



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 06:57 AM UTC

PDB ID : 3EAN / pdb\_00003ean  
Title : Crystal structure of recombinant rat selenoprotein thioredoxin reductase 1 with reduced C-terminal tail  
Authors : Sandalova, T.; Cheng, Q.; Lindqvist, Y.; Arner, E.  
Deposited on : 2008-08-26  
Resolution : 2.75 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

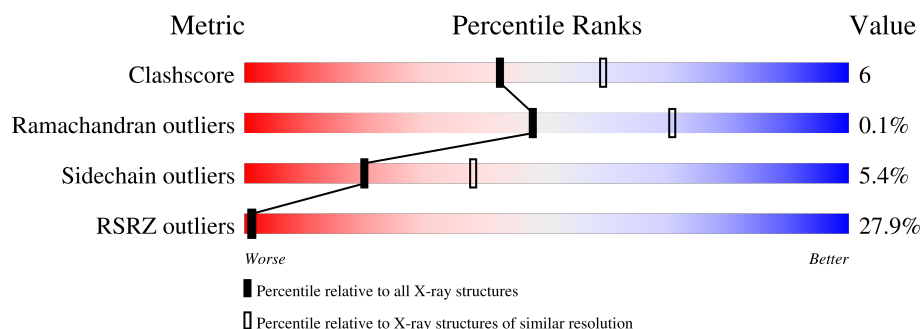
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1044 (2.76-2.76)                                      |
| Ramachandran outliers | 187476                      | 1024 (2.76-2.76)                                      |
| Sidechain outliers    | 187428                      | 1024 (2.76-2.76)                                      |
| RSRZ outliers         | 180081                      | 1009 (2.76-2.76)                                      |

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     | 499    | <div> <div>13%</div> <div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div> |
| 1   | B     | 499    | <div> <div>10%</div> <div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div> |
| 1   | C     | 499    | <div> <div>45%</div> <div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div> |
| 1   | D     | 499    | <div> <div>25%</div> <div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div> |
| 1   | E     | 499    | <div> <div>22%</div> <div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div> |
| 1   | F     | 499    | <div> <div>48%</div> <div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

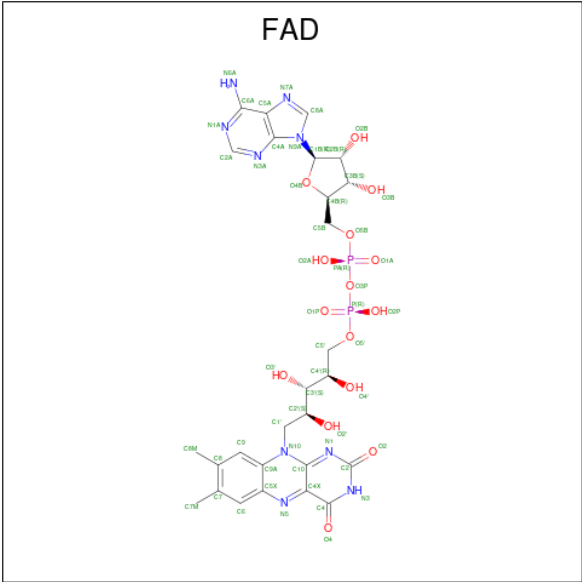
- Molecule 1 is a protein called Thioredoxin reductase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|----|---------|---------|-------|
| 1   | A     | 490      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3768  | 2393 | 637 | 716 | 21 | 1  |         |         |       |
| 1   | B     | 490      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3768  | 2393 | 637 | 716 | 21 | 1  |         |         |       |
| 1   | C     | 486      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3731  | 2368 | 633 | 708 | 21 | 1  |         |         |       |
| 1   | D     | 491      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3777  | 2399 | 639 | 717 | 21 | 1  |         |         |       |
| 1   | E     | 490      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3768  | 2393 | 637 | 716 | 21 | 1  |         |         |       |
| 1   | F     | 489      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3762  | 2390 | 636 | 714 | 21 | 1  |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

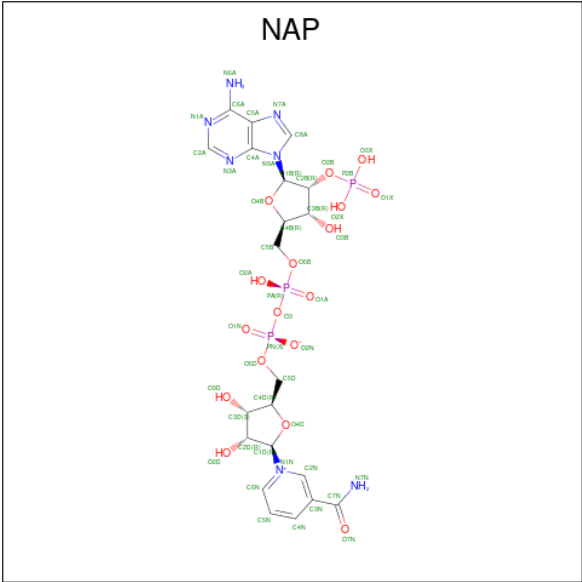
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 52      | ARG      | ASN    | conflict | UNP O89049 |
| A     | 53      | TRP      | GLY    | conflict | UNP O89049 |
| B     | 52      | ARG      | ASN    | conflict | UNP O89049 |
| B     | 53      | TRP      | GLY    | conflict | UNP O89049 |
| C     | 52      | ARG      | ASN    | conflict | UNP O89049 |
| C     | 53      | TRP      | GLY    | conflict | UNP O89049 |
| D     | 52      | ARG      | ASN    | conflict | UNP O89049 |
| D     | 53      | TRP      | GLY    | conflict | UNP O89049 |
| E     | 52      | ARG      | ASN    | conflict | UNP O89049 |
| E     | 53      | TRP      | GLY    | conflict | UNP O89049 |
| F     | 52      | ARG      | ASN    | conflict | UNP O89049 |
| F     | 53      | TRP      | GLY    | conflict | UNP O89049 |

- 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   | 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   | D     | 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   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |         |
| 3   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |         |
| 3   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 11 | 5 | 13 | 3 |         |         |

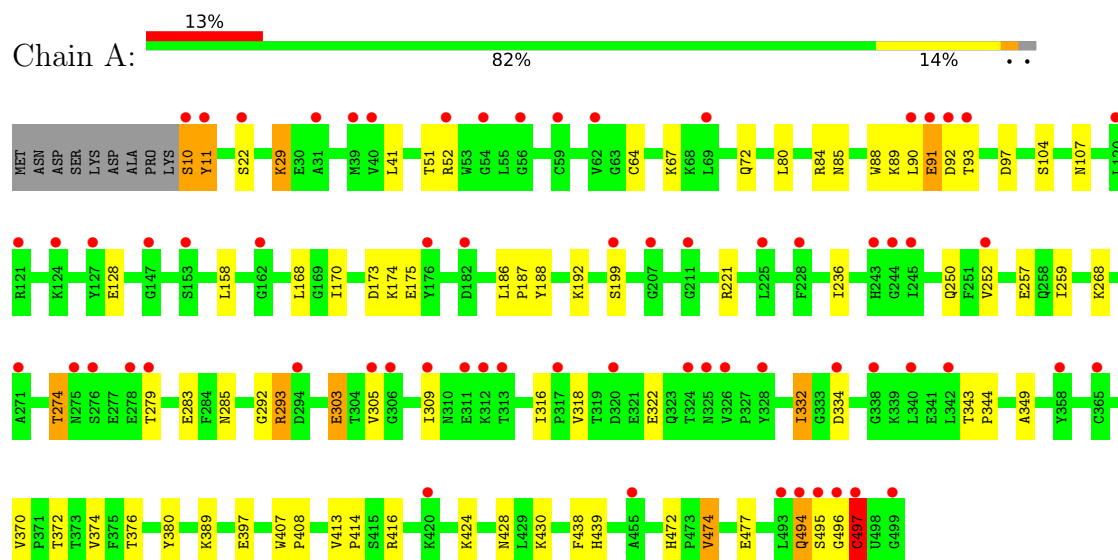
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 4   | B     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 4   | C     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 4   | D     | 35       | Total | O  | 0       | 0       |
|     |       |          | 35    | 35 |         |         |
| 4   | E     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 4   | F     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |

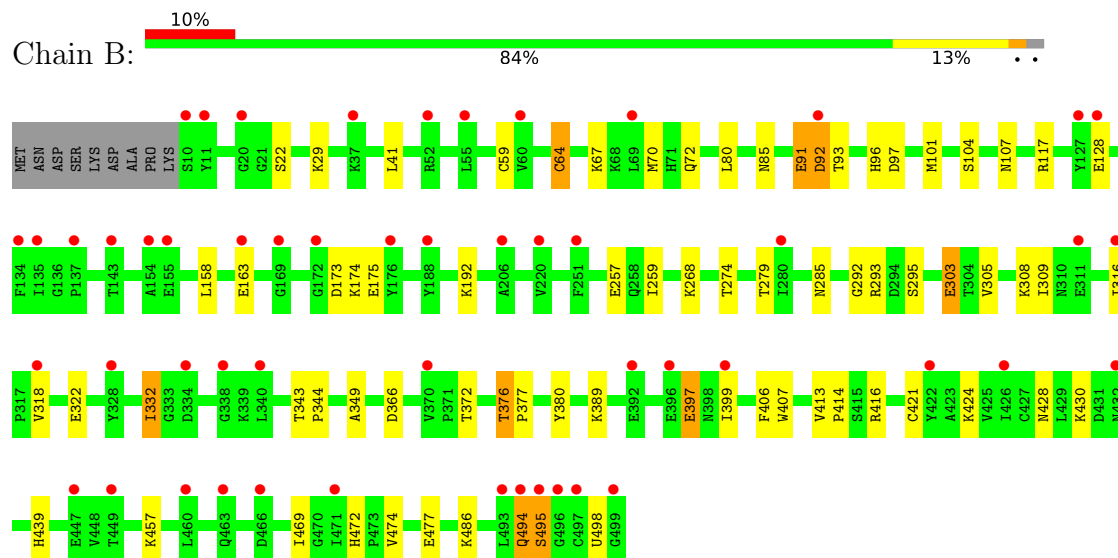
### 3 Residue-property plots [i](#)

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.

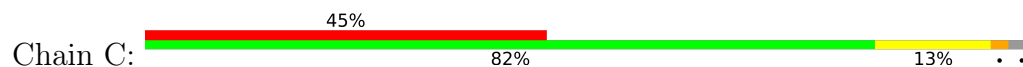
#### • Molecule 1: Thioredoxin reductase 1

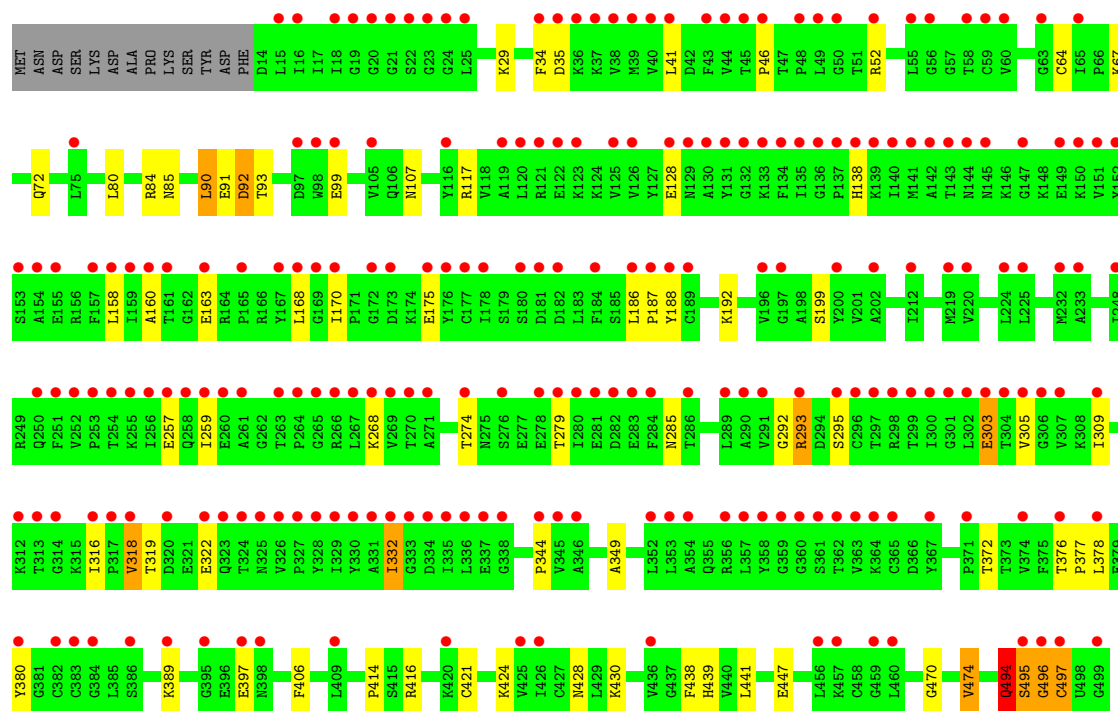


#### • Molecule 1: Thioredoxin reductase 1

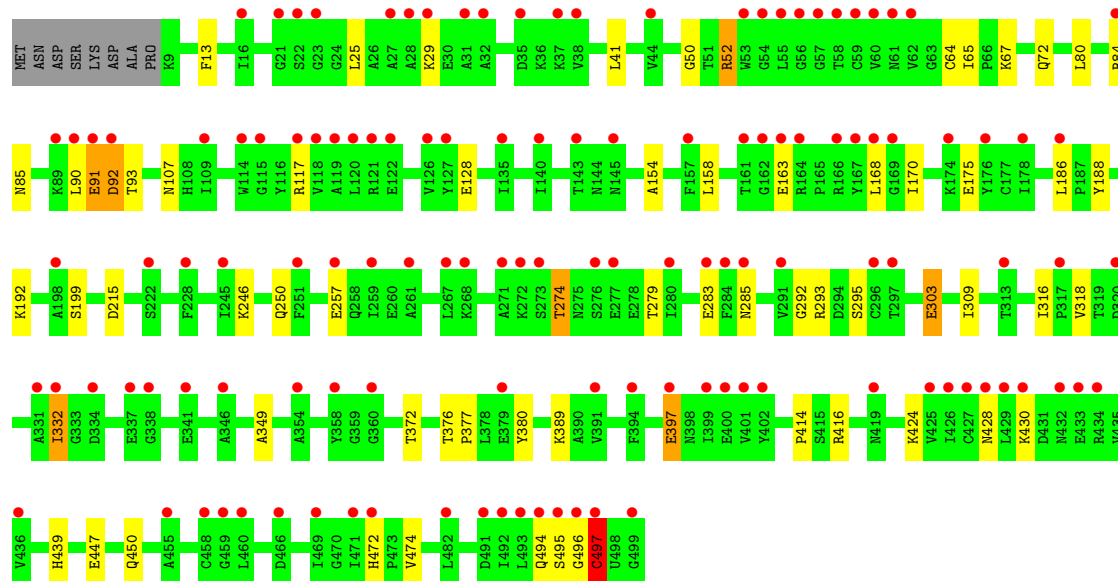
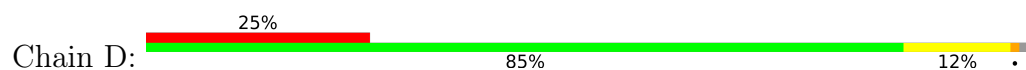


#### • Molecule 1: Thioredoxin reductase 1

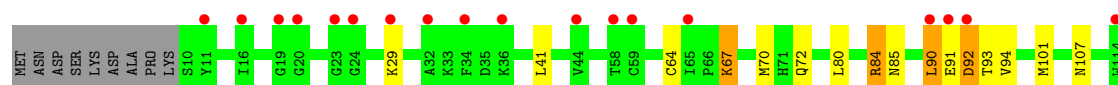
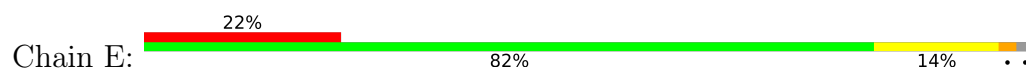


