              |
| 1:B:72:THR:HG21  | 1:B:412:ARG:H    | 1.66                     | 0.60              |
| 1:F:72:THR:HG21  | 1:F:412:ARG:H    | 1.66                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:309:GLN:HE22 | 1:B:39:PRO:HG2   | 1.67                     | 0.60              |
| 1:A:39:PRO:HG2   | 1:D:309:GLN:HE22 | 1.67                     | 0.60              |
| 1:C:309:GLN:HE22 | 1:D:39:PRO:HG2   | 1.67                     | 0.60              |
| 1:E:39:PRO:HG2   | 1:H:309:GLN:HE22 | 1.67                     | 0.60              |
| 1:E:309:GLN:HE22 | 1:F:39:PRO:HG2   | 1.67                     | 0.60              |
| 1:A:72:THR:HG21  | 1:A:412:ARG:H    | 1.66                     | 0.59              |
| 1:C:228:LYS:NZ   | 1:E:164:ASP:O    | 2.35                     | 0.59              |
| 1:B:164:ASP:O    | 1:F:228:LYS:NZ   | 2.35                     | 0.59              |
| 1:E:72:THR:HG21  | 1:E:412:ARG:H    | 1.66                     | 0.59              |
| 1:F:309:GLN:HE22 | 1:G:39:PRO:HG2   | 1.67                     | 0.59              |
| 1:A:343:GLN:NE2  | 1:A:364:ASP:O    | 2.37                     | 0.58              |
| 1:B:228:LYS:O    | 1:B:231:ARG:NH1  | 2.36                     | 0.58              |
| 1:B:228:LYS:NZ   | 1:F:164:ASP:O    | 2.37                     | 0.58              |
| 1:B:309:GLN:HE22 | 1:C:39:PRO:HG2   | 1.68                     | 0.58              |
| 1:C:164:ASP:O    | 1:E:228:LYS:NZ   | 2.36                     | 0.58              |
| 1:E:343:GLN:NE2  | 1:E:364:ASP:O    | 2.37                     | 0.58              |
| 1:D:343:GLN:NE2  | 1:D:364:ASP:O    | 2.37                     | 0.58              |
| 1:F:228:LYS:O    | 1:F:231:ARG:NH1  | 2.36                     | 0.58              |
| 1:G:343:GLN:NE2  | 1:G:364:ASP:O    | 2.37                     | 0.58              |
| 1:H:343:GLN:NE2  | 1:H:364:ASP:O    | 2.37                     | 0.58              |
| 1:C:343:GLN:NE2  | 1:C:364:ASP:O    | 2.37                     | 0.58              |
| 1:D:228:LYS:O    | 1:D:231:ARG:NH1  | 2.36                     | 0.58              |
| 1:H:228:LYS:O    | 1:H:231:ARG:NH1  | 2.36                     | 0.58              |
| 1:G:228:LYS:O    | 1:G:231:ARG:NH1  | 2.36                     | 0.57              |
| 1:E:195:LYS:HA   | 1:E:198:ASN:HD22 | 1.69                     | 0.57              |
| 1:E:228:LYS:O    | 1:E:231:ARG:NH1  | 2.36                     | 0.57              |
| 1:F:195:LYS:HA   | 1:F:198:ASN:HD22 | 1.69                     | 0.57              |
| 1:F:343:GLN:NE2  | 1:F:364:ASP:O    | 2.37                     | 0.57              |
| 1:A:228:LYS:O    | 1:A:231:ARG:NH1  | 2.36                     | 0.57              |
| 1:B:195:LYS:HA   | 1:B:198:ASN:HD22 | 1.69                     | 0.57              |
| 1:B:343:GLN:NE2  | 1:B:364:ASP:O    | 2.37                     | 0.57              |
| 1:A:195:LYS:HA   | 1:A:198:ASN:HD22 | 1.69                     | 0.57              |
| 1:H:195:LYS:HA   | 1:H:198:ASN:HD22 | 1.69                     | 0.57              |
| 1:D:228:LYS:NZ   | 1:H:164:ASP:O    | 2.37                     | 0.57              |
| 1:E:161:ARG:HD3  | 2:E:601:ATP:H5'1 | 1.87                     | 0.57              |
| 1:A:161:ARG:HD3  | 2:A:601:ATP:H5'1 | 1.87                     | 0.57              |
| 1:D:164:ASP:O    | 1:H:228:LYS:NZ   | 2.37                     | 0.57              |
| 1:D:195:LYS:HA   | 1:D:198:ASN:HD22 | 1.69                     | 0.57              |
| 1:D:161:ARG:HD3  | 2:D:601:ATP:H5'1 | 1.87                     | 0.57              |
| 1:H:161:ARG:HD3  | 2:H:601:ATP:H5'1 | 1.87                     | 0.57              |
| 1:G:195:LYS:HA   | 1:G:198:ASN:HD22 | 1.69                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:161:ARG:HD3  | 2:F:601:ATP:H5'1 | 1.87                     | 0.56              |
| 1:B:161:ARG:HD3  | 2:B:601:ATP:H5'1 | 1.87                     | 0.56              |
| 1:C:195:LYS:HA   | 1:C:198:ASN:HD22 | 1.69                     | 0.56              |
| 1:C:228:LYS:O    | 1:C:231:ARG:NH1  | 2.36                     | 0.56              |
| 1:A:246:CYS:SG   | 1:A:247:GLY:N    | 2.79                     | 0.56              |
| 1:C:161:ARG:HD3  | 2:C:601:ATP:H5'1 | 1.87                     | 0.56              |
| 1:E:246:CYS:SG   | 1:E:247:GLY:N    | 2.79                     | 0.56              |
| 1:G:161:ARG:HD3  | 2:G:601:ATP:H5'1 | 1.87                     | 0.56              |
| 1:A:228:LYS:NZ   | 1:G:164:ASP:O    | 2.38                     | 0.56              |
| 1:B:246:CYS:SG   | 1:B:247:GLY:N    | 2.79                     | 0.56              |
| 1:A:164:ASP:O    | 1:G:228:LYS:NZ   | 2.39                     | 0.56              |
| 1:B:205:LYS:NZ   | 1:F:162:ASP:OD1  | 2.32                     | 0.56              |
| 1:F:246:CYS:SG   | 1:F:247:GLY:N    | 2.79                     | 0.56              |
| 1:C:246:CYS:SG   | 1:C:247:GLY:N    | 2.79                     | 0.55              |
| 1:G:246:CYS:SG   | 1:G:247:GLY:N    | 2.79                     | 0.55              |
| 1:H:246:CYS:SG   | 1:H:247:GLY:N    | 2.79                     | 0.55              |
| 1:D:246:CYS:SG   | 1:D:247:GLY:N    | 2.79                     | 0.55              |
| 1:B:144:ILE:N    | 1:B:156:GLY:O    | 2.38                     | 0.54              |
| 1:F:144:ILE:N    | 1:F:156:GLY:O    | 2.38                     | 0.54              |
| 1:H:144:ILE:N    | 1:H:156:GLY:O    | 2.38                     | 0.54              |
| 1:D:144:ILE:N    | 1:D:156:GLY:O    | 2.38                     | 0.54              |
| 1:E:144:ILE:N    | 1:E:156:GLY:O    | 2.38                     | 0.54              |
| 1:C:452:SER:OG   | 1:C:453:ILE:N    | 2.41                     | 0.53              |
| 1:A:144:ILE:N    | 1:A:156:GLY:O    | 2.38                     | 0.53              |
| 1:G:452:SER:OG   | 1:G:453:ILE:N    | 2.41                     | 0.53              |
| 1:G:144:ILE:N    | 1:G:156:GLY:O    | 2.38                     | 0.53              |
| 1:B:361:VAL:HG13 | 1:B:381:ALA:HA   | 1.90                     | 0.53              |
| 1:C:361:VAL:HG13 | 1:C:381:ALA:HA   | 1.90                     | 0.53              |
| 1:F:361:VAL:HG13 | 1:F:381:ALA:HA   | 1.90                     | 0.53              |
| 1:G:83:ALA:O     | 1:G:237:SER:OG   | 2.26                     | 0.53              |
| 1:G:364:ASP:OD2  | 3:G:603:IMP:O2'  | 2.27                     | 0.53              |
| 1:A:364:ASP:OD2  | 3:A:603:IMP:O2'  | 2.27                     | 0.53              |
| 1:C:83:ALA:O     | 1:C:237:SER:OG   | 2.26                     | 0.53              |
| 1:C:364:ASP:OD2  | 3:C:603:IMP:O2'  | 2.27                     | 0.53              |
| 1:G:361:VAL:HG13 | 1:G:381:ALA:HA   | 1.90                     | 0.53              |
| 1:C:144:ILE:N    | 1:C:156:GLY:O    | 2.38                     | 0.53              |
| 1:E:364:ASP:OD2  | 3:E:603:IMP:O2'  | 2.27                     | 0.53              |
| 1:A:452:SER:OG   | 1:A:453:ILE:N    | 2.41                     | 0.52              |
| 1:E:452:SER:OG   | 1:E:453:ILE:N    | 2.41                     | 0.52              |
| 1:B:162:ASP:OD1  | 1:F:205:LYS:NZ   | 2.36                     | 0.52              |
| 1:D:361:VAL:HG13 | 1:D:381:ALA:HA   | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:162:ASP:OD1  | 1:E:205:LYS:NZ   | 2.32                     | 0.52              |
| 1:H:364:ASP:OD2  | 3:H:603:IMP:O2'  | 2.27                     | 0.52              |
| 1:A:361:VAL:HG13 | 1:A:381:ALA:HA   | 1.90                     | 0.52              |
| 1:D:364:ASP:OD2  | 3:D:603:IMP:O2'  | 2.27                     | 0.52              |
| 1:E:361:VAL:HG13 | 1:E:381:ALA:HA   | 1.90                     | 0.52              |
| 1:H:361:VAL:HG13 | 1:H:381:ALA:HA   | 1.90                     | 0.52              |
| 1:B:364:ASP:OD2  | 3:B:603:IMP:O2'  | 2.27                     | 0.51              |
| 1:B:207:GLY:HA2  | 1:B:224:ARG:HD2  | 1.93                     | 0.51              |
| 1:B:452:SER:OG   | 1:B:453:ILE:N    | 2.41                     | 0.51              |
| 1:F:364:ASP:OD2  | 3:F:603:IMP:O2'  | 2.27                     | 0.51              |
| 1:G:377:LEU:HD13 | 1:G:476:LEU:HD21 | 1.93                     | 0.51              |
| 1:C:207:GLY:HA2  | 1:C:224:ARG:HD2  | 1.93                     | 0.51              |
| 1:C:377:LEU:HD13 | 1:C:476:LEU:HD21 | 1.93                     | 0.51              |
| 1:D:83:ALA:O     | 1:D:237:SER:OG   | 2.26                     | 0.51              |
| 1:F:452:SER:OG   | 1:F:453:ILE:N    | 2.41                     | 0.51              |
| 1:B:277:GLN:HE22 | 1:B:279:ASN:HB3  | 1.76                     | 0.51              |
| 1:F:207:GLY:HA2  | 1:F:224:ARG:HD2  | 1.93                     | 0.51              |
| 1:F:277:GLN:HE22 | 1:F:279:ASN:HB3  | 1.76                     | 0.51              |
| 1:G:207:GLY:HA2  | 1:G:224:ARG:HD2  | 1.93                     | 0.51              |
| 1:H:83:ALA:O     | 1:H:237:SER:OG   | 2.26                     | 0.51              |
| 1:A:162:ASP:OD1  | 1:G:205:LYS:NZ   | 2.35                     | 0.51              |
| 1:D:377:LEU:HD13 | 1:D:476:LEU:HD21 | 1.93                     | 0.51              |
| 1:F:83:ALA:O     | 1:F:237:SER:OG   | 2.26                     | 0.51              |
| 1:H:377:LEU:HD13 | 1:H:476:LEU:HD21 | 1.93                     | 0.51              |
| 1:B:83:ALA:O     | 1:B:237:SER:OG   | 2.26                     | 0.51              |
| 1:B:377:LEU:HD13 | 1:B:476:LEU:HD21 | 1.93                     | 0.51              |
| 1:D:452:SER:OG   | 1:D:453:ILE:N    | 2.41                     | 0.51              |
| 1:H:452:SER:OG   | 1:H:453:ILE:N    | 2.41                     | 0.51              |
| 1:F:377:LEU:HD13 | 1:F:476:LEU:HD21 | 1.93                     | 0.51              |
| 1:A:207:GLY:HA2  | 1:A:224:ARG:HD2  | 1.93                     | 0.51              |
| 1:D:187:VAL:HG11 | 1:D:212:VAL:HG23 | 1.93                     | 0.51              |
| 1:E:83:ALA:O     | 1:E:237:SER:OG   | 2.26                     | 0.51              |
| 1:H:187:VAL:HG11 | 1:H:212:VAL:HG23 | 1.93                     | 0.51              |
| 1:C:187:VAL:HG11 | 1:C:212:VAL:HG23 | 1.93                     | 0.50              |
| 1:F:187:VAL:HG11 | 1:F:212:VAL:HG23 | 1.93                     | 0.50              |
| 1:A:83:ALA:O     | 1:A:237:SER:OG   | 2.26                     | 0.50              |
| 1:B:187:VAL:HG11 | 1:B:212:VAL:HG23 | 1.93                     | 0.50              |
| 1:D:277:GLN:HE22 | 1:D:279:ASN:HB3  | 1.76                     | 0.50              |
| 1:E:207:GLY:HA2  | 1:E:224:ARG:HD2  | 1.93                     | 0.50              |
| 1:G:187:VAL:HG11 | 1:G:212:VAL:HG23 | 1.93                     | 0.50              |
| 1:A:187:VAL:HG11 | 1:A:212:VAL:HG23 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:277:GLN:HE22 | 1:H:279:ASN:HB3  | 1.76                     | 0.50              |
| 1:A:277:GLN:HE22 | 1:A:279:ASN:HB3  | 1.76                     | 0.50              |
| 1:E:187:VAL:HG11 | 1:E:212:VAL:HG23 | 1.93                     | 0.50              |
| 1:E:277:GLN:HE22 | 1:E:279:ASN:HB3  | 1.76                     | 0.50              |
| 1:G:277:GLN:HE22 | 1:G:279:ASN:HB3  | 1.76                     | 0.50              |
| 1:A:377:LEU:HD13 | 1:A:476:LEU:HD21 | 1.92                     | 0.50              |
| 1:C:277:GLN:HE22 | 1:C:279:ASN:HB3  | 1.76                     | 0.50              |
| 1:E:377:LEU:HD13 | 1:E:476:LEU:HD21 | 1.93                     | 0.50              |
| 1:C:325:MET:HG3  | 1:C:340:GLY:HA2  | 1.94                     | 0.50              |
| 1:D:207:GLY:HA2  | 1:D:224:ARG:HD2  | 1.93                     | 0.50              |
| 1:G:325:MET:HG3  | 1:G:340:GLY:HA2  | 1.94                     | 0.50              |
| 1:F:325:MET:HG3  | 1:F:340:GLY:HA2  | 1.94                     | 0.50              |
| 1:A:61:LEU:HD21  | 1:A:88:ILE:HB    | 1.93                     | 0.50              |
| 1:B:325:MET:HG3  | 1:B:340:GLY:HA2  | 1.94                     | 0.50              |
| 1:H:207:GLY:HA2  | 1:H:224:ARG:HD2  | 1.93                     | 0.50              |
| 1:D:144:ILE:HG22 | 1:D:155:VAL:HB   | 1.94                     | 0.50              |
| 1:E:61:LEU:HD21  | 1:E:88:ILE:HB    | 1.94                     | 0.50              |
| 1:E:72:THR:OG1   | 1:E:410:LYS:O    | 2.29                     | 0.50              |
| 1:H:325:MET:HA   | 4:H:604:NAD:H4N  | 1.94                     | 0.50              |
| 1:D:325:MET:HG3  | 1:D:340:GLY:HA2  | 1.94                     | 0.49              |
| 1:D:325:MET:HA   | 4:D:604:NAD:H4N  | 1.94                     | 0.49              |
| 1:G:144:ILE:HG22 | 1:G:155:VAL:HB   | 1.94                     | 0.49              |
| 1:H:144:ILE:HG22 | 1:H:155:VAL:HB   | 1.94                     | 0.49              |
| 1:H:325:MET:HG3  | 1:H:340:GLY:HA2  | 1.94                     | 0.49              |
| 1:A:325:MET:HA   | 4:A:604:NAD:H4N  | 1.94                     | 0.49              |
| 1:C:144:ILE:HG22 | 1:C:155:VAL:HB   | 1.94                     | 0.49              |
| 1:C:325:MET:HA   | 4:C:604:NAD:H4N  | 1.94                     | 0.49              |
| 1:G:325:MET:HA   | 4:G:604:NAD:H4N  | 1.94                     | 0.49              |
| 1:E:325:MET:HA   | 4:E:604:NAD:H4N  | 1.94                     | 0.49              |
| 1:A:325:MET:HG3  | 1:A:340:GLY:HA2  | 1.94                     | 0.49              |
| 1:B:61:LEU:HD21  | 1:B:88:ILE:HB    | 1.94                     | 0.49              |
| 1:B:144:ILE:HG22 | 1:B:155:VAL:HB   | 1.94                     | 0.49              |
| 1:C:61:LEU:HD21  | 1:C:88:ILE:HB    | 1.94                     | 0.49              |
| 1:F:144:ILE:HG22 | 1:F:155:VAL:HB   | 1.94                     | 0.49              |
| 1:G:61:LEU:HD21  | 1:G:88:ILE:HB    | 1.94                     | 0.49              |
| 1:A:205:LYS:NZ   | 1:G:162:ASP:OD1  | 2.35                     | 0.49              |
| 1:E:325:MET:HG3  | 1:E:340:GLY:HA2  | 1.94                     | 0.49              |
| 1:F:61:LEU:HD21  | 1:F:88:ILE:HB    | 1.94                     | 0.49              |
| 1:D:61:LEU:HD21  | 1:D:88:ILE:HB    | 1.94                     | 0.49              |
| 1:F:325:MET:HA   | 4:F:604:NAD:H4N  | 1.94                     | 0.48              |
| 1:H:61:LEU:HD21  | 1:H:88:ILE:HB    | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:370:VAL:HG11 | 1:A:463:GLY:HA3  | 1.95                     | 0.48              |
| 1:B:31:THR:OG1   | 1:B:32:TYR:N     | 2.46                     | 0.48              |
| 1:B:325:MET:HA   | 4:B:604:NAD:H4N  | 1.94                     | 0.48              |
| 1:F:31:THR:OG1   | 1:F:32:TYR:N     | 2.46                     | 0.48              |
| 1:C:31:THR:OG1   | 1:C:32:TYR:N     | 2.46                     | 0.48              |
| 1:D:205:LYS:NZ   | 1:H:162:ASP:OD1  | 2.34                     | 0.48              |
| 1:E:370:VAL:HG11 | 1:E:463:GLY:HA3  | 1.95                     | 0.48              |
| 1:D:394:THR:OG1  | 1:D:395:GLU:OE1  | 2.28                     | 0.48              |
| 1:E:144:ILE:HG22 | 1:E:155:VAL:HB   | 1.94                     | 0.48              |
| 1:G:31:THR:OG1   | 1:G:32:TYR:N     | 2.46                     | 0.48              |
| 1:A:78:MET:HE2   | 1:A:453:ILE:HD11 | 1.96                     | 0.48              |
| 1:E:78:MET:HE2   | 1:E:453:ILE:HD11 | 1.96                     | 0.48              |
| 1:G:78:MET:HE2   | 1:G:453:ILE:HD11 | 1.96                     | 0.48              |
| 1:A:144:ILE:HG22 | 1:A:155:VAL:HB   | 1.94                     | 0.48              |
| 1:B:370:VAL:HG11 | 1:B:463:GLY:HA3  | 1.95                     | 0.48              |
| 1:C:78:MET:HE2   | 1:C:453:ILE:HD11 | 1.96                     | 0.48              |
| 1:F:370:VAL:HG11 | 1:F:463:GLY:HA3  | 1.95                     | 0.48              |
| 1:B:78:MET:HE2   | 1:B:453:ILE:HD11 | 1.96                     | 0.48              |
| 1:D:78:MET:HE2   | 1:D:453:ILE:HD11 | 1.96                     | 0.48              |
| 1:D:162:ASP:OD1  | 1:H:205:LYS:NZ   | 2.34                     | 0.48              |
| 1:F:78:MET:HE2   | 1:F:453:ILE:HD11 | 1.96                     | 0.48              |
| 1:H:78:MET:HE2   | 1:H:453:ILE:HD11 | 1.96                     | 0.48              |
| 3:G:603:IMP:O2'  | 4:G:604:NAD:O7N  | 2.33                     | 0.47              |
| 1:D:409:LYS:HE2  | 1:D:409:LYS:HB2  | 1.46                     | 0.47              |
| 1:A:326:GLY:HA3  | 1:A:334:GLN:HG3  | 1.97                     | 0.47              |
| 1:C:370:VAL:HG11 | 1:C:463:GLY:HA3  | 1.95                     | 0.47              |
| 1:C:386:MET:HE3  | 1:C:386:MET:HB2  | 1.77                     | 0.47              |
| 1:D:31:THR:OG1   | 1:D:32:TYR:N     | 2.46                     | 0.47              |
| 1:E:326:GLY:HA3  | 1:E:334:GLN:HG3  | 1.97                     | 0.47              |
| 1:G:370:VAL:HG11 | 1:G:463:GLY:HA3  | 1.95                     | 0.47              |
| 1:F:326:GLY:HA3  | 1:F:334:GLN:HG3  | 1.97                     | 0.47              |
| 1:H:31:THR:OG1   | 1:H:32:TYR:N     | 2.47                     | 0.47              |
| 1:B:326:GLY:HA3  | 1:B:334:GLN:HG3  | 1.97                     | 0.47              |
| 1:D:326:GLY:HA3  | 1:D:334:GLN:HG3  | 1.97                     | 0.47              |
| 1:D:370:VAL:HG11 | 1:D:463:GLY:HA3  | 1.95                     | 0.47              |
| 1:H:326:GLY:HA3  | 1:H:334:GLN:HG3  | 1.97                     | 0.47              |
| 1:G:72:THR:OG1   | 1:G:410:LYS:O    | 2.29                     | 0.47              |
| 1:G:386:MET:HE3  | 1:G:386:MET:HB2  | 1.77                     | 0.47              |
| 1:H:370:VAL:HG11 | 1:H:463:GLY:HA3  | 1.95                     | 0.47              |
| 1:C:326:GLY:HA3  | 1:C:334:GLN:HG3  | 1.97                     | 0.47              |
| 1:D:55:LEU:HB2   | 1:D:61:LEU:HD13  | 1.98                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:55:LEU:HB2   | 1:G:61:LEU:HD13  | 1.98                     | 0.47              |
| 1:G:326:GLY:HA3  | 1:G:334:GLN:HG3  | 1.97                     | 0.47              |
| 1:H:55:LEU:HB2   | 1:H:61:LEU:HD13  | 1.98                     | 0.46              |
| 1:D:72:THR:OG1   | 1:D:410:LYS:O    | 2.29                     | 0.46              |
| 1:H:409:LYS:HB2  | 1:H:409:LYS:HE2  | 1.47                     | 0.46              |
| 1:C:55:LEU:HB2   | 1:C:61:LEU:HD13  | 1.98                     | 0.46              |
| 1:C:205:LYS:NZ   | 1:E:162:ASP:OD1  | 2.35                     | 0.46              |
| 1:A:31:THR:OG1   | 1:A:32:TYR:N     | 2.46                     | 0.46              |
| 1:L:5:LEU:HD21   | 1:D:52:THR:HG22  | 1.97                     | 0.46              |
| 1:H:72:THR:OG1   | 1:H:410:LYS:O    | 2.29                     | 0.46              |
| 1:B:239:ASP:OD1  | 1:B:243:GLN:N    | 2.42                     | 0.46              |
| 1:H:70:MET:HB2   | 1:H:414:MET:HE3  | 1.98                     | 0.46              |
| 1:D:70:MET:HB2   | 1:D:414:MET:HE3  | 1.98                     | 0.46              |
| 1:D:373:ILE:HG23 | 1:D:384:VAL:HG21 | 1.98                     | 0.46              |
| 1:E:31:THR:OG1   | 1:E:32:TYR:N     | 2.46                     | 0.46              |
| 1:H:373:ILE:HG23 | 1:H:384:VAL:HG21 | 1.98                     | 0.46              |
| 1:B:55:LEU:HB2   | 1:B:61:LEU:HD13  | 1.98                     | 0.46              |
| 1:F:55:LEU:HB2   | 1:F:61:LEU:HD13  | 1.98                     | 0.46              |
| 1:F:239:ASP:OD1  | 1:F:243:GLN:N    | 2.42                     | 0.46              |
| 1:B:70:MET:HB2   | 1:B:414:MET:HE3  | 1.98                     | 0.46              |
| 1:D:260:LEU:HD13 | 1:D:286:MET:HE1  | 1.98                     | 0.46              |
| 1:H:260:LEU:HD13 | 1:H:286:MET:HE1  | 1.98                     | 0.46              |
| 1:F:70:MET:HB2   | 1:F:414:MET:HE3  | 1.98                     | 0.46              |
| 1:G:260:LEU:HD13 | 1:G:286:MET:HE1  | 1.98                     | 0.46              |
| 1:A:394:THR:OG1  | 1:A:395:GLU:OE1  | 2.27                     | 0.45              |
| 1:B:381:ALA:O    | 1:B:480:ARG:NH1  | 2.49                     | 0.45              |
| 1:C:260:LEU:HD13 | 1:C:286:MET:HE1  | 1.98                     | 0.45              |
| 1:D:386:MET:HB2  | 1:D:386:MET:HE3  | 1.77                     | 0.45              |
| 1:F:381:ALA:O    | 1:F:480:ARG:NH1  | 2.49                     | 0.45              |
| 1:A:55:LEU:HB2   | 1:A:61:LEU:HD13  | 1.98                     | 0.45              |
| 1:A:239:ASP:OD1  | 1:A:243:GLN:N    | 2.43                     | 0.45              |
| 1:C:51:LEU:HD11  | 1:C:465:GLN:HB3  | 1.99                     | 0.45              |
| 1:E:55:LEU:HB2   | 1:E:61:LEU:HD13  | 1.98                     | 0.45              |
| 1:G:51:LEU:HD11  | 1:G:465:GLN:HB3  | 1.99                     | 0.45              |
| 1:A:373:ILE:HG23 | 1:A:384:VAL:HG21 | 1.98                     | 0.45              |
| 1:B:373:ILE:HG23 | 1:B:384:VAL:HG21 | 1.98                     | 0.45              |
| 1:F:373:ILE:HG23 | 1:F:384:VAL:HG21 | 1.98                     | 0.45              |
| 1:G:381:ALA:O    | 1:G:480:ARG:NH1  | 2.49                     | 0.45              |
| 1:A:381:ALA:O    | 1:A:480:ARG:NH1  | 2.49                     | 0.45              |
| 1:C:373:ILE:HG23 | 1:C:384:VAL:HG21 | 1.98                     | 0.45              |
| 1:C:381:ALA:O    | 1:C:480:ARG:NH1  | 2.49                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:381:ALA:O    | 1:E:480:ARG:NH1  | 2.50                     | 0.45              |
| 1:G:373:ILE:HG23 | 1:G:384:VAL:HG21 | 1.98                     | 0.45              |
| 1:H:386:MET:HB2  | 1:H:386:MET:HE3  | 1.77                     | 0.45              |
| 1:B:51:LEU:HD11  | 1:B:465:GLN:HB3  | 1.99                     | 0.45              |
| 1:C:70:MET:HB2   | 1:C:414:MET:HE3  | 1.98                     | 0.45              |
| 1:C:164:ASP:OD2  | 1:E:224:ARG:NH2  | 2.48                     | 0.45              |
| 1:E:239:ASP:OD1  | 1:E:243:GLN:N    | 2.43                     | 0.45              |
| 1:E:373:ILE:HG23 | 1:E:384:VAL:HG21 | 1.98                     | 0.45              |
| 1:F:51:LEU:HD11  | 1:F:465:GLN:HB3  | 1.99                     | 0.45              |
| 1:G:70:MET:HB2   | 1:G:414:MET:HE3  | 1.98                     | 0.45              |
| 1:G:303:ASN:HD21 | 1:G:322:ARG:NH1  | 2.15                     | 0.45              |
| 1:E:51:LEU:HD11  | 1:E:465:GLN:HB3  | 1.99                     | 0.45              |
| 1:A:51:LEU:HD11  | 1:A:465:GLN:HB3  | 1.99                     | 0.45              |
| 1:C:303:ASN:HD21 | 1:C:322:ARG:NH1  | 2.15                     | 0.45              |
| 1:F:260:LEU:HD13 | 1:F:286:MET:HE1  | 1.98                     | 0.45              |
| 1:A:260:LEU:HD13 | 1:A:286:MET:HE1  | 1.98                     | 0.45              |
| 1:B:260:LEU:HD13 | 1:B:286:MET:HE1  | 1.98                     | 0.45              |
| 1:D:51:LEU:HD11  | 1:D:465:GLN:HB3  | 1.99                     | 0.45              |
| 1:E:260:LEU:HD13 | 1:E:286:MET:HE1  | 1.98                     | 0.45              |
| 1:A:70:MET:HB2   | 1:A:414:MET:HE3  | 1.98                     | 0.45              |
| 1:A:72:THR:OG1   | 1:A:410:LYS:O    | 2.29                     | 0.45              |
| 1:B:72:THR:OG1   | 1:B:410:LYS:O    | 2.29                     | 0.45              |
| 1:H:51:LEU:HD11  | 1:H:465:GLN:HB3  | 1.99                     | 0.45              |
| 1:B:76:ALA:HA    | 1:B:79:ALA:HB3   | 1.99                     | 0.44              |
| 1:B:394:THR:OG1  | 1:B:395:GLU:OE1  | 2.28                     | 0.44              |
| 1:C:72:THR:OG1   | 1:C:410:LYS:O    | 2.29                     | 0.44              |
| 1:E:70:MET:HB2   | 1:E:414:MET:HE3  | 1.98                     | 0.44              |
| 1:F:76:ALA:HA    | 1:F:79:ALA:HB3   | 1.99                     | 0.44              |
| 1:H:303:ASN:HD21 | 1:H:322:ARG:NH1  | 2.15                     | 0.44              |
| 1:D:303:ASN:HD21 | 1:D:322:ARG:NH1  | 2.15                     | 0.44              |
| 1:F:303:ASN:HD21 | 1:F:322:ARG:NH1  | 2.15                     | 0.44              |
| 1:F:409:LYS:HE2  | 1:F:409:LYS:HB2  | 1.47                     | 0.44              |
| 1:B:386:MET:HE3  | 1:B:386:MET:HB2  | 1.77                     | 0.44              |
| 1:D:381:ALA:O    | 1:D:480:ARG:NH1  | 2.49                     | 0.44              |
| 1:F:72:THR:OG1   | 1:F:410:LYS:O    | 2.29                     | 0.44              |
| 1:B:303:ASN:HD21 | 1:B:322:ARG:NH1  | 2.15                     | 0.44              |
| 1:C:409:LYS:HB2  | 1:C:409:LYS:HE2  | 1.47                     | 0.44              |
| 1:G:181:LYS:HE2  | 1:G:181:LYS:HB2  | 1.81                     | 0.44              |
| 1:H:381:ALA:O    | 1:H:480:ARG:NH1  | 2.49                     | 0.44              |
| 1:B:272:VAL:HA   | 1:B:300:ILE:HB   | 2.00                     | 0.44              |
| 1:E:329:SER:OG   | 3:E:603:IMP:O1P  | 2.34                     | 0.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:272:VAL:HA   | 1:F:300:ILE:HB  | 2.00                     | 0.44              |
| 1:H:73:VAL:HG13  | 1:H:74:THR:HG22 | 1.99                     | 0.44              |
| 1:A:329:SER:OG   | 3:A:603:IMP:O3P | 2.34                     | 0.44              |
| 1:D:73:VAL:HG13  | 1:D:74:THR:HG22 | 1.99                     | 0.44              |
| 1:H:201:LEU:HD22 | 1:H:201:LEU:HA  | 1.86                     | 0.44              |
| 1:A:76:ALA:HA    | 1:A:79:ALA:HB3  | 1.99                     | 0.44              |
| 1:D:76:ALA:HA    | 1:D:79:ALA:HB3  | 1.99                     | 0.44              |
| 1:D:201:LEU:HD22 | 1:D:201:LEU:HA  | 1.86                     | 0.44              |
| 1:H:76:ALA:HA    | 1:H:79:ALA:HB3  | 1.99                     | 0.44              |
| 1:B:409:LYS:HE2  | 1:B:409:LYS:HB2 | 1.46                     | 0.44              |
| 1:C:76:ALA:HA    | 1:C:79:ALA:HB3  | 1.99                     | 0.44              |
| 1:E:76:ALA:HA    | 1:E:79:ALA:HB3  | 1.99                     | 0.44              |
| 1:G:76:ALA:HA    | 1:G:79:ALA:HB3  | 1.99                     | 0.44              |
| 1:A:272:VAL:HA   | 1:A:300:ILE:HB  | 2.00                     | 0.43              |
| 1:C:272:VAL:HA   | 1:C:300:ILE:HB  | 2.00                     | 0.43              |
| 1:E:73:VAL:HG13  | 1:E:74:THR:HG22 | 1.99                     | 0.43              |
| 1:G:272:VAL:HA   | 1:G:300:ILE:HB  | 2.00                     | 0.43              |
| 1:G:409:LYS:HB2  | 1:G:409:LYS:HE2 | 1.47                     | 0.43              |
| 1:A:73:VAL:HG13  | 1:A:74:THR:HG22 | 1.99                     | 0.43              |
| 1:B:415:GLY:N    | 3:B:603:IMP:O6  | 2.41                     | 0.43              |
| 1:C:181:LYS:HE2  | 1:C:181:LYS:HB2 | 1.81                     | 0.43              |
| 1:E:272:VAL:HA   | 1:E:300:ILE:HB  | 2.00                     | 0.43              |
| 1:H:181:LYS:HE2  | 1:H:181:LYS:HB2 | 1.81                     | 0.43              |
| 1:A:303:ASN:HD21 | 1:A:322:ARG:NH1 | 2.15                     | 0.43              |
| 1:E:303:ASN:HD21 | 1:E:322:ARG:NH1 | 2.15                     | 0.43              |
| 1:F:415:GLY:N    | 3:F:603:IMP:O6  | 2.41                     | 0.43              |
| 1:H:388:SER:N    | 3:H:603:IMP:O2P | 2.47                     | 0.43              |
| 1:C:73:VAL:HG13  | 1:C:74:THR:HG22 | 1.99                     | 0.43              |
| 1:C:239:ASP:OD1  | 1:C:243:GLN:N   | 2.42                     | 0.43              |
| 1:G:73:VAL:HG13  | 1:G:74:THR:HG22 | 1.99                     | 0.43              |
| 1:N:5:LEU:HD21   | 1:F:52:THR:HG22 | 2.00                     | 0.43              |
| 1:F:128:ARG:HH22 | 1:F:172:ASP:H   | 1.66                     | 0.43              |
| 1:E:283:GLN:NE2  | 1:E:302:GLY:O   | 2.42                     | 0.43              |
| 1:F:73:VAL:HG13  | 1:F:74:THR:HG22 | 1.99                     | 0.43              |
| 1:I:10:THR:OG1   | 1:I:11:SER:N    | 2.52                     | 0.43              |
| 1:B:73:VAL:HG13  | 1:B:74:THR:HG22 | 1.99                     | 0.43              |
| 1:B:128:ARG:HH22 | 1:B:172:ASP:H   | 1.66                     | 0.43              |
| 1:D:181:LYS:HE2  | 1:D:181:LYS:HB2 | 1.81                     | 0.43              |
| 1:D:388:SER:N    | 3:D:603:IMP:O2P | 2.47                     | 0.43              |
| 1:P:10:THR:OG1   | 1:P:11:SER:N    | 2.52                     | 0.43              |
| 1:H:128:ARG:HH22 | 1:H:172:ASP:H   | 1.66                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:364:ASP:HB3  | 1:A:385:MET:HB3  | 2.01                     | 0.43              |
| 1:D:63:THR:HG23  | 1:D:65:LEU:HD23  | 2.01                     | 0.43              |
| 1:M:10:THR:OG1   | 1:M:11:SER:N     | 2.52                     | 0.43              |
| 1:E:364:ASP:HB3  | 1:E:385:MET:HB3  | 2.01                     | 0.43              |
| 1:G:239:ASP:OD1  | 1:G:243:GLN:N    | 2.42                     | 0.43              |
| 1:A:63:THR:HG23  | 1:A:65:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:181:LYS:HB2  | 1:A:181:LYS:HE2  | 1.81                     | 0.42              |
| 1:B:364:ASP:HB3  | 1:B:385:MET:HB3  | 2.01                     | 0.42              |
| 1:L:10:THR:OG1   | 1:L:11:SER:N     | 2.52                     | 0.42              |
| 1:D:128:ARG:HH22 | 1:D:172:ASP:H    | 1.66                     | 0.42              |
| 1:F:364:ASP:HB3  | 1:F:385:MET:HB3  | 2.01                     | 0.42              |
| 1:H:63:THR:HG23  | 1:H:65:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:283:GLN:NE2  | 1:A:302:GLY:O    | 2.42                     | 0.42              |
| 1:B:116:THR:OG1  | 1:B:117:ASP:N    | 2.53                     | 0.42              |
| 1:E:63:THR:HG23  | 1:E:65:LEU:HD23  | 2.02                     | 0.42              |
| 1:H:71:ASP:OD2   | 1:H:412:ARG:NH1  | 2.52                     | 0.42              |
| 1:A:409:LYS:HB2  | 1:A:409:LYS:HE2  | 1.47                     | 0.42              |
| 1:D:71:ASP:OD2   | 1:D:412:ARG:NH1  | 2.52                     | 0.42              |
| 1:F:71:ASP:OD2   | 1:F:412:ARG:NH1  | 2.52                     | 0.42              |
| 1:H:226:ASP:OD1  | 1:H:226:ASP:N    | 2.52                     | 0.42              |
| 1:B:63:THR:HG23  | 1:B:65:LEU:HD23  | 2.01                     | 0.42              |
| 1:B:71:ASP:OD2   | 1:B:412:ARG:NH1  | 2.52                     | 0.42              |
| 1:C:116:THR:OG1  | 1:C:117:ASP:N    | 2.53                     | 0.42              |
| 1:F:63:THR:HG23  | 1:F:65:LEU:HD23  | 2.01                     | 0.42              |
| 1:F:116:THR:OG1  | 1:F:117:ASP:N    | 2.53                     | 0.42              |
| 1:H:272:VAL:HA   | 1:H:300:ILE:HB   | 2.00                     | 0.42              |
| 1:A:331:CYS:HB3  | 1:A:333:THR:HG23 | 2.01                     | 0.42              |
| 1:B:329:SER:N    | 3:B:603:IMP:O1P  | 2.52                     | 0.42              |
| 1:C:71:ASP:OD2   | 1:C:412:ARG:NH1  | 2.52                     | 0.42              |
| 1:C:129:ASP:OD1  | 1:C:129:ASP:N    | 2.52                     | 0.42              |
| 1:D:226:ASP:OD1  | 1:D:226:ASP:N    | 2.52                     | 0.42              |
| 1:D:272:VAL:HA   | 1:D:300:ILE:HB   | 2.00                     | 0.42              |
| 1:E:181:LYS:HB2  | 1:E:181:LYS:HE2  | 1.81                     | 0.42              |
| 1:E:331:CYS:HB3  | 1:E:333:THR:HG23 | 2.01                     | 0.42              |
| 1:F:329:SER:N    | 3:F:603:IMP:O3P  | 2.52                     | 0.42              |
| 1:G:116:THR:OG1  | 1:G:117:ASP:N    | 2.53                     | 0.42              |
| 1:H:128:ARG:H    | 1:H:128:ARG:HD2  | 1.85                     | 0.42              |
| 1:A:209:LEU:HB3  | 1:A:222:ILE:HB   | 2.02                     | 0.42              |
| 1:A:226:ASP:N    | 1:A:226:ASP:OD1  | 2.52                     | 0.42              |
| 1:C:63:THR:HG23  | 1:C:65:LEU:HD23  | 2.01                     | 0.42              |
| 1:E:226:ASP:N    | 1:E:226:ASP:OD1  | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:63:THR:HG23  | 1:G:65:LEU:HD23  | 2.01                     | 0.42              |
| 1:G:71:ASP:OD2   | 1:G:412:ARG:NH1  | 2.52                     | 0.42              |
| 1:G:129:ASP:N    | 1:G:129:ASP:OD1  | 2.52                     | 0.42              |
| 1:C:226:ASP:N    | 1:C:226:ASP:OD1  | 2.52                     | 0.42              |
| 1:D:128:ARG:H    | 1:D:128:ARG:HD2  | 1.85                     | 0.42              |
| 1:E:209:LEU:HB3  | 1:E:222:ILE:HB   | 2.02                     | 0.42              |
| 1:A:128:ARG:HH22 | 1:A:172:ASP:H    | 1.66                     | 0.42              |
| 1:B:331:CYS:HB3  | 1:B:333:THR:HG23 | 2.01                     | 0.42              |
| 1:E:128:ARG:HH22 | 1:E:172:ASP:H    | 1.66                     | 0.42              |
| 1:G:226:ASP:N    | 1:G:226:ASP:OD1  | 2.52                     | 0.42              |
| 1:E:329:SER:N    | 3:E:603:IMP:O3P  | 2.52                     | 0.42              |
| 1:A:329:SER:N    | 3:A:603:IMP:O1P  | 2.52                     | 0.42              |
| 1:B:128:ARG:H    | 1:B:128:ARG:HD2  | 1.85                     | 0.42              |
| 1:C:331:CYS:HB3  | 1:C:333:THR:HG23 | 2.01                     | 0.42              |
| 1:D:364:ASP:HB3  | 1:D:385:MET:HB3  | 2.01                     | 0.42              |
| 1:E:128:ARG:H    | 1:E:128:ARG:HD2  | 1.85                     | 0.42              |
| 1:F:128:ARG:H    | 1:F:128:ARG:HD2  | 1.85                     | 0.42              |
| 1:F:226:ASP:N    | 1:F:226:ASP:OD1  | 2.52                     | 0.42              |
| 1:F:329:SER:OG   | 3:F:603:IMP:O1P  | 2.34                     | 0.42              |
| 1:F:331:CYS:HB3  | 1:F:333:THR:HG23 | 2.01                     | 0.42              |
| 1:G:128:ARG:HH22 | 1:G:172:ASP:H    | 1.66                     | 0.42              |
| 1:H:364:ASP:HB3  | 1:H:385:MET:HB3  | 2.01                     | 0.42              |
| 1:A:128:ARG:H    | 1:A:128:ARG:HD2  | 1.85                     | 0.41              |
| 1:C:364:ASP:HB3  | 1:C:385:MET:HB3  | 2.01                     | 0.41              |
| 1:G:364:ASP:HB3  | 1:G:385:MET:HB3  | 2.01                     | 0.41              |
| 1:B:209:LEU:HB3  | 1:B:222:ILE:HB   | 2.02                     | 0.41              |
| 1:C:128:ARG:H    | 1:C:128:ARG:HD2  | 1.85                     | 0.41              |
| 1:C:128:ARG:HH22 | 1:C:172:ASP:H    | 1.66                     | 0.41              |
| 1:C:329:SER:N    | 3:C:603:IMP:O1P  | 2.52                     | 0.41              |
| 1:D:329:SER:N    | 3:D:603:IMP:O1P  | 2.52                     | 0.41              |
| 1:D:331:CYS:HB3  | 1:D:333:THR:HG23 | 2.01                     | 0.41              |
| 1:E:71:ASP:OD2   | 1:E:412:ARG:NH1  | 2.52                     | 0.41              |
| 1:E:409:LYS:HB2  | 1:E:409:LYS:HE2  | 1.46                     | 0.41              |
| 1:G:128:ARG:H    | 1:G:128:ARG:HD2  | 1.85                     | 0.41              |
| 1:G:329:SER:N    | 3:G:603:IMP:O3P  | 2.52                     | 0.41              |
| 1:H:394:THR:OG1  | 1:H:395:GLU:OE1  | 2.27                     | 0.41              |
| 1:A:71:ASP:OD2   | 1:A:412:ARG:NH1  | 2.52                     | 0.41              |
| 1:A:224:ARG:NH2  | 1:G:164:ASP:OD2  | 2.51                     | 0.41              |
| 1:B:224:ARG:NH2  | 1:F:164:ASP:OD2  | 2.49                     | 0.41              |
| 1:F:47:ASP:OD1   | 1:F:47:ASP:N     | 2.53                     | 0.41              |
| 1:G:331:CYS:HB3  | 1:G:333:THR:HG23 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:209:LEU:HB3  | 1:H:222:ILE:HB   | 2.02                     | 0.41              |
| 1:H:331:CYS:HB3  | 1:H:333:THR:HG23 | 2.01                     | 0.41              |
| 1:A:116:THR:OG1  | 1:A:117:ASP:N    | 2.53                     | 0.41              |
| 1:B:47:ASP:OD1   | 1:B:47:ASP:N     | 2.53                     | 0.41              |
| 1:D:209:LEU:HB3  | 1:D:222:ILE:HB   | 2.02                     | 0.41              |
| 1:D:239:ASP:OD1  | 1:D:243:GLN:N    | 2.42                     | 0.41              |
| 1:F:209:LEU:HB3  | 1:F:222:ILE:HB   | 2.02                     | 0.41              |
| 1:F:386:MET:HE3  | 1:F:386:MET:HB2  | 1.77                     | 0.41              |
| 1:H:329:SER:N    | 3:H:603:IMP:O3P  | 2.52                     | 0.41              |
| 1:I:5:LEU:HD21   | 1:A:52:THR:HG22  | 2.03                     | 0.41              |
| 1:O:10:THR:OG1   | 1:O:11:SER:N     | 2.52                     | 0.41              |
| 1:G:394:THR:OG1  | 1:G:395:GLU:OE1  | 2.28                     | 0.41              |
| 1:E:341:ARG:HA   | 1:F:36:LEU:HD11  | 2.03                     | 0.41              |
| 1:H:239:ASP:OD1  | 1:H:243:GLN:N    | 2.42                     | 0.41              |
| 1:A:341:ARG:HA   | 1:B:36:LEU:HD11  | 2.03                     | 0.41              |
| 1:J:5:LEU:HD21   | 1:B:52:THR:HG22  | 2.03                     | 0.41              |
| 1:C:209:LEU:HB3  | 1:C:222:ILE:HB   | 2.02                     | 0.41              |
| 1:C:394:THR:OG1  | 1:C:395:GLU:OE1  | 2.28                     | 0.41              |
| 1:D:208:LYS:HD3  | 1:D:208:LYS:HA   | 1.94                     | 0.41              |
| 1:E:388:SER:N    | 3:E:603:IMP:O2P  | 2.47                     | 0.41              |
| 1:G:209:LEU:HB3  | 1:G:222:ILE:HB   | 2.02                     | 0.41              |
| 1:G:281:ILE:H    | 1:G:281:ILE:HG13 | 1.75                     | 0.41              |
| 1:H:47:ASP:OD1   | 1:H:47:ASP:N     | 2.53                     | 0.41              |
| 1:D:47:ASP:OD1   | 1:D:47:ASP:N     | 2.53                     | 0.40              |
| 1:D:116:THR:OG1  | 1:D:117:ASP:N    | 2.53                     | 0.40              |
| 1:H:116:THR:OG1  | 1:H:117:ASP:N    | 2.53                     | 0.40              |
| 1:A:72:THR:HG21  | 1:A:412:ARG:N    | 2.35                     | 0.40              |
| 1:A:388:SER:N    | 3:A:603:IMP:O2P  | 2.47                     | 0.40              |
| 1:C:281:ILE:H    | 1:C:281:ILE:HG13 | 1.75                     | 0.40              |
| 1:F:341:ARG:HA   | 1:G:36:LEU:HD11  | 2.03                     | 0.40              |
| 1:G:201:LEU:HD22 | 1:G:201:LEU:HA   | 1.86                     | 0.40              |
| 1:G:388:SER:N    | 3:G:603:IMP:O2P  | 2.47                     | 0.40              |
| 1:E:72:THR:HG21  | 1:E:412:ARG:N    | 2.35                     | 0.40              |
| 1:F:194:LEU:HD13 | 1:F:194:LEU:HA   | 1.96                     | 0.40              |
| 1:F:394:THR:OG1  | 1:F:395:GLU:OE1  | 2.28                     | 0.40              |
| 1:H:208:LYS:HD3  | 1:H:208:LYS:HA   | 1.94                     | 0.40              |
| 1:D:462:ALA:HA   | 1:D:465:GLN:HG2  | 2.03                     | 0.40              |
| 1:E:36:LEU:HD11  | 1:H:341:ARG:HA   | 2.03                     | 0.40              |
| 1:H:462:ALA:HA   | 1:H:465:GLN:HG2  | 2.03                     | 0.40              |
| 1:B:341:ARG:HA   | 1:C:36:LEU:HD11  | 2.04                     | 0.40              |
| 1:E:116:THR:OG1  | 1:E:117:ASP:N    | 2.53                     | 0.40              |

