



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:58 AM UTC

PDB ID : 6SE3 / pdb\_00006se3  
Title : Crystal Structure of Ancestral Flavin-containing monooxygenase (FMO) 3-6  
Authors : Nicoll, C.; Bailleul, G.; Fiorentini, F.; Mascotti, M.L.; Fraaije, M.; Mattevi, A.  
Deposited on : 2019-07-29  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

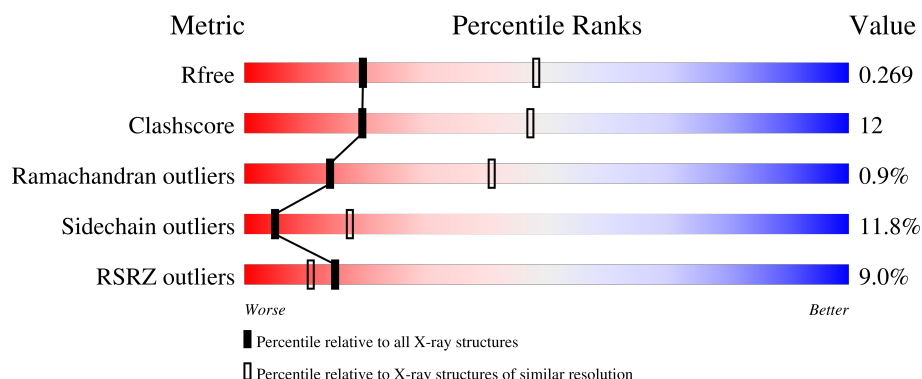
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                    |
|-----|-------|--------|-----------------------------------------------------|
| 1   | A     | 532    | <div> <div>35%</div> <div>68% 25% 6% .</div> </div> |
| 1   | B     | 532    | <div> <div>3%</div> <div>78% 16% 5% .</div> </div>  |
| 1   | C     | 532    | <div> <div>3%</div> <div>77% 16% 5% ..</div> </div> |
| 1   | D     | 532    | <div> <div>3%</div> <div>77% 17% 5% ..</div> </div> |
| 1   | E     | 532    | <div> <div>5%</div> <div>78% 17% . .</div> </div>   |

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| Mol | Chain | Length | Quality of chain                                                                |
|-----|-------|--------|---------------------------------------------------------------------------------|
| 1   | F     | 532    | <div><div></div><div>4%</div><div>78%</div><div>16%</div><div>5% ..</div></div> |

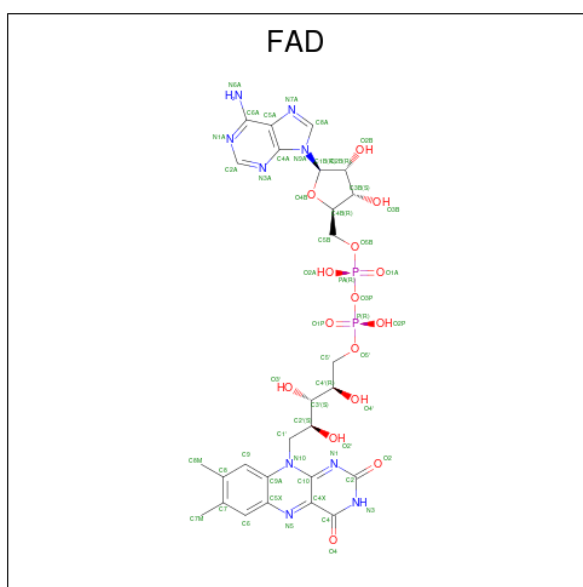


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ancestral Flavin-containing monooxygenase (FMO) 3-6.

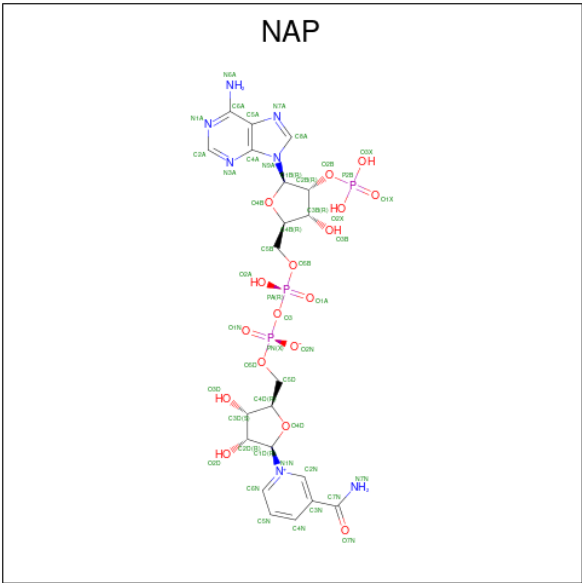
| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 1   | D     | 528      | Total<br>4198 | C<br>2718 | N<br>689 | O<br>767 | S<br>24 | 0       | 0       | 0     |
| 1   | A     | 528      | Total<br>4198 | C<br>2718 | N<br>689 | O<br>767 | S<br>24 | 0       | 0       | 0     |
| 1   | B     | 528      | Total<br>4198 | C<br>2718 | N<br>689 | O<br>767 | S<br>24 | 0       | 0       | 0     |
| 1   | C     | 528      | Total<br>4198 | C<br>2718 | N<br>689 | O<br>767 | S<br>24 | 0       | 0       | 0     |
| 1   | E     | 528      | Total<br>4198 | C<br>2718 | N<br>689 | O<br>767 | S<br>24 | 0       | 0       | 0     |
| 1   | F     | 528      | Total<br>4198 | C<br>2718 | N<br>689 | O<br>767 | S<br>24 | 0       | 0       | 0     |

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



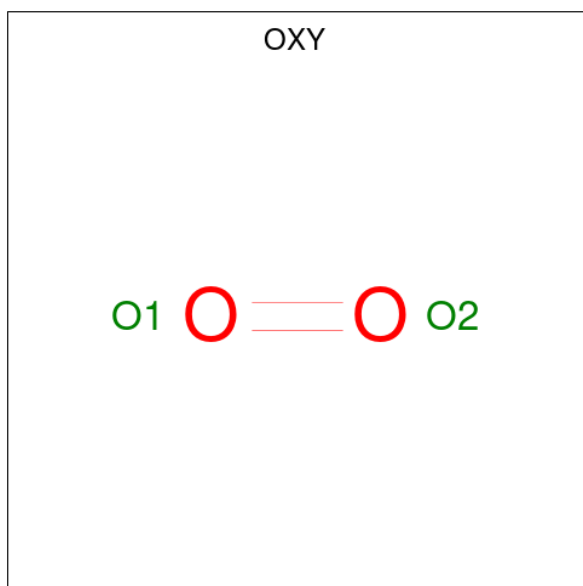
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |         |
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |         |
| 3   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |         |

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4   | D     | 1        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | A     | 1        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | B     | 1        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | C     | 1        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | E     | 1        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | F     | 1        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | D     | 74       | Total | O  | 0       | 0       |
|     |       |          | 74    | 74 |         |         |
| 5   | A     | 32       | Total | O  | 0       | 0       |
|     |       |          | 32    | 32 |         |         |

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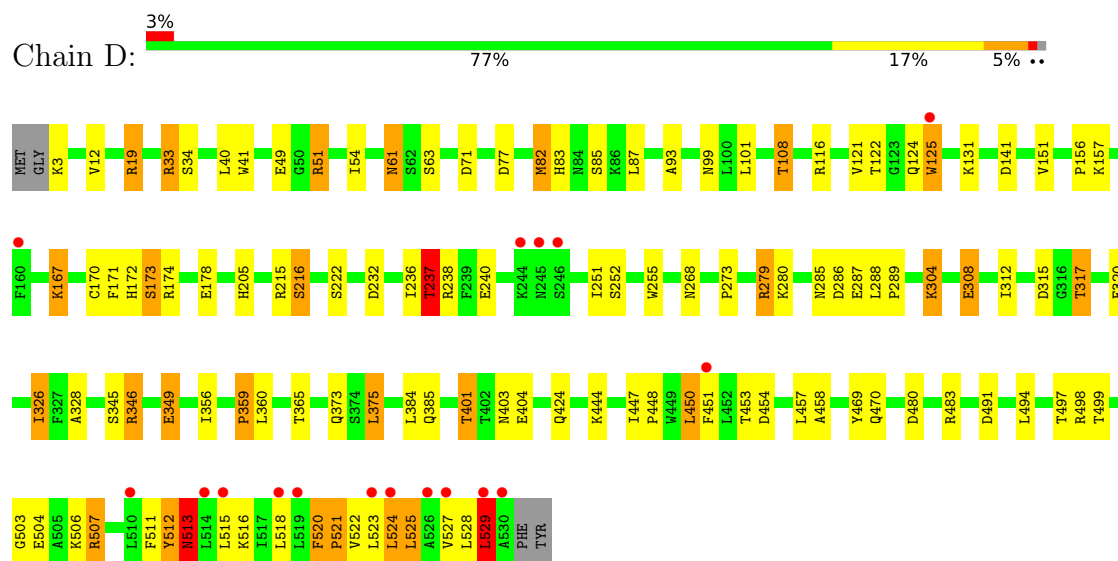
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 5   | B     | 52       | Total<br>52 | O<br>52 | 0       | 0       |
| 5   | C     | 75       | Total<br>75 | O<br>75 | 0       | 0       |
| 5   | E     | 56       | Total<br>56 | O<br>56 | 0       | 0       |
| 5   | F     | 68       | Total<br>68 | O<br>68 | 0       | 0       |

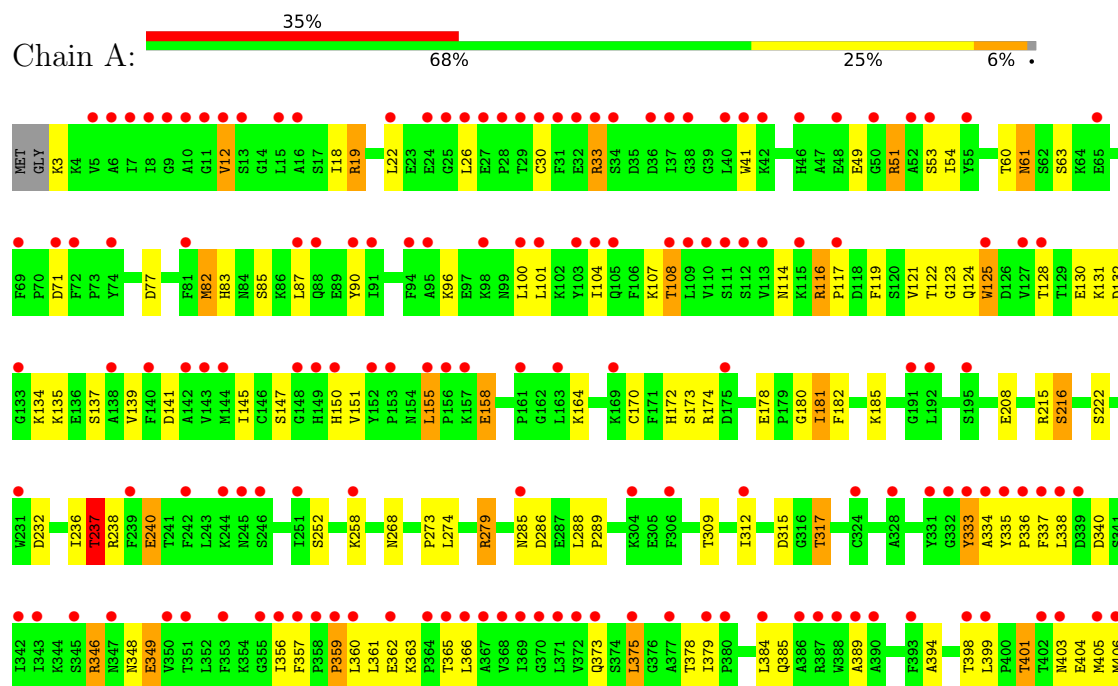
### 3 Residue-property plots [i](#)

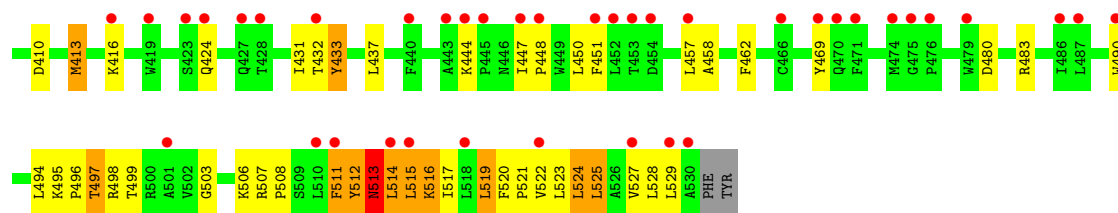
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6



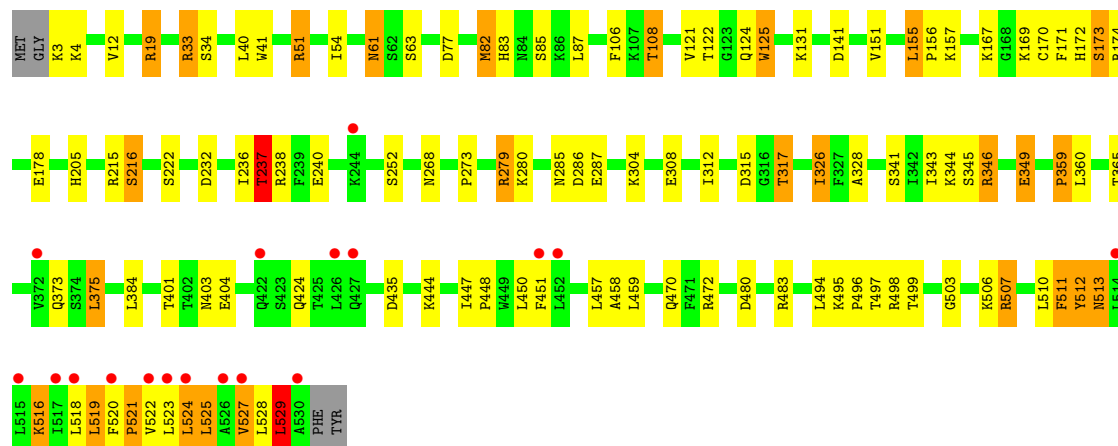
#### • Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6





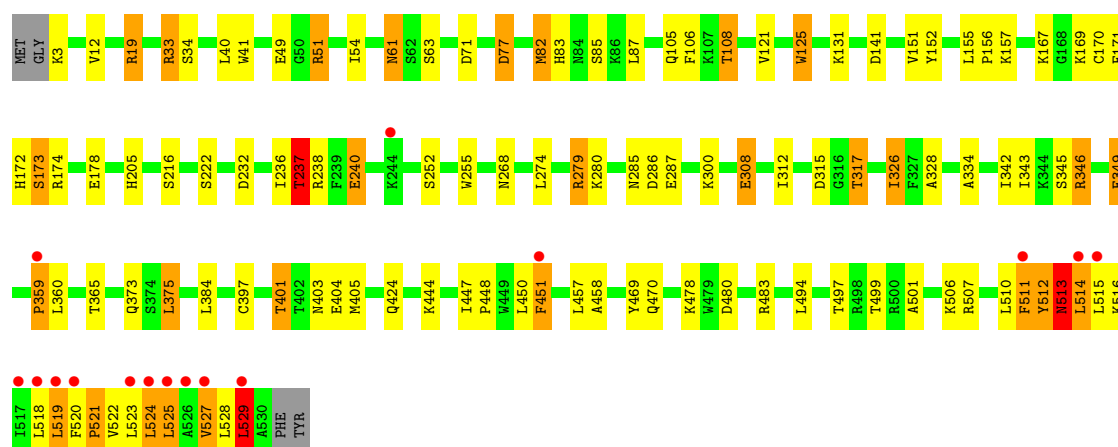
• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6

Chain B: 3% 78% 16% 5% .



• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6

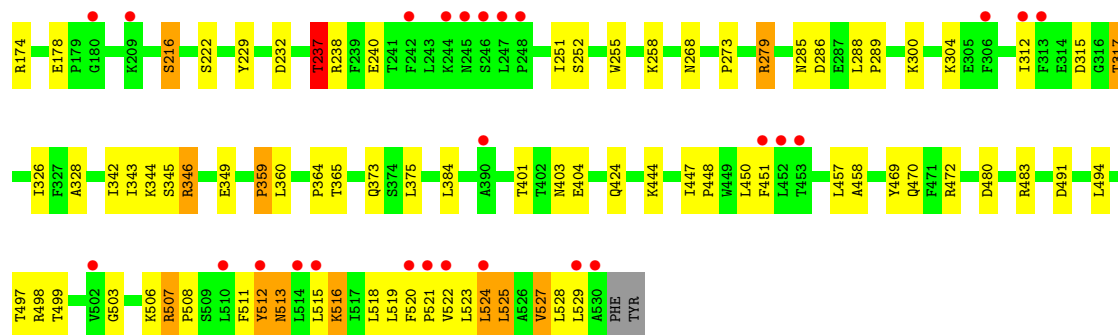
Chain C: 3% 77% 16% 5% ..



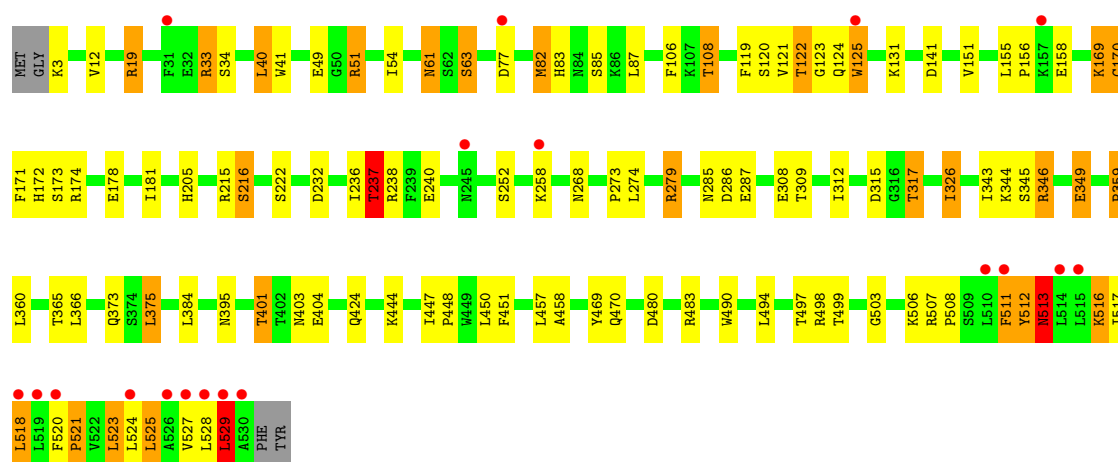
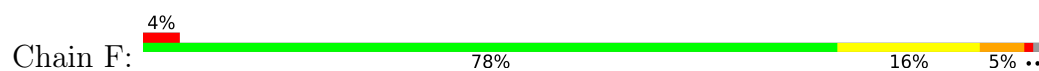
• Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6

Chain E: 5% 78% 17% . .





● Molecule 1: Ancestral Flavin-containing monooxygenase (FMO) 3-6



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 31 2 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 156.09Å 156.09Å 370.61Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 49.30 – 2.80<br>49.30 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (49.30-2.80)<br>100.0 (49.30-2.80)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.23                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.56 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0230                                             | Depositor        |
| R, $R_{free}$                                                           | 0.217 , 0.266<br>0.220 , 0.269                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 6492 reflections (5.02%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 63.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.028                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 33.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.023 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 26163                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 73.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAP, OXY

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     | 0.81         | 2/4312 (0.0%)  | 1.10        | 6/5843 (0.1%)   |
| 1   | B     | 0.82         | 1/4312 (0.0%)  | 1.07        | 6/5843 (0.1%)   |
| 1   | C     | 0.80         | 1/4312 (0.0%)  | 1.08        | 11/5843 (0.2%)  |
| 1   | D     | 0.79         | 0/4312         | 1.05        | 6/5843 (0.1%)   |
| 1   | E     | 0.80         | 0/4312         | 1.06        | 4/5843 (0.1%)   |
| 1   | F     | 0.81         | 2/4312 (0.0%)  | 1.07        | 6/5843 (0.1%)   |
| All | All   | 0.80         | 6/25872 (0.0%) | 1.07        | 39/35058 (0.1%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 507 | ARG  | C-N   | 13.12 | 1.50        | 1.33     |
| 1   | F     | 523 | LEU  | N-CA  | 5.90  | 1.53        | 1.46     |
| 1   | A     | 389 | ALA  | C-O   | -5.48 | 1.17        | 1.24     |
| 1   | F     | 170 | CYS  | C-O   | -5.29 | 1.17        | 1.23     |
| 1   | C     | 523 | LEU  | N-CA  | 5.13  | 1.52        | 1.46     |
| 1   | A     | 337 | PHE  | C-O   | 5.04  | 1.30        | 1.24     |

All (39) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 507 | ARG  | CA-C-N   | 11.99 | 131.96      | 119.85   |
| 1   | B     | 507 | ARG  | C-N-CA   | 11.99 | 131.96      | 119.85   |
| 1   | C     | 511 | PHE  | CA-CB-CG | 10.83 | 124.63      | 113.80   |
| 1   | F     | 359 | PRO  | N-CA-C   | -6.46 | 101.50      | 111.13   |
| 1   | B     | 359 | PRO  | N-CA-C   | -6.45 | 101.53      | 111.13   |
| 1   | D     | 359 | PRO  | N-CA-C   | -6.42 | 101.57      | 111.13   |
| 1   | A     | 359 | PRO  | N-CA-C   | -6.34 | 101.68      | 111.13   |
| 1   | C     | 513 | ASN  | CA-C-N   | 6.32  | 129.91      | 120.31   |
| 1   | C     | 513 | ASN  | C-N-CA   | 6.32  | 129.91      | 120.31   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 359 | PRO  | N-CA-C    | -6.31 | 101.73      | 111.13   |
| 1   | B     | 215 | ARG  | CB-CA-C   | -6.29 | 100.92      | 110.92   |
| 1   | D     | 215 | ARG  | CB-CA-C   | -6.07 | 101.26      | 110.92   |
| 1   | C     | 501 | ALA  | CA-C-N    | -5.85 | 116.96      | 123.16   |
| 1   | C     | 501 | ALA  | C-N-CA    | -5.85 | 116.96      | 123.16   |
| 1   | D     | 237 | THR  | CA-CB-OG1 | -5.80 | 100.89      | 109.60   |
| 1   | D     | 469 | TYR  | CA-C-N    | 5.77  | 128.81      | 120.38   |
| 1   | D     | 469 | TYR  | C-N-CA    | 5.77  | 128.81      | 120.38   |
| 1   | C     | 359 | PRO  | N-CA-C    | -5.73 | 102.60      | 111.13   |
| 1   | F     | 237 | THR  | CA-CB-OG1 | -5.66 | 101.10      | 109.60   |
| 1   | A     | 237 | THR  | CA-CB-OG1 | -5.57 | 101.25      | 109.60   |
| 1   | E     | 237 | THR  | CA-CB-OG1 | -5.47 | 101.39      | 109.60   |
| 1   | F     | 169 | LYS  | CB-CA-C   | 5.44  | 119.46      | 109.46   |
| 1   | C     | 451 | PHE  | CA-CB-CG  | 5.34  | 119.14      | 113.80   |
| 1   | F     | 521 | PRO  | N-CA-C    | 5.31  | 120.52      | 113.40   |
| 1   | A     | 77  | ASP  | CA-CB-CG  | 5.30  | 117.90      | 112.60   |
| 1   | E     | 469 | TYR  | CA-C-N    | 5.20  | 127.97      | 120.38   |
| 1   | E     | 469 | TYR  | C-N-CA    | 5.20  | 127.97      | 120.38   |
| 1   | C     | 237 | THR  | CA-CB-OG1 | -5.18 | 101.83      | 109.60   |
| 1   | F     | 469 | TYR  | CA-C-N    | 5.16  | 127.91      | 120.38   |
| 1   | F     | 469 | TYR  | C-N-CA    | 5.16  | 127.91      | 120.38   |
| 1   | C     | 521 | PRO  | N-CA-C    | 5.15  | 120.30      | 113.40   |
| 1   | C     | 469 | TYR  | CA-C-N    | 5.13  | 127.86      | 120.38   |
| 1   | C     | 469 | TYR  | C-N-CA    | 5.13  | 127.86      | 120.38   |
| 1   | A     | 469 | TYR  | CA-C-N    | 5.12  | 127.85      | 120.38   |
| 1   | A     | 469 | TYR  | C-N-CA    | 5.12  | 127.85      | 120.38   |
| 1   | A     | 511 | PHE  | CA-CB-CG  | 5.08  | 118.88      | 113.80   |
| 1   | B     | 237 | THR  | CA-CB-OG1 | -5.07 | 101.99      | 109.60   |
| 1   | D     | 521 | PRO  | N-CA-C    | 5.06  | 120.19      | 113.40   |
| 1   | B     | 521 | PRO  | N-CA-C    | 5.00  | 120.10      | 113.40   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4198  | 0        | 4172     | 151     | 0            |
| 1   | B     | 4198  | 0        | 4172     | 95      | 0            |
| 1   | C     | 4198  | 0        | 4172     | 101     | 0            |
| 1   | D     | 4198  | 0        | 4172     | 99      | 0            |
| 1   | E     | 4198  | 0        | 4172     | 71      | 0            |
| 1   | F     | 4198  | 0        | 4172     | 89      | 0            |
| 2   | A     | 53    | 0        | 31       | 16      | 0            |
| 2   | B     | 53    | 0        | 31       | 1       | 0            |
| 2   | C     | 53    | 0        | 31       | 4       | 0            |
| 2   | D     | 53    | 0        | 31       | 1       | 0            |
| 2   | E     | 53    | 0        | 31       | 4       | 0            |
| 2   | F     | 53    | 0        | 31       | 4       | 0            |
| 3   | A     | 48    | 0        | 25       | 2       | 0            |
| 3   | B     | 48    | 0        | 25       | 2       | 0            |
| 3   | C     | 48    | 0        | 25       | 2       | 0            |
| 3   | D     | 48    | 0        | 25       | 4       | 0            |
| 3   | E     | 48    | 0        | 25       | 2       | 0            |
| 3   | F     | 48    | 0        | 25       | 3       | 0            |
| 4   | A     | 2     | 0        | 0        | 0       | 0            |
| 4   | B     | 2     | 0        | 0        | 0       | 0            |
| 4   | C     | 2     | 0        | 0        | 0       | 0            |
| 4   | D     | 2     | 0        | 0        | 0       | 0            |
| 4   | E     | 2     | 0        | 0        | 0       | 0            |
| 4   | F     | 2     | 0        | 0        | 0       | 0            |
| 5   | A     | 32    | 0        | 0        | 19      | 0            |
| 5   | B     | 52    | 0        | 0        | 6       | 0            |
| 5   | C     | 75    | 0        | 0        | 11      | 0            |
| 5   | D     | 74    | 0        | 0        | 8       | 0            |
| 5   | E     | 56    | 0        | 0        | 2       | 0            |
| 5   | F     | 68    | 0        | 0        | 6       | 0            |
| All | All   | 26163 | 0        | 25368    | 595     | 0            |