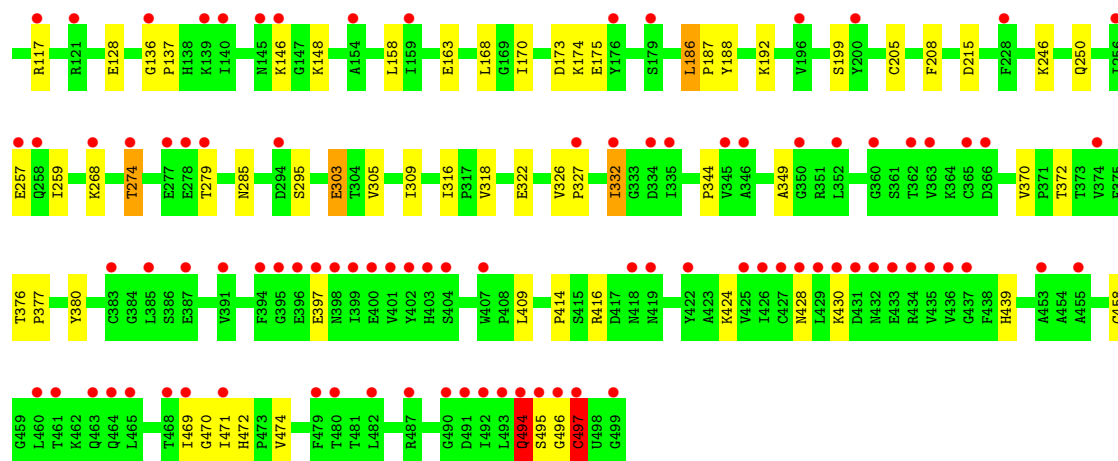


• Molecule 1: Thioredoxin reductase 1

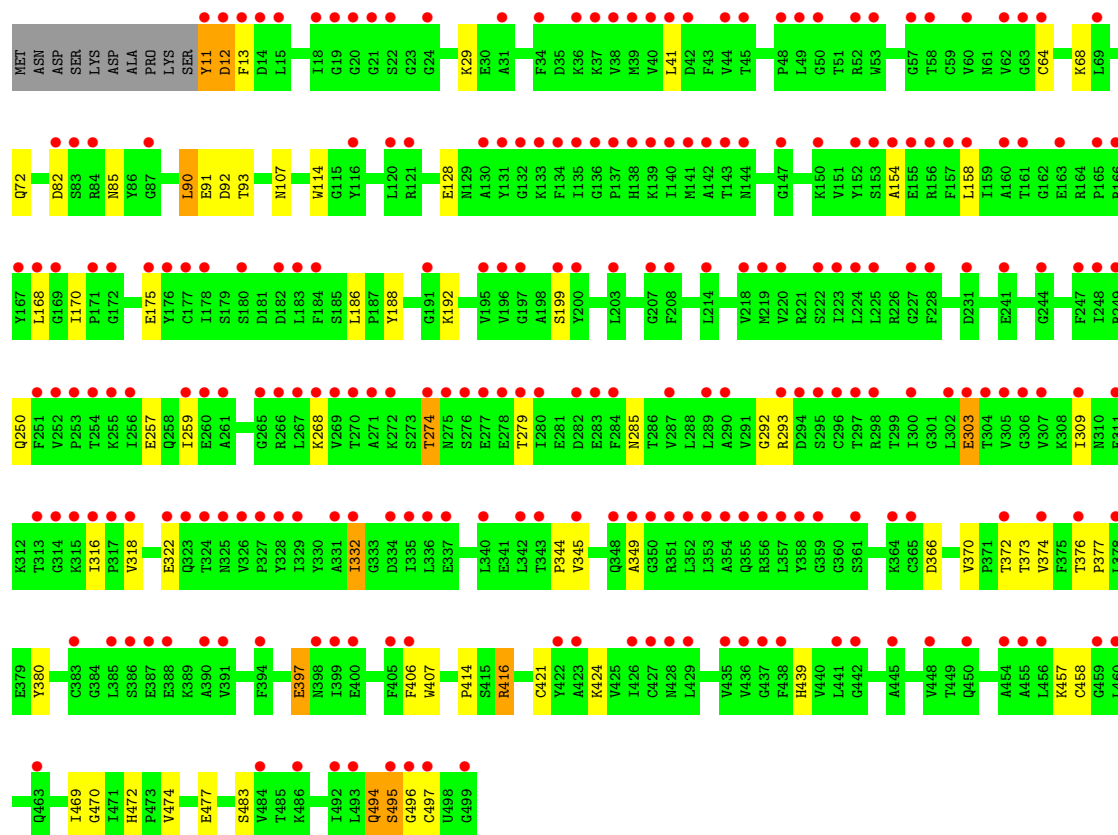
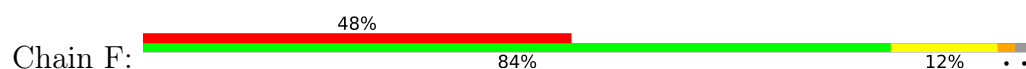


• Molecule 1: Thioredoxin reductase 1





• Molecule 1: Thioredoxin reductase 1





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 78.57Å 140.67Å 171.17Å<br>90.00° 94.50° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 29.74 – 2.75<br>29.74 – 2.75                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (29.74-2.75)<br>99.4 (29.74-2.75)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.52 (at 2.76Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.206 , 0.236<br>0.276 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 55.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.210                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 35.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.88                                                        | EDS              |
| Total number of atoms                                                   | 23214                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 63.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: NAP, FAD, SEC

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     | 0.88         | 0/3835         | 0.96        | 2/5185 (0.0%)   |
| 1   | B     | 0.89         | 1/3835 (0.0%)  | 0.97        | 2/5185 (0.0%)   |
| 1   | C     | 0.80         | 1/3796 (0.0%)  | 0.93        | 4/5132 (0.1%)   |
| 1   | D     | 0.94         | 1/3844 (0.0%)  | 0.96        | 4/5196 (0.1%)   |
| 1   | E     | 0.87         | 0/3835         | 0.96        | 4/5185 (0.1%)   |
| 1   | F     | 0.73         | 3/3829 (0.1%)  | 0.90        | 2/5177 (0.0%)   |
| All | All   | 0.85         | 6/22974 (0.0%) | 0.94        | 18/31060 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | C     | 0                   | 2                   |
| 1   | E     | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 407 | TRP  | C-O   | -6.50 | 1.19        | 1.25     |
| 1   | F     | 11  | TYR  | N-CA  | 6.30  | 1.58        | 1.46     |
| 1   | F     | 11  | TYR  | C-N   | 5.90  | 1.42        | 1.33     |
| 1   | D     | 52  | ARG  | C-O   | -5.65 | 1.16        | 1.23     |
| 1   | C     | 495 | SER  | CA-C  | 5.56  | 1.60        | 1.53     |
| 1   | B     | 407 | TRP  | C-O   | -5.51 | 1.20        | 1.25     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 92  | ASP  | N-CA-C   | 10.69 | 124.27      | 111.33   |
| 1   | E     | 92  | ASP  | N-CA-C   | 10.60 | 124.16      | 111.33   |
| 1   | F     | 92  | ASP  | N-CA-C   | 9.38  | 122.71      | 111.82   |
| 1   | F     | 114 | TRP  | CA-CB-CG | -7.26 | 99.81       | 113.60   |
| 1   | B     | 92  | ASP  | N-CA-C   | 6.68  | 119.57      | 111.82   |
| 1   | E     | 117 | ARG  | N-CA-C   | -6.65 | 104.03      | 111.28   |
| 1   | D     | 92  | ASP  | N-CA-C   | 6.57  | 121.38      | 113.23   |
| 1   | D     | 117 | ARG  | N-CA-C   | -6.17 | 104.64      | 111.36   |
| 1   | D     | 65  | ILE  | CA-C-N   | -5.80 | 113.04      | 119.19   |
| 1   | D     | 65  | ILE  | C-N-CA   | -5.80 | 113.04      | 119.19   |
| 1   | C     | 496 | GLY  | CA-C-N   | 5.77  | 132.09      | 121.70   |
| 1   | C     | 496 | GLY  | C-N-CA   | 5.77  | 132.09      | 121.70   |
| 1   | B     | 117 | ARG  | N-CA-C   | -5.43 | 105.36      | 111.28   |
| 1   | A     | 11  | TYR  | CB-CA-C  | 5.30  | 119.40      | 109.86   |
| 1   | C     | 117 | ARG  | N-CA-C   | -5.30 | 105.51      | 111.28   |
| 1   | E     | 186 | LEU  | CA-C-N   | 5.20  | 125.28      | 119.87   |
| 1   | E     | 186 | LEU  | C-N-CA   | 5.20  | 125.28      | 119.87   |
| 1   | A     | 236 | ILE  | N-CA-C   | -5.13 | 105.49      | 110.42   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 494 | GLN  | Peptide   |
| 1   | C     | 496 | GLY  | Peptide   |
| 1   | E     | 494 | GLN  | Peptide   |
| 1   | F     | 11  | TYR  | Mainchain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3768  | 0        | 3767     | 62      | 0            |
| 1   | B     | 3768  | 0        | 3769     | 53      | 0            |
| 1   | C     | 3731  | 0        | 3740     | 60      | 0            |
| 1   | D     | 3777  | 0        | 3780     | 37      | 0            |
| 1   | E     | 3768  | 0        | 3767     | 57      | 0            |
| 1   | F     | 3762  | 0        | 3762     | 49      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | A     | 53    | 0        | 31       | 1       | 0            |
| 2   | B     | 53    | 0        | 31       | 0       | 0            |
| 2   | C     | 53    | 0        | 31       | 0       | 0            |
| 2   | D     | 53    | 0        | 31       | 0       | 0            |
| 2   | E     | 53    | 0        | 31       | 0       | 0            |
| 2   | F     | 53    | 0        | 31       | 0       | 0            |
| 3   | A     | 32    | 0        | 11       | 1       | 0            |
| 3   | B     | 32    | 0        | 11       | 2       | 0            |
| 3   | C     | 32    | 0        | 11       | 1       | 0            |
| 3   | D     | 32    | 0        | 11       | 1       | 0            |
| 3   | E     | 32    | 0        | 11       | 1       | 0            |
| 3   | F     | 32    | 0        | 11       | 1       | 0            |
| 4   | A     | 23    | 0        | 0        | 2       | 0            |
| 4   | B     | 20    | 0        | 0        | 5       | 0            |
| 4   | C     | 14    | 0        | 0        | 7       | 0            |
| 4   | D     | 35    | 0        | 0        | 0       | 0            |
| 4   | E     | 26    | 0        | 0        | 0       | 0            |
| 4   | F     | 12    | 0        | 0        | 1       | 0            |
| All | All   | 23214 | 0        | 22837    | 288     | 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 6.