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| Atom-1          | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------|--------------------------|-------------------|
| 1:E:184:ASP:OD1 | 1:E:184:ASP:N | 2.54                     | 0.40              |
| 1:G:47:ASP:OD1  | 1:G:47:ASP:N  | 2.53                     | 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     | 484/519 (93%)   | 447 (92%)  | 35 (7%)  | 2 (0%)   | 30          | 60  |
| 1   | B     | 484/519 (93%)   | 447 (92%)  | 35 (7%)  | 2 (0%)   | 30          | 60  |
| 1   | C     | 484/519 (93%)   | 447 (92%)  | 35 (7%)  | 2 (0%)   | 30          | 60  |
| 1   | D     | 484/519 (93%)   | 447 (92%)  | 35 (7%)  | 2 (0%)   | 30          | 60  |
| 1   | E     | 484/519 (93%)   | 447 (92%)  | 35 (7%)  | 2 (0%)   | 30          | 60  |
| 1   | F     | 484/519 (93%)   | 447 (92%)  | 35 (7%)  | 2 (0%)   | 30          | 60  |
| 1   | G     | 484/519 (93%)   | 447 (92%)  | 35 (7%)  | 2 (0%)   | 30          | 60  |
| 1   | H     | 484/519 (93%)   | 447 (92%)  | 35 (7%)  | 2 (0%)   | 30          | 60  |
| 1   | I     | 12/519 (2%)     | 6 (50%)    | 6 (50%)  | 0        | 100         | 100 |
| 1   | J     | 12/519 (2%)     | 6 (50%)    | 6 (50%)  | 0        | 100         | 100 |
| 1   | K     | 12/519 (2%)     | 6 (50%)    | 6 (50%)  | 0        | 100         | 100 |
| 1   | L     | 12/519 (2%)     | 6 (50%)    | 6 (50%)  | 0        | 100         | 100 |
| 1   | M     | 12/519 (2%)     | 6 (50%)    | 6 (50%)  | 0        | 100         | 100 |
| 1   | N     | 12/519 (2%)     | 6 (50%)    | 6 (50%)  | 0        | 100         | 100 |
| 1   | O     | 12/519 (2%)     | 6 (50%)    | 6 (50%)  | 0        | 100         | 100 |
| 1   | P     | 12/519 (2%)     | 6 (50%)    | 6 (50%)  | 0        | 100         | 100 |
| All | All   | 3968/8304 (48%) | 3624 (91%) | 328 (8%) | 16 (0%)  | 31          | 60  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 110 | TYR  |
| 1   | B     | 110 | TYR  |
| 1   | C     | 110 | TYR  |
| 1   | D     | 110 | TYR  |
| 1   | E     | 110 | TYR  |
| 1   | F     | 110 | TYR  |
| 1   | G     | 110 | TYR  |
| 1   | H     | 110 | TYR  |
| 1   | A     | 111 | GLU  |
| 1   | B     | 111 | GLU  |
| 1   | C     | 111 | GLU  |
| 1   | D     | 111 | GLU  |
| 1   | E     | 111 | GLU  |
| 1   | F     | 111 | GLU  |
| 1   | G     | 111 | GLU  |
| 1   | H     | 111 | GLU  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 398/425 (94%) | 363 (91%) | 35 (9%)  | 9           | 32 |
| 1   | B     | 398/425 (94%) | 363 (91%) | 35 (9%)  | 9           | 32 |
| 1   | C     | 398/425 (94%) | 363 (91%) | 35 (9%)  | 9           | 32 |
| 1   | D     | 398/425 (94%) | 363 (91%) | 35 (9%)  | 9           | 32 |
| 1   | E     | 398/425 (94%) | 363 (91%) | 35 (9%)  | 9           | 32 |
| 1   | F     | 398/425 (94%) | 363 (91%) | 35 (9%)  | 9           | 32 |
| 1   | G     | 398/425 (94%) | 363 (91%) | 35 (9%)  | 9           | 32 |
| 1   | H     | 398/425 (94%) | 363 (91%) | 35 (9%)  | 9           | 32 |
| 1   | I     | 11/425 (3%)   | 9 (82%)   | 2 (18%)  | 2           | 8  |
| 1   | J     | 11/425 (3%)   | 9 (82%)   | 2 (18%)  | 2           | 8  |
| 1   | K     | 11/425 (3%)   | 9 (82%)   | 2 (18%)  | 2           | 8  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | L     | 11/425 (3%)     | 9 (82%)    | 2 (18%)  | 2           | 8  |
| 1   | M     | 11/425 (3%)     | 9 (82%)    | 2 (18%)  | 2           | 8  |
| 1   | N     | 11/425 (3%)     | 9 (82%)    | 2 (18%)  | 2           | 8  |
| 1   | O     | 11/425 (3%)     | 9 (82%)    | 2 (18%)  | 2           | 8  |
| 1   | P     | 11/425 (3%)     | 9 (82%)    | 2 (18%)  | 2           | 8  |
| All | All   | 3272/6800 (48%) | 2976 (91%) | 296 (9%) | 11          | 31 |

All (296) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 11  | SER  |
| 1   | I     | 13  | VAL  |
| 1   | A     | 36  | LEU  |
| 1   | A     | 49  | VAL  |
| 1   | A     | 59  | ILE  |
| 1   | A     | 63  | THR  |
| 1   | A     | 66  | VAL  |
| 1   | A     | 80  | ILE  |
| 1   | A     | 107 | VAL  |
| 1   | A     | 108 | LYS  |
| 1   | A     | 124 | LYS  |
| 1   | A     | 126 | ARG  |
| 1   | A     | 132 | GLU  |
| 1   | A     | 144 | ILE  |
| 1   | A     | 175 | LEU  |
| 1   | A     | 186 | VAL  |
| 1   | A     | 199 | GLU  |
| 1   | A     | 200 | ILE  |
| 1   | A     | 201 | LEU  |
| 1   | A     | 205 | LYS  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 235 | LEU  |
| 1   | A     | 241 | LYS  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 262 | LEU  |
| 1   | A     | 281 | ILE  |
| 1   | A     | 287 | ILE  |
| 1   | A     | 318 | VAL  |
| 1   | A     | 323 | VAL  |
| 1   | A     | 337 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 361 | VAL  |
| 1   | A     | 362 | ILE  |
| 1   | A     | 389 | LEU  |
| 1   | A     | 399 | GLU  |
| 1   | A     | 409 | LYS  |
| 1   | A     | 448 | GLN  |
| 1   | A     | 453 | ILE  |
| 1   | J     | 11  | SER  |
| 1   | J     | 13  | VAL  |
| 1   | B     | 36  | LEU  |
| 1   | B     | 49  | VAL  |
| 1   | B     | 59  | ILE  |
| 1   | B     | 63  | THR  |
| 1   | B     | 66  | VAL  |
| 1   | B     | 80  | ILE  |
| 1   | B     | 107 | VAL  |
| 1   | B     | 108 | LYS  |
| 1   | B     | 124 | LYS  |
| 1   | B     | 126 | ARG  |
| 1   | B     | 132 | GLU  |
| 1   | B     | 144 | ILE  |
| 1   | B     | 175 | LEU  |
| 1   | B     | 186 | VAL  |
| 1   | B     | 199 | GLU  |
| 1   | B     | 200 | ILE  |
| 1   | B     | 201 | LEU  |
| 1   | B     | 205 | LYS  |
| 1   | B     | 218 | LEU  |
| 1   | B     | 235 | LEU  |
| 1   | B     | 241 | LYS  |
| 1   | B     | 244 | LEU  |
| 1   | B     | 262 | LEU  |
| 1   | B     | 281 | ILE  |
| 1   | B     | 287 | ILE  |
| 1   | B     | 318 | VAL  |
| 1   | B     | 323 | VAL  |
| 1   | B     | 337 | LEU  |
| 1   | B     | 361 | VAL  |
| 1   | B     | 362 | ILE  |
| 1   | B     | 389 | LEU  |
| 1   | B     | 399 | GLU  |
| 1   | B     | 409 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 448 | GLN  |
| 1   | B     | 453 | ILE  |
| 1   | K     | 11  | SER  |
| 1   | K     | 13  | VAL  |
| 1   | C     | 36  | LEU  |
| 1   | C     | 49  | VAL  |
| 1   | C     | 59  | ILE  |
| 1   | C     | 63  | THR  |
| 1   | C     | 66  | VAL  |
| 1   | C     | 80  | ILE  |
| 1   | C     | 107 | VAL  |
| 1   | C     | 108 | LYS  |
| 1   | C     | 124 | LYS  |
| 1   | C     | 126 | ARG  |
| 1   | C     | 132 | GLU  |
| 1   | C     | 144 | ILE  |
| 1   | C     | 175 | LEU  |
| 1   | C     | 186 | VAL  |
| 1   | C     | 199 | GLU  |
| 1   | C     | 200 | ILE  |
| 1   | C     | 201 | LEU  |
| 1   | C     | 205 | LYS  |
| 1   | C     | 218 | LEU  |
| 1   | C     | 235 | LEU  |
| 1   | C     | 241 | LYS  |
| 1   | C     | 244 | LEU  |
| 1   | C     | 262 | LEU  |
| 1   | C     | 281 | ILE  |
| 1   | C     | 287 | ILE  |
| 1   | C     | 318 | VAL  |
| 1   | C     | 323 | VAL  |
| 1   | C     | 337 | LEU  |
| 1   | C     | 361 | VAL  |
| 1   | C     | 362 | ILE  |
| 1   | C     | 389 | LEU  |
| 1   | C     | 399 | GLU  |
| 1   | C     | 409 | LYS  |
| 1   | C     | 448 | GLN  |
| 1   | C     | 453 | ILE  |
| 1   | L     | 11  | SER  |
| 1   | L     | 13  | VAL  |
| 1   | D     | 36  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 49  | VAL  |
| 1   | D     | 59  | ILE  |
| 1   | D     | 63  | THR  |
| 1   | D     | 66  | VAL  |
| 1   | D     | 80  | ILE  |
| 1   | D     | 107 | VAL  |
| 1   | D     | 108 | LYS  |
| 1   | D     | 124 | LYS  |
| 1   | D     | 126 | ARG  |
| 1   | D     | 132 | GLU  |
| 1   | D     | 144 | ILE  |
| 1   | D     | 175 | LEU  |
| 1   | D     | 186 | VAL  |
| 1   | D     | 199 | GLU  |
| 1   | D     | 200 | ILE  |
| 1   | D     | 201 | LEU  |
| 1   | D     | 205 | LYS  |
| 1   | D     | 218 | LEU  |
| 1   | D     | 235 | LEU  |
| 1   | D     | 241 | LYS  |
| 1   | D     | 244 | LEU  |
| 1   | D     | 262 | LEU  |
| 1   | D     | 281 | ILE  |
| 1   | D     | 287 | ILE  |
| 1   | D     | 318 | VAL  |
| 1   | D     | 323 | VAL  |
| 1   | D     | 337 | LEU  |
| 1   | D     | 361 | VAL  |
| 1   | D     | 362 | ILE  |
| 1   | D     | 389 | LEU  |
| 1   | D     | 399 | GLU  |
| 1   | D     | 409 | LYS  |
| 1   | D     | 448 | GLN  |
| 1   | D     | 453 | ILE  |
| 1   | M     | 11  | SER  |
| 1   | M     | 13  | VAL  |
| 1   | E     | 36  | LEU  |
| 1   | E     | 49  | VAL  |
| 1   | E     | 59  | ILE  |
| 1   | E     | 63  | THR  |
| 1   | E     | 66  | VAL  |
| 1   | E     | 80  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 107 | VAL  |
| 1   | E     | 108 | LYS  |
| 1   | E     | 124 | LYS  |
| 1   | E     | 126 | ARG  |
| 1   | E     | 132 | GLU  |
| 1   | E     | 144 | ILE  |
| 1   | E     | 175 | LEU  |
| 1   | E     | 186 | VAL  |
| 1   | E     | 199 | GLU  |
| 1   | E     | 200 | ILE  |
| 1   | E     | 201 | LEU  |
| 1   | E     | 205 | LYS  |
| 1   | E     | 218 | LEU  |
| 1   | E     | 235 | LEU  |
| 1   | E     | 241 | LYS  |
| 1   | E     | 244 | LEU  |
| 1   | E     | 262 | LEU  |
| 1   | E     | 281 | ILE  |
| 1   | E     | 287 | ILE  |
| 1   | E     | 318 | VAL  |
| 1   | E     | 323 | VAL  |
| 1   | E     | 337 | LEU  |
| 1   | E     | 361 | VAL  |
| 1   | E     | 362 | ILE  |
| 1   | E     | 389 | LEU  |
| 1   | E     | 399 | GLU  |
| 1   | E     | 409 | LYS  |
| 1   | E     | 448 | GLN  |
| 1   | E     | 453 | ILE  |
| 1   | N     | 11  | SER  |
| 1   | N     | 13  | VAL  |
| 1   | F     | 36  | LEU  |
| 1   | F     | 49  | VAL  |
| 1   | F     | 59  | ILE  |
| 1   | F     | 63  | THR  |
| 1   | F     | 66  | VAL  |
| 1   | F     | 80  | ILE  |
| 1   | F     | 107 | VAL  |
| 1   | F     | 108 | LYS  |
| 1   | F     | 124 | LYS  |
| 1   | F     | 126 | ARG  |
| 1   | F     | 132 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 144 | ILE  |
| 1   | F     | 175 | LEU  |
| 1   | F     | 186 | VAL  |
| 1   | F     | 199 | GLU  |
| 1   | F     | 200 | ILE  |
| 1   | F     | 201 | LEU  |
| 1   | F     | 205 | LYS  |
| 1   | F     | 218 | LEU  |
| 1   | F     | 235 | LEU  |
| 1   | F     | 241 | LYS  |
| 1   | F     | 244 | LEU  |
| 1   | F     | 262 | LEU  |
| 1   | F     | 281 | ILE  |
| 1   | F     | 287 | ILE  |
| 1   | F     | 318 | VAL  |
| 1   | F     | 323 | VAL  |
| 1   | F     | 337 | LEU  |
| 1   | F     | 361 | VAL  |
| 1   | F     | 362 | ILE  |
| 1   | F     | 389 | LEU  |
| 1   | F     | 399 | GLU  |
| 1   | F     | 409 | LYS  |
| 1   | F     | 448 | GLN  |
| 1   | F     | 453 | ILE  |
| 1   | O     | 11  | SER  |
| 1   | O     | 13  | VAL  |
| 1   | G     | 36  | LEU  |
| 1   | G     | 49  | VAL  |
| 1   | G     | 59  | ILE  |
| 1   | G     | 63  | THR  |
| 1   | G     | 66  | VAL  |
| 1   | G     | 80  | ILE  |
| 1   | G     | 107 | VAL  |
| 1   | G     | 108 | LYS  |
| 1   | G     | 124 | LYS  |
| 1   | G     | 126 | ARG  |
| 1   | G     | 132 | GLU  |
| 1   | G     | 144 | ILE  |
| 1   | G     | 175 | LEU  |
| 1   | G     | 186 | VAL  |
| 1   | G     | 199 | GLU  |
| 1   | G     | 200 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 201 | LEU  |
| 1   | G     | 205 | LYS  |
| 1   | G     | 218 | LEU  |
| 1   | G     | 235 | LEU  |
| 1   | G     | 241 | LYS  |
| 1   | G     | 244 | LEU  |
| 1   | G     | 262 | LEU  |
| 1   | G     | 281 | ILE  |
| 1   | G     | 287 | ILE  |
| 1   | G     | 318 | VAL  |
| 1   | G     | 323 | VAL  |
| 1   | G     | 337 | LEU  |
| 1   | G     | 361 | VAL  |
| 1   | G     | 362 | ILE  |
| 1   | G     | 389 | LEU  |
| 1   | G     | 399 | GLU  |
| 1   | G     | 409 | LYS  |
| 1   | G     | 448 | GLN  |
| 1   | G     | 453 | ILE  |
| 1   | P     | 11  | SER  |
| 1   | P     | 13  | VAL  |
| 1   | H     | 36  | LEU  |
| 1   | H     | 49  | VAL  |
| 1   | H     | 59  | ILE  |
| 1   | H     | 63  | THR  |
| 1   | H     | 66  | VAL  |
| 1   | H     | 80  | ILE  |
| 1   | H     | 107 | VAL  |
| 1   | H     | 108 | LYS  |
| 1   | H     | 124 | LYS  |
| 1   | H     | 126 | ARG  |
| 1   | H     | 132 | GLU  |
| 1   | H     | 144 | ILE  |
| 1   | H     | 175 | LEU  |
| 1   | H     | 186 | VAL  |
| 1   | H     | 199 | GLU  |
| 1   | H     | 200 | ILE  |
| 1   | H     | 201 | LEU  |
| 1   | H     | 205 | LYS  |
| 1   | H     | 218 | LEU  |
| 1   | H     | 235 | LEU  |
| 1   | H     | 241 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 244 | LEU  |
| 1   | H     | 262 | LEU  |
| 1   | H     | 281 | ILE  |
| 1   | H     | 287 | ILE  |
| 1   | H     | 318 | VAL  |
| 1   | H     | 323 | VAL  |
| 1   | H     | 337 | LEU  |
| 1   | H     | 361 | VAL  |
| 1   | H     | 362 | ILE  |
| 1   | H     | 389 | LEU  |
| 1   | H     | 399 | GLU  |
| 1   | H     | 409 | LYS  |
| 1   | H     | 448 | GLN  |
| 1   | H     | 453 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | GLN  |
| 1   | A     | 198 | ASN  |
| 1   | A     | 277 | GLN  |
| 1   | A     | 279 | ASN  |
| 1   | A     | 285 | ASN  |
| 1   | A     | 303 | ASN  |
| 1   | A     | 343 | GLN  |
| 1   | A     | 478 | GLN  |
| 1   | B     | 198 | ASN  |
| 1   | B     | 277 | GLN  |
| 1   | B     | 279 | ASN  |
| 1   | B     | 285 | ASN  |
| 1   | B     | 303 | ASN  |
| 1   | B     | 309 | GLN  |
| 1   | B     | 343 | GLN  |
| 1   | B     | 478 | GLN  |
| 1   | C     | 198 | ASN  |
| 1   | C     | 277 | GLN  |
| 1   | C     | 279 | ASN  |
| 1   | C     | 285 | ASN  |
| 1   | C     | 303 | ASN  |
| 1   | C     | 309 | GLN  |
| 1   | C     | 343 | GLN  |
| 1   | C     | 478 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 198 | ASN  |
| 1   | D     | 277 | GLN  |
| 1   | D     | 279 | ASN  |
| 1   | D     | 285 | ASN  |
| 1   | D     | 303 | ASN  |
| 1   | D     | 309 | GLN  |
| 1   | D     | 343 | GLN  |
| 1   | D     | 478 | GLN  |
| 1   | E     | 21  | GLN  |
| 1   | E     | 198 | ASN  |
| 1   | E     | 277 | GLN  |
| 1   | E     | 279 | ASN  |
| 1   | E     | 285 | ASN  |
| 1   | E     | 303 | ASN  |
| 1   | E     | 309 | GLN  |
| 1   | E     | 343 | GLN  |
| 1   | E     | 478 | GLN  |
| 1   | F     | 21  | GLN  |
| 1   | F     | 198 | ASN  |
| 1   | F     | 277 | GLN  |
| 1   | F     | 279 | ASN  |
| 1   | F     | 285 | ASN  |
| 1   | F     | 303 | ASN  |
| 1   | F     | 309 | GLN  |
| 1   | F     | 343 | GLN  |
| 1   | F     | 478 | GLN  |
| 1   | G     | 198 | ASN  |
| 1   | G     | 277 | GLN  |
| 1   | G     | 279 | ASN  |
| 1   | G     | 285 | ASN  |
| 1   | G     | 303 | ASN  |
| 1   | G     | 309 | GLN  |
| 1   | G     | 343 | GLN  |
| 1   | G     | 478 | GLN  |
| 1   | H     | 198 | ASN  |
| 1   | H     | 277 | GLN  |
| 1   | H     | 279 | ASN  |
| 1   | H     | 285 | ASN  |
| 1   | H     | 303 | ASN  |
| 1   | H     | 309 | GLN  |
| 1   | H     | 343 | GLN  |
| 1   | H     | 478 | GLN  |

### 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 | $\# Z  > 2$ |
| 2   | ATP  | B     | 601 | -    | 32,33,33     | 3.16 | 17 (53%)    | 48,52,52    | 2.95 | 13 (27%)    |
| 2   | ATP  | F     | 601 | -    | 32,33,33     | 3.17 | 16 (50%)    | 48,52,52    | 2.95 | 13 (27%)    |
| 4   | NAD  | A     | 604 | -    | 46,48,48     | 3.56 | 21 (45%)    | 64,73,73    | 2.56 | 19 (29%)    |
| 3   | IMP  | G     | 603 | -    | 25,25,25     | 2.63 | 7 (28%)     | 37,38,38    | 2.16 | 9 (24%)     |
| 4   | NAD  | G     | 604 | -    | 46,48,48     | 3.56 | 21 (45%)    | 64,73,73    | 2.56 | 19 (29%)    |
| 2   | ATP  | A     | 602 | -    | 32,33,33     | 3.24 | 16 (50%)    | 48,52,52    | 2.89 | 11 (22%)    |
| 3   | IMP  | F     | 603 | -    | 25,25,25     | 2.62 | 7 (28%)     | 37,38,38    | 2.16 | 9 (24%)     |
| 2   | ATP  | G     | 602 | -    | 32,33,33     | 3.24 | 16 (50%)    | 48,52,52    | 2.89 | 11 (22%)    |
| 2   | ATP  | B     | 602 | -    | 32,33,33     | 3.24 | 17 (53%)    | 48,52,52    | 2.88 | 12 (25%)    |
| 4   | NAD  | H     | 604 | -    | 46,48,48     | 3.56 | 21 (45%)    | 64,73,73    | 2.56 | 19 (29%)    |
| 3   | IMP  | C     | 603 | -    | 25,25,25     | 2.62 | 7 (28%)     | 37,38,38    | 2.13 | 9 (24%)     |
| 2   | ATP  | F     | 602 | -    | 32,33,33     | 3.24 | 17 (53%)    | 48,52,52    | 2.88 | 12 (25%)    |
| 2   | ATP  | C     | 601 | -    | 32,33,33     | 3.17 | 17 (53%)    | 48,52,52    | 2.95 | 12 (25%)    |
| 3   | IMP  | D     | 603 | -    | 25,25,25     | 2.63 | 7 (28%)     | 37,38,38    | 2.13 | 9 (24%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAD  | C     | 604 | -    | 46,48,48     | 3.56 | 21 (45%) | 64,73,73    | 2.56 | 19 (29%) |
| 4   | NAD  | E     | 604 | -    | 46,48,48     | 3.56 | 21 (45%) | 64,73,73    | 2.56 | 19 (29%) |
| 2   | ATP  | A     | 601 | -    | 32,33,33     | 3.17 | 17 (53%) | 48,52,52    | 2.94 | 13 (27%) |
| 4   | NAD  | B     | 604 | -    | 46,48,48     | 3.57 | 21 (45%) | 64,73,73    | 2.56 | 19 (29%) |
| 2   | ATP  | H     | 602 | -    | 32,33,33     | 3.23 | 17 (53%) | 48,52,52    | 2.88 | 11 (22%) |
| 2   | ATP  | D     | 601 | -    | 32,33,33     | 3.18 | 17 (53%) | 48,52,52    | 2.94 | 12 (25%) |
| 2   | ATP  | E     | 602 | -    | 32,33,33     | 3.24 | 17 (53%) | 48,52,52    | 2.88 | 11 (22%) |
| 3   | IMP  | E     | 603 | -    | 25,25,25     | 2.62 | 7 (28%)  | 37,38,38    | 2.16 | 9 (24%)  |
| 2   | ATP  | E     | 601 | -    | 32,33,33     | 3.17 | 18 (56%) | 48,52,52    | 2.94 | 13 (27%) |
| 2   | ATP  | C     | 602 | -    | 32,33,33     | 3.24 | 16 (50%) | 48,52,52    | 2.89 | 11 (22%) |
| 2   | ATP  | D     | 602 | -    | 32,33,33     | 3.25 | 17 (53%) | 48,52,52    | 2.89 | 11 (22%) |
| 3   | IMP  | H     | 603 | -    | 25,25,25     | 2.62 | 7 (28%)  | 37,38,38    | 2.16 | 9 (24%)  |
| 4   | NAD  | D     | 604 | -    | 46,48,48     | 3.56 | 21 (45%) | 64,73,73    | 2.56 | 19 (29%) |
| 4   | NAD  | F     | 604 | -    | 46,48,48     | 3.57 | 21 (45%) | 64,73,73    | 2.56 | 19 (29%) |
| 2   | ATP  | G     | 601 | -    | 32,33,33     | 3.18 | 17 (53%) | 48,52,52    | 2.94 | 12 (25%) |
| 3   | IMP  | A     | 603 | -    | 25,25,25     | 2.62 | 7 (28%)  | 37,38,38    | 2.13 | 9 (24%)  |
| 2   | ATP  | H     | 601 | -    | 32,33,33     | 3.17 | 16 (50%) | 48,52,52    | 2.94 | 13 (27%) |
| 3   | IMP  | B     | 603 | -    | 25,25,25     | 2.63 | 7 (28%)  | 37,38,38    | 2.13 | 9 (24%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | ATP  | B     | 601 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 2   | ATP  | F     | 601 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 4   | NAD  | A     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 3   | IMP  | G     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 4   | NAD  | G     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 2   | ATP  | A     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 3   | IMP  | F     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 2   | ATP  | G     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 2   | ATP  | B     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 4   | NAD  | H     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 3   | IMP  | C     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | ATP  | F     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 2   | ATP  | C     | 601 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 3   | IMP  | D     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 4   | NAD  | C     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 4   | NAD  | E     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 2   | ATP  | A     | 601 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 4   | NAD  | B     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 2   | ATP  | H     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 2   | ATP  | D     | 601 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 2   | ATP  | E     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 3   | IMP  | E     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 2   | ATP  | E     | 601 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 2   | ATP  | C     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 2   | ATP  | D     | 602 | -    | -       | 9/22/38/38  | 0/3/3/3 |
| 3   | IMP  | H     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |
| 4   | NAD  | D     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 4   | NAD  | F     | 604 | -    | -       | 13/30/62/62 | 0/5/5/5 |
| 2   | ATP  | G     | 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 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 3   | IMP  | B     | 603 | -    | -       | 5/10/26/26  | 0/3/3/3 |