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

All (595) 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:A:145:ILE:CG2  | 1:A:335:TYR:HE1 | 1.61                     | 1.14              |
| 1:A:145:ILE:CG2  | 1:A:335:TYR:CE1 | 2.34                     | 1.10              |
| 1:C:238:ARG:HE   | 1:C:470:GLN:NE2 | 1.51                     | 1.08              |
| 1:A:145:ILE:HG21 | 1:A:335:TYR:CE1 | 1.89                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:359:PRO:HB3  | 1:C:405:MET:HE3  | 1.34                     | 1.06              |
| 1:A:145:ILE:HG22 | 1:A:335:TYR:HE1  | 1.16                     | 1.05              |
| 1:A:51:ARG:HH11  | 1:A:51:ARG:HB3   | 1.24                     | 1.03              |
| 1:E:238:ARG:HE   | 1:E:470:GLN:NE2  | 1.59                     | 1.00              |
| 1:C:268:ASN:O    | 1:F:497:THR:HG23 | 1.61                     | 1.00              |
| 1:D:238:ARG:HH11 | 1:D:470:GLN:HE21 | 1.07                     | 0.98              |
| 1:B:33:ARG:HH11  | 1:B:33:ARG:HG3   | 1.29                     | 0.98              |
| 1:F:19:ARG:HG2   | 1:F:19:ARG:HH11  | 1.30                     | 0.97              |
| 1:F:238:ARG:HE   | 1:F:470:GLN:NE2  | 1.66                     | 0.94              |
| 1:F:521:PRO:HA   | 5:F:713:HOH:O    | 1.67                     | 0.93              |
| 1:D:33:ARG:HG3   | 1:D:33:ARG:HH11  | 1.34                     | 0.92              |
| 1:A:33:ARG:HB2   | 1:A:33:ARG:HH11  | 1.35                     | 0.92              |
| 1:F:19:ARG:HG2   | 1:F:19:ARG:NH1   | 1.83                     | 0.90              |
| 1:D:497:THR:HG23 | 1:B:268:ASN:O    | 1.73                     | 0.89              |
| 1:C:300:LYS:HE3  | 5:C:752:HOH:O    | 1.72                     | 0.88              |
| 1:A:33:ARG:CD    | 2:A:601:FAD:C5A  | 2.51                     | 0.87              |
| 1:F:238:ARG:HH11 | 1:F:470:GLN:HE21 | 1.19                     | 0.86              |
| 1:A:33:ARG:HD3   | 2:A:601:FAD:C4A  | 2.06                     | 0.86              |
| 1:A:497:THR:HG23 | 1:E:268:ASN:O    | 1.76                     | 0.85              |
| 1:A:51:ARG:HH11  | 1:A:51:ARG:CB    | 1.88                     | 0.85              |
| 1:A:33:ARG:HH11  | 1:A:33:ARG:CB    | 1.89                     | 0.85              |
| 1:C:238:ARG:HE   | 1:C:470:GLN:HE21 | 1.18                     | 0.85              |
| 1:D:238:ARG:NH1  | 1:D:470:GLN:HE21 | 1.74                     | 0.84              |
| 1:F:19:ARG:HH11  | 1:F:19:ARG:CG    | 1.90                     | 0.84              |
| 1:D:167:LYS:HD2  | 1:D:308:GLU:HG3  | 1.60                     | 0.84              |
| 1:A:145:ILE:HG21 | 1:A:335:TYR:CD1  | 2.13                     | 0.83              |
| 1:C:238:ARG:NE   | 1:C:470:GLN:NE2  | 2.28                     | 0.82              |
| 1:B:125:TRP:HZ3  | 1:B:365:THR:HG1  | 1.25                     | 0.82              |
| 1:E:238:ARG:HE   | 1:E:470:GLN:HE21 | 1.26                     | 0.80              |
| 1:F:309:THR:HG23 | 5:F:710:HOH:O    | 1.81                     | 0.79              |
| 1:A:33:ARG:HD2   | 2:A:601:FAD:C5A  | 2.12                     | 0.79              |
| 1:A:268:ASN:O    | 1:E:497:THR:HG23 | 1.82                     | 0.79              |
| 1:C:359:PRO:HB3  | 1:C:405:MET:CE   | 2.13                     | 0.79              |
| 1:A:145:ILE:HG22 | 1:A:335:TYR:CE1  | 2.07                     | 0.78              |
| 1:B:19:ARG:HH12  | 1:B:472:ARG:NH2  | 1.82                     | 0.77              |
| 1:E:524:LEU:O    | 1:E:528:LEU:HD23 | 1.84                     | 0.77              |
| 1:D:99:ASN:HB2   | 5:D:753:HOH:O    | 1.85                     | 0.77              |
| 1:A:19:ARG:HG2   | 1:A:19:ARG:HH11  | 1.51                     | 0.76              |
| 1:A:33:ARG:CD    | 2:A:601:FAD:C4A  | 2.64                     | 0.76              |
| 1:E:33:ARG:HG3   | 1:E:33:ARG:HH11  | 1.50                     | 0.76              |
| 1:D:33:ARG:HG3   | 1:D:33:ARG:NH1   | 1.99                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:237:THR:HG22 | 1:B:240:GLU:H    | 1.51                     | 0.75              |
| 1:F:237:THR:HG22 | 1:F:240:GLU:H    | 1.51                     | 0.75              |
| 1:D:237:THR:HG22 | 1:D:240:GLU:H    | 1.52                     | 0.75              |
| 1:C:238:ARG:HG2  | 1:C:238:ARG:HH21 | 1.51                     | 0.74              |
| 1:E:237:THR:HG22 | 1:E:240:GLU:H    | 1.52                     | 0.74              |
| 1:E:108:THR:HG22 | 1:E:131:LYS:HD3  | 1.67                     | 0.74              |
| 1:A:51:ARG:HB3   | 1:A:51:ARG:NH1   | 2.01                     | 0.73              |
| 1:C:237:THR:HG22 | 1:C:240:GLU:H    | 1.52                     | 0.73              |
| 1:A:447:ILE:HB   | 1:A:448:PRO:HD3  | 1.71                     | 0.73              |
| 2:A:601:FAD:C6   | 3:A:602:NAP:C2N  | 2.66                     | 0.73              |
| 1:E:125:TRP:HZ3  | 1:E:365:THR:HG1  | 1.33                     | 0.73              |
| 1:A:237:THR:HG22 | 1:A:240:GLU:H    | 1.52                     | 0.73              |
| 1:F:524:LEU:O    | 1:F:528:LEU:HD12 | 1.89                     | 0.73              |
| 1:D:268:ASN:O    | 1:B:497:THR:HG23 | 1.88                     | 0.72              |
| 1:F:238:ARG:NH1  | 1:F:470:GLN:HE21 | 1.87                     | 0.72              |
| 1:B:33:ARG:HG3   | 1:B:33:ARG:NH1   | 1.99                     | 0.72              |
| 1:A:33:ARG:HD3   | 2:A:601:FAD:N9A  | 2.04                     | 0.72              |
| 1:C:497:THR:HG23 | 1:F:268:ASN:O    | 1.90                     | 0.72              |
| 1:A:128:THR:HG23 | 5:A:722:HOH:O    | 1.90                     | 0.71              |
| 1:C:77:ASP:CB    | 5:C:746:HOH:O    | 2.38                     | 0.71              |
| 1:F:524:LEU:O    | 1:F:528:LEU:HB2  | 1.90                     | 0.71              |
| 1:D:529:LEU:HD11 | 1:F:518:LEU:HD13 | 1.72                     | 0.71              |
| 1:B:457:LEU:HD22 | 1:B:483:ARG:HG3  | 1.73                     | 0.71              |
| 1:D:498:ARG:NH2  | 1:D:503:GLY:O    | 2.23                     | 0.70              |
| 1:A:19:ARG:HH11  | 1:A:19:ARG:CG    | 2.04                     | 0.70              |
| 1:E:457:LEU:HD22 | 1:E:483:ARG:HG3  | 1.73                     | 0.70              |
| 1:C:125:TRP:HZ3  | 1:C:365:THR:HG1  | 1.40                     | 0.70              |
| 1:A:512:TYR:CZ   | 5:A:701:HOH:O    | 2.44                     | 0.70              |
| 1:A:60:THR:HG21  | 1:A:82:MET:HE2   | 1.73                     | 0.69              |
| 1:A:524:LEU:O    | 1:A:528:LEU:HB2  | 1.92                     | 0.69              |
| 1:F:457:LEU:HD22 | 1:F:483:ARG:HG3  | 1.74                     | 0.69              |
| 1:D:457:LEU:HD22 | 1:D:483:ARG:HG3  | 1.74                     | 0.69              |
| 1:A:498:ARG:NH2  | 1:A:503:GLY:O    | 2.25                     | 0.69              |
| 1:B:19:ARG:HH12  | 1:B:472:ARG:HH21 | 1.37                     | 0.69              |
| 1:B:19:ARG:NH1   | 1:B:472:ARG:NH2  | 2.41                     | 0.69              |
| 1:A:119:PHE:CE2  | 1:A:362:GLU:HB2  | 2.27                     | 0.69              |
| 1:F:106:PHE:O    | 1:F:108:THR:HG23 | 1.93                     | 0.69              |
| 1:A:19:ARG:NH2   | 1:A:71:ASP:OD2   | 2.25                     | 0.68              |
| 1:A:33:ARG:HD3   | 2:A:601:FAD:C8A  | 2.23                     | 0.68              |
| 1:B:519:LEU:HD13 | 1:B:519:LEU:H    | 1.59                     | 0.68              |
| 1:D:524:LEU:O    | 1:D:528:LEU:HG   | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:130:GLU:HB2  | 1:A:135:LYS:NZ   | 2.09                     | 0.68              |
| 1:A:433:TYR:HE2  | 1:A:437:LEU:HD22 | 1.58                     | 0.68              |
| 1:C:457:LEU:HD22 | 1:C:483:ARG:HG3  | 1.75                     | 0.68              |
| 1:A:33:ARG:HH11  | 1:A:33:ARG:CG    | 2.05                     | 0.68              |
| 1:F:63:SER:HB3   | 1:F:232:ASP:OD1  | 1.94                     | 0.67              |
| 1:A:181:ILE:HD13 | 1:A:181:ILE:H    | 1.60                     | 0.67              |
| 1:C:172:HIS:HD2  | 1:C:174:ARG:HB2  | 1.58                     | 0.67              |
| 1:F:450:LEU:HB3  | 1:F:458:ALA:HB2  | 1.77                     | 0.67              |
| 1:A:51:ARG:HH11  | 1:A:51:ARG:CG    | 2.07                     | 0.67              |
| 1:A:515:LEU:C    | 1:A:519:LEU:HD21 | 2.19                     | 0.66              |
| 1:D:167:LYS:CD   | 1:D:308:GLU:HG3  | 2.25                     | 0.66              |
| 1:A:130:GLU:HB2  | 1:A:135:LYS:HZ1  | 1.60                     | 0.66              |
| 1:C:106:PHE:O    | 1:C:108:THR:HG23 | 1.95                     | 0.66              |
| 1:A:309:THR:HG22 | 5:A:711:HOH:O    | 1.95                     | 0.66              |
| 1:A:457:LEU:HD22 | 1:A:483:ARG:HG3  | 1.76                     | 0.66              |
| 1:A:361:LEU:HD23 | 1:A:363:LYS:O    | 1.95                     | 0.66              |
| 1:E:106:PHE:O    | 1:E:108:THR:HG23 | 1.95                     | 0.66              |
| 1:F:122:THR:HB   | 1:F:124:GLN:HG3  | 1.76                     | 0.66              |
| 1:F:125:TRP:HZ3  | 1:F:365:THR:HG1  | 1.41                     | 0.66              |
| 1:C:238:ARG:HG2  | 1:C:238:ARG:NH2  | 2.11                     | 0.65              |
| 1:B:279:ARG:CG   | 1:B:279:ARG:HH11 | 2.10                     | 0.65              |
| 1:B:106:PHE:O    | 1:B:108:THR:HG23 | 1.96                     | 0.65              |
| 1:D:450:LEU:HB3  | 1:D:458:ALA:HB2  | 1.78                     | 0.65              |
| 1:C:450:LEU:HB3  | 1:C:458:ALA:HB2  | 1.77                     | 0.65              |
| 1:C:513:ASN:HB3  | 1:C:516:LYS:HB3  | 1.79                     | 0.65              |
| 1:D:447:ILE:HB   | 1:D:448:PRO:HD3  | 1.79                     | 0.65              |
| 1:C:279:ARG:HH11 | 1:C:279:ARG:CG   | 2.09                     | 0.64              |
| 1:F:238:ARG:NE   | 1:F:470:GLN:NE2  | 2.40                     | 0.64              |
| 1:D:122:THR:HB   | 1:D:124:GLN:HG3  | 1.80                     | 0.64              |
| 1:B:519:LEU:HD22 | 1:B:520:PHE:H    | 1.62                     | 0.64              |
| 1:E:513:ASN:HB3  | 1:E:516:LYS:HB3  | 1.81                     | 0.63              |
| 1:D:521:PRO:HB2  | 5:D:711:HOH:O    | 1.97                     | 0.63              |
| 1:A:410:ASP:HA   | 5:A:712:HOH:O    | 1.97                     | 0.63              |
| 1:F:279:ARG:HH11 | 1:F:279:ARG:CG   | 2.11                     | 0.63              |
| 1:A:19:ARG:HG2   | 1:A:19:ARG:NH1   | 2.11                     | 0.63              |
| 1:A:119:PHE:HE2  | 1:A:362:GLU:HB2  | 1.61                     | 0.63              |
| 1:C:519:LEU:HD13 | 1:C:519:LEU:N    | 2.14                     | 0.63              |
| 1:E:33:ARG:HG3   | 1:E:33:ARG:NH1   | 2.11                     | 0.63              |
| 1:F:172:HIS:HD2  | 1:F:174:ARG:HB2  | 1.64                     | 0.63              |
| 1:E:172:HIS:HD2  | 1:E:174:ARG:HB2  | 1.63                     | 0.62              |
| 1:D:172:HIS:HD2  | 1:D:174:ARG:HB2  | 1.63                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:518:LEU:HD13 | 1:C:529:LEU:HD13 | 1.81                     | 0.62              |
| 1:D:516:LYS:HD2  | 5:D:719:HOH:O    | 1.98                     | 0.62              |
| 1:D:279:ARG:HH11 | 1:D:279:ARG:CG   | 2.12                     | 0.62              |
| 1:B:172:HIS:HD2  | 1:B:174:ARG:HB2  | 1.64                     | 0.62              |
| 1:D:524:LEU:O    | 1:D:528:LEU:CG   | 2.47                     | 0.62              |
| 1:B:519:LEU:HD13 | 1:B:519:LEU:N    | 2.15                     | 0.62              |
| 1:A:19:ARG:HH22  | 1:A:71:ASP:CG    | 2.08                     | 0.62              |
| 1:E:279:ARG:HH11 | 1:E:279:ARG:CG   | 2.13                     | 0.62              |
| 1:D:238:ARG:HE   | 1:D:470:GLN:NE2  | 1.97                     | 0.61              |
| 1:A:416:LYS:HG3  | 5:A:730:HOH:O    | 2.00                     | 0.61              |
| 1:B:516:LYS:HA   | 1:B:519:LEU:HD21 | 1.82                     | 0.61              |
| 1:A:33:ARG:HD3   | 2:A:601:FAD:C5A  | 2.28                     | 0.61              |
| 1:C:447:ILE:HB   | 1:C:448:PRO:HD3  | 1.82                     | 0.61              |
| 1:E:450:LEU:HB3  | 1:E:458:ALA:HB2  | 1.81                     | 0.61              |
| 1:D:19:ARG:HH11  | 1:D:19:ARG:CG    | 2.14                     | 0.61              |
| 1:A:12:VAL:HG11  | 1:A:379:ILE:HG12 | 1.82                     | 0.61              |
| 1:D:156:PRO:HG2  | 3:D:602:NAP:N6A  | 2.16                     | 0.61              |
| 1:F:238:ARG:HE   | 1:F:470:GLN:HE22 | 1.44                     | 0.61              |
| 1:A:238:ARG:HH21 | 1:A:431:ILE:HG23 | 1.65                     | 0.60              |
| 1:E:447:ILE:HB   | 1:E:448:PRO:HD3  | 1.82                     | 0.60              |
| 1:A:238:ARG:HH21 | 1:A:431:ILE:CG2  | 2.14                     | 0.60              |
| 1:B:450:LEU:HB3  | 1:B:458:ALA:HB2  | 1.82                     | 0.60              |
| 1:C:359:PRO:CB   | 1:C:405:MET:HE3  | 2.23                     | 0.60              |
| 1:F:516:LYS:HE2  | 5:F:762:HOH:O    | 1.99                     | 0.60              |
| 1:E:255:TRP:HZ2  | 1:E:515:LEU:HD13 | 1.65                     | 0.60              |
| 1:A:450:LEU:HB3  | 1:A:458:ALA:HB2  | 1.82                     | 0.60              |
| 1:F:447:ILE:HB   | 1:F:448:PRO:HD3  | 1.84                     | 0.60              |
| 1:A:498:ARG:O    | 1:A:498:ARG:HG2  | 2.02                     | 0.60              |
| 1:A:333:TYR:CD1  | 1:A:333:TYR:N    | 2.68                     | 0.59              |
| 1:B:82:MET:HE1   | 1:B:87:LEU:HA    | 1.84                     | 0.59              |
| 1:C:82:MET:HE1   | 1:C:87:LEU:HA    | 1.84                     | 0.59              |
| 1:D:525:LEU:C    | 1:D:525:LEU:HD22 | 2.28                     | 0.59              |
| 1:A:238:ARG:HG3  | 1:A:462:PHE:HA   | 1.84                     | 0.59              |
| 1:A:525:LEU:C    | 1:A:525:LEU:HD22 | 2.28                     | 0.59              |
| 1:F:525:LEU:C    | 1:F:525:LEU:HD22 | 2.28                     | 0.59              |
| 1:C:40:LEU:HD11  | 2:C:601:FAD:HM83 | 1.85                     | 0.59              |
| 1:D:349:GLU:HG3  | 1:D:424:GLN:HE22 | 1.67                     | 0.59              |
| 1:E:525:LEU:HD22 | 1:E:525:LEU:C    | 2.28                     | 0.59              |
| 1:E:82:MET:HE1   | 1:E:87:LEU:HA    | 1.84                     | 0.59              |
| 1:D:82:MET:HE1   | 1:D:87:LEU:HA    | 1.85                     | 0.59              |
| 1:A:399:LEU:HD22 | 1:A:405:MET:SD   | 2.42                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:ARG:HH11 | 1:A:279:ARG:CG   | 2.16                     | 0.59              |
| 1:B:525:LEU:C    | 1:B:525:LEU:HD22 | 2.28                     | 0.59              |
| 1:F:82:MET:HE1   | 1:F:87:LEU:HA    | 1.84                     | 0.58              |
| 1:F:222:SER:HB2  | 1:F:286:ASP:OD1  | 2.03                     | 0.58              |
| 1:F:498:ARG:NH2  | 1:F:503:GLY:O    | 2.37                     | 0.58              |
| 1:D:255:TRP:HZ2  | 1:D:515:LEU:HD13 | 1.68                     | 0.58              |
| 1:A:516:LYS:O    | 1:A:521:PRO:HD3  | 2.03                     | 0.58              |
| 1:D:222:SER:HB2  | 1:D:286:ASP:OD1  | 2.03                     | 0.58              |
| 1:B:315:ASP:OD1  | 1:B:317:THR:OG1  | 2.21                     | 0.58              |
| 1:B:451:PHE:HD1  | 1:B:458:ALA:HB1  | 1.67                     | 0.58              |
| 1:A:182:PHE:HA   | 1:A:185:LYS:HD2  | 1.86                     | 0.57              |
| 1:A:222:SER:HB2  | 1:A:286:ASP:OD1  | 2.04                     | 0.57              |
| 1:B:447:ILE:HB   | 1:B:448:PRO:HD3  | 1.85                     | 0.57              |
| 1:E:222:SER:HB2  | 1:E:286:ASP:OD1  | 2.04                     | 0.57              |
| 1:B:349:GLU:HG3  | 1:B:424:GLN:HE22 | 1.68                     | 0.57              |
| 1:C:222:SER:HB2  | 1:C:286:ASP:OD1  | 2.04                     | 0.57              |
| 1:A:520:PHE:O    | 1:A:524:LEU:HB2  | 2.05                     | 0.57              |
| 1:D:167:LYS:HD2  | 1:D:308:GLU:CG   | 2.33                     | 0.57              |
| 1:A:433:TYR:C    | 1:A:433:TYR:CD2  | 2.81                     | 0.57              |
| 1:B:451:PHE:CD1  | 1:B:458:ALA:HB1  | 2.40                     | 0.57              |
| 1:C:255:TRP:CZ2  | 1:C:515:LEU:HD22 | 2.40                     | 0.57              |
| 1:A:333:TYR:N    | 1:A:333:TYR:HD1  | 2.02                     | 0.57              |
| 1:A:336:PRO:HA   | 5:A:717:HOH:O    | 2.04                     | 0.57              |
| 1:B:238:ARG:HH22 | 1:B:435:ASP:CG   | 2.12                     | 0.57              |
| 1:A:108:THR:HG23 | 1:A:131:LYS:HD3  | 1.86                     | 0.56              |
| 1:E:520:PHE:O    | 1:E:524:LEU:HB2  | 2.05                     | 0.56              |
| 1:D:125:TRP:HZ3  | 1:D:365:THR:OG1  | 1.88                     | 0.56              |
| 1:B:518:LEU:HD13 | 1:C:529:LEU:CD1  | 2.35                     | 0.56              |
| 1:A:33:ARG:HD2   | 2:A:601:FAD:C4A  | 2.35                     | 0.56              |
| 1:A:180:GLY:N    | 5:A:704:HOH:O    | 2.31                     | 0.56              |
| 1:E:125:TRP:HZ3  | 1:E:365:THR:OG1  | 1.88                     | 0.56              |
| 1:D:453:THR:HB   | 5:D:706:HOH:O    | 2.06                     | 0.56              |
| 1:B:19:ARG:HH11  | 1:B:19:ARG:CG    | 2.17                     | 0.56              |
| 1:B:222:SER:HB2  | 1:B:286:ASP:OD1  | 2.04                     | 0.56              |
| 1:C:19:ARG:NH2   | 1:C:71:ASP:OD1   | 2.38                     | 0.56              |
| 1:F:34:SER:HB3   | 1:F:51:ARG:HE    | 1.71                     | 0.56              |
| 1:F:520:PHE:O    | 1:F:524:LEU:HB2  | 2.06                     | 0.56              |
| 1:D:61:ASN:C     | 1:D:61:ASN:HD22  | 2.14                     | 0.56              |
| 1:C:34:SER:HB3   | 1:C:51:ARG:HE    | 1.70                     | 0.56              |
| 1:C:238:ARG:NH2  | 5:C:703:HOH:O    | 2.39                     | 0.56              |
| 1:F:61:ASN:C     | 1:F:61:ASN:HD22  | 2.14                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:359:PRO:O    | 1:B:360:LEU:HB2  | 2.05                     | 0.56              |
| 1:E:524:LEU:O    | 1:E:528:LEU:HB2  | 2.06                     | 0.56              |
| 1:F:513:ASN:HB3  | 1:F:516:LYS:HB3  | 1.88                     | 0.56              |
| 1:C:506:LYS:HE3  | 5:C:725:HOH:O    | 2.05                     | 0.56              |
| 1:E:172:HIS:CD2  | 1:E:174:ARG:H    | 2.24                     | 0.56              |
| 1:A:172:HIS:CD2  | 1:A:174:ARG:H    | 2.24                     | 0.55              |
| 1:B:172:HIS:CD2  | 1:B:174:ARG:H    | 2.24                     | 0.55              |
| 1:F:172:HIS:CD2  | 1:F:174:ARG:H    | 2.24                     | 0.55              |
| 1:C:125:TRP:HZ3  | 1:C:365:THR:OG1  | 1.89                     | 0.55              |
| 1:D:359:PRO:O    | 1:D:360:LEU:HB2  | 2.06                     | 0.55              |
| 1:F:315:ASP:OD1  | 1:F:317:THR:OG1  | 2.25                     | 0.55              |
| 1:D:172:HIS:CD2  | 1:D:174:ARG:H    | 2.25                     | 0.55              |
| 1:A:349:GLU:CD   | 1:A:424:GLN:HE22 | 2.15                     | 0.55              |
| 1:B:238:ARG:HD3  | 5:B:747:HOH:O    | 2.07                     | 0.55              |
| 1:A:18:ILE:HD11  | 1:A:30:CYS:HB2   | 1.89                     | 0.55              |
| 1:C:172:HIS:CD2  | 1:C:174:ARG:H    | 2.25                     | 0.55              |
| 1:D:527:VAL:O    | 1:D:528:LEU:HD23 | 2.06                     | 0.55              |
| 1:A:334:ALA:O    | 1:A:335:TYR:HB2  | 2.07                     | 0.55              |
| 1:A:19:ARG:NH2   | 1:A:71:ASP:CG    | 2.65                     | 0.55              |
| 1:B:122:THR:HB   | 1:B:124:GLN:HG3  | 1.88                     | 0.55              |
| 1:F:125:TRP:HZ3  | 1:F:365:THR:OG1  | 1.90                     | 0.55              |
| 1:A:348:ASN:HA   | 5:A:703:HOH:O    | 2.06                     | 0.54              |
| 1:A:490:TRP:CE2  | 1:A:508:PRO:HG2  | 2.41                     | 0.54              |
| 1:E:315:ASP:OD1  | 1:E:317:THR:OG1  | 2.24                     | 0.54              |
| 1:E:359:PRO:O    | 1:E:360:LEU:HB2  | 2.06                     | 0.54              |
| 1:F:527:VAL:HG12 | 1:F:527:VAL:O    | 2.07                     | 0.54              |
| 1:A:61:ASN:HD22  | 1:A:61:ASN:C     | 2.15                     | 0.54              |
| 1:C:359:PRO:CB   | 1:C:405:MET:CE   | 2.85                     | 0.54              |
| 1:E:497:THR:HG21 | 5:E:705:HOH:O    | 2.07                     | 0.54              |
| 1:A:433:TYR:C    | 1:A:433:TYR:HD2  | 2.15                     | 0.54              |
| 1:B:524:LEU:O    | 1:B:528:LEU:HB2  | 2.07                     | 0.54              |
| 1:E:34:SER:HB3   | 1:E:51:ARG:HE    | 1.73                     | 0.54              |
| 1:E:19:ARG:NH2   | 1:E:71:ASP:OD1   | 2.41                     | 0.54              |
| 1:A:82:MET:HE1   | 1:A:87:LEU:HD13  | 1.90                     | 0.54              |
| 1:A:150:HIS:HD2  | 2:A:601:FAD:O2'  | 1.90                     | 0.54              |
| 1:E:527:VAL:HG12 | 1:E:527:VAL:O    | 2.08                     | 0.54              |
| 1:A:125:TRP:HZ3  | 1:A:365:THR:OG1  | 1.91                     | 0.54              |
| 1:D:527:VAL:O    | 1:D:527:VAL:HG12 | 2.08                     | 0.54              |
| 1:B:34:SER:HB3   | 1:B:51:ARG:HE    | 1.73                     | 0.54              |
| 1:B:525:LEU:HD21 | 1:C:522:VAL:HG21 | 1.90                     | 0.54              |
| 1:C:527:VAL:HG12 | 1:C:527:VAL:O    | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:51:ARG:HH11  | 1:D:51:ARG:HB3   | 1.72                     | 0.54              |
| 1:A:117:PRO:HA   | 5:A:713:HOH:O    | 2.08                     | 0.54              |
| 1:F:40:LEU:HD11  | 2:F:601:FAD:HM83 | 1.90                     | 0.54              |
| 1:A:527:VAL:HG12 | 1:A:527:VAL:O    | 2.08                     | 0.53              |
| 1:B:279:ARG:HH11 | 1:B:279:ARG:HG2  | 1.73                     | 0.53              |
| 1:D:19:ARG:NH2   | 1:D:71:ASP:OD1   | 2.42                     | 0.53              |
| 1:D:315:ASP:OD1  | 1:D:317:THR:OG1  | 2.27                     | 0.53              |
| 1:A:515:LEU:HD13 | 1:A:519:LEU:HD22 | 1.91                     | 0.53              |
| 1:B:61:ASN:C     | 1:B:61:ASN:HD22  | 2.16                     | 0.53              |
| 1:A:522:VAL:HA   | 1:A:525:LEU:CD1  | 2.38                     | 0.53              |
| 1:C:19:ARG:CG    | 1:C:19:ARG:HH11  | 2.20                     | 0.53              |
| 1:E:527:VAL:O    | 1:E:528:LEU:HD22 | 2.09                     | 0.53              |
| 1:D:34:SER:HB3   | 1:D:51:ARG:HE    | 1.73                     | 0.53              |
| 1:A:18:ILE:HD11  | 1:A:30:CYS:CB    | 2.39                     | 0.53              |
| 1:B:525:LEU:HD21 | 1:C:522:VAL:CG2  | 2.39                     | 0.53              |
| 1:A:135:LYS:CG   | 5:A:716:HOH:O    | 2.56                     | 0.53              |
| 1:C:61:ASN:C     | 1:C:61:ASN:HD22  | 2.16                     | 0.53              |
| 1:A:90:TYR:HA    | 5:A:728:HOH:O    | 2.08                     | 0.53              |
| 1:A:145:ILE:CG2  | 1:A:335:TYR:CD1  | 2.85                     | 0.53              |
| 1:C:349:GLU:HG3  | 1:C:424:GLN:HE22 | 1.73                     | 0.53              |
| 1:D:19:ARG:HG2   | 1:D:19:ARG:NH1   | 2.24                     | 0.52              |
| 1:C:524:LEU:HA   | 1:C:528:LEU:HD23 | 1.91                     | 0.52              |
| 1:B:125:TRP:HZ3  | 1:B:365:THR:OG1  | 1.89                     | 0.52              |
| 1:C:512:TYR:CE1  | 1:C:514:LEU:HB2  | 2.45                     | 0.52              |
| 1:A:359:PRO:O    | 1:A:360:LEU:HB2  | 2.09                     | 0.52              |
| 1:E:61:ASN:C     | 1:E:61:ASN:HD22  | 2.16                     | 0.52              |
| 1:C:524:LEU:O    | 1:C:528:LEU:HB2  | 2.10                     | 0.52              |
| 1:F:401:THR:HG22 | 1:F:404:GLU:CG   | 2.39                     | 0.52              |
| 1:C:359:PRO:O    | 1:C:360:LEU:HB2  | 2.08                     | 0.52              |
| 1:E:51:ARG:HH11  | 1:E:51:ARG:HB3   | 1.75                     | 0.52              |
| 1:F:119:PHE:CD1  | 1:F:123:GLY:HA2  | 2.45                     | 0.52              |
| 1:B:527:VAL:HG12 | 1:B:527:VAL:O    | 2.10                     | 0.52              |
| 1:F:108:THR:HG22 | 1:F:131:LYS:HD3  | 1.92                     | 0.52              |
| 1:D:401:THR:HG22 | 1:D:404:GLU:CG   | 2.40                     | 0.52              |
| 1:A:346:ARG:NH1  | 1:A:406:MET:HE3  | 2.25                     | 0.52              |
| 1:C:300:LYS:CE   | 5:C:752:HOH:O    | 2.45                     | 0.52              |
| 1:C:167:LYS:HD2  | 1:C:308:GLU:HG2  | 1.92                     | 0.51              |
| 1:C:315:ASP:OD1  | 1:C:317:THR:OG1  | 2.27                     | 0.51              |
| 1:A:33:ARG:HB2   | 1:A:33:ARG:NH1   | 2.16                     | 0.51              |
| 1:C:156:PRO:HG3  | 3:C:602:NAP:N6A  | 2.26                     | 0.51              |
| 1:A:53:SER:OG    | 1:A:174:ARG:O    | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:HIS:HD2  | 1:A:174:ARG:H    | 1.59                     | 0.51              |
| 1:C:401:THR:HG22 | 1:C:404:GLU:CG   | 2.41                     | 0.51              |
| 1:B:51:ARG:HB3   | 1:B:51:ARG:HH11  | 1.76                     | 0.51              |
| 1:A:33:ARG:HD2   | 2:A:601:FAD:C6A  | 2.40                     | 0.51              |
| 1:A:401:THR:HG22 | 1:A:404:GLU:CG   | 2.40                     | 0.51              |
| 1:B:19:ARG:NH1   | 1:B:19:ARG:CG    | 2.73                     | 0.51              |
| 1:B:108:THR:HG22 | 1:B:131:LYS:HD3  | 1.93                     | 0.51              |
| 1:C:255:TRP:HZ2  | 1:C:515:LEU:HD22 | 1.75                     | 0.51              |
| 1:D:522:VAL:HG23 | 5:D:711:HOH:O    | 2.10                     | 0.51              |
| 1:A:315:ASP:OD1  | 1:A:317:THR:OG1  | 2.29                     | 0.51              |
| 1:B:401:THR:HG22 | 1:B:404:GLU:CG   | 2.41                     | 0.51              |
| 1:C:41:TRP:CD2   | 1:C:87:LEU:HD23  | 2.45                     | 0.51              |
| 1:E:229:TYR:CE2  | 1:E:508:PRO:HG3  | 2.46                     | 0.51              |
| 1:F:41:TRP:CD2   | 1:F:87:LEU:HD23  | 2.46                     | 0.51              |
| 1:D:167:LYS:CD   | 1:D:308:GLU:CG   | 2.88                     | 0.50              |
| 1:D:41:TRP:CD2   | 1:D:87:LEU:HD23  | 2.46                     | 0.50              |
| 1:D:524:LEU:O    | 1:D:528:LEU:HD12 | 2.11                     | 0.50              |
| 1:A:279:ARG:HH11 | 1:A:279:ARG:HG3  | 1.76                     | 0.50              |
| 1:E:19:ARG:CG    | 1:E:19:ARG:HH11  | 2.23                     | 0.50              |
| 1:E:41:TRP:CD2   | 1:E:87:LEU:HD23  | 2.46                     | 0.50              |
| 1:E:401:THR:HG22 | 1:E:404:GLU:CG   | 2.40                     | 0.50              |
| 1:E:522:VAL:HA   | 1:E:525:LEU:CD1  | 2.41                     | 0.50              |
| 1:F:172:HIS:HD2  | 1:F:174:ARG:H    | 1.59                     | 0.50              |
| 1:F:490:TRP:CZ2  | 1:F:508:PRO:HG2  | 2.47                     | 0.50              |
| 1:A:3:LYS:N      | 1:A:141:ASP:OD2  | 2.45                     | 0.50              |
| 1:A:33:ARG:CG    | 1:A:33:ARG:NH1   | 2.72                     | 0.50              |
| 1:B:155:LEU:CD2  | 1:B:172:HIS:HB2  | 2.42                     | 0.50              |
| 1:E:40:LEU:HD11  | 2:E:601:FAD:HM83 | 1.92                     | 0.50              |
| 1:B:41:TRP:CD2   | 1:B:87:LEU:HD23  | 2.45                     | 0.50              |
| 1:B:516:LYS:HG2  | 1:B:519:LEU:HD21 | 1.92                     | 0.50              |
| 1:F:156:PRO:HG2  | 3:F:602:NAP:H61A | 1.77                     | 0.50              |
| 1:F:359:PRO:O    | 1:F:360:LEU:HB2  | 2.11                     | 0.50              |
| 2:D:601:FAD:C6   | 3:D:602:NAP:C2N  | 2.90                     | 0.50              |
| 1:C:108:THR:HG22 | 1:C:131:LYS:HD3  | 1.94                     | 0.50              |
| 1:F:51:ARG:HH11  | 1:F:51:ARG:HB3   | 1.77                     | 0.50              |
| 1:A:19:ARG:HD2   | 1:A:19:ARG:O     | 2.12                     | 0.50              |
| 1:A:490:TRP:CZ2  | 1:A:508:PRO:HG2  | 2.46                     | 0.50              |
| 1:C:519:LEU:HD13 | 1:C:519:LEU:H    | 1.77                     | 0.50              |
| 1:D:238:ARG:NE   | 1:D:470:GLN:NE2  | 2.60                     | 0.50              |
| 1:A:114:ASN:HB2  | 5:A:706:HOH:O    | 2.12                     | 0.50              |
| 1:F:524:LEU:HB2  | 5:F:713:HOH:O    | 2.10                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:527:VAL:O    | 1:A:528:LEU:HD22 | 2.12                     | 0.49              |
| 1:C:238:ARG:NE   | 1:C:470:GLN:HE21 | 1.96                     | 0.49              |
| 1:E:172:HIS:HD2  | 1:E:174:ARG:H    | 1.60                     | 0.49              |
| 1:C:51:ARG:HH11  | 1:C:51:ARG:HB3   | 1.76                     | 0.49              |
| 1:F:215:ARG:NH1  | 5:F:703:HOH:O    | 2.42                     | 0.49              |
| 1:A:41:TRP:CD2   | 1:A:87:LEU:HD23  | 2.47                     | 0.49              |
| 1:B:238:ARG:NH2  | 1:B:435:ASP:OD2  | 2.45                     | 0.49              |
| 1:A:346:ARG:HD3  | 1:A:406:MET:HE1  | 1.95                     | 0.49              |
| 1:D:518:LEU:CD2  | 1:F:525:LEU:HD23 | 2.43                     | 0.49              |
| 1:F:345:SER:O    | 1:F:346:ARG:HB2  | 2.13                     | 0.49              |
| 1:A:51:ARG:NH1   | 1:A:51:ARG:CG    | 2.72                     | 0.49              |
| 2:B:601:FAD:C6   | 3:B:602:NAP:C2N  | 2.91                     | 0.49              |
| 1:E:238:ARG:HE   | 1:E:470:GLN:HE22 | 1.51                     | 0.49              |
| 1:D:172:HIS:HD2  | 1:D:174:ARG:H    | 1.60                     | 0.49              |
| 1:C:172:HIS:HD2  | 1:C:174:ARG:H    | 1.60                     | 0.49              |
| 1:B:238:ARG:HH11 | 1:B:470:GLN:HE21 | 1.59                     | 0.48              |
| 1:C:527:VAL:O    | 1:C:528:LEU:HD22 | 2.12                     | 0.48              |
| 1:A:123:GLY:O    | 1:A:141:ASP:O    | 2.30                     | 0.48              |
| 1:F:238:ARG:HE   | 1:F:470:GLN:HE21 | 1.58                     | 0.48              |
| 1:F:401:THR:HG22 | 1:F:404:GLU:HG3  | 1.95                     | 0.48              |
| 1:A:180:GLY:CA   | 5:A:704:HOH:O    | 2.60                     | 0.48              |
| 1:A:522:VAL:HA   | 1:A:525:LEU:HD12 | 1.95                     | 0.48              |
| 1:B:451:PHE:HD1  | 1:B:458:ALA:CB   | 2.26                     | 0.48              |
| 1:C:172:HIS:CD2  | 1:C:174:ARG:HB2  | 2.45                     | 0.48              |
| 1:D:516:LYS:O    | 1:D:521:PRO:HD3  | 2.13                     | 0.48              |
| 1:E:491:ASP:OD1  | 1:E:507:ARG:NH2  | 2.40                     | 0.48              |
| 1:D:108:THR:HG23 | 1:D:131:LYS:HD3  | 1.94                     | 0.48              |
| 1:D:518:LEU:HD13 | 1:F:529:LEU:CD1  | 2.44                     | 0.48              |
| 1:B:172:HIS:HD2  | 1:B:174:ARG:H    | 1.59                     | 0.48              |
| 1:C:522:VAL:HG23 | 5:C:747:HOH:O    | 2.14                     | 0.48              |
| 1:D:518:LEU:HD22 | 1:F:529:LEU:HD13 | 1.96                     | 0.48              |
| 1:A:356:ILE:HD11 | 1:A:385:GLN:HG2  | 1.96                     | 0.48              |
| 1:B:510:LEU:HD21 | 5:B:712:HOH:O    | 2.13                     | 0.48              |
| 1:A:348:ASN:CA   | 5:A:703:HOH:O    | 2.61                     | 0.47              |
| 1:C:77:ASP:HB3   | 5:C:746:HOH:O    | 2.06                     | 0.47              |
| 1:C:238:ARG:NE   | 1:C:470:GLN:HE22 | 2.07                     | 0.47              |
| 1:C:519:LEU:HD22 | 1:C:520:PHE:H    | 1.78                     | 0.47              |
| 1:E:401:THR:HG22 | 1:E:404:GLU:HB2  | 1.96                     | 0.47              |
| 1:A:137:SER:HB2  | 5:A:722:HOH:O    | 2.14                     | 0.47              |
| 1:F:156:PRO:HG2  | 3:F:602:NAP:N6A  | 2.29                     | 0.47              |
| 1:C:279:ARG:HH11 | 1:C:279:ARG:HG2  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:19:ARG:CG    | 1:D:19:ARG:NH1   | 2.73                     | 0.47              |
| 1:F:349:GLU:HG3  | 1:F:424:GLN:HE22 | 1.80                     | 0.47              |
| 1:D:520:PHE:N    | 1:D:521:PRO:CD   | 2.78                     | 0.47              |
| 1:B:33:ARG:HH11  | 1:B:33:ARG:CG    | 2.10                     | 0.47              |
| 1:C:512:TYR:CD2  | 1:C:513:ASN:N    | 2.83                     | 0.47              |
| 1:A:33:ARG:NE    | 2:A:601:FAD:N7A  | 2.62                     | 0.47              |
| 2:C:601:FAD:C6   | 3:C:602:NAP:C2N  | 2.93                     | 0.47              |
| 1:F:279:ARG:CG   | 1:F:279:ARG:NH1  | 2.78                     | 0.47              |
| 1:A:101:LEU:HA   | 1:A:104:ILE:HD12 | 1.96                     | 0.47              |
| 1:B:401:THR:HG22 | 1:B:404:GLU:HB2  | 1.97                     | 0.47              |
| 5:B:715:HOH:O    | 1:C:529:LEU:HD21 | 2.14                     | 0.47              |
| 2:E:601:FAD:HM73 | 3:E:602:NAP:C5N  | 2.45                     | 0.47              |
| 1:D:101:LEU:HD12 | 5:D:774:HOH:O    | 2.15                     | 0.47              |
| 1:D:345:SER:O    | 1:D:346:ARG:HB2  | 2.15                     | 0.47              |
| 1:A:150:HIS:CD2  | 2:A:601:FAD:O2'  | 2.67                     | 0.47              |
| 1:C:397:CYS:HA   | 5:C:713:HOH:O    | 2.15                     | 0.47              |
| 1:E:512:TYR:CD2  | 1:E:513:ASN:N    | 2.82                     | 0.47              |
| 1:D:522:VAL:HA   | 1:D:525:LEU:CD1  | 2.45                     | 0.46              |
| 1:B:4:LYS:NZ     | 5:B:702:HOH:O    | 2.38                     | 0.46              |
| 1:B:527:VAL:O    | 1:B:528:LEU:HD22 | 2.14                     | 0.46              |
| 1:D:454:ASP:N    | 5:D:706:HOH:O    | 2.47                     | 0.46              |
| 1:D:3:LYS:N      | 1:D:141:ASP:OD2  | 2.48                     | 0.46              |
| 1:D:156:PRO:HG2  | 3:D:602:NAP:H61A | 1.79                     | 0.46              |
| 1:D:516:LYS:O    | 1:D:516:LYS:HG2  | 2.14                     | 0.46              |
| 1:A:236:ILE:HD11 | 1:A:375:LEU:HB3  | 1.98                     | 0.46              |
| 1:C:40:LEU:HD11  | 2:C:601:FAD:C8M  | 2.46                     | 0.46              |
| 1:B:522:VAL:HA   | 1:B:525:LEU:CD1  | 2.45                     | 0.46              |
| 1:C:345:SER:O    | 1:C:346:ARG:HB2  | 2.15                     | 0.46              |
| 1:D:304:LYS:HA   | 1:D:304:LYS:HD2  | 1.76                     | 0.46              |
| 1:D:216:SER:OG   | 3:D:602:NAP:O2X  | 2.34                     | 0.46              |
| 1:D:401:THR:HG22 | 1:D:404:GLU:HG3  | 1.97                     | 0.46              |
| 1:A:399:LEU:HD13 | 1:A:405:MET:HE1  | 1.97                     | 0.46              |
| 1:B:520:PHE:O    | 1:B:524:LEU:HB2  | 2.15                     | 0.46              |
| 1:F:512:TYR:CD2  | 1:F:513:ASN:N    | 2.82                     | 0.46              |
| 1:E:238:ARG:NE   | 1:E:470:GLN:NE2  | 2.43                     | 0.46              |
| 1:D:512:TYR:CD2  | 1:D:513:ASN:N    | 2.83                     | 0.46              |
| 1:B:512:TYR:CD2  | 1:B:513:ASN:N    | 2.83                     | 0.46              |
| 1:B:519:LEU:HD22 | 1:B:520:PHE:N    | 2.30                     | 0.46              |
| 1:C:279:ARG:CG   | 1:C:279:ARG:NH1  | 2.76                     | 0.46              |
| 2:E:601:FAD:C6   | 3:E:602:NAP:C2N  | 2.93                     | 0.46              |
| 1:D:524:LEU:O    | 1:D:528:LEU:CD1  | 2.64                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:19:ARG:CG    | 1:C:19:ARG:NH1   | 2.78                     | 0.46              |
| 1:E:229:TYR:CZ   | 1:E:508:PRO:HG3  | 2.51                     | 0.46              |
| 1:B:156:PRO:HG2  | 3:B:602:NAP:H61A | 1.80                     | 0.45              |
| 1:B:82:MET:HE2   | 1:B:87:LEU:HB2   | 1.98                     | 0.45              |
| 1:B:345:SER:O    | 1:B:346:ARG:HB2  | 2.16                     | 0.45              |
| 1:D:49:GLU:OE2   | 1:D:49:GLU:HA    | 2.16                     | 0.45              |
| 1:A:512:TYR:CE1  | 1:A:514:LEU:HB2  | 2.51                     | 0.45              |
| 1:C:521:PRO:HB2  | 5:C:747:HOH:O    | 2.16                     | 0.45              |
| 1:A:33:ARG:CD    | 2:A:601:FAD:N7A  | 2.79                     | 0.45              |
| 1:A:512:TYR:CD2  | 1:A:513:ASN:N    | 2.83                     | 0.45              |
| 1:E:401:THR:HG22 | 1:E:404:GLU:HG3  | 1.99                     | 0.45              |
| 1:A:401:THR:HG22 | 1:A:404:GLU:HG3  | 1.99                     | 0.45              |
| 1:D:83:HIS:HD2   | 1:D:85:SER:OG    | 2.00                     | 0.45              |
| 1:D:401:THR:HG22 | 1:D:404:GLU:HB2  | 1.98                     | 0.45              |
| 1:A:60:THR:CG2   | 1:A:82:MET:HE2   | 2.46                     | 0.45              |
| 1:B:173:SER:HB3  | 1:B:328:ALA:HA   | 1.99                     | 0.45              |
| 1:C:33:ARG:HG2   | 2:C:601:FAD:C4A  | 2.46                     | 0.45              |
| 1:F:158:GLU:O    | 1:F:158:GLU:HG3  | 2.17                     | 0.45              |
| 1:C:3:LYS:N      | 1:C:141:ASP:OD2  | 2.50                     | 0.45              |
| 1:C:516:LYS:HA   | 1:C:519:LEU:HD21 | 1.99                     | 0.45              |
| 1:B:516:LYS:HA   | 1:B:519:LEU:HD11 | 1.99                     | 0.45              |
| 1:E:498:ARG:NH2  | 1:E:503:GLY:O    | 2.50                     | 0.45              |
| 1:D:19:ARG:HH11  | 1:D:19:ARG:HG2   | 1.82                     | 0.44              |
| 1:D:63:SER:HB3   | 1:D:232:ASP:OD1  | 2.17                     | 0.44              |
| 1:A:119:PHE:O    | 1:A:122:THR:O    | 2.34                     | 0.44              |
| 1:B:520:PHE:N    | 1:B:521:PRO:CD   | 2.80                     | 0.44              |
| 1:D:450:LEU:O    | 1:D:451:PHE:C    | 2.60                     | 0.44              |
| 1:B:529:LEU:CD1  | 1:C:518:LEU:HD22 | 2.48                     | 0.44              |
| 1:E:122:THR:HB   | 1:E:124:GLN:HG3  | 1.98                     | 0.44              |
| 1:A:357:PHE:CD2  | 1:A:399:LEU:HD21 | 2.52                     | 0.44              |
| 1:C:19:ARG:NH1   | 1:C:19:ARG:HG2   | 2.33                     | 0.44              |
| 1:C:401:THR:HG22 | 1:C:404:GLU:HB2  | 1.98                     | 0.44              |
| 1:B:529:LEU:HD22 | 5:C:757:HOH:O    | 2.17                     | 0.44              |
| 1:E:522:VAL:HA   | 1:E:525:LEU:HD12 | 1.98                     | 0.44              |
| 1:F:171:PHE:CZ   | 1:F:326:ILE:HD13 | 2.52                     | 0.44              |
| 1:F:401:THR:HG22 | 1:F:404:GLU:HB2  | 2.00                     | 0.44              |
| 1:C:205:HIS:HE1  | 1:C:287:GLU:OE1  | 2.01                     | 0.44              |
| 1:E:19:ARG:CG    | 1:E:19:ARG:NH1   | 2.79                     | 0.44              |
| 2:F:601:FAD:C6   | 3:F:602:NAP:C2N  | 2.95                     | 0.44              |
| 1:A:63:SER:HB3   | 1:A:232:ASP:OD1  | 2.18                     | 0.44              |
| 1:B:63:SER:HB3   | 1:B:232:ASP:OD1  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:173:SER:HB3  | 1:E:328:ALA:HA   | 2.00                     | 0.44              |
| 1:D:279:ARG:HH11 | 1:D:279:ARG:HG2  | 1.81                     | 0.44              |
| 1:A:181:ILE:H    | 1:A:181:ILE:CD1  | 2.21                     | 0.44              |
| 3:A:602:NAP:O2A  | 3:A:602:NAP:O5D  | 2.35                     | 0.44              |
| 1:C:63:SER:HB3   | 1:C:232:ASP:OD1  | 2.18                     | 0.44              |
| 1:C:520:PHE:O    | 1:C:524:LEU:HB2  | 2.18                     | 0.44              |
| 1:E:345:SER:O    | 1:E:346:ARG:HB2  | 2.18                     | 0.44              |
| 1:E:520:PHE:N    | 1:E:521:PRO:CD   | 2.81                     | 0.44              |
| 1:F:524:LEU:CB   | 5:F:713:HOH:O    | 2.66                     | 0.44              |
| 1:A:135:LYS:HB2  | 5:A:716:HOH:O    | 2.18                     | 0.43              |
| 1:A:401:THR:HG22 | 1:A:404:GLU:HB2  | 2.00                     | 0.43              |
| 1:E:3:LYS:N      | 1:E:141:ASP:OD2  | 2.51                     | 0.43              |
| 1:B:3:LYS:N      | 1:B:141:ASP:OD2  | 2.51                     | 0.43              |
| 1:D:93:ALA:HA    | 5:D:758:HOH:O    | 2.16                     | 0.43              |
| 1:B:495:LYS:HB3  | 1:B:496:PRO:HD3  | 2.00                     | 0.43              |
| 5:B:715:HOH:O    | 1:C:529:LEU:CD2  | 2.65                     | 0.43              |
| 1:E:83:HIS:HD2   | 1:E:85:SER:OG    | 2.01                     | 0.43              |
| 1:D:173:SER:HB3  | 1:D:328:ALA:HA   | 1.99                     | 0.43              |
| 1:D:238:ARG:CZ   | 1:D:470:GLN:HE21 | 2.29                     | 0.43              |
| 1:F:279:ARG:HH11 | 1:F:279:ARG:HG2  | 1.80                     | 0.43              |
| 1:D:529:LEU:CD1  | 1:F:518:LEU:HD13 | 2.45                     | 0.43              |
| 1:B:516:LYS:HA   | 1:B:519:LEU:CD2  | 2.46                     | 0.43              |
| 1:B:345:SER:HB3  | 5:B:704:HOH:O    | 2.19                     | 0.43              |
| 1:E:82:MET:HE2   | 1:E:87:LEU:HB2   | 2.00                     | 0.43              |
| 1:F:450:LEU:O    | 1:F:451:PHE:C    | 2.61                     | 0.43              |
| 1:B:359:PRO:O    | 1:B:360:LEU:CB   | 2.66                     | 0.43              |
| 1:F:238:ARG:CZ   | 1:F:470:GLN:HE21 | 2.32                     | 0.43              |
| 1:F:401:THR:HG22 | 1:F:404:GLU:CB   | 2.49                     | 0.43              |
| 1:B:519:LEU:N    | 1:B:519:LEU:CD1  | 2.79                     | 0.43              |
| 1:E:63:SER:HB3   | 1:E:232:ASP:OD1  | 2.18                     | 0.43              |
| 1:A:26:LEU:HD21  | 1:A:394:ALA:HB2  | 2.00                     | 0.43              |
| 1:B:236:ILE:HD11 | 1:B:375:LEU:HB3  | 2.01                     | 0.43              |
| 1:C:401:THR:HG22 | 1:C:404:GLU:HG3  | 2.00                     | 0.43              |
| 1:D:529:LEU:HD11 | 1:F:518:LEU:CD1  | 2.45                     | 0.43              |
| 1:B:401:THR:HG22 | 1:B:404:GLU:CB   | 2.48                     | 0.43              |
| 1:E:288:LEU:HB3  | 1:E:289:PRO:HD3  | 2.01                     | 0.43              |
| 1:F:238:ARG:NE   | 1:F:470:GLN:HE22 | 2.12                     | 0.43              |
| 1:B:19:ARG:NH1   | 1:B:19:ARG:HG2   | 2.33                     | 0.42              |
| 1:E:279:ARG:CG   | 1:E:279:ARG:NH1  | 2.79                     | 0.42              |
| 1:E:359:PRO:O    | 1:E:360:LEU:CB   | 2.67                     | 0.42              |
| 1:E:450:LEU:O    | 1:E:451:PHE:C    | 2.61                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:83:HIS:HD2   | 1:F:85:SER:OG    | 2.02                     | 0.42              |
| 1:F:216:SER:O    | 1:F:273:PRO:HA   | 2.19                     | 0.42              |
| 1:D:33:ARG:HH11  | 1:D:33:ARG:CG    | 2.12                     | 0.42              |
| 1:D:288:LEU:HB3  | 1:D:289:PRO:HD3  | 2.01                     | 0.42              |
| 1:D:520:PHE:O    | 1:D:524:LEU:HB2  | 2.19                     | 0.42              |
| 1:E:19:ARG:NH1   | 1:E:472:ARG:NH2  | 2.67                     | 0.42              |
| 1:F:520:PHE:N    | 1:F:521:PRO:CD   | 2.82                     | 0.42              |
| 1:A:83:HIS:HD2   | 1:A:85:SER:OG    | 2.02                     | 0.42              |
| 1:C:173:SER:HB3  | 1:C:328:ALA:HA   | 2.01                     | 0.42              |
| 1:C:516:LYS:HA   | 1:C:519:LEU:CD2  | 2.49                     | 0.42              |
| 1:E:401:THR:HG22 | 1:E:404:GLU:CB   | 2.48                     | 0.42              |
| 1:D:401:THR:HG22 | 1:D:404:GLU:CB   | 2.48                     | 0.42              |
| 1:A:520:PHE:N    | 1:A:521:PRO:CD   | 2.82                     | 0.42              |
| 1:D:205:HIS:HE1  | 1:D:287:GLU:OE1  | 2.03                     | 0.42              |
| 1:B:83:HIS:HD2   | 1:B:85:SER:OG    | 2.02                     | 0.42              |
| 1:B:401:THR:HG22 | 1:B:404:GLU:HG3  | 2.00                     | 0.42              |
| 1:F:33:ARG:HG2   | 2:F:601:FAD:C4A  | 2.49                     | 0.42              |
| 1:F:172:HIS:CD2  | 1:F:174:ARG:HB2  | 2.50                     | 0.42              |
| 1:F:205:HIS:HE1  | 1:F:287:GLU:OE1  | 2.02                     | 0.42              |
| 1:F:513:ASN:O    | 1:F:517:ILE:HD13 | 2.19                     | 0.42              |
| 1:D:359:PRO:O    | 1:D:360:LEU:CB   | 2.67                     | 0.42              |
| 1:F:3:LYS:N      | 1:F:141:ASP:OD2  | 2.53                     | 0.42              |
| 1:F:158:GLU:O    | 1:F:158:GLU:CG   | 2.67                     | 0.42              |
| 1:A:450:LEU:O    | 1:A:451:PHE:C    | 2.62                     | 0.42              |
| 1:B:155:LEU:C    | 1:B:155:LEU:HD12 | 2.43                     | 0.42              |
| 1:B:172:HIS:CD2  | 1:B:174:ARG:HB2  | 2.50                     | 0.42              |
| 1:C:83:HIS:HD2   | 1:C:85:SER:OG    | 2.03                     | 0.42              |
| 1:C:401:THR:HG22 | 1:C:404:GLU:CB   | 2.49                     | 0.42              |
| 1:A:359:PRO:O    | 1:A:360:LEU:CB   | 2.68                     | 0.42              |
| 1:E:364:PRO:HA   | 5:E:741:HOH:O    | 2.19                     | 0.42              |
| 1:F:236:ILE:HD11 | 1:F:375:LEU:HB3  | 2.02                     | 0.42              |
| 1:A:135:LYS:CB   | 5:A:716:HOH:O    | 2.68                     | 0.42              |
| 1:B:498:ARG:NH2  | 1:B:503:GLY:O    | 2.53                     | 0.42              |
| 1:C:105:GLN:HG3  | 5:C:739:HOH:O    | 2.20                     | 0.42              |
| 1:C:520:PHE:N    | 1:C:521:PRO:CD   | 2.83                     | 0.42              |
| 1:D:171:PHE:CZ   | 1:D:326:ILE:HD13 | 2.55                     | 0.41              |
| 1:D:236:ILE:HD11 | 1:D:375:LEU:HB3  | 2.01                     | 0.41              |
| 1:A:18:ILE:HG22  | 1:A:100:LEU:HD22 | 2.01                     | 0.41              |
| 1:A:401:THR:HG22 | 1:A:404:GLU:CB   | 2.50                     | 0.41              |
| 1:A:495:LYS:N    | 1:A:496:PRO:HD2  | 2.35                     | 0.41              |
| 1:A:507:ARG:H    | 1:A:507:ARG:HG2  | 1.47                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:349:GLU:CD   | 1:E:424:GLN:HE22 | 2.28                     | 0.41              |
| 1:F:125:TRP:CH2  | 1:F:366:LEU:HB2  | 2.55                     | 0.41              |
| 1:F:82:MET:HE2   | 1:F:87:LEU:HB2   | 2.02                     | 0.41              |
| 1:A:116:ARG:NH2  | 1:A:139:VAL:HG21 | 2.35                     | 0.41              |
| 1:B:33:ARG:NH1   | 1:B:33:ARG:CG    | 2.73                     | 0.41              |
| 1:D:116:ARG:HG3  | 1:D:124:GLN:HB2  | 2.03                     | 0.41              |
| 1:B:529:LEU:HD13 | 1:C:518:LEU:HD22 | 2.01                     | 0.41              |
| 1:A:116:ARG:HB2  | 1:A:124:GLN:O    | 2.21                     | 0.41              |
| 1:F:279:ARG:HH11 | 1:F:279:ARG:HG3  | 1.85                     | 0.41              |
| 1:D:216:SER:O    | 1:D:273:PRO:HA   | 2.21                     | 0.41              |
| 1:D:491:ASP:HA   | 1:D:507:ARG:HH12 | 1.86                     | 0.41              |
| 1:A:19:ARG:CD    | 1:A:19:ARG:C     | 2.94                     | 0.41              |
| 1:A:349:GLU:OE2  | 1:A:413:MET:HE2  | 2.19                     | 0.41              |
| 1:A:378:THR:HG21 | 2:A:601:FAD:C5'  | 2.50                     | 0.41              |
| 1:C:82:MET:HE2   | 1:C:87:LEU:HB2   | 2.02                     | 0.41              |
| 1:C:83:HIS:CD2   | 1:C:85:SER:H     | 2.39                     | 0.41              |
| 1:E:279:ARG:HH11 | 1:E:279:ARG:HG3  | 1.85                     | 0.41              |
| 1:D:522:VAL:HA   | 1:D:525:LEU:HD12 | 2.03                     | 0.41              |
| 1:A:155:LEU:CD2  | 1:A:172:HIS:HB2  | 2.50                     | 0.41              |
| 1:A:288:LEU:HB3  | 1:A:289:PRO:HD3  | 2.02                     | 0.41              |
| 1:B:495:LYS:N    | 1:B:496:PRO:HD2  | 2.36                     | 0.41              |
| 1:C:236:ILE:HD11 | 1:C:375:LEU:HB3  | 2.03                     | 0.41              |
| 1:F:49:GLU:OE2   | 1:F:49:GLU:HA    | 2.21                     | 0.41              |
| 1:A:512:TYR:OH   | 5:A:701:HOH:O    | 2.22                     | 0.41              |
| 1:B:205:HIS:HE1  | 1:B:287:GLU:OE1  | 2.02                     | 0.41              |
| 1:B:279:ARG:HG2  | 1:B:279:ARG:NH1  | 2.34                     | 0.41              |
| 1:E:83:HIS:CD2   | 1:E:85:SER:H     | 2.39                     | 0.41              |
| 1:D:82:MET:HE2   | 1:D:87:LEU:HB2   | 2.02                     | 0.41              |
| 1:D:356:ILE:HD11 | 1:D:385:GLN:HG2  | 2.03                     | 0.41              |
| 1:B:216:SER:O    | 1:B:273:PRO:HA   | 2.20                     | 0.41              |
| 1:B:516:LYS:HE3  | 1:B:516:LYS:HB3  | 1.92                     | 0.41              |
| 1:C:49:GLU:OE2   | 1:C:49:GLU:HA    | 2.20                     | 0.41              |
| 1:C:152:TYR:CE2  | 1:C:334:ALA:HB3  | 2.56                     | 0.41              |
| 1:C:450:LEU:O    | 1:C:451:PHE:C    | 2.62                     | 0.41              |
| 1:E:216:SER:O    | 1:E:273:PRO:HA   | 2.20                     | 0.41              |
| 1:F:516:LYS:O    | 1:F:516:LYS:HG2  | 2.21                     | 0.41              |
| 1:B:451:PHE:CE1  | 1:B:459:LEU:HD23 | 2.56                     | 0.41              |
| 1:F:238:ARG:NE   | 1:F:470:GLN:HE21 | 2.16                     | 0.41              |
| 1:A:158:GLU:O    | 1:A:158:GLU:CG   | 2.68                     | 0.40              |
| 1:A:216:SER:O    | 1:A:273:PRO:HA   | 2.21                     | 0.40              |
| 1:A:519:LEU:HD23 | 1:A:519:LEU:N    | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:171:PHE:CZ   | 1:B:326:ILE:HD13 | 2.56                     | 0.40              |
| 1:C:359:PRO:HA   | 1:C:405:MET:HE1  | 2.02                     | 0.40              |
| 1:D:41:TRP:CE2   | 1:D:87:LEU:HD23  | 2.56                     | 0.40              |
| 1:A:125:TRP:CH2  | 1:A:366:LEU:HB2  | 2.56                     | 0.40              |
| 1:C:279:ARG:HH11 | 1:C:279:ARG:HG3  | 1.83                     | 0.40              |
| 1:D:504:GLU:O    | 1:D:506:LYS:HD3  | 2.21                     | 0.40              |
| 1:A:125:TRP:HH2  | 1:A:361:LEU:HD21 | 1.85                     | 0.40              |
| 1:D:238:ARG:NH1  | 1:D:470:GLN:NE2  | 2.56                     | 0.40              |
| 1:D:529:LEU:CD1  | 1:F:518:LEU:CD1  | 2.99                     | 0.40              |
| 1:A:33:ARG:NE    | 2:A:601:FAD:C5A  | 2.85                     | 0.40              |
| 1:A:164:LYS:HE3  | 5:A:727:HOH:O    | 2.21                     | 0.40              |
| 1:C:510:LEU:O    | 1:C:512:TYR:N    | 2.54                     | 0.40              |
| 1:F:359:PRO:O    | 1:F:360:LEU:CB   | 2.69                     | 0.40              |
| 1:B:518:LEU:HD21 | 1:C:525:LEU:HD12 | 2.04                     | 0.40              |
| 1:C:171:PHE:CZ   | 1:C:326:ILE:HD13 | 2.56                     | 0.40              |
| 1:E:150:HIS:HD2  | 2:E:601:FAD:O2'  | 2.04                     | 0.40              |
| 2:F:601:FAD:H5'1 | 2:F:601:FAD:O2'  | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 526/532 (99%)   | 481 (91%)  | 41 (8%)  | 4 (1%)   | 16          | 44 |
| 1   | B     | 526/532 (99%)   | 487 (93%)  | 34 (6%)  | 5 (1%)   | 12          | 38 |
| 1   | C     | 526/532 (99%)   | 489 (93%)  | 32 (6%)  | 5 (1%)   | 12          | 38 |
| 1   | D     | 526/532 (99%)   | 484 (92%)  | 38 (7%)  | 4 (1%)   | 16          | 44 |
| 1   | E     | 526/532 (99%)   | 487 (93%)  | 34 (6%)  | 5 (1%)   | 12          | 38 |
| 1   | F     | 526/532 (99%)   | 485 (92%)  | 37 (7%)  | 4 (1%)   | 16          | 44 |
| All | All   | 3156/3192 (99%) | 2913 (92%) | 216 (7%) | 27 (1%)  | 14          | 41 |