All (288) 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:C:192:LYS:H    | 1:C:285:ASN:HD22 | 1.24                     | 0.85              |
| 1:E:496:GLY:N    | 1:E:497:CYS:HB2  | 1.92                     | 0.84              |
| 1:B:380:TYR:OH   | 1:B:439:HIS:HD2  | 1.62                     | 0.83              |
| 1:A:10:SER:O     | 1:A:11:TYR:CG    | 2.35                     | 0.80              |
| 1:B:192:LYS:H    | 1:B:285:ASN:HD22 | 1.28                     | 0.78              |
| 1:E:380:TYR:OH   | 1:E:439:HIS:HD2  | 1.64                     | 0.78              |
| 1:A:192:LYS:H    | 1:A:285:ASN:HD22 | 1.28                     | 0.77              |
| 1:A:10:SER:O     | 1:A:11:TYR:CD1   | 2.38                     | 0.77              |
| 1:E:192:LYS:H    | 1:E:285:ASN:HD22 | 1.30                     | 0.76              |
| 1:C:380:TYR:OH   | 1:C:439:HIS:HD2  | 1.70                     | 0.75              |
| 1:C:494:GLN:HE21 | 1:C:494:GLN:HA   | 1.52                     | 0.74              |
| 1:A:380:TYR:OH   | 1:A:439:HIS:HD2  | 1.71                     | 0.74              |
| 1:A:472:HIS:HB2  | 1:B:344:PRO:HG3  | 1.70                     | 0.73              |
| 1:E:469:ILE:HB   | 1:F:370:VAL:HG13 | 1.70                     | 0.72              |
| 1:D:192:LYS:H    | 1:D:285:ASN:HD22 | 1.38                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:221:ARG:HG3  | 1:A:252:VAL:CG2  | 2.21                     | 0.70              |
| 1:C:84:ARG:HH22  | 1:C:90:LEU:HB3   | 1.57                     | 0.70              |
| 1:C:46:PRO:HB3   | 1:C:52:ARG:NH1   | 2.06                     | 0.69              |
| 1:C:138:HIS:HB3  | 4:C:613:HOH:O    | 1.93                     | 0.69              |
| 1:C:84:ARG:NH2   | 1:C:90:LEU:HB3   | 2.07                     | 0.69              |
| 1:C:90:LEU:HD11  | 1:D:90:LEU:HD11  | 1.75                     | 0.69              |
| 1:A:494:GLN:HB3  | 1:A:495:SER:HA   | 1.76                     | 0.68              |
| 1:D:380:TYR:OH   | 1:D:439:HIS:HD2  | 1.77                     | 0.68              |
| 1:F:192:LYS:H    | 1:F:285:ASN:HD22 | 1.42                     | 0.67              |
| 1:E:72:GLN:HA    | 1:E:72:GLN:NE2   | 2.10                     | 0.67              |
| 1:D:84:ARG:NH2   | 1:D:90:LEU:HB3   | 2.11                     | 0.66              |
| 1:C:494:GLN:HA   | 1:C:494:GLN:NE2  | 2.10                     | 0.66              |
| 1:E:496:GLY:H    | 1:E:497:CYS:CB   | 2.09                     | 0.66              |
| 1:C:494:GLN:HE21 | 1:C:494:GLN:CA   | 2.09                     | 0.65              |
| 1:B:494:GLN:HE21 | 1:B:494:GLN:HA   | 1.61                     | 0.65              |
| 1:E:72:GLN:HA    | 1:E:72:GLN:HE21  | 1.60                     | 0.65              |
| 1:D:50:GLY:O     | 1:D:52:ARG:NH1   | 2.30                     | 0.64              |
| 1:F:494:GLN:HB3  | 1:F:495:SER:HB2  | 1.79                     | 0.64              |
| 1:F:380:TYR:OH   | 1:F:439:HIS:HD2  | 1.80                     | 0.64              |
| 1:A:91:GLU:CD    | 1:A:92:ASP:H     | 2.07                     | 0.63              |
| 1:E:496:GLY:H    | 1:E:497:CYS:HB2  | 1.62                     | 0.63              |
| 1:E:84:ARG:NH2   | 1:E:90:LEU:HB3   | 2.15                     | 0.62              |
| 1:F:494:GLN:HE21 | 1:F:494:GLN:HA   | 1.65                     | 0.61              |
| 1:D:186:LEU:HD11 | 1:D:188:TYR:CZ   | 2.35                     | 0.61              |
| 1:B:486:LYS:CE   | 4:B:603:HOH:O    | 2.47                     | 0.61              |
| 1:C:46:PRO:CG    | 1:C:52:ARG:NH1   | 2.65                     | 0.60              |
| 1:C:158:LEU:HD11 | 1:C:332:ILE:HG12 | 1.82                     | 0.60              |
| 1:E:344:PRO:HG3  | 1:F:472:HIS:HB2  | 1.85                     | 0.59              |
| 1:D:84:ARG:HH22  | 1:D:90:LEU:HB3   | 1.67                     | 0.59              |
| 1:E:84:ARG:HH22  | 1:E:90:LEU:HB3   | 1.68                     | 0.58              |
| 1:A:158:LEU:HD11 | 1:A:332:ILE:HG12 | 1.86                     | 0.58              |
| 1:E:332:ILE:HD12 | 1:E:349:ALA:HB1  | 1.86                     | 0.58              |
| 1:F:85:ASN:HD22  | 1:F:414:PRO:HA   | 1.69                     | 0.57              |
| 1:E:380:TYR:OH   | 1:E:439:HIS:CD2  | 2.54                     | 0.57              |
| 1:C:192:LYS:N    | 1:C:285:ASN:HD22 | 2.00                     | 0.57              |
| 1:A:85:ASN:HD22  | 1:A:414:PRO:HA   | 1.70                     | 0.57              |
| 1:C:46:PRO:CB    | 1:C:52:ARG:NH1   | 2.68                     | 0.56              |
| 1:A:344:PRO:HG3  | 1:B:472:HIS:HB2  | 1.86                     | 0.56              |
| 1:B:332:ILE:HD12 | 1:B:349:ALA:CB   | 2.35                     | 0.56              |
| 1:D:309:ILE:HG22 | 1:D:316:ILE:HG12 | 1.87                     | 0.56              |
| 1:C:344:PRO:HG3  | 1:D:472:HIS:HB2  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:158:LEU:HD11 | 1:F:332:ILE:HG12 | 1.88                     | 0.56              |
| 1:B:332:ILE:HD12 | 1:B:349:ALA:HB1  | 1.86                     | 0.56              |
| 1:E:309:ILE:HG22 | 1:E:316:ILE:HG12 | 1.88                     | 0.55              |
| 1:E:496:GLY:N    | 1:E:497:CYS:CB   | 2.64                     | 0.55              |
| 3:B:601:NAP:H51A | 4:B:612:HOH:O    | 2.05                     | 0.55              |
| 1:F:332:ILE:HD12 | 1:F:349:ALA:HB1  | 1.89                     | 0.55              |
| 1:B:380:TYR:OH   | 1:B:439:HIS:CD2  | 2.51                     | 0.55              |
| 1:C:406:PHE:CZ   | 1:C:421:CYS:HB3  | 2.42                     | 0.55              |
| 1:F:309:ILE:HG22 | 1:F:316:ILE:HG12 | 1.89                     | 0.55              |
| 3:B:601:NAP:C5B  | 4:B:612:HOH:O    | 2.55                     | 0.54              |
| 1:D:158:LEU:HD11 | 1:D:332:ILE:HG12 | 1.89                     | 0.54              |
| 1:A:72:GLN:HA    | 1:A:72:GLN:NE2   | 2.23                     | 0.54              |
| 1:B:486:LYS:HE3  | 4:B:603:HOH:O    | 2.06                     | 0.54              |
| 1:A:221:ARG:HG3  | 1:A:252:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:22:SER:OG    | 1:B:343:THR:HG23 | 2.07                     | 0.54              |
| 1:D:91:GLU:CD    | 1:D:92:ASP:H     | 2.15                     | 0.54              |
| 1:A:84:ARG:NH2   | 1:A:90:LEU:HB3   | 2.23                     | 0.54              |
| 1:D:84:ARG:CZ    | 1:D:84:ARG:HB2   | 2.38                     | 0.54              |
| 1:E:192:LYS:N    | 1:E:285:ASN:HD22 | 2.04                     | 0.54              |
| 1:A:259:ILE:HD11 | 1:A:268:LYS:HB2  | 1.89                     | 0.54              |
| 1:B:332:ILE:CD1  | 1:B:349:ALA:HB1  | 2.37                     | 0.54              |
| 1:C:72:GLN:HA    | 1:C:72:GLN:NE2   | 2.22                     | 0.53              |
| 1:C:138:HIS:CB   | 4:C:613:HOH:O    | 2.55                     | 0.53              |
| 1:D:303:GLU:CD   | 1:D:303:GLU:H    | 2.17                     | 0.53              |
| 1:B:70:MET:HE2   | 1:B:101:MET:HE3  | 1.91                     | 0.53              |
| 1:D:199:SER:HB3  | 3:D:601:NAP:O1N  | 2.09                     | 0.52              |
| 1:F:332:ILE:HD12 | 1:F:349:ALA:CB   | 2.39                     | 0.52              |
| 1:E:332:ILE:HD12 | 1:E:349:ALA:CB   | 2.39                     | 0.52              |
| 1:E:85:ASN:HD22  | 1:E:414:PRO:HA   | 1.74                     | 0.52              |
| 1:A:29:LYS:NZ    | 1:B:498:SEC:SE   | 2.93                     | 0.52              |
| 1:C:72:GLN:HA    | 1:C:72:GLN:HE21  | 1.75                     | 0.52              |
| 1:C:380:TYR:OH   | 1:C:439:HIS:CD2  | 2.57                     | 0.52              |
| 1:C:428:ASN:ND2  | 1:C:430:LYS:H    | 2.07                     | 0.52              |
| 1:B:308:LYS:HD2  | 4:B:614:HOH:O    | 2.09                     | 0.51              |
| 1:B:259:ILE:HD11 | 1:B:268:LYS:HB2  | 1.92                     | 0.51              |
| 1:F:72:GLN:NE2   | 1:F:72:GLN:HA    | 2.25                     | 0.51              |
| 1:A:168:LEU:HB2  | 1:A:170:ILE:HG12 | 1.92                     | 0.51              |
| 1:C:199:SER:HB3  | 3:C:601:NAP:O1N  | 2.10                     | 0.51              |
| 1:A:380:TYR:OH   | 1:A:439:HIS:CD2  | 2.60                     | 0.51              |
| 1:D:496:GLY:N    | 1:D:497:CYS:HB2  | 2.25                     | 0.51              |
| 1:C:84:ARG:HB2   | 1:C:84:ARG:CZ    | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:494:GLN:HE21 | 1:F:494:GLN:CA   | 2.23                     | 0.51              |
| 1:A:374:VAL:HG12 | 1:A:376:THR:HG23 | 1.93                     | 0.51              |
| 1:E:332:ILE:CD1  | 1:E:349:ALA:HB1  | 2.40                     | 0.51              |
| 1:A:89:LYS:HE3   | 1:B:97:ASP:HB2   | 1.93                     | 0.51              |
| 1:C:46:PRO:HG3   | 1:C:52:ARG:NH1   | 2.26                     | 0.51              |
| 1:B:59:CYS:CB    | 1:B:64:CYS:HG    | 2.23                     | 0.50              |
| 1:E:303:GLU:CD   | 1:E:303:GLU:H    | 2.19                     | 0.50              |
| 1:F:494:GLN:HB3  | 1:F:495:SER:CB   | 2.41                     | 0.50              |
| 1:F:13:PHE:O     | 1:F:154:ALA:HA   | 2.11                     | 0.50              |
| 1:C:309:ILE:HG22 | 1:C:316:ILE:HG12 | 1.94                     | 0.50              |
| 1:E:70:MET:HE2   | 1:E:101:MET:HE3  | 1.92                     | 0.50              |
| 1:F:406:PHE:CZ   | 1:F:421:CYS:HB3  | 2.47                     | 0.50              |
| 1:B:72:GLN:HA    | 1:B:72:GLN:NE2   | 2.26                     | 0.50              |
| 1:C:259:ILE:HD11 | 1:C:268:LYS:HB2  | 1.93                     | 0.50              |
| 1:A:84:ARG:HB2   | 1:A:84:ARG:CZ    | 2.41                     | 0.49              |
| 1:B:91:GLU:CD    | 1:B:92:ASP:H     | 2.20                     | 0.49              |
| 1:A:104:SER:HB3  | 1:B:413:VAL:HG13 | 1.94                     | 0.49              |
| 1:E:163:GLU:HG2  | 1:E:295:SER:HA   | 1.94                     | 0.49              |
| 1:B:494:GLN:HE21 | 1:B:494:GLN:CA   | 2.24                     | 0.49              |
| 1:F:374:VAL:HG12 | 1:F:376:THR:HG23 | 1.94                     | 0.49              |
| 1:F:494:GLN:HA   | 1:F:494:GLN:NE2  | 2.26                     | 0.49              |
| 1:A:41:LEU:HD23  | 1:A:128:GLU:HB3  | 1.95                     | 0.49              |
| 1:B:85:ASN:HD22  | 1:B:414:PRO:HA   | 1.77                     | 0.49              |
| 1:A:303:GLU:CD   | 1:A:303:GLU:H    | 2.21                     | 0.48              |
| 1:F:72:GLN:HA    | 1:F:72:GLN:HE21  | 1.78                     | 0.48              |
| 1:B:366:ASP:OD2  | 1:B:457:LYS:HE3  | 2.13                     | 0.48              |
| 1:D:13:PHE:O     | 1:D:154:ALA:HA   | 2.14                     | 0.48              |
| 1:D:85:ASN:HD22  | 1:D:414:PRO:HA   | 1.78                     | 0.48              |
| 1:C:186:LEU:HD11 | 1:C:188:TYR:CZ   | 2.48                     | 0.47              |
| 1:B:292:GLY:C    | 1:B:293:ARG:HG2  | 2.39                     | 0.47              |
| 1:B:474:VAL:O    | 1:B:477:GLU:HG2  | 2.14                     | 0.47              |
| 1:F:168:LEU:HB2  | 1:F:170:ILE:HG12 | 1.95                     | 0.47              |
| 1:A:67:LYS:HE2   | 1:A:67:LYS:HB3   | 1.75                     | 0.47              |
| 1:A:428:ASN:ND2  | 1:A:430:LYS:H    | 2.13                     | 0.47              |
| 1:F:41:LEU:HD23  | 1:F:128:GLU:HB3  | 1.95                     | 0.47              |
| 1:C:168:LEU:HB2  | 1:C:170:ILE:HG12 | 1.97                     | 0.47              |
| 1:D:292:GLY:C    | 1:D:293:ARG:HG2  | 2.40                     | 0.47              |
| 1:E:471:ILE:HG21 | 1:F:373:THR:OG1  | 2.14                     | 0.47              |
| 1:A:199:SER:HB3  | 3:A:601:NAP:O1N  | 2.15                     | 0.46              |
| 1:D:332:ILE:HD12 | 1:D:349:ALA:HB1  | 1.97                     | 0.46              |
| 1:A:494:GLN:HE21 | 1:A:494:GLN:N    | 2.13                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:46:PRO:CG    | 1:C:52:ARG:HH12  | 2.28                     | 0.46              |
| 1:C:41:LEU:HD23  | 1:C:128:GLU:HB3  | 1.98                     | 0.46              |
| 1:B:332:ILE:HD13 | 1:B:332:ILE:HA   | 1.70                     | 0.46              |
| 1:B:376:THR:O    | 1:B:377:PRO:C    | 2.59                     | 0.46              |
| 1:D:84:ARG:NH2   | 1:D:84:ARG:HB2   | 2.31                     | 0.46              |
| 1:F:474:VAL:O    | 1:F:477:GLU:HG2  | 2.16                     | 0.46              |
| 1:D:376:THR:O    | 1:D:377:PRO:C    | 2.57                     | 0.46              |
| 1:F:332:ILE:CD1  | 1:F:349:ALA:HB1  | 2.45                     | 0.46              |
| 1:A:22:SER:OG    | 1:A:343:THR:HG23 | 2.16                     | 0.46              |
| 1:A:332:ILE:HD12 | 1:A:349:ALA:HB1  | 1.97                     | 0.46              |