All (492) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | B     | 601 | ATP  | C2'-C3' | -10.62 | 1.24        | 1.53     |
| 2   | E     | 601 | ATP  | C2'-C3' | -10.62 | 1.24        | 1.53     |
| 2   | G     | 601 | ATP  | C2'-C3' | -10.62 | 1.24        | 1.53     |
| 2   | D     | 601 | ATP  | C2'-C3' | -10.61 | 1.24        | 1.53     |
| 2   | C     | 601 | ATP  | C2'-C3' | -10.60 | 1.24        | 1.53     |
| 2   | F     | 601 | ATP  | C2'-C3' | -10.60 | 1.24        | 1.53     |
| 2   | A     | 601 | ATP  | C2'-C3' | -10.59 | 1.24        | 1.53     |
| 2   | H     | 601 | ATP  | C2'-C3' | -10.58 | 1.24        | 1.53     |
| 2   | B     | 602 | ATP  | C2'-C3' | -10.47 | 1.25        | 1.53     |
| 2   | F     | 602 | ATP  | C2'-C3' | -10.47 | 1.25        | 1.53     |
| 2   | A     | 602 | ATP  | C2'-C3' | -10.46 | 1.25        | 1.53     |
| 2   | D     | 602 | ATP  | C2'-C3' | -10.46 | 1.25        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | E     | 602 | ATP  | C2'-C3' | -10.46 | 1.25        | 1.53     |
| 2   | G     | 602 | ATP  | C2'-C3' | -10.46 | 1.25        | 1.53     |
| 2   | H     | 602 | ATP  | C2'-C3' | -10.46 | 1.25        | 1.53     |
| 2   | C     | 602 | ATP  | C2'-C3' | -10.45 | 1.25        | 1.53     |
| 4   | E     | 604 | NAD  | C3D-C4D | -9.11  | 1.29        | 1.53     |
| 4   | F     | 604 | NAD  | C3D-C4D | -9.11  | 1.29        | 1.53     |
| 4   | B     | 604 | NAD  | C3D-C4D | -9.10  | 1.29        | 1.53     |
| 4   | C     | 604 | NAD  | C3D-C4D | -9.10  | 1.29        | 1.53     |
| 4   | D     | 604 | NAD  | C3D-C4D | -9.10  | 1.29        | 1.53     |
| 4   | H     | 604 | NAD  | C3D-C4D | -9.10  | 1.29        | 1.53     |
| 4   | A     | 604 | NAD  | C3D-C4D | -9.07  | 1.30        | 1.53     |
| 4   | G     | 604 | NAD  | C3D-C4D | -9.07  | 1.30        | 1.53     |
| 4   | A     | 604 | NAD  | C3B-C4B | -9.04  | 1.30        | 1.53     |
| 4   | B     | 604 | NAD  | C3B-C4B | -9.04  | 1.30        | 1.53     |
| 4   | H     | 604 | NAD  | C3B-C4B | -9.04  | 1.30        | 1.53     |
| 4   | C     | 604 | NAD  | C3B-C4B | -9.04  | 1.30        | 1.53     |
| 4   | D     | 604 | NAD  | C3B-C4B | -9.01  | 1.30        | 1.53     |
| 4   | G     | 604 | NAD  | C3B-C4B | -9.01  | 1.30        | 1.53     |
| 4   | E     | 604 | NAD  | C3B-C4B | -9.01  | 1.30        | 1.53     |
| 4   | F     | 604 | NAD  | C3B-C4B | -9.01  | 1.30        | 1.53     |
| 3   | B     | 603 | IMP  | C2-N3   | 8.44   | 1.45        | 1.30     |
| 3   | G     | 603 | IMP  | C2-N3   | 8.44   | 1.45        | 1.30     |
| 3   | D     | 603 | IMP  | C2-N3   | 8.43   | 1.45        | 1.30     |
| 3   | A     | 603 | IMP  | C2-N3   | 8.41   | 1.45        | 1.30     |
| 3   | H     | 603 | IMP  | C2-N3   | 8.41   | 1.45        | 1.30     |
| 3   | C     | 603 | IMP  | C2-N3   | 8.40   | 1.45        | 1.30     |
| 3   | E     | 603 | IMP  | C2-N3   | 8.40   | 1.45        | 1.30     |
| 3   | F     | 603 | IMP  | C2-N3   | 8.39   | 1.45        | 1.30     |
| 4   | A     | 604 | NAD  | O4D-C1D | -8.13  | 1.30        | 1.40     |
| 4   | D     | 604 | NAD  | O4D-C1D | -8.13  | 1.30        | 1.40     |
| 4   | B     | 604 | NAD  | O4D-C1D | -8.12  | 1.30        | 1.40     |
| 4   | E     | 604 | NAD  | O4D-C1D | -8.12  | 1.30        | 1.40     |
| 4   | G     | 604 | NAD  | O4D-C1D | -8.12  | 1.30        | 1.40     |
| 4   | F     | 604 | NAD  | O4D-C1D | -8.09  | 1.30        | 1.40     |
| 4   | C     | 604 | NAD  | O4D-C1D | -8.08  | 1.30        | 1.40     |
| 4   | H     | 604 | NAD  | O4D-C1D | -8.03  | 1.30        | 1.40     |
| 4   | A     | 604 | NAD  | O4B-C4B | 7.78   | 1.62        | 1.45     |
| 4   | C     | 604 | NAD  | O4B-C4B | 7.78   | 1.62        | 1.45     |
| 4   | E     | 604 | NAD  | O4B-C4B | 7.78   | 1.62        | 1.45     |
| 4   | H     | 604 | NAD  | O4B-C4B | 7.78   | 1.62        | 1.45     |
| 4   | F     | 604 | NAD  | O4B-C4B | 7.76   | 1.62        | 1.45     |
| 4   | G     | 604 | NAD  | O4B-C4B | 7.76   | 1.62        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4   | B     | 604 | NAD  | O4B-C4B | 7.75 | 1.62        | 1.45     |
| 4   | D     | 604 | NAD  | O4B-C4B | 7.75 | 1.62        | 1.45     |
| 4   | G     | 604 | NAD  | C7N-N7N | 7.60 | 1.47        | 1.33     |
| 4   | B     | 604 | NAD  | C7N-N7N | 7.58 | 1.46        | 1.33     |
| 4   | D     | 604 | NAD  | C7N-N7N | 7.55 | 1.46        | 1.33     |
| 4   | A     | 604 | NAD  | C7N-N7N | 7.53 | 1.46        | 1.33     |
| 4   | E     | 604 | NAD  | C7N-N7N | 7.53 | 1.46        | 1.33     |
| 4   | F     | 604 | NAD  | C7N-N7N | 7.53 | 1.46        | 1.33     |
| 4   | H     | 604 | NAD  | C7N-N7N | 7.53 | 1.46        | 1.33     |
| 4   | C     | 604 | NAD  | C7N-N7N | 7.51 | 1.46        | 1.33     |
| 4   | B     | 604 | NAD  | O4D-C4D | 7.47 | 1.61        | 1.45     |
| 4   | C     | 604 | NAD  | O4D-C4D | 7.44 | 1.61        | 1.45     |
| 4   | E     | 604 | NAD  | O4D-C4D | 7.44 | 1.61        | 1.45     |
| 4   | F     | 604 | NAD  | O4D-C4D | 7.44 | 1.61        | 1.45     |
| 4   | H     | 604 | NAD  | O4D-C4D | 7.44 | 1.61        | 1.45     |
| 4   | A     | 604 | NAD  | O4D-C4D | 7.44 | 1.61        | 1.45     |
| 4   | D     | 604 | NAD  | O4D-C4D | 7.44 | 1.61        | 1.45     |
| 4   | G     | 604 | NAD  | O4D-C4D | 7.41 | 1.61        | 1.45     |
| 2   | D     | 602 | ATP  | PA-O3A  | 6.33 | 1.66        | 1.59     |
| 2   | E     | 602 | ATP  | PA-O3A  | 6.33 | 1.66        | 1.59     |
| 2   | G     | 602 | ATP  | PA-O3A  | 6.31 | 1.66        | 1.59     |
| 2   | C     | 602 | ATP  | PA-O3A  | 6.28 | 1.66        | 1.59     |
| 2   | F     | 602 | ATP  | PA-O3A  | 6.27 | 1.66        | 1.59     |
| 2   | A     | 602 | ATP  | PA-O3A  | 6.25 | 1.66        | 1.59     |
| 2   | H     | 602 | ATP  | PA-O3A  | 6.24 | 1.66        | 1.59     |
| 2   | B     | 602 | ATP  | PA-O3A  | 6.21 | 1.66        | 1.59     |
| 2   | B     | 602 | ATP  | PB-O3A  | 6.04 | 1.66        | 1.59     |
| 2   | F     | 602 | ATP  | PB-O3A  | 6.04 | 1.66        | 1.59     |
| 2   | D     | 602 | ATP  | PB-O3A  | 6.02 | 1.66        | 1.59     |
| 2   | C     | 602 | ATP  | PB-O3A  | 5.99 | 1.66        | 1.59     |
| 2   | E     | 602 | ATP  | PB-O3A  | 5.97 | 1.65        | 1.59     |
| 2   | G     | 602 | ATP  | PB-O3A  | 5.97 | 1.65        | 1.59     |
| 2   | H     | 602 | ATP  | PB-O3A  | 5.97 | 1.65        | 1.59     |
| 2   | A     | 602 | ATP  | PB-O3A  | 5.95 | 1.65        | 1.59     |
| 2   | A     | 601 | ATP  | PA-O3A  | 5.51 | 1.65        | 1.59     |
| 2   | D     | 601 | ATP  | PA-O3A  | 5.51 | 1.65        | 1.59     |
| 2   | G     | 601 | ATP  | PA-O3A  | 5.51 | 1.65        | 1.59     |
| 2   | H     | 601 | ATP  | PA-O3A  | 5.51 | 1.65        | 1.59     |
| 2   | C     | 601 | ATP  | PA-O3A  | 5.49 | 1.65        | 1.59     |
| 3   | A     | 603 | IMP  | C4-N3   | 5.48 | 1.46        | 1.35     |
| 2   | F     | 601 | ATP  | PA-O3A  | 5.47 | 1.65        | 1.59     |
| 3   | C     | 603 | IMP  | C4-N3   | 5.46 | 1.46        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | D     | 603 | IMP  | C4-N3   | 5.46  | 1.46        | 1.35     |
| 3   | G     | 603 | IMP  | C4-N3   | 5.46  | 1.46        | 1.35     |
| 2   | E     | 601 | ATP  | PA-O3A  | 5.44  | 1.65        | 1.59     |
| 3   | B     | 603 | IMP  | C4-N3   | 5.44  | 1.46        | 1.35     |
| 3   | E     | 603 | IMP  | C4-N3   | 5.44  | 1.46        | 1.35     |
| 3   | F     | 603 | IMP  | C4-N3   | 5.44  | 1.46        | 1.35     |
| 3   | H     | 603 | IMP  | C4-N3   | 5.44  | 1.46        | 1.35     |
| 2   | B     | 601 | ATP  | PA-O3A  | 5.42  | 1.65        | 1.59     |
| 4   | F     | 604 | NAD  | O4B-C1B | -5.13 | 1.30        | 1.42     |
| 4   | C     | 604 | NAD  | O4B-C1B | -5.12 | 1.30        | 1.42     |
| 4   | B     | 604 | NAD  | O4B-C1B | -5.09 | 1.30        | 1.42     |
| 4   | A     | 604 | NAD  | O4B-C1B | -5.08 | 1.30        | 1.42     |
| 4   | D     | 604 | NAD  | O4B-C1B | -5.08 | 1.30        | 1.42     |
| 4   | E     | 604 | NAD  | O4B-C1B | -5.08 | 1.30        | 1.42     |
| 4   | G     | 604 | NAD  | O4B-C1B | -5.08 | 1.30        | 1.42     |
| 4   | H     | 604 | NAD  | O4B-C1B | -5.08 | 1.30        | 1.42     |
| 2   | D     | 601 | ATP  | PB-O3A  | 4.95  | 1.64        | 1.59     |
| 2   | G     | 601 | ATP  | PB-O3A  | 4.95  | 1.64        | 1.59     |
| 2   | A     | 601 | ATP  | PB-O3A  | 4.94  | 1.64        | 1.59     |
| 2   | C     | 601 | ATP  | PB-O3A  | 4.90  | 1.64        | 1.59     |
| 2   | B     | 601 | ATP  | PB-O3A  | 4.86  | 1.64        | 1.59     |
| 2   | F     | 601 | ATP  | PB-O3A  | 4.86  | 1.64        | 1.59     |
| 2   | H     | 601 | ATP  | PB-O3A  | 4.86  | 1.64        | 1.59     |
| 2   | E     | 601 | ATP  | PB-O3A  | 4.86  | 1.64        | 1.59     |
| 2   | D     | 601 | ATP  | O4'-C1' | -4.62 | 1.31        | 1.42     |
| 2   | A     | 601 | ATP  | O4'-C1' | -4.60 | 1.31        | 1.42     |
| 2   | B     | 601 | ATP  | O4'-C1' | -4.59 | 1.31        | 1.42     |
| 2   | C     | 601 | ATP  | O4'-C1' | -4.59 | 1.31        | 1.42     |
| 2   | E     | 601 | ATP  | O4'-C1' | -4.59 | 1.31        | 1.42     |
| 2   | F     | 601 | ATP  | O4'-C1' | -4.59 | 1.31        | 1.42     |
| 2   | H     | 601 | ATP  | O4'-C1' | -4.58 | 1.31        | 1.42     |
| 2   | G     | 601 | ATP  | O4'-C1' | -4.57 | 1.31        | 1.42     |
| 3   | F     | 603 | IMP  | C2-N1   | 4.30  | 1.43        | 1.35     |
| 3   | D     | 603 | IMP  | C2-N1   | 4.27  | 1.42        | 1.35     |
| 3   | E     | 603 | IMP  | C2-N1   | 4.27  | 1.42        | 1.35     |
| 3   | C     | 603 | IMP  | C2-N1   | 4.26  | 1.42        | 1.35     |
| 3   | A     | 603 | IMP  | C2-N1   | 4.25  | 1.42        | 1.35     |
| 3   | B     | 603 | IMP  | C2-N1   | 4.25  | 1.42        | 1.35     |
| 3   | G     | 603 | IMP  | C2-N1   | 4.25  | 1.42        | 1.35     |
| 3   | H     | 603 | IMP  | C2-N1   | 4.25  | 1.42        | 1.35     |
| 4   | F     | 604 | NAD  | PA-O3   | 4.24  | 1.64        | 1.59     |
| 4   | C     | 604 | NAD  | C6A-N6A | 4.24  | 1.45        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | H     | 604 | NAD  | C6A-N6A | 4.24  | 1.45        | 1.34     |
| 4   | B     | 604 | NAD  | C6A-N6A | 4.23  | 1.45        | 1.34     |
| 4   | D     | 604 | NAD  | C6A-N6A | 4.23  | 1.45        | 1.34     |
| 4   | E     | 604 | NAD  | C6A-N6A | 4.23  | 1.45        | 1.34     |
| 4   | F     | 604 | NAD  | C6A-N6A | 4.23  | 1.45        | 1.34     |
| 4   | G     | 604 | NAD  | C6A-N6A | 4.23  | 1.45        | 1.34     |
| 4   | D     | 604 | NAD  | PA-O3   | 4.22  | 1.64        | 1.59     |
| 4   | A     | 604 | NAD  | C6A-N6A | 4.20  | 1.44        | 1.34     |
| 4   | A     | 604 | NAD  | PA-O3   | 4.18  | 1.64        | 1.59     |
| 2   | A     | 602 | ATP  | O4'-C1' | -4.17 | 1.32        | 1.42     |
| 2   | H     | 602 | ATP  | O4'-C1' | -4.16 | 1.32        | 1.42     |
| 4   | B     | 604 | NAD  | PA-O3   | 4.15  | 1.64        | 1.59     |
| 4   | C     | 604 | NAD  | PA-O3   | 4.15  | 1.64        | 1.59     |
| 4   | E     | 604 | NAD  | PA-O3   | 4.15  | 1.64        | 1.59     |
| 2   | B     | 602 | ATP  | O4'-C1' | -4.14 | 1.32        | 1.42     |
| 2   | C     | 602 | ATP  | O4'-C1' | -4.14 | 1.32        | 1.42     |
| 2   | D     | 602 | ATP  | O4'-C1' | -4.14 | 1.32        | 1.42     |
| 2   | E     | 602 | ATP  | O4'-C1' | -4.14 | 1.32        | 1.42     |
| 2   | F     | 602 | ATP  | O4'-C1' | -4.14 | 1.32        | 1.42     |
| 2   | G     | 602 | ATP  | O4'-C1' | -4.14 | 1.32        | 1.42     |
| 4   | H     | 604 | NAD  | PA-O3   | 4.11  | 1.63        | 1.59     |
| 4   | G     | 604 | NAD  | PA-O3   | 4.09  | 1.63        | 1.59     |
| 2   | D     | 602 | ATP  | C2'-C1' | 4.06  | 1.66        | 1.53     |
| 2   | G     | 602 | ATP  | C2'-C1' | 4.04  | 1.66        | 1.53     |
| 2   | B     | 602 | ATP  | C2'-C1' | 4.04  | 1.66        | 1.53     |
| 2   | E     | 602 | ATP  | C2'-C1' | 4.04  | 1.66        | 1.53     |
| 2   | H     | 602 | ATP  | C2'-C1' | 4.04  | 1.66        | 1.53     |
| 2   | C     | 602 | ATP  | C2'-C1' | 4.02  | 1.66        | 1.53     |
| 2   | A     | 602 | ATP  | C2'-C1' | 4.02  | 1.66        | 1.53     |
| 2   | F     | 602 | ATP  | C2'-C1' | 4.01  | 1.66        | 1.53     |
| 3   | C     | 603 | IMP  | C5-N7   | -3.97 | 1.31        | 1.39     |
| 3   | A     | 603 | IMP  | C5-N7   | -3.94 | 1.31        | 1.39     |
| 3   | G     | 603 | IMP  | C5-N7   | -3.94 | 1.31        | 1.39     |
| 3   | B     | 603 | IMP  | C5-N7   | -3.93 | 1.31        | 1.39     |
| 3   | E     | 603 | IMP  | C5-N7   | -3.93 | 1.31        | 1.39     |
| 3   | H     | 603 | IMP  | C5-N7   | -3.93 | 1.31        | 1.39     |
| 3   | D     | 603 | IMP  | C5-N7   | -3.91 | 1.31        | 1.39     |
| 3   | F     | 603 | IMP  | C5-N7   | -3.91 | 1.31        | 1.39     |
| 2   | A     | 601 | ATP  | C5'-C4' | -3.79 | 1.40        | 1.51     |
| 2   | B     | 601 | ATP  | C5'-C4' | -3.79 | 1.40        | 1.51     |
| 2   | C     | 601 | ATP  | C5'-C4' | -3.79 | 1.40        | 1.51     |
| 2   | D     | 601 | ATP  | C5'-C4' | -3.79 | 1.40        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 601 | ATP  | C5'-C4' | -3.79 | 1.40        | 1.51     |
| 2   | F     | 601 | ATP  | C5'-C4' | -3.79 | 1.40        | 1.51     |
| 2   | G     | 601 | ATP  | C5'-C4' | -3.79 | 1.40        | 1.51     |
| 2   | H     | 601 | ATP  | C5'-C4' | -3.78 | 1.40        | 1.51     |
| 2   | E     | 601 | ATP  | C6-N6   | 3.71  | 1.43        | 1.34     |
| 2   | B     | 601 | ATP  | C6-N6   | 3.71  | 1.43        | 1.34     |
| 2   | C     | 602 | ATP  | C5'-C4' | -3.70 | 1.40        | 1.51     |
| 2   | D     | 602 | ATP  | C5'-C4' | -3.69 | 1.40        | 1.51     |
| 2   | F     | 602 | ATP  | C5'-C4' | -3.69 | 1.40        | 1.51     |
| 2   | B     | 602 | ATP  | C5'-C4' | -3.68 | 1.40        | 1.51     |
| 2   | D     | 601 | ATP  | C6-N6   | 3.68  | 1.43        | 1.34     |
| 2   | C     | 601 | ATP  | C6-N6   | 3.67  | 1.43        | 1.34     |
| 2   | F     | 601 | ATP  | C6-N6   | 3.67  | 1.43        | 1.34     |
| 2   | A     | 602 | ATP  | C5'-C4' | -3.67 | 1.40        | 1.51     |
| 2   | E     | 602 | ATP  | C5'-C4' | -3.67 | 1.40        | 1.51     |
| 2   | G     | 602 | ATP  | C5'-C4' | -3.67 | 1.40        | 1.51     |
| 2   | H     | 602 | ATP  | C5'-C4' | -3.67 | 1.40        | 1.51     |
| 2   | A     | 601 | ATP  | C6-N6   | 3.67  | 1.43        | 1.34     |
| 2   | G     | 601 | ATP  | C6-N6   | 3.67  | 1.43        | 1.34     |
| 2   | H     | 601 | ATP  | C6-N6   | 3.67  | 1.43        | 1.34     |
| 2   | B     | 602 | ATP  | C6-N6   | 3.62  | 1.43        | 1.34     |
| 2   | A     | 602 | ATP  | C6-N6   | 3.62  | 1.43        | 1.34     |
| 2   | D     | 602 | ATP  | C6-N6   | 3.62  | 1.43        | 1.34     |
| 2   | D     | 601 | ATP  | C2'-C1' | 3.61  | 1.64        | 1.53     |
| 2   | F     | 601 | ATP  | C2'-C1' | 3.61  | 1.64        | 1.53     |
| 2   | G     | 601 | ATP  | C2'-C1' | 3.61  | 1.64        | 1.53     |
| 2   | A     | 601 | ATP  | C2'-C1' | 3.60  | 1.64        | 1.53     |
| 2   | C     | 601 | ATP  | C2'-C1' | 3.59  | 1.64        | 1.53     |
| 2   | H     | 601 | ATP  | C2'-C1' | 3.59  | 1.64        | 1.53     |
| 2   | E     | 602 | ATP  | C6-N6   | 3.59  | 1.43        | 1.34     |
| 2   | G     | 602 | ATP  | C6-N6   | 3.59  | 1.43        | 1.34     |
| 2   | H     | 602 | ATP  | C6-N6   | 3.59  | 1.43        | 1.34     |
| 2   | C     | 602 | ATP  | C6-N6   | 3.59  | 1.43        | 1.34     |
| 2   | F     | 602 | ATP  | C6-N6   | 3.59  | 1.43        | 1.34     |
| 2   | F     | 601 | ATP  | C5-C4   | -3.59 | 1.32        | 1.39     |
| 2   | H     | 601 | ATP  | C5-C4   | -3.59 | 1.32        | 1.39     |
| 2   | B     | 601 | ATP  | C2'-C1' | 3.59  | 1.64        | 1.53     |
| 2   | E     | 601 | ATP  | C2'-C1' | 3.59  | 1.64        | 1.53     |
| 2   | A     | 601 | ATP  | C5-C4   | -3.58 | 1.32        | 1.39     |
| 2   | D     | 601 | ATP  | C5-C4   | -3.57 | 1.32        | 1.39     |
| 2   | G     | 601 | ATP  | C5-C4   | -3.57 | 1.32        | 1.39     |
| 2   | B     | 601 | ATP  | C5-C4   | -3.54 | 1.32        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 601 | ATP  | C5-C4   | -3.53 | 1.32        | 1.39     |
| 2   | E     | 601 | ATP  | C5-C4   | -3.53 | 1.32        | 1.39     |
| 2   | B     | 602 | ATP  | C5-C4   | -3.47 | 1.32        | 1.39     |
| 2   | C     | 602 | ATP  | C5-C4   | -3.47 | 1.32        | 1.39     |
| 2   | E     | 602 | ATP  | C5-C4   | -3.47 | 1.32        | 1.39     |
| 2   | F     | 602 | ATP  | C5-C4   | -3.47 | 1.32        | 1.39     |
| 2   | G     | 602 | ATP  | C5-C4   | -3.47 | 1.32        | 1.39     |
| 2   | H     | 602 | ATP  | C5-C4   | -3.47 | 1.32        | 1.39     |
| 2   | A     | 602 | ATP  | C5-C4   | -3.45 | 1.32        | 1.39     |
| 2   | D     | 602 | ATP  | C5-C4   | -3.45 | 1.32        | 1.39     |
| 4   | H     | 604 | NAD  | PN-O3   | 3.43  | 1.63        | 1.59     |
| 4   | E     | 604 | NAD  | C5A-C4A | -3.39 | 1.33        | 1.39     |
| 4   | F     | 604 | NAD  | C5A-C4A | -3.39 | 1.33        | 1.39     |
| 4   | C     | 604 | NAD  | PN-O3   | 3.36  | 1.63        | 1.59     |
| 4   | F     | 604 | NAD  | PN-O3   | 3.36  | 1.63        | 1.59     |
| 4   | A     | 604 | NAD  | PN-O3   | 3.34  | 1.63        | 1.59     |
| 4   | D     | 604 | NAD  | PN-O3   | 3.34  | 1.63        | 1.59     |
| 4   | B     | 604 | NAD  | O7N-C7N | -3.34 | 1.17        | 1.24     |
| 4   | F     | 604 | NAD  | O7N-C7N | -3.34 | 1.17        | 1.24     |
| 4   | G     | 604 | NAD  | O7N-C7N | -3.34 | 1.17        | 1.24     |
| 4   | B     | 604 | NAD  | C5A-C4A | -3.34 | 1.33        | 1.39     |
| 4   | D     | 604 | NAD  | C5A-C4A | -3.34 | 1.33        | 1.39     |
| 4   | G     | 604 | NAD  | C5A-C4A | -3.34 | 1.33        | 1.39     |
| 4   | C     | 604 | NAD  | O7N-C7N | -3.34 | 1.17        | 1.24     |
| 4   | B     | 604 | NAD  | PN-O3   | 3.34  | 1.63        | 1.59     |
| 4   | E     | 604 | NAD  | PN-O3   | 3.34  | 1.63        | 1.59     |
| 4   | C     | 604 | NAD  | C5A-C4A | -3.34 | 1.33        | 1.39     |
| 4   | H     | 604 | NAD  | C5A-C4A | -3.33 | 1.33        | 1.39     |
| 4   | A     | 604 | NAD  | C5A-C4A | -3.32 | 1.33        | 1.39     |
| 4   | D     | 604 | NAD  | O7N-C7N | -3.32 | 1.17        | 1.24     |
| 4   | G     | 604 | NAD  | PN-O3   | 3.32  | 1.63        | 1.59     |
| 4   | A     | 604 | NAD  | O7N-C7N | -3.32 | 1.17        | 1.24     |
| 4   | H     | 604 | NAD  | O7N-C7N | -3.32 | 1.17        | 1.24     |
| 4   | E     | 604 | NAD  | O7N-C7N | -3.30 | 1.18        | 1.24     |
| 2   | D     | 602 | ATP  | PB-O3B  | 3.23  | 1.63        | 1.59     |
| 2   | B     | 601 | ATP  | C8-N9   | -3.23 | 1.32        | 1.37     |
| 2   | F     | 601 | ATP  | C8-N9   | -3.23 | 1.32        | 1.37     |
| 3   | D     | 603 | IMP  | O6-C6   | -3.23 | 1.17        | 1.23     |
| 2   | A     | 601 | ATP  | C8-N9   | -3.23 | 1.32        | 1.37     |
| 2   | E     | 601 | ATP  | C8-N9   | -3.23 | 1.32        | 1.37     |
| 2   | G     | 601 | ATP  | C8-N9   | -3.22 | 1.32        | 1.37     |
| 2   | C     | 601 | ATP  | C8-N9   | -3.19 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 604 | NAD  | O2D-C2D | -3.19 | 1.35        | 1.43     |
| 2   | H     | 601 | ATP  | C8-N9   | -3.19 | 1.32        | 1.37     |
| 3   | A     | 603 | IMP  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 3   | B     | 603 | IMP  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 3   | C     | 603 | IMP  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 3   | E     | 603 | IMP  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 3   | F     | 603 | IMP  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 3   | G     | 603 | IMP  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 3   | H     | 603 | IMP  | O6-C6   | -3.19 | 1.17        | 1.23     |
| 2   | D     | 601 | ATP  | C8-N9   | -3.18 | 1.32        | 1.37     |
| 4   | F     | 604 | NAD  | O2D-C2D | -3.17 | 1.35        | 1.43     |
| 4   | C     | 604 | NAD  | O2D-C2D | -3.16 | 1.35        | 1.43     |
| 4   | E     | 604 | NAD  | O2D-C2D | -3.16 | 1.35        | 1.43     |
| 4   | A     | 604 | NAD  | O2D-C2D | -3.16 | 1.35        | 1.43     |
| 3   | A     | 603 | IMP  | C4-N9   | -3.14 | 1.30        | 1.38     |
| 2   | G     | 602 | ATP  | PB-O3B  | 3.14  | 1.62        | 1.59     |
| 4   | B     | 604 | NAD  | O2D-C2D | -3.14 | 1.35        | 1.43     |
| 4   | G     | 604 | NAD  | O2D-C2D | -3.14 | 1.35        | 1.43     |
| 4   | H     | 604 | NAD  | O2D-C2D | -3.14 | 1.35        | 1.43     |
| 2   | A     | 602 | ATP  | PB-O3B  | 3.13  | 1.62        | 1.59     |
| 2   | H     | 602 | ATP  | PB-O3B  | 3.13  | 1.62        | 1.59     |
| 2   | C     | 602 | ATP  | PB-O3B  | 3.13  | 1.62        | 1.59     |
| 3   | B     | 603 | IMP  | C4-N9   | -3.12 | 1.30        | 1.38     |
| 3   | D     | 603 | IMP  | C4-N9   | -3.12 | 1.30        | 1.38     |
| 3   | E     | 603 | IMP  | C4-N9   | -3.12 | 1.30        | 1.38     |
| 3   | F     | 603 | IMP  | C4-N9   | -3.12 | 1.30        | 1.38     |
| 3   | G     | 603 | IMP  | C4-N9   | -3.12 | 1.30        | 1.38     |
| 3   | H     | 603 | IMP  | C4-N9   | -3.12 | 1.30        | 1.38     |
| 2   | B     | 602 | ATP  | PB-O3B  | 3.12  | 1.62        | 1.59     |
| 2   | E     | 602 | ATP  | PB-O3B  | 3.12  | 1.62        | 1.59     |
| 2   | F     | 602 | ATP  | PB-O3B  | 3.12  | 1.62        | 1.59     |
| 3   | C     | 603 | IMP  | C4-N9   | -3.12 | 1.30        | 1.38     |
| 4   | B     | 604 | NAD  | O2B-C2B | -3.06 | 1.35        | 1.43     |
| 4   | C     | 604 | NAD  | O2B-C2B | -3.06 | 1.35        | 1.43     |
| 4   | F     | 604 | NAD  | O2B-C2B | -3.06 | 1.35        | 1.43     |
| 4   | A     | 604 | NAD  | O2B-C2B | -3.05 | 1.35        | 1.43     |
| 4   | D     | 604 | NAD  | O2B-C2B | -3.05 | 1.35        | 1.43     |
| 4   | E     | 604 | NAD  | O2B-C2B | -3.05 | 1.35        | 1.43     |
| 4   | G     | 604 | NAD  | O2B-C2B | -3.05 | 1.35        | 1.43     |
| 4   | H     | 604 | NAD  | O2B-C2B | -3.05 | 1.35        | 1.43     |
| 2   | F     | 601 | ATP  | O3'-C3' | 2.97  | 1.50        | 1.43     |
| 2   | A     | 601 | ATP  | O3'-C3' | 2.95  | 1.50        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 601 | ATP  | O3'-C3' | 2.95  | 1.50        | 1.43     |
| 2   | H     | 601 | ATP  | O3'-C3' | 2.95  | 1.50        | 1.43     |
| 2   | B     | 601 | ATP  | O3'-C3' | 2.94  | 1.50        | 1.43     |
| 2   | C     | 601 | ATP  | O3'-C3' | 2.94  | 1.50        | 1.43     |
| 2   | E     | 601 | ATP  | O3'-C3' | 2.94  | 1.50        | 1.43     |
| 2   | G     | 601 | ATP  | O3'-C3' | 2.94  | 1.50        | 1.43     |
| 4   | A     | 604 | NAD  | C5A-N7A | -2.93 | 1.33        | 1.39     |
| 4   | D     | 604 | NAD  | C5A-N7A | -2.93 | 1.33        | 1.39     |
| 4   | G     | 604 | NAD  | C5A-N7A | -2.93 | 1.33        | 1.39     |
| 4   | H     | 604 | NAD  | C5A-N7A | -2.93 | 1.33        | 1.39     |
| 4   | B     | 604 | NAD  | C5A-N7A | -2.92 | 1.33        | 1.39     |
| 4   | C     | 604 | NAD  | C5A-N7A | -2.92 | 1.33        | 1.39     |
| 2   | B     | 602 | ATP  | O3'-C3' | 2.91  | 1.50        | 1.43     |
| 2   | E     | 602 | ATP  | O3'-C3' | 2.91  | 1.50        | 1.43     |
| 2   | D     | 602 | ATP  | O3'-C3' | 2.90  | 1.50        | 1.43     |
| 2   | F     | 602 | ATP  | O3'-C3' | 2.90  | 1.50        | 1.43     |
| 2   | G     | 602 | ATP  | O3'-C3' | 2.90  | 1.50        | 1.43     |
| 2   | H     | 602 | ATP  | O3'-C3' | 2.90  | 1.50        | 1.43     |
| 2   | A     | 602 | ATP  | O3'-C3' | 2.89  | 1.50        | 1.43     |
| 2   | E     | 601 | ATP  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 2   | A     | 601 | ATP  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 2   | C     | 601 | ATP  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 2   | D     | 601 | ATP  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 2   | F     | 601 | ATP  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 2   | G     | 601 | ATP  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 2   | C     | 602 | ATP  | O3'-C3' | 2.86  | 1.50        | 1.43     |
| 4   | E     | 604 | NAD  | C5A-N7A | -2.85 | 1.33        | 1.39     |
| 4   | F     | 604 | NAD  | C5A-N7A | -2.85 | 1.33        | 1.39     |
| 4   | C     | 604 | NAD  | C8A-N9A | -2.84 | 1.32        | 1.37     |
| 4   | F     | 604 | NAD  | C8A-N9A | -2.84 | 1.32        | 1.37     |
| 2   | G     | 602 | ATP  | PA-O5'  | 2.83  | 1.70        | 1.59     |
| 2   | B     | 601 | ATP  | C5-N7   | -2.83 | 1.33        | 1.39     |
| 2   | B     | 602 | ATP  | PA-O5'  | 2.83  | 1.70        | 1.59     |
| 2   | C     | 602 | ATP  | C3'-C4' | 2.83  | 1.60        | 1.53     |
| 2   | H     | 601 | ATP  | C5-N7   | -2.83 | 1.33        | 1.39     |
| 2   | H     | 601 | ATP  | PA-O5'  | 2.83  | 1.70        | 1.59     |
| 2   | C     | 601 | ATP  | PA-O5'  | 2.82  | 1.70        | 1.59     |
| 2   | B     | 602 | ATP  | C3'-C4' | 2.82  | 1.60        | 1.53     |
| 2   | A     | 602 | ATP  | PA-O5'  | 2.82  | 1.70        | 1.59     |
| 2   | A     | 602 | ATP  | C8-N9   | -2.82 | 1.32        | 1.37     |
| 2   | D     | 602 | ATP  | C8-N9   | -2.82 | 1.32        | 1.37     |
| 2   | G     | 602 | ATP  | C8-N9   | -2.82 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 601 | ATP  | PA-O5'  | 2.82  | 1.70        | 1.59     |
| 2   | D     | 602 | ATP  | PA-O5'  | 2.82  | 1.70        | 1.59     |
| 2   | C     | 602 | ATP  | PA-O5'  | 2.81  | 1.70        | 1.59     |
| 2   | E     | 602 | ATP  | PA-O5'  | 2.81  | 1.70        | 1.59     |
| 2   | F     | 602 | ATP  | PA-O5'  | 2.81  | 1.70        | 1.59     |
| 2   | D     | 601 | ATP  | PA-O5'  | 2.81  | 1.70        | 1.59     |
| 4   | H     | 604 | NAD  | C8A-N9A | -2.81 | 1.32        | 1.37     |
| 2   | A     | 601 | ATP  | PA-O5'  | 2.80  | 1.70        | 1.59     |
| 2   | E     | 601 | ATP  | PA-O5'  | 2.80  | 1.70        | 1.59     |
| 2   | G     | 601 | ATP  | PA-O5'  | 2.80  | 1.70        | 1.59     |
| 2   | H     | 602 | ATP  | PA-O5'  | 2.80  | 1.70        | 1.59     |
| 2   | F     | 601 | ATP  | PA-O5'  | 2.80  | 1.70        | 1.59     |
| 4   | B     | 604 | NAD  | C8A-N9A | -2.79 | 1.32        | 1.37     |
| 2   | A     | 602 | ATP  | C3'-C4' | 2.78  | 1.60        | 1.53     |
| 2   | E     | 602 | ATP  | C3'-C4' | 2.78  | 1.60        | 1.53     |
| 2   | F     | 602 | ATP  | C3'-C4' | 2.78  | 1.60        | 1.53     |
| 2   | D     | 602 | ATP  | C3'-C4' | 2.78  | 1.60        | 1.53     |
| 2   | G     | 602 | ATP  | C3'-C4' | 2.78  | 1.60        | 1.53     |
| 2   | H     | 602 | ATP  | C3'-C4' | 2.78  | 1.60        | 1.53     |
| 4   | A     | 604 | NAD  | C3N-C7N | 2.78  | 1.54        | 1.50     |
| 4   | H     | 604 | NAD  | C3N-C7N | 2.78  | 1.54        | 1.50     |
| 2   | B     | 602 | ATP  | C8-N9   | -2.78 | 1.32        | 1.37     |
| 2   | C     | 602 | ATP  | C8-N9   | -2.78 | 1.32        | 1.37     |
| 2   | F     | 602 | ATP  | C8-N9   | -2.78 | 1.32        | 1.37     |
| 4   | A     | 604 | NAD  | C8A-N9A | -2.77 | 1.32        | 1.37     |
| 4   | D     | 604 | NAD  | C8A-N9A | -2.77 | 1.32        | 1.37     |
| 4   | E     | 604 | NAD  | C8A-N9A | -2.77 | 1.32        | 1.37     |
| 4   | G     | 604 | NAD  | C8A-N9A | -2.77 | 1.32        | 1.37     |
| 2   | E     | 602 | ATP  | C8-N9   | -2.76 | 1.32        | 1.37     |
| 4   | B     | 604 | NAD  | C3N-C7N | 2.76  | 1.54        | 1.50     |
| 4   | D     | 604 | NAD  | C3N-C7N | 2.76  | 1.54        | 1.50     |
| 4   | F     | 604 | NAD  | C3N-C7N | 2.76  | 1.54        | 1.50     |
| 4   | C     | 604 | NAD  | C3N-C7N | 2.76  | 1.54        | 1.50     |
| 2   | H     | 602 | ATP  | C8-N9   | -2.74 | 1.32        | 1.37     |
| 4   | G     | 604 | NAD  | C3N-C7N | 2.73  | 1.54        | 1.50     |
| 4   | E     | 604 | NAD  | C3N-C7N | 2.73  | 1.54        | 1.50     |
| 4   | A     | 604 | NAD  | C4N-C3N | -2.72 | 1.35        | 1.39     |
| 4   | G     | 604 | NAD  | C4N-C3N | -2.72 | 1.35        | 1.39     |
| 4   | H     | 604 | NAD  | C4N-C3N | -2.72 | 1.35        | 1.39     |
| 4   | B     | 604 | NAD  | C4N-C3N | -2.70 | 1.35        | 1.39     |
| 4   | D     | 604 | NAD  | C4N-C3N | -2.70 | 1.35        | 1.39     |
| 4   | E     | 604 | NAD  | C4N-C3N | -2.70 | 1.35        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | F     | 604 | NAD  | C4N-C3N | -2.70 | 1.35        | 1.39     |
| 2   | B     | 602 | ATP  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 2   | E     | 602 | ATP  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 2   | A     | 602 | ATP  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 2   | G     | 602 | ATP  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 2   | H     | 602 | ATP  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 2   | B     | 602 | ATP  | O4'-C4' | 2.66  | 1.50        | 1.45     |
| 2   | E     | 602 | ATP  | O4'-C4' | 2.66  | 1.50        | 1.45     |
| 2   | F     | 602 | ATP  | O4'-C4' | 2.66  | 1.50        | 1.45     |
| 2   | H     | 602 | ATP  | O4'-C4' | 2.66  | 1.50        | 1.45     |
| 2   | D     | 602 | ATP  | O4'-C4' | 2.66  | 1.50        | 1.45     |
| 2   | C     | 602 | ATP  | C5-N7   | -2.66 | 1.34        | 1.39     |
| 2   | A     | 602 | ATP  | O4'-C4' | 2.64  | 1.50        | 1.45     |
| 2   | D     | 602 | ATP  | C5-N7   | -2.64 | 1.34        | 1.39     |
| 2   | F     | 602 | ATP  | C5-N7   | -2.64 | 1.34        | 1.39     |
| 2   | B     | 601 | ATP  | C3'-C4' | 2.63  | 1.59        | 1.53     |
| 2   | C     | 601 | ATP  | C3'-C4' | 2.63  | 1.59        | 1.53     |
| 2   | E     | 601 | ATP  | C3'-C4' | 2.63  | 1.59        | 1.53     |
| 2   | G     | 601 | ATP  | C3'-C4' | 2.63  | 1.59        | 1.53     |
| 2   | A     | 601 | ATP  | C3'-C4' | 2.63  | 1.59        | 1.53     |
| 2   | D     | 601 | ATP  | C3'-C4' | 2.63  | 1.59        | 1.53     |
| 2   | F     | 601 | ATP  | C3'-C4' | 2.63  | 1.59        | 1.53     |
| 4   | C     | 604 | NAD  | C4N-C3N | -2.62 | 1.35        | 1.39     |
| 2   | C     | 602 | ATP  | O4'-C4' | 2.61  | 1.50        | 1.45     |
| 2   | G     | 602 | ATP  | O4'-C4' | 2.61  | 1.50        | 1.45     |
| 2   | H     | 601 | ATP  | C3'-C4' | 2.59  | 1.59        | 1.53     |
| 4   | F     | 604 | NAD  | O3B-C3B | 2.54  | 1.49        | 1.43     |
| 4   | H     | 604 | NAD  | O3B-C3B | 2.54  | 1.49        | 1.43     |
| 2   | A     | 601 | ATP  | O4'-C4' | 2.54  | 1.50        | 1.45     |
| 2   | H     | 601 | ATP  | O4'-C4' | 2.54  | 1.50        | 1.45     |
| 2   | C     | 601 | ATP  | PB-O3B  | 2.54  | 1.62        | 1.59     |
| 2   | E     | 601 | ATP  | PB-O3B  | 2.54  | 1.62        | 1.59     |
| 4   | A     | 604 | NAD  | O3B-C3B | 2.53  | 1.49        | 1.43     |
| 2   | D     | 601 | ATP  | O4'-C4' | 2.53  | 1.50        | 1.45     |
| 2   | E     | 601 | ATP  | O4'-C4' | 2.53  | 1.50        | 1.45     |
| 2   | F     | 601 | ATP  | O4'-C4' | 2.53  | 1.50        | 1.45     |
| 4   | E     | 604 | NAD  | O3B-C3B | 2.52  | 1.49        | 1.43     |
| 2   | A     | 601 | ATP  | PB-O3B  | 2.51  | 1.62        | 1.59     |
| 2   | G     | 601 | ATP  | PB-O3B  | 2.51  | 1.62        | 1.59     |
| 2   | H     | 601 | ATP  | PB-O3B  | 2.51  | 1.62        | 1.59     |
| 4   | B     | 604 | NAD  | O3B-C3B | 2.51  | 1.49        | 1.43     |
| 4   | C     | 604 | NAD  | O3B-C3B | 2.51  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 604 | NAD  | O3B-C3B | 2.51  | 1.49        | 1.43     |
| 4   | G     | 604 | NAD  | O3B-C3B | 2.51  | 1.49        | 1.43     |
| 2   | G     | 601 | ATP  | O4'-C4' | 2.51  | 1.50        | 1.45     |
| 2   | H     | 601 | ATP  | C1'-N9  | -2.50 | 1.39        | 1.46     |
| 2   | B     | 601 | ATP  | O4'-C4' | 2.49  | 1.50        | 1.45     |
| 2   | C     | 601 | ATP  | O4'-C4' | 2.49  | 1.50        | 1.45     |
| 2   | F     | 601 | ATP  | PB-O3B  | 2.47  | 1.62        | 1.59     |
| 2   | C     | 601 | ATP  | C1'-N9  | -2.47 | 1.39        | 1.46     |
| 2   | D     | 601 | ATP  | C1'-N9  | -2.47 | 1.39        | 1.46     |
| 2   | E     | 601 | ATP  | C1'-N9  | -2.47 | 1.39        | 1.46     |
| 2   | G     | 601 | ATP  | C1'-N9  | -2.47 | 1.39        | 1.46     |
| 2   | A     | 601 | ATP  | C1'-N9  | -2.46 | 1.39        | 1.46     |
| 2   | B     | 601 | ATP  | C1'-N9  | -2.46 | 1.39        | 1.46     |
| 2   | F     | 601 | ATP  | C1'-N9  | -2.46 | 1.39        | 1.46     |
| 4   | C     | 604 | NAD  | O3D-C3D | 2.45  | 1.49        | 1.43     |
| 4   | H     | 604 | NAD  | O3D-C3D | 2.45  | 1.49        | 1.43     |
| 2   | D     | 601 | ATP  | PB-O3B  | 2.45  | 1.62        | 1.59     |
| 4   | D     | 604 | NAD  | O3D-C3D | 2.43  | 1.49        | 1.43     |
| 4   | B     | 604 | NAD  | O3D-C3D | 2.43  | 1.49        | 1.43     |
| 4   | A     | 604 | NAD  | O3D-C3D | 2.41  | 1.48        | 1.43     |
| 4   | G     | 604 | NAD  | O3D-C3D | 2.41  | 1.48        | 1.43     |
| 2   | B     | 601 | ATP  | PB-O3B  | 2.41  | 1.62        | 1.59     |
| 4   | E     | 604 | NAD  | O3D-C3D | 2.41  | 1.48        | 1.43     |
| 4   | F     | 604 | NAD  | O3D-C3D | 2.41  | 1.48        | 1.43     |
| 4   | A     | 604 | NAD  | C4A-N9A | -2.36 | 1.32        | 1.37     |
| 4   | B     | 604 | NAD  | C4A-N9A | -2.36 | 1.32        | 1.37     |
| 4   | C     | 604 | NAD  | C4A-N9A | -2.36 | 1.32        | 1.37     |
| 4   | F     | 604 | NAD  | C4A-N9A | -2.36 | 1.32        | 1.37     |
| 4   | H     | 604 | NAD  | C4A-N9A | -2.36 | 1.32        | 1.37     |
| 4   | E     | 604 | NAD  | C4A-N9A | -2.36 | 1.32        | 1.37     |
| 4   | D     | 604 | NAD  | C4A-N9A | -2.32 | 1.32        | 1.37     |
| 4   | G     | 604 | NAD  | C4A-N9A | -2.32 | 1.32        | 1.37     |
| 2   | D     | 602 | ATP  | O2'-C2' | 2.28  | 1.48        | 1.43     |
| 2   | F     | 602 | ATP  | O2'-C2' | 2.28  | 1.48        | 1.43     |
| 2   | A     | 602 | ATP  | O2'-C2' | 2.28  | 1.48        | 1.43     |
| 2   | B     | 602 | ATP  | O2'-C2' | 2.27  | 1.48        | 1.43     |
| 2   | C     | 602 | ATP  | O2'-C2' | 2.27  | 1.48        | 1.43     |
| 2   | H     | 602 | ATP  | O2'-C2' | 2.27  | 1.48        | 1.43     |
| 2   | E     | 602 | ATP  | O2'-C2' | 2.25  | 1.48        | 1.43     |
| 2   | G     | 602 | ATP  | O2'-C2' | 2.23  | 1.48        | 1.43     |
| 3   | A     | 603 | IMP  | C8-N9   | -2.09 | 1.32        | 1.37     |
| 3   | B     | 603 | IMP  | C8-N9   | -2.09 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | G     | 603 | IMP  | C8-N9   | -2.09 | 1.32        | 1.37     |
| 3   | H     | 603 | IMP  | C8-N9   | -2.09 | 1.32        | 1.37     |
| 3   | E     | 603 | IMP  | C8-N9   | -2.07 | 1.32        | 1.37     |
| 3   | F     | 603 | IMP  | C8-N9   | -2.06 | 1.32        | 1.37     |
| 3   | D     | 603 | IMP  | C8-N9   | -2.06 | 1.32        | 1.37     |
| 2   | A     | 601 | ATP  | O2'-C2' | 2.04  | 1.48        | 1.43     |
| 2   | B     | 601 | ATP  | O2'-C2' | 2.04  | 1.48        | 1.43     |
| 2   | E     | 601 | ATP  | O2'-C2' | 2.04  | 1.48        | 1.43     |
| 2   | G     | 601 | ATP  | O2'-C2' | 2.04  | 1.48        | 1.43     |
| 3   | C     | 603 | IMP  | C8-N9   | -2.04 | 1.32        | 1.37     |
| 2   | H     | 602 | ATP  | C1'-N9  | -2.03 | 1.40        | 1.46     |
| 2   | B     | 602 | ATP  | C1'-N9  | -2.03 | 1.40        | 1.46     |
| 2   | D     | 602 | ATP  | C1'-N9  | -2.03 | 1.40        | 1.46     |
| 2   | E     | 602 | ATP  | C1'-N9  | -2.03 | 1.40        | 1.46     |
| 2   | F     | 602 | ATP  | C1'-N9  | -2.03 | 1.40        | 1.46     |
| 2   | D     | 601 | ATP  | O2'-C2' | 2.02  | 1.48        | 1.43     |
| 2   | C     | 601 | ATP  | O2'-C2' | 2.01  | 1.47        | 1.43     |
| 2   | E     | 601 | ATP  | C4-N9   | -2.00 | 1.33        | 1.37     |