All (27) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 511 | PHE  |
| 1   | A     | 511 | PHE  |
| 1   | B     | 511 | PHE  |
| 1   | C     | 511 | PHE  |
| 1   | E     | 511 | PHE  |
| 1   | D     | 346 | ARG  |
| 1   | D     | 529 | LEU  |
| 1   | A     | 529 | LEU  |
| 1   | B     | 346 | ARG  |
| 1   | B     | 529 | LEU  |
| 1   | C     | 346 | ARG  |
| 1   | C     | 529 | LEU  |
| 1   | E     | 346 | ARG  |
| 1   | E     | 529 | LEU  |
| 1   | F     | 346 | ARG  |
| 1   | F     | 511 | PHE  |
| 1   | F     | 529 | LEU  |
| 1   | B     | 513 | ASN  |
| 1   | C     | 513 | ASN  |
| 1   | E     | 513 | ASN  |
| 1   | D     | 513 | ASN  |
| 1   | A     | 513 | ASN  |
| 1   | A     | 346 | ARG  |
| 1   | F     | 513 | ASN  |
| 1   | E     | 527 | VAL  |
| 1   | C     | 527 | VAL  |
| 1   | B     | 527 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 459/462 (99%) | 393 (86%) | 66 (14%) | 3           | 11 |
| 1   | B     | 459/462 (99%) | 406 (88%) | 53 (12%) | 5           | 18 |
| 1   | C     | 459/462 (99%) | 408 (89%) | 51 (11%) | 6           | 20 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | D     | 459/462 (99%)   | 409 (89%)  | 50 (11%)  | 6           | 21 |
| 1   | E     | 459/462 (99%)   | 409 (89%)  | 50 (11%)  | 6           | 21 |
| 1   | F     | 459/462 (99%)   | 403 (88%)  | 56 (12%)  | 5           | 16 |
| All | All   | 2754/2772 (99%) | 2428 (88%) | 326 (12%) | 5           | 17 |