| 1:B:158:LEU:HD11 | 1:B:332:ILE:HG12 | 1.98                     | 0.46              |
| 1:D:72:GLN:HA    | 1:D:72:GLN:NE2   | 2.31                     | 0.46              |
| 1:C:332:ILE:HD12 | 1:C:349:ALA:HB1  | 1.98                     | 0.46              |
| 1:D:72:GLN:HA    | 1:D:72:GLN:HE21  | 1.79                     | 0.46              |
| 1:C:35:ASP:CB    | 4:C:614:HOH:O    | 2.63                     | 0.46              |
| 1:A:413:VAL:HG13 | 1:B:104:SER:HB3  | 1.98                     | 0.45              |
| 1:B:91:GLU:CD    | 1:B:92:ASP:N     | 2.74                     | 0.45              |
| 1:D:250:GLN:HB3  | 1:D:274:THR:HB   | 1.97                     | 0.45              |
| 1:D:397:GLU:O    | 1:D:397:GLU:HG2  | 2.16                     | 0.45              |
| 1:E:322:GLU:HG2  | 1:E:332:ILE:CD1  | 2.46                     | 0.45              |
| 1:E:496:GLY:H    | 1:E:497:CYS:HB3  | 1.80                     | 0.45              |
| 1:A:370:VAL:HG13 | 1:B:469:ILE:HB   | 1.99                     | 0.45              |
| 1:B:67:LYS:HB3   | 1:B:67:LYS:HE2   | 1.82                     | 0.45              |
| 1:E:158:LEU:HD11 | 1:E:332:ILE:HG12 | 1.97                     | 0.45              |
| 1:F:250:GLN:HB3  | 1:F:274:THR:HB   | 1.98                     | 0.45              |
| 1:B:322:GLU:HG2  | 1:B:332:ILE:HD13 | 1.98                     | 0.45              |
| 1:C:67:LYS:HB3   | 1:C:67:LYS:HE2   | 1.67                     | 0.45              |
| 1:C:160:ALA:HB1  | 4:C:605:HOH:O    | 2.16                     | 0.45              |
| 1:A:84:ARG:HH22  | 1:A:90:LEU:HB3   | 1.79                     | 0.45              |
| 1:B:406:PHE:CZ   | 1:B:421:CYS:HB3  | 2.51                     | 0.45              |
| 1:A:80:LEU:HD23  | 1:B:80:LEU:HD23  | 1.99                     | 0.45              |
| 1:B:309:ILE:HG22 | 1:B:316:ILE:HG12 | 1.98                     | 0.45              |
| 1:C:34:PHE:C     | 4:C:614:HOH:O    | 2.60                     | 0.45              |
| 1:E:322:GLU:HG2  | 1:E:332:ILE:HD13 | 1.98                     | 0.45              |
| 1:A:332:ILE:HD12 | 1:A:349:ALA:CB   | 2.46                     | 0.45              |
| 1:B:173:ASP:OD1  | 1:B:174:LYS:N    | 2.50                     | 0.45              |
| 1:B:494:GLN:HB3  | 1:B:495:SER:HA   | 1.99                     | 0.45              |
| 1:E:84:ARG:HB2   | 1:E:84:ARG:CZ    | 2.47                     | 0.44              |
| 1:B:163:GLU:HG2  | 1:B:295:SER:HA   | 2.00                     | 0.44              |
| 1:E:205:CYS:HA   | 1:E:208:PHE:CE2  | 2.52                     | 0.44              |
| 1:E:332:ILE:HD13 | 1:E:332:ILE:HA   | 1.70                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:376:THR:O    | 1:E:377:PRO:C    | 2.59                     | 0.44              |
| 1:A:91:GLU:CD    | 1:A:92:ASP:N     | 2.74                     | 0.44              |
| 1:A:186:LEU:HD11 | 1:A:188:TYR:CZ   | 2.53                     | 0.44              |
| 1:A:389:LYS:HD2  | 1:A:389:LYS:HA   | 1.82                     | 0.44              |
| 1:E:173:ASP:OD1  | 1:E:174:LYS:N    | 2.51                     | 0.44              |
| 1:E:250:GLN:HB3  | 1:E:274:THR:HB   | 1.99                     | 0.44              |
| 1:E:494:GLN:HB3  | 1:E:495:SER:HA   | 2.00                     | 0.44              |
| 1:B:303:GLU:H    | 1:B:303:GLU:CD   | 2.25                     | 0.44              |
| 1:C:99:GLU:OE1   | 1:E:148:LYS:HE3  | 2.18                     | 0.44              |
| 1:B:322:GLU:HG2  | 1:B:332:ILE:CD1  | 2.47                     | 0.44              |
| 1:C:303:GLU:CD   | 1:C:303:GLU:H    | 2.24                     | 0.43              |
| 1:C:322:GLU:HG2  | 1:C:332:ILE:CD1  | 2.48                     | 0.43              |
| 1:D:168:LEU:HB2  | 1:D:170:ILE:HG12 | 2.00                     | 0.43              |
| 1:E:67:LYS:HB3   | 1:E:67:LYS:HE2   | 1.67                     | 0.43              |
| 1:E:469:ILE:HG21 | 1:F:345:VAL:HG23 | 1.99                     | 0.43              |
| 1:A:84:ARG:NH2   | 1:A:84:ARG:HB2   | 2.33                     | 0.43              |
| 1:B:41:LEU:HD23  | 1:B:128:GLU:HB3  | 2.00                     | 0.43              |
| 1:E:458:CYS:HB2  | 1:F:458:CYS:HB2  | 2.01                     | 0.43              |
| 1:A:173:ASP:OD1  | 1:A:174:LYS:N    | 2.51                     | 0.43              |
| 1:C:187:PRO:HB3  | 1:E:146:LYS:NZ   | 2.34                     | 0.43              |
| 1:E:370:VAL:HG13 | 1:F:469:ILE:HB   | 2.00                     | 0.43              |
| 1:E:469:ILE:CB   | 1:F:370:VAL:HG13 | 2.44                     | 0.43              |
| 1:F:186:LEU:HD11 | 1:F:188:TYR:CZ   | 2.52                     | 0.43              |
| 1:A:72:GLN:HA    | 1:A:72:GLN:HE21  | 1.81                     | 0.43              |
| 1:A:494:GLN:HB3  | 1:A:495:SER:CA   | 2.44                     | 0.43              |
| 1:B:72:GLN:HA    | 1:B:72:GLN:HE21  | 1.83                     | 0.43              |
| 1:B:389:LYS:HD2  | 1:B:389:LYS:HA   | 1.78                     | 0.43              |
| 1:C:292:GLY:C    | 1:C:293:ARG:HG2  | 2.42                     | 0.43              |
| 1:E:428:ASN:ND2  | 1:E:430:LYS:H    | 2.16                     | 0.43              |
| 1:F:292:GLY:C    | 1:F:293:ARG:HG2  | 2.43                     | 0.43              |
| 1:A:250:GLN:HB3  | 1:A:274:THR:HB   | 2.01                     | 0.43              |
| 1:C:85:ASN:HD22  | 1:C:414:PRO:HA   | 1.83                     | 0.43              |
| 1:C:318:VAL:HG13 | 1:C:319:THR:O    | 2.19                     | 0.43              |
| 1:C:428:ASN:C    | 1:C:428:ASN:HD22 | 2.25                     | 0.43              |
| 1:F:199:SER:HB3  | 3:F:601:NAP:O1N  | 2.19                     | 0.43              |
| 1:F:397:GLU:O    | 1:F:397:GLU:HG2  | 2.17                     | 0.43              |
| 1:C:80:LEU:HD23  | 1:D:80:LEU:HD23  | 2.00                     | 0.43              |
| 1:C:186:LEU:HA   | 1:C:187:PRO:HD3  | 1.80                     | 0.43              |
| 1:D:41:LEU:HD23  | 1:D:128:GLU:HB3  | 1.99                     | 0.43              |
| 1:D:428:ASN:ND2  | 1:D:430:LYS:H    | 2.16                     | 0.43              |
| 1:E:472:HIS:HB2  | 1:F:344:PRO:HG3  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:303:GLU:CD   | 1:F:303:GLU:H    | 2.26                     | 0.43              |
| 1:F:322:GLU:HG2  | 1:F:332:ILE:HD13 | 2.00                     | 0.43              |
| 1:C:35:ASP:HB2   | 4:C:614:HOH:O    | 2.19                     | 0.43              |
| 1:F:259:ILE:HD11 | 1:F:268:LYS:HB2  | 2.01                     | 0.43              |
| 1:A:283:GLU:HG3  | 4:A:620:HOH:O    | 2.18                     | 0.43              |
| 1:C:138:HIS:CG   | 4:C:613:HOH:O    | 2.71                     | 0.43              |
| 1:A:309:ILE:HG22 | 1:A:316:ILE:HG12 | 2.01                     | 0.43              |
| 1:D:25:LEU:HD23  | 1:D:25:LEU:HA    | 1.88                     | 0.43              |
| 1:A:438:PHE:CD2  | 1:A:438:PHE:C    | 2.97                     | 0.42              |
| 1:D:163:GLU:HG2  | 1:D:295:SER:HA   | 2.01                     | 0.42              |
| 1:E:90:LEU:HD11  | 1:F:90:LEU:HD11  | 2.01                     | 0.42              |
| 1:C:474:VAL:HG13 | 1:D:447:GLU:CD   | 2.43                     | 0.42              |
| 1:A:292:GLY:C    | 1:A:293:ARG:HG2  | 2.44                     | 0.42              |
| 1:C:163:GLU:HG2  | 1:C:295:SER:HA   | 2.01                     | 0.42              |
| 1:E:41:LEU:HD23  | 1:E:128:GLU:HB3  | 2.02                     | 0.42              |
| 1:F:483:SER:N    | 4:F:606:HOH:O    | 2.50                     | 0.42              |
| 1:F:496:GLY:N    | 1:F:497:CYS:HB3  | 2.34                     | 0.42              |
| 1:A:97:ASP:OD1   | 1:A:97:ASP:C     | 2.62                     | 0.42              |
| 1:A:322:GLU:HG2  | 1:A:332:ILE:CD1  | 2.50                     | 0.42              |
| 1:C:376:THR:O    | 1:C:377:PRO:C    | 2.60                     | 0.42              |
| 1:C:389:LYS:HD2  | 1:C:389:LYS:HA   | 1.82                     | 0.42              |
| 1:E:470:GLY:O    | 1:F:344:PRO:HG2  | 2.20                     | 0.42              |
| 1:B:428:ASN:ND2  | 1:B:430:LYS:H    | 2.18                     | 0.42              |
| 1:C:322:GLU:HG2  | 1:C:332:ILE:HD13 | 2.01                     | 0.42              |
| 1:E:215:ASP:OD1  | 1:E:246:LYS:NZ   | 2.52                     | 0.42              |
| 1:C:332:ILE:HD13 | 1:C:332:ILE:HA   | 1.76                     | 0.42              |
| 1:E:186:LEU:HA   | 1:E:187:PRO:HD3  | 1.73                     | 0.42              |
| 1:A:332:ILE:CD1  | 1:A:349:ALA:HB1  | 2.50                     | 0.41              |
| 1:E:199:SER:HB3  | 3:E:601:NAP:O1N  | 2.20                     | 0.41              |
| 1:F:366:ASP:OD2  | 1:F:457:LYS:HE3  | 2.20                     | 0.41              |
| 1:F:376:THR:O    | 1:F:377:PRO:C    | 2.62                     | 0.41              |
| 1:E:259:ILE:HD11 | 1:E:268:LYS:HB2  | 2.02                     | 0.41              |
| 1:A:407:TRP:O    | 1:A:408:PRO:C    | 2.62                     | 0.41              |
| 1:C:378:LEU:CD2  | 1:C:441:LEU:HG   | 2.50                     | 0.41              |
| 1:E:326:VAL:HA   | 1:E:327:PRO:HD3  | 1.93                     | 0.41              |
| 1:E:168:LEU:HB2  | 1:E:170:ILE:HG12 | 2.03                     | 0.41              |
| 1:A:186:LEU:HA   | 1:A:187:PRO:HD3  | 1.81                     | 0.41              |
| 1:B:380:TYR:HH   | 1:B:439:HIS:HD2  | 1.62                     | 0.41              |
| 1:C:46:PRO:CB    | 1:C:52:ARG:HH12  | 2.32                     | 0.41              |
| 1:A:51:THR:HA    | 4:A:611:HOH:O    | 2.19                     | 0.41              |
| 1:B:397:GLU:O    | 1:B:397:GLU:HG2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:215:ASP:OD1  | 1:D:246:LYS:NZ   | 2.53                     | 0.41              |
| 1:D:389:LYS:HD2  | 1:D:389:LYS:HA   | 1.82                     | 0.41              |
| 1:E:136:GLY:O    | 1:E:137:PRO:C    | 2.62                     | 0.41              |
| 1:E:409:LEU:HD23 | 1:F:68:LYS:HG2   | 2.02                     | 0.41              |
| 1:E:186:LEU:HD11 | 1:E:188:TYR:CZ   | 2.55                     | 0.41              |
| 1:A:29:LYS:HZ3   | 1:B:498:SEC:SE   | 2.53                     | 0.41              |
| 1:C:332:ILE:HD12 | 1:C:349:ALA:CB   | 2.50                     | 0.41              |
| 1:A:29:LYS:HZ2   | 1:B:498:SEC:SE   | 2.54                     | 0.41              |
| 1:A:80:LEU:CD2   | 1:B:80:LEU:HD23  | 2.51                     | 0.41              |
| 1:A:496:GLY:H    | 1:A:497:CYS:HB3  | 1.85                     | 0.41              |
| 1:F:12:ASP:HB3   | 1:F:13:PHE:CD2   | 2.56                     | 0.40              |
| 1:A:88:TRP:CZ3   | 1:B:96:HIS:HB2   | 2.56                     | 0.40              |
| 1:A:474:VAL:O    | 1:A:477:GLU:HG2  | 2.22                     | 0.40              |
| 1:C:46:PRO:HG3   | 1:C:52:ARG:CZ    | 2.50                     | 0.40              |
| 1:C:447:GLU:CD   | 1:D:474:VAL:HG13 | 2.46                     | 0.40              |
| 1:C:470:GLY:HA2  | 1:D:450:GLN:OE1  | 2.21                     | 0.40              |
| 1:F:322:GLU:HG2  | 1:F:332:ILE:CD1  | 2.51                     | 0.40              |
| 1:A:259:ILE:CD1  | 1:A:268:LYS:HB2  | 2.51                     | 0.40              |
| 1:E:344:PRO:HG2  | 1:F:470:GLY:O    | 2.21                     | 0.40              |
| 1:A:322:GLU:HG2  | 1:A:332:ILE:HD13 | 2.02                     | 0.40              |
| 1:B:399:ILE:HD13 | 1:B:399:ILE:HA   | 1.91                     | 0.40              |
| 1:D:91:GLU:CD    | 1:D:92:ASP:N     | 2.80                     | 0.40              |
| 1:A:334:ASP:CG   | 2:A:600:FAD:HO3' | 2.29                     | 0.40              |
| 1:C:438:PHE:CD2  | 1:C:438:PHE:C    | 2.99                     | 0.40              |
| 1:E:80:LEU:HD13  | 1:E:94:VAL:HG21  | 2.04                     | 0.40              |
| 1:F:82:ASP:OD2   | 1:F:416:ARG:NH1  | 2.55                     | 0.40              |
| 1:F:332:ILE:HD13 | 1:F:332:ILE:HA   | 1.81                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 487/499 (98%)   | 460 (94%)  | 26 (5%)  | 1 (0%)   | 43          | 64  |
| 1   | B     | 487/499 (98%)   | 463 (95%)  | 24 (5%)  | 0        | 100         | 100 |
| 1   | C     | 483/499 (97%)   | 456 (94%)  | 26 (5%)  | 1 (0%)   | 43          | 64  |
| 1   | D     | 488/499 (98%)   | 461 (94%)  | 26 (5%)  | 1 (0%)   | 43          | 64  |
| 1   | E     | 487/499 (98%)   | 462 (95%)  | 24 (5%)  | 1 (0%)   | 43          | 64  |
| 1   | F     | 486/499 (97%)   | 461 (95%)  | 25 (5%)  | 0        | 100         | 100 |
| All | All   | 2918/2994 (98%) | 2763 (95%) | 151 (5%) | 4 (0%)   | 48          | 71  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 497 | CYS  |
| 1   | D     | 497 | CYS  |
| 1   | E     | 497 | CYS  |
| 1   | A     | 497 | CYS  |