All (415) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | E     | 601 | ATP  | N6-C6-N1 | -9.54 | 97.13       | 118.38   |
| 2   | B     | 601 | ATP  | N6-C6-N1 | -9.52 | 97.17       | 118.38   |
| 2   | F     | 601 | ATP  | N6-C6-N1 | -9.52 | 97.18       | 118.38   |
| 2   | A     | 601 | ATP  | N6-C6-N1 | -9.51 | 97.20       | 118.38   |
| 2   | H     | 601 | ATP  | N6-C6-N1 | -9.51 | 97.20       | 118.38   |
| 2   | C     | 601 | ATP  | N6-C6-N1 | -9.50 | 97.21       | 118.38   |
| 2   | D     | 601 | ATP  | N6-C6-N1 | -9.50 | 97.22       | 118.38   |
| 2   | G     | 601 | ATP  | N6-C6-N1 | -9.48 | 97.26       | 118.38   |
| 2   | E     | 602 | ATP  | N6-C6-N1 | -9.38 | 97.49       | 118.38   |
| 2   | A     | 602 | ATP  | N6-C6-N1 | -9.38 | 97.49       | 118.38   |
| 2   | D     | 602 | ATP  | N6-C6-N1 | -9.38 | 97.49       | 118.38   |
| 2   | G     | 602 | ATP  | N6-C6-N1 | -9.37 | 97.52       | 118.38   |
| 2   | H     | 602 | ATP  | N6-C6-N1 | -9.37 | 97.52       | 118.38   |
| 2   | B     | 602 | ATP  | N6-C6-N1 | -9.36 | 97.54       | 118.38   |
| 2   | F     | 602 | ATP  | N6-C6-N1 | -9.35 | 97.55       | 118.38   |
| 2   | C     | 602 | ATP  | N6-C6-N1 | -9.35 | 97.55       | 118.38   |
| 2   | F     | 601 | ATP  | C5-C6-N6 | 7.88  | 142.79      | 123.29   |
| 2   | C     | 601 | ATP  | C5-C6-N6 | 7.88  | 142.79      | 123.29   |
| 2   | D     | 601 | ATP  | C5-C6-N6 | 7.88  | 142.79      | 123.29   |
| 2   | H     | 601 | ATP  | C5-C6-N6 | 7.87  | 142.78      | 123.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 601 | ATP  | C5-C6-N6    | 7.87  | 142.78      | 123.29   |
| 2   | A     | 601 | ATP  | C5-C6-N6    | 7.86  | 142.75      | 123.29   |
| 2   | G     | 601 | ATP  | C5-C6-N6    | 7.86  | 142.75      | 123.29   |
| 2   | E     | 601 | ATP  | C5-C6-N6    | 7.86  | 142.74      | 123.29   |
| 2   | D     | 602 | ATP  | C5-C6-N6    | 7.60  | 142.11      | 123.29   |
| 2   | E     | 602 | ATP  | C5-C6-N6    | 7.59  | 142.09      | 123.29   |
| 2   | G     | 602 | ATP  | C5-C6-N6    | 7.59  | 142.08      | 123.29   |
| 2   | H     | 602 | ATP  | C5-C6-N6    | 7.59  | 142.08      | 123.29   |
| 2   | C     | 602 | ATP  | C5-C6-N6    | 7.58  | 142.06      | 123.29   |
| 2   | F     | 602 | ATP  | C5-C6-N6    | 7.58  | 142.06      | 123.29   |
| 2   | A     | 602 | ATP  | C5-C6-N6    | 7.58  | 142.05      | 123.29   |
| 2   | B     | 602 | ATP  | C5-C6-N6    | 7.57  | 142.04      | 123.29   |
| 2   | B     | 601 | ATP  | C4-N9-C1'   | -7.29 | 109.59      | 126.63   |
| 2   | F     | 601 | ATP  | C4-N9-C1'   | -7.29 | 109.59      | 126.63   |
| 2   | C     | 601 | ATP  | C4-N9-C1'   | -7.27 | 109.63      | 126.63   |
| 2   | D     | 601 | ATP  | C4-N9-C1'   | -7.27 | 109.63      | 126.63   |
| 2   | G     | 601 | ATP  | C4-N9-C1'   | -7.27 | 109.63      | 126.63   |
| 2   | E     | 601 | ATP  | C4-N9-C1'   | -7.26 | 109.66      | 126.63   |
| 2   | H     | 601 | ATP  | C4-N9-C1'   | -7.25 | 109.69      | 126.63   |
| 2   | A     | 601 | ATP  | C4-N9-C1'   | -7.24 | 109.69      | 126.63   |
| 4   | C     | 604 | NAD  | N6A-C6A-N1A | -6.98 | 102.82      | 118.38   |
| 4   | B     | 604 | NAD  | N6A-C6A-N1A | -6.96 | 102.87      | 118.38   |
| 4   | A     | 604 | NAD  | N6A-C6A-N1A | -6.95 | 102.89      | 118.38   |
| 4   | D     | 604 | NAD  | N6A-C6A-N1A | -6.95 | 102.89      | 118.38   |
| 4   | G     | 604 | NAD  | N6A-C6A-N1A | -6.95 | 102.89      | 118.38   |
| 4   | E     | 604 | NAD  | N6A-C6A-N1A | -6.95 | 102.90      | 118.38   |
| 4   | F     | 604 | NAD  | N6A-C6A-N1A | -6.95 | 102.90      | 118.38   |
| 4   | H     | 604 | NAD  | N6A-C6A-N1A | -6.95 | 102.90      | 118.38   |
| 2   | G     | 602 | ATP  | C4-N9-C1'   | -6.89 | 110.51      | 126.63   |
| 2   | A     | 602 | ATP  | C4-N9-C1'   | -6.89 | 110.52      | 126.63   |
| 2   | D     | 602 | ATP  | C4-N9-C1'   | -6.87 | 110.55      | 126.63   |
| 2   | C     | 602 | ATP  | C4-N9-C1'   | -6.87 | 110.57      | 126.63   |
| 2   | B     | 602 | ATP  | C4-N9-C1'   | -6.86 | 110.58      | 126.63   |
| 2   | E     | 602 | ATP  | C4-N9-C1'   | -6.86 | 110.58      | 126.63   |
| 2   | F     | 602 | ATP  | C4-N9-C1'   | -6.86 | 110.58      | 126.63   |
| 2   | H     | 602 | ATP  | C4-N9-C1'   | -6.86 | 110.59      | 126.63   |
| 3   | C     | 603 | IMP  | C5-C6-N1    | 6.78  | 120.53      | 110.78   |
| 3   | A     | 603 | IMP  | C5-C6-N1    | 6.78  | 120.52      | 110.78   |
| 3   | G     | 603 | IMP  | C5-C6-N1    | 6.77  | 120.51      | 110.78   |
| 3   | E     | 603 | IMP  | C5-C6-N1    | 6.76  | 120.50      | 110.78   |
| 4   | F     | 604 | NAD  | C4D-O4D-C1D | -6.76 | 103.73      | 109.92   |
| 3   | B     | 603 | IMP  | C5-C6-N1    | 6.76  | 120.50      | 110.78   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | H     | 604 | NAD  | C4D-O4D-C1D | -6.76 | 103.74      | 109.92   |
| 4   | C     | 604 | NAD  | C4D-O4D-C1D | -6.75 | 103.75      | 109.92   |
| 3   | F     | 603 | IMP  | C5-C6-N1    | 6.75  | 120.48      | 110.78   |
| 3   | H     | 603 | IMP  | C5-C6-N1    | 6.74  | 120.47      | 110.78   |
| 3   | D     | 603 | IMP  | C5-C6-N1    | 6.73  | 120.45      | 110.78   |
| 4   | E     | 604 | NAD  | C4D-O4D-C1D | -6.72 | 103.77      | 109.92   |
| 4   | G     | 604 | NAD  | C4D-O4D-C1D | -6.69 | 103.79      | 109.92   |
| 4   | B     | 604 | NAD  | C4D-O4D-C1D | -6.69 | 103.80      | 109.92   |
| 4   | A     | 604 | NAD  | C4D-O4D-C1D | -6.68 | 103.81      | 109.92   |
| 4   | D     | 604 | NAD  | C4D-O4D-C1D | -6.68 | 103.81      | 109.92   |
| 4   | C     | 604 | NAD  | C4A-N9A-C1B | -6.54 | 111.33      | 126.63   |
| 4   | F     | 604 | NAD  | C4A-N9A-C1B | -6.54 | 111.33      | 126.63   |
| 4   | H     | 604 | NAD  | C4A-N9A-C1B | -6.54 | 111.33      | 126.63   |
| 4   | D     | 604 | NAD  | C4A-N9A-C1B | -6.54 | 111.34      | 126.63   |
| 4   | G     | 604 | NAD  | C4A-N9A-C1B | -6.54 | 111.34      | 126.63   |
| 4   | B     | 604 | NAD  | C4A-N9A-C1B | -6.54 | 111.34      | 126.63   |
| 4   | A     | 604 | NAD  | C4A-N9A-C1B | -6.54 | 111.35      | 126.63   |
| 4   | E     | 604 | NAD  | C4A-N9A-C1B | -6.52 | 111.39      | 126.63   |
| 2   | D     | 602 | ATP  | N3-C2-N1    | -6.09 | 119.36      | 128.58   |
| 2   | G     | 602 | ATP  | N3-C2-N1    | -6.08 | 119.38      | 128.58   |
| 2   | C     | 602 | ATP  | N3-C2-N1    | -6.08 | 119.38      | 128.58   |
| 2   | A     | 602 | ATP  | N3-C2-N1    | -6.08 | 119.38      | 128.58   |
| 2   | H     | 602 | ATP  | N3-C2-N1    | -6.07 | 119.39      | 128.58   |
| 2   | F     | 602 | ATP  | N3-C2-N1    | -6.06 | 119.41      | 128.58   |
| 2   | E     | 602 | ATP  | N3-C2-N1    | -6.06 | 119.42      | 128.58   |
| 2   | B     | 602 | ATP  | N3-C2-N1    | -6.05 | 119.43      | 128.58   |
| 2   | G     | 601 | ATP  | N9-C8-N7    | -5.90 | 105.56      | 113.94   |
| 2   | D     | 601 | ATP  | N9-C8-N7    | -5.89 | 105.58      | 113.94   |
| 2   | C     | 601 | ATP  | N9-C8-N7    | -5.88 | 105.59      | 113.94   |
| 2   | A     | 601 | ATP  | N9-C8-N7    | -5.87 | 105.60      | 113.94   |
| 2   | E     | 601 | ATP  | N9-C8-N7    | -5.87 | 105.60      | 113.94   |
| 2   | F     | 601 | ATP  | N9-C8-N7    | -5.87 | 105.60      | 113.94   |
| 2   | H     | 601 | ATP  | N9-C8-N7    | -5.87 | 105.61      | 113.94   |
| 2   | F     | 601 | ATP  | N3-C2-N1    | -5.85 | 119.72      | 128.58   |
| 2   | B     | 601 | ATP  | N9-C8-N7    | -5.85 | 105.64      | 113.94   |
| 2   | C     | 601 | ATP  | N3-C2-N1    | -5.83 | 119.75      | 128.58   |
| 2   | D     | 601 | ATP  | N3-C2-N1    | -5.83 | 119.75      | 128.58   |
| 2   | G     | 601 | ATP  | N3-C2-N1    | -5.83 | 119.75      | 128.58   |
| 2   | A     | 601 | ATP  | N3-C2-N1    | -5.79 | 119.82      | 128.58   |
| 2   | H     | 601 | ATP  | N3-C2-N1    | -5.79 | 119.82      | 128.58   |
| 2   | B     | 601 | ATP  | N3-C2-N1    | -5.79 | 119.82      | 128.58   |
| 2   | E     | 601 | ATP  | N3-C2-N1    | -5.78 | 119.83      | 128.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | F     | 604 | NAD  | N3A-C2A-N1A | -5.71 | 119.95      | 128.58   |
| 4   | C     | 604 | NAD  | N3A-C2A-N1A | -5.69 | 119.97      | 128.58   |
| 4   | E     | 604 | NAD  | N3A-C2A-N1A | -5.69 | 119.97      | 128.58   |
| 4   | H     | 604 | NAD  | N3A-C2A-N1A | -5.68 | 119.98      | 128.58   |
| 4   | A     | 604 | NAD  | N3A-C2A-N1A | -5.67 | 119.99      | 128.58   |
| 4   | G     | 604 | NAD  | N3A-C2A-N1A | -5.67 | 120.00      | 128.58   |
| 4   | D     | 604 | NAD  | N3A-C2A-N1A | -5.67 | 120.00      | 128.58   |
| 4   | B     | 604 | NAD  | N3A-C2A-N1A | -5.65 | 120.03      | 128.58   |
| 4   | C     | 604 | NAD  | C3N-C7N-N7N | 5.58  | 124.61      | 117.74   |
| 4   | E     | 604 | NAD  | C3N-C7N-N7N | 5.57  | 124.61      | 117.74   |
| 4   | D     | 604 | NAD  | C3N-C7N-N7N | 5.57  | 124.61      | 117.74   |
| 4   | H     | 604 | NAD  | C3N-C7N-N7N | 5.57  | 124.61      | 117.74   |
| 4   | F     | 604 | NAD  | C3N-C7N-N7N | 5.55  | 124.58      | 117.74   |
| 4   | B     | 604 | NAD  | C3N-C7N-N7N | 5.55  | 124.58      | 117.74   |
| 4   | C     | 604 | NAD  | C5A-C6A-N6A | 5.55  | 137.03      | 123.29   |
| 4   | G     | 604 | NAD  | C3N-C7N-N7N | 5.55  | 124.58      | 117.74   |
| 2   | B     | 601 | ATP  | C1'-N9-C8   | 5.55  | 139.41      | 127.09   |
| 2   | F     | 601 | ATP  | C1'-N9-C8   | 5.55  | 139.41      | 127.09   |
| 4   | E     | 604 | NAD  | C5A-C6A-N6A | 5.55  | 137.02      | 123.29   |
| 4   | F     | 604 | NAD  | C5A-C6A-N6A | 5.55  | 137.02      | 123.29   |
| 4   | A     | 604 | NAD  | C3N-C7N-N7N | 5.53  | 124.55      | 117.74   |
| 4   | A     | 604 | NAD  | C5A-C6A-N6A | 5.53  | 136.97      | 123.29   |
| 2   | B     | 602 | ATP  | N9-C8-N7    | -5.53 | 106.09      | 113.94   |
| 2   | C     | 602 | ATP  | N9-C8-N7    | -5.53 | 106.10      | 113.94   |
| 4   | D     | 604 | NAD  | C5A-C6A-N6A | 5.53  | 136.97      | 123.29   |
| 4   | G     | 604 | NAD  | C5A-C6A-N6A | 5.53  | 136.97      | 123.29   |
| 4   | H     | 604 | NAD  | C5A-C6A-N6A | 5.52  | 136.96      | 123.29   |
| 4   | B     | 604 | NAD  | C5A-C6A-N6A | 5.52  | 136.96      | 123.29   |
| 2   | H     | 601 | ATP  | C1'-N9-C8   | 5.52  | 139.34      | 127.09   |
| 2   | D     | 601 | ATP  | C1'-N9-C8   | 5.52  | 139.34      | 127.09   |
| 2   | C     | 601 | ATP  | C1'-N9-C8   | 5.52  | 139.34      | 127.09   |
| 2   | A     | 602 | ATP  | N9-C8-N7    | -5.51 | 106.12      | 113.94   |
| 2   | H     | 602 | ATP  | N9-C8-N7    | -5.51 | 106.12      | 113.94   |
| 2   | F     | 602 | ATP  | N9-C8-N7    | -5.51 | 106.12      | 113.94   |
| 2   | A     | 601 | ATP  | C1'-N9-C8   | 5.50  | 139.31      | 127.09   |
| 2   | G     | 601 | ATP  | C1'-N9-C8   | 5.50  | 139.31      | 127.09   |
| 2   | E     | 601 | ATP  | C1'-N9-C8   | 5.50  | 139.31      | 127.09   |
| 2   | E     | 602 | ATP  | N9-C8-N7    | -5.50 | 106.13      | 113.94   |
| 2   | G     | 602 | ATP  | N9-C8-N7    | -5.49 | 106.15      | 113.94   |
| 2   | D     | 602 | ATP  | N9-C8-N7    | -5.46 | 106.19      | 113.94   |
| 2   | G     | 602 | ATP  | C1'-N9-C8   | 5.35  | 138.96      | 127.09   |
| 2   | D     | 602 | ATP  | C1'-N9-C8   | 5.34  | 138.96      | 127.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 602 | ATP  | C1'-N9-C8   | 5.34  | 138.94      | 127.09   |
| 2   | A     | 602 | ATP  | C1'-N9-C8   | 5.33  | 138.93      | 127.09   |
| 2   | H     | 602 | ATP  | C1'-N9-C8   | 5.33  | 138.93      | 127.09   |
| 2   | C     | 602 | ATP  | C1'-N9-C8   | 5.32  | 138.91      | 127.09   |
| 2   | B     | 602 | ATP  | C1'-N9-C8   | 5.32  | 138.91      | 127.09   |
| 2   | F     | 602 | ATP  | C1'-N9-C8   | 5.32  | 138.91      | 127.09   |
| 4   | A     | 604 | NAD  | C1B-N9A-C8A | 5.29  | 138.83      | 127.09   |
| 4   | D     | 604 | NAD  | C1B-N9A-C8A | 5.29  | 138.83      | 127.09   |
| 4   | G     | 604 | NAD  | C1B-N9A-C8A | 5.29  | 138.83      | 127.09   |
| 4   | E     | 604 | NAD  | C1B-N9A-C8A | 5.29  | 138.83      | 127.09   |
| 4   | C     | 604 | NAD  | C1B-N9A-C8A | 5.28  | 138.81      | 127.09   |
| 4   | F     | 604 | NAD  | C1B-N9A-C8A | 5.28  | 138.81      | 127.09   |
| 4   | H     | 604 | NAD  | C1B-N9A-C8A | 5.26  | 138.78      | 127.09   |
| 4   | B     | 604 | NAD  | C1B-N9A-C8A | 5.26  | 138.77      | 127.09   |
| 4   | H     | 604 | NAD  | N9A-C8A-N7A | -5.05 | 106.77      | 113.94   |
| 4   | B     | 604 | NAD  | N9A-C8A-N7A | -5.05 | 106.77      | 113.94   |
| 2   | G     | 601 | ATP  | C4-N9-C8    | 5.04  | 111.03      | 105.74   |
| 4   | D     | 604 | NAD  | N9A-C8A-N7A | -5.04 | 106.79      | 113.94   |
| 4   | G     | 604 | NAD  | N9A-C8A-N7A | -5.04 | 106.79      | 113.94   |
| 4   | A     | 604 | NAD  | N9A-C8A-N7A | -5.03 | 106.80      | 113.94   |
| 4   | C     | 604 | NAD  | N9A-C8A-N7A | -5.03 | 106.80      | 113.94   |
| 2   | E     | 601 | ATP  | C4-N9-C8    | 5.02  | 111.01      | 105.74   |
| 2   | C     | 601 | ATP  | C4-N9-C8    | 5.01  | 111.00      | 105.74   |
| 2   | D     | 601 | ATP  | C4-N9-C8    | 5.01  | 111.00      | 105.74   |
| 4   | F     | 604 | NAD  | N9A-C8A-N7A | -5.00 | 106.84      | 113.94   |
| 4   | E     | 604 | NAD  | N9A-C8A-N7A | -4.99 | 106.86      | 113.94   |
| 2   | A     | 601 | ATP  | C4-N9-C8    | 4.99  | 110.97      | 105.74   |
| 2   | B     | 601 | ATP  | C4-N9-C8    | 4.98  | 110.97      | 105.74   |
| 2   | F     | 601 | ATP  | C4-N9-C8    | 4.98  | 110.97      | 105.74   |
| 2   | H     | 601 | ATP  | C4-N9-C8    | 4.96  | 110.94      | 105.74   |
| 2   | D     | 602 | ATP  | C5-C4-N3    | -4.84 | 120.06      | 126.72   |
| 2   | G     | 602 | ATP  | C5-C4-N3    | -4.82 | 120.08      | 126.72   |
| 2   | B     | 602 | ATP  | C5-C4-N3    | -4.81 | 120.09      | 126.72   |
| 2   | E     | 602 | ATP  | C5-C4-N3    | -4.81 | 120.09      | 126.72   |
| 2   | A     | 602 | ATP  | C5-C4-N3    | -4.81 | 120.09      | 126.72   |
| 2   | C     | 602 | ATP  | C5-C4-N3    | -4.81 | 120.09      | 126.72   |
| 3   | C     | 603 | IMP  | C2-N1-C6    | -4.80 | 118.52      | 125.09   |
| 2   | F     | 602 | ATP  | C5-C4-N3    | -4.79 | 120.12      | 126.72   |
| 2   | H     | 602 | ATP  | C5-C4-N3    | -4.79 | 120.12      | 126.72   |
| 3   | B     | 603 | IMP  | C2-N1-C6    | -4.79 | 118.53      | 125.09   |
| 3   | H     | 603 | IMP  | C2-N1-C6    | -4.77 | 118.56      | 125.09   |
| 3   | A     | 603 | IMP  | C2-N1-C6    | -4.76 | 118.56      | 125.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | E     | 603 | IMP  | C2-N1-C6    | -4.76 | 118.57      | 125.09   |
| 3   | G     | 603 | IMP  | C2-N1-C6    | -4.75 | 118.57      | 125.09   |
| 3   | F     | 603 | IMP  | C2-N1-C6    | -4.75 | 118.58      | 125.09   |
| 3   | D     | 603 | IMP  | C2-N1-C6    | -4.72 | 118.62      | 125.09   |
| 2   | A     | 602 | ATP  | C4-N9-C8    | 4.58  | 110.55      | 105.74   |
| 2   | G     | 602 | ATP  | C4-N9-C8    | 4.56  | 110.52      | 105.74   |
| 2   | B     | 602 | ATP  | C4-N9-C8    | 4.55  | 110.52      | 105.74   |
| 2   | C     | 602 | ATP  | C4-N9-C8    | 4.55  | 110.52      | 105.74   |
| 2   | F     | 602 | ATP  | C4-N9-C8    | 4.55  | 110.52      | 105.74   |
| 2   | D     | 602 | ATP  | C4-N9-C8    | 4.52  | 110.49      | 105.74   |
| 2   | E     | 602 | ATP  | C4-N9-C8    | 4.52  | 110.48      | 105.74   |
| 2   | H     | 602 | ATP  | C4-N9-C8    | 4.52  | 110.48      | 105.74   |
| 3   | A     | 603 | IMP  | C5-C4-N3    | -4.48 | 120.67      | 127.27   |
| 3   | B     | 603 | IMP  | C5-C4-N3    | -4.46 | 120.71      | 127.27   |
| 3   | D     | 603 | IMP  | C5-C4-N3    | -4.46 | 120.71      | 127.27   |
| 3   | F     | 603 | IMP  | C5-C4-N3    | -4.46 | 120.71      | 127.27   |
| 3   | H     | 603 | IMP  | C5-C4-N3    | -4.46 | 120.71      | 127.27   |
| 3   | E     | 603 | IMP  | C5-C4-N3    | -4.43 | 120.75      | 127.27   |
| 3   | G     | 603 | IMP  | C5-C4-N3    | -4.42 | 120.76      | 127.27   |
| 3   | C     | 603 | IMP  | C5-C4-N3    | -4.42 | 120.77      | 127.27   |
| 3   | F     | 603 | IMP  | C2-N3-C4    | 4.39  | 119.25      | 111.53   |
| 3   | A     | 603 | IMP  | C2-N3-C4    | 4.38  | 119.24      | 111.53   |
| 3   | H     | 603 | IMP  | C2-N3-C4    | 4.37  | 119.22      | 111.53   |
| 3   | D     | 603 | IMP  | C2-N3-C4    | 4.37  | 119.22      | 111.53   |
| 3   | B     | 603 | IMP  | C2-N3-C4    | 4.37  | 119.21      | 111.53   |
| 3   | E     | 603 | IMP  | C2-N3-C4    | 4.36  | 119.19      | 111.53   |
| 4   | E     | 604 | NAD  | C5A-C4A-N3A | -4.34 | 120.73      | 126.72   |
| 4   | F     | 604 | NAD  | C5A-C4A-N3A | -4.34 | 120.73      | 126.72   |
| 4   | C     | 604 | NAD  | C5A-C4A-N3A | -4.34 | 120.74      | 126.72   |
| 3   | C     | 603 | IMP  | C2-N3-C4    | 4.34  | 119.17      | 111.53   |
| 3   | G     | 603 | IMP  | C2-N3-C4    | 4.34  | 119.16      | 111.53   |
| 4   | A     | 604 | NAD  | C5A-C4A-N3A | -4.34 | 120.74      | 126.72   |
| 4   | D     | 604 | NAD  | C5A-C4A-N3A | -4.31 | 120.78      | 126.72   |
| 4   | B     | 604 | NAD  | C5A-C4A-N3A | -4.31 | 120.78      | 126.72   |
| 4   | G     | 604 | NAD  | C5A-C4A-N3A | -4.31 | 120.78      | 126.72   |
| 4   | H     | 604 | NAD  | C5A-C4A-N3A | -4.31 | 120.78      | 126.72   |
| 2   | B     | 601 | ATP  | C5-C4-N3    | -4.30 | 120.80      | 126.72   |
| 2   | F     | 601 | ATP  | C5-C4-N3    | -4.29 | 120.81      | 126.72   |
| 2   | H     | 601 | ATP  | C5-C4-N3    | -4.29 | 120.81      | 126.72   |
| 2   | E     | 601 | ATP  | C5-C4-N3    | -4.27 | 120.84      | 126.72   |
| 2   | A     | 601 | ATP  | C5-C4-N3    | -4.26 | 120.85      | 126.72   |
| 2   | C     | 601 | ATP  | C5-C4-N3    | -4.25 | 120.86      | 126.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 601 | ATP  | C5-C4-N3    | -4.22 | 120.91      | 126.72   |
| 2   | G     | 601 | ATP  | C5-C4-N3    | -4.22 | 120.91      | 126.72   |
| 3   | D     | 603 | IMP  | N1-C2-N3    | -4.22 | 120.64      | 125.50   |
| 3   | F     | 603 | IMP  | N1-C2-N3    | -4.22 | 120.64      | 125.50   |
| 3   | A     | 603 | IMP  | N1-C2-N3    | -4.18 | 120.68      | 125.50   |
| 3   | H     | 603 | IMP  | N1-C2-N3    | -4.18 | 120.68      | 125.50   |
| 3   | E     | 603 | IMP  | N1-C2-N3    | -4.17 | 120.69      | 125.50   |
| 3   | B     | 603 | IMP  | N1-C2-N3    | -4.17 | 120.69      | 125.50   |
| 3   | G     | 603 | IMP  | N1-C2-N3    | -4.17 | 120.69      | 125.50   |
| 3   | C     | 603 | IMP  | N1-C2-N3    | -4.14 | 120.73      | 125.50   |
| 4   | H     | 604 | NAD  | C4A-N9A-C8A | 3.96  | 109.89      | 105.74   |
| 4   | B     | 604 | NAD  | C4A-N9A-C8A | 3.94  | 109.88      | 105.74   |
| 2   | G     | 602 | ATP  | N3-C4-N9    | 3.94  | 133.87      | 127.17   |
| 2   | A     | 602 | ATP  | N3-C4-N9    | 3.93  | 133.86      | 127.17   |
| 4   | C     | 604 | NAD  | C4A-N9A-C8A | 3.92  | 109.86      | 105.74   |
| 4   | F     | 604 | NAD  | C4A-N9A-C8A | 3.92  | 109.86      | 105.74   |
| 2   | D     | 602 | ATP  | N3-C4-N9    | 3.92  | 133.83      | 127.17   |
| 2   | B     | 602 | ATP  | N3-C4-N9    | 3.91  | 133.81      | 127.17   |
| 2   | E     | 602 | ATP  | N3-C4-N9    | 3.91  | 133.81      | 127.17   |
| 2   | C     | 602 | ATP  | N3-C4-N9    | 3.90  | 133.81      | 127.17   |
| 2   | H     | 602 | ATP  | N3-C4-N9    | 3.90  | 133.79      | 127.17   |
| 4   | D     | 604 | NAD  | C4A-N9A-C8A | 3.90  | 109.83      | 105.74   |
| 4   | G     | 604 | NAD  | C4A-N9A-C8A | 3.90  | 109.83      | 105.74   |
| 2   | F     | 602 | ATP  | N3-C4-N9    | 3.89  | 133.78      | 127.17   |
| 4   | A     | 604 | NAD  | C4A-N9A-C8A | 3.89  | 109.82      | 105.74   |
| 4   | G     | 604 | NAD  | O7N-C7N-N7N | -3.85 | 117.06      | 122.62   |
| 4   | E     | 604 | NAD  | C4A-N9A-C8A | 3.85  | 109.78      | 105.74   |
| 4   | E     | 604 | NAD  | O7N-C7N-N7N | -3.84 | 117.07      | 122.62   |
| 4   | F     | 604 | NAD  | O7N-C7N-N7N | -3.83 | 117.08      | 122.62   |
| 4   | B     | 604 | NAD  | O7N-C7N-N7N | -3.83 | 117.08      | 122.62   |
| 4   | D     | 604 | NAD  | O7N-C7N-N7N | -3.82 | 117.09      | 122.62   |
| 4   | A     | 604 | NAD  | O7N-C7N-N7N | -3.81 | 117.10      | 122.62   |
| 4   | H     | 604 | NAD  | O7N-C7N-N7N | -3.81 | 117.10      | 122.62   |
| 4   | C     | 604 | NAD  | O7N-C7N-N7N | -3.77 | 117.17      | 122.62   |
| 2   | G     | 602 | ATP  | C2-N3-C4    | 3.47  | 120.30      | 111.83   |
| 2   | A     | 602 | ATP  | C2-N3-C4    | 3.46  | 120.29      | 111.83   |
| 2   | B     | 601 | ATP  | C5-N7-C8    | 3.46  | 108.89      | 103.45   |
| 2   | D     | 602 | ATP  | C2-N3-C4    | 3.46  | 120.28      | 111.83   |
| 2   | H     | 601 | ATP  | C5-N7-C8    | 3.46  | 108.88      | 103.45   |
| 2   | D     | 601 | ATP  | C5-N7-C8    | 3.45  | 108.88      | 103.45   |
| 2   | F     | 601 | ATP  | C5-N7-C8    | 3.45  | 108.88      | 103.45   |
| 2   | E     | 602 | ATP  | C2-N3-C4    | 3.45  | 120.26      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 602 | ATP  | C2-N3-C4    | 3.45  | 120.26      | 111.83   |
| 2   | H     | 602 | ATP  | C2-N3-C4    | 3.45  | 120.25      | 111.83   |
| 2   | E     | 601 | ATP  | C5-N7-C8    | 3.44  | 108.86      | 103.45   |
| 2   | G     | 601 | ATP  | C5-N7-C8    | 3.44  | 108.86      | 103.45   |
| 2   | C     | 601 | ATP  | C5-N7-C8    | 3.44  | 108.86      | 103.45   |
| 2   | F     | 602 | ATP  | C2-N3-C4    | 3.44  | 120.23      | 111.83   |
| 2   | A     | 601 | ATP  | C5-N7-C8    | 3.44  | 108.86      | 103.45   |
| 2   | B     | 602 | ATP  | C2-N3-C4    | 3.44  | 120.22      | 111.83   |
| 2   | B     | 601 | ATP  | N3-C4-N9    | 3.39  | 132.94      | 127.17   |
| 2   | F     | 601 | ATP  | N3-C4-N9    | 3.39  | 132.94      | 127.17   |
| 2   | C     | 601 | ATP  | N3-C4-N9    | 3.38  | 132.92      | 127.17   |
| 2   | E     | 601 | ATP  | N3-C4-N9    | 3.38  | 132.91      | 127.17   |
| 2   | D     | 601 | ATP  | N3-C4-N9    | 3.36  | 132.88      | 127.17   |
| 2   | G     | 601 | ATP  | N3-C4-N9    | 3.36  | 132.88      | 127.17   |
| 2   | H     | 601 | ATP  | N3-C4-N9    | 3.36  | 132.88      | 127.17   |
| 2   | A     | 601 | ATP  | N3-C4-N9    | 3.35  | 132.87      | 127.17   |
| 2   | F     | 601 | ATP  | C2-N3-C4    | 3.25  | 119.77      | 111.83   |
| 4   | F     | 604 | NAD  | C2A-N3A-C4A | 3.24  | 119.74      | 111.83   |
| 4   | D     | 604 | NAD  | C2A-N3A-C4A | 3.23  | 119.73      | 111.83   |
| 4   | A     | 604 | NAD  | C2A-N3A-C4A | 3.23  | 119.73      | 111.83   |
| 2   | C     | 601 | ATP  | C2-N3-C4    | 3.23  | 119.72      | 111.83   |
| 4   | G     | 604 | NAD  | C2A-N3A-C4A | 3.23  | 119.72      | 111.83   |
| 4   | C     | 604 | NAD  | C2A-N3A-C4A | 3.23  | 119.71      | 111.83   |
| 4   | E     | 604 | NAD  | C2A-N3A-C4A | 3.23  | 119.71      | 111.83   |
| 2   | E     | 601 | ATP  | C2-N3-C4    | 3.23  | 119.71      | 111.83   |
| 2   | H     | 601 | ATP  | C2-N3-C4    | 3.23  | 119.71      | 111.83   |
| 2   | A     | 601 | ATP  | C2-N3-C4    | 3.23  | 119.71      | 111.83   |
| 2   | B     | 601 | ATP  | C2-N3-C4    | 3.23  | 119.71      | 111.83   |
| 4   | H     | 604 | NAD  | C2A-N3A-C4A | 3.23  | 119.71      | 111.83   |
| 4   | B     | 604 | NAD  | C2A-N3A-C4A | 3.22  | 119.70      | 111.83   |
| 2   | D     | 601 | ATP  | C2-N3-C4    | 3.22  | 119.68      | 111.83   |
| 2   | G     | 601 | ATP  | C2-N3-C4    | 3.22  | 119.68      | 111.83   |
| 2   | C     | 602 | ATP  | C5-N7-C8    | 3.17  | 108.44      | 103.45   |
| 3   | A     | 603 | IMP  | O6-C6-C5    | -3.16 | 118.19      | 126.53   |
| 3   | G     | 603 | IMP  | O6-C6-C5    | -3.16 | 118.19      | 126.53   |
| 2   | A     | 602 | ATP  | C5-N7-C8    | 3.15  | 108.41      | 103.45   |
| 2   | H     | 602 | ATP  | C5-N7-C8    | 3.15  | 108.41      | 103.45   |
| 3   | C     | 603 | IMP  | O6-C6-C5    | -3.15 | 118.21      | 126.53   |
| 2   | B     | 602 | ATP  | C5-N7-C8    | 3.15  | 108.40      | 103.45   |
| 2   | E     | 602 | ATP  | C5-N7-C8    | 3.15  | 108.40      | 103.45   |
| 3   | E     | 603 | IMP  | O6-C6-C5    | -3.15 | 118.22      | 126.53   |
| 3   | F     | 603 | IMP  | O6-C6-C5    | -3.15 | 118.22      | 126.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | D     | 603 | IMP  | O6-C6-C5    | -3.15 | 118.23      | 126.53   |
| 3   | B     | 603 | IMP  | O6-C6-C5    | -3.14 | 118.24      | 126.53   |
| 3   | H     | 603 | IMP  | O6-C6-C5    | -3.14 | 118.24      | 126.53   |
| 3   | E     | 603 | IMP  | O3P-P-O2P   | 3.14  | 119.56      | 107.80   |
| 3   | H     | 603 | IMP  | O3P-P-O2P   | 3.13  | 119.56      | 107.80   |
| 2   | G     | 602 | ATP  | C5-N7-C8    | 3.13  | 108.38      | 103.45   |
| 3   | G     | 603 | IMP  | O3P-P-O2P   | 3.13  | 119.55      | 107.80   |
| 2   | F     | 602 | ATP  | C5-N7-C8    | 3.13  | 108.37      | 103.45   |
| 3   | F     | 603 | IMP  | O3P-P-O2P   | 3.13  | 119.54      | 107.80   |
| 2   | D     | 602 | ATP  | C5-N7-C8    | 3.12  | 108.36      | 103.45   |
| 3   | C     | 603 | IMP  | N9-C8-N7    | -3.12 | 107.61      | 113.40   |
| 3   | D     | 603 | IMP  | N9-C8-N7    | -3.10 | 107.66      | 113.40   |
| 3   | E     | 603 | IMP  | N9-C8-N7    | -3.10 | 107.66      | 113.40   |
| 4   | H     | 604 | NAD  | N3A-C4A-N9A | 3.08  | 132.41      | 127.17   |
| 4   | D     | 604 | NAD  | N3A-C4A-N9A | 3.08  | 132.41      | 127.17   |
| 3   | A     | 603 | IMP  | N9-C8-N7    | -3.08 | 107.69      | 113.40   |
| 3   | B     | 603 | IMP  | N9-C8-N7    | -3.08 | 107.69      | 113.40   |
| 3   | G     | 603 | IMP  | N9-C8-N7    | -3.08 | 107.69      | 113.40   |
| 3   | H     | 603 | IMP  | N9-C8-N7    | -3.08 | 107.69      | 113.40   |
| 4   | C     | 604 | NAD  | N3A-C4A-N9A | 3.08  | 132.41      | 127.17   |
| 4   | F     | 604 | NAD  | N3A-C4A-N9A | 3.08  | 132.41      | 127.17   |
| 4   | G     | 604 | NAD  | N3A-C4A-N9A | 3.08  | 132.40      | 127.17   |
| 4   | A     | 604 | NAD  | N3A-C4A-N9A | 3.07  | 132.39      | 127.17   |
| 4   | B     | 604 | NAD  | N3A-C4A-N9A | 3.07  | 132.39      | 127.17   |
| 3   | F     | 603 | IMP  | N9-C8-N7    | -3.07 | 107.70      | 113.40   |
| 4   | E     | 604 | NAD  | N3A-C4A-N9A | 3.05  | 132.35      | 127.17   |
| 4   | D     | 604 | NAD  | C5A-N7A-C8A | 2.97  | 108.11      | 103.45   |
| 4   | G     | 604 | NAD  | C5A-N7A-C8A | 2.97  | 108.11      | 103.45   |
| 4   | A     | 604 | NAD  | C5A-N7A-C8A | 2.96  | 108.10      | 103.45   |
| 4   | H     | 604 | NAD  | C5A-N7A-C8A | 2.94  | 108.07      | 103.45   |
| 4   | B     | 604 | NAD  | C5A-N7A-C8A | 2.94  | 108.06      | 103.45   |
| 4   | C     | 604 | NAD  | C5A-N7A-C8A | 2.94  | 108.06      | 103.45   |
| 4   | E     | 604 | NAD  | C5A-N7A-C8A | 2.90  | 108.01      | 103.45   |
| 4   | F     | 604 | NAD  | C5A-N7A-C8A | 2.90  | 108.01      | 103.45   |
| 4   | B     | 604 | NAD  | O4B-C1B-C2B | -2.90 | 100.42      | 106.62   |
| 4   | A     | 604 | NAD  | O4B-C1B-C2B | -2.89 | 100.43      | 106.62   |
| 4   | H     | 604 | NAD  | O4B-C1B-C2B | -2.89 | 100.43      | 106.62   |
| 4   | G     | 604 | NAD  | O4B-C1B-C2B | -2.89 | 100.44      | 106.62   |
| 4   | F     | 604 | NAD  | O4B-C1B-C2B | -2.88 | 100.46      | 106.62   |
| 4   | E     | 604 | NAD  | O4B-C1B-C2B | -2.87 | 100.47      | 106.62   |
| 4   | D     | 604 | NAD  | O4B-C1B-C2B | -2.87 | 100.47      | 106.62   |
| 4   | C     | 604 | NAD  | O4B-C1B-C2B | -2.86 | 100.51      | 106.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 603 | IMP  | N9-C4-N3    | 2.32  | 132.18      | 126.90   |
| 3   | B     | 603 | IMP  | N9-C4-N3    | 2.30  | 132.14      | 126.90   |
| 3   | E     | 603 | IMP  | N9-C4-N3    | 2.30  | 132.14      | 126.90   |
| 3   | F     | 603 | IMP  | N9-C4-N3    | 2.30  | 132.14      | 126.90   |
| 3   | H     | 603 | IMP  | N9-C4-N3    | 2.30  | 132.14      | 126.90   |
| 4   | D     | 604 | NAD  | C4B-O4B-C1B | -2.30 | 104.39      | 109.47   |
| 3   | D     | 603 | IMP  | N9-C4-N3    | 2.29  | 132.12      | 126.90   |
| 4   | A     | 604 | NAD  | C4B-O4B-C1B | -2.29 | 104.42      | 109.47   |
| 4   | E     | 604 | NAD  | C4B-O4B-C1B | -2.29 | 104.42      | 109.47   |
| 4   | H     | 604 | NAD  | C4B-O4B-C1B | -2.29 | 104.42      | 109.47   |
| 4   | B     | 604 | NAD  | C4B-O4B-C1B | -2.29 | 104.42      | 109.47   |
| 4   | C     | 604 | NAD  | C4B-O4B-C1B | -2.28 | 104.42      | 109.47   |
| 4   | G     | 604 | NAD  | C4B-O4B-C1B | -2.28 | 104.43      | 109.47   |
| 3   | G     | 603 | IMP  | N9-C4-N3    | 2.28  | 132.09      | 126.90   |
| 3   | C     | 603 | IMP  | N9-C4-N3    | 2.27  | 132.08      | 126.90   |
| 4   | F     | 604 | NAD  | C4B-O4B-C1B | -2.27 | 104.46      | 109.47   |
| 3   | B     | 603 | IMP  | O2P-P-O1P   | 2.24  | 119.58      | 110.83   |
| 3   | D     | 603 | IMP  | O2P-P-O1P   | 2.24  | 119.55      | 110.83   |
| 3   | A     | 603 | IMP  | O2P-P-O1P   | 2.23  | 119.53      | 110.83   |
| 3   | C     | 603 | IMP  | O2P-P-O1P   | 2.23  | 119.51      | 110.83   |
| 4   | F     | 604 | NAD  | O4B-C1B-N9A | 2.18  | 112.27      | 108.09   |
| 4   | A     | 604 | NAD  | O4B-C1B-N9A | 2.17  | 112.26      | 108.09   |
| 4   | C     | 604 | NAD  | O4B-C1B-N9A | 2.17  | 112.26      | 108.09   |
| 4   | H     | 604 | NAD  | O4B-C1B-N9A | 2.17  | 112.25      | 108.09   |
| 4   | B     | 604 | NAD  | O4B-C1B-N9A | 2.15  | 112.22      | 108.09   |
| 4   | E     | 604 | NAD  | O4B-C1B-N9A | 2.15  | 112.22      | 108.09   |
| 4   | D     | 604 | NAD  | O4B-C1B-N9A | 2.15  | 112.21      | 108.09   |
| 4   | G     | 604 | NAD  | O4B-C1B-N9A | 2.15  | 112.21      | 108.09   |
| 2   | C     | 601 | ATP  | O3G-PG-O3B  | 2.09  | 111.64      | 104.64   |
| 2   | B     | 601 | ATP  | O3G-PG-O3B  | 2.09  | 111.64      | 104.64   |
| 2   | D     | 601 | ATP  | O3G-PG-O3B  | 2.08  | 111.63      | 104.64   |
| 2   | E     | 601 | ATP  | O3G-PG-O3B  | 2.08  | 111.62      | 104.64   |
| 2   | G     | 601 | ATP  | O3G-PG-O3B  | 2.08  | 111.60      | 104.64   |
| 2   | A     | 601 | ATP  | O3G-PG-O3B  | 2.07  | 111.59      | 104.64   |
| 2   | H     | 601 | ATP  | O3G-PG-O3B  | 2.07  | 111.59      | 104.64   |
| 2   | F     | 601 | ATP  | O3G-PG-O3B  | 2.07  | 111.57      | 104.64   |
| 2   | B     | 601 | ATP  | C4-C5-N7    | -2.05 | 108.23      | 110.58   |
| 4   | D     | 604 | NAD  | C5B-C4B-C3B | -2.05 | 107.85      | 115.21   |
| 4   | G     | 604 | NAD  | C5B-C4B-C3B | -2.05 | 107.85      | 115.21   |
| 2   | H     | 601 | ATP  | C4-C5-N7    | -2.04 | 108.25      | 110.58   |
| 4   | B     | 604 | NAD  | C5B-C4B-C3B | -2.04 | 107.88      | 115.21   |
| 4   | D     | 604 | NAD  | C2B-C1B-N9A | -2.04 | 108.25      | 113.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | F     | 604 | NAD  | C5B-C4B-C3B | -2.03 | 107.89      | 115.21   |
| 4   | E     | 604 | NAD  | C5B-C4B-C3B | -2.03 | 107.89      | 115.21   |
| 4   | G     | 604 | NAD  | C2B-C1B-N9A | -2.03 | 108.26      | 113.30   |
| 4   | F     | 604 | NAD  | C2B-C1B-N9A | -2.03 | 108.26      | 113.30   |
| 4   | C     | 604 | NAD  | C2B-C1B-N9A | -2.03 | 108.27      | 113.30   |
| 4   | A     | 604 | NAD  | C5B-C4B-C3B | -2.03 | 107.91      | 115.21   |
| 4   | H     | 604 | NAD  | C5B-C4B-C3B | -2.03 | 107.91      | 115.21   |
| 2   | F     | 602 | ATP  | C3'-C2'-C1' | 2.03  | 105.30      | 101.46   |
| 4   | C     | 604 | NAD  | C5B-C4B-C3B | -2.02 | 107.93      | 115.21   |
| 4   | B     | 604 | NAD  | C2B-C1B-N9A | -2.02 | 108.28      | 113.30   |
| 4   | H     | 604 | NAD  | C2B-C1B-N9A | -2.02 | 108.28      | 113.30   |
| 4   | A     | 604 | NAD  | C2B-C1B-N9A | -2.02 | 108.29      | 113.30   |
| 4   | E     | 604 | NAD  | C2B-C1B-N9A | -2.02 | 108.29      | 113.30   |
| 2   | B     | 602 | ATP  | C3'-C2'-C1' | 2.02  | 105.28      | 101.46   |
| 2   | E     | 601 | ATP  | C4-C5-N7    | -2.01 | 108.28      | 110.58   |
| 2   | F     | 601 | ATP  | C4-C5-N7    | -2.01 | 108.29      | 110.58   |
| 2   | A     | 601 | ATP  | C4-C5-N7    | -2.00 | 108.29      | 110.58   |

There are no chirality outliers.