All (326) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 12  | VAL  |
| 1   | D     | 19  | ARG  |
| 1   | D     | 33  | ARG  |
| 1   | D     | 40  | LEU  |
| 1   | D     | 51  | ARG  |
| 1   | D     | 54  | ILE  |
| 1   | D     | 61  | ASN  |
| 1   | D     | 77  | ASP  |
| 1   | D     | 82  | MET  |
| 1   | D     | 108 | THR  |
| 1   | D     | 121 | VAL  |
| 1   | D     | 125 | TRP  |
| 1   | D     | 151 | VAL  |
| 1   | D     | 157 | LYS  |
| 1   | D     | 167 | LYS  |
| 1   | D     | 170 | CYS  |
| 1   | D     | 173 | SER  |
| 1   | D     | 178 | GLU  |
| 1   | D     | 216 | SER  |
| 1   | D     | 237 | THR  |
| 1   | D     | 251 | ILE  |
| 1   | D     | 252 | SER  |
| 1   | D     | 279 | ARG  |
| 1   | D     | 280 | LYS  |
| 1   | D     | 285 | ASN  |
| 1   | D     | 304 | LYS  |
| 1   | D     | 308 | GLU  |
| 1   | D     | 312 | ILE  |
| 1   | D     | 317 | THR  |
| 1   | D     | 320 | GLU  |
| 1   | D     | 326 | ILE  |
| 1   | D     | 349 | GLU  |
| 1   | D     | 373 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 375 | LEU  |
| 1   | D     | 384 | LEU  |
| 1   | D     | 401 | THR  |
| 1   | D     | 403 | ASN  |
| 1   | D     | 444 | LYS  |
| 1   | D     | 450 | LEU  |
| 1   | D     | 480 | ASP  |
| 1   | D     | 494 | LEU  |
| 1   | D     | 499 | THR  |
| 1   | D     | 507 | ARG  |
| 1   | D     | 512 | TYR  |
| 1   | D     | 513 | ASN  |
| 1   | D     | 520 | PHE  |
| 1   | D     | 523 | LEU  |
| 1   | D     | 524 | LEU  |
| 1   | D     | 525 | LEU  |
| 1   | D     | 529 | LEU  |
| 1   | A     | 12  | VAL  |
| 1   | A     | 19  | ARG  |
| 1   | A     | 22  | LEU  |
| 1   | A     | 33  | ARG  |
| 1   | A     | 49  | GLU  |
| 1   | A     | 51  | ARG  |
| 1   | A     | 54  | ILE  |
| 1   | A     | 61  | ASN  |
| 1   | A     | 82  | MET  |
| 1   | A     | 96  | LYS  |
| 1   | A     | 107 | LYS  |
| 1   | A     | 108 | THR  |
| 1   | A     | 116 | ARG  |
| 1   | A     | 121 | VAL  |
| 1   | A     | 125 | TRP  |
| 1   | A     | 132 | ASP  |
| 1   | A     | 134 | LYS  |
| 1   | A     | 147 | SER  |
| 1   | A     | 151 | VAL  |
| 1   | A     | 155 | LEU  |
| 1   | A     | 158 | GLU  |
| 1   | A     | 170 | CYS  |
| 1   | A     | 173 | SER  |
| 1   | A     | 178 | GLU  |
| 1   | A     | 181 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 208 | GLU  |
| 1   | A     | 215 | ARG  |
| 1   | A     | 216 | SER  |
| 1   | A     | 237 | THR  |
| 1   | A     | 240 | GLU  |
| 1   | A     | 252 | SER  |
| 1   | A     | 258 | LYS  |
| 1   | A     | 274 | LEU  |
| 1   | A     | 279 | ARG  |
| 1   | A     | 285 | ASN  |
| 1   | A     | 312 | ILE  |
| 1   | A     | 317 | THR  |
| 1   | A     | 333 | TYR  |
| 1   | A     | 338 | LEU  |
| 1   | A     | 340 | ASP  |
| 1   | A     | 349 | GLU  |
| 1   | A     | 373 | GLN  |
| 1   | A     | 375 | LEU  |
| 1   | A     | 384 | LEU  |
| 1   | A     | 398 | THR  |
| 1   | A     | 401 | THR  |
| 1   | A     | 403 | ASN  |
| 1   | A     | 413 | MET  |
| 1   | A     | 432 | THR  |
| 1   | A     | 433 | TYR  |
| 1   | A     | 444 | LYS  |
| 1   | A     | 480 | ASP  |
| 1   | A     | 494 | LEU  |
| 1   | A     | 497 | THR  |
| 1   | A     | 499 | THR  |
| 1   | A     | 506 | LYS  |
| 1   | A     | 512 | TYR  |
| 1   | A     | 513 | ASN  |
| 1   | A     | 514 | LEU  |
| 1   | A     | 515 | LEU  |
| 1   | A     | 516 | LYS  |
| 1   | A     | 517 | ILE  |
| 1   | A     | 519 | LEU  |
| 1   | A     | 523 | LEU  |
| 1   | A     | 524 | LEU  |
| 1   | A     | 525 | LEU  |
| 1   | B     | 12  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 19  | ARG  |
| 1   | B     | 33  | ARG  |
| 1   | B     | 40  | LEU  |
| 1   | B     | 51  | ARG  |
| 1   | B     | 54  | ILE  |
| 1   | B     | 61  | ASN  |
| 1   | B     | 77  | ASP  |
| 1   | B     | 82  | MET  |
| 1   | B     | 108 | THR  |
| 1   | B     | 121 | VAL  |
| 1   | B     | 125 | TRP  |
| 1   | B     | 151 | VAL  |
| 1   | B     | 155 | LEU  |
| 1   | B     | 157 | LYS  |
| 1   | B     | 167 | LYS  |
| 1   | B     | 169 | LYS  |
| 1   | B     | 170 | CYS  |
| 1   | B     | 173 | SER  |
| 1   | B     | 178 | GLU  |
| 1   | B     | 216 | SER  |
| 1   | B     | 237 | THR  |
| 1   | B     | 252 | SER  |
| 1   | B     | 279 | ARG  |
| 1   | B     | 280 | LYS  |
| 1   | B     | 285 | ASN  |
| 1   | B     | 304 | LYS  |
| 1   | B     | 308 | GLU  |
| 1   | B     | 312 | ILE  |
| 1   | B     | 317 | THR  |
| 1   | B     | 326 | ILE  |
| 1   | B     | 341 | SER  |
| 1   | B     | 343 | ILE  |
| 1   | B     | 344 | LYS  |
| 1   | B     | 349 | GLU  |
| 1   | B     | 373 | GLN  |
| 1   | B     | 375 | LEU  |
| 1   | B     | 384 | LEU  |
| 1   | B     | 403 | ASN  |
| 1   | B     | 444 | LYS  |
| 1   | B     | 480 | ASP  |
| 1   | B     | 494 | LEU  |
| 1   | B     | 499 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 506 | LYS  |
| 1   | B     | 507 | ARG  |
| 1   | B     | 511 | PHE  |
| 1   | B     | 512 | TYR  |
| 1   | B     | 516 | LYS  |
| 1   | B     | 519 | LEU  |
| 1   | B     | 523 | LEU  |
| 1   | B     | 524 | LEU  |
| 1   | B     | 525 | LEU  |
| 1   | B     | 529 | LEU  |
| 1   | C     | 12  | VAL  |
| 1   | C     | 19  | ARG  |
| 1   | C     | 33  | ARG  |
| 1   | C     | 51  | ARG  |
| 1   | C     | 54  | ILE  |
| 1   | C     | 61  | ASN  |
| 1   | C     | 77  | ASP  |
| 1   | C     | 82  | MET  |
| 1   | C     | 108 | THR  |
| 1   | C     | 121 | VAL  |
| 1   | C     | 125 | TRP  |
| 1   | C     | 151 | VAL  |
| 1   | C     | 155 | LEU  |
| 1   | C     | 157 | LYS  |
| 1   | C     | 169 | LYS  |
| 1   | C     | 170 | CYS  |
| 1   | C     | 173 | SER  |
| 1   | C     | 178 | GLU  |
| 1   | C     | 216 | SER  |
| 1   | C     | 237 | THR  |
| 1   | C     | 240 | GLU  |
| 1   | C     | 252 | SER  |
| 1   | C     | 274 | LEU  |
| 1   | C     | 279 | ARG  |
| 1   | C     | 280 | LYS  |
| 1   | C     | 285 | ASN  |
| 1   | C     | 308 | GLU  |
| 1   | C     | 312 | ILE  |
| 1   | C     | 317 | THR  |
| 1   | C     | 326 | ILE  |
| 1   | C     | 342 | ILE  |
| 1   | C     | 343 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 349 | GLU  |
| 1   | C     | 373 | GLN  |
| 1   | C     | 375 | LEU  |
| 1   | C     | 384 | LEU  |
| 1   | C     | 401 | THR  |
| 1   | C     | 403 | ASN  |
| 1   | C     | 444 | LYS  |
| 1   | C     | 478 | LYS  |
| 1   | C     | 480 | ASP  |
| 1   | C     | 494 | LEU  |
| 1   | C     | 499 | THR  |
| 1   | C     | 507 | ARG  |
| 1   | C     | 512 | TYR  |
| 1   | C     | 513 | ASN  |
| 1   | C     | 514 | LEU  |
| 1   | C     | 519 | LEU  |
| 1   | C     | 524 | LEU  |
| 1   | C     | 525 | LEU  |
| 1   | C     | 529 | LEU  |
| 1   | E     | 12  | VAL  |
| 1   | E     | 19  | ARG  |
| 1   | E     | 33  | ARG  |
| 1   | E     | 40  | LEU  |
| 1   | E     | 51  | ARG  |
| 1   | E     | 54  | ILE  |
| 1   | E     | 61  | ASN  |
| 1   | E     | 82  | MET  |
| 1   | E     | 108 | THR  |
| 1   | E     | 121 | VAL  |
| 1   | E     | 125 | TRP  |
| 1   | E     | 151 | VAL  |
| 1   | E     | 155 | LEU  |
| 1   | E     | 157 | LYS  |
| 1   | E     | 167 | LYS  |
| 1   | E     | 170 | CYS  |
| 1   | E     | 173 | SER  |
| 1   | E     | 178 | GLU  |
| 1   | E     | 216 | SER  |
| 1   | E     | 237 | THR  |
| 1   | E     | 251 | ILE  |
| 1   | E     | 252 | SER  |
| 1   | E     | 258 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 279 | ARG  |
| 1   | E     | 285 | ASN  |
| 1   | E     | 300 | LYS  |
| 1   | E     | 304 | LYS  |
| 1   | E     | 312 | ILE  |
| 1   | E     | 317 | THR  |
| 1   | E     | 326 | ILE  |
| 1   | E     | 342 | ILE  |
| 1   | E     | 343 | ILE  |
| 1   | E     | 344 | LYS  |
| 1   | E     | 373 | GLN  |
| 1   | E     | 375 | LEU  |
| 1   | E     | 384 | LEU  |
| 1   | E     | 403 | ASN  |
| 1   | E     | 444 | LYS  |
| 1   | E     | 480 | ASP  |
| 1   | E     | 494 | LEU  |
| 1   | E     | 499 | THR  |
| 1   | E     | 506 | LYS  |
| 1   | E     | 507 | ARG  |
| 1   | E     | 512 | TYR  |
| 1   | E     | 516 | LYS  |
| 1   | E     | 518 | LEU  |
| 1   | E     | 519 | LEU  |
| 1   | E     | 523 | LEU  |
| 1   | E     | 524 | LEU  |
| 1   | E     | 525 | LEU  |
| 1   | F     | 12  | VAL  |
| 1   | F     | 19  | ARG  |
| 1   | F     | 33  | ARG  |
| 1   | F     | 40  | LEU  |
| 1   | F     | 51  | ARG  |
| 1   | F     | 54  | ILE  |
| 1   | F     | 61  | ASN  |
| 1   | F     | 63  | SER  |
| 1   | F     | 77  | ASP  |
| 1   | F     | 82  | MET  |
| 1   | F     | 108 | THR  |
| 1   | F     | 120 | SER  |
| 1   | F     | 121 | VAL  |
| 1   | F     | 122 | THR  |
| 1   | F     | 125 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 151 | VAL  |
| 1   | F     | 155 | LEU  |
| 1   | F     | 169 | LYS  |
| 1   | F     | 170 | CYS  |
| 1   | F     | 173 | SER  |
| 1   | F     | 178 | GLU  |
| 1   | F     | 181 | ILE  |
| 1   | F     | 216 | SER  |
| 1   | F     | 237 | THR  |
| 1   | F     | 252 | SER  |
| 1   | F     | 258 | LYS  |
| 1   | F     | 274 | LEU  |
| 1   | F     | 279 | ARG  |
| 1   | F     | 285 | ASN  |
| 1   | F     | 308 | GLU  |
| 1   | F     | 312 | ILE  |
| 1   | F     | 317 | THR  |
| 1   | F     | 326 | ILE  |
| 1   | F     | 343 | ILE  |
| 1   | F     | 344 | LYS  |
| 1   | F     | 349 | GLU  |
| 1   | F     | 373 | GLN  |
| 1   | F     | 375 | LEU  |
| 1   | F     | 384 | LEU  |
| 1   | F     | 395 | ASN  |
| 1   | F     | 401 | THR  |
| 1   | F     | 403 | ASN  |
| 1   | F     | 444 | LYS  |
| 1   | F     | 480 | ASP  |
| 1   | F     | 494 | LEU  |
| 1   | F     | 499 | THR  |
| 1   | F     | 506 | LYS  |
| 1   | F     | 507 | ARG  |
| 1   | F     | 511 | PHE  |
| 1   | F     | 512 | TYR  |
| 1   | F     | 513 | ASN  |
| 1   | F     | 516 | LYS  |
| 1   | F     | 518 | LEU  |
| 1   | F     | 523 | LEU  |
| 1   | F     | 525 | LEU  |
| 1   | F     | 529 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 56  | GLN  |
| 1   | D     | 61  | ASN  |
| 1   | D     | 83  | HIS  |
| 1   | D     | 150 | HIS  |
| 1   | D     | 172 | HIS  |
| 1   | D     | 205 | HIS  |
| 1   | D     | 285 | ASN  |
| 1   | D     | 373 | GLN  |
| 1   | D     | 470 | GLN  |
| 1   | A     | 56  | GLN  |
| 1   | A     | 83  | HIS  |
| 1   | A     | 150 | HIS  |
| 1   | A     | 172 | HIS  |
| 1   | A     | 205 | HIS  |
| 1   | A     | 285 | ASN  |
| 1   | A     | 373 | GLN  |
| 1   | A     | 513 | ASN  |
| 1   | B     | 56  | GLN  |
| 1   | B     | 61  | ASN  |
| 1   | B     | 83  | HIS  |
| 1   | B     | 150 | HIS  |
| 1   | B     | 172 | HIS  |
| 1   | B     | 205 | HIS  |
| 1   | B     | 285 | ASN  |
| 1   | B     | 373 | GLN  |
| 1   | B     | 470 | GLN  |
| 1   | B     | 513 | ASN  |
| 1   | C     | 56  | GLN  |
| 1   | C     | 61  | ASN  |
| 1   | C     | 83  | HIS  |
| 1   | C     | 150 | HIS  |
| 1   | C     | 172 | HIS  |
| 1   | C     | 205 | HIS  |
| 1   | C     | 285 | ASN  |
| 1   | C     | 373 | GLN  |
| 1   | C     | 470 | GLN  |
| 1   | E     | 56  | GLN  |
| 1   | E     | 61  | ASN  |
| 1   | E     | 83  | HIS  |
| 1   | E     | 150 | HIS  |
| 1   | E     | 172 | HIS  |
| 1   | E     | 205 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 285 | ASN  |
| 1   | E     | 373 | GLN  |
| 1   | E     | 424 | GLN  |
| 1   | E     | 470 | GLN  |
| 1   | F     | 56  | GLN  |
| 1   | F     | 61  | ASN  |
| 1   | F     | 83  | HIS  |
| 1   | F     | 124 | GLN  |
| 1   | F     | 150 | HIS  |
| 1   | F     | 172 | HIS  |
| 1   | F     | 205 | HIS  |
| 1   | F     | 285 | ASN  |
| 1   | F     | 373 | GLN  |
| 1   | F     | 470 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | OXY  | C     | 603 | -    | 1,1,1        | 0.03 | 0        | -           |      |          |
| 4   | OXY  | F     | 603 | -    | 1,1,1        | 0.05 | 0        | -           |      |          |
| 2   | FAD  | A     | 601 | -    | 58,58,58     | 2.21 | 11 (18%) | 85,89,89    | 2.31 | 33 (38%) |
| 3   | NAP  | C     | 602 | -    | 50,52,52     | 1.10 | 5 (10%)  | 71,80,80    | 2.14 | 24 (33%) |
| 2   | FAD  | E     | 601 | -    | 58,58,58     | 1.42 | 9 (15%)  | 85,89,89    | 1.65 | 17 (20%) |
| 3   | NAP  | D     | 602 | -    | 50,52,52     | 1.37 | 5 (10%)  | 71,80,80    | 1.67 | 13 (18%) |
| 3   | NAP  | B     | 602 | -    | 50,52,52     | 1.30 | 5 (10%)  | 71,80,80    | 1.86 | 13 (18%) |
| 3   | NAP  | F     | 602 | -    | 50,52,52     | 1.43 | 5 (10%)  | 71,80,80    | 1.87 | 23 (32%) |
| 2   | FAD  | D     | 601 | -    | 58,58,58     | 1.65 | 11 (18%) | 85,89,89    | 1.90 | 20 (23%) |
| 4   | OXY  | B     | 603 | -    | 1,1,1        | 0.06 | 0        | -           |      |          |
| 2   | FAD  | F     | 601 | -    | 58,58,58     | 1.57 | 14 (24%) | 85,89,89    | 1.82 | 20 (23%) |
| 3   | NAP  | A     | 602 | -    | 50,52,52     | 1.41 | 5 (10%)  | 71,80,80    | 2.09 | 25 (35%) |
| 4   | OXY  | E     | 603 | -    | 1,1,1        | 0.05 | 0        | -           |      |          |
| 3   | NAP  | E     | 602 | -    | 50,52,52     | 1.35 | 7 (14%)  | 71,80,80    | 1.94 | 21 (29%) |
| 4   | OXY  | D     | 603 | -    | 1,1,1        | 0.14 | 0        | -           |      |          |
| 2   | FAD  | B     | 601 | -    | 58,58,58     | 1.70 | 14 (24%) | 85,89,89    | 1.86 | 22 (25%) |
| 4   | OXY  | A     | 603 | -    | 1,1,1        | 0.04 | 0        | -           |      |          |
| 2   | FAD  | C     | 601 | -    | 58,58,58     | 1.65 | 15 (25%) | 85,89,89    | 1.68 | 22 (25%) |

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   | FAD  | A     | 601 | -    | -       | 17/34/50/50 | 0/6/6/6 |
| 3   | NAP  | C     | 602 | -    | -       | 7/35/67/67  | 0/5/5/5 |
| 2   | FAD  | E     | 601 | -    | -       | 6/34/50/50  | 0/6/6/6 |
| 3   | NAP  | D     | 602 | -    | -       | 2/35/67/67  | 0/5/5/5 |
| 3   | NAP  | B     | 602 | -    | -       | 4/35/67/67  | 0/5/5/5 |
| 3   | NAP  | F     | 602 | -    | -       | 5/35/67/67  | 0/5/5/5 |
| 2   | FAD  | D     | 601 | -    | -       | 7/34/50/50  | 0/6/6/6 |
| 2   | FAD  | F     | 601 | -    | -       | 7/34/50/50  | 0/6/6/6 |
| 3   | NAP  | A     | 602 | -    | -       | 7/35/67/67  | 0/5/5/5 |
| 3   | NAP  | E     | 602 | -    | -       | 6/35/67/67  | 0/5/5/5 |
| 2   | FAD  | B     | 601 | -    | -       | 4/34/50/50  | 0/6/6/6 |
| 2   | FAD  | C     | 601 | -    | -       | 6/34/50/50  | 0/6/6/6 |

All (106) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 601 | FAD  | P-O3P   | 8.38  | 1.68        | 1.59     |
| 3   | F     | 602 | NAP  | PN-O3   | 6.01  | 1.66        | 1.59     |
| 2   | A     | 601 | FAD  | C9A-C5X | 5.86  | 1.50        | 1.41     |
| 2   | A     | 601 | FAD  | C5A-C4A | 5.74  | 1.49        | 1.39     |
| 2   | C     | 601 | FAD  | C9A-C5X | 5.53  | 1.50        | 1.41     |
| 2   | A     | 601 | FAD  | PA-O3P  | 5.41  | 1.65        | 1.59     |
| 2   | E     | 601 | FAD  | C9A-C5X | 5.01  | 1.49        | 1.41     |
| 3   | A     | 602 | NAP  | C5A-C4A | 4.90  | 1.47        | 1.39     |
| 2   | A     | 601 | FAD  | C5'-C4' | 4.75  | 1.58        | 1.51     |
| 3   | D     | 602 | NAP  | C5A-C4A | 4.74  | 1.47        | 1.39     |
| 2   | B     | 601 | FAD  | C9A-C5X | 4.67  | 1.48        | 1.41     |
| 3   | B     | 602 | NAP  | C5A-C4A | 4.59  | 1.47        | 1.39     |
| 2   | D     | 601 | FAD  | C5A-C4A | 4.50  | 1.47        | 1.39     |
| 2   | D     | 601 | FAD  | C9A-C5X | 4.28  | 1.48        | 1.41     |
| 2   | D     | 601 | FAD  | PA-O3P  | 4.21  | 1.64        | 1.59     |
| 2   | B     | 601 | FAD  | C5A-C4A | 4.13  | 1.46        | 1.39     |
| 2   | F     | 601 | FAD  | C5A-C4A | 4.09  | 1.46        | 1.39     |
| 3   | F     | 602 | NAP  | C5A-C4A | 3.92  | 1.46        | 1.39     |
| 2   | C     | 601 | FAD  | C8-C7   | 3.82  | 1.50        | 1.40     |
| 3   | E     | 602 | NAP  | C5A-C4A | 3.80  | 1.45        | 1.39     |
| 2   | E     | 601 | FAD  | C5A-C4A | 3.78  | 1.45        | 1.39     |
| 2   | F     | 601 | FAD  | C9A-C5X | 3.76  | 1.47        | 1.41     |
| 3   | B     | 602 | NAP  | PN-O3   | 3.65  | 1.63        | 1.59     |
| 2   | B     | 601 | FAD  | P-O3P   | 3.64  | 1.63        | 1.59     |
| 2   | A     | 601 | FAD  | C8-C7   | 3.63  | 1.49        | 1.40     |
| 2   | E     | 601 | FAD  | C5A-N7A | -3.60 | 1.32        | 1.39     |
| 3   | A     | 602 | NAP  | C8A-N7A | 3.58  | 1.38        | 1.31     |
| 3   | D     | 602 | NAP  | PA-O3   | 3.54  | 1.63        | 1.59     |
| 3   | A     | 602 | NAP  | C5A-C6A | 3.45  | 1.50        | 1.41     |
| 2   | B     | 601 | FAD  | C5X-N5  | -3.42 | 1.33        | 1.39     |
| 2   | F     | 601 | FAD  | P-O3P   | 3.38  | 1.63        | 1.59     |
| 3   | C     | 602 | NAP  | C5A-C4A | 3.28  | 1.44        | 1.39     |
| 2   | C     | 601 | FAD  | C5A-C4A | 3.25  | 1.44        | 1.39     |
| 2   | A     | 601 | FAD  | C5A-C6A | 3.24  | 1.50        | 1.41     |
| 2   | B     | 601 | FAD  | C4-N3   | -3.23 | 1.32        | 1.38     |
| 2   | D     | 601 | FAD  | C5A-N7A | -3.22 | 1.33        | 1.39     |
| 3   | A     | 602 | NAP  | O4D-C1D | 3.17  | 1.45        | 1.40     |
| 2   | F     | 601 | FAD  | C8A-N7A | 3.08  | 1.37        | 1.31     |
| 2   | C     | 601 | FAD  | C5A-N7A | -3.04 | 1.33        | 1.39     |
| 2   | B     | 601 | FAD  | C6-C5X  | -2.97 | 1.35        | 1.40     |
| 3   | E     | 602 | NAP  | C4A-N9A | -2.97 | 1.31        | 1.37     |
| 2   | C     | 601 | FAD  | C5X-N5  | -2.95 | 1.34        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | D     | 602 | NAP  | C5A-C6A | 2.94  | 1.49        | 1.41     |
| 2   | D     | 601 | FAD  | C4-N3   | -2.92 | 1.33        | 1.38     |
| 3   | E     | 602 | NAP  | O4D-C1D | 2.91  | 1.44        | 1.40     |
| 2   | D     | 601 | FAD  | C6-C7   | -2.89 | 1.35        | 1.39     |
| 3   | E     | 602 | NAP  | C5A-N7A | -2.80 | 1.34        | 1.39     |
| 2   | C     | 601 | FAD  | C4A-N9A | -2.78 | 1.31        | 1.37     |
| 2   | F     | 601 | FAD  | C5X-N5  | -2.75 | 1.34        | 1.39     |
| 2   | B     | 601 | FAD  | C8A-N7A | 2.72  | 1.36        | 1.31     |
| 2   | F     | 601 | FAD  | C6-C5X  | -2.70 | 1.35        | 1.40     |
| 2   | B     | 601 | FAD  | C5A-C6A | 2.70  | 1.48        | 1.41     |
| 3   | B     | 602 | NAP  | C5A-C6A | 2.68  | 1.48        | 1.41     |
| 3   | D     | 602 | NAP  | C4A-N9A | -2.61 | 1.32        | 1.37     |
| 3   | E     | 602 | NAP  | PN-O3   | 2.60  | 1.62        | 1.59     |
| 2   | E     | 601 | FAD  | C8-C7   | 2.57  | 1.47        | 1.40     |
| 2   | D     | 601 | FAD  | C8A-N7A | 2.56  | 1.36        | 1.31     |
| 2   | B     | 601 | FAD  | C5A-N7A | -2.55 | 1.34        | 1.39     |
| 2   | A     | 601 | FAD  | C8A-N7A | 2.53  | 1.36        | 1.31     |
| 2   | D     | 601 | FAD  | C8-C7   | 2.51  | 1.47        | 1.40     |
| 3   | C     | 602 | NAP  | C4A-N9A | -2.51 | 1.32        | 1.37     |
| 2   | D     | 601 | FAD  | C2-N3   | -2.47 | 1.33        | 1.39     |
| 2   | B     | 601 | FAD  | C4A-N9A | -2.47 | 1.32        | 1.37     |
| 2   | C     | 601 | FAD  | C10-N10 | 2.45  | 1.42        | 1.37     |
| 2   | C     | 601 | FAD  | C4'-C3' | -2.44 | 1.49        | 1.53     |
| 3   | C     | 602 | NAP  | C5A-C6A | 2.42  | 1.47        | 1.41     |
| 2   | A     | 601 | FAD  | C4A-N3A | 2.41  | 1.38        | 1.34     |
| 2   | F     | 601 | FAD  | PA-O3P  | 2.40  | 1.62        | 1.59     |
| 3   | B     | 602 | NAP  | C8A-N7A | 2.39  | 1.36        | 1.31     |
| 2   | C     | 601 | FAD  | C4X-N5  | 2.38  | 1.35        | 1.30     |
| 2   | F     | 601 | FAD  | C5A-N7A | -2.36 | 1.34        | 1.39     |
| 2   | B     | 601 | FAD  | C8A-N9A | -2.35 | 1.33        | 1.37     |
| 3   | E     | 602 | NAP  | C8A-N9A | -2.34 | 1.33        | 1.37     |
| 3   | F     | 602 | NAP  | C5A-N7A | -2.32 | 1.34        | 1.39     |
| 2   | C     | 601 | FAD  | P-O3P   | 2.31  | 1.62        | 1.59     |
| 2   | F     | 601 | FAD  | C5A-C6A | 2.30  | 1.47        | 1.41     |
| 2   | B     | 601 | FAD  | C8-C7   | 2.29  | 1.46        | 1.40     |
| 3   | C     | 602 | NAP  | C2D-C3D | -2.29 | 1.47        | 1.53     |
| 3   | E     | 602 | NAP  | C5D-C4D | 2.28  | 1.58        | 1.51     |
| 3   | F     | 602 | NAP  | C5A-C6A | 2.27  | 1.47        | 1.41     |
| 2   | F     | 601 | FAD  | C9-C8   | -2.27 | 1.36        | 1.39     |
| 2   | F     | 601 | FAD  | C6-C7   | -2.22 | 1.36        | 1.39     |
| 2   | C     | 601 | FAD  | C10-N1  | 2.22  | 1.37        | 1.33     |
| 2   | D     | 601 | FAD  | C5'-C4' | 2.21  | 1.54        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 601 | FAD  | C2'-C3' | 2.18  | 1.57        | 1.53     |
| 2   | B     | 601 | FAD  | C5'-C4' | 2.18  | 1.54        | 1.51     |
| 2   | E     | 601 | FAD  | C8A-N9A | -2.18 | 1.33        | 1.37     |
| 2   | E     | 601 | FAD  | C5A-C6A | 2.16  | 1.47        | 1.41     |
| 3   | D     | 602 | NAP  | C5A-N7A | -2.15 | 1.35        | 1.39     |
| 2   | F     | 601 | FAD  | C8-C7   | 2.15  | 1.46        | 1.40     |
| 3   | F     | 602 | NAP  | C4A-N9A | -2.14 | 1.33        | 1.37     |
| 2   | E     | 601 | FAD  | PA-O3P  | 2.12  | 1.61        | 1.59     |
| 3   | A     | 602 | NAP  | PN-O5D  | 2.12  | 1.67        | 1.59     |
| 2   | A     | 601 | FAD  | C4X-N5  | 2.11  | 1.35        | 1.30     |
| 3   | C     | 602 | NAP  | C8A-N7A | 2.11  | 1.35        | 1.31     |
| 2   | D     | 601 | FAD  | C4'-C3' | 2.10  | 1.57        | 1.53     |
| 2   | E     | 601 | FAD  | C4A-N9A | -2.10 | 1.33        | 1.37     |
| 2   | C     | 601 | FAD  | O4-C4   | 2.09  | 1.27        | 1.23     |
| 2   | E     | 601 | FAD  | C8A-N7A | 2.08  | 1.35        | 1.31     |
| 2   | F     | 601 | FAD  | C4X-N5  | 2.06  | 1.35        | 1.30     |
| 2   | C     | 601 | FAD  | C8A-N7A | 2.06  | 1.35        | 1.31     |
| 2   | C     | 601 | FAD  | O2-C2   | 2.04  | 1.28        | 1.24     |
| 2   | F     | 601 | FAD  | C9-C9A  | -2.02 | 1.36        | 1.39     |
| 2   | C     | 601 | FAD  | PA-O3P  | 2.01  | 1.61        | 1.59     |
| 3   | B     | 602 | NAP  | C4A-N9A | -2.01 | 1.33        | 1.37     |
| 2   | B     | 601 | FAD  | C4X-N5  | 2.00  | 1.35        | 1.30     |