### 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     | 405/413 (98%)   | 382 (94%)  | 23 (6%)  | 18          | 35 |
| 1   | B     | 405/413 (98%)   | 385 (95%)  | 20 (5%)  | 22          | 43 |
| 1   | C     | 401/413 (97%)   | 377 (94%)  | 24 (6%)  | 17          | 32 |
| 1   | D     | 406/413 (98%)   | 385 (95%)  | 21 (5%)  | 21          | 39 |
| 1   | E     | 405/413 (98%)   | 381 (94%)  | 24 (6%)  | 18          | 33 |
| 1   | F     | 404/413 (98%)   | 384 (95%)  | 20 (5%)  | 22          | 42 |
| All | All   | 2426/2478 (98%) | 2294 (95%) | 132 (5%) | 20          | 38 |

All (132) residues with a non-rotameric sidechain are listed below:

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

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | LYS  |
| 1   | A     | 52  | ARG  |
| 1   | A     | 64  | CYS  |
| 1   | A     | 91  | GLU  |
| 1   | A     | 93  | THR  |
| 1   | A     | 107 | ASN  |
| 1   | A     | 175 | GLU  |
| 1   | A     | 257 | GLU  |
| 1   | A     | 274 | THR  |
| 1   | A     | 279 | THR  |
| 1   | A     | 293 | ARG  |
| 1   | A     | 303 | GLU  |
| 1   | A     | 305 | VAL  |
| 1   | A     | 318 | VAL  |
| 1   | A     | 332 | ILE  |
| 1   | A     | 372 | THR  |
| 1   | A     | 397 | GLU  |
| 1   | A     | 416 | ARG  |
| 1   | A     | 424 | LYS  |
| 1   | A     | 474 | VAL  |
| 1   | A     | 494 | GLN  |
| 1   | A     | 497 | CYS  |
| 1   | B     | 29  | LYS  |
| 1   | B     | 64  | CYS  |
| 1   | B     | 91  | GLU  |
| 1   | B     | 93  | THR  |
| 1   | B     | 107 | ASN  |
| 1   | B     | 175 | GLU  |
| 1   | B     | 257 | GLU  |
| 1   | B     | 274 | THR  |
| 1   | B     | 279 | THR  |
| 1   | B     | 303 | GLU  |
| 1   | B     | 305 | VAL  |
| 1   | B     | 318 | VAL  |
| 1   | B     | 332 | ILE  |
| 1   | B     | 372 | THR  |
| 1   | B     | 376 | THR  |
| 1   | B     | 397 | GLU  |
| 1   | B     | 416 | ARG  |
| 1   | B     | 424 | LYS  |
| 1   | B     | 494 | GLN  |
| 1   | B     | 495 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 29  | LYS  |
| 1   | C     | 64  | CYS  |
| 1   | C     | 90  | LEU  |
| 1   | C     | 91  | GLU  |
| 1   | C     | 92  | ASP  |
| 1   | C     | 93  | THR  |
| 1   | C     | 107 | ASN  |
| 1   | C     | 175 | GLU  |
| 1   | C     | 257 | GLU  |
| 1   | C     | 274 | THR  |
| 1   | C     | 279 | THR  |
| 1   | C     | 293 | ARG  |
| 1   | C     | 303 | GLU  |
| 1   | C     | 305 | VAL  |
| 1   | C     | 318 | VAL  |
| 1   | C     | 332 | ILE  |
| 1   | C     | 372 | THR  |
| 1   | C     | 397 | GLU  |
| 1   | C     | 416 | ARG  |
| 1   | C     | 424 | LYS  |
| 1   | C     | 474 | VAL  |
| 1   | C     | 494 | GLN  |
| 1   | C     | 495 | SER  |
| 1   | C     | 497 | CYS  |
| 1   | D     | 29  | LYS  |
| 1   | D     | 64  | CYS  |
| 1   | D     | 67  | LYS  |
| 1   | D     | 91  | GLU  |
| 1   | D     | 93  | THR  |
| 1   | D     | 107 | ASN  |
| 1   | D     | 175 | GLU  |
| 1   | D     | 257 | GLU  |
| 1   | D     | 274 | THR  |
| 1   | D     | 279 | THR  |
| 1   | D     | 283 | GLU  |
| 1   | D     | 303 | GLU  |
| 1   | D     | 318 | VAL  |
| 1   | D     | 332 | ILE  |
| 1   | D     | 372 | THR  |
| 1   | D     | 397 | GLU  |
| 1   | D     | 416 | ARG  |
| 1   | D     | 424 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 494 | GLN  |
| 1   | D     | 495 | SER  |
| 1   | D     | 497 | CYS  |
| 1   | E     | 29  | LYS  |
| 1   | E     | 64  | CYS  |
| 1   | E     | 67  | LYS  |
| 1   | E     | 84  | ARG  |
| 1   | E     | 90  | LEU  |
| 1   | E     | 91  | GLU  |
| 1   | E     | 92  | ASP  |
| 1   | E     | 93  | THR  |
| 1   | E     | 107 | ASN  |
| 1   | E     | 175 | GLU  |
| 1   | E     | 257 | GLU  |
| 1   | E     | 274 | THR  |
| 1   | E     | 279 | THR  |
| 1   | E     | 303 | GLU  |
| 1   | E     | 305 | VAL  |
| 1   | E     | 318 | VAL  |
| 1   | E     | 332 | ILE  |
| 1   | E     | 372 | THR  |
| 1   | E     | 397 | GLU  |
| 1   | E     | 416 | ARG  |
| 1   | E     | 424 | LYS  |
| 1   | E     | 474 | VAL  |
| 1   | E     | 494 | GLN  |
| 1   | E     | 497 | CYS  |
| 1   | F     | 12  | ASP  |
| 1   | F     | 29  | LYS  |
| 1   | F     | 64  | CYS  |
| 1   | F     | 90  | LEU  |
| 1   | F     | 91  | GLU  |
| 1   | F     | 93  | THR  |
| 1   | F     | 107 | ASN  |
| 1   | F     | 175 | GLU  |
| 1   | F     | 257 | GLU  |
| 1   | F     | 274 | THR  |
| 1   | F     | 279 | THR  |
| 1   | F     | 303 | GLU  |
| 1   | F     | 318 | VAL  |
| 1   | F     | 332 | ILE  |
| 1   | F     | 372 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 397 | GLU  |
| 1   | F     | 416 | ARG  |
| 1   | F     | 424 | LYS  |
| 1   | F     | 494 | GLN  |
| 1   | F     | 495 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 61  | ASN  |
| 1   | A     | 72  | GLN  |
| 1   | A     | 113 | ASN  |
| 1   | A     | 258 | GLN  |
| 1   | A     | 285 | ASN  |
| 1   | A     | 355 | GLN  |
| 1   | A     | 428 | ASN  |
| 1   | A     | 439 | HIS  |
| 1   | A     | 494 | GLN  |
| 1   | B     | 61  | ASN  |
| 1   | B     | 72  | GLN  |
| 1   | B     | 106 | GLN  |
| 1   | B     | 113 | ASN  |
| 1   | B     | 129 | ASN  |
| 1   | B     | 258 | GLN  |
| 1   | B     | 285 | ASN  |
| 1   | B     | 428 | ASN  |
| 1   | B     | 439 | HIS  |
| 1   | B     | 494 | GLN  |
| 1   | C     | 72  | GLN  |
| 1   | C     | 113 | ASN  |
| 1   | C     | 285 | ASN  |
| 1   | C     | 428 | ASN  |
| 1   | C     | 439 | HIS  |
| 1   | C     | 494 | GLN  |
| 1   | D     | 61  | ASN  |
| 1   | D     | 72  | GLN  |
| 1   | D     | 113 | ASN  |
| 1   | D     | 258 | GLN  |
| 1   | D     | 285 | ASN  |
| 1   | D     | 355 | GLN  |
| 1   | D     | 428 | ASN  |
| 1   | D     | 439 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 72  | GLN  |
| 1   | E     | 96  | HIS  |
| 1   | E     | 113 | ASN  |
| 1   | E     | 129 | ASN  |
| 1   | E     | 258 | GLN  |
| 1   | E     | 285 | ASN  |
| 1   | E     | 428 | ASN  |
| 1   | E     | 439 | HIS  |
| 1   | E     | 494 | GLN  |
| 1   | F     | 72  | GLN  |
| 1   | F     | 113 | ASN  |
| 1   | F     | 285 | ASN  |
| 1   | F     | 355 | GLN  |
| 1   | F     | 428 | ASN  |
| 1   | F     | 439 | HIS  |
| 1   | F     | 494 | 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](#)

12 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | FAD  | E     | 600 | -    | 58,58,58     | 1.42 | 7 (12%)  | 85,89,89    | 1.71 | 23 (27%) |
| 3   | NAP  | D     | 601 | -    | 34,34,52     | 3.88 | 6 (17%)  | 50,53,80    | 1.89 | 11 (22%) |
| 2   | FAD  | D     | 600 | -    | 58,58,58     | 1.55 | 6 (10%)  | 85,89,89    | 1.68 | 18 (21%) |
| 2   | FAD  | C     | 600 | -    | 58,58,58     | 1.36 | 6 (10%)  | 85,89,89    | 1.56 | 17 (20%) |
| 3   | NAP  | C     | 601 | -    | 34,34,52     | 2.84 | 6 (17%)  | 50,53,80    | 1.78 | 10 (20%) |
| 2   | FAD  | A     | 600 | -    | 58,58,58     | 1.32 | 7 (12%)  | 85,89,89    | 1.60 | 16 (18%) |
| 3   | NAP  | E     | 601 | -    | 34,34,52     | 3.43 | 6 (17%)  | 50,53,80    | 1.74 | 9 (18%)  |
| 3   | NAP  | B     | 601 | -    | 34,34,52     | 3.11 | 7 (20%)  | 50,53,80    | 1.93 | 9 (18%)  |
| 2   | FAD  | F     | 600 | -    | 58,58,58     | 1.43 | 7 (12%)  | 85,89,89    | 1.58 | 16 (18%) |
| 3   | NAP  | A     | 601 | -    | 34,34,52     | 2.93 | 5 (14%)  | 50,53,80    | 1.91 | 11 (22%) |
| 2   | FAD  | B     | 600 | -    | 58,58,58     | 1.52 | 6 (10%)  | 85,89,89    | 1.62 | 19 (22%) |
| 3   | NAP  | F     | 601 | -    | 34,34,52     | 2.89 | 4 (11%)  | 50,53,80    | 1.76 | 9 (18%)  |

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  | E     | 600 | -    | -       | 3/34/50/50  | 0/6/6/6 |
| 3   | NAP  | D     | 601 | -    | -       | 8/24/40/67  | 0/3/3/5 |
| 2   | FAD  | D     | 600 | -    | -       | 3/34/50/50  | 0/6/6/6 |
| 2   | FAD  | C     | 600 | -    | -       | 3/34/50/50  | 0/6/6/6 |
| 3   | NAP  | C     | 601 | -    | -       | 11/24/40/67 | 0/3/3/5 |
| 2   | FAD  | A     | 600 | -    | -       | 2/34/50/50  | 0/6/6/6 |
| 3   | NAP  | E     | 601 | -    | -       | 8/24/40/67  | 0/3/3/5 |
| 3   | NAP  | B     | 601 | -    | -       | 8/24/40/67  | 0/3/3/5 |
| 2   | FAD  | F     | 600 | -    | -       | 3/34/50/50  | 0/6/6/6 |
| 3   | NAP  | A     | 601 | -    | -       | 6/24/40/67  | 0/3/3/5 |
| 2   | FAD  | B     | 600 | -    | -       | 3/34/50/50  | 0/6/6/6 |
| 3   | NAP  | F     | 601 | -    | -       | 7/24/40/67  | 0/3/3/5 |

All (73) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | D     | 601 | NAP  | PA-O3 | 15.10 | 1.75        | 1.59     |
| 3   | D     | 601 | NAP  | PN-O3 | 15.02 | 1.75        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | B     | 601 | NAP  | PN-O3   | 14.20 | 1.74        | 1.59     |
| 3   | E     | 601 | NAP  | PN-O3   | 14.14 | 1.74        | 1.59     |
| 3   | C     | 601 | NAP  | PN-O3   | 12.51 | 1.73        | 1.59     |
| 3   | E     | 601 | NAP  | PA-O3   | 11.53 | 1.71        | 1.59     |
| 3   | F     | 601 | NAP  | PN-O3   | 11.35 | 1.71        | 1.59     |
| 3   | A     | 601 | NAP  | PN-O3   | 11.22 | 1.71        | 1.59     |
| 3   | A     | 601 | NAP  | PA-O3   | 10.37 | 1.70        | 1.59     |
| 3   | F     | 601 | NAP  | PA-O3   | 10.00 | 1.70        | 1.59     |
| 3   | B     | 601 | NAP  | PA-O3   | 8.40  | 1.68        | 1.59     |
| 3   | C     | 601 | NAP  | PA-O3   | 7.95  | 1.68        | 1.59     |
| 2   | D     | 600 | FAD  | PA-O3P  | 5.53  | 1.65        | 1.59     |
| 2   | E     | 600 | FAD  | C4X-N5  | 5.53  | 1.42        | 1.30     |
| 2   | D     | 600 | FAD  | C4X-N5  | 5.22  | 1.42        | 1.30     |
| 2   | B     | 600 | FAD  | C4X-N5  | 5.06  | 1.41        | 1.30     |
| 2   | B     | 600 | FAD  | P-O3P   | 5.06  | 1.65        | 1.59     |
| 2   | C     | 600 | FAD  | C4X-N5  | 4.94  | 1.41        | 1.30     |
| 2   | F     | 600 | FAD  | C4X-N5  | 4.81  | 1.41        | 1.30     |
| 3   | E     | 601 | NAP  | PN-O5D  | 4.73  | 1.74        | 1.58     |
| 2   | F     | 600 | FAD  | C10-N1  | 4.60  | 1.42        | 1.33     |
| 2   | A     | 600 | FAD  | C4X-N5  | 4.46  | 1.40        | 1.30     |
| 3   | A     | 601 | NAP  | PN-O5D  | 4.03  | 1.72        | 1.58     |
| 3   | F     | 601 | NAP  | P2B-O1X | 3.96  | 1.62        | 1.50     |
| 2   | C     | 600 | FAD  | C10-N1  | 3.91  | 1.41        | 1.33     |
| 3   | B     | 601 | NAP  | P2B-O1X | 3.89  | 1.62        | 1.50     |
| 2   | A     | 600 | FAD  | C10-N1  | 3.80  | 1.40        | 1.33     |
| 3   | C     | 601 | NAP  | P2B-O1X | 3.65  | 1.61        | 1.50     |
| 2   | E     | 600 | FAD  | C5A-N7A | -3.59 | 1.32        | 1.39     |
| 2   | F     | 600 | FAD  | P-O3P   | 3.49  | 1.63        | 1.59     |
| 2   | E     | 600 | FAD  | C10-N1  | 3.42  | 1.40        | 1.33     |
| 2   | F     | 600 | FAD  | C5A-N7A | -3.41 | 1.32        | 1.39     |
| 3   | D     | 601 | NAP  | C5A-N7A | -3.38 | 1.32        | 1.39     |
| 3   | E     | 601 | NAP  | P2B-O1X | 3.30  | 1.60        | 1.50     |
| 3   | D     | 601 | NAP  | PN-O5D  | 3.29  | 1.69        | 1.58     |
| 2   | B     | 600 | FAD  | O4B-C1B | 3.27  | 1.49        | 1.42     |
| 2   | D     | 600 | FAD  | C5A-N7A | -3.27 | 1.33        | 1.39     |
| 3   | C     | 601 | NAP  | C5A-N7A | -3.18 | 1.33        | 1.39     |
| 3   | D     | 601 | NAP  | P2B-O1X | 3.16  | 1.60        | 1.50     |
| 2   | A     | 600 | FAD  | C5A-N7A | -3.15 | 1.33        | 1.39     |
| 2   | B     | 600 | FAD  | C5A-N7A | -3.15 | 1.33        | 1.39     |
| 2   | B     | 600 | FAD  | C10-N1  | 3.14  | 1.39        | 1.33     |
| 3   | F     | 601 | NAP  | C5A-N7A | -3.13 | 1.33        | 1.39     |
| 3   | B     | 601 | NAP  | C5A-N7A | -3.09 | 1.33        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 600 | FAD  | C10-N1  | 3.08  | 1.39        | 1.33     |
| 3   | A     | 601 | NAP  | C5A-N7A | -3.06 | 1.33        | 1.39     |
| 3   | B     | 601 | NAP  | PN-O5D  | 3.00  | 1.68        | 1.58     |
| 2   | C     | 600 | FAD  | C5A-N7A | -2.97 | 1.33        | 1.39     |
| 2   | F     | 600 | FAD  | C2-N1   | 2.96  | 1.43        | 1.36     |
| 3   | E     | 601 | NAP  | C5A-N7A | -2.87 | 1.33        | 1.39     |
| 2   | D     | 600 | FAD  | C4A-N9A | -2.77 | 1.31        | 1.37     |
| 2   | C     | 600 | FAD  | P-O3P   | 2.69  | 1.62        | 1.59     |
| 3   | C     | 601 | NAP  | PN-O5D  | 2.54  | 1.67        | 1.58     |
| 2   | E     | 600 | FAD  | P-O3P   | 2.53  | 1.62        | 1.59     |
| 2   | A     | 600 | FAD  | C8A-N9A | -2.52 | 1.33        | 1.37     |
| 2   | C     | 600 | FAD  | C1'-C2' | 2.41  | 1.56        | 1.52     |
| 2   | A     | 600 | FAD  | C4A-N9A | -2.40 | 1.32        | 1.37     |
| 3   | A     | 601 | NAP  | P2B-O1X | 2.39  | 1.57        | 1.50     |
| 2   | E     | 600 | FAD  | C1B-N9A | 2.37  | 1.52        | 1.46     |
| 3   | B     | 601 | NAP  | C4A-N9A | -2.37 | 1.32        | 1.37     |
| 2   | F     | 600 | FAD  | C8A-N9A | -2.31 | 1.33        | 1.37     |
| 3   | E     | 601 | NAP  | C4A-N9A | -2.26 | 1.33        | 1.37     |
| 2   | C     | 600 | FAD  | C4A-N9A | -2.24 | 1.33        | 1.37     |
| 3   | D     | 601 | NAP  | P2B-O3X | -2.23 | 1.46        | 1.54     |
| 2   | D     | 600 | FAD  | O4B-C1B | 2.22  | 1.47        | 1.42     |
| 2   | A     | 600 | FAD  | PA-O3P  | 2.20  | 1.61        | 1.59     |
| 2   | E     | 600 | FAD  | O4B-C1B | 2.17  | 1.47        | 1.42     |
| 2   | A     | 600 | FAD  | C10-N10 | 2.14  | 1.42        | 1.37     |
| 2   | F     | 600 | FAD  | C4A-N9A | -2.14 | 1.33        | 1.37     |
| 2   | B     | 600 | FAD  | C7M-C7  | 2.10  | 1.54        | 1.51     |
| 3   | B     | 601 | NAP  | P2B-O3X | -2.07 | 1.47        | 1.54     |
| 2   | E     | 600 | FAD  | C4A-N9A | -2.04 | 1.33        | 1.37     |
| 3   | C     | 601 | NAP  | C4A-N9A | -2.00 | 1.33        | 1.37     |