All (264) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | A     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | A     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | A     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 2   | B     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | B     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | B     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | B     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 2   | C     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | C     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | C     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | C     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 2   | D     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | D     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | D     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | D     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 2   | E     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | E     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | E     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | E     | 602 | ATP  | C5'-O5'-PA-O3A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | F     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | F     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | F     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | F     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 2   | G     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | G     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 2   | G     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 2   | G     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 2   | H     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 2   | H     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 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   | C     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | C     | 603 | IMP  | C5'-O5'-P-O3P   |
| 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-O1P   |
| 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   | G     | 603 | IMP  | C5'-O5'-P-O1P   |
| 3   | G     | 603 | IMP  | C5'-O5'-P-O2P   |
| 3   | G     | 603 | IMP  | C5'-O5'-P-O3P   |
| 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  | O4B-C4B-C5B-O5B |
| 4   | A     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | B     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | B     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | C     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | C     | 604 | NAD  | C2B-C1B-N9A-C8A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | D     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | D     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | E     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | E     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | F     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | F     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | G     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | G     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 4   | H     | 604 | NAD  | O4B-C4B-C5B-O5B |
| 4   | H     | 604 | NAD  | C2B-C1B-N9A-C8A |
| 3   | A     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | B     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | C     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | D     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | E     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | F     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | G     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | H     | 603 | IMP  | C3'-C4'-C5'-O5' |
| 3   | A     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | B     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | C     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | D     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | E     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | F     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | G     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 3   | H     | 603 | IMP  | O4'-C4'-C5'-O5' |
| 4   | A     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 4   | B     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 4   | C     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 4   | D     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 4   | E     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 4   | F     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 4   | G     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 4   | H     | 604 | NAD  | C2B-C1B-N9A-C4A |
| 4   | A     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | B     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | C     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | D     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | E     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | F     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | G     | 604 | NAD  | C3B-C4B-C5B-O5B |
| 4   | H     | 604 | NAD  | C3B-C4B-C5B-O5B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | B     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | C     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | D     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | E     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | F     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | G     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | H     | 602 | ATP  | C3'-C4'-C5'-O5' |
| 2   | A     | 602 | ATP  | C4'-C5'-O5'-PA  |
| 2   | B     | 602 | ATP  | C4'-C5'-O5'-PA  |
| 2   | C     | 602 | ATP  | C4'-C5'-O5'-PA  |
| 2   | D     | 602 | ATP  | C4'-C5'-O5'-PA  |
| 2   | E     | 602 | ATP  | C4'-C5'-O5'-PA  |
| 2   | F     | 602 | ATP  | C4'-C5'-O5'-PA  |
| 2   | G     | 602 | ATP  | C4'-C5'-O5'-PA  |
| 2   | H     | 602 | ATP  | C4'-C5'-O5'-PA  |
| 2   | A     | 602 | ATP  | PB-O3A-PA-O5'   |
| 2   | B     | 602 | ATP  | PB-O3A-PA-O5'   |
| 2   | C     | 602 | ATP  | PB-O3A-PA-O5'   |
| 2   | D     | 602 | ATP  | PB-O3A-PA-O5'   |
| 2   | E     | 602 | ATP  | PB-O3A-PA-O5'   |
| 2   | F     | 602 | ATP  | PB-O3A-PA-O5'   |
| 2   | G     | 602 | ATP  | PB-O3A-PA-O5'   |
| 2   | H     | 602 | ATP  | PB-O3A-PA-O5'   |
| 2   | A     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | B     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | C     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | D     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | E     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | F     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | G     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | H     | 602 | ATP  | PA-O3A-PB-O1B   |
| 2   | A     | 601 | ATP  | C5'-O5'-PA-O1A  |
| 2   | A     | 601 | ATP  | C5'-O5'-PA-O2A  |
| 2   | A     | 601 | ATP  | C5'-O5'-PA-O3A  |
| 2   | A     | 602 | ATP  | C5'-O5'-PA-O1A  |
| 2   | B     | 601 | ATP  | C5'-O5'-PA-O1A  |
| 2   | B     | 601 | ATP  | C5'-O5'-PA-O2A  |
| 2   | B     | 601 | ATP  | C5'-O5'-PA-O3A  |
| 2   | B     | 602 | ATP  | C5'-O5'-PA-O1A  |
| 2   | C     | 601 | ATP  | C5'-O5'-PA-O1A  |
| 2   | C     | 601 | ATP  | C5'-O5'-PA-O2A  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | C     | 601 | ATP  | C5'-O5'-PA-O3A |
| 2   | C     | 602 | ATP  | C5'-O5'-PA-O1A |
| 2   | D     | 601 | ATP  | C5'-O5'-PA-O1A |
| 2   | D     | 601 | ATP  | C5'-O5'-PA-O2A |
| 2   | D     | 601 | ATP  | C5'-O5'-PA-O3A |
| 2   | D     | 602 | ATP  | C5'-O5'-PA-O1A |
| 2   | E     | 601 | ATP  | C5'-O5'-PA-O1A |
| 2   | E     | 601 | ATP  | C5'-O5'-PA-O2A |
| 2   | E     | 601 | ATP  | C5'-O5'-PA-O3A |
| 2   | E     | 602 | ATP  | C5'-O5'-PA-O1A |
| 2   | F     | 601 | ATP  | C5'-O5'-PA-O1A |
| 2   | F     | 601 | ATP  | C5'-O5'-PA-O2A |
| 2   | F     | 601 | ATP  | C5'-O5'-PA-O3A |
| 2   | F     | 602 | ATP  | C5'-O5'-PA-O1A |
| 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   | 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-O1A |
| 4   | A     | 604 | NAD  | C5B-O5B-PA-O1A |
| 4   | A     | 604 | NAD  | C5B-O5B-PA-O2A |
| 4   | A     | 604 | NAD  | C5B-O5B-PA-O3  |
| 4   | A     | 604 | NAD  | C5D-O5D-PN-O2N |
| 4   | B     | 604 | NAD  | C5B-O5B-PA-O1A |
| 4   | B     | 604 | NAD  | C5B-O5B-PA-O2A |
| 4   | B     | 604 | NAD  | C5B-O5B-PA-O3  |
| 4   | B     | 604 | NAD  | C5D-O5D-PN-O2N |
| 4   | C     | 604 | NAD  | C5B-O5B-PA-O1A |
| 4   | C     | 604 | NAD  | C5B-O5B-PA-O2A |
| 4   | C     | 604 | NAD  | C5B-O5B-PA-O3  |
| 4   | C     | 604 | NAD  | C5D-O5D-PN-O2N |
| 4   | D     | 604 | NAD  | C5B-O5B-PA-O1A |
| 4   | D     | 604 | NAD  | C5B-O5B-PA-O2A |
| 4   | D     | 604 | NAD  | C5B-O5B-PA-O3  |
| 4   | D     | 604 | NAD  | C5D-O5D-PN-O2N |
| 4   | E     | 604 | NAD  | C5B-O5B-PA-O1A |
| 4   | E     | 604 | NAD  | C5B-O5B-PA-O2A |
| 4   | E     | 604 | NAD  | C5B-O5B-PA-O3  |
| 4   | E     | 604 | NAD  | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | F     | 604 | NAD  | C5B-O5B-PA-O1A  |
| 4   | F     | 604 | NAD  | C5B-O5B-PA-O2A  |
| 4   | F     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | F     | 604 | NAD  | C5D-O5D-PN-O2N  |
| 4   | G     | 604 | NAD  | C5B-O5B-PA-O1A  |
| 4   | G     | 604 | NAD  | C5B-O5B-PA-O2A  |
| 4   | G     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | G     | 604 | NAD  | C5D-O5D-PN-O2N  |
| 4   | H     | 604 | NAD  | C5B-O5B-PA-O1A  |
| 4   | H     | 604 | NAD  | C5B-O5B-PA-O2A  |
| 4   | H     | 604 | NAD  | C5B-O5B-PA-O3   |
| 4   | H     | 604 | NAD  | C5D-O5D-PN-O2N  |
| 4   | A     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | A     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | B     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | B     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | C     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | C     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | D     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | D     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | E     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | E     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | F     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | F     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | G     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | G     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 4   | H     | 604 | NAD  | C2D-C1D-N1N-C2N |
| 4   | H     | 604 | NAD  | C2D-C1D-N1N-C6N |
| 2   | A     | 602 | ATP  | PB-O3B-PG-O1G   |
| 2   | B     | 602 | ATP  | PB-O3B-PG-O1G   |
| 2   | C     | 602 | ATP  | PB-O3B-PG-O1G   |
| 2   | D     | 602 | ATP  | PB-O3B-PG-O1G   |
| 2   | E     | 602 | ATP  | PB-O3B-PG-O1G   |
| 2   | F     | 602 | ATP  | PB-O3B-PG-O1G   |
| 2   | G     | 602 | ATP  | PB-O3B-PG-O1G   |
| 2   | H     | 602 | ATP  | PB-O3B-PG-O1G   |
| 4   | A     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 4   | A     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | B     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 4   | B     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | C     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 4   | C     | 604 | NAD  | C4D-C5D-O5D-PN  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | D     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 4   | D     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | E     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 4   | E     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | F     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 4   | F     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | G     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 4   | G     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | H     | 604 | NAD  | C4B-C5B-O5B-PA  |
| 4   | H     | 604 | NAD  | C4D-C5D-O5D-PN  |
| 4   | A     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 4   | B     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 4   | C     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 4   | D     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 4   | E     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 4   | F     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 4   | G     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 4   | H     | 604 | NAD  | O4B-C1B-N9A-C8A |
| 2   | A     | 601 | ATP  | PG-O3B-PB-O2B   |
| 2   | A     | 602 | ATP  | PA-O3A-PB-O2B   |
| 2   | B     | 601 | ATP  | PG-O3B-PB-O2B   |
| 2   | B     | 602 | ATP  | PA-O3A-PB-O2B   |
| 2   | C     | 601 | ATP  | PG-O3B-PB-O2B   |
| 2   | C     | 602 | ATP  | PA-O3A-PB-O2B   |
| 2   | D     | 601 | ATP  | PG-O3B-PB-O2B   |
| 2   | D     | 602 | ATP  | PA-O3A-PB-O2B   |
| 2   | E     | 601 | ATP  | PG-O3B-PB-O2B   |
| 2   | E     | 602 | ATP  | PA-O3A-PB-O2B   |
| 2   | F     | 601 | ATP  | PG-O3B-PB-O2B   |
| 2   | F     | 602 | ATP  | PA-O3A-PB-O2B   |
| 2   | G     | 601 | ATP  | PG-O3B-PB-O2B   |
| 2   | G     | 602 | ATP  | PA-O3A-PB-O2B   |
| 2   | H     | 601 | ATP  | PG-O3B-PB-O2B   |
| 2   | H     | 602 | ATP  | PA-O3A-PB-O2B   |

There are no ring outliers.

24 monomers are involved in 43 short contacts:

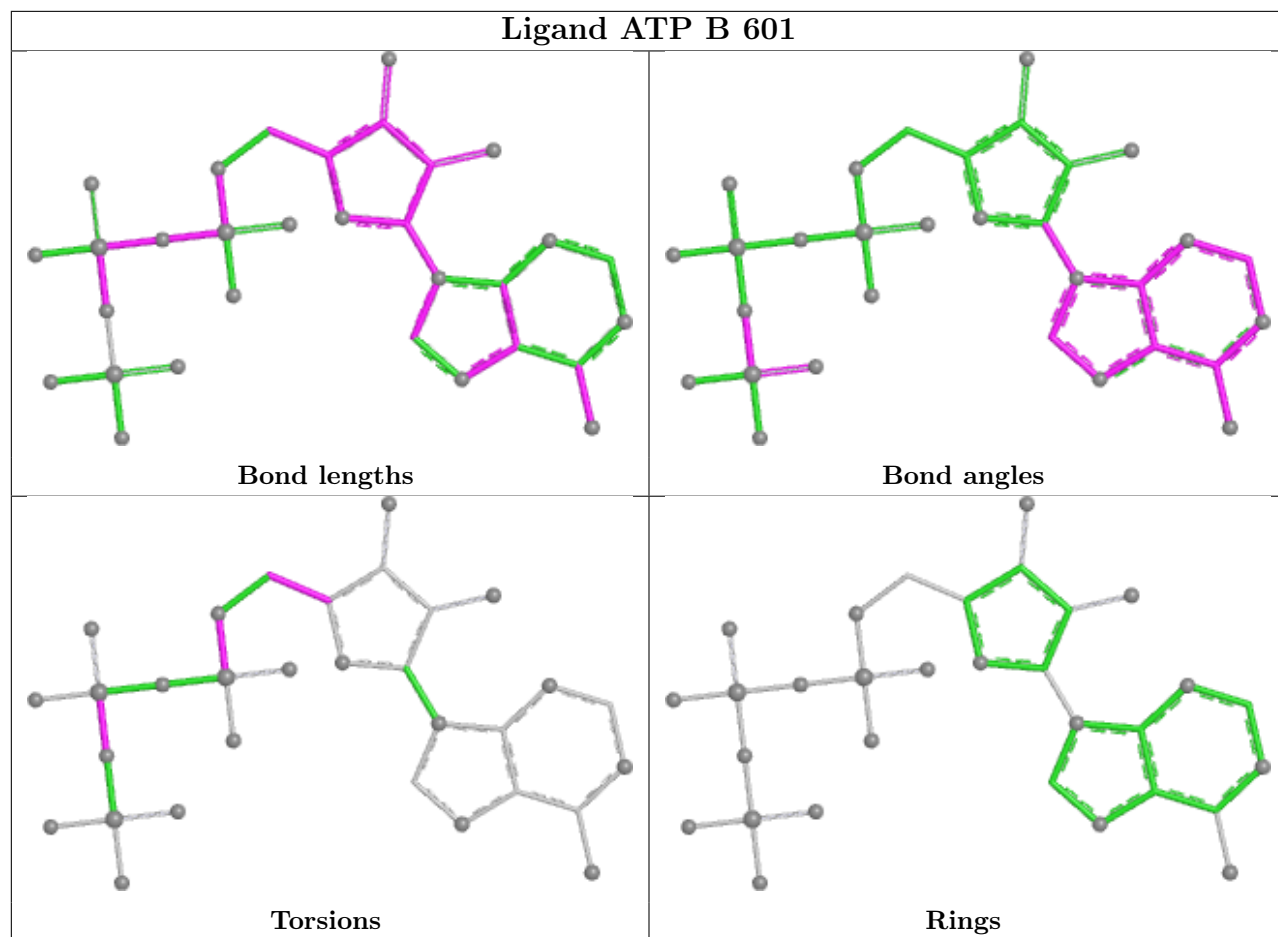
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 601 | ATP  | 1       | 0            |
| 2   | F     | 601 | ATP  | 1       | 0            |
| 4   | A     | 604 | NAD  | 1       | 0            |

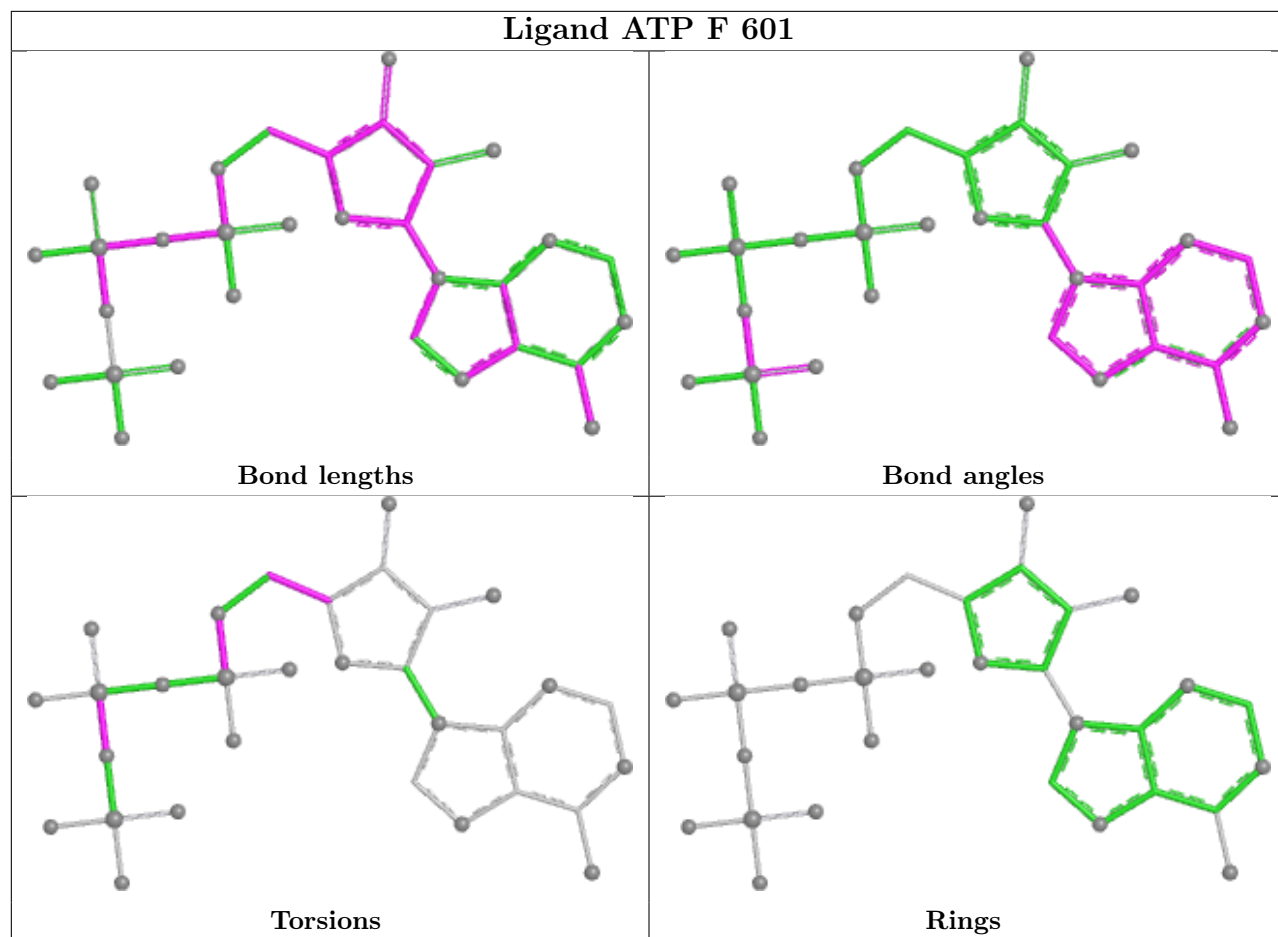
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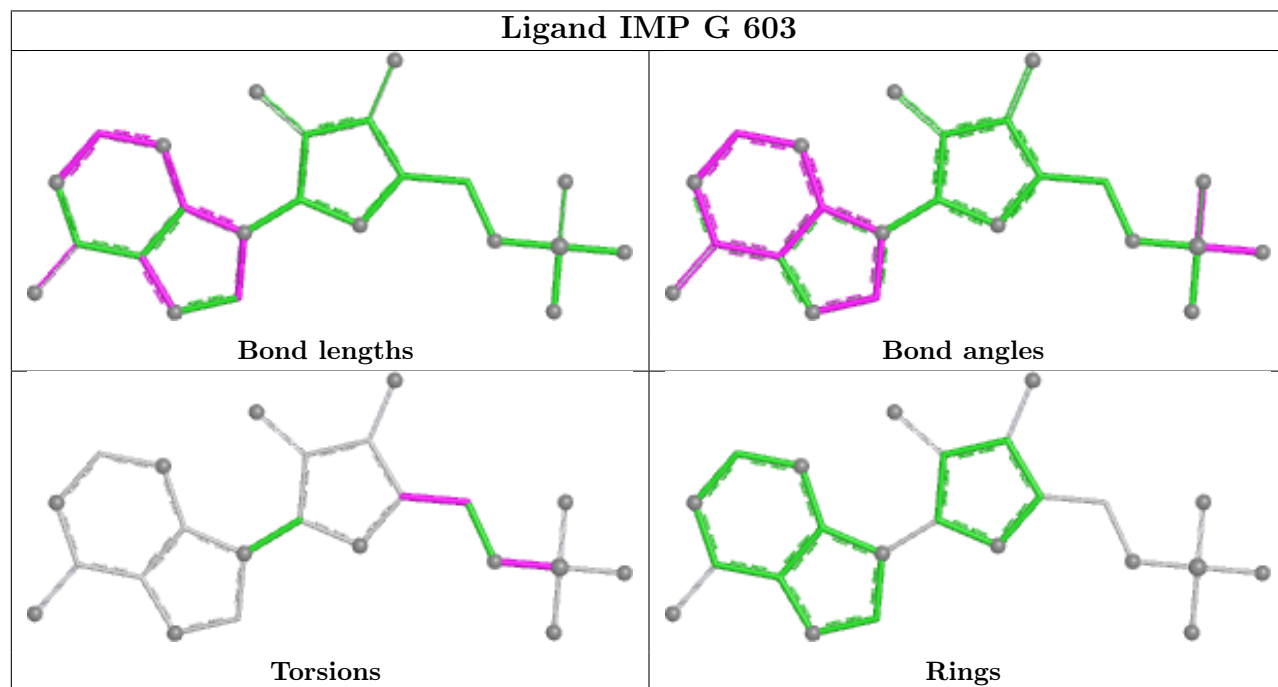
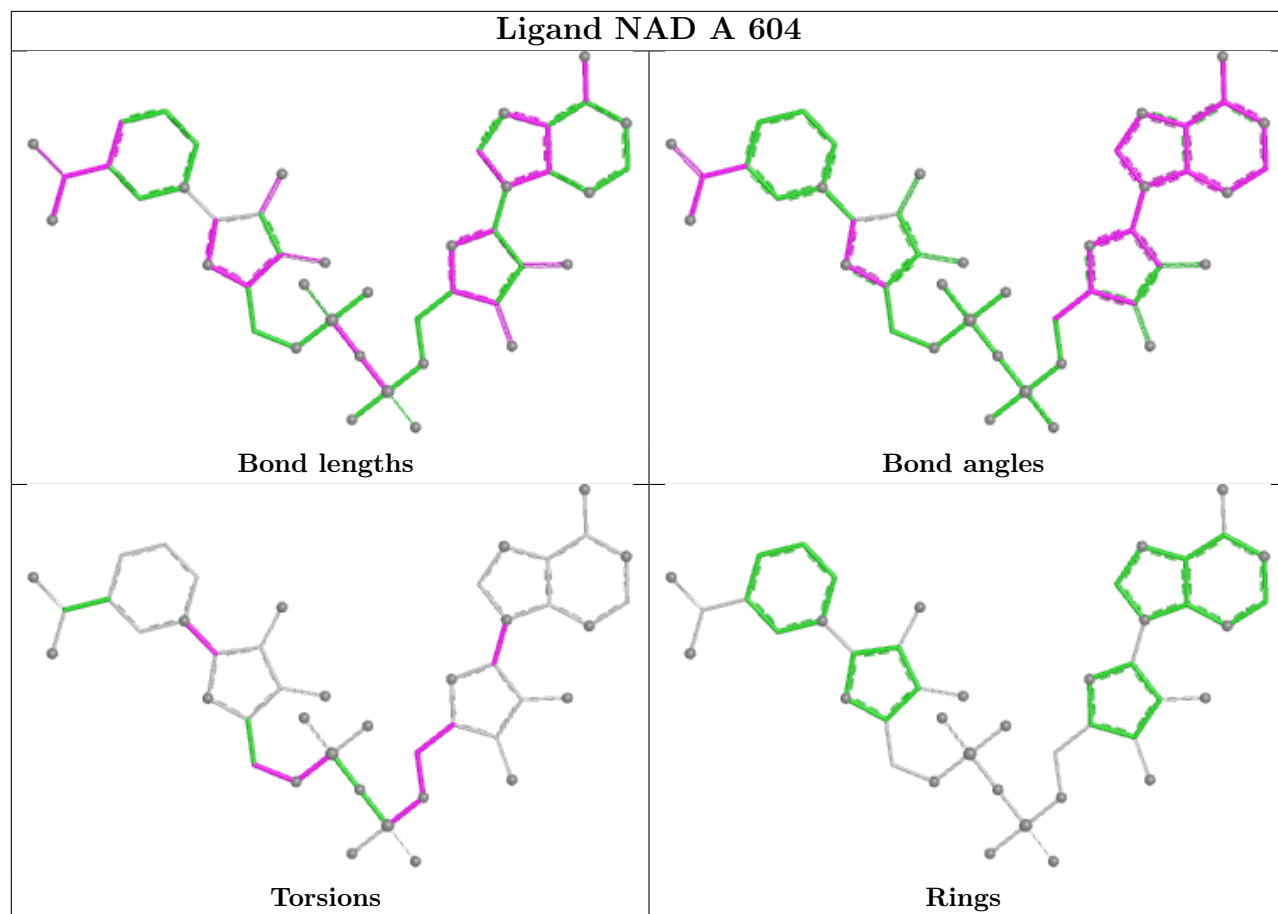
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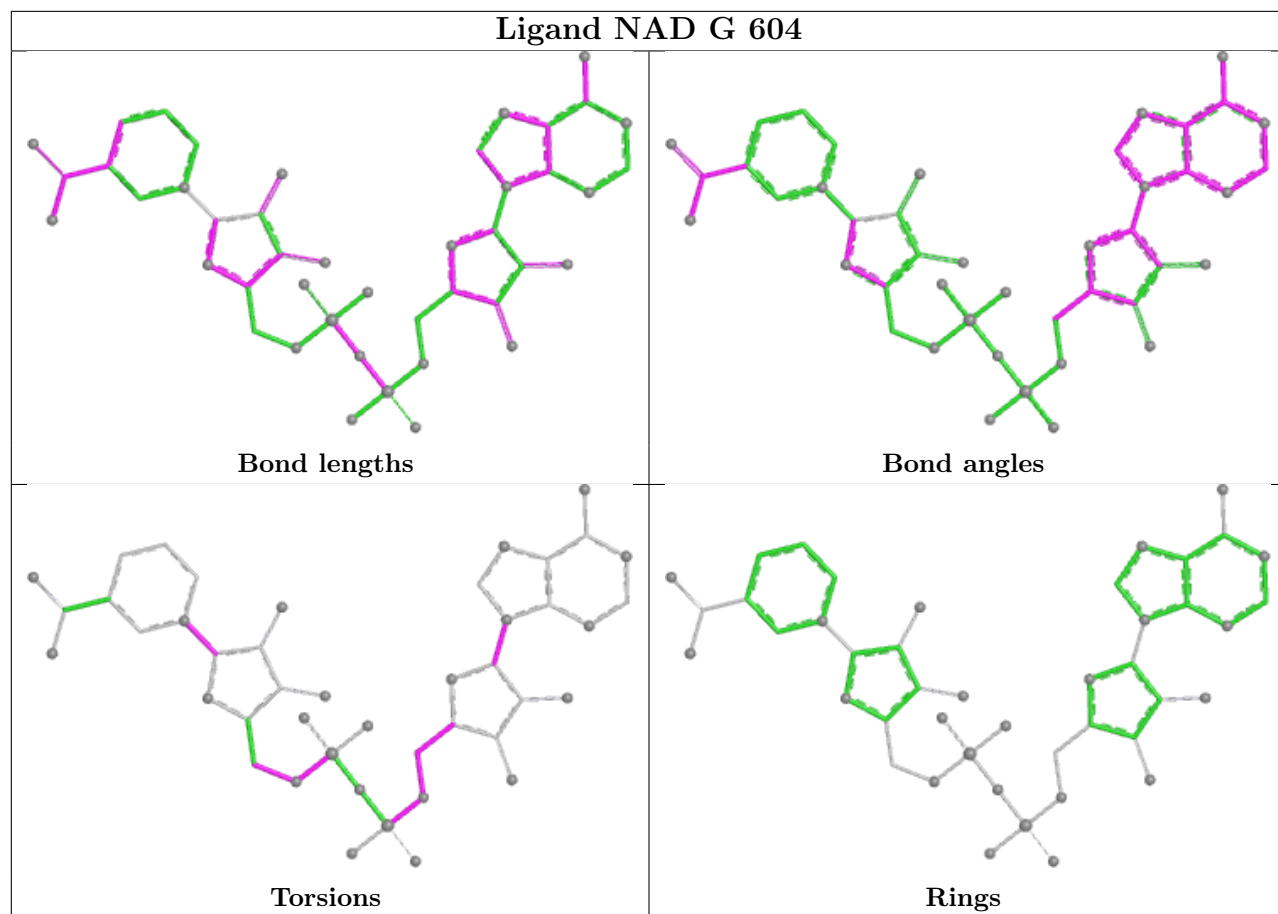
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | G     | 603 | IMP  | 4       | 0            |
| 4   | G     | 604 | NAD  | 2       | 0            |
| 3   | F     | 603 | IMP  | 4       | 0            |
| 4   | H     | 604 | NAD  | 1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