All (253) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 601 | FAD  | C5A-C4A-N3A | -6.25 | 118.11      | 126.72   |
| 2   | A     | 601 | FAD  | O4B-C1B-N9A | 6.09  | 119.79      | 108.09   |
| 2   | D     | 601 | FAD  | C5A-C4A-N3A | -6.06 | 118.37      | 126.72   |
| 3   | E     | 602 | NAP  | C4A-N9A-C8A | 5.88  | 111.91      | 105.74   |
| 2   | D     | 601 | FAD  | C4-C4X-N5   | 5.74  | 126.13      | 118.21   |
| 2   | F     | 601 | FAD  | C5A-C4A-N3A | -5.54 | 119.09      | 126.72   |
| 3   | C     | 602 | NAP  | O7N-C7N-C3N | -5.45 | 112.94      | 119.60   |
| 3   | A     | 602 | NAP  | C5A-C4A-N3A | -5.36 | 119.33      | 126.72   |
| 3   | B     | 602 | NAP  | C5A-C4A-N3A | -5.30 | 119.42      | 126.72   |
| 3   | A     | 602 | NAP  | N3A-C2A-N1A | -5.23 | 120.66      | 128.58   |
| 2   | B     | 601 | FAD  | C5A-C4A-N3A | -5.23 | 119.52      | 126.72   |
| 2   | A     | 601 | FAD  | C4A-N9A-C8A | 5.21  | 111.21      | 105.74   |
| 2   | A     | 601 | FAD  | O5'-C5'-C4' | 5.14  | 123.08      | 109.36   |
| 3   | C     | 602 | NAP  | C4A-N9A-C8A | 5.09  | 111.08      | 105.74   |
| 2   | A     | 601 | FAD  | N3A-C2A-N1A | -5.07 | 120.91      | 128.58   |
| 2   | F     | 601 | FAD  | N3A-C2A-N1A | -5.00 | 121.02      | 128.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | F     | 602 | NAP  | C4A-N9A-C8A | 4.91  | 110.89      | 105.74   |
| 2   | C     | 601 | FAD  | N3A-C2A-N1A | -4.79 | 121.34      | 128.58   |
| 3   | E     | 602 | NAP  | N3A-C2A-N1A | -4.76 | 121.38      | 128.58   |
| 3   | D     | 602 | NAP  | C5A-C4A-N3A | -4.73 | 120.21      | 126.72   |
| 3   | A     | 602 | NAP  | C2A-N3A-C4A | 4.71  | 123.33      | 111.83   |
| 3   | C     | 602 | NAP  | C5A-C4A-N3A | -4.69 | 120.25      | 126.72   |
| 2   | F     | 601 | FAD  | O4-C4-C4X   | -4.66 | 114.22      | 126.53   |
| 2   | E     | 601 | FAD  | N3A-C4A-N9A | 4.66  | 135.09      | 127.17   |
| 3   | B     | 602 | NAP  | N3A-C4A-N9A | 4.60  | 134.99      | 127.17   |
| 2   | D     | 601 | FAD  | N3A-C4A-N9A | 4.58  | 134.95      | 127.17   |
| 3   | D     | 602 | NAP  | N3A-C4A-N9A | 4.55  | 134.91      | 127.17   |
| 2   | F     | 601 | FAD  | C2A-N3A-C4A | 4.50  | 122.83      | 111.83   |
| 2   | A     | 601 | FAD  | O5'-P-O1P   | -4.50 | 91.08       | 108.94   |
| 3   | C     | 602 | NAP  | N3A-C2A-N1A | -4.50 | 121.77      | 128.58   |
| 3   | E     | 602 | NAP  | N3A-C4A-N9A | 4.45  | 134.73      | 127.17   |
| 2   | B     | 601 | FAD  | C4A-C5A-N7A | -4.42 | 105.53      | 110.58   |
| 3   | C     | 602 | NAP  | N3A-C4A-N9A | 4.34  | 134.56      | 127.17   |
| 3   | C     | 602 | NAP  | O3-PA-O1A   | -4.30 | 97.78       | 110.70   |
| 3   | B     | 602 | NAP  | N3A-C2A-N1A | -4.28 | 122.11      | 128.58   |
| 3   | F     | 602 | NAP  | N3A-C2A-N1A | -4.26 | 122.13      | 128.58   |
| 3   | F     | 602 | NAP  | N3A-C4A-N9A | 4.24  | 134.37      | 127.17   |
| 3   | B     | 602 | NAP  | C2A-N3A-C4A | 4.20  | 122.10      | 111.83   |
| 3   | C     | 602 | NAP  | C2A-N3A-C4A | 4.19  | 122.07      | 111.83   |
| 2   | A     | 601 | FAD  | O2'-C2'-C3' | 4.19  | 119.05      | 109.25   |
| 2   | F     | 601 | FAD  | N3A-C4A-N9A | 4.19  | 134.28      | 127.17   |
| 2   | B     | 601 | FAD  | C4-C4X-N5   | 4.13  | 123.91      | 118.21   |
| 3   | D     | 602 | NAP  | N3A-C2A-N1A | -4.12 | 122.35      | 128.58   |
| 2   | C     | 601 | FAD  | C5A-C4A-N3A | -4.12 | 121.05      | 126.72   |
| 3   | B     | 602 | NAP  | O2N-PN-O3   | -4.04 | 96.34       | 107.27   |
| 2   | D     | 601 | FAD  | C10-C4X-N5  | -4.02 | 116.60      | 124.81   |
| 2   | A     | 601 | FAD  | N3A-C4A-N9A | 4.01  | 133.99      | 127.17   |
| 2   | A     | 601 | FAD  | C2A-N1A-C6A | 3.99  | 125.29      | 118.73   |
| 3   | A     | 602 | NAP  | C3N-C7N-N7N | 3.95  | 122.61      | 117.74   |
| 3   | A     | 602 | NAP  | C6N-N1N-C2N | -3.95 | 118.52      | 121.88   |
| 3   | A     | 602 | NAP  | C4A-C5A-N7A | -3.94 | 106.08      | 110.58   |
| 2   | B     | 601 | FAD  | N3A-C4A-N9A | 3.87  | 133.75      | 127.17   |
| 3   | C     | 602 | NAP  | O4B-C1B-N9A | 3.87  | 115.53      | 108.09   |
| 2   | B     | 601 | FAD  | C4A-N9A-C8A | 3.84  | 109.77      | 105.74   |
| 2   | B     | 601 | FAD  | C5'-C4'-C3' | 3.79  | 119.36      | 112.22   |
| 3   | C     | 602 | NAP  | N9A-C8A-N7A | -3.78 | 108.57      | 113.94   |
| 3   | A     | 602 | NAP  | C6A-C5A-N7A | 3.78  | 139.38      | 132.09   |
| 2   | D     | 601 | FAD  | C4X-C10-N10 | 3.78  | 121.89      | 116.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 601 | FAD  | N3A-C4A-N9A | 3.73  | 133.50      | 127.17   |
| 2   | D     | 601 | FAD  | O2-C2-N1    | -3.70 | 115.65      | 121.80   |
| 3   | D     | 602 | NAP  | C2A-N3A-C4A | 3.68  | 120.81      | 111.83   |
| 3   | D     | 602 | NAP  | C4A-N9A-C8A | 3.65  | 109.57      | 105.74   |
| 2   | A     | 601 | FAD  | O4-C4-C4X   | -3.64 | 116.91      | 126.53   |
| 3   | F     | 602 | NAP  | C5A-C4A-N3A | -3.63 | 121.72      | 126.72   |
| 2   | E     | 601 | FAD  | C4A-C5A-N7A | -3.61 | 106.45      | 110.58   |
| 2   | A     | 601 | FAD  | C4-C4X-N5   | 3.59  | 123.16      | 118.21   |
| 3   | E     | 602 | NAP  | C2A-N1A-C6A | 3.55  | 124.56      | 118.73   |
| 2   | C     | 601 | FAD  | C2A-N3A-C4A | 3.51  | 120.40      | 111.83   |
| 2   | D     | 601 | FAD  | C5X-N5-C4X  | 3.50  | 123.75      | 118.09   |
| 2   | A     | 601 | FAD  | C5A-C4A-N3A | -3.50 | 121.90      | 126.72   |
| 3   | A     | 602 | NAP  | N3A-C4A-N9A | 3.44  | 133.01      | 127.17   |
| 2   | C     | 601 | FAD  | O4-C4-C4X   | -3.43 | 117.47      | 126.53   |
| 2   | A     | 601 | FAD  | C2A-N3A-C4A | 3.41  | 120.16      | 111.83   |
| 2   | B     | 601 | FAD  | O4'-C4'-C5' | -3.41 | 102.47      | 109.99   |
| 3   | C     | 602 | NAP  | C6A-C5A-N7A | 3.41  | 138.66      | 132.09   |
| 2   | B     | 601 | FAD  | C2A-N3A-C4A | 3.40  | 120.14      | 111.83   |
| 2   | C     | 601 | FAD  | C10-N1-C2   | 3.39  | 124.19      | 116.85   |
| 3   | E     | 602 | NAP  | C5A-C4A-N3A | -3.38 | 122.06      | 126.72   |
| 2   | E     | 601 | FAD  | O4-C4-C4X   | -3.34 | 117.73      | 126.53   |
| 3   | B     | 602 | NAP  | C3N-C7N-N7N | 3.34  | 121.85      | 117.74   |
| 2   | B     | 601 | FAD  | C5A-N7A-C8A | 3.29  | 108.62      | 103.45   |
| 3   | F     | 602 | NAP  | C4A-N9A-C1B | -3.28 | 118.97      | 126.63   |
| 3   | B     | 602 | NAP  | O4B-C1B-N9A | 3.27  | 114.36      | 108.09   |
| 3   | F     | 602 | NAP  | C2A-N3A-C4A | 3.26  | 119.80      | 111.83   |
| 2   | E     | 601 | FAD  | C2A-N3A-C4A | 3.26  | 119.79      | 111.83   |
| 2   | B     | 601 | FAD  | N9A-C8A-N7A | -3.24 | 109.34      | 113.94   |
| 2   | A     | 601 | FAD  | O3'-C3'-C2' | 3.22  | 116.24      | 108.93   |
| 3   | E     | 602 | NAP  | N9A-C8A-N7A | -3.20 | 109.39      | 113.94   |
| 3   | D     | 602 | NAP  | C5N-C4N-C3N | -3.18 | 117.23      | 120.36   |
| 3   | B     | 602 | NAP  | C4A-N9A-C8A | 3.17  | 109.07      | 105.74   |
| 3   | A     | 602 | NAP  | O7N-C7N-C3N | -3.17 | 115.73      | 119.60   |
| 2   | B     | 601 | FAD  | C4X-C4-N3   | 3.16  | 121.31      | 113.25   |
| 3   | F     | 602 | NAP  | N9A-C8A-N7A | -3.15 | 109.46      | 113.94   |
| 2   | A     | 601 | FAD  | C4A-N9A-C1B | -3.14 | 119.28      | 126.63   |
| 2   | A     | 601 | FAD  | N9A-C8A-N7A | -3.14 | 109.48      | 113.94   |
| 3   | C     | 602 | NAP  | C4A-N9A-C1B | -3.13 | 119.31      | 126.63   |
| 2   | D     | 601 | FAD  | O4'-C4'-C5' | -3.12 | 103.11      | 109.99   |
| 3   | C     | 602 | NAP  | O3X-P2B-O2X | 3.11  | 119.45      | 107.80   |
| 2   | B     | 601 | FAD  | C1'-C2'-C3' | 3.09  | 118.03      | 109.66   |
| 2   | D     | 601 | FAD  | C4A-C5A-N7A | -3.05 | 107.09      | 110.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 601 | FAD  | C4'-C3'-C2' | -3.05 | 108.50      | 113.57   |
| 2   | A     | 601 | FAD  | C3B-C2B-C1B | -3.03 | 95.73       | 101.46   |
| 2   | F     | 601 | FAD  | C4X-C4-N3   | 3.03  | 120.97      | 113.25   |
| 3   | A     | 602 | NAP  | C5A-N7A-C8A | 3.01  | 108.19      | 103.45   |
| 3   | B     | 602 | NAP  | C4D-O4D-C1D | -3.01 | 107.17      | 109.92   |
| 2   | D     | 601 | FAD  | C5'-C4'-C3' | 3.00  | 117.89      | 112.22   |
| 2   | D     | 601 | FAD  | C2A-N3A-C4A | 2.99  | 119.12      | 111.83   |
| 3   | E     | 602 | NAP  | C2A-N3A-C4A | 2.98  | 119.10      | 111.83   |
| 3   | F     | 602 | NAP  | C4D-O4D-C1D | -2.96 | 107.22      | 109.92   |
| 2   | B     | 601 | FAD  | N3A-C2A-N1A | -2.96 | 124.11      | 128.58   |
| 2   | A     | 601 | FAD  | O2A-PA-O5B  | -2.94 | 94.24       | 107.57   |
| 3   | A     | 602 | NAP  | O3X-P2B-O2X | 2.94  | 118.81      | 107.80   |
| 2   | C     | 601 | FAD  | C2A-N1A-C6A | 2.91  | 123.52      | 118.73   |
| 2   | E     | 601 | FAD  | O2'-C2'-C1' | -2.91 | 98.24       | 110.20   |
| 3   | A     | 602 | NAP  | N9A-C8A-N7A | -2.88 | 109.84      | 113.94   |
| 2   | E     | 601 | FAD  | C5A-N7A-C8A | 2.87  | 107.96      | 103.45   |
| 2   | E     | 601 | FAD  | C4-C4X-N5   | 2.86  | 122.16      | 118.21   |
| 2   | A     | 601 | FAD  | C9A-C5X-N5  | -2.85 | 119.43      | 122.45   |
| 2   | C     | 601 | FAD  | C5'-C4'-C3' | 2.85  | 117.59      | 112.22   |
| 2   | F     | 601 | FAD  | C6A-C5A-N7A | 2.83  | 137.55      | 132.09   |
| 3   | C     | 602 | NAP  | O7N-C7N-N7N | 2.81  | 126.68      | 122.62   |
| 3   | F     | 602 | NAP  | O3X-P2B-O2B | -2.80 | 94.95       | 105.85   |
| 3   | B     | 602 | NAP  | C6A-C5A-N7A | 2.80  | 137.48      | 132.09   |
| 3   | C     | 602 | NAP  | O3X-P2B-O2B | -2.79 | 94.97       | 105.85   |
| 3   | E     | 602 | NAP  | N6A-C6A-N1A | 2.78  | 124.56      | 118.38   |
| 2   | B     | 601 | FAD  | C6A-C5A-N7A | 2.78  | 137.44      | 132.09   |
| 3   | C     | 602 | NAP  | C4A-C5A-N7A | -2.77 | 107.42      | 110.58   |
| 3   | A     | 602 | NAP  | O2N-PN-O3   | -2.75 | 99.84       | 107.27   |
| 2   | F     | 601 | FAD  | C4-N3-C2    | -2.75 | 120.76      | 125.64   |
| 2   | A     | 601 | FAD  | C6A-C5A-N7A | 2.75  | 137.39      | 132.09   |
| 3   | E     | 602 | NAP  | O4B-C4B-C3B | 2.75  | 110.60      | 105.15   |
| 3   | F     | 602 | NAP  | O3X-P2B-O1X | 2.72  | 121.44      | 110.83   |
| 3   | C     | 602 | NAP  | C5A-N7A-C8A | 2.72  | 107.73      | 103.45   |
| 3   | E     | 602 | NAP  | C4A-N9A-C1B | -2.70 | 120.32      | 126.63   |
| 2   | A     | 601 | FAD  | C4X-C4-N3   | 2.70  | 120.11      | 113.25   |
| 2   | B     | 601 | FAD  | O4-C4-C4X   | -2.69 | 119.43      | 126.53   |
| 2   | A     | 601 | FAD  | C7M-C7-C6   | 2.69  | 124.31      | 119.57   |
| 2   | E     | 601 | FAD  | C10-N1-C2   | 2.69  | 122.67      | 116.85   |
| 2   | E     | 601 | FAD  | O2'-C2'-C3' | 2.68  | 115.52      | 109.25   |
| 3   | A     | 602 | NAP  | O5D-C5D-C4D | 2.68  | 118.10      | 108.99   |
| 3   | A     | 602 | NAP  | C3B-C2B-C1B | 2.67  | 107.92      | 102.81   |
| 2   | F     | 601 | FAD  | C4'-C3'-C2' | -2.67 | 109.12      | 113.57   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | D     | 602 | NAP  | O3X-P2B-O2X | 2.67  | 117.81      | 107.80   |
| 3   | F     | 602 | NAP  | O7N-C7N-C3N | -2.67 | 116.34      | 119.60   |
| 2   | A     | 601 | FAD  | O2-C2-N1    | -2.66 | 117.37      | 121.80   |
| 2   | B     | 601 | FAD  | C1'-N10-C9A | 2.65  | 125.78      | 120.63   |
| 2   | D     | 601 | FAD  | C4X-C10-N1  | -2.65 | 118.10      | 124.59   |
| 2   | D     | 601 | FAD  | C5A-N7A-C8A | 2.64  | 107.59      | 103.45   |
| 3   | E     | 602 | NAP  | O2A-PA-O1A  | 2.63  | 124.70      | 112.44   |
| 3   | C     | 602 | NAP  | C2N-C3N-C4N | 2.63  | 121.31      | 118.26   |
| 3   | C     | 602 | NAP  | O3-PN-O1N   | -2.62 | 102.82      | 110.70   |
| 2   | F     | 601 | FAD  | C10-N1-C2   | 2.61  | 122.51      | 116.85   |
| 2   | A     | 601 | FAD  | C1'-N10-C9A | 2.61  | 125.70      | 120.63   |
| 2   | A     | 601 | FAD  | C5A-N7A-C8A | 2.60  | 107.54      | 103.45   |
| 3   | F     | 602 | NAP  | O2A-PA-O1A  | 2.58  | 124.44      | 112.44   |
| 2   | A     | 601 | FAD  | C4A-C5A-N7A | -2.57 | 107.64      | 110.58   |
| 2   | E     | 601 | FAD  | O4B-C4B-C3B | 2.57  | 110.25      | 105.15   |
| 2   | A     | 601 | FAD  | O3P-PA-O1A  | 2.56  | 118.40      | 110.70   |
| 2   | F     | 601 | FAD  | C2A-N1A-C6A | 2.54  | 122.91      | 118.73   |
| 3   | C     | 602 | NAP  | C2B-C1B-N9A | -2.51 | 109.61      | 113.75   |
| 2   | C     | 601 | FAD  | O2'-C2'-C1' | -2.51 | 99.89       | 110.20   |
| 3   | B     | 602 | NAP  | C4A-C5A-N7A | -2.50 | 107.72      | 110.58   |
| 2   | F     | 601 | FAD  | O4-C4-N3    | 2.50  | 124.81      | 120.11   |
| 3   | A     | 602 | NAP  | C4A-N9A-C1B | -2.50 | 120.79      | 126.63   |
| 3   | F     | 602 | NAP  | O4D-C4D-C3D | 2.50  | 110.11      | 105.15   |
| 2   | B     | 601 | FAD  | O2'-C2'-C1' | -2.49 | 99.97       | 110.20   |
| 3   | F     | 602 | NAP  | O2B-P2B-O1X | -2.47 | 100.54      | 109.33   |
| 3   | B     | 602 | NAP  | O3X-P2B-O1X | 2.47  | 120.44      | 110.83   |
| 2   | D     | 601 | FAD  | N3A-C2A-N1A | -2.46 | 124.86      | 128.58   |
| 2   | C     | 601 | FAD  | C4A-N9A-C8A | 2.45  | 108.31      | 105.74   |
| 3   | E     | 602 | NAP  | O3B-C3B-C2B | 2.44  | 118.00      | 111.19   |
| 3   | D     | 602 | NAP  | C6N-N1N-C2N | -2.43 | 119.81      | 121.88   |
| 2   | B     | 601 | FAD  | C2B-C1B-N9A | 2.42  | 119.33      | 113.30   |
| 2   | C     | 601 | FAD  | C2'-C1'-N10 | 2.42  | 121.64      | 110.20   |
| 2   | F     | 601 | FAD  | C4A-C5A-N7A | -2.42 | 107.82      | 110.58   |
| 3   | C     | 602 | NAP  | O2A-PA-O1A  | 2.41  | 123.64      | 112.44   |
| 3   | F     | 602 | NAP  | C5A-N7A-C8A | 2.40  | 107.22      | 103.45   |
| 3   | C     | 602 | NAP  | O5D-PN-O1N  | 2.40  | 118.43      | 108.94   |
| 3   | E     | 602 | NAP  | C5A-C4A-N9A | -2.39 | 103.21      | 105.81   |
| 3   | C     | 602 | NAP  | C6A-C5A-C4A | -2.39 | 113.92      | 117.18   |
| 2   | C     | 601 | FAD  | O4'-C4'-C5' | -2.38 | 104.73      | 109.99   |
| 3   | A     | 602 | NAP  | C4A-N9A-C8A | 2.38  | 108.24      | 105.74   |
| 3   | F     | 602 | NAP  | C6A-C5A-N7A | 2.38  | 136.67      | 132.09   |
| 2   | C     | 601 | FAD  | O2P-P-O3P   | -2.37 | 100.86      | 107.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 601 | FAD  | C4-C4X-N5   | 2.37  | 121.48      | 118.21   |
| 2   | F     | 601 | FAD  | O2A-PA-O1A  | 2.37  | 123.45      | 112.44   |
| 2   | D     | 601 | FAD  | C1'-N10-C9A | 2.37  | 125.23      | 120.63   |
| 2   | C     | 601 | FAD  | C4X-C10-N1  | -2.35 | 118.83      | 124.59   |
| 3   | A     | 602 | NAP  | O2N-PN-O5D  | 2.34  | 118.19      | 107.57   |
| 2   | B     | 601 | FAD  | O2P-P-O3P   | -2.33 | 100.97      | 107.27   |
| 3   | A     | 602 | NAP  | O2X-P2B-O2B | -2.33 | 96.76       | 105.85   |
| 3   | F     | 602 | NAP  | C5A-C6A-N6A | -2.33 | 117.53      | 123.29   |
| 2   | A     | 601 | FAD  | O2'-C2'-C1' | -2.32 | 100.67      | 110.20   |
| 2   | D     | 601 | FAD  | C2B-C1B-N9A | 2.29  | 118.99      | 113.30   |
| 2   | B     | 601 | FAD  | O2A-PA-O3P  | 2.28  | 113.44      | 107.27   |
| 2   | D     | 601 | FAD  | N3-C2-N1    | 2.28  | 124.35      | 119.50   |
| 3   | E     | 602 | NAP  | O7N-C7N-N7N | 2.28  | 125.91      | 122.62   |
| 2   | C     | 601 | FAD  | O3P-P-O1P   | 2.28  | 117.57      | 110.70   |
| 2   | C     | 601 | FAD  | O2A-PA-O1A  | 2.28  | 123.04      | 112.44   |
| 2   | C     | 601 | FAD  | C4X-C4-N3   | 2.27  | 119.04      | 113.25   |
| 2   | D     | 601 | FAD  | C8M-C8-C7   | -2.27 | 116.13      | 120.76   |
| 2   | C     | 601 | FAD  | O2P-P-O1P   | 2.26  | 122.98      | 112.44   |
| 3   | E     | 602 | NAP  | C5A-N7A-C8A | 2.26  | 107.01      | 103.45   |
| 3   | F     | 602 | NAP  | O2B-C2B-C1B | -2.26 | 102.10      | 110.05   |
| 2   | E     | 601 | FAD  | C4X-C4-N3   | 2.26  | 119.00      | 113.25   |
| 3   | D     | 602 | NAP  | C4A-C5A-N7A | -2.25 | 108.00      | 110.58   |
| 2   | F     | 601 | FAD  | C5'-C4'-C3' | 2.25  | 116.45      | 112.22   |
| 2   | D     | 601 | FAD  | C9-C9A-N10  | 2.24  | 124.87      | 121.85   |
| 2   | B     | 601 | FAD  | C10-N1-C2   | 2.23  | 121.68      | 116.85   |
| 3   | D     | 602 | NAP  | C6A-C5A-N7A | 2.23  | 136.39      | 132.09   |
| 2   | A     | 601 | FAD  | C10-N1-C2   | 2.22  | 121.66      | 116.85   |
| 3   | D     | 602 | NAP  | C2A-N1A-C6A | 2.22  | 122.38      | 118.73   |
| 3   | E     | 602 | NAP  | O4B-C4B-C5B | -2.22 | 102.23      | 109.33   |
| 3   | B     | 602 | NAP  | C4A-N9A-C1B | -2.21 | 121.45      | 126.63   |
| 2   | F     | 601 | FAD  | O3P-PA-O1A  | -2.20 | 104.07      | 110.70   |
| 3   | E     | 602 | NAP  | C2B-C1B-N9A | -2.20 | 110.13      | 113.75   |
| 3   | F     | 602 | NAP  | N6A-C6A-N1A | 2.20  | 123.28      | 118.38   |
| 3   | F     | 602 | NAP  | C2A-N1A-C6A | 2.20  | 122.34      | 118.73   |
| 2   | F     | 601 | FAD  | O5'-C5'-C4' | -2.19 | 103.52      | 109.36   |
| 3   | F     | 602 | NAP  | O3X-P2B-O2X | 2.19  | 116.00      | 107.80   |
| 2   | D     | 601 | FAD  | O3P-P-O1P   | 2.18  | 117.28      | 110.70   |
| 2   | A     | 601 | FAD  | O5B-C5B-C4B | 2.18  | 116.42      | 108.99   |
| 2   | F     | 601 | FAD  | C4X-C10-N1  | -2.18 | 119.25      | 124.59   |
| 3   | A     | 602 | NAP  | P2B-O2B-C2B | -2.17 | 117.64      | 123.43   |
| 3   | A     | 602 | NAP  | O4B-C1B-C2B | -2.17 | 102.85      | 106.59   |
| 2   | C     | 601 | FAD  | C1'-C2'-C3' | 2.16  | 115.52      | 109.66   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 601 | FAD  | C7M-C7-C8   | -2.16 | 116.34      | 120.76   |
| 2   | A     | 601 | FAD  | O2A-PA-O1A  | 2.16  | 122.50      | 112.44   |
| 2   | E     | 601 | FAD  | N9A-C8A-N7A | -2.16 | 110.87      | 113.94   |
| 3   | F     | 602 | NAP  | C2B-C1B-N9A | 2.16  | 117.30      | 113.75   |
| 3   | E     | 602 | NAP  | C4D-O4D-C1D | 2.15  | 111.90      | 109.92   |
| 3   | A     | 602 | NAP  | O2D-C2D-C3D | 2.15  | 118.70      | 111.82   |
| 2   | C     | 601 | FAD  | N6A-C6A-N1A | 2.13  | 123.13      | 118.38   |
| 3   | A     | 602 | NAP  | O3-PA-O1A   | -2.13 | 104.30      | 110.70   |
| 3   | E     | 602 | NAP  | C4B-O4B-C1B | -2.12 | 104.78      | 109.47   |
| 2   | B     | 601 | FAD  | C4-C4X-C10  | -2.12 | 113.30      | 116.93   |
| 2   | E     | 601 | FAD  | C3B-C2B-C1B | 2.12  | 105.47      | 101.46   |
| 2   | E     | 601 | FAD  | N3A-C2A-N1A | -2.11 | 125.38      | 128.58   |
| 3   | D     | 602 | NAP  | O3X-P2B-O2B | -2.11 | 97.62       | 105.85   |
| 3   | A     | 602 | NAP  | C2A-N1A-C6A | 2.11  | 122.19      | 118.73   |
| 2   | F     | 601 | FAD  | O2'-C2'-C1' | -2.11 | 101.54      | 110.20   |
| 3   | A     | 602 | NAP  | C4D-O4D-C1D | 2.09  | 111.84      | 109.92   |
| 3   | C     | 602 | NAP  | C5N-C4N-C3N | -2.08 | 118.32      | 120.36   |
| 3   | F     | 602 | NAP  | O7N-C7N-N7N | 2.08  | 125.62      | 122.62   |
| 2   | E     | 601 | FAD  | C9A-C5X-N5  | -2.07 | 120.26      | 122.45   |
| 2   | F     | 601 | FAD  | C2B-C1B-N9A | 2.06  | 118.43      | 113.30   |
| 3   | E     | 602 | NAP  | C2D-C3D-C4D | 2.06  | 106.60      | 102.61   |
| 3   | E     | 602 | NAP  | C5A-C6A-N6A | -2.04 | 118.23      | 123.29   |
| 2   | E     | 601 | FAD  | C4A-N9A-C8A | 2.04  | 107.88      | 105.74   |
| 3   | C     | 602 | NAP  | C3N-C7N-N7N | 2.02  | 120.23      | 117.74   |
| 2   | A     | 601 | FAD  | O2-C2-N3    | 2.01  | 122.45      | 118.58   |
| 3   | D     | 602 | NAP  | O2B-C2B-C3B | -2.00 | 104.49      | 111.68   |
| 2   | A     | 601 | FAD  | N6A-C6A-N1A | 2.00  | 122.83      | 118.38   |

There are no chirality outliers.