All (168) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | B     | 601 | NAP  | N3A-C2A-N1A | -5.72 | 119.93      | 128.58   |
| 3   | D     | 601 | NAP  | N3A-C2A-N1A | -5.49 | 120.27      | 128.58   |
| 2   | F     | 600 | FAD  | C5A-C4A-N3A | -5.14 | 119.63      | 126.72   |
| 2   | A     | 600 | FAD  | N3A-C2A-N1A | -5.08 | 120.89      | 128.58   |
| 2   | C     | 600 | FAD  | C5A-C4A-N3A | -5.07 | 119.74      | 126.72   |
| 3   | C     | 601 | NAP  | C5A-C4A-N3A | -5.06 | 119.75      | 126.72   |
| 3   | F     | 601 | NAP  | C5A-C4A-N3A | -5.03 | 119.78      | 126.72   |
| 3   | A     | 601 | NAP  | N3A-C2A-N1A | -4.98 | 121.04      | 128.58   |
| 3   | F     | 601 | NAP  | N3A-C2A-N1A | -4.98 | 121.05      | 128.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 600 | FAD  | N3A-C2A-N1A | -4.94 | 121.10      | 128.58   |
| 3   | E     | 601 | NAP  | N3A-C2A-N1A | -4.93 | 121.11      | 128.58   |
| 2   | D     | 600 | FAD  | C5A-C4A-N3A | -4.91 | 119.95      | 126.72   |
| 3   | C     | 601 | NAP  | N3A-C2A-N1A | -4.79 | 121.33      | 128.58   |
| 3   | B     | 601 | NAP  | C5A-C4A-N3A | -4.74 | 120.19      | 126.72   |
| 2   | A     | 600 | FAD  | C5A-C4A-N3A | -4.73 | 120.20      | 126.72   |
| 2   | E     | 600 | FAD  | N9A-C8A-N7A | -4.73 | 107.23      | 113.94   |
| 2   | F     | 600 | FAD  | N3A-C2A-N1A | -4.71 | 121.46      | 128.58   |
| 2   | E     | 600 | FAD  | C5A-C4A-N3A | -4.61 | 120.37      | 126.72   |
| 2   | C     | 600 | FAD  | N3A-C2A-N1A | -4.59 | 121.64      | 128.58   |
| 2   | B     | 600 | FAD  | N3A-C2A-N1A | -4.48 | 121.80      | 128.58   |
| 3   | A     | 601 | NAP  | C5A-C4A-N3A | -4.42 | 120.63      | 126.72   |
| 3   | D     | 601 | NAP  | C5A-C4A-N3A | -4.39 | 120.68      | 126.72   |
| 3   | E     | 601 | NAP  | C5A-C4A-N3A | -4.38 | 120.68      | 126.72   |
| 2   | B     | 600 | FAD  | C5A-C4A-N3A | -4.23 | 120.89      | 126.72   |
| 3   | A     | 601 | NAP  | N9A-C8A-N7A | -4.19 | 107.99      | 113.94   |
| 3   | D     | 601 | NAP  | N9A-C8A-N7A | -4.11 | 108.11      | 113.94   |
| 3   | A     | 601 | NAP  | C2B-C1B-N9A | -4.02 | 107.13      | 113.75   |
| 3   | B     | 601 | NAP  | N9A-C8A-N7A | -4.01 | 108.25      | 113.94   |
| 3   | B     | 601 | NAP  | N3A-C4A-N9A | 3.94  | 133.87      | 127.17   |
| 2   | E     | 600 | FAD  | C5A-N7A-C8A | 3.94  | 109.64      | 103.45   |
| 3   | B     | 601 | NAP  | C2A-N3A-C4A | 3.90  | 121.35      | 111.83   |
| 2   | F     | 600 | FAD  | N3A-C4A-N9A | 3.88  | 133.77      | 127.17   |
| 3   | D     | 601 | NAP  | N3A-C4A-N9A | 3.88  | 133.77      | 127.17   |
| 2   | E     | 600 | FAD  | N3A-C2A-N1A | -3.88 | 122.72      | 128.58   |
| 3   | F     | 601 | NAP  | N3A-C4A-N9A | 3.82  | 133.66      | 127.17   |
| 3   | C     | 601 | NAP  | N3A-C4A-N9A | 3.71  | 133.48      | 127.17   |
| 3   | A     | 601 | NAP  | N3A-C4A-N9A | 3.70  | 133.47      | 127.17   |
| 2   | B     | 600 | FAD  | N3A-C4A-N9A | 3.69  | 133.44      | 127.17   |
| 2   | A     | 600 | FAD  | N3A-C4A-N9A | 3.68  | 133.42      | 127.17   |
| 2   | B     | 600 | FAD  | N9A-C8A-N7A | -3.68 | 108.72      | 113.94   |
| 2   | A     | 600 | FAD  | C2A-N3A-C4A | 3.61  | 120.66      | 111.83   |
| 3   | A     | 601 | NAP  | C4A-N9A-C8A | 3.61  | 109.53      | 105.74   |
| 3   | B     | 601 | NAP  | C4A-N9A-C8A | 3.58  | 109.50      | 105.74   |
| 3   | E     | 601 | NAP  | N3A-C4A-N9A | 3.58  | 133.25      | 127.17   |
| 2   | C     | 600 | FAD  | N3A-C4A-N9A | 3.57  | 133.24      | 127.17   |
| 2   | B     | 600 | FAD  | C5B-C4B-C3B | -3.56 | 102.41      | 115.21   |
| 2   | D     | 600 | FAD  | C2A-N3A-C4A | 3.54  | 120.49      | 111.83   |
| 3   | D     | 601 | NAP  | C2A-N3A-C4A | 3.51  | 120.41      | 111.83   |
| 2   | D     | 600 | FAD  | O4B-C1B-C2B | -3.51 | 99.10       | 106.62   |
| 3   | C     | 601 | NAP  | C2A-N3A-C4A | 3.50  | 120.39      | 111.83   |
| 2   | D     | 600 | FAD  | O4B-C1B-N9A | -3.50 | 101.37      | 108.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | D     | 601 | NAP  | C4A-N9A-C8A | 3.47  | 109.38      | 105.74   |
| 3   | F     | 601 | NAP  | C2A-N3A-C4A | 3.46  | 120.28      | 111.83   |
| 3   | A     | 601 | NAP  | C5A-N7A-C8A | 3.45  | 108.88      | 103.45   |
| 2   | F     | 600 | FAD  | C2A-N3A-C4A | 3.42  | 120.18      | 111.83   |
| 2   | C     | 600 | FAD  | C2A-N3A-C4A | 3.39  | 120.11      | 111.83   |
| 2   | C     | 600 | FAD  | O4B-C1B-N9A | -3.37 | 101.62      | 108.09   |
| 3   | C     | 601 | NAP  | N9A-C8A-N7A | -3.36 | 109.16      | 113.94   |
| 3   | F     | 601 | NAP  | N9A-C8A-N7A | -3.33 | 109.22      | 113.94   |
| 3   | E     | 601 | NAP  | N9A-C8A-N7A | -3.28 | 109.28      | 113.94   |
| 2   | A     | 600 | FAD  | O4B-C1B-N9A | -3.26 | 101.82      | 108.09   |
| 2   | E     | 600 | FAD  | N3A-C4A-N9A | 3.22  | 132.64      | 127.17   |
| 2   | B     | 600 | FAD  | C4A-N9A-C8A | 3.18  | 109.08      | 105.74   |
| 2   | F     | 600 | FAD  | O4B-C1B-N9A | -3.18 | 101.99      | 108.09   |
| 3   | A     | 601 | NAP  | C2A-N3A-C4A | 3.16  | 119.56      | 111.83   |
| 3   | E     | 601 | NAP  | C2A-N3A-C4A | 3.14  | 119.50      | 111.83   |
| 2   | E     | 600 | FAD  | C2A-N3A-C4A | 3.13  | 119.48      | 111.83   |
| 2   | D     | 600 | FAD  | N3A-C4A-N9A | 3.13  | 132.49      | 127.17   |
| 2   | B     | 600 | FAD  | O4B-C1B-N9A | -3.11 | 102.11      | 108.09   |
| 2   | D     | 600 | FAD  | C9A-C5X-N5  | -3.08 | 119.19      | 122.45   |
| 2   | A     | 600 | FAD  | C4X-C10-N10 | 3.05  | 120.85      | 116.48   |
| 3   | E     | 601 | NAP  | C4A-N9A-C8A | 3.03  | 108.92      | 105.74   |
| 2   | D     | 600 | FAD  | C4X-C4-N3   | 3.03  | 120.97      | 113.25   |
| 3   | D     | 601 | NAP  | C5A-N7A-C8A | 3.03  | 108.21      | 103.45   |
| 2   | F     | 600 | FAD  | N9A-C8A-N7A | -2.95 | 109.74      | 113.94   |
| 2   | A     | 600 | FAD  | N9A-C8A-N7A | -2.95 | 109.75      | 113.94   |
| 3   | C     | 601 | NAP  | C2B-C1B-N9A | -2.92 | 108.95      | 113.75   |
| 2   | D     | 600 | FAD  | C4X-C10-N10 | 2.91  | 120.65      | 116.48   |
| 2   | E     | 600 | FAD  | C4X-C4-N3   | 2.91  | 120.65      | 113.25   |
| 2   | C     | 600 | FAD  | N9A-C8A-N7A | -2.90 | 109.83      | 113.94   |
| 2   | C     | 600 | FAD  | C9A-C5X-N5  | -2.90 | 119.38      | 122.45   |
| 2   | E     | 600 | FAD  | O3'-C3'-C2' | -2.89 | 102.36      | 108.93   |
| 2   | E     | 600 | FAD  | C4A-N9A-C8A | 2.88  | 108.77      | 105.74   |
| 2   | F     | 600 | FAD  | C9A-C5X-N5  | -2.86 | 119.42      | 122.45   |
| 2   | E     | 600 | FAD  | C4A-C5A-N7A | -2.84 | 107.33      | 110.58   |
| 2   | B     | 600 | FAD  | C2A-N3A-C4A | 2.82  | 118.73      | 111.83   |
| 2   | F     | 600 | FAD  | C4X-C4-N3   | 2.82  | 120.42      | 113.25   |
| 3   | C     | 601 | NAP  | C5A-N7A-C8A | 2.82  | 107.88      | 103.45   |
| 2   | E     | 600 | FAD  | C4-N3-C2    | -2.78 | 120.70      | 125.64   |
| 2   | C     | 600 | FAD  | C4-N3-C2    | -2.77 | 120.72      | 125.64   |
| 2   | A     | 600 | FAD  | C5'-C4'-C3' | -2.76 | 107.00      | 112.22   |
| 2   | E     | 600 | FAD  | O4B-C1B-N9A | -2.75 | 102.81      | 108.09   |
| 2   | D     | 600 | FAD  | C4-N3-C2    | -2.74 | 120.77      | 125.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 600 | FAD  | C5A-N7A-C8A | 2.71  | 107.70      | 103.45   |
| 3   | B     | 601 | NAP  | C5A-N7A-C8A | 2.68  | 107.66      | 103.45   |
| 2   | B     | 600 | FAD  | O3B-C3B-C4B | -2.67 | 103.40      | 111.08   |
| 3   | B     | 601 | NAP  | O3X-P2B-O2X | 2.63  | 117.67      | 107.80   |
| 3   | F     | 601 | NAP  | C5A-N7A-C8A | 2.62  | 107.56      | 103.45   |
| 2   | C     | 600 | FAD  | C10-C4X-N5  | -2.61 | 119.47      | 124.81   |
| 3   | F     | 601 | NAP  | C4A-N9A-C8A | 2.61  | 108.47      | 105.74   |
| 2   | A     | 600 | FAD  | C4A-N9A-C8A | 2.60  | 108.47      | 105.74   |
| 2   | C     | 600 | FAD  | C4X-C4-N3   | 2.60  | 119.86      | 113.25   |
| 2   | B     | 600 | FAD  | C9A-C5X-N5  | -2.56 | 119.74      | 122.45   |
| 3   | A     | 601 | NAP  | C4A-C5A-N7A | -2.54 | 107.68      | 110.58   |
| 2   | C     | 600 | FAD  | C5'-C4'-C3' | -2.51 | 107.49      | 112.22   |
| 3   | F     | 601 | NAP  | C2B-C1B-N9A | -2.50 | 109.63      | 113.75   |
| 2   | A     | 600 | FAD  | C4X-C4-N3   | 2.50  | 119.62      | 113.25   |
| 2   | C     | 600 | FAD  | C4X-C10-N10 | 2.49  | 120.05      | 116.48   |
| 3   | D     | 601 | NAP  | O3X-P2B-O2B | 2.49  | 115.56      | 105.85   |
| 2   | F     | 600 | FAD  | C4-N3-C2    | -2.44 | 121.30      | 125.64   |
| 2   | D     | 600 | FAD  | C10-C4X-N5  | -2.44 | 119.82      | 124.81   |
| 2   | E     | 600 | FAD  | C10-C4X-N5  | -2.44 | 119.82      | 124.81   |
| 2   | F     | 600 | FAD  | C5A-N7A-C8A | 2.43  | 107.27      | 103.45   |
| 2   | D     | 600 | FAD  | N9A-C8A-N7A | -2.43 | 110.49      | 113.94   |
| 2   | F     | 600 | FAD  | C5B-C4B-C3B | -2.40 | 106.56      | 115.21   |
| 2   | E     | 600 | FAD  | C9A-C5X-N5  | -2.40 | 119.91      | 122.45   |
| 2   | F     | 600 | FAD  | O4B-C1B-C2B | -2.38 | 101.52      | 106.62   |
| 3   | E     | 601 | NAP  | C5A-N7A-C8A | 2.38  | 107.19      | 103.45   |
| 2   | E     | 600 | FAD  | C4X-C10-N10 | 2.37  | 119.88      | 116.48   |
| 2   | B     | 600 | FAD  | C4X-C4-N3   | 2.37  | 119.29      | 113.25   |
| 2   | E     | 600 | FAD  | O4-C4-C4X   | -2.37 | 120.28      | 126.53   |
| 3   | C     | 601 | NAP  | C4A-N9A-C8A | 2.35  | 108.21      | 105.74   |
| 2   | F     | 600 | FAD  | C4A-N9A-C8A | 2.34  | 108.19      | 105.74   |
| 2   | F     | 600 | FAD  | C10-C4X-N5  | -2.33 | 120.04      | 124.81   |
| 3   | D     | 601 | NAP  | O5B-PA-O1A  | -2.33 | 99.69       | 108.94   |
| 2   | E     | 600 | FAD  | O2P-P-O1P   | 2.33  | 123.28      | 112.44   |
| 2   | F     | 600 | FAD  | O4-C4-C4X   | -2.33 | 120.39      | 126.53   |
| 2   | D     | 600 | FAD  | C5B-C4B-C3B | -2.31 | 106.88      | 115.21   |
| 2   | B     | 600 | FAD  | C5'-C4'-C3' | -2.31 | 107.86      | 112.22   |
| 2   | D     | 600 | FAD  | O3'-C3'-C2' | -2.31 | 103.68      | 108.93   |
| 2   | B     | 600 | FAD  | C10-C4X-N5  | -2.31 | 120.09      | 124.81   |
| 2   | B     | 600 | FAD  | C2B-C1B-N9A | 2.31  | 119.03      | 113.30   |
| 2   | B     | 600 | FAD  | N6A-C6A-N1A | 2.29  | 123.47      | 118.38   |
| 2   | A     | 600 | FAD  | C5B-C4B-C3B | -2.28 | 106.99      | 115.21   |
| 2   | C     | 600 | FAD  | C5B-C4B-C3B | -2.28 | 107.02      | 115.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | C     | 601 | NAP  | C4A-C5A-N7A | -2.28 | 107.98      | 110.58   |
| 2   | E     | 600 | FAD  | O4'-C4'-C3' | 2.26  | 114.54      | 109.25   |
| 2   | B     | 600 | FAD  | C4X-C10-N10 | 2.26  | 119.72      | 116.48   |
| 2   | B     | 600 | FAD  | C4-N3-C2    | -2.25 | 121.64      | 125.64   |
| 2   | A     | 600 | FAD  | O2P-P-O1P   | 2.24  | 122.86      | 112.44   |
| 2   | D     | 600 | FAD  | C4X-C10-N1  | -2.22 | 119.15      | 124.59   |
| 2   | C     | 600 | FAD  | C5A-N7A-C8A | 2.20  | 106.91      | 103.45   |
| 2   | D     | 600 | FAD  | O2P-P-O1P   | 2.20  | 122.68      | 112.44   |
| 2   | A     | 600 | FAD  | C5A-N7A-C8A | 2.19  | 106.89      | 103.45   |
| 2   | E     | 600 | FAD  | O2'-C2'-C3' | 2.18  | 114.36      | 109.25   |
| 3   | D     | 601 | NAP  | C2B-C1B-N9A | -2.14 | 110.23      | 113.75   |
| 2   | E     | 600 | FAD  | O3B-C3B-C4B | -2.13 | 104.95      | 111.08   |
| 2   | E     | 600 | FAD  | C5'-C4'-C3' | -2.13 | 108.19      | 112.22   |
| 2   | D     | 600 | FAD  | O3'-C3'-C4' | -2.13 | 104.09      | 108.93   |
| 2   | A     | 600 | FAD  | C10-C4X-N5  | -2.13 | 120.45      | 124.81   |
| 3   | D     | 601 | NAP  | O2A-PA-O1A  | 2.12  | 122.28      | 112.44   |
| 3   | E     | 601 | NAP  | O3X-P2B-O2X | 2.11  | 115.71      | 107.80   |
| 3   | F     | 601 | NAP  | C4A-C5A-N7A | -2.10 | 108.19      | 110.58   |
| 2   | D     | 600 | FAD  | C2B-C1B-N9A | 2.09  | 118.50      | 113.30   |
| 2   | F     | 600 | FAD  | C4A-C5A-N7A | -2.09 | 108.19      | 110.58   |
| 2   | E     | 600 | FAD  | C5B-C4B-C3B | -2.09 | 107.70      | 115.21   |
| 3   | C     | 601 | NAP  | O2A-PA-O1A  | 2.09  | 122.15      | 112.44   |
| 2   | E     | 600 | FAD  | C4-C4X-N5   | 2.08  | 121.09      | 118.21   |
| 2   | B     | 600 | FAD  | C5A-C6A-N6A | -2.08 | 118.13      | 123.29   |
| 2   | C     | 600 | FAD  | C4A-N9A-C8A | 2.06  | 107.91      | 105.74   |
| 2   | A     | 600 | FAD  | C4-N3-C2    | -2.04 | 122.02      | 125.64   |
| 2   | C     | 600 | FAD  | C4-C4X-N5   | 2.04  | 121.02      | 118.21   |
| 3   | E     | 601 | NAP  | C2B-C1B-N9A | -2.03 | 110.41      | 113.75   |
| 2   | A     | 600 | FAD  | C2B-C1B-N9A | 2.03  | 118.34      | 113.30   |
| 3   | A     | 601 | NAP  | C3B-C2B-C1B | -2.01 | 98.95       | 102.81   |
| 3   | B     | 601 | NAP  | O2A-PA-O1A  | 2.01  | 121.79      | 112.44   |
| 3   | A     | 601 | NAP  | O3X-P2B-O2X | 2.01  | 115.32      | 107.80   |
| 2   | C     | 600 | FAD  | O4-C4-C4X   | -2.00 | 121.24      | 126.53   |