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

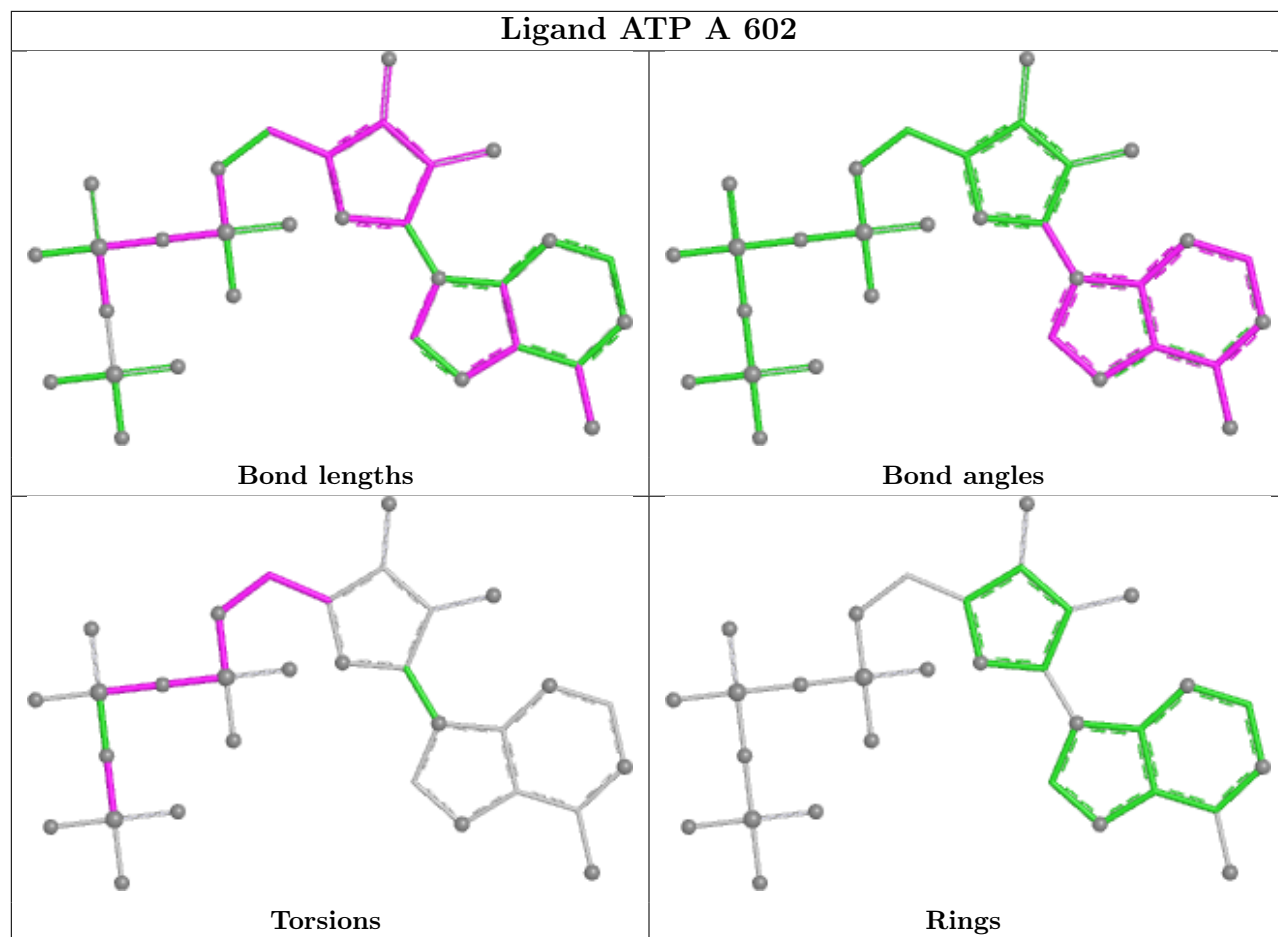




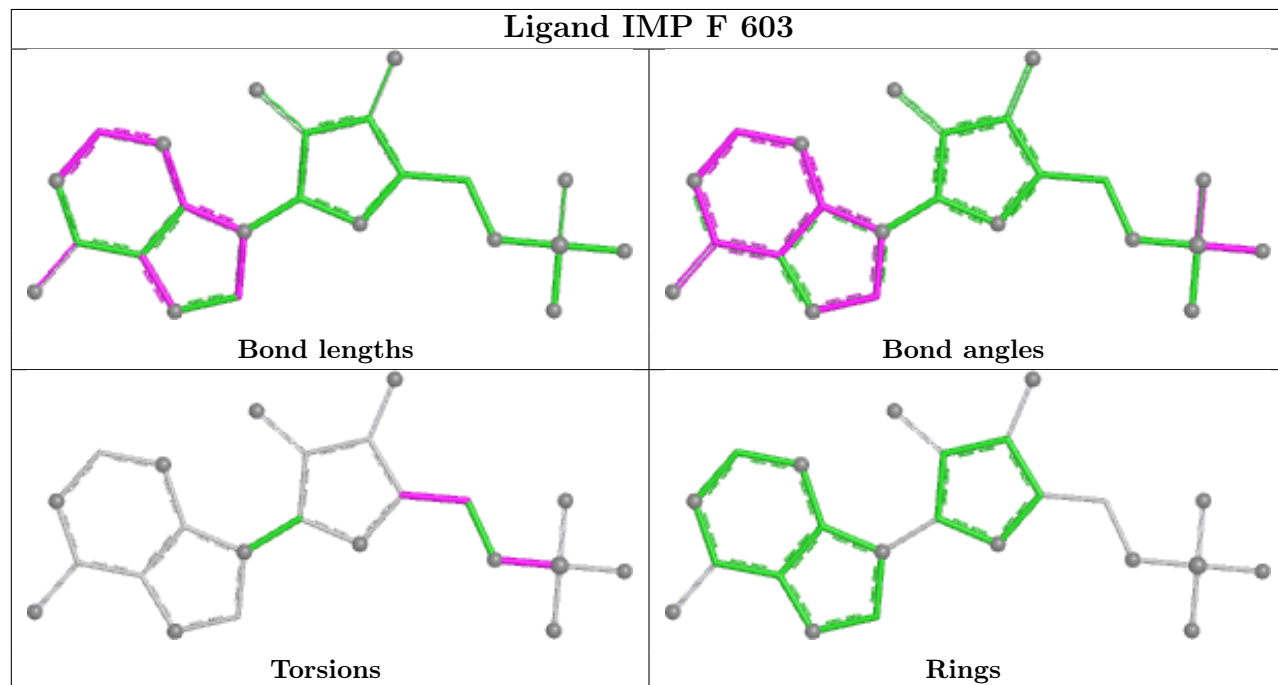


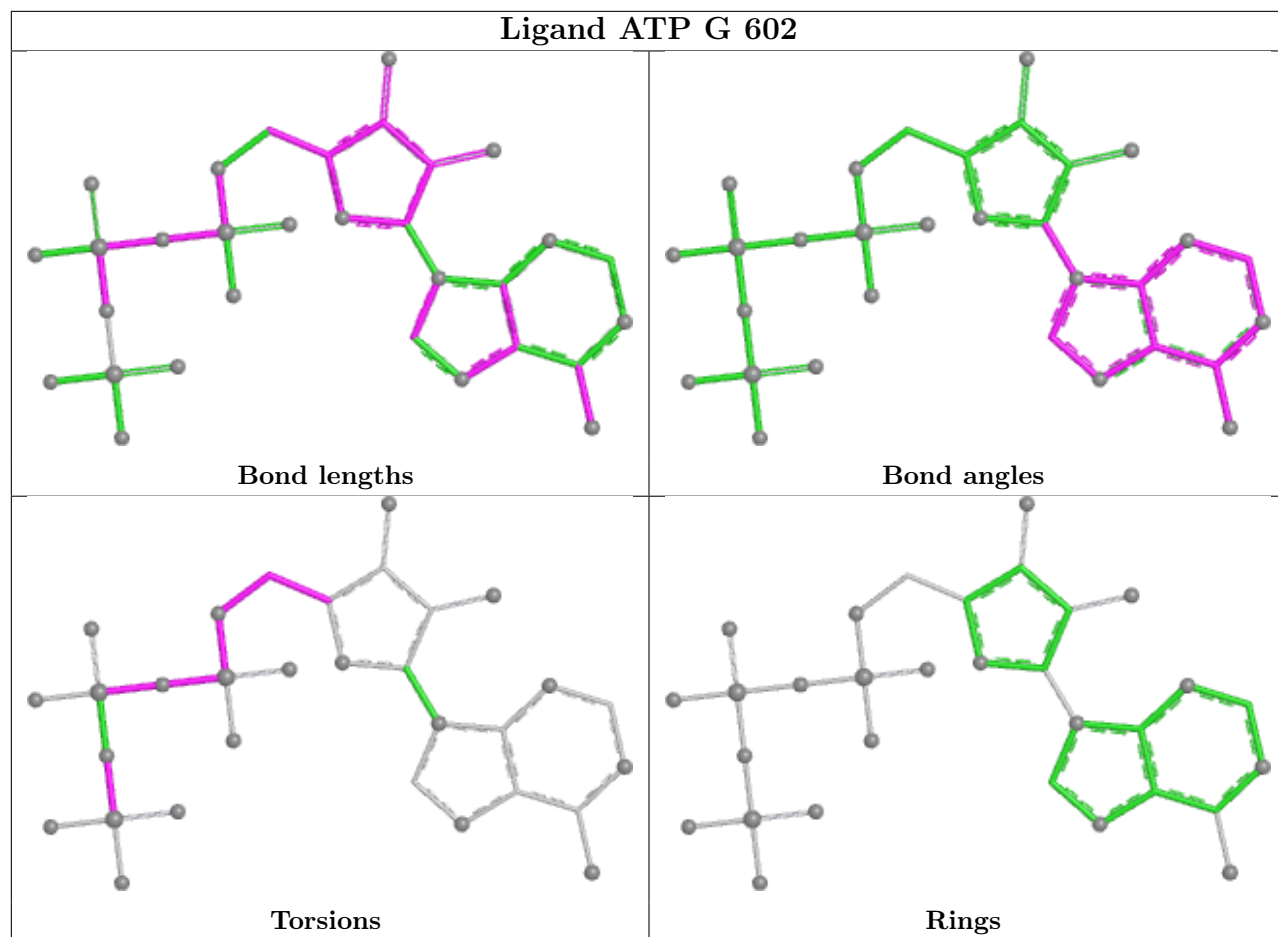


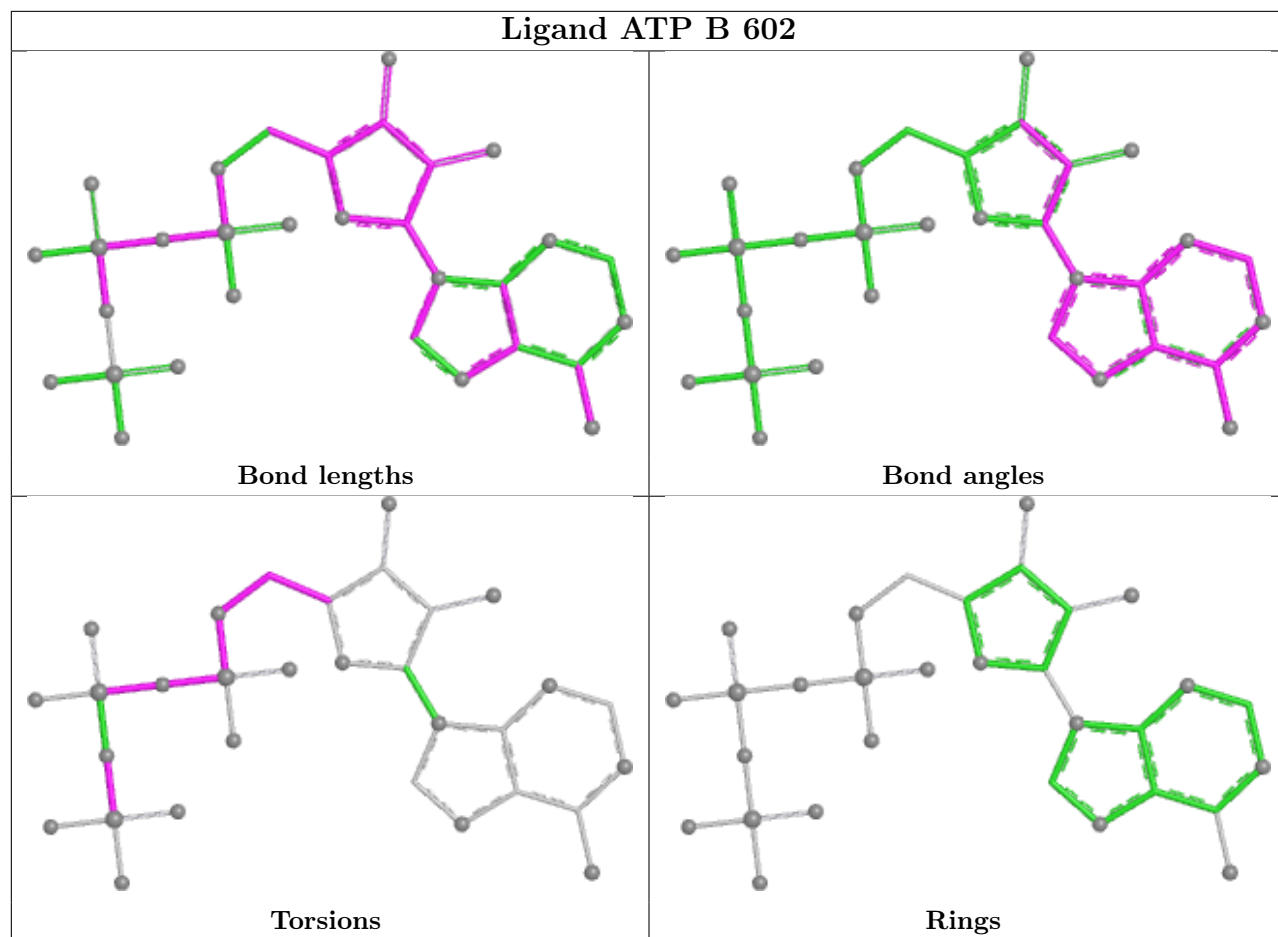
## Ligand ATP A 602

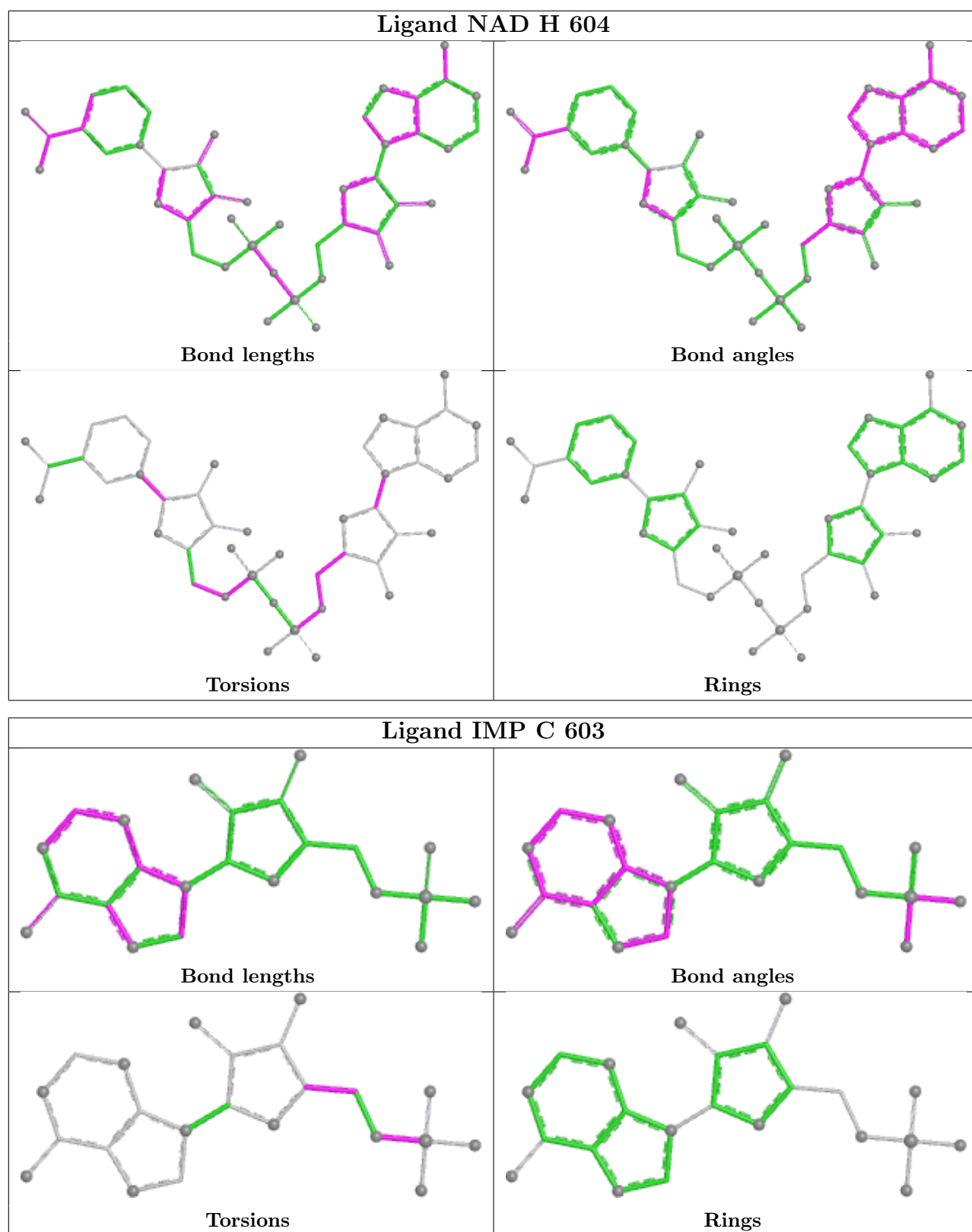


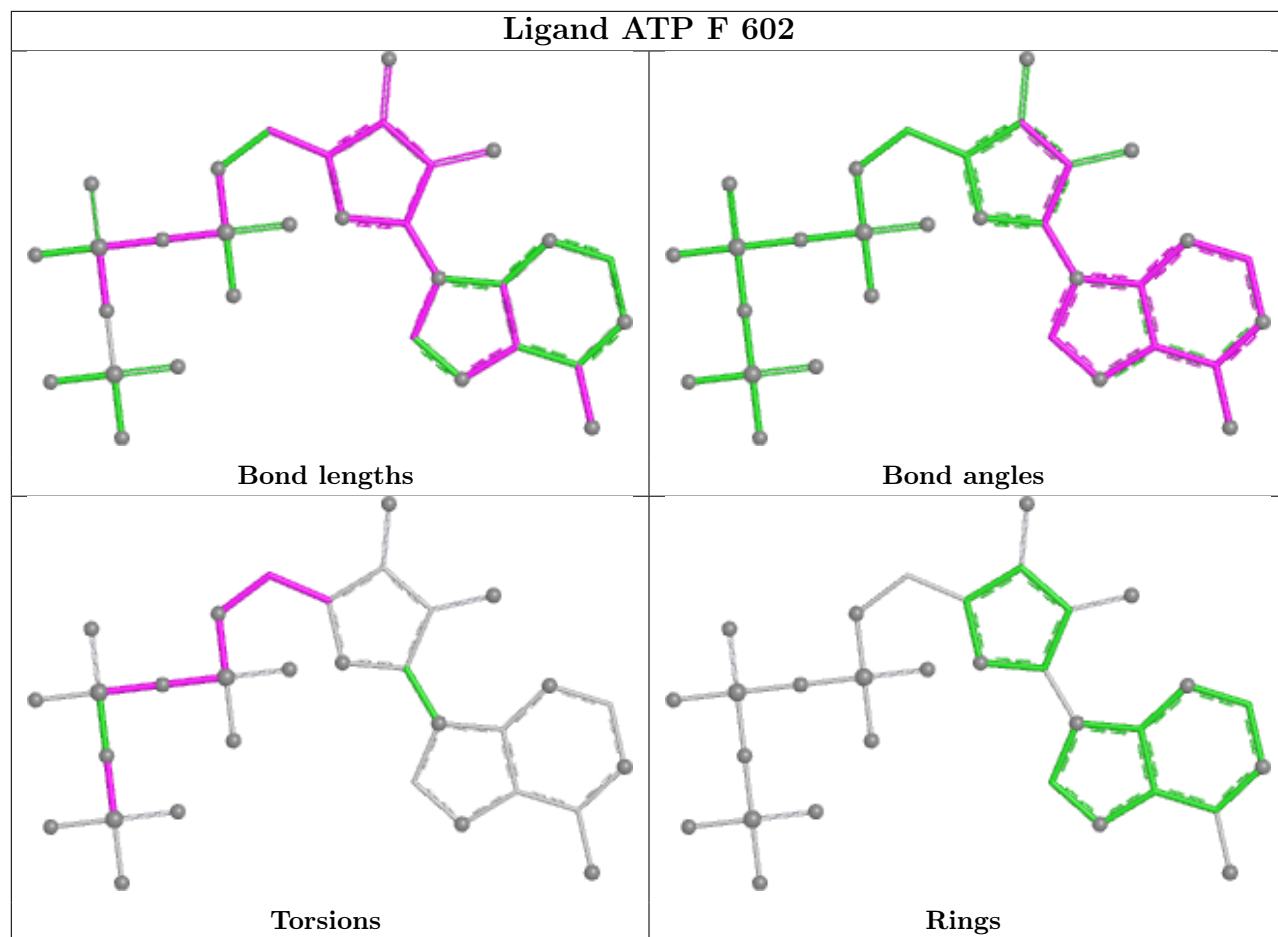
## Ligand IMP F 603



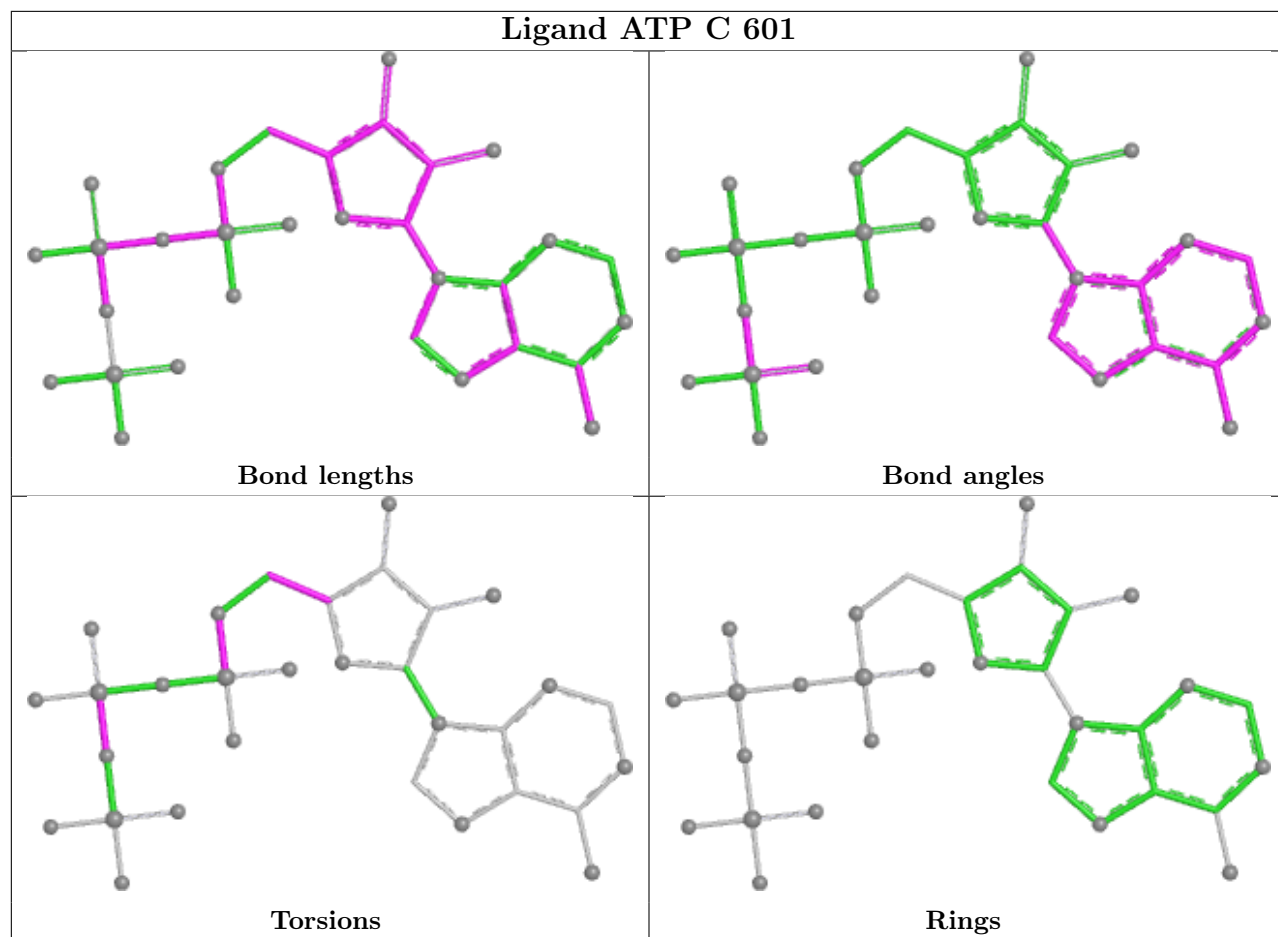




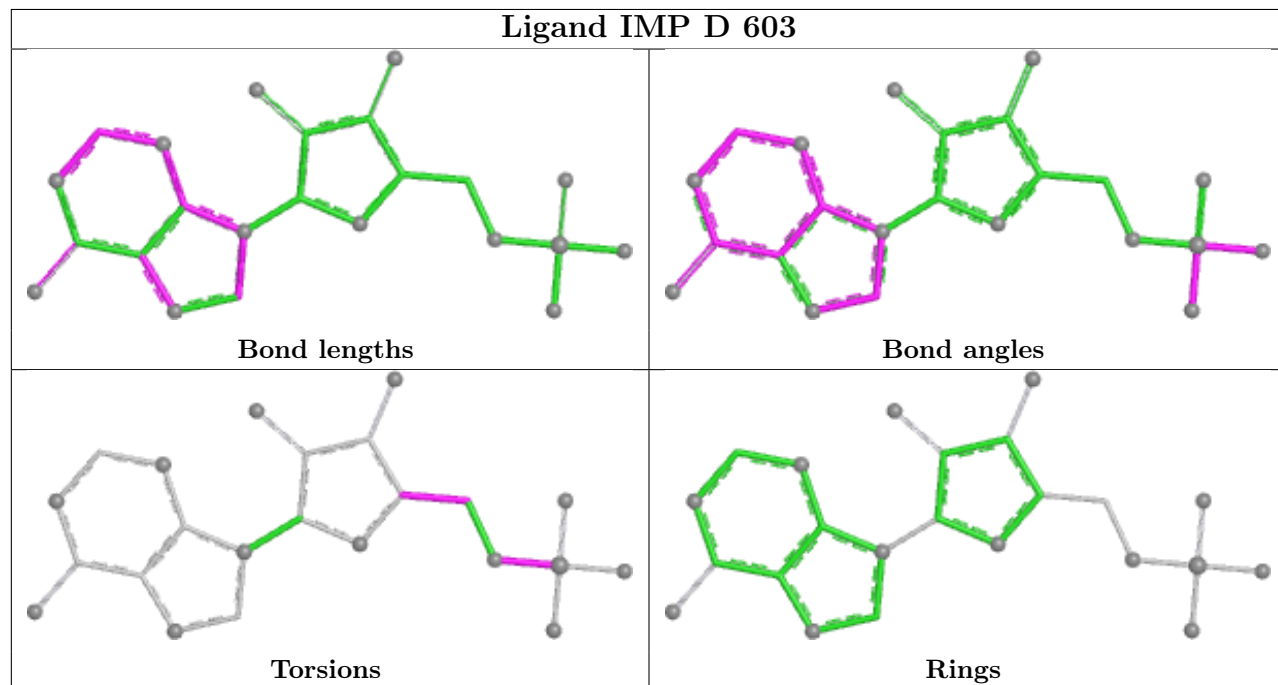


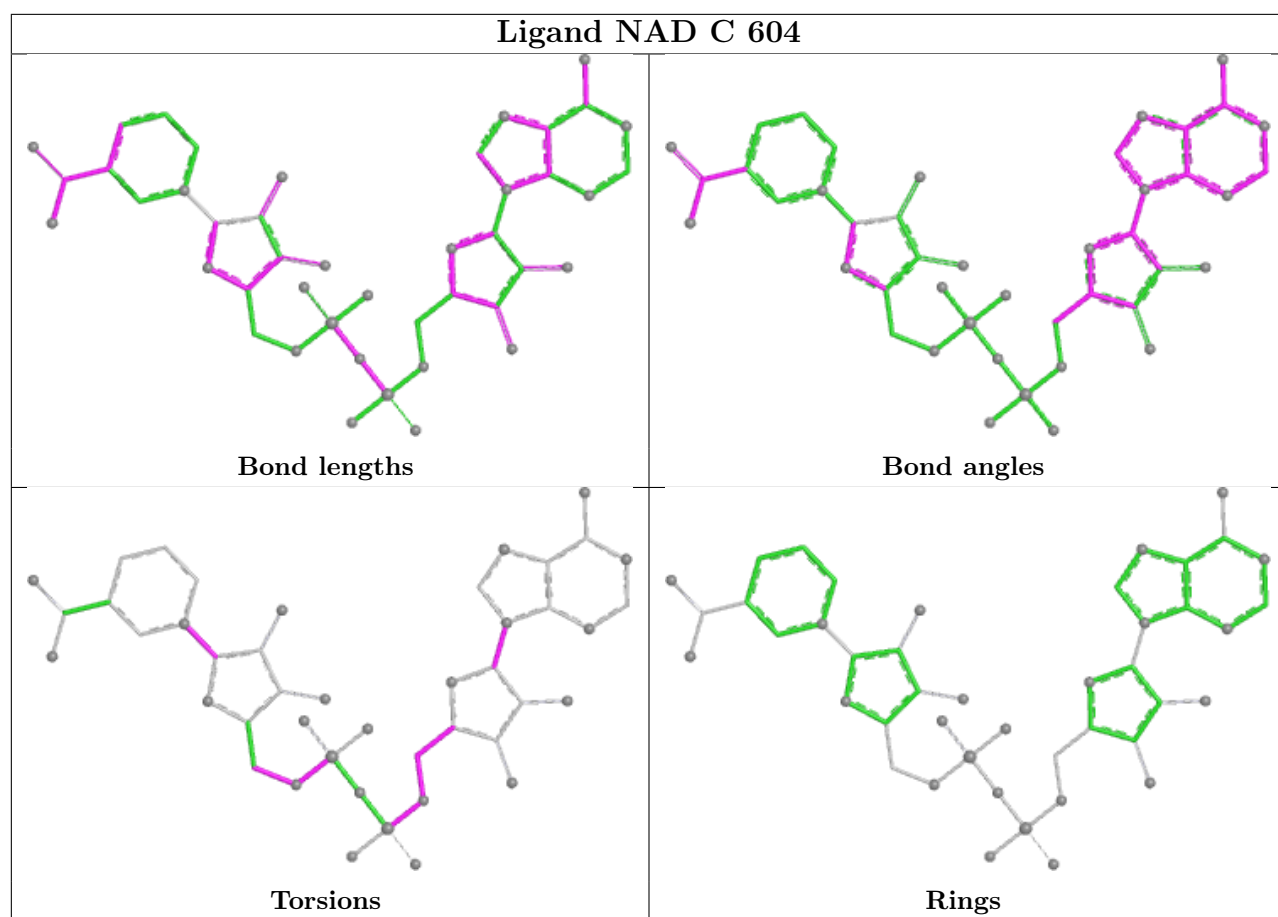


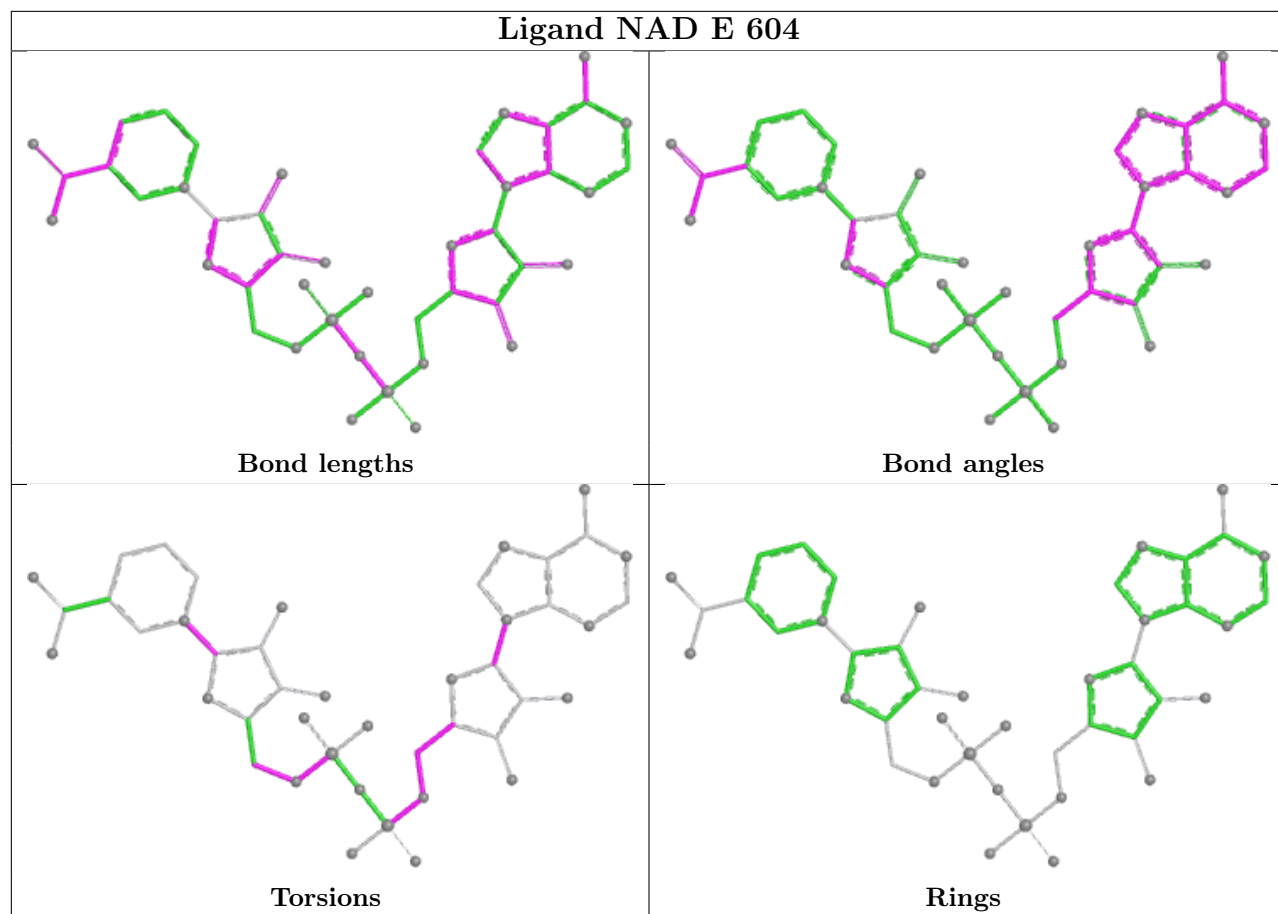
## Ligand ATP C 601

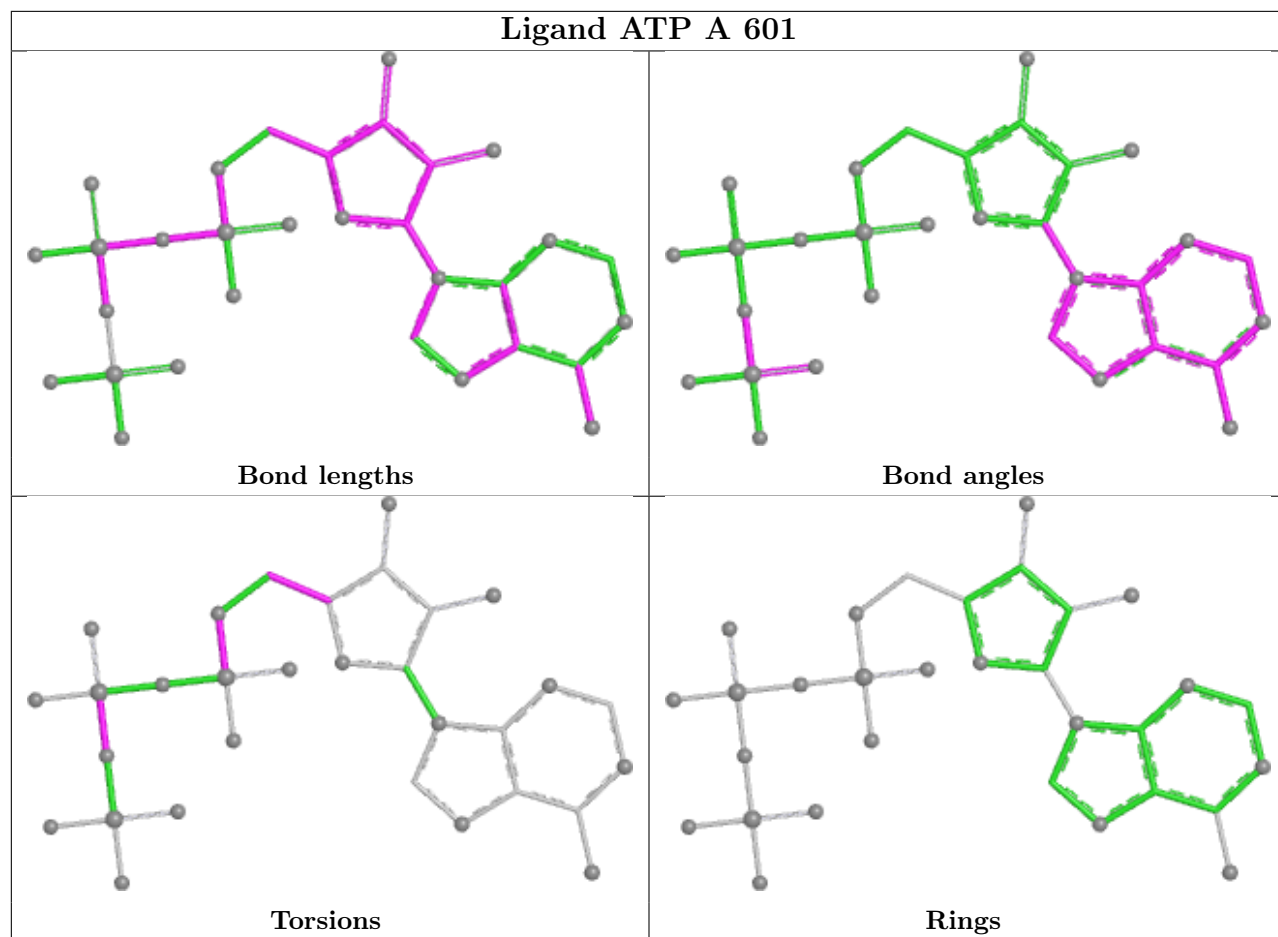


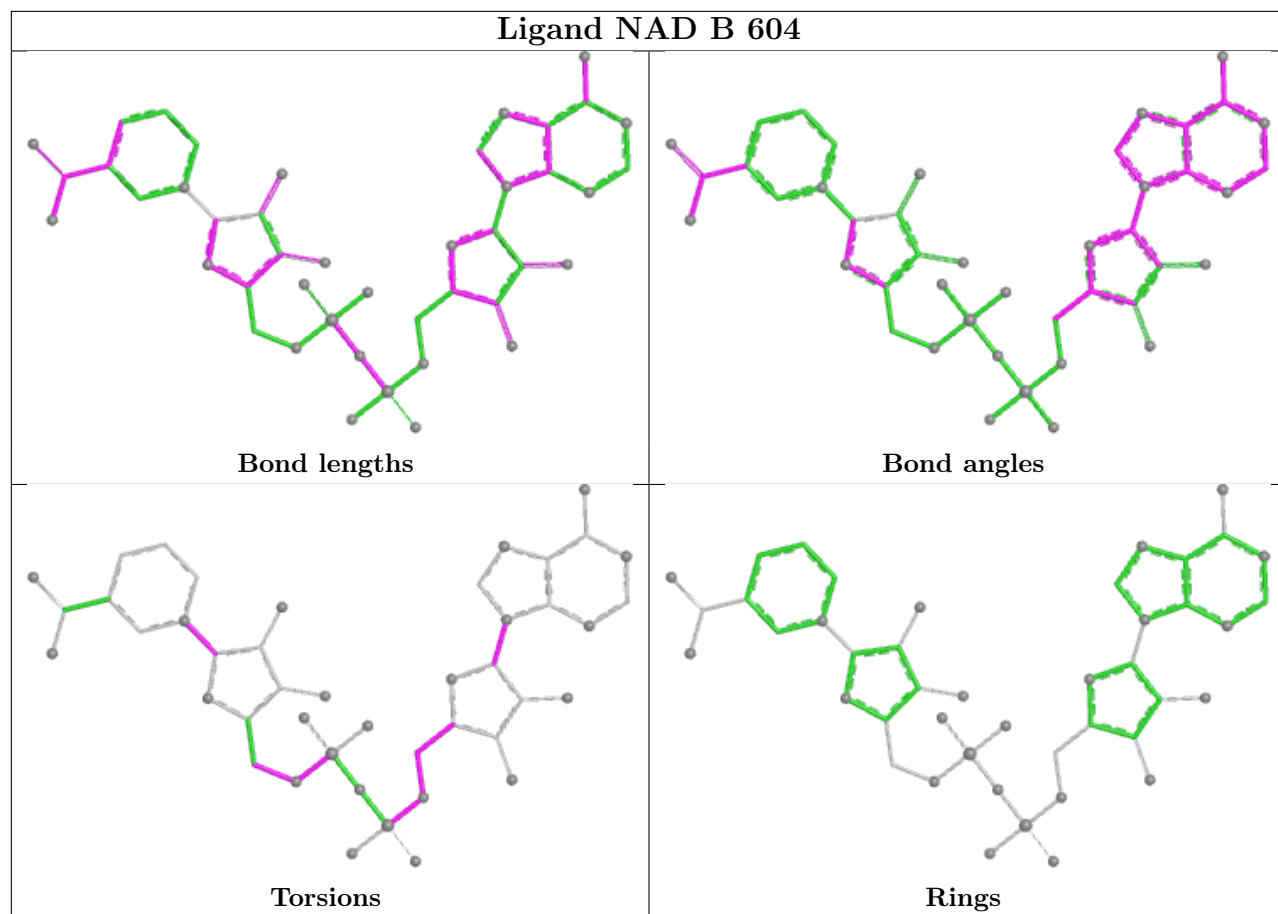
## Ligand IMP D 603

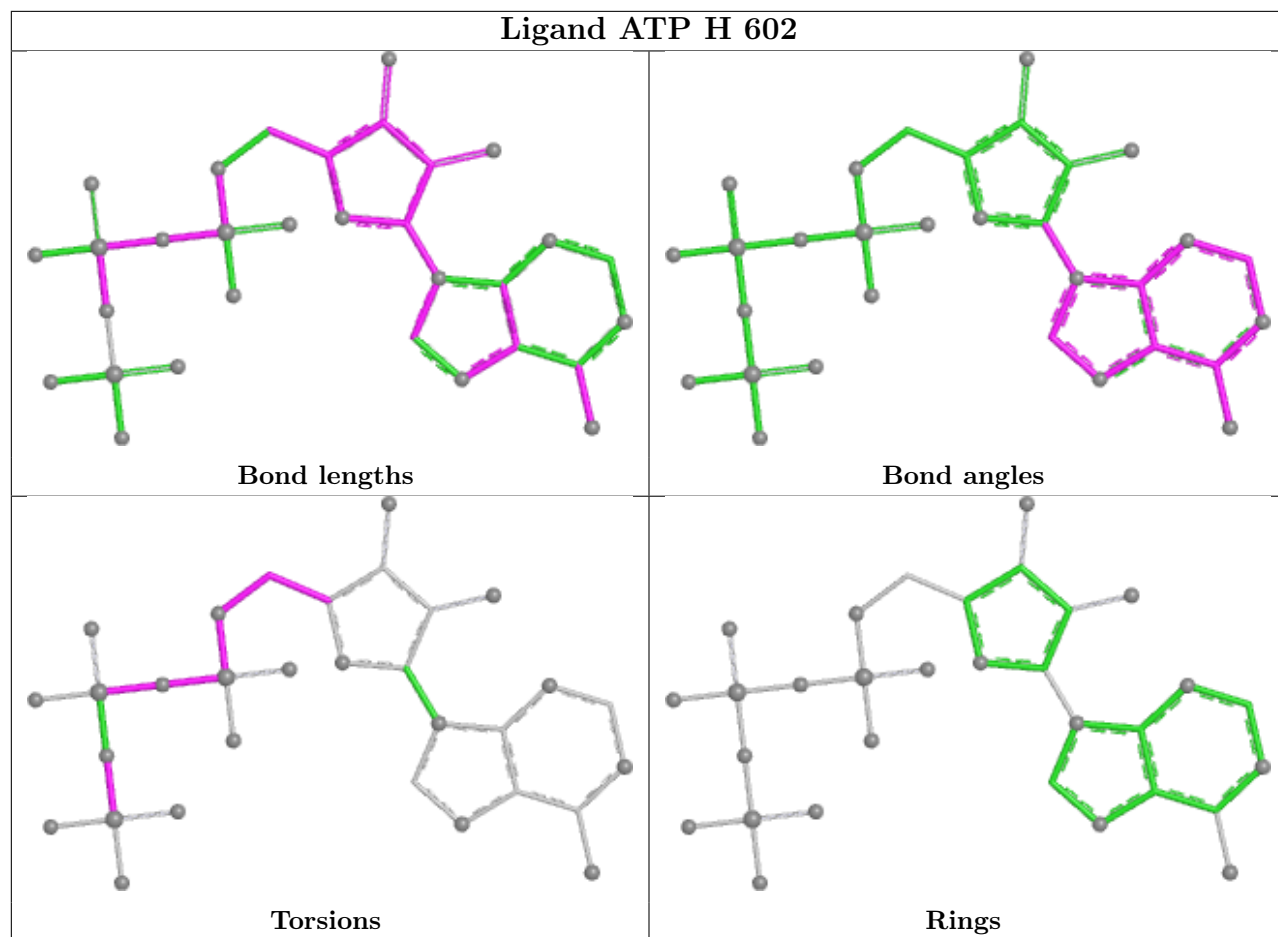


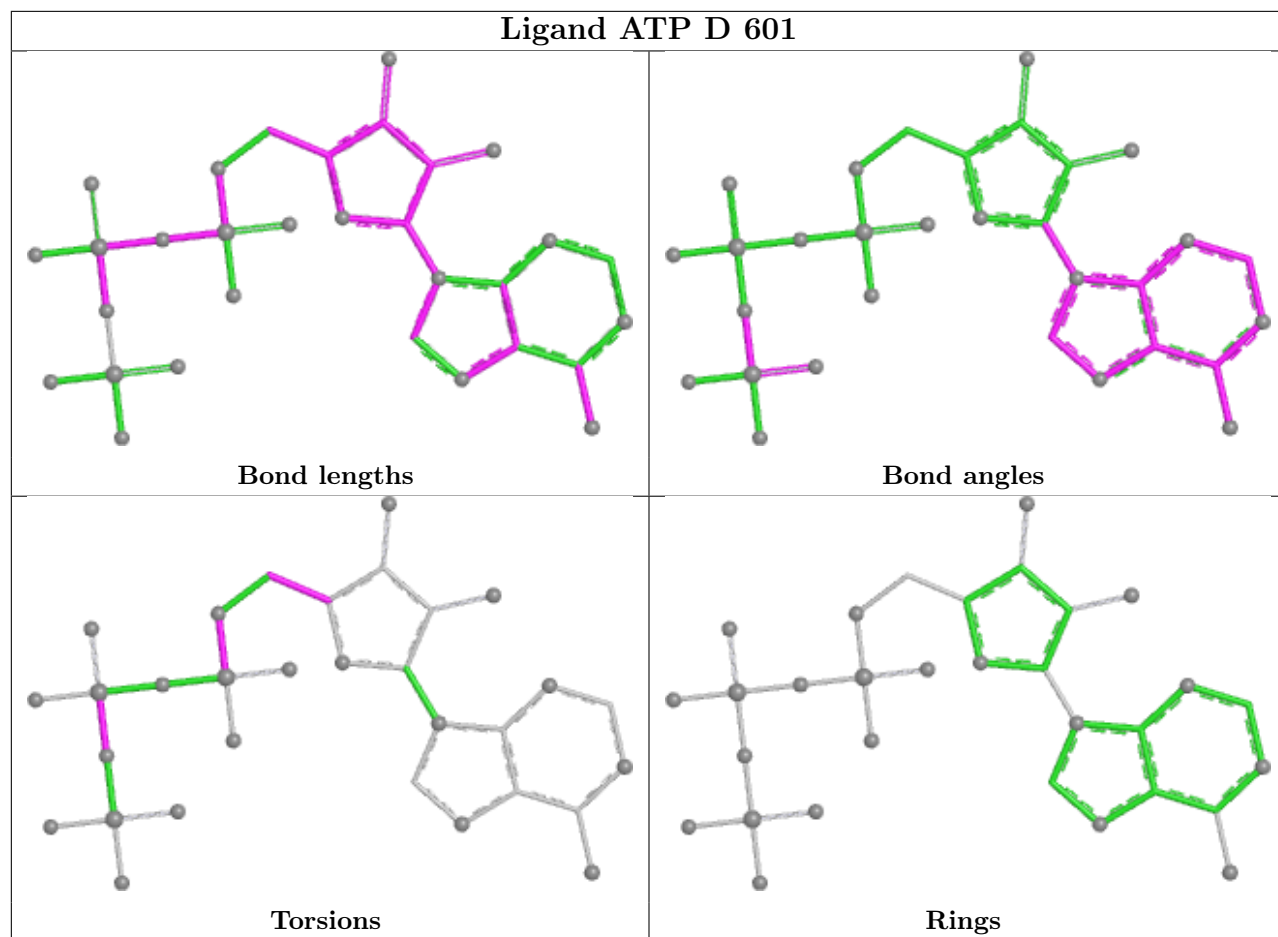




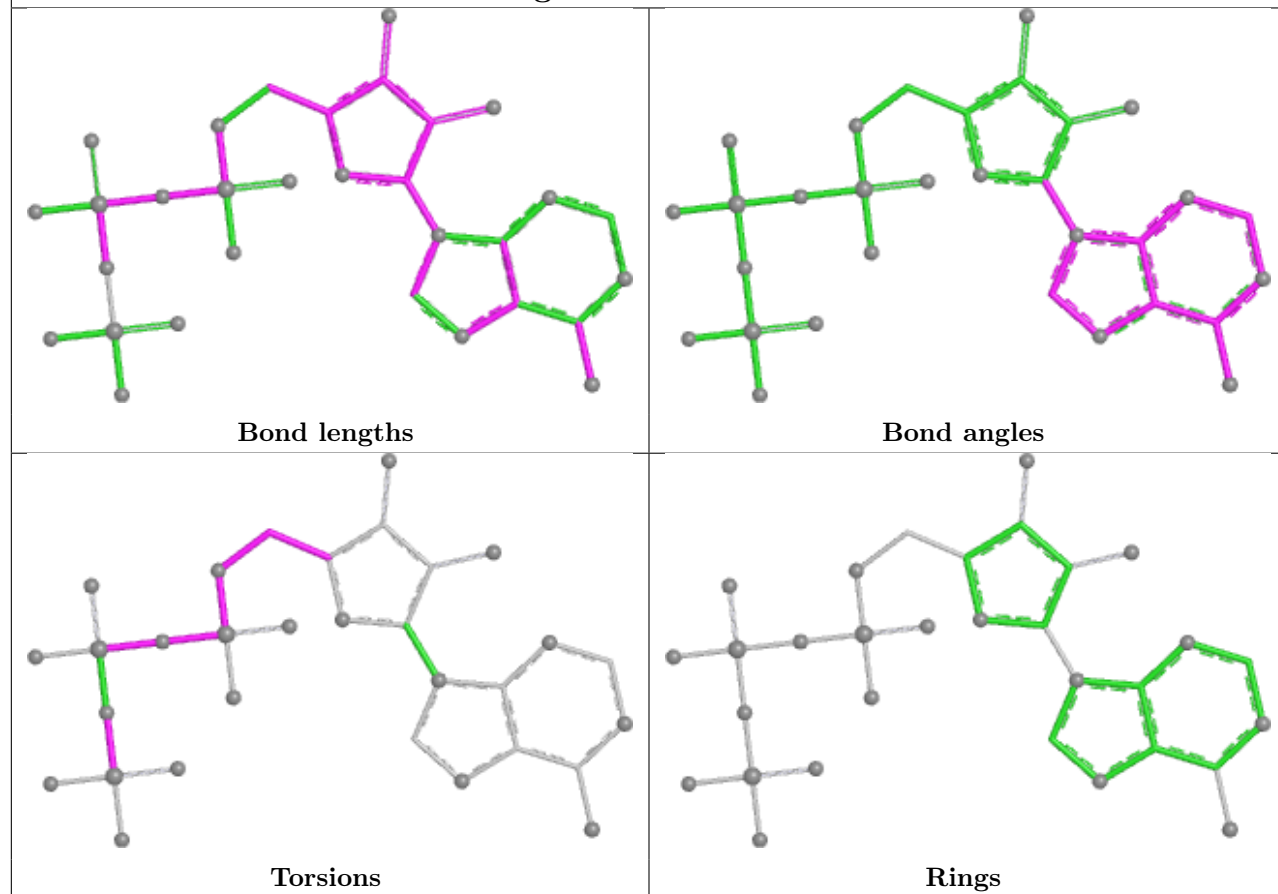




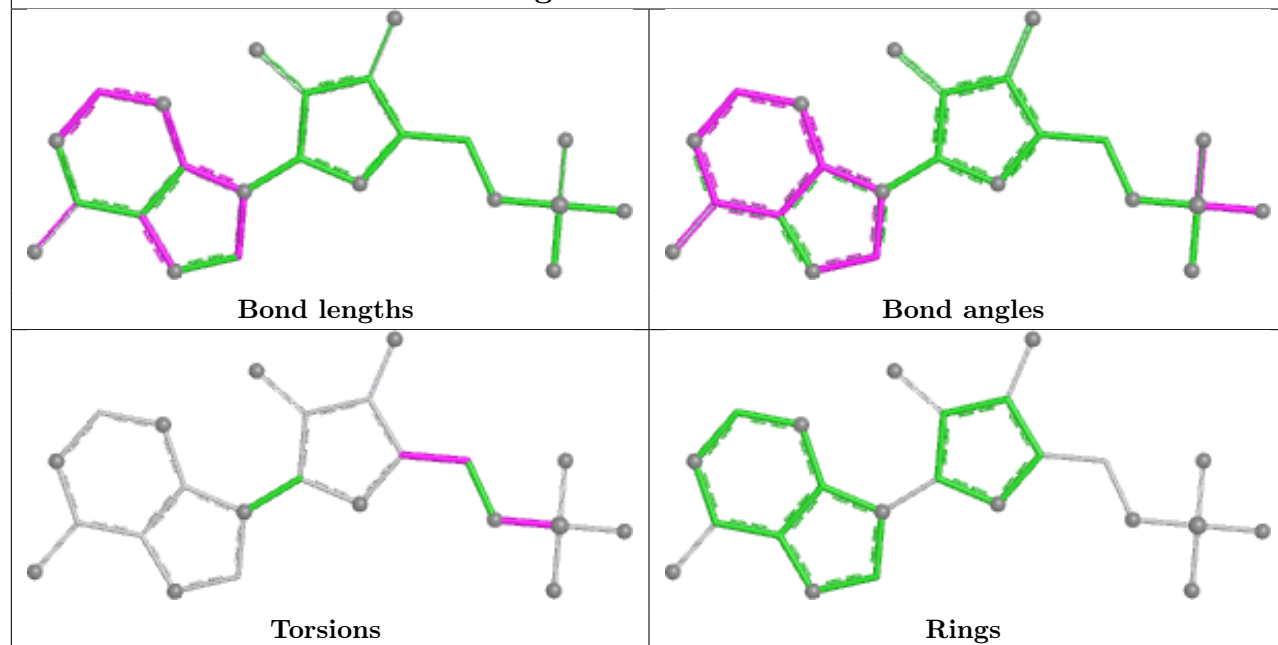




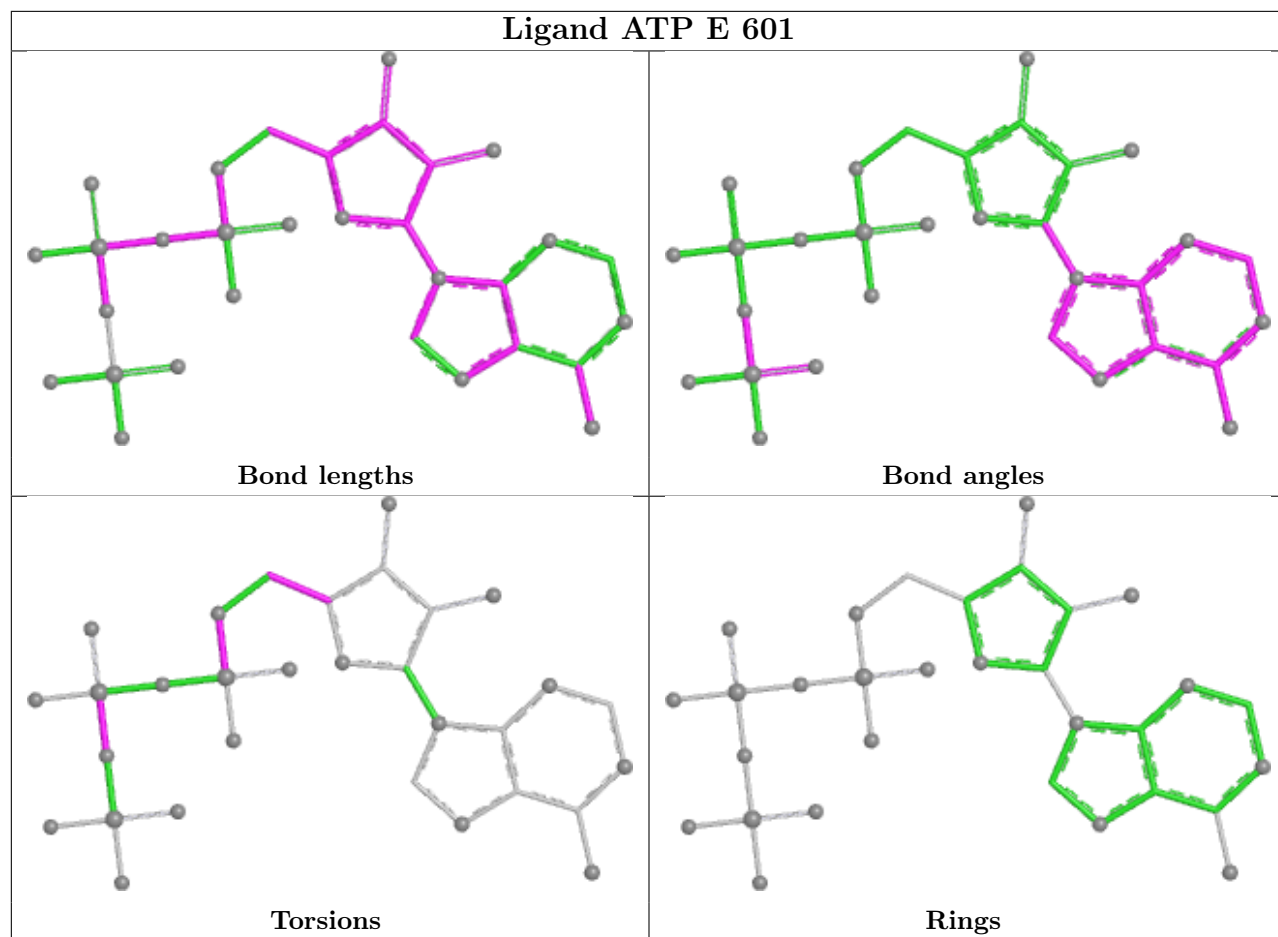
## Ligand ATP E 602

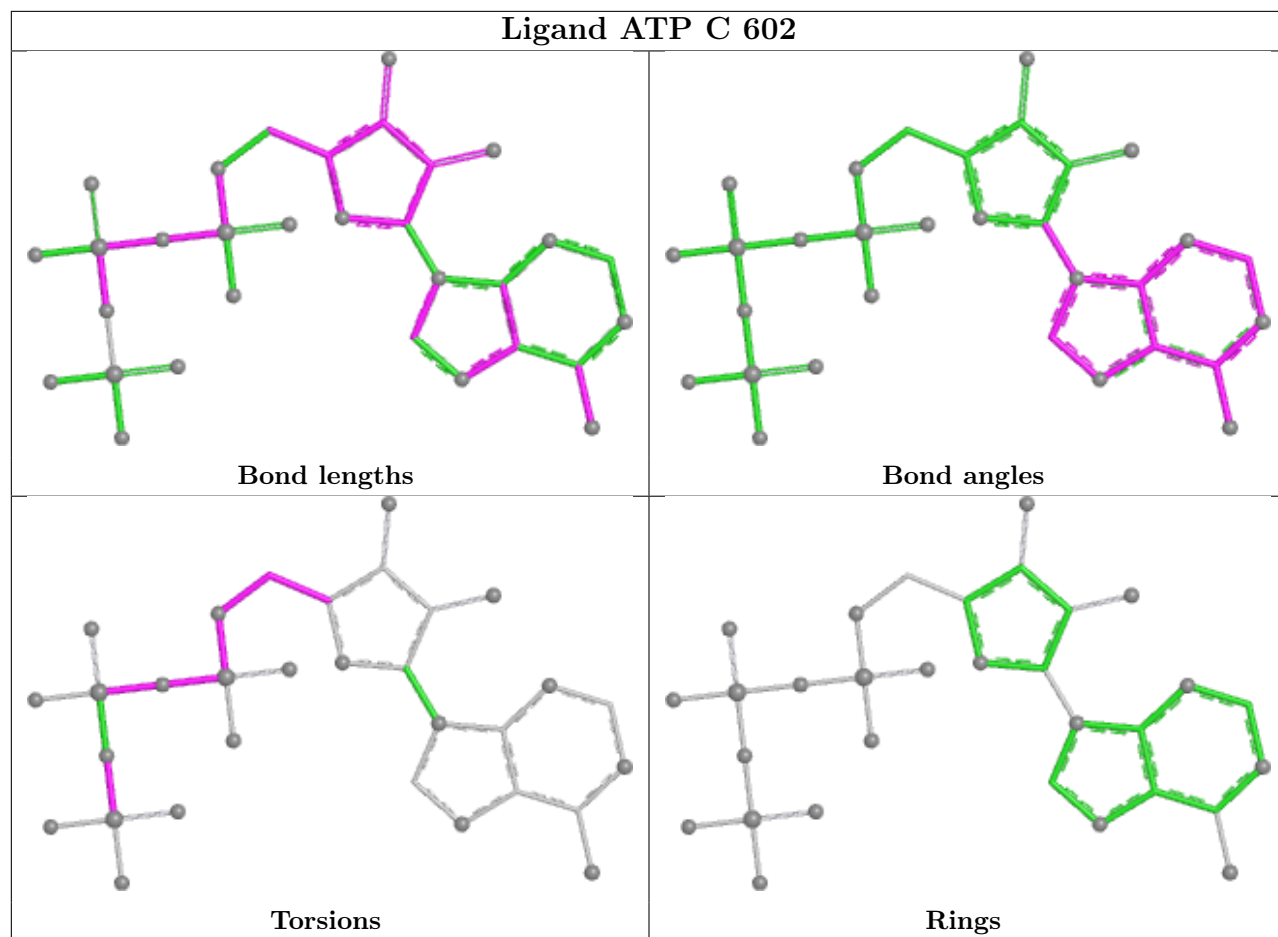


## Ligand IMP E 603

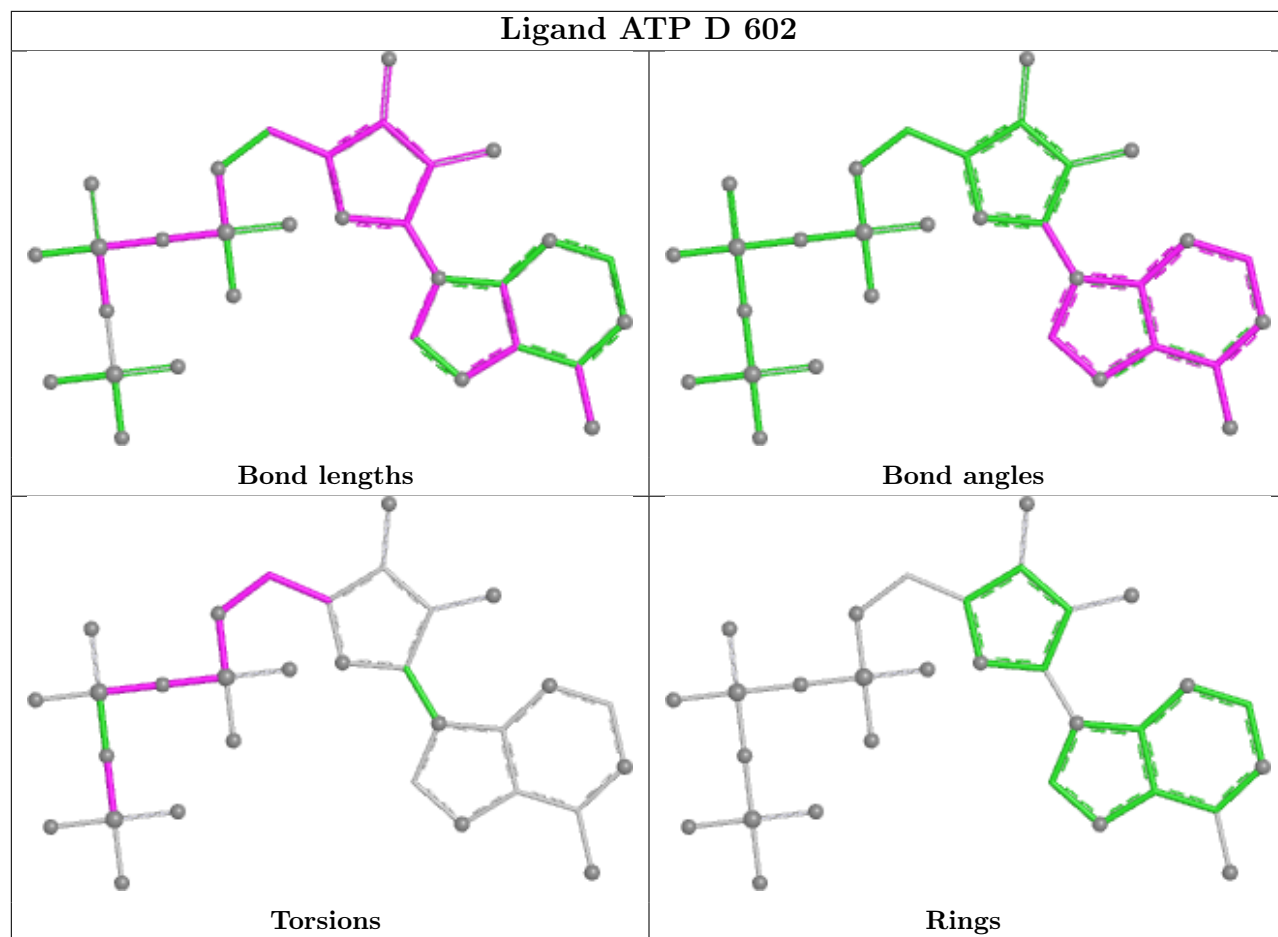