All (78) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | D     | 601 | FAD  | C5B-O5B-PA-O1A  |
| 2   | D     | 601 | FAD  | C5B-O5B-PA-O3P  |
| 2   | D     | 601 | FAD  | N10-C1'-C2'-O2' |
| 2   | D     | 601 | FAD  | N10-C1'-C2'-C3' |
| 2   | A     | 601 | FAD  | C5B-O5B-PA-O1A  |
| 2   | A     | 601 | FAD  | C5B-O5B-PA-O3P  |
| 2   | A     | 601 | FAD  | N10-C1'-C2'-O2' |
| 2   | A     | 601 | FAD  | N10-C1'-C2'-C3' |
| 2   | A     | 601 | FAD  | C2'-C3'-C4'-O4' |
| 2   | A     | 601 | FAD  | C2'-C3'-C4'-C5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 601 | FAD  | N10-C1'-C2'-O2' |
| 2   | B     | 601 | FAD  | N10-C1'-C2'-C3' |
| 2   | C     | 601 | FAD  | C5B-O5B-PA-O1A  |
| 2   | C     | 601 | FAD  | N10-C1'-C2'-O2' |
| 2   | C     | 601 | FAD  | N10-C1'-C2'-C3' |
| 2   | E     | 601 | FAD  | C5B-O5B-PA-O1A  |
| 2   | E     | 601 | FAD  | N10-C1'-C2'-O2' |
| 2   | E     | 601 | FAD  | N10-C1'-C2'-C3' |
| 2   | F     | 601 | FAD  | N10-C1'-C2'-O2' |
| 2   | F     | 601 | FAD  | N10-C1'-C2'-C3' |
| 2   | F     | 601 | FAD  | C5'-O5'-P-O2P   |
| 2   | F     | 601 | FAD  | PA-O3P-P-O5'    |
| 3   | A     | 602 | NAP  | O4D-C4D-C5D-O5D |
| 3   | F     | 602 | NAP  | C5B-O5B-PA-O1A  |
| 3   | F     | 602 | NAP  | C5B-O5B-PA-O3   |
| 3   | A     | 602 | NAP  | C3D-C4D-C5D-O5D |
| 2   | A     | 601 | FAD  | O3'-C3'-C4'-O4' |
| 2   | A     | 601 | FAD  | O3'-C3'-C4'-C5' |
| 3   | A     | 602 | NAP  | C3B-C2B-O2B-P2B |
| 3   | B     | 602 | NAP  | C3B-C2B-O2B-P2B |
| 2   | E     | 601 | FAD  | O4B-C4B-C5B-O5B |
| 3   | B     | 602 | NAP  | C1B-C2B-O2B-P2B |
| 2   | E     | 601 | FAD  | C3B-C4B-C5B-O5B |
| 2   | A     | 601 | FAD  | C2B-C1B-N9A-C8A |
| 2   | C     | 601 | FAD  | O4B-C4B-C5B-O5B |
| 2   | D     | 601 | FAD  | O4B-C4B-C5B-O5B |
| 2   | C     | 601 | FAD  | C3B-C4B-C5B-O5B |
| 2   | F     | 601 | FAD  | P-O3P-PA-O1A    |
| 3   | C     | 602 | NAP  | PN-O3-PA-O1A    |
| 2   | A     | 601 | FAD  | C4'-C5'-O5'-P   |
| 3   | C     | 602 | NAP  | C2N-C3N-C7N-O7N |
| 2   | A     | 601 | FAD  | P-O3P-PA-O5B    |
| 2   | B     | 601 | FAD  | PA-O3P-P-O5'    |
| 3   | A     | 602 | NAP  | PA-O3-PN-O5D    |
| 3   | B     | 602 | NAP  | PA-O3-PN-O5D    |
| 3   | C     | 602 | NAP  | PA-O3-PN-O5D    |
| 3   | E     | 602 | NAP  | C4N-C3N-C7N-N7N |
| 2   | D     | 601 | FAD  | C3B-C4B-C5B-O5B |
| 2   | A     | 601 | FAD  | PA-O3P-P-O1P    |
| 3   | E     | 602 | NAP  | C4N-C3N-C7N-O7N |
| 3   | E     | 602 | NAP  | C2N-C3N-C7N-N7N |
| 2   | D     | 601 | FAD  | C5B-O5B-PA-O2A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 601 | FAD  | C5B-O5B-PA-O2A  |
| 2   | E     | 601 | FAD  | C5B-O5B-PA-O3P  |
| 3   | A     | 602 | NAP  | C5B-O5B-PA-O1A  |
| 3   | F     | 602 | NAP  | C5B-O5B-PA-O2A  |
| 2   | F     | 601 | FAD  | P-O3P-PA-O2A    |
| 2   | A     | 601 | FAD  | C2B-C1B-N9A-C4A |
| 2   | A     | 601 | FAD  | O4B-C4B-C5B-O5B |
| 2   | A     | 601 | FAD  | C3B-C4B-C5B-O5B |
| 3   | F     | 602 | NAP  | O4B-C4B-C5B-O5B |
| 3   | D     | 602 | NAP  | C2B-O2B-P2B-O1X |
| 3   | A     | 602 | NAP  | C2B-O2B-P2B-O1X |
| 3   | C     | 602 | NAP  | C2B-O2B-P2B-O1X |
| 2   | C     | 601 | FAD  | O4'-C4'-C5'-O5' |
| 3   | E     | 602 | NAP  | C2N-C3N-C7N-O7N |
| 3   | A     | 602 | NAP  | C1B-C2B-O2B-P2B |
| 3   | C     | 602 | NAP  | C4N-C3N-C7N-O7N |
| 3   | B     | 602 | NAP  | O4B-C4B-C5B-O5B |
| 2   | A     | 601 | FAD  | PA-O3P-P-O2P    |
| 3   | C     | 602 | NAP  | PN-O3-PA-O2A    |
| 2   | B     | 601 | FAD  | O4B-C4B-C5B-O5B |
| 3   | E     | 602 | NAP  | O4B-C4B-C5B-O5B |
| 3   | D     | 602 | NAP  | O4B-C4B-C5B-O5B |
| 3   | F     | 602 | NAP  | C2B-O2B-P2B-O1X |
| 3   | C     | 602 | NAP  | C2N-C3N-C7N-N7N |
| 3   | E     | 602 | NAP  | PN-O3-PA-O2A    |
| 2   | F     | 601 | FAD  | O4B-C4B-C5B-O5B |

There are no ring outliers.

12 monomers are involved in 38 short contacts:

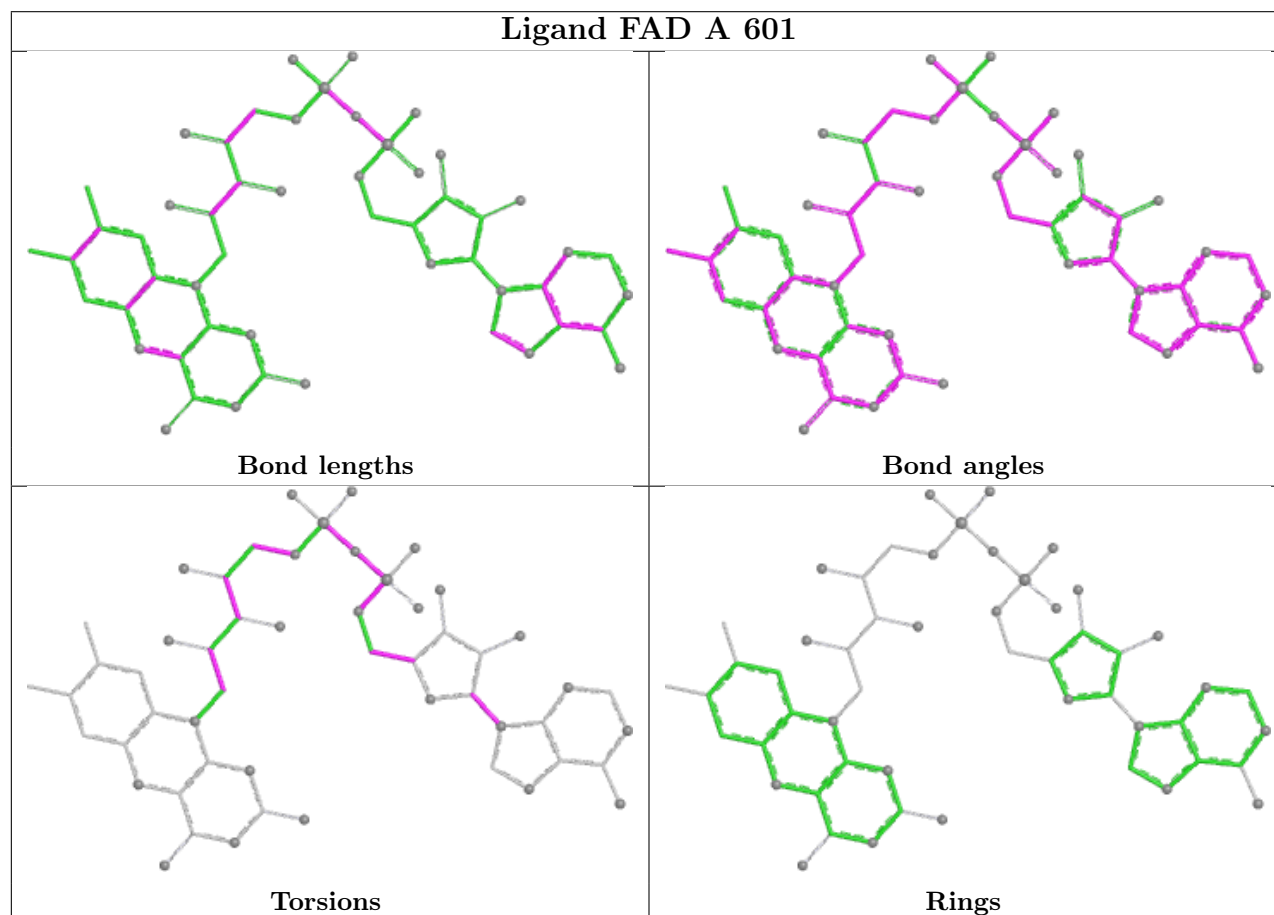
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 601 | FAD  | 16      | 0            |
| 3   | C     | 602 | NAP  | 2       | 0            |
| 2   | E     | 601 | FAD  | 4       | 0            |
| 3   | D     | 602 | NAP  | 4       | 0            |
| 3   | B     | 602 | NAP  | 2       | 0            |
| 3   | F     | 602 | NAP  | 3       | 0            |
| 2   | D     | 601 | FAD  | 1       | 0            |
| 2   | F     | 601 | FAD  | 4       | 0            |
| 3   | A     | 602 | NAP  | 2       | 0            |
| 3   | E     | 602 | NAP  | 2       | 0            |
| 2   | B     | 601 | FAD  | 1       | 0            |

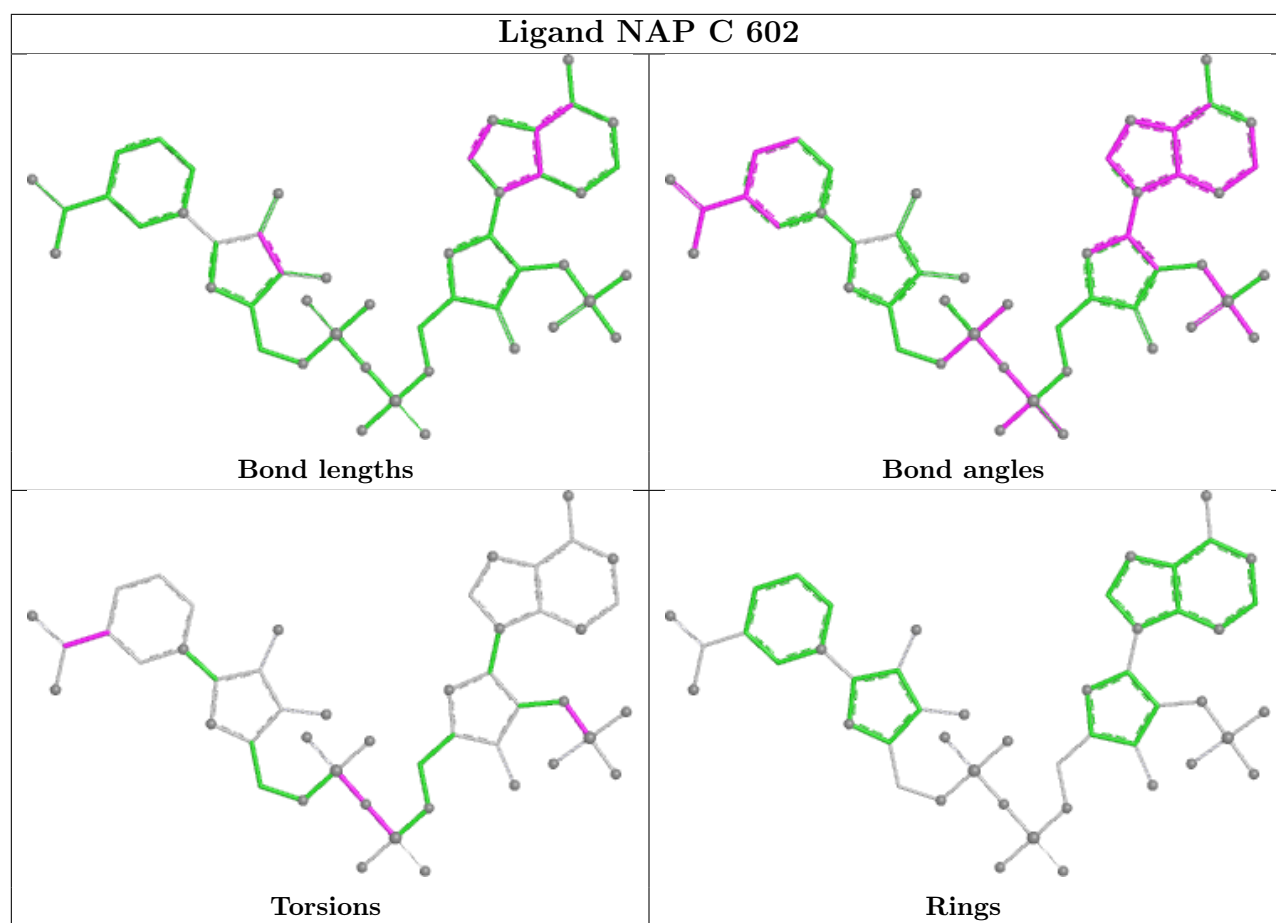
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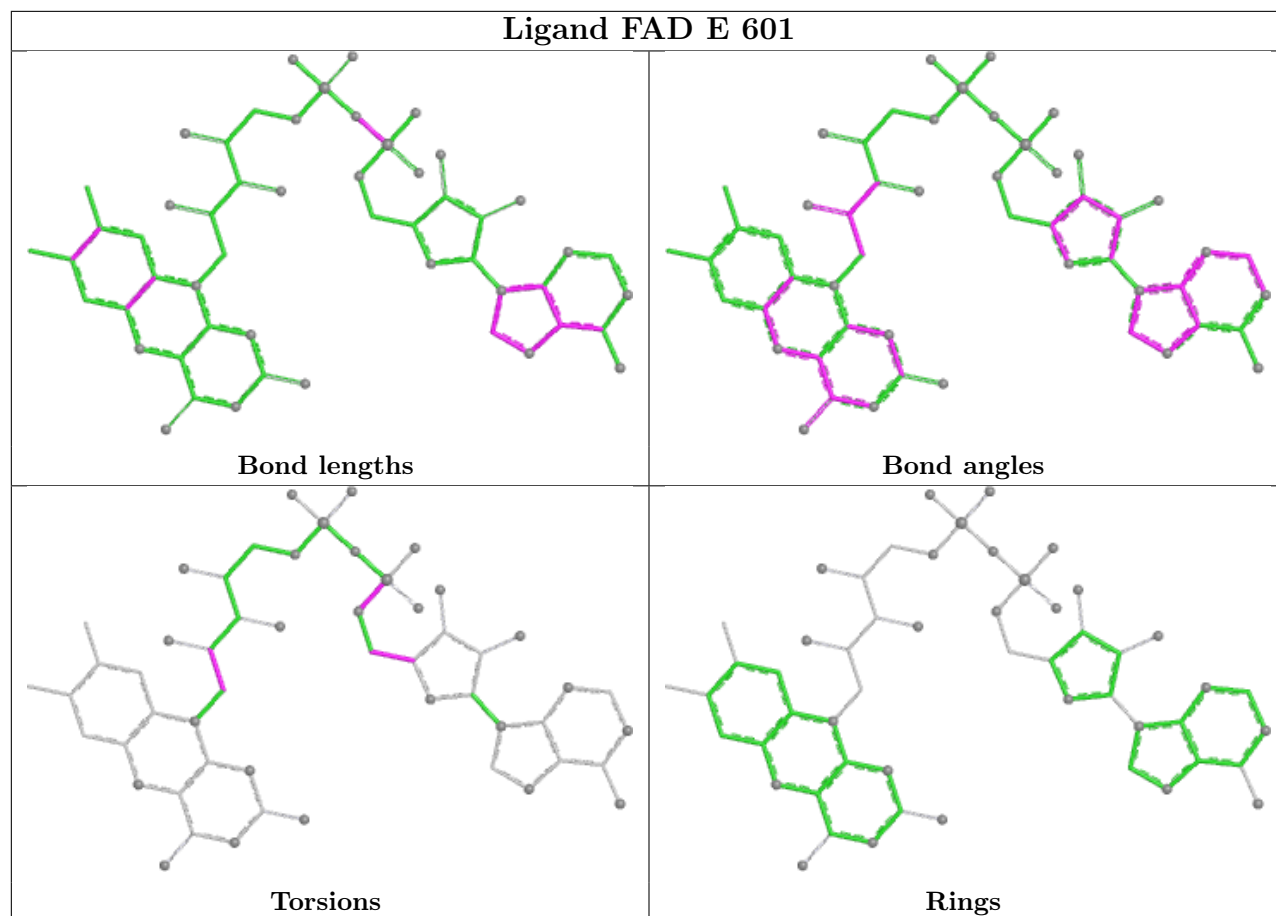
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 601 | FAD  | 4       | 0            |

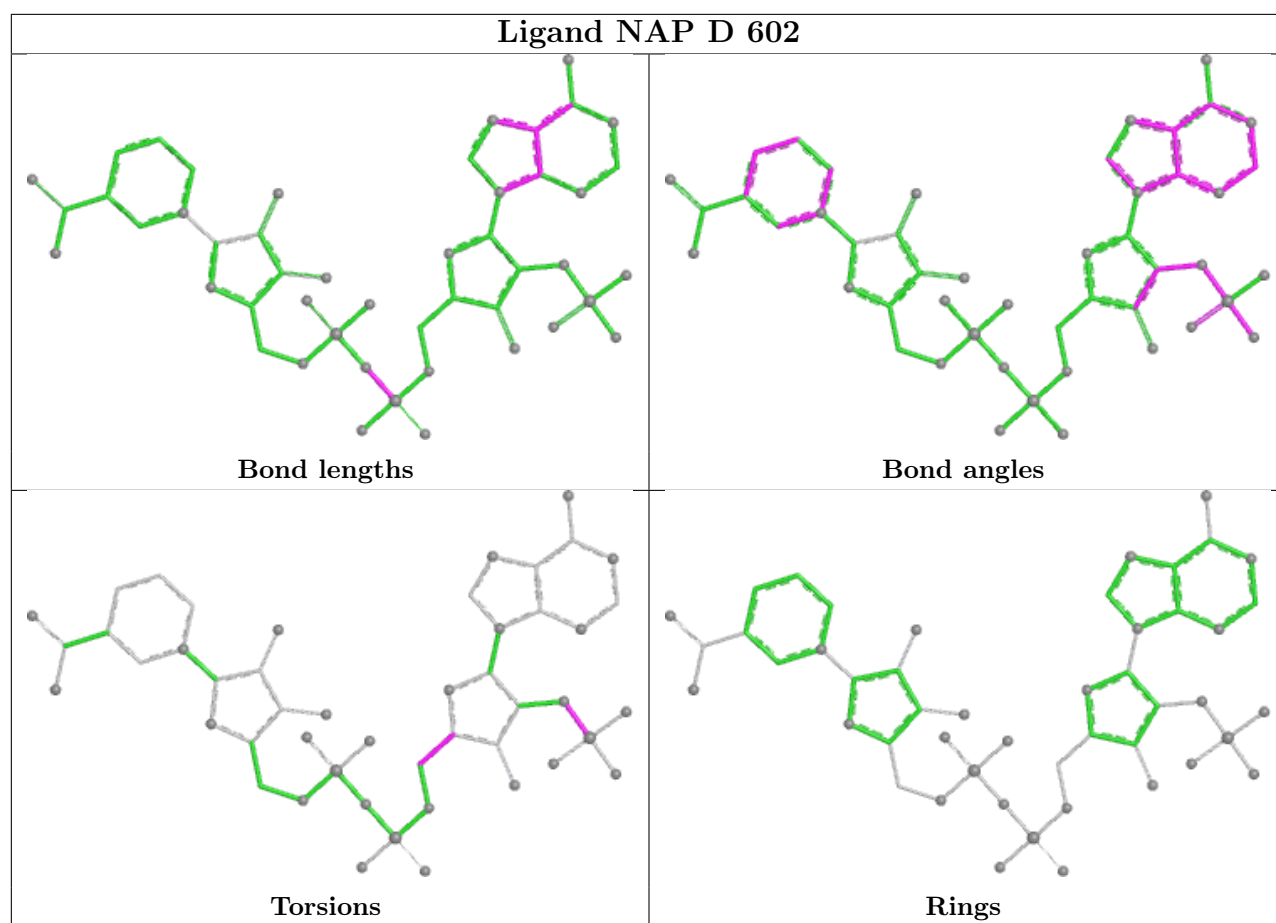
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