There are no chirality outliers.

All (65) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | A     | 601 | NAP  | C5B-O5B-PA-O1A |
| 3   | B     | 601 | NAP  | C5B-O5B-PA-O1A |
| 3   | B     | 601 | NAP  | C5B-O5B-PA-O3  |
| 3   | C     | 601 | NAP  | C5B-O5B-PA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | D     | 601 | NAP  | C5B-O5B-PA-O1A  |
| 3   | E     | 601 | NAP  | C5B-O5B-PA-O1A  |
| 3   | F     | 601 | NAP  | C5B-O5B-PA-O1A  |
| 2   | B     | 600 | FAD  | O4B-C4B-C5B-O5B |
| 2   | A     | 600 | FAD  | C3B-C4B-C5B-O5B |
| 2   | B     | 600 | FAD  | C3B-C4B-C5B-O5B |
| 2   | C     | 600 | FAD  | C3B-C4B-C5B-O5B |
| 2   | D     | 600 | FAD  | C3B-C4B-C5B-O5B |
| 2   | E     | 600 | FAD  | C3B-C4B-C5B-O5B |
| 2   | F     | 600 | FAD  | C3B-C4B-C5B-O5B |
| 3   | A     | 601 | NAP  | C5D-O5D-PN-O1N  |
| 3   | B     | 601 | NAP  | C5D-O5D-PN-O1N  |
| 3   | C     | 601 | NAP  | C5D-O5D-PN-O1N  |
| 3   | D     | 601 | NAP  | C5D-O5D-PN-O1N  |
| 3   | E     | 601 | NAP  | C5D-O5D-PN-O1N  |
| 3   | F     | 601 | NAP  | C5D-O5D-PN-O1N  |
| 2   | A     | 600 | FAD  | O4B-C4B-C5B-O5B |
| 2   | C     | 600 | FAD  | O4B-C4B-C5B-O5B |
| 2   | D     | 600 | FAD  | O4B-C4B-C5B-O5B |
| 2   | E     | 600 | FAD  | O4B-C4B-C5B-O5B |
| 2   | F     | 600 | FAD  | O4B-C4B-C5B-O5B |
| 3   | A     | 601 | NAP  | PA-O3-PN-O5D    |
| 3   | B     | 601 | NAP  | PA-O3-PN-O5D    |
| 3   | C     | 601 | NAP  | PA-O3-PN-O5D    |
| 3   | D     | 601 | NAP  | PA-O3-PN-O5D    |
| 3   | E     | 601 | NAP  | PA-O3-PN-O5D    |
| 3   | F     | 601 | NAP  | PA-O3-PN-O5D    |
| 3   | A     | 601 | NAP  | C2B-O2B-P2B-O1X |
| 3   | B     | 601 | NAP  | C2B-O2B-P2B-O1X |
| 3   | C     | 601 | NAP  | C2B-O2B-P2B-O1X |
| 3   | D     | 601 | NAP  | C2B-O2B-P2B-O1X |
| 3   | F     | 601 | NAP  | C2B-O2B-P2B-O1X |
| 3   | B     | 601 | NAP  | C5B-O5B-PA-O2A  |
| 3   | C     | 601 | NAP  | C5B-O5B-PA-O2A  |
| 3   | C     | 601 | NAP  | C5B-O5B-PA-O3   |
| 3   | D     | 601 | NAP  | C5B-O5B-PA-O2A  |
| 3   | D     | 601 | NAP  | C5B-O5B-PA-O3   |
| 2   | D     | 600 | FAD  | C2B-C1B-N9A-C8A |
| 3   | D     | 601 | NAP  | PN-O3-PA-O2A    |
| 2   | C     | 600 | FAD  | C2B-C1B-N9A-C8A |
| 2   | F     | 600 | FAD  | C2B-C1B-N9A-C8A |
| 3   | B     | 601 | NAP  | PN-O3-PA-O1A    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 601 | NAP  | PN-O3-PA-O2A    |
| 3   | E     | 601 | NAP  | PN-O3-PA-O1A    |
| 3   | F     | 601 | NAP  | PN-O3-PA-O1A    |
| 3   | B     | 601 | NAP  | O4B-C4B-C5B-O5B |
| 3   | E     | 601 | NAP  | O4B-C4B-C5B-O5B |
| 3   | A     | 601 | NAP  | C2B-O2B-P2B-O3X |
| 3   | C     | 601 | NAP  | C2B-O2B-P2B-O3X |
| 3   | D     | 601 | NAP  | C2B-O2B-P2B-O3X |
| 3   | E     | 601 | NAP  | C2B-O2B-P2B-O2X |
| 3   | E     | 601 | NAP  | C2B-O2B-P2B-O3X |
| 2   | E     | 600 | FAD  | C2B-C1B-N9A-C8A |
| 3   | E     | 601 | NAP  | C2B-O2B-P2B-O1X |
| 2   | B     | 600 | FAD  | C2B-C1B-N9A-C8A |
| 3   | C     | 601 | NAP  | C5D-O5D-PN-O3   |
| 3   | A     | 601 | NAP  | PN-O3-PA-O1A    |
| 3   | C     | 601 | NAP  | PN-O3-PA-O1A    |
| 3   | F     | 601 | NAP  | PN-O3-PA-O2A    |
| 3   | C     | 601 | NAP  | O4B-C4B-C5B-O5B |
| 3   | F     | 601 | NAP  | O4B-C4B-C5B-O5B |

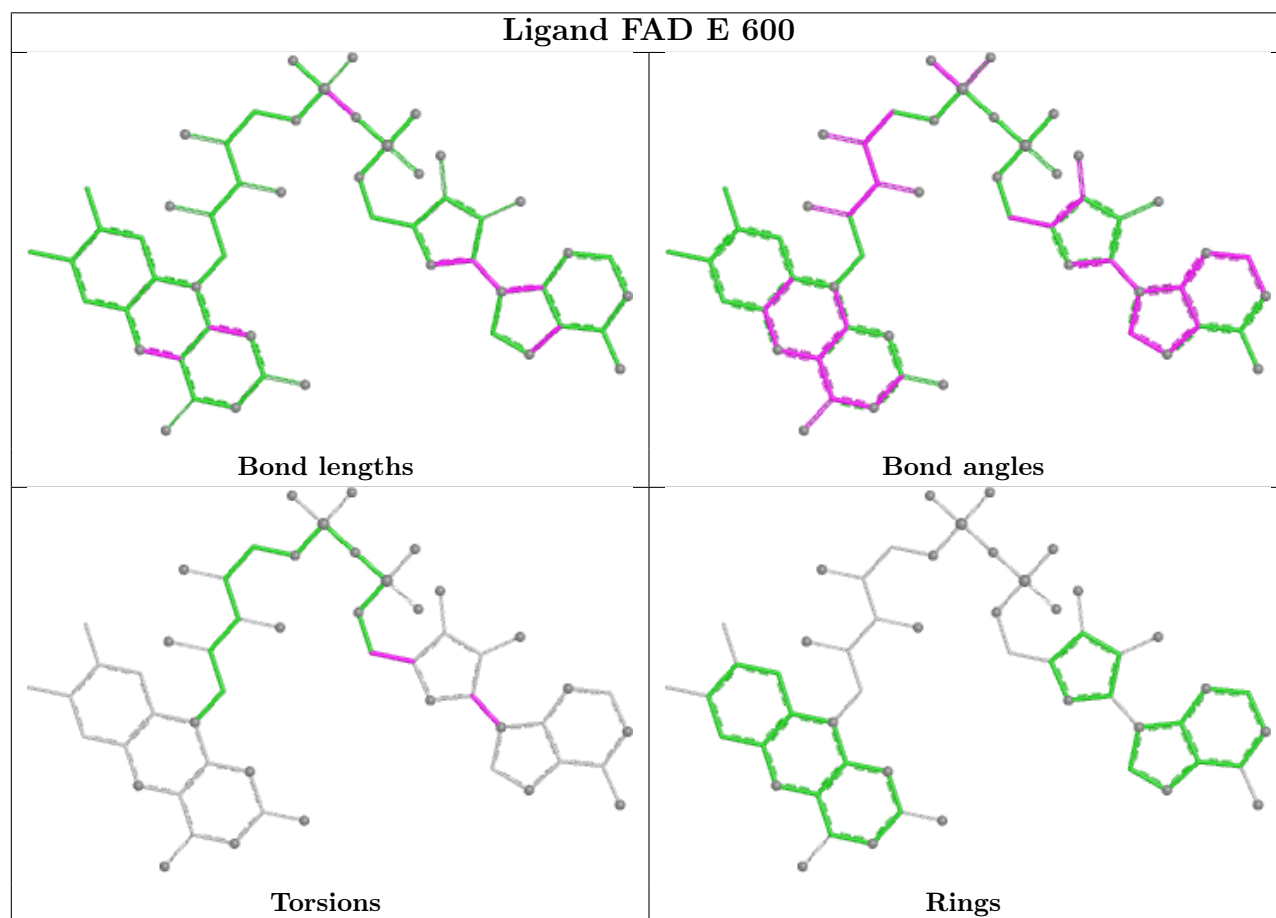
There are no ring outliers.