## Ligand ATP E 601

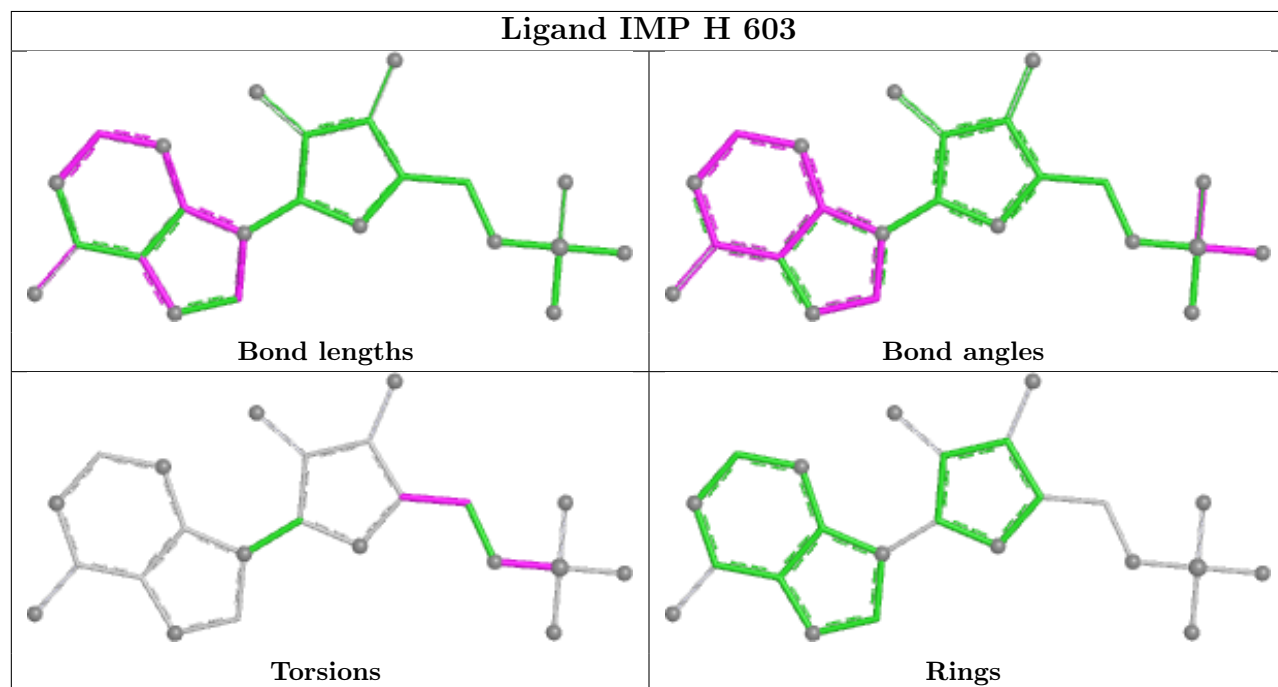


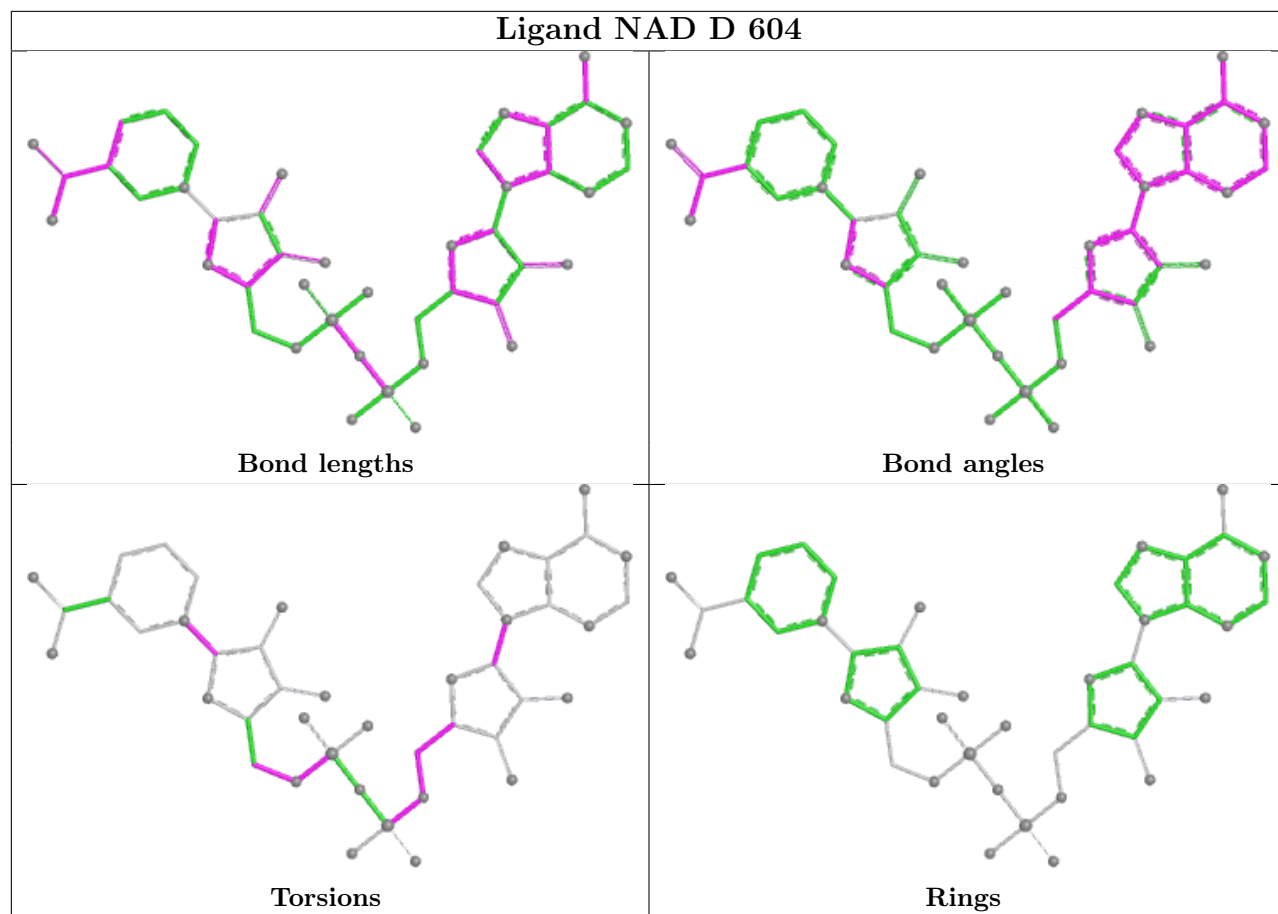


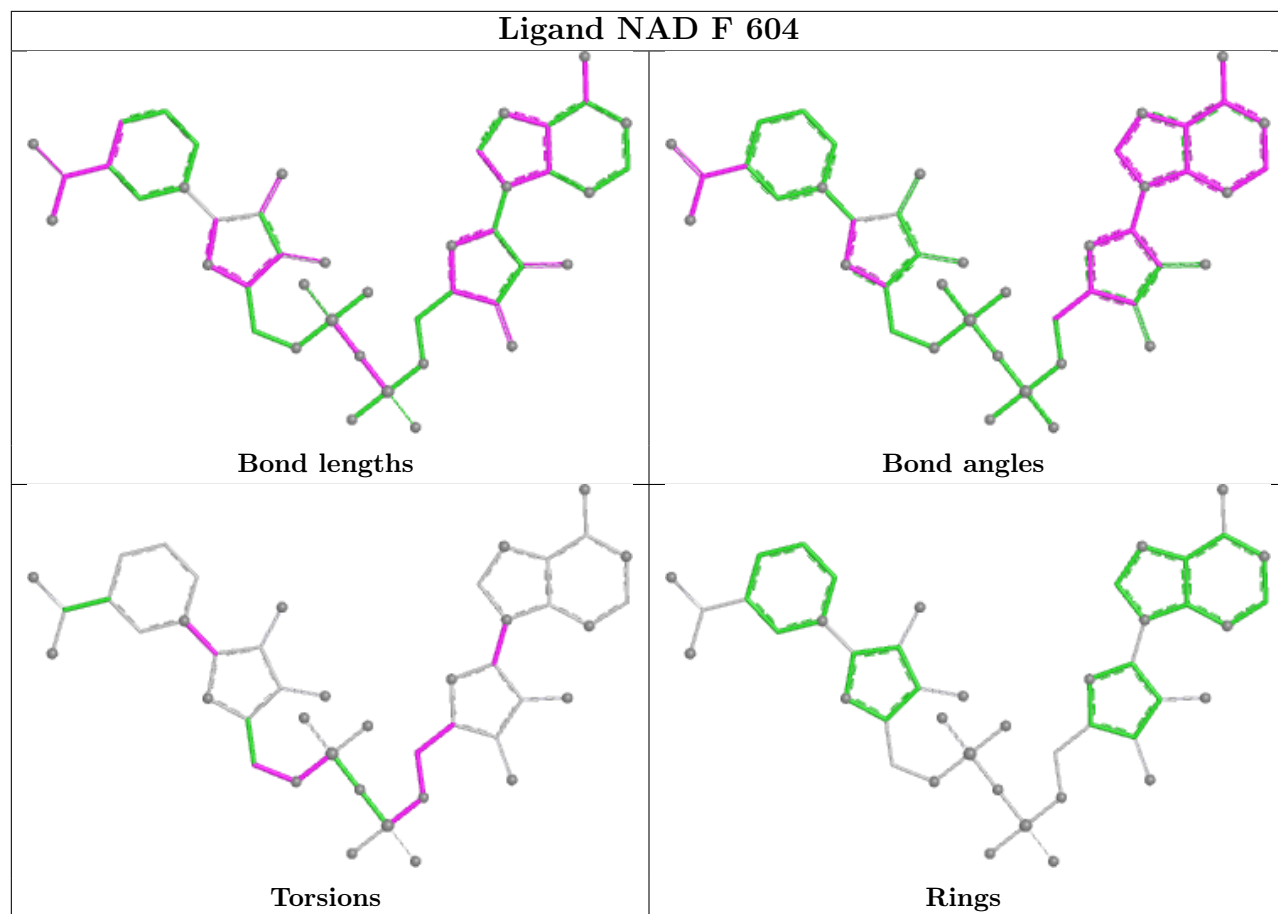
## Ligand ATP D 602



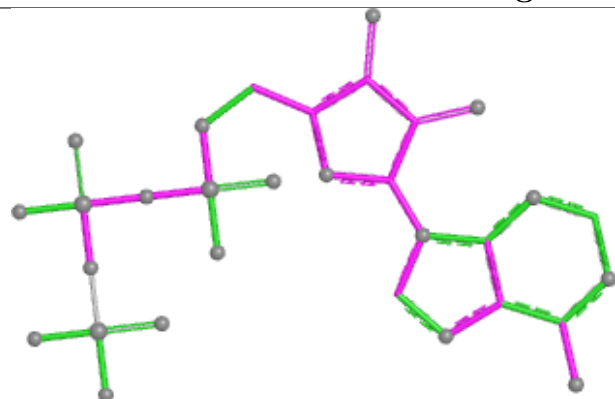
## Ligand IMP H 603



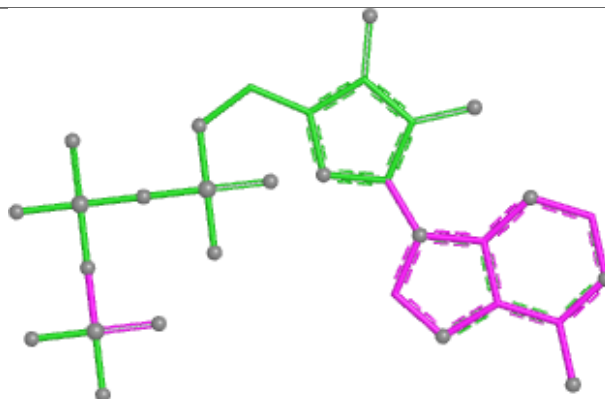




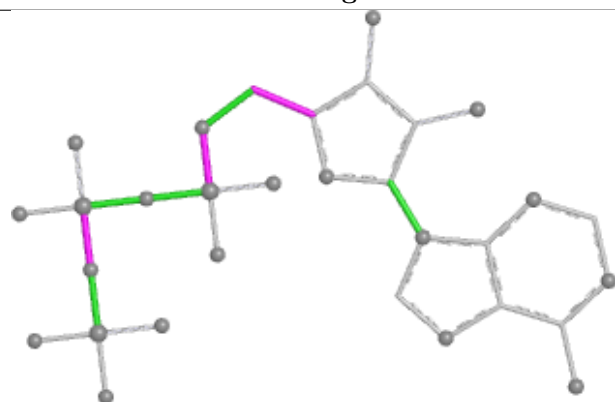
## Ligand ATP G 601



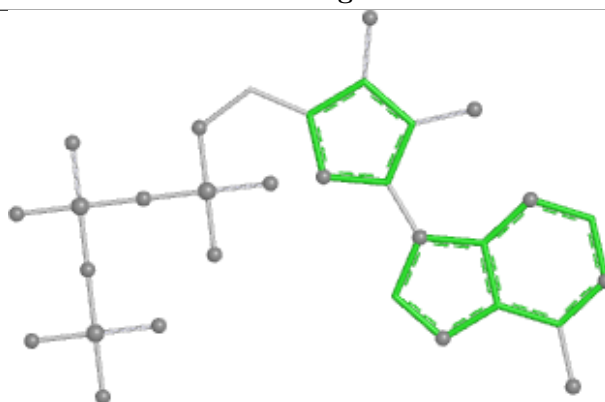
Bond lengths



Bond angles

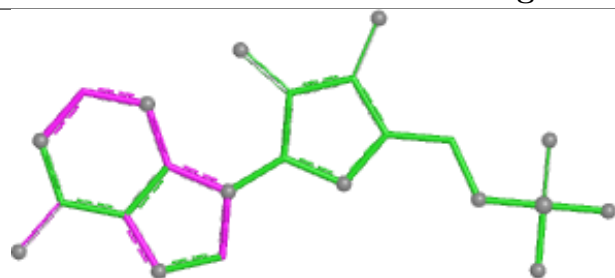


Torsions

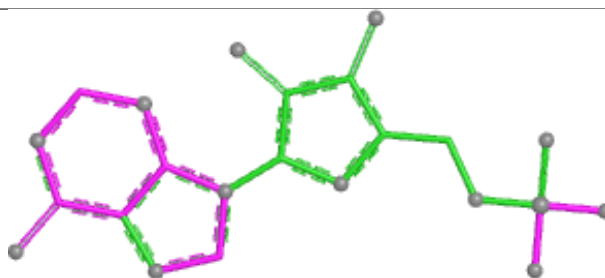


Rings

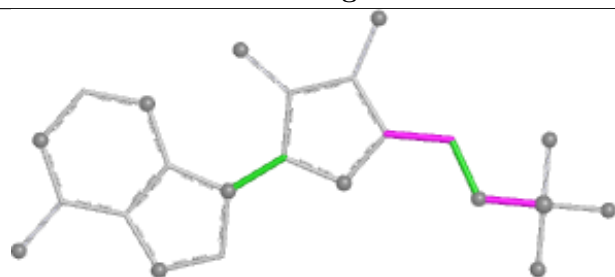
## Ligand IMP A 603



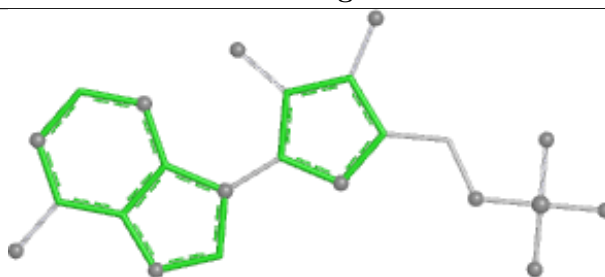
Bond lengths



Bond angles

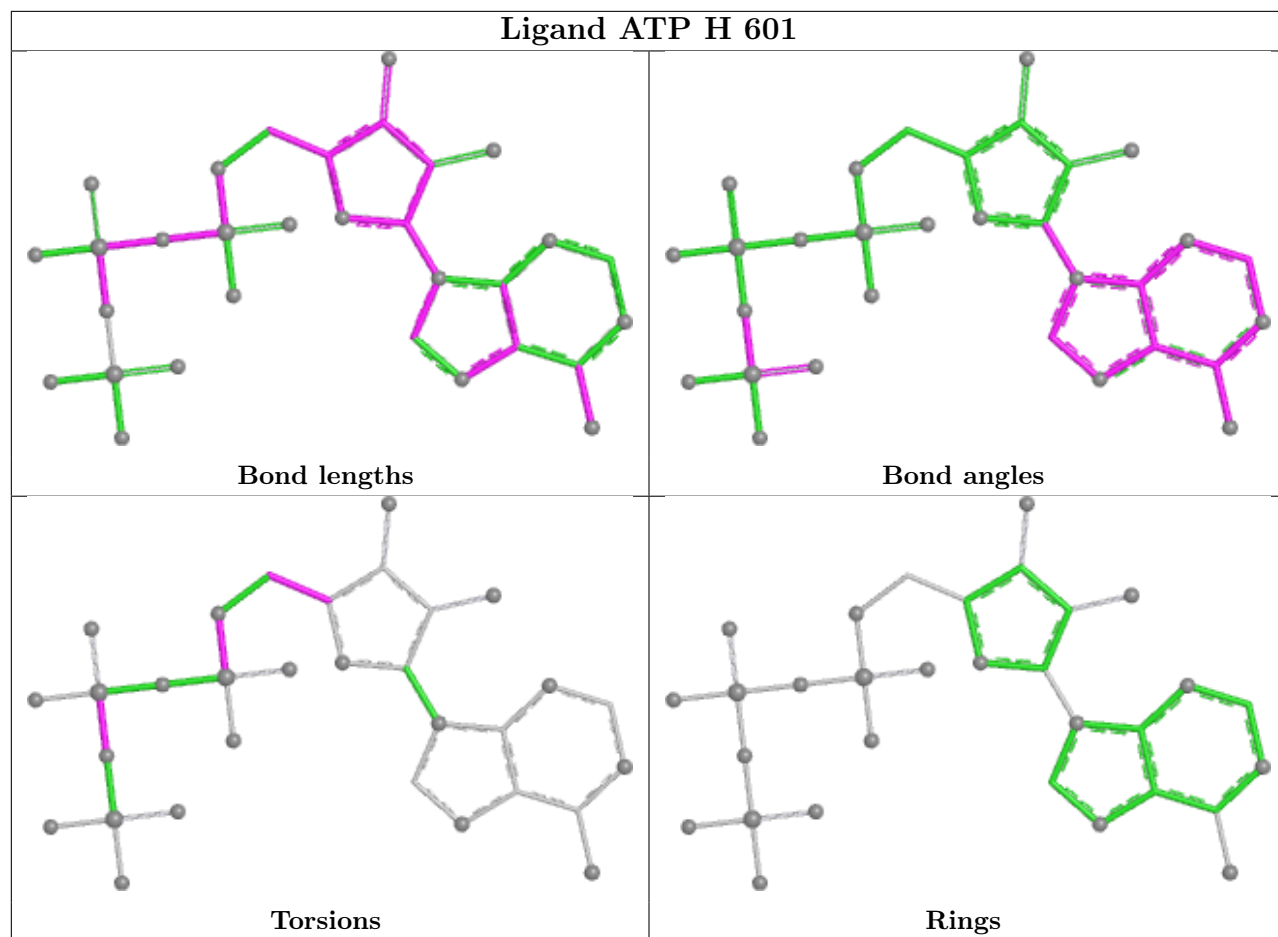


Torsions

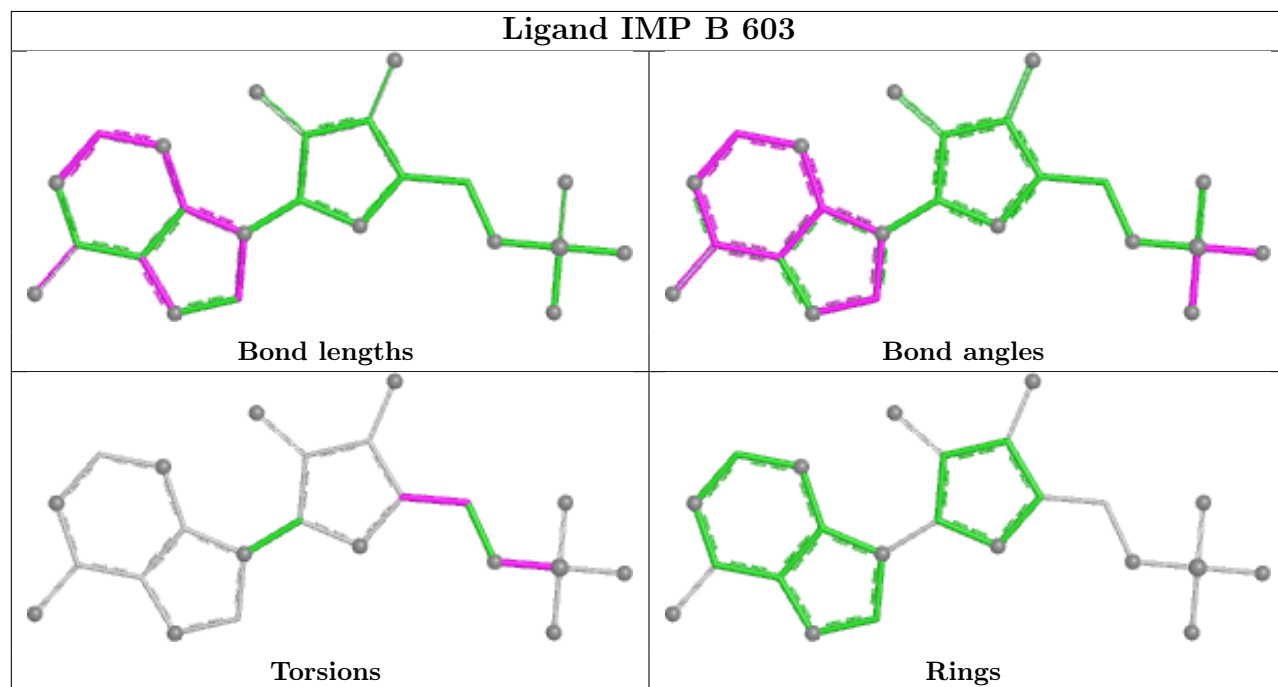


Rings

## Ligand ATP H 601



## Ligand IMP B 603



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

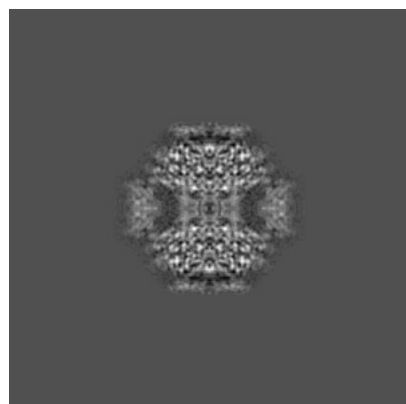
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20688. These allow visual inspection of the internal detail of the map and identification of artifacts.