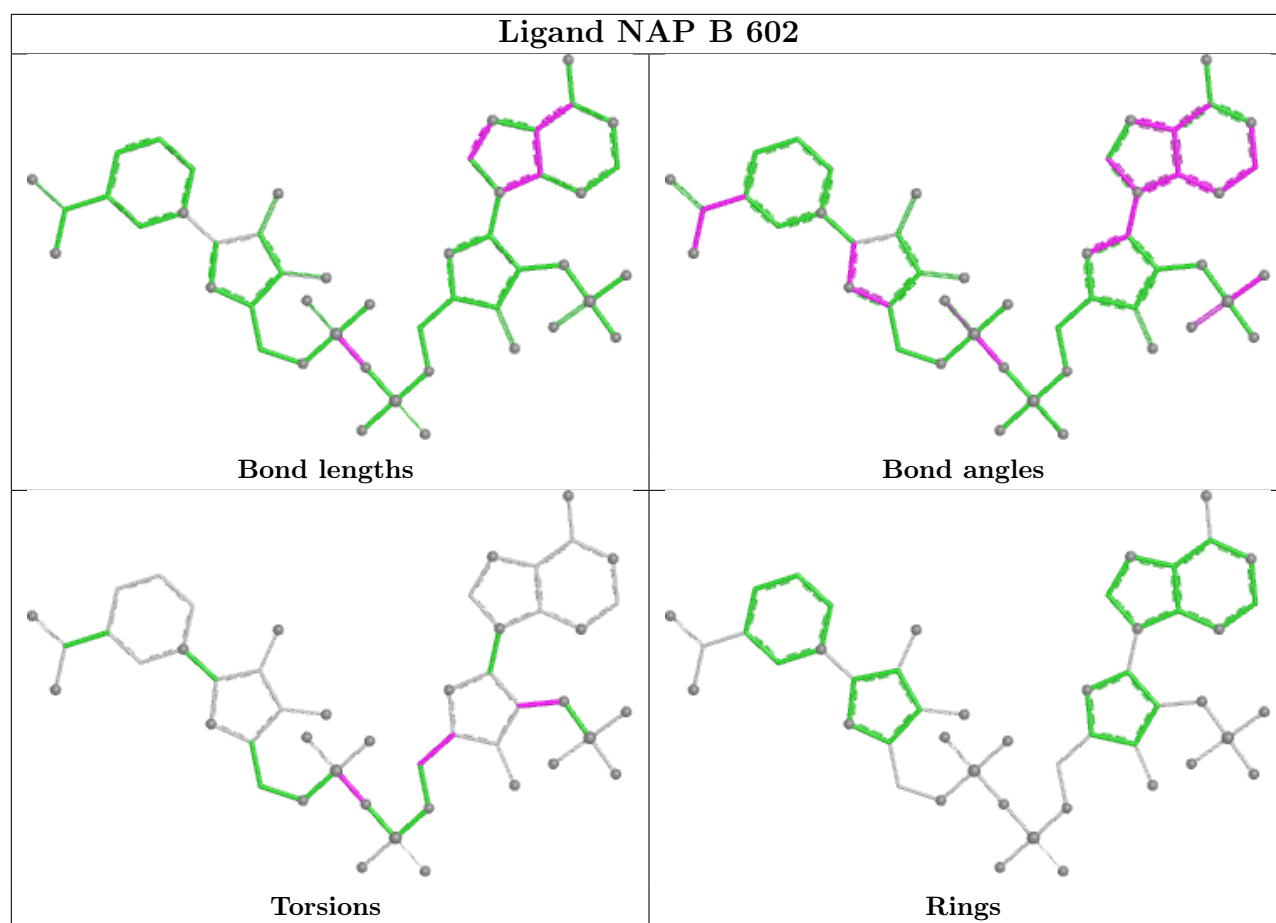


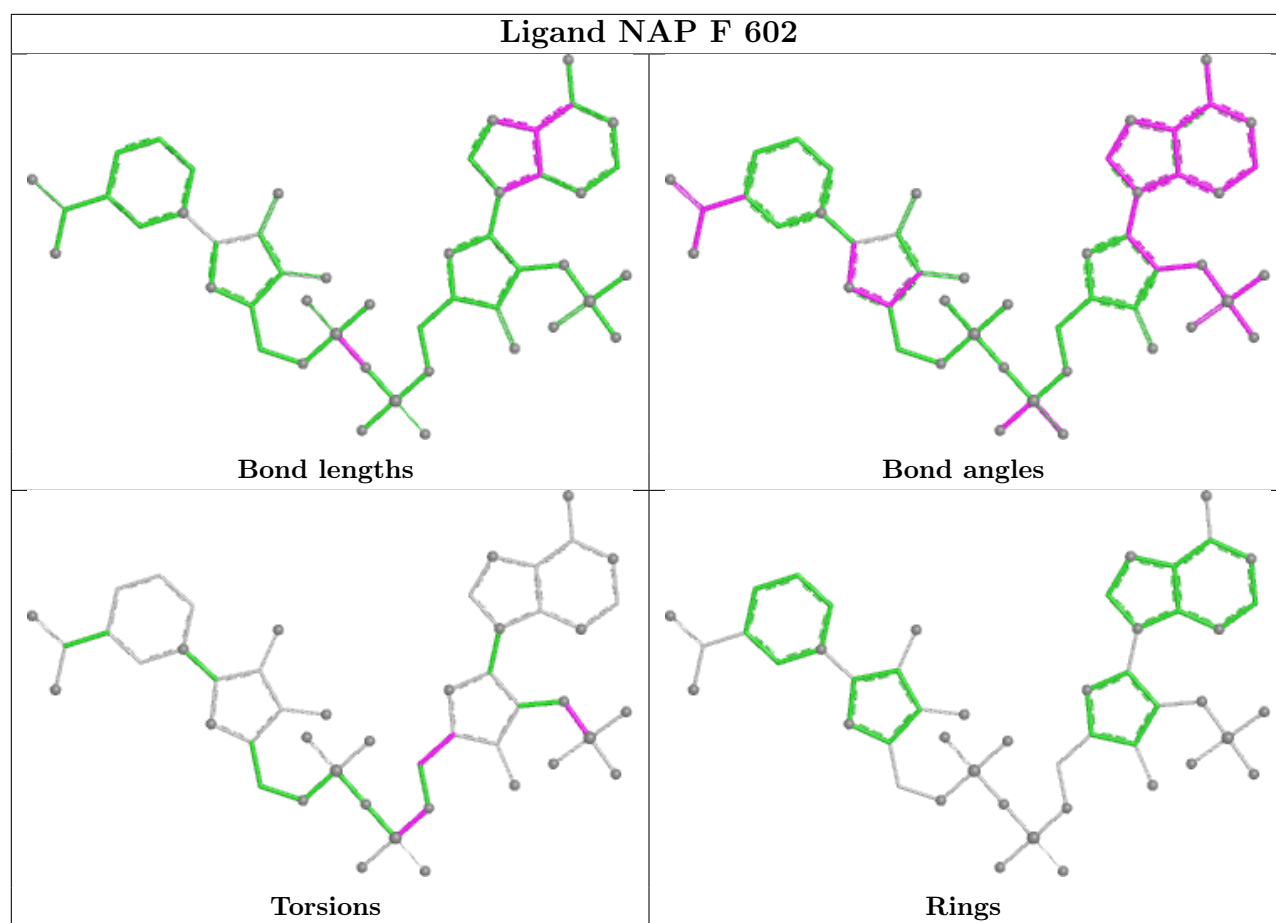


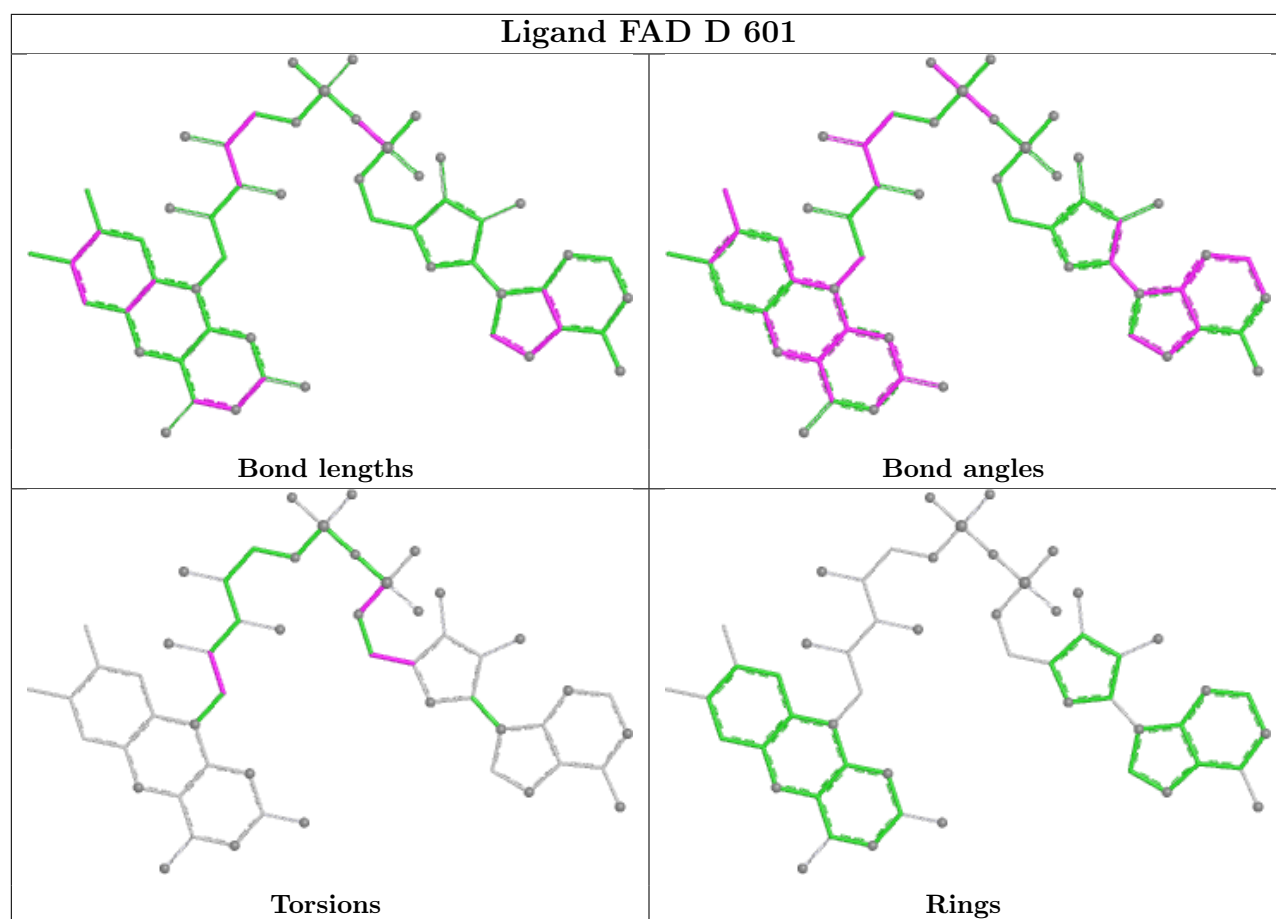
## Ligand FAD E 601

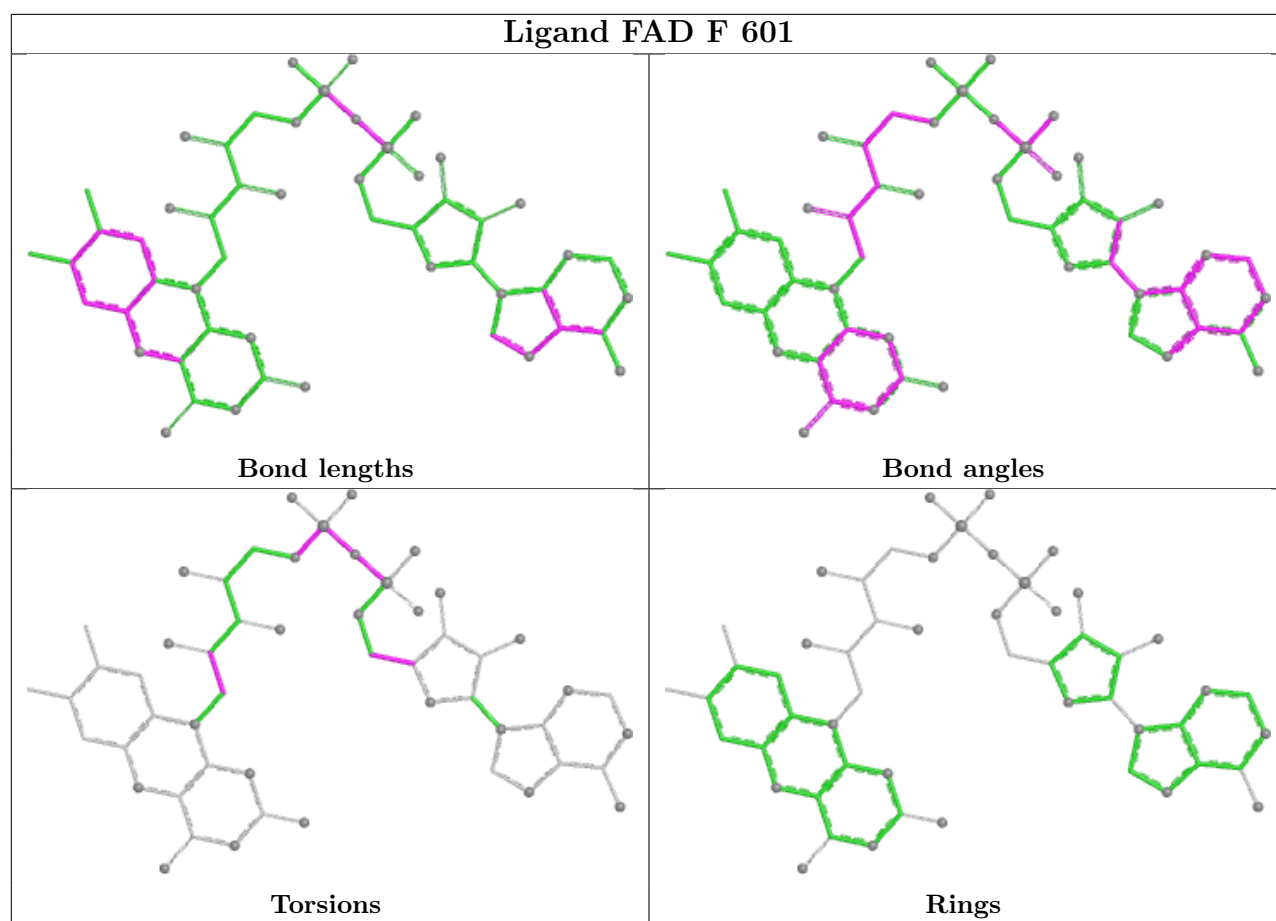


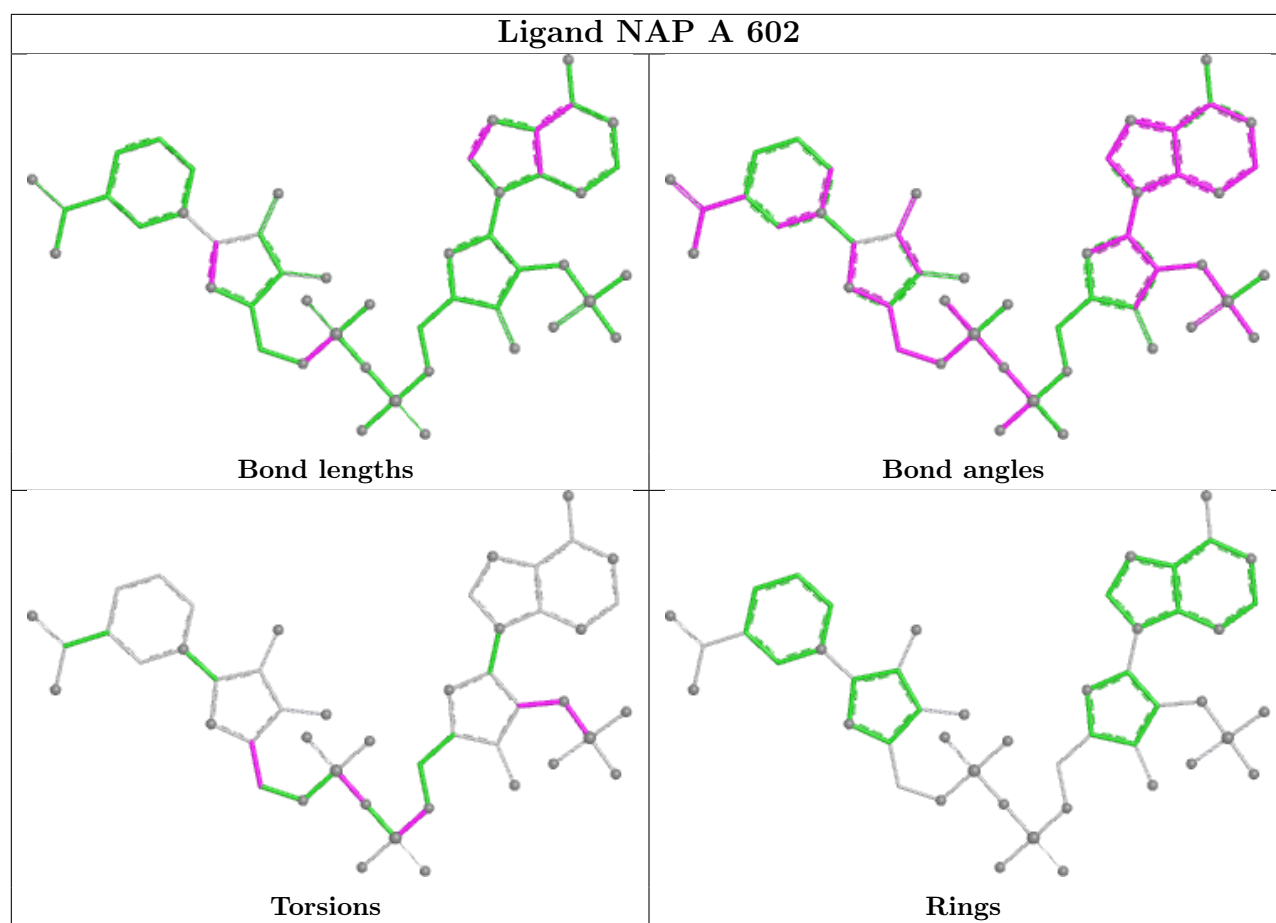


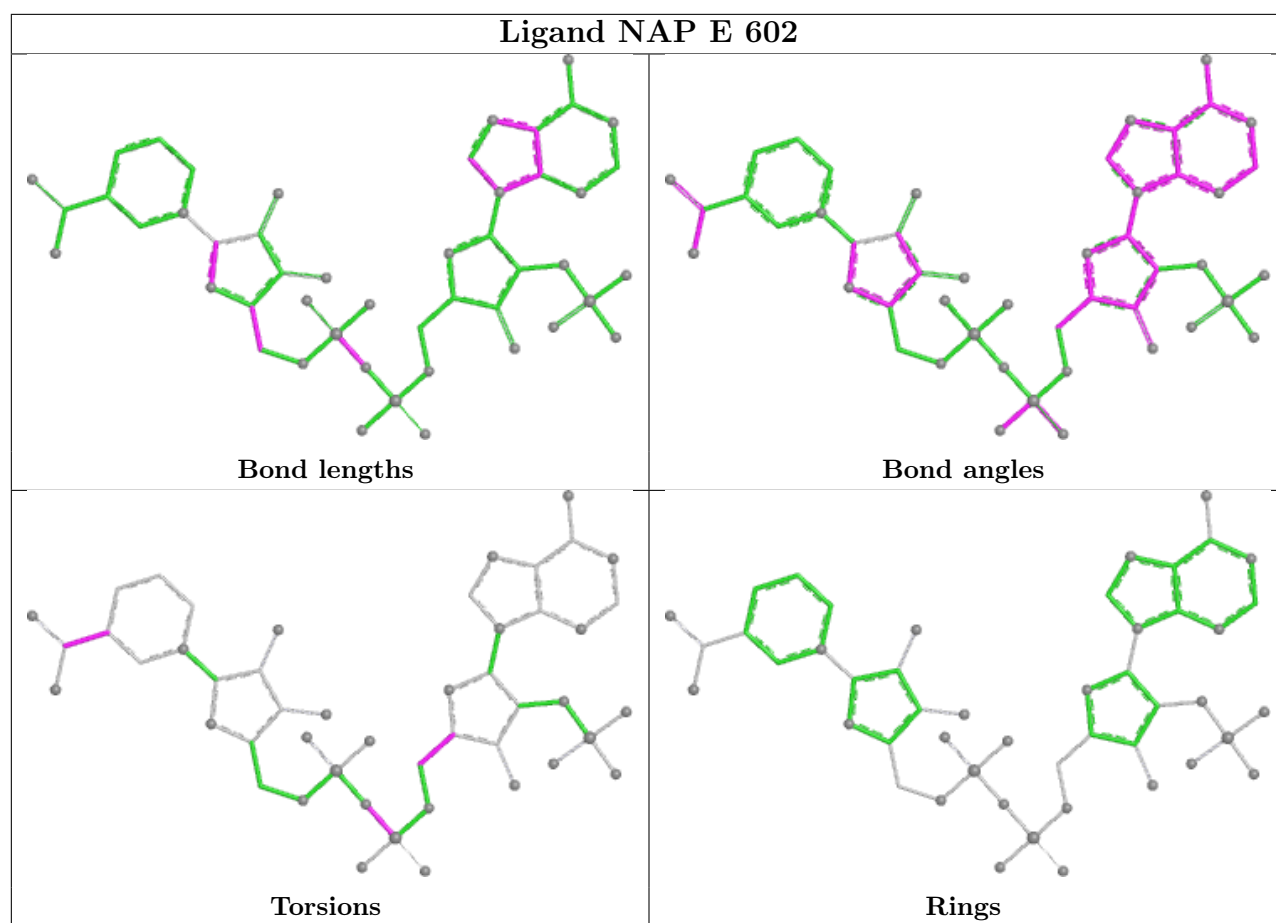


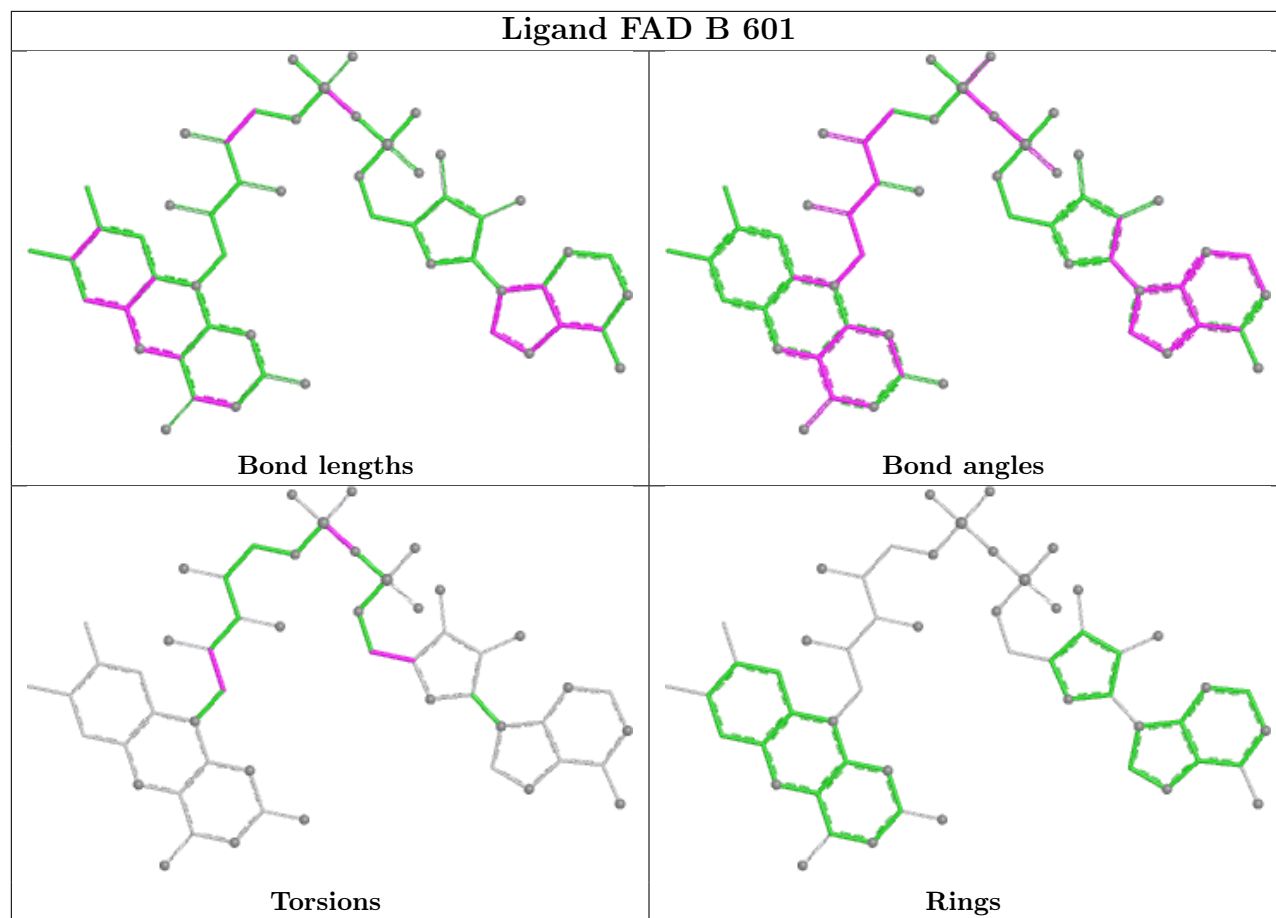


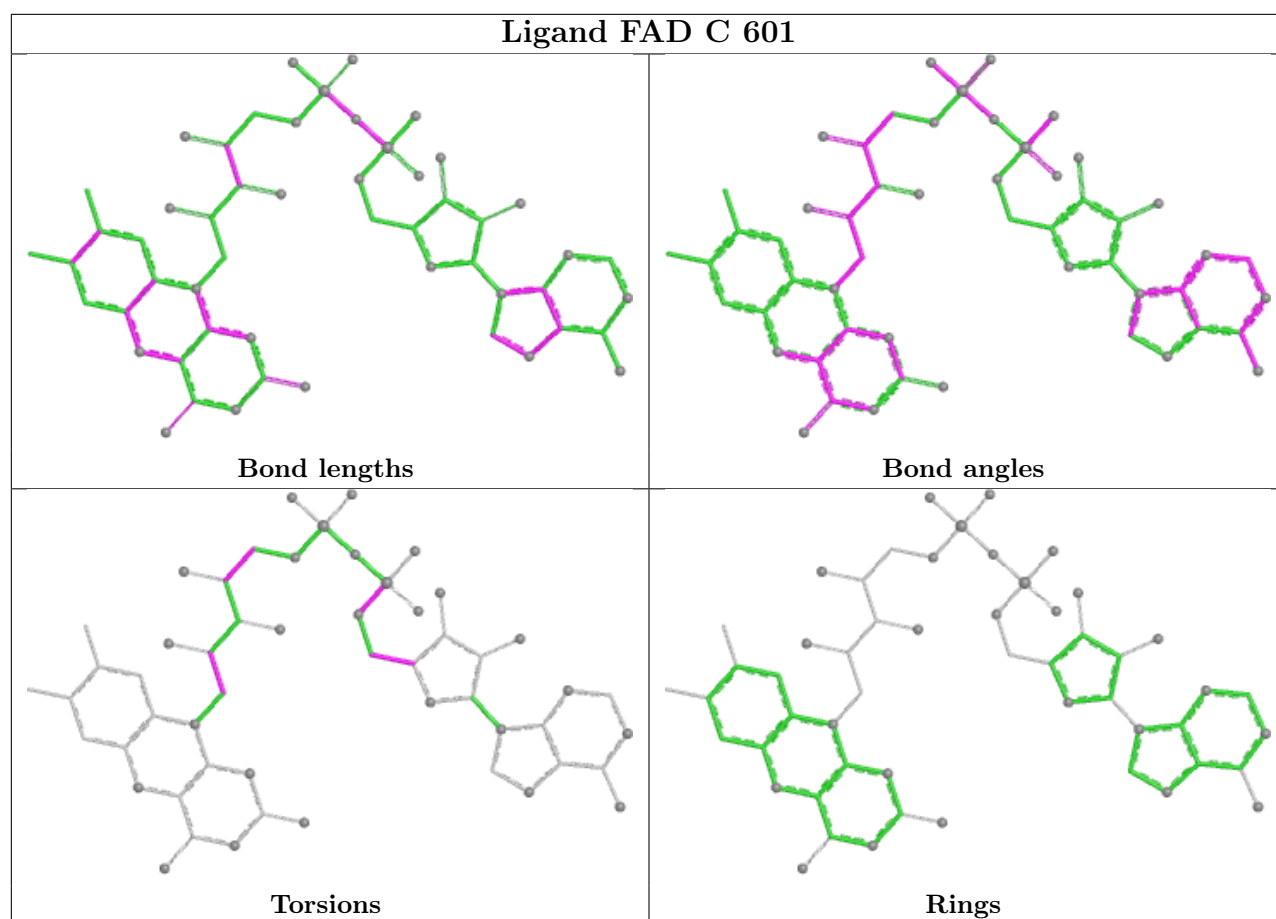












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|------------------------------|-----------------------|-------|
| 1   | A     | 528/532 (99%)   | 1.77   | 188 (35%) <b>1</b> <b>0</b>  | 44, 110, 162, 232     | 0     |
| 1   | B     | 528/532 (99%)   | 0.18   | 18 (3%) 48 39                | 41, 65, 112, 180      | 0     |
| 1   | C     | 528/532 (99%)   | 0.01   | 16 (3%) 52 42                | 35, 59, 100, 163      | 0     |
| 1   | D     | 528/532 (99%)   | 0.08   | 17 (3%) 50 40                | 39, 62, 115, 155      | 0     |
| 1   | E     | 528/532 (99%)   | 0.24   | 27 (5%) 33 25                | 37, 62, 111, 184      | 0     |
| 1   | F     | 528/532 (99%)   | 0.07   | 19 (3%) 46 37                | 36, 59, 100, 169      | 0     |
| All | All   | 3168/3192 (99%) | 0.39   | 285 (8%) <b>15</b> <b>11</b> | 35, 65, 139, 232      | 0     |

All (285) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 367 | ALA  | 7.5  |
| 1   | A     | 113 | VAL  | 6.9  |
| 1   | A     | 10  | ALA  | 6.8  |
| 1   | A     | 359 | PRO  | 6.6  |
| 1   | A     | 335 | TYR  | 6.4  |
| 1   | A     | 333 | TYR  | 6.2  |
| 1   | A     | 364 | PRO  | 5.8  |
| 1   | A     | 343 | ILE  | 5.7  |
| 1   | A     | 338 | LEU  | 5.5  |
| 1   | E     | 245 | ASN  | 5.1  |
| 1   | F     | 514 | LEU  | 5.1  |
| 1   | A     | 94  | PHE  | 5.1  |
| 1   | A     | 337 | PHE  | 5.0  |
| 1   | C     | 518 | LEU  | 5.0  |
| 1   | A     | 142 | ALA  | 5.0  |
| 1   | A     | 366 | LEU  | 4.9  |
| 1   | A     | 331 | TYR  | 4.9  |
| 1   | C     | 514 | LEU  | 4.9  |
| 1   | A     | 46  | HIS  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 368 | VAL  | 4.8  |
| 1   | A     | 41  | TRP  | 4.8  |
| 1   | A     | 342 | ILE  | 4.7  |
| 1   | A     | 31  | PHE  | 4.5  |
| 1   | B     | 514 | LEU  | 4.5  |
| 1   | A     | 5   | VAL  | 4.4  |
| 1   | A     | 351 | THR  | 4.3  |
| 1   | A     | 372 | VAL  | 4.3  |
| 1   | A     | 143 | VAL  | 4.3  |
| 1   | A     | 360 | LEU  | 4.3  |
| 1   | A     | 334 | ALA  | 4.3  |
| 1   | D     | 515 | LEU  | 4.3  |
| 1   | E     | 246 | SER  | 4.2  |
| 1   | A     | 101 | LEU  | 4.2  |
| 1   | A     | 125 | TRP  | 4.1  |
| 1   | D     | 514 | LEU  | 4.1  |
| 1   | A     | 28  | PRO  | 4.1  |
| 1   | A     | 6   | ALA  | 4.1  |
| 1   | F     | 245 | ASN  | 4.1  |
| 1   | A     | 355 | GLY  | 4.0  |
| 1   | A     | 336 | PRO  | 4.0  |
| 1   | F     | 515 | LEU  | 3.9  |
| 1   | A     | 332 | GLY  | 3.9  |
| 1   | A     | 110 | VAL  | 3.9  |
| 1   | A     | 353 | PHE  | 3.9  |
| 1   | A     | 357 | PHE  | 3.8  |
| 1   | A     | 12  | VAL  | 3.8  |
| 1   | A     | 38  | GLY  | 3.8  |
| 1   | A     | 443 | ALA  | 3.8  |
| 1   | A     | 111 | SER  | 3.8  |
| 1   | B     | 244 | LYS  | 3.8  |
| 1   | C     | 244 | LYS  | 3.7  |
| 1   | A     | 358 | PRO  | 3.7  |
| 1   | A     | 390 | ALA  | 3.7  |
| 1   | A     | 304 | LYS  | 3.6  |
| 1   | A     | 152 | TYR  | 3.6  |
| 1   | A     | 445 | PRO  | 3.6  |
| 1   | A     | 55  | TYR  | 3.6  |
| 1   | A     | 371 | LEU  | 3.6  |
| 1   | B     | 372 | VAL  | 3.5  |
| 1   | C     | 523 | LEU  | 3.5  |
| 1   | A     | 72  | PHE  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 519 | LEU  | 3.5  |
| 1   | A     | 157 | LYS  | 3.5  |
| 1   | A     | 52  | ALA  | 3.5  |
| 1   | A     | 530 | ALA  | 3.5  |
| 1   | A     | 427 | GLN  | 3.4  |
| 1   | D     | 246 | SER  | 3.4  |
| 1   | A     | 150 | HIS  | 3.4  |
| 1   | A     | 7   | ILE  | 3.4  |
| 1   | D     | 510 | LEU  | 3.4  |
| 1   | A     | 515 | LEU  | 3.3  |
| 1   | A     | 133 | GLY  | 3.3  |
| 1   | A     | 474 | MET  | 3.3  |
| 1   | A     | 26  | LEU  | 3.3  |
| 1   | B     | 526 | ALA  | 3.3  |
| 1   | A     | 88  | GLN  | 3.3  |
| 1   | A     | 251 | ILE  | 3.3  |
| 1   | B     | 515 | LEU  | 3.3  |
| 1   | A     | 50  | GLY  | 3.3  |
| 1   | A     | 384 | LEU  | 3.3  |
| 1   | A     | 514 | LEU  | 3.3  |
| 1   | B     | 523 | LEU  | 3.3  |
| 1   | E     | 524 | LEU  | 3.3  |
| 1   | F     | 528 | LEU  | 3.3  |
| 1   | B     | 522 | VAL  | 3.3  |
| 1   | A     | 246 | SER  | 3.3  |
| 1   | A     | 8   | ILE  | 3.2  |
| 1   | A     | 328 | ALA  | 3.2  |
| 1   | A     | 452 | LEU  | 3.2  |
| 1   | A     | 25  | GLY  | 3.2  |
| 1   | F     | 157 | LYS  | 3.2  |
| 1   | A     | 347 | ASN  | 3.2  |
| 1   | A     | 356 | ILE  | 3.2  |
| 1   | A     | 365 | THR  | 3.2  |
| 1   | A     | 406 | MET  | 3.2  |
| 1   | A     | 447 | ILE  | 3.2  |
| 1   | C     | 517 | ILE  | 3.2  |
| 1   | F     | 510 | LEU  | 3.1  |
| 1   | A     | 138 | ALA  | 3.1  |
| 1   | E     | 514 | LEU  | 3.1  |
| 1   | D     | 245 | ASN  | 3.1  |
| 1   | A     | 16  | ALA  | 3.1  |
| 1   | A     | 350 | VAL  | 3.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | C            | 524        | LEU         | 3.1         |
| 1          | A            | 36         | ASP         | 3.1         |
| 1          | A            | 148        | GLY         | 3.1         |
| 1          | A            | 22         | LEU         | 3.1         |
| 1          | F            | 529        | LEU         | 3.1         |
| 1          | E            | 515        | LEU         | 3.0         |
| 1          | A            | 510        | LEU         | 3.0         |
| 1          | A            | 428        | THR         | 3.0         |
| 1          | A            | 100        | LEU         | 3.0         |
| 1          | A            | 244        | LYS         | 3.0         |
| 1          | A            | 40         | LEU         | 3.0         |
| 1          | B            | 427        | GLN         | 3.0         |
| 1          | A            | 393        | PHE         | 3.0         |
| 1          | A            | 32         | GLU         | 2.9         |
| 1          | A            | 405        | MET         | 2.9         |
| 1          | B            | 520        | PHE         | 2.9         |
| 1          | A            | 386        | ALA         | 2.9         |
| 1          | A            | 453        | THR         | 2.9         |
| 1          | A            | 511        | PHE         | 2.9         |
| 1          | A            | 37         | ILE         | 2.9         |
| 1          | A            | 312        | ILE         | 2.9         |
| 1          | E            | 520        | PHE         | 2.9         |
| 1          | C            | 515        | LEU         | 2.9         |
| 1          | D            | 530        | ALA         | 2.9         |
| 1          | A            | 69         | PHE         | 2.9         |
| 1          | A            | 140        | PHE         | 2.9         |
| 1          | C            | 511        | PHE         | 2.9         |
| 1          | A            | 469        | TYR         | 2.8         |
| 1          | A            | 127        | VAL         | 2.8         |
| 1          | D            | 451        | PHE         | 2.8         |
| 1          | E            | 242        | PHE         | 2.8         |
| 1          | A            | 149        | HIS         | 2.8         |
| 1          | A            | 369        | ILE         | 2.8         |
| 1          | A            | 399        | LEU         | 2.8         |
| 1          | B            | 452        | LEU         | 2.8         |
| 1          | A            | 471        | PHE         | 2.8         |
| 1          | B            | 426        | LEU         | 2.8         |
| 1          | A            | 34         | SER         | 2.8         |
| 1          | D            | 529        | LEU         | 2.8         |
| 1          | B            | 524        | LEU         | 2.8         |
| 1          | A            | 398        | THR         | 2.8         |
| 1          | E            | 244        | LYS         | 2.8         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 153 | PRO  | 2.8  |
| 1   | A     | 387 | ARG  | 2.7  |
| 1   | A     | 466 | CYS  | 2.7  |
| 1   | E     | 312 | ILE  | 2.7  |
| 1   | A     | 175 | ASP  | 2.7  |
| 1   | E     | 522 | VAL  | 2.7  |
| 1   | A     | 424 | GLN  | 2.7  |
| 1   | A     | 377 | ALA  | 2.7  |
| 1   | B     | 530 | ALA  | 2.7  |
| 1   | A     | 245 | ASN  | 2.7  |
| 1   | A     | 48  | GLU  | 2.7  |
| 1   | E     | 452 | LEU  | 2.7  |
| 1   | A     | 440 | PHE  | 2.6  |
| 1   | A     | 11  | GLY  | 2.6  |
| 1   | A     | 192 | LEU  | 2.6  |
| 1   | A     | 487 | LEU  | 2.6  |
| 1   | F     | 518 | LEU  | 2.6  |
| 1   | A     | 370 | GLY  | 2.6  |
| 1   | D     | 519 | LEU  | 2.6  |
| 1   | A     | 15  | LEU  | 2.6  |
| 1   | A     | 155 | LEU  | 2.6  |
| 1   | A     | 13  | SER  | 2.6  |
| 1   | A     | 112 | SER  | 2.5  |
| 1   | A     | 169 | LYS  | 2.5  |
| 1   | A     | 529 | LEU  | 2.5  |
| 1   | A     | 104 | ILE  | 2.5  |
| 1   | A     | 29  | THR  | 2.5  |
| 1   | A     | 285 | ASN  | 2.5  |
| 1   | A     | 345 | SER  | 2.5  |
| 1   | A     | 9   | GLY  | 2.5  |
| 1   | F     | 520 | PHE  | 2.5  |
| 1   | A     | 71  | ASP  | 2.5  |
| 1   | D     | 523 | LEU  | 2.5  |
| 1   | A     | 522 | VAL  | 2.5  |
| 1   | D     | 526 | ALA  | 2.5  |
| 1   | E     | 390 | ALA  | 2.5  |
| 1   | E     | 530 | ALA  | 2.5  |
| 1   | A     | 109 | LEU  | 2.5  |
| 1   | A     | 451 | PHE  | 2.5  |
| 1   | E     | 512 | TYR  | 2.5  |
| 1   | A     | 87  | LEU  | 2.4  |
| 1   | A     | 144 | MET  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 518 | LEU  | 2.4  |
| 1   | A     | 161 | PRO  | 2.4  |
| 1   | D     | 527 | VAL  | 2.4  |
| 1   | A     | 231 | TRP  | 2.4  |
| 1   | E     | 306 | PHE  | 2.4  |
| 1   | A     | 432 | THR  | 2.4  |
| 1   | A     | 490 | TRP  | 2.4  |
| 1   | F     | 530 | ALA  | 2.4  |
| 1   | A     | 42  | LYS  | 2.4  |
| 1   | A     | 423 | SER  | 2.4  |
| 1   | A     | 388 | TRP  | 2.4  |
| 1   | E     | 453 | THR  | 2.4  |
| 1   | E     | 529 | LEU  | 2.4  |
| 1   | A     | 380 | PRO  | 2.4  |
| 1   | E     | 248 | PRO  | 2.4  |
| 1   | A     | 527 | VAL  | 2.3  |
| 1   | A     | 242 | PHE  | 2.3  |
| 1   | B     | 451 | PHE  | 2.3  |
| 1   | A     | 24  | GLU  | 2.3  |
| 1   | A     | 95  | ALA  | 2.3  |
| 1   | A     | 375 | LEU  | 2.3  |
| 1   | C     | 519 | LEU  | 2.3  |
| 1   | B     | 517 | ILE  | 2.3  |
| 1   | C     | 527 | VAL  | 2.3  |
| 1   | A     | 27  | GLU  | 2.3  |
| 1   | B     | 518 | LEU  | 2.3  |
| 1   | A     | 108 | THR  | 2.3  |
| 1   | A     | 476 | PRO  | 2.3  |
| 1   | E     | 451 | PHE  | 2.3  |
| 1   | D     | 524 | LEU  | 2.3  |
| 1   | B     | 422 | GLN  | 2.3  |
| 1   | D     | 244 | LYS  | 2.3  |
| 1   | A     | 98  | LYS  | 2.3  |
| 1   | A     | 195 | SER  | 2.3  |
| 1   | A     | 479 | TRP  | 2.3  |
| 1   | A     | 306 | PHE  | 2.3  |
| 1   | F     | 511 | PHE  | 2.3  |
| 1   | A     | 362 | GLU  | 2.3  |
| 1   | A     | 501 | ALA  | 2.3  |
| 1   | A     | 373 | GLN  | 2.3  |
| 1   | A     | 470 | GLN  | 2.3  |
| 1   | A     | 486 | ILE  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 103 | TYR  | 2.3  |
| 1   | A     | 448 | PRO  | 2.3  |
| 1   | A     | 258 | LYS  | 2.2  |
| 1   | A     | 444 | LYS  | 2.2  |
| 1   | E     | 209 | LYS  | 2.2  |
| 1   | A     | 379 | ILE  | 2.2  |
| 1   | A     | 33  | ARG  | 2.2  |
| 1   | A     | 90  | TYR  | 2.2  |
| 1   | A     | 239 | PHE  | 2.2  |
| 1   | F     | 526 | ALA  | 2.2  |
| 1   | A     | 91  | ILE  | 2.2  |
| 1   | F     | 77  | ASP  | 2.2  |
| 1   | A     | 128 | THR  | 2.2  |
| 1   | B     | 527 | VAL  | 2.2  |
| 1   | A     | 191 | GLY  | 2.2  |
| 1   | C     | 525 | LEU  | 2.2  |
| 1   | E     | 247 | LEU  | 2.2  |
| 1   | E     | 510 | LEU  | 2.2  |
| 1   | A     | 115 | LYS  | 2.2  |
| 1   | E     | 180 | GLY  | 2.2  |
| 1   | A     | 74  | TYR  | 2.2  |
| 1   | C     | 451 | PHE  | 2.2  |
| 1   | C     | 520 | PHE  | 2.2  |
| 1   | C     | 526 | ALA  | 2.2  |
| 1   | D     | 125 | TRP  | 2.1  |
| 1   | A     | 419 | TRP  | 2.1  |
| 1   | A     | 324 | CYS  | 2.1  |
| 1   | C     | 529 | LEU  | 2.1  |
| 1   | E     | 119 | PHE  | 2.1  |
| 1   | A     | 30  | CYS  | 2.1  |
| 1   | A     | 403 | ASN  | 2.1  |
| 1   | F     | 527 | VAL  | 2.1  |
| 1   | A     | 163 | LEU  | 2.1  |
| 1   | A     | 475 | GLY  | 2.1  |
| 1   | D     | 160 | PHE  | 2.1  |
| 1   | A     | 339 | ASP  | 2.1  |
| 1   | A     | 389 | ALA  | 2.1  |
| 1   | A     | 65  | GLU  | 2.1  |
| 1   | F     | 258 | LYS  | 2.1  |
| 1   | D     | 518 | LEU  | 2.1  |
| 1   | A     | 457 | LEU  | 2.1  |
| 1   | E     | 313 | PHE  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 402 | THR  | 2.1  |
| 1   | F     | 125 | TRP  | 2.1  |
| 1   | A     | 105 | GLN  | 2.0  |
| 1   | E     | 502 | VAL  | 2.0  |
| 1   | E     | 521 | PRO  | 2.0  |
| 1   | A     | 81  | PHE  | 2.0  |
| 1   | A     | 454 | ASP  | 2.0  |
| 1   | A     | 53  | SER  | 2.0  |
| 1   | A     | 117 | PRO  | 2.0  |
| 1   | A     | 156 | PRO  | 2.0  |
| 1   | C     | 359 | PRO  | 2.0  |
| 1   | F     | 524 | LEU  | 2.0  |
| 1   | F     | 31  | PHE  | 2.0  |
| 1   | A     | 416 | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