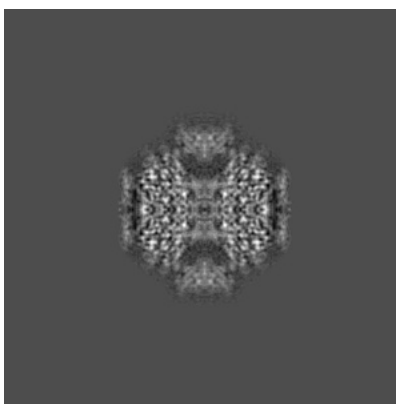
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

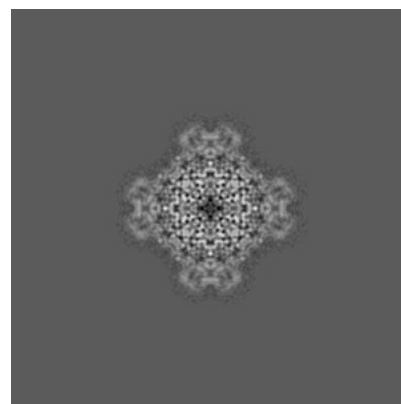
#### 6.1.1 Primary map



X

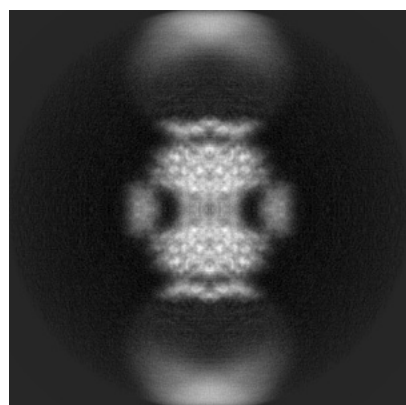


Y

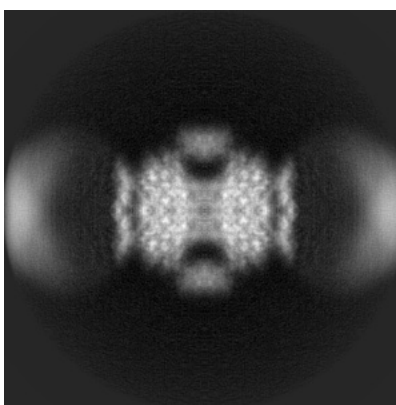


Z

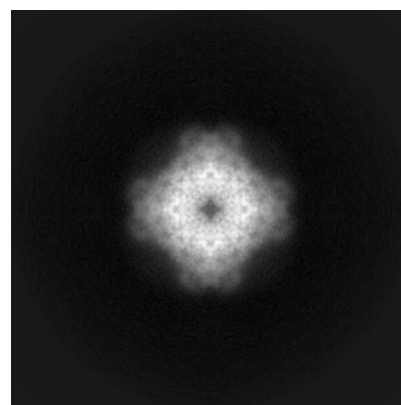
#### 6.1.2 Raw map



X



Y

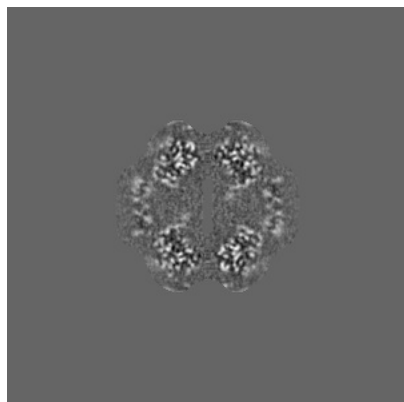


Z

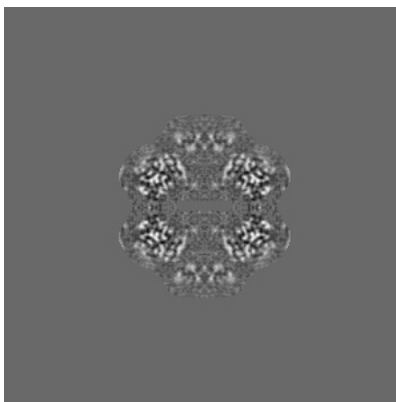
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

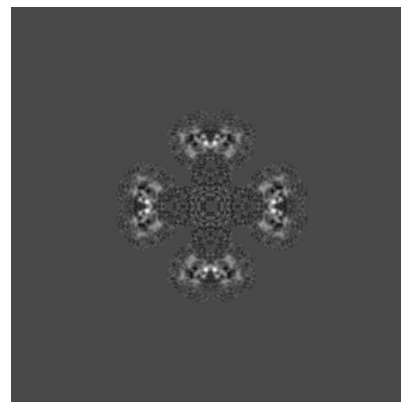
### 6.2.1 Primary map



X Index: 160

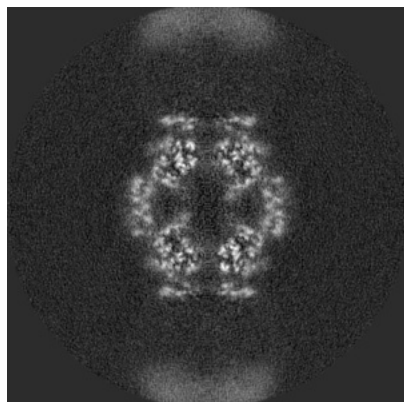


Y Index: 160

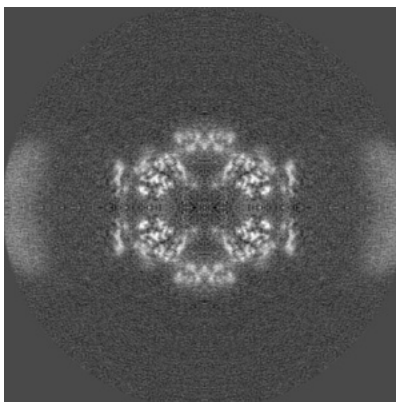


Z Index: 160

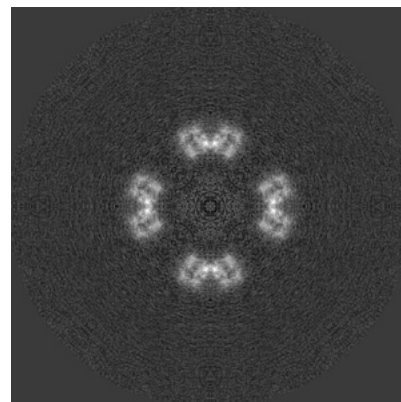
### 6.2.2 Raw map



X Index: 160



Y Index: 160

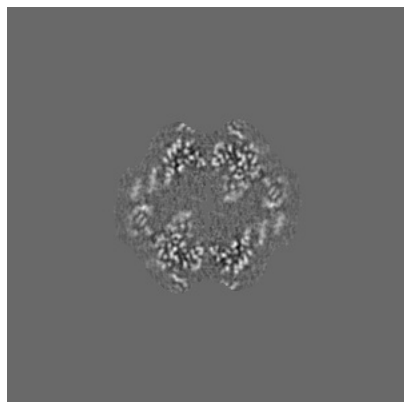


Z Index: 160

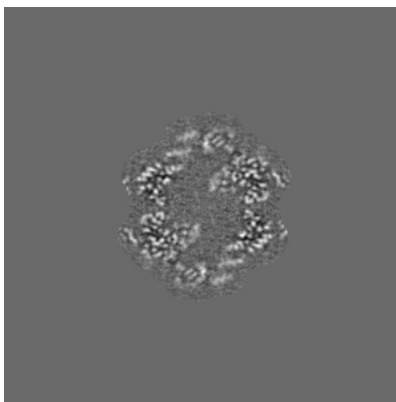
The images above show central slices of the map in three orthogonal directions.

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

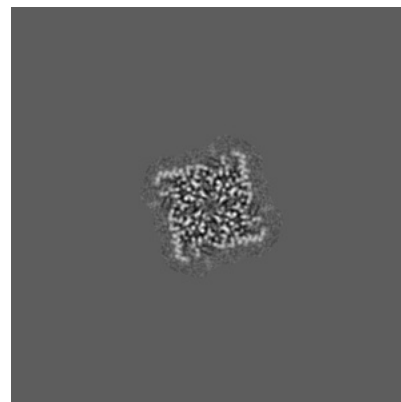
### 6.3.1 Primary map



X Index: 163

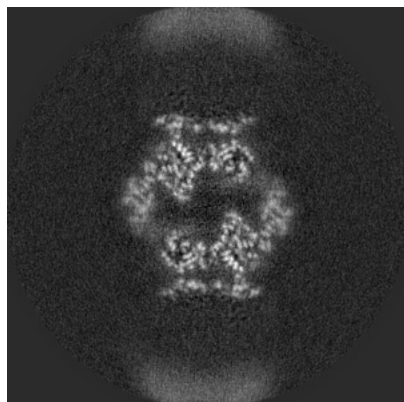


Y Index: 156

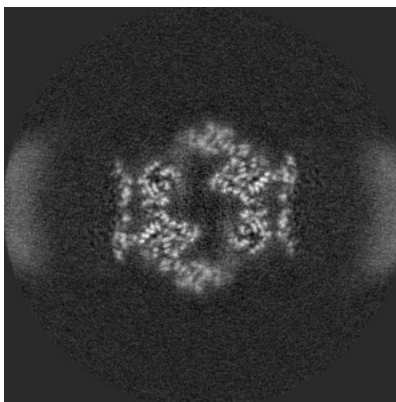


Z Index: 202

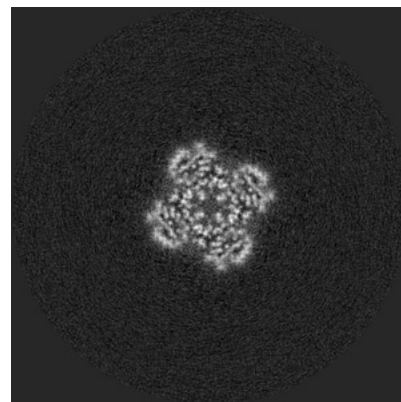
### 6.3.2 Raw map



X Index: 152



Y Index: 153

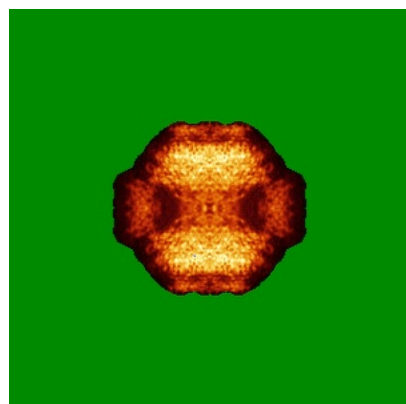


Z Index: 129

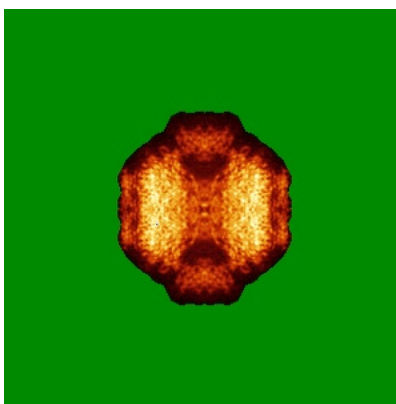
The images above show the largest variance slices of the map in three orthogonal directions.

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

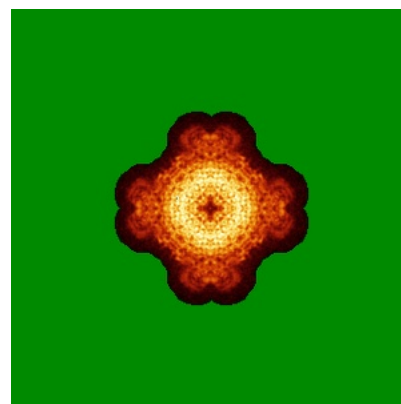
### 6.4.1 Primary map



X

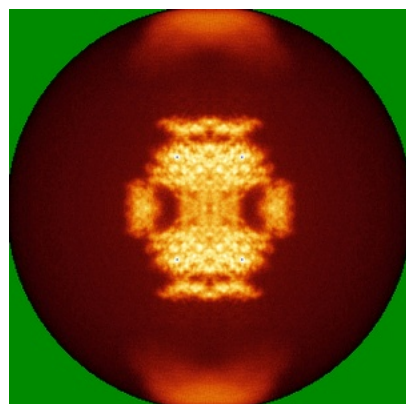


Y

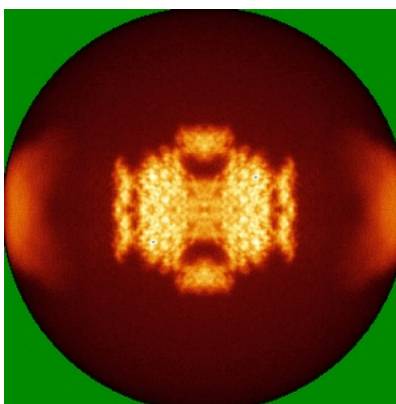


Z

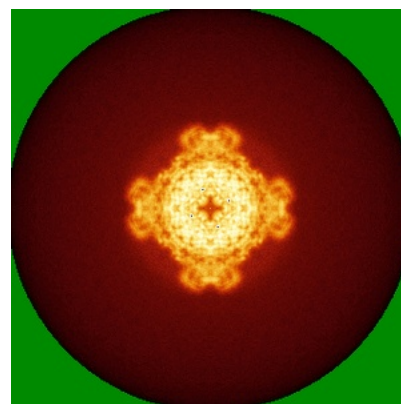
### 6.4.2 Raw map



X



Y

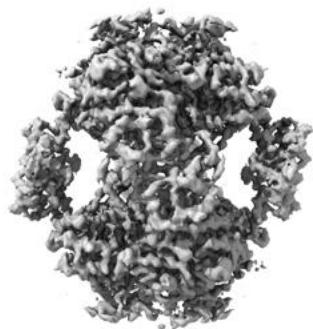


Z

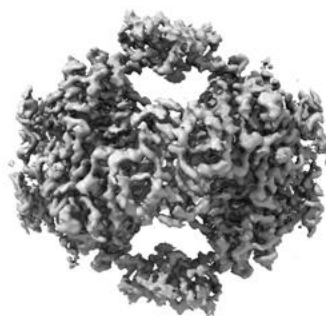
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

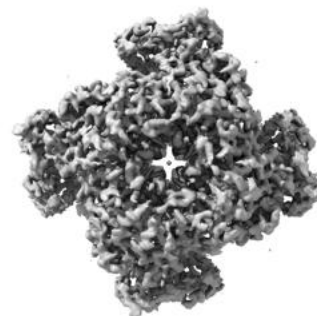
### 6.5.1 Primary map



X



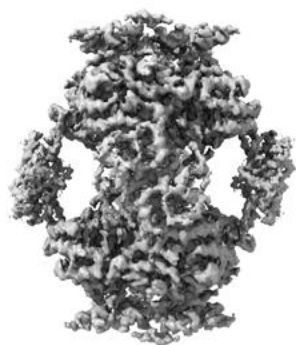
Y



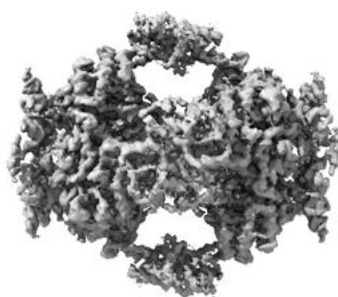
Z

The images above show the 3D surface view of the map at the recommended contour level 17.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

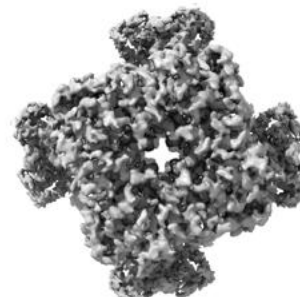
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

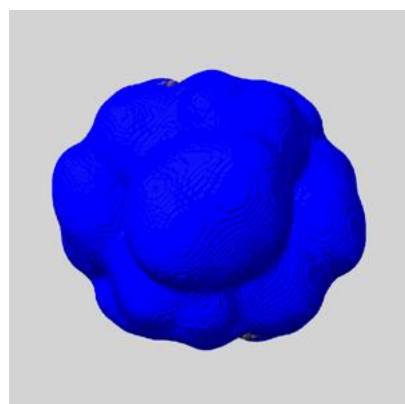
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

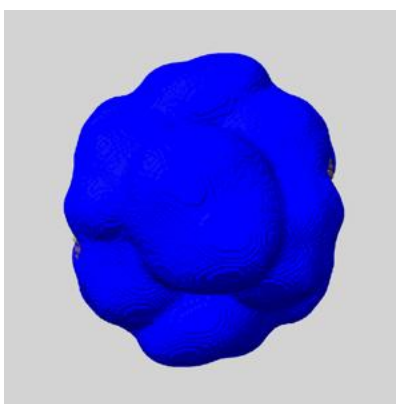
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

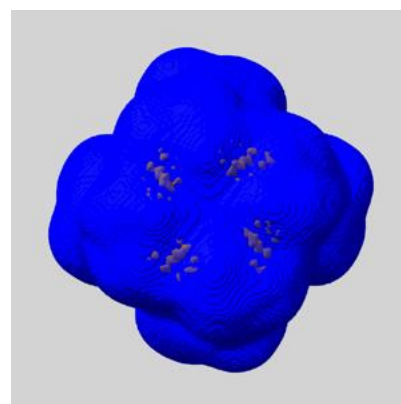
### 6.6.1 emd\_20688\_msk\_1.map [i](#)



X



Y

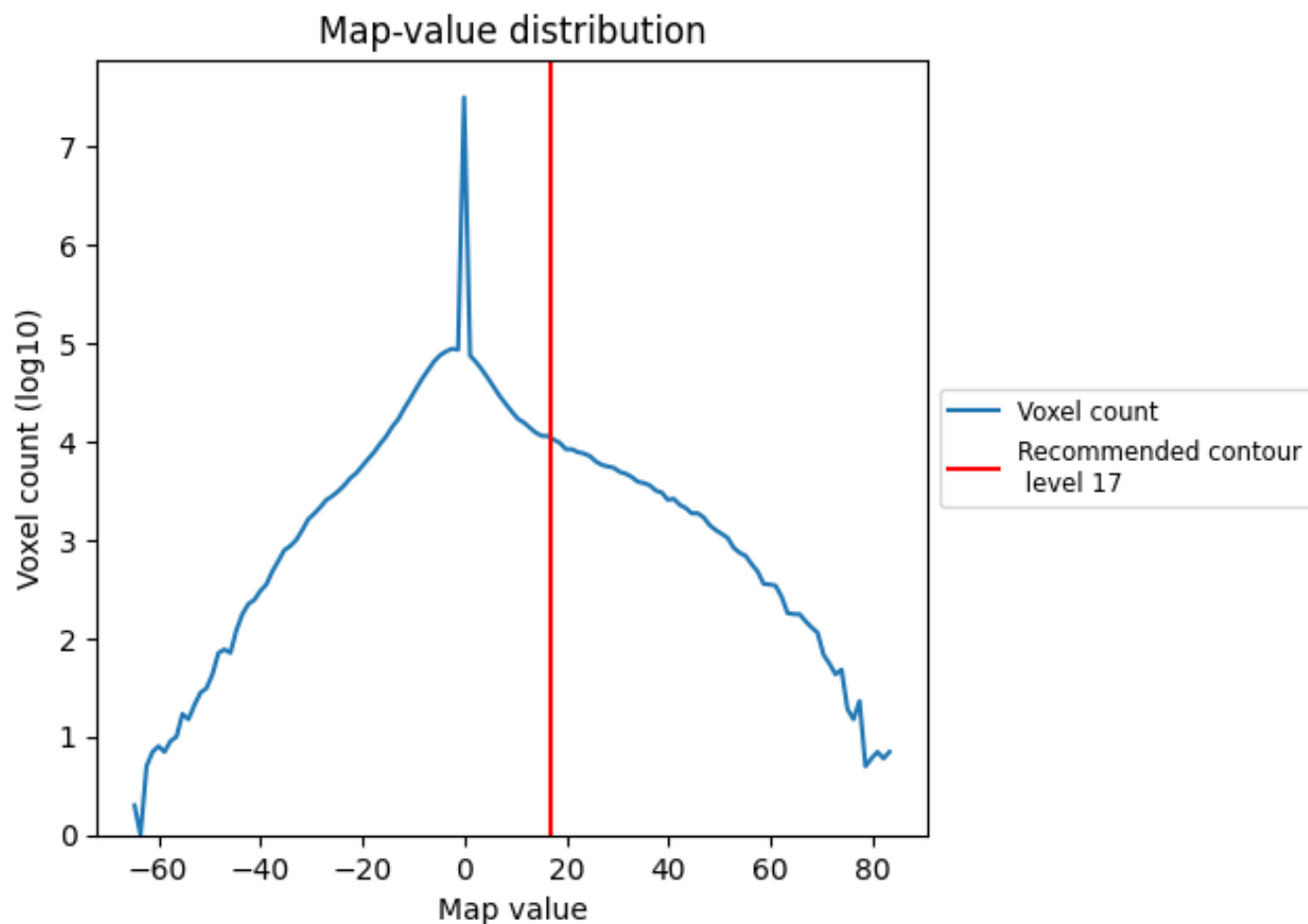


Z

## 7 Map analysis [i](#)

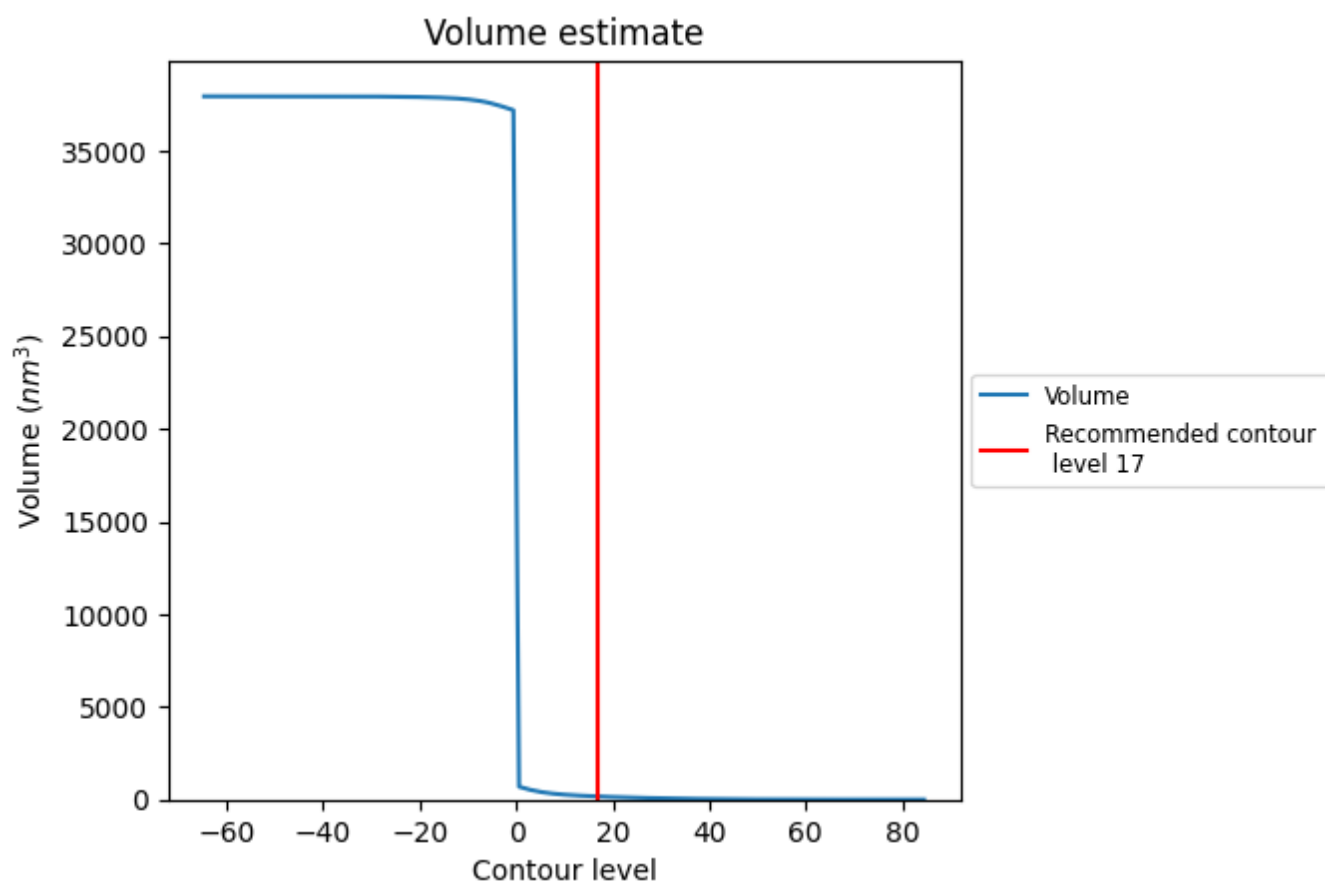
This section contains the results of statistical analysis of the map.

### 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.

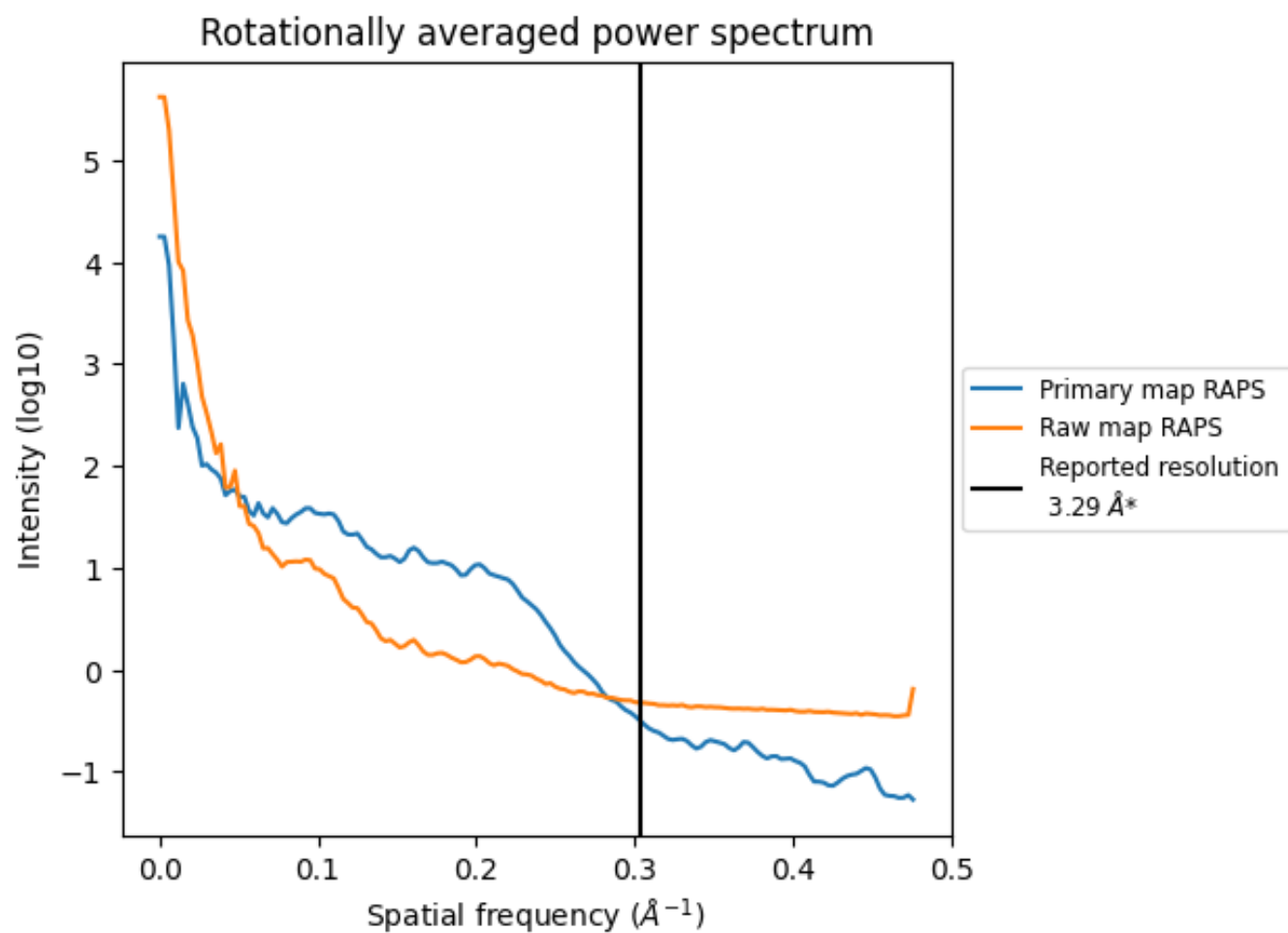
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm<sup>3</sup>; this corresponds to an approximate mass of 151 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 ⓘ

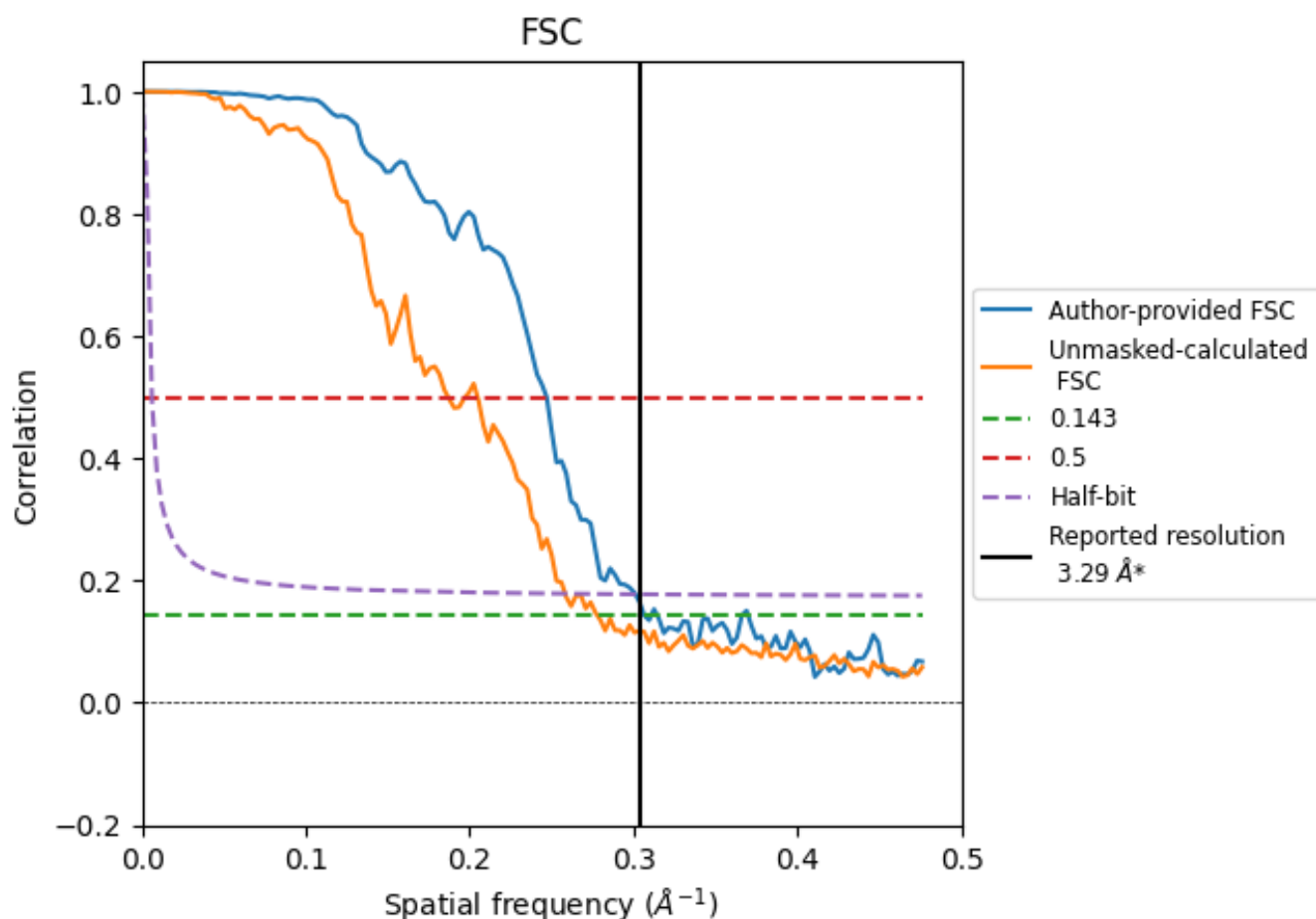


\*Reported resolution corresponds to spatial frequency of 0.304 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.304  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

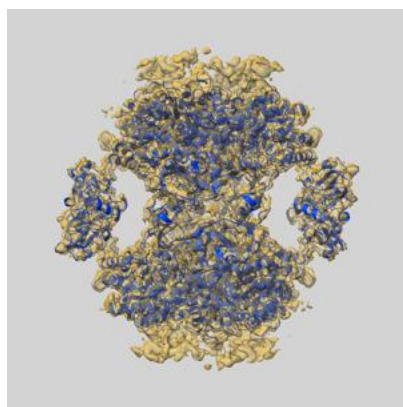
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.29                               | -    | -        |
| Author-provided FSC curve | 3.26                               | 4.05 | 3.32     |
| Unmasked-calculated*      | 3.60                               | 5.35 | 3.87     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

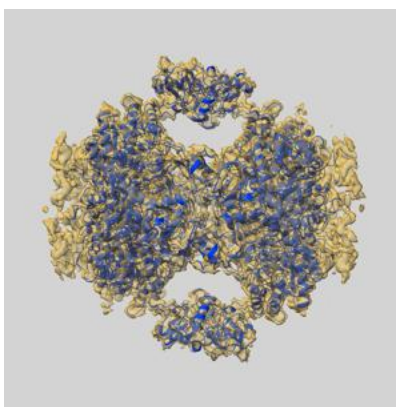
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20688 and PDB model 6U8N. Per-residue inclusion information can be found in section [3](#) on page [8](#).

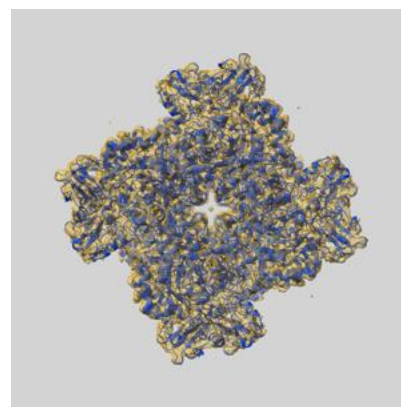
### 9.1 Map-model overlay [i](#)



X



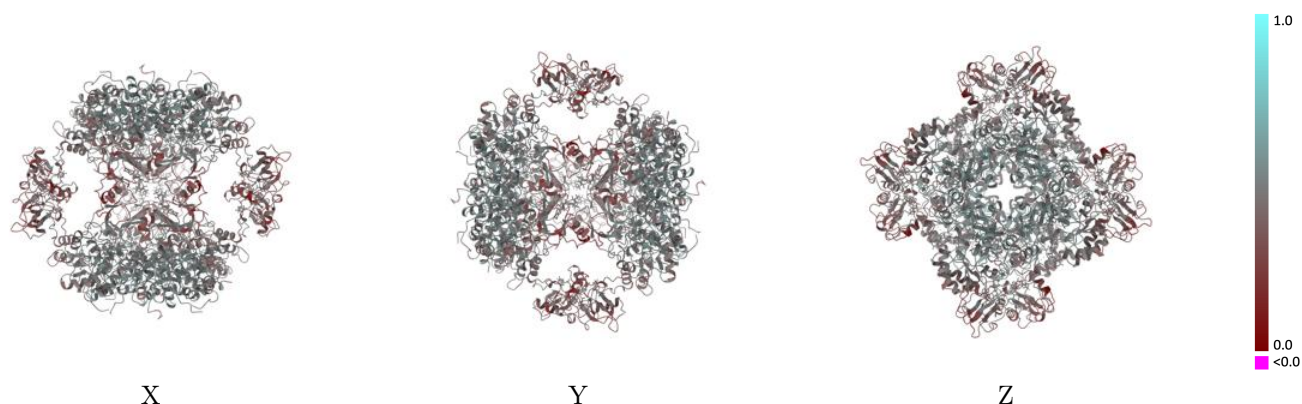
Y



Z

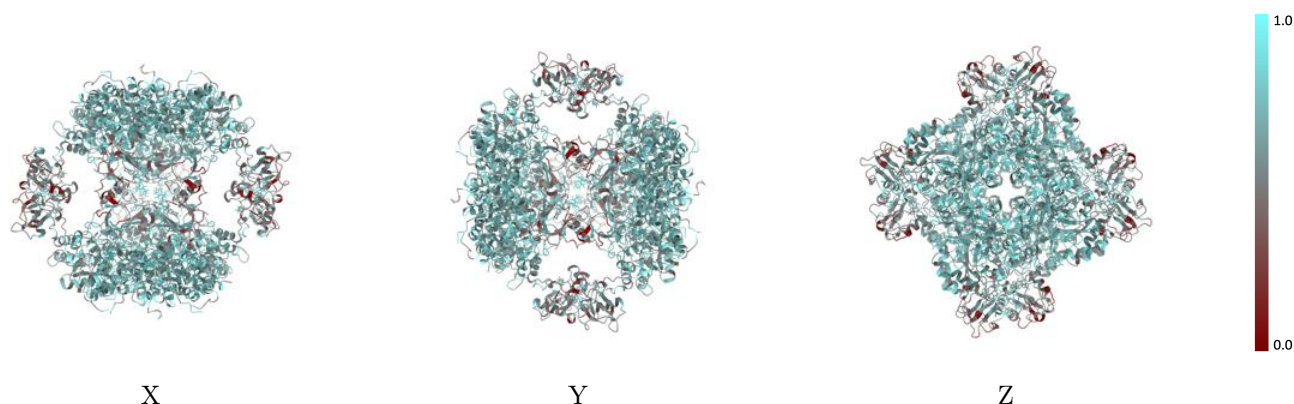
The images above show the 3D surface view of the map at the recommended contour level 17.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



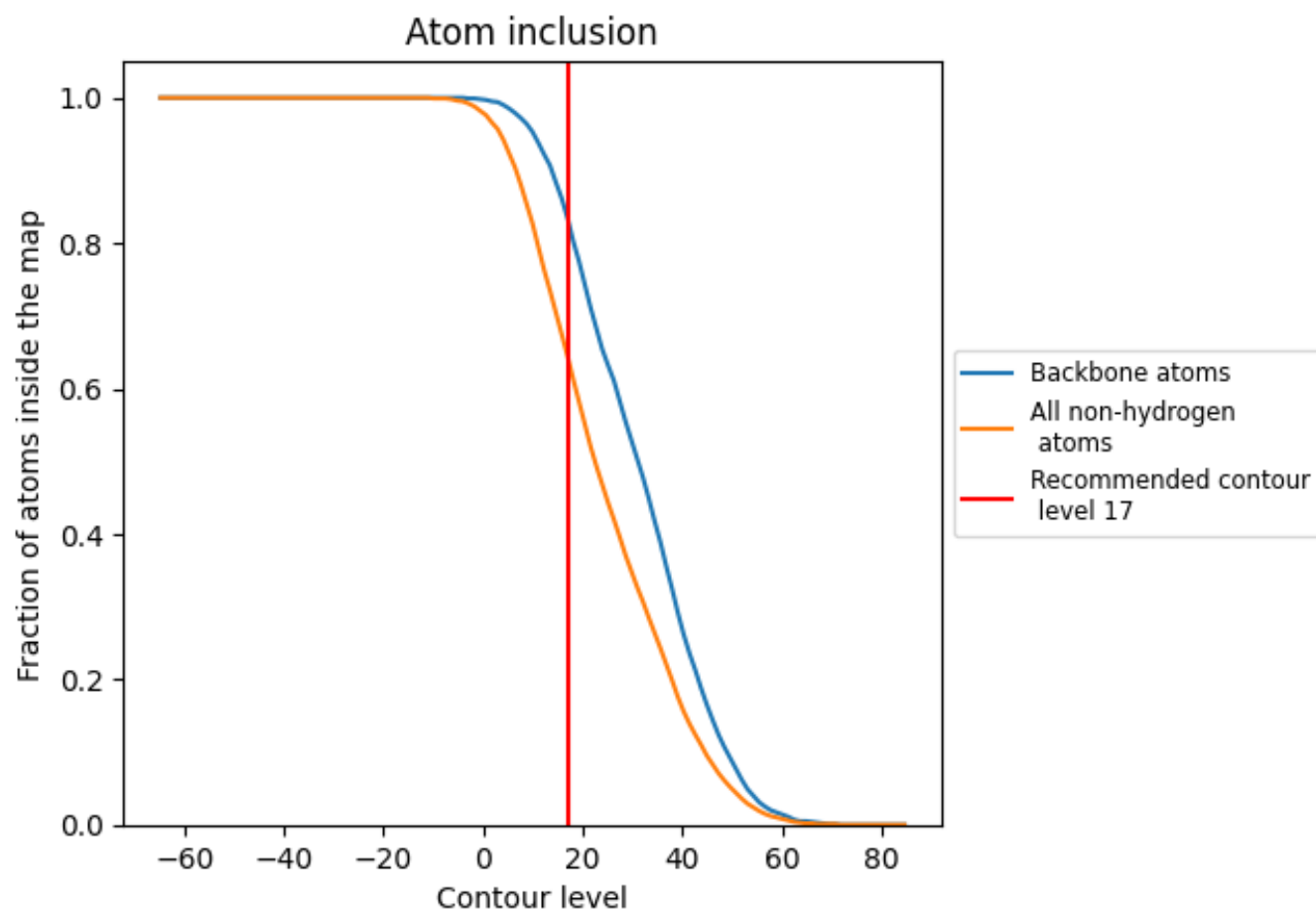
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (17).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 64% 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 (17) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6430 | <div></div> 0.4470 |
| A     | <div></div> 0.6380 | <div></div> 0.4470 |
| B     | <div></div> 0.6460 | <div></div> 0.4480 |
| C     | <div></div> 0.6420 | <div></div> 0.4470 |
| D     | <div></div> 0.6470 | <div></div> 0.4460 |
| E     | <div></div> 0.6410 | <div></div> 0.4460 |
| F     | <div></div> 0.6460 | <div></div> 0.4460 |
| G     | <div></div> 0.6400 | <div></div> 0.4480 |
| H     | <div></div> 0.6480 | <div></div> 0.4490 |
| I     | <div></div> 0.6400 | <div></div> 0.4560 |
| J     | <div></div> 0.6300 | <div></div> 0.4610 |
| K     | <div></div> 0.6100 | <div></div> 0.4550 |
| L     | <div></div> 0.6500 | <div></div> 0.4590 |
| M     | <div></div> 0.6200 | <div></div> 0.4540 |
| N     | <div></div> 0.6400 | <div></div> 0.4510 |
| O     | <div></div> 0.6200 | <div></div> 0.4630 |
| P     | <div></div> 0.6500 | <div></div> 0.4590 |

1.0

0.0

<0.0