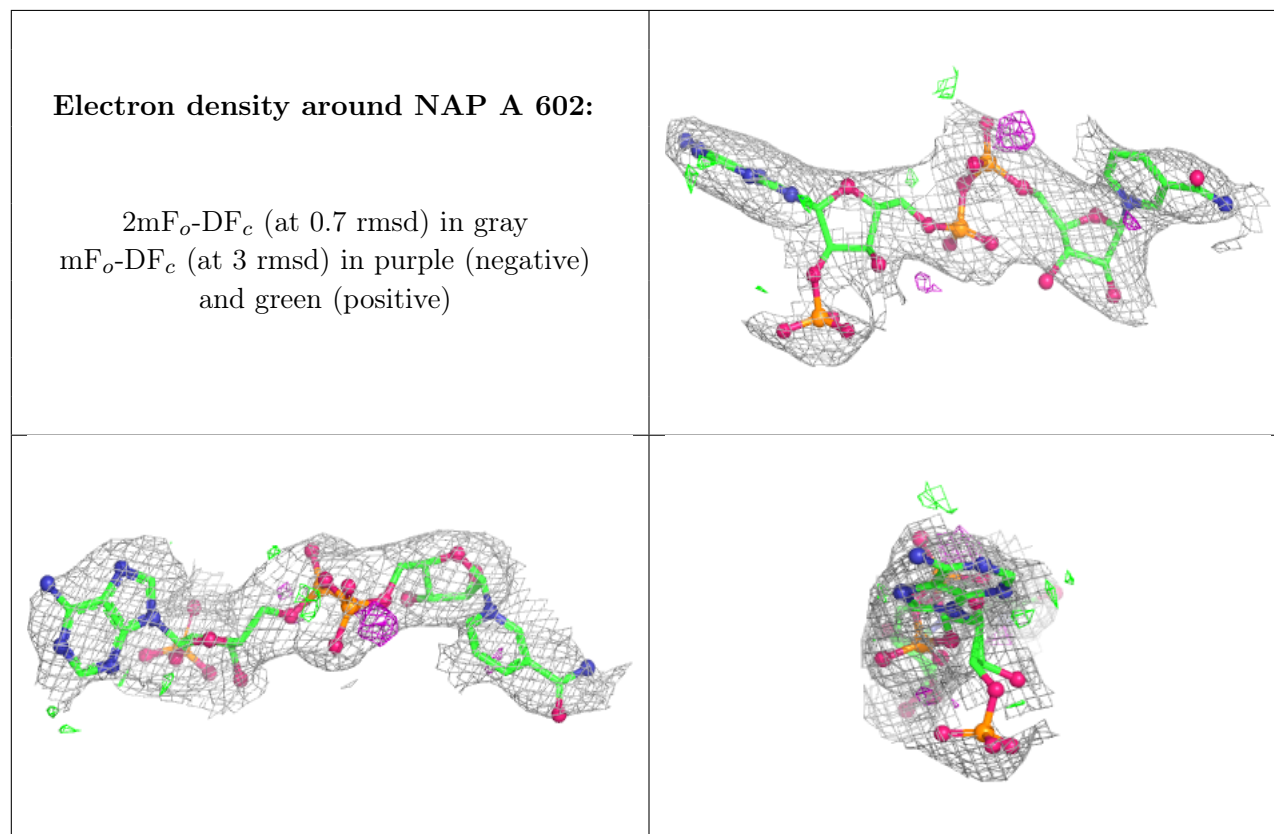
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | NAP  | A     | 602 | 48/48 | 0.86 | 0.11 | 65,94,126,138               | 0     |
| 2   | FAD  | A     | 601 | 53/53 | 0.88 | 0.14 | 55,88,147,158               | 0     |
| 4   | OXY  | E     | 603 | 2/2   | 0.90 | 0.18 | 52,52,52,56                 | 0     |
| 4   | OXY  | A     | 603 | 2/2   | 0.92 | 0.11 | 72,72,72,74                 | 0     |
| 4   | OXY  | C     | 603 | 2/2   | 0.93 | 0.09 | 52,52,52,56                 | 0     |
| 4   | OXY  | D     | 603 | 2/2   | 0.93 | 0.17 | 54,54,54,60                 | 0     |
| 4   | OXY  | B     | 603 | 2/2   | 0.94 | 0.09 | 58,58,58,59                 | 0     |
| 3   | NAP  | D     | 602 | 48/48 | 0.95 | 0.07 | 45,64,86,94                 | 0     |
| 3   | NAP  | E     | 602 | 48/48 | 0.96 | 0.08 | 45,67,99,105                | 0     |

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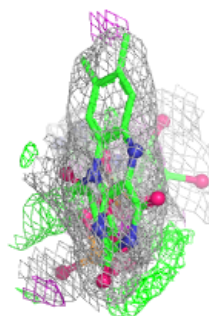
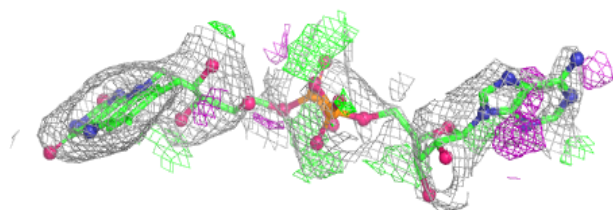
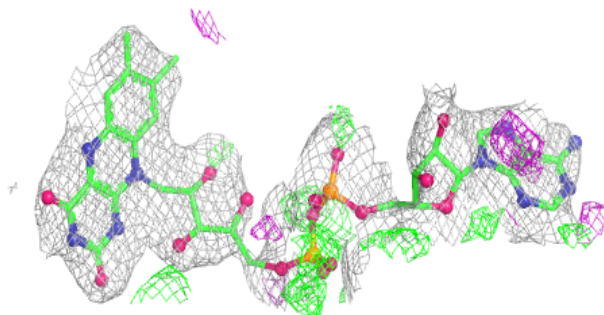
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | NAP  | B     | 602 | 48/48 | 0.96 | 0.07 | 45,57,75,77                 | 0     |
| 2   | FAD  | C     | 601 | 53/53 | 0.97 | 0.07 | 32,50,63,69                 | 0     |
| 2   | FAD  | F     | 601 | 53/53 | 0.97 | 0.06 | 39,47,56,61                 | 0     |
| 3   | NAP  | C     | 602 | 48/48 | 0.97 | 0.06 | 47,57,72,79                 | 0     |
| 2   | FAD  | B     | 601 | 53/53 | 0.97 | 0.06 | 44,54,62,69                 | 0     |
| 3   | NAP  | F     | 602 | 48/48 | 0.97 | 0.06 | 35,55,74,79                 | 0     |
| 4   | OXY  | F     | 603 | 2/2   | 0.97 | 0.08 | 47,47,47,51                 | 0     |
| 2   | FAD  | E     | 601 | 53/53 | 0.98 | 0.05 | 33,42,50,52                 | 0     |
| 2   | FAD  | D     | 601 | 53/53 | 0.98 | 0.06 | 37,48,62,67                 | 0     |

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

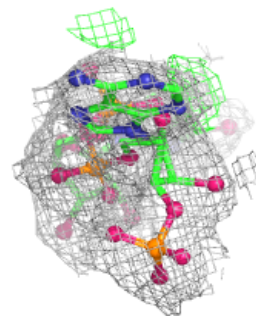
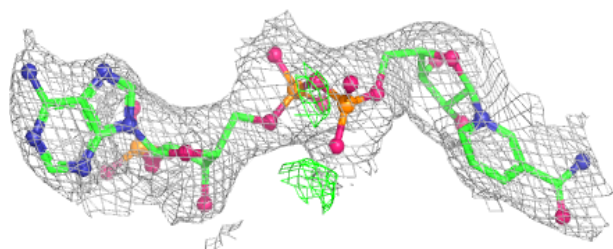
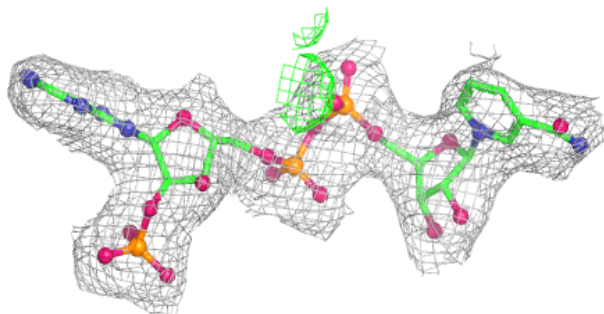


**Electron density around FAD A 601:**

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

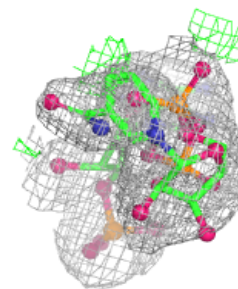
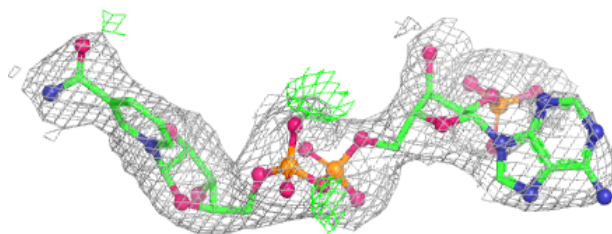
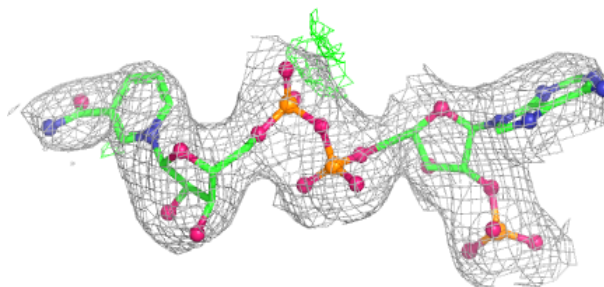
**Electron density around NAP D 602:**

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

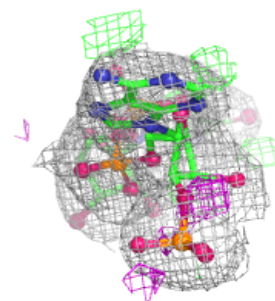
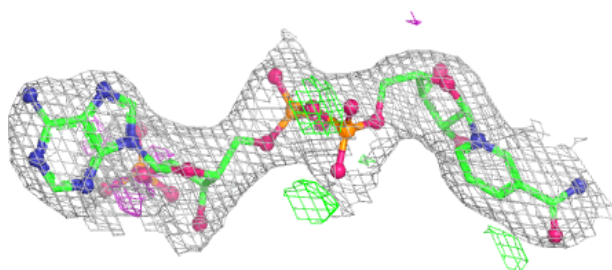
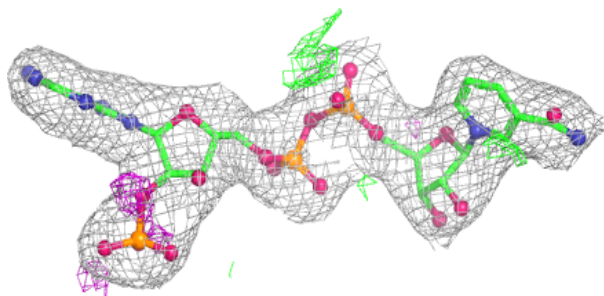


**Electron density around NAP E 602:**

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

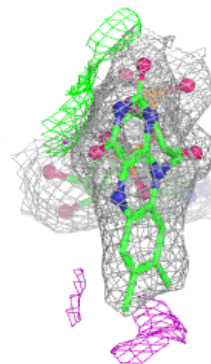
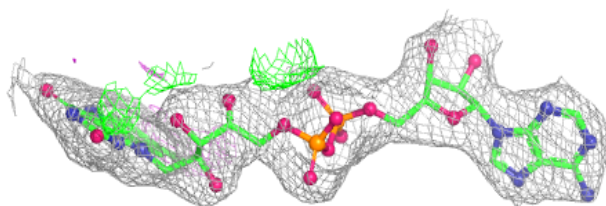
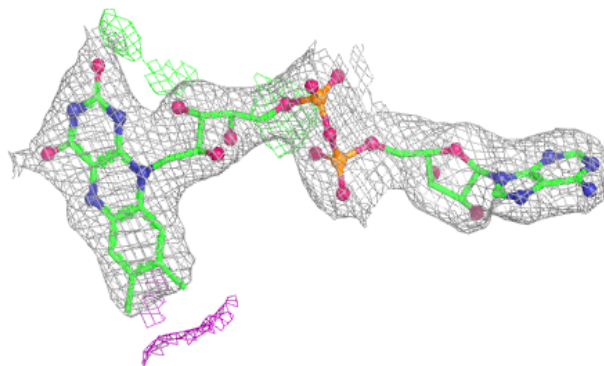
**Electron density around NAP B 602:**

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

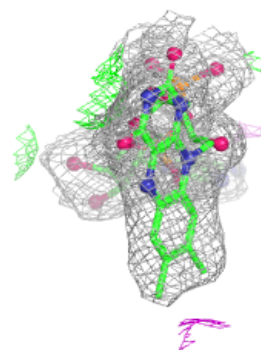
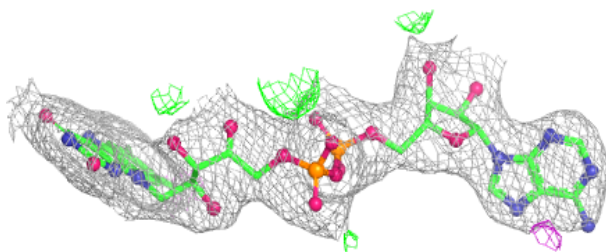
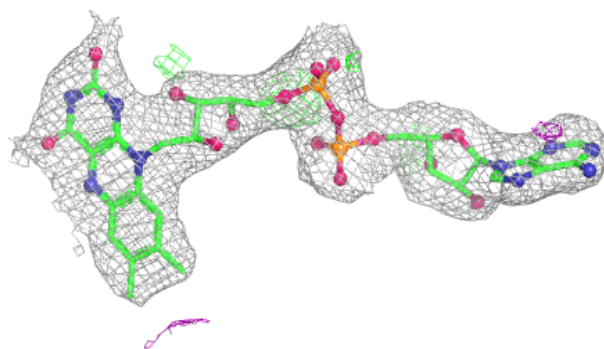


**Electron density around FAD C 601:**

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

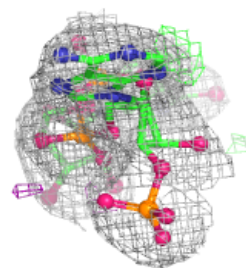
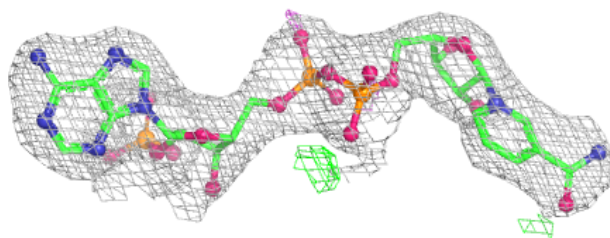
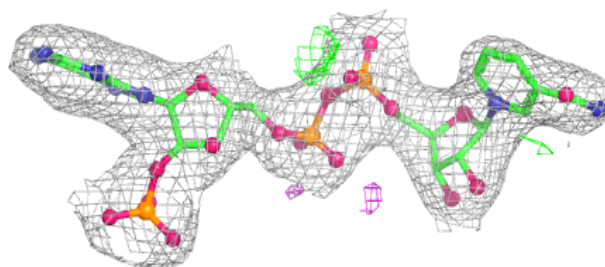
**Electron density around FAD F 601:**

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

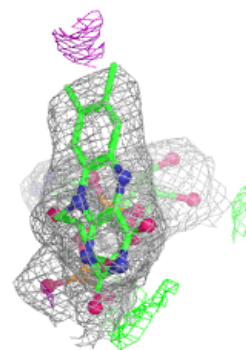
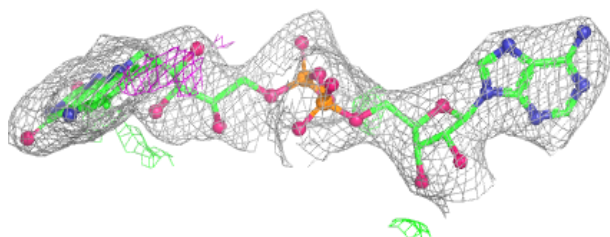
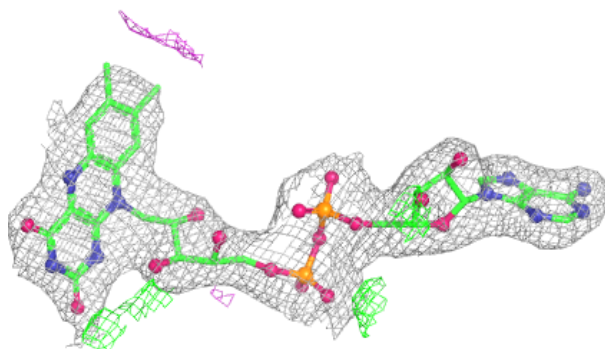


**Electron density around NAP C 602:**

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

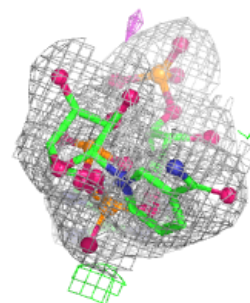
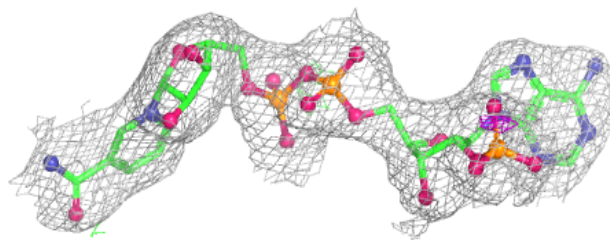
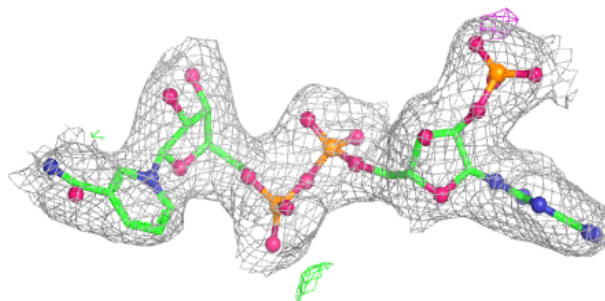
**Electron density around FAD B 601:**

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

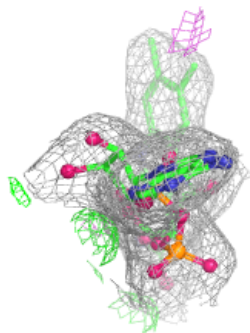
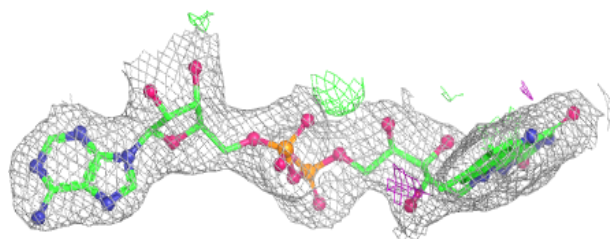
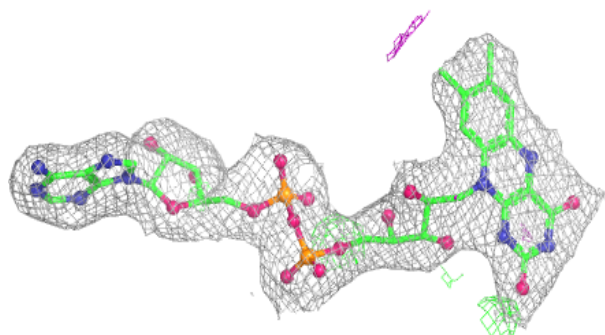


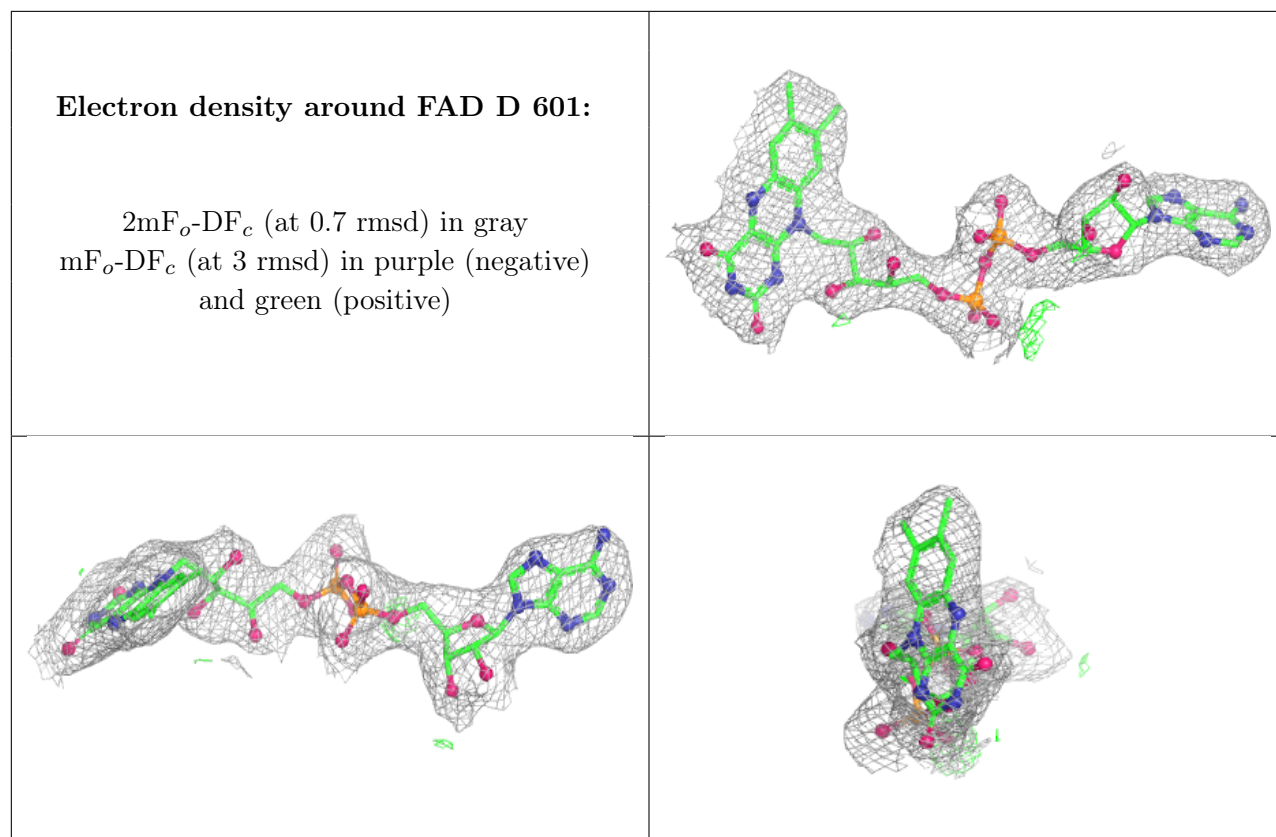
**Electron density around NAP F 602:**

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

**Electron density around FAD E 601:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.