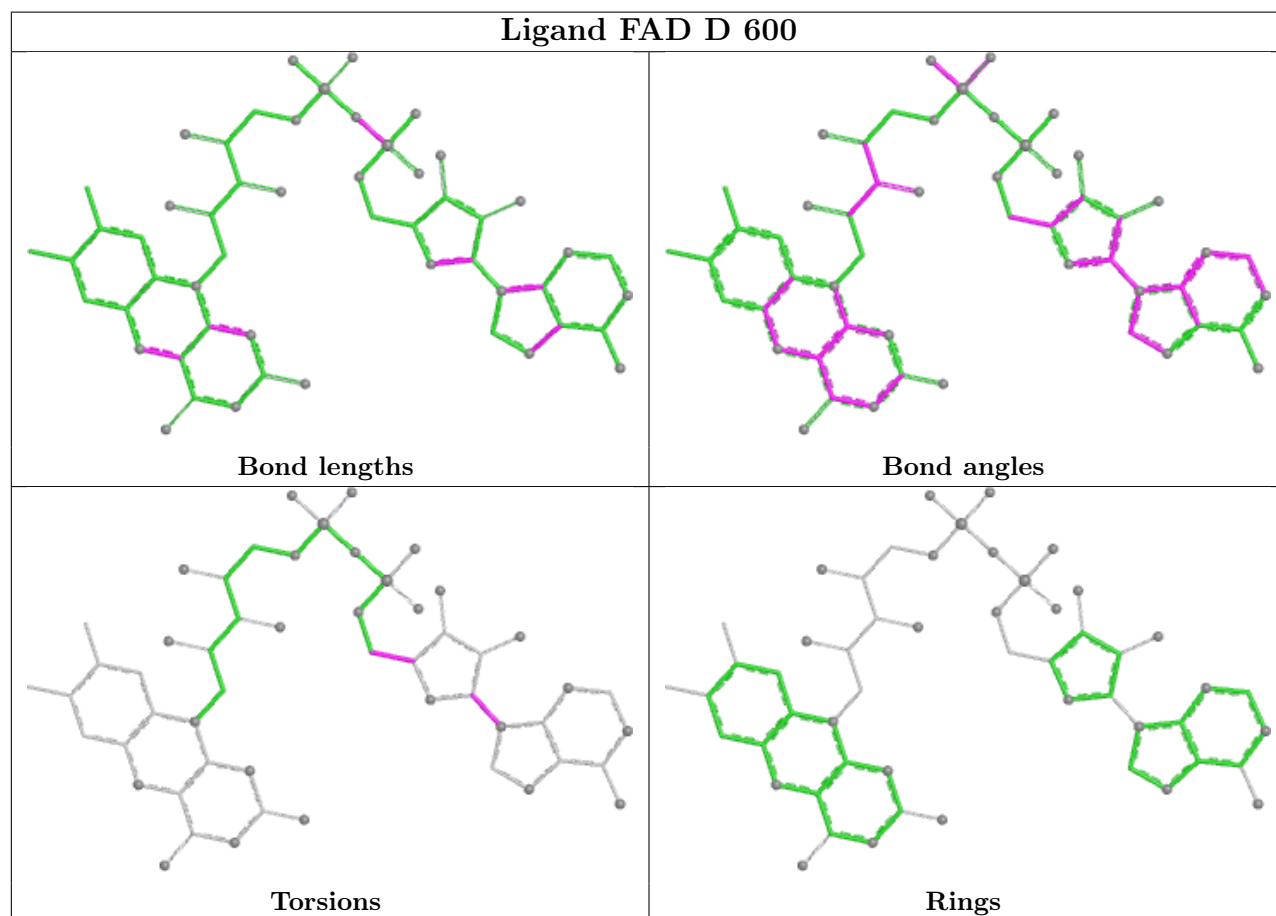
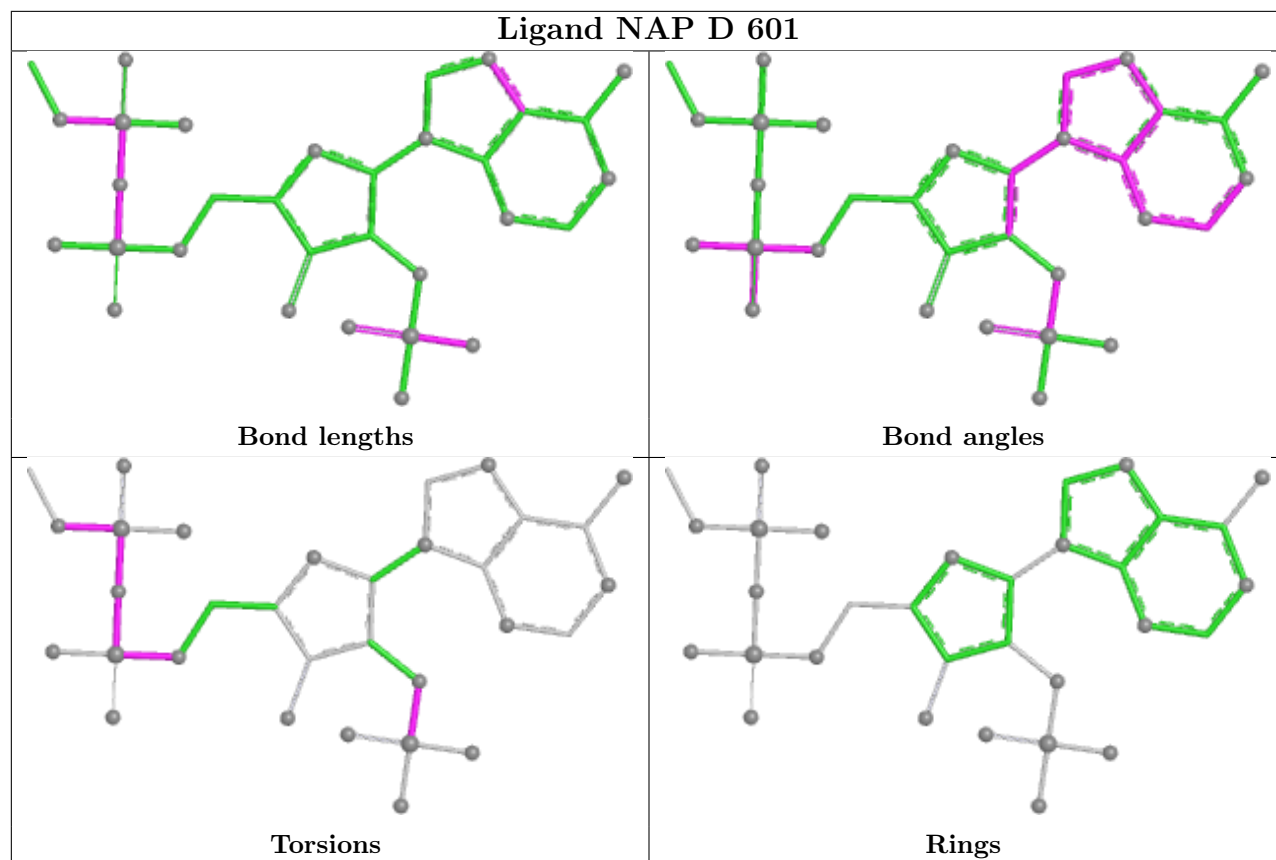
7 monomers are involved in 8 short contacts:

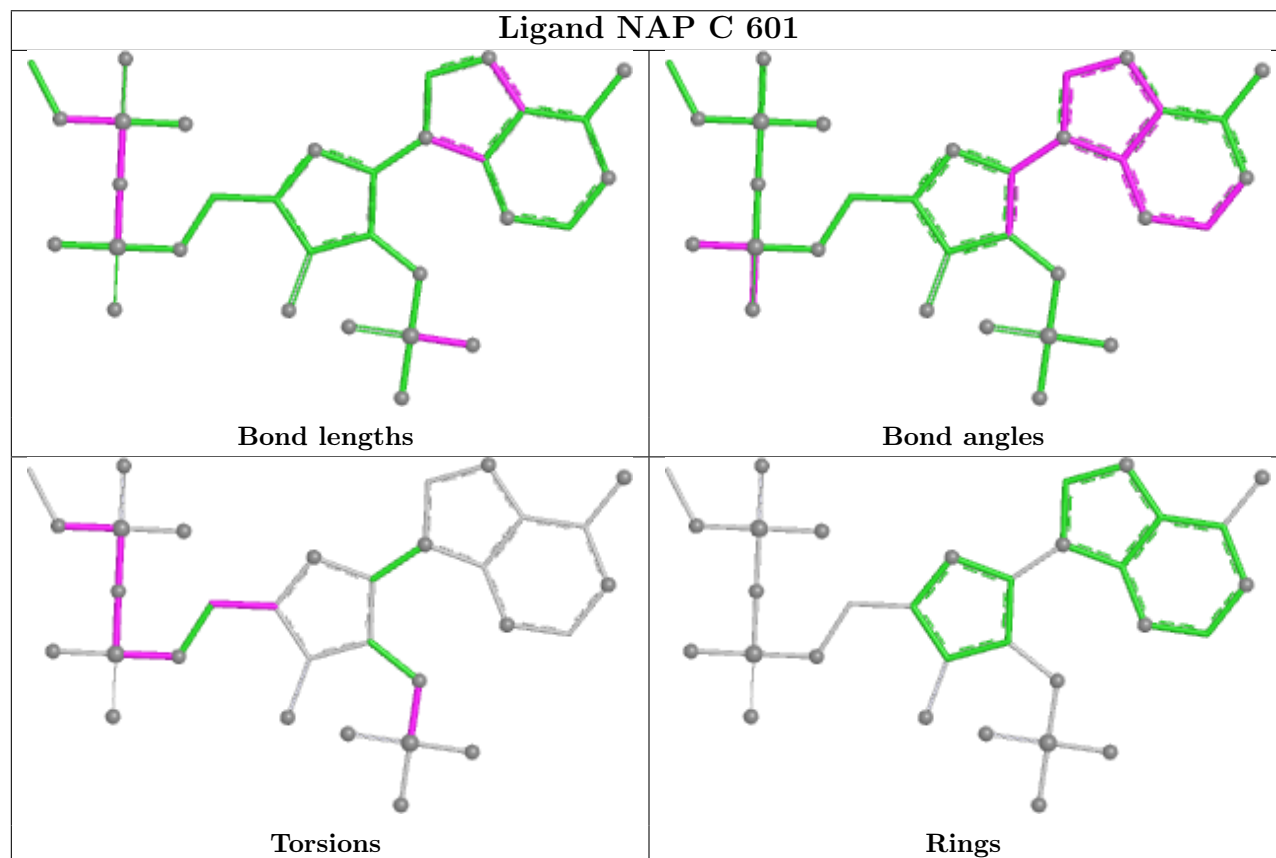
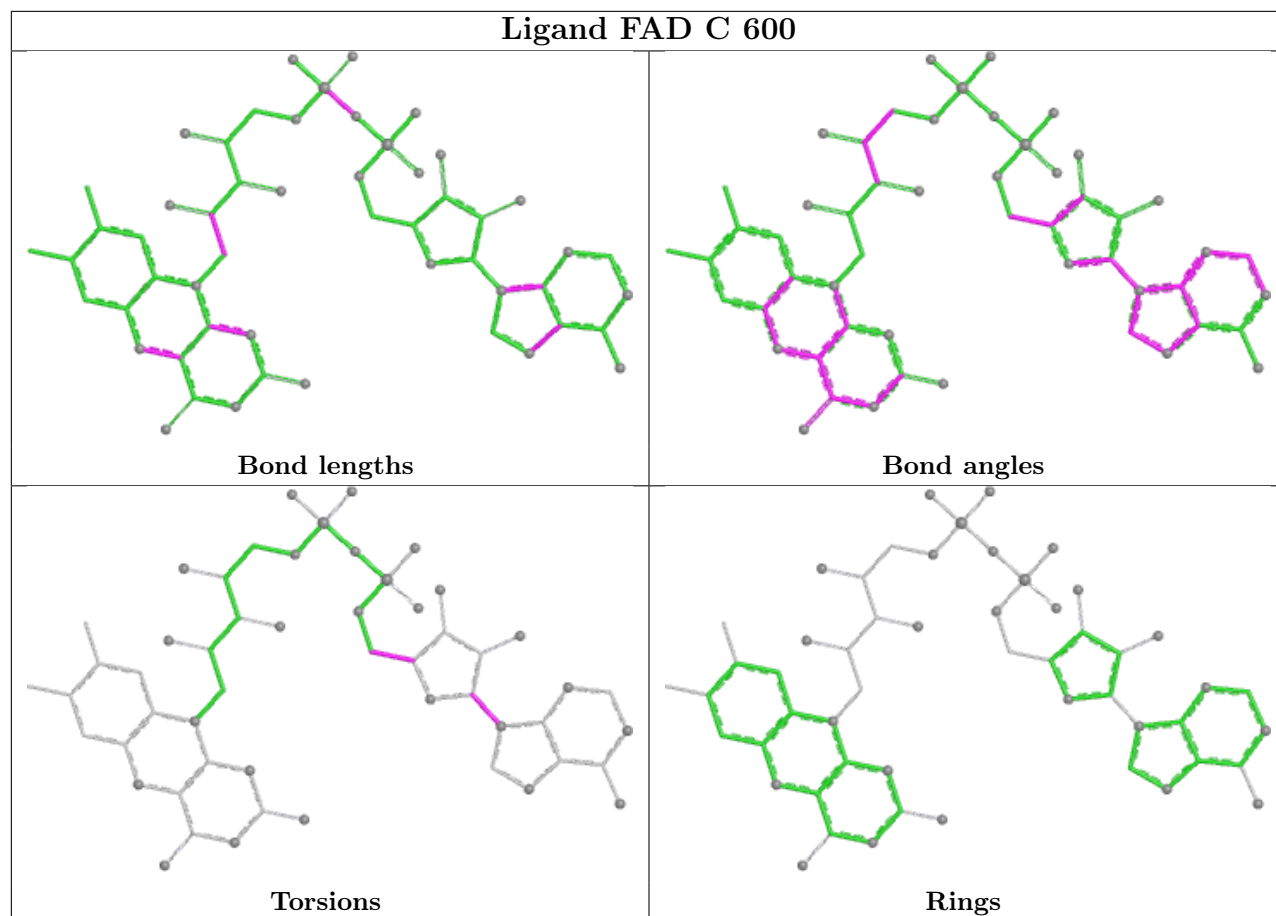
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | D     | 601 | NAP  | 1       | 0            |
| 3   | C     | 601 | NAP  | 1       | 0            |
| 2   | A     | 600 | FAD  | 1       | 0            |
| 3   | E     | 601 | NAP  | 1       | 0            |
| 3   | B     | 601 | NAP  | 2       | 0            |
| 3   | A     | 601 | NAP  | 1       | 0            |
| 3   | F     | 601 | NAP  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

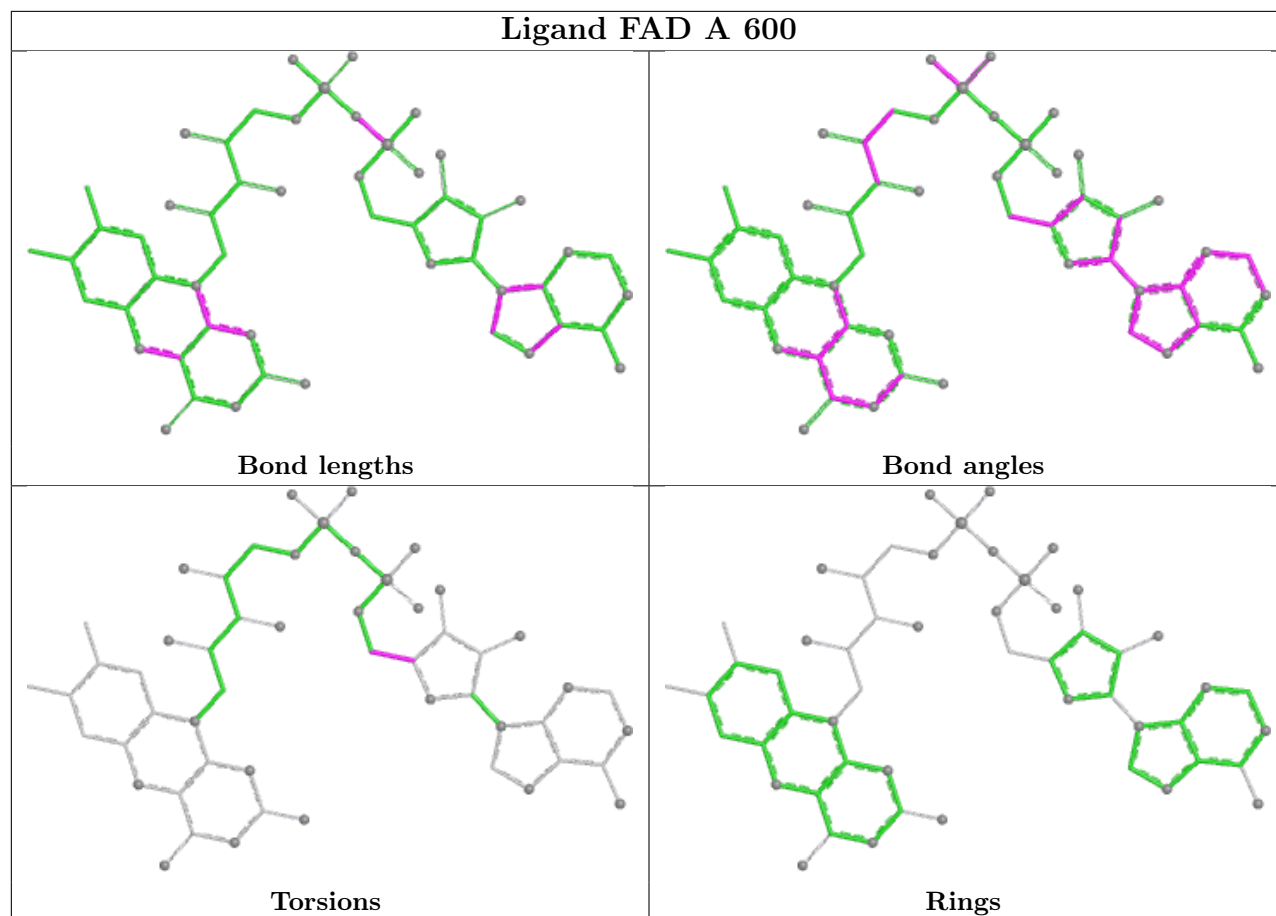
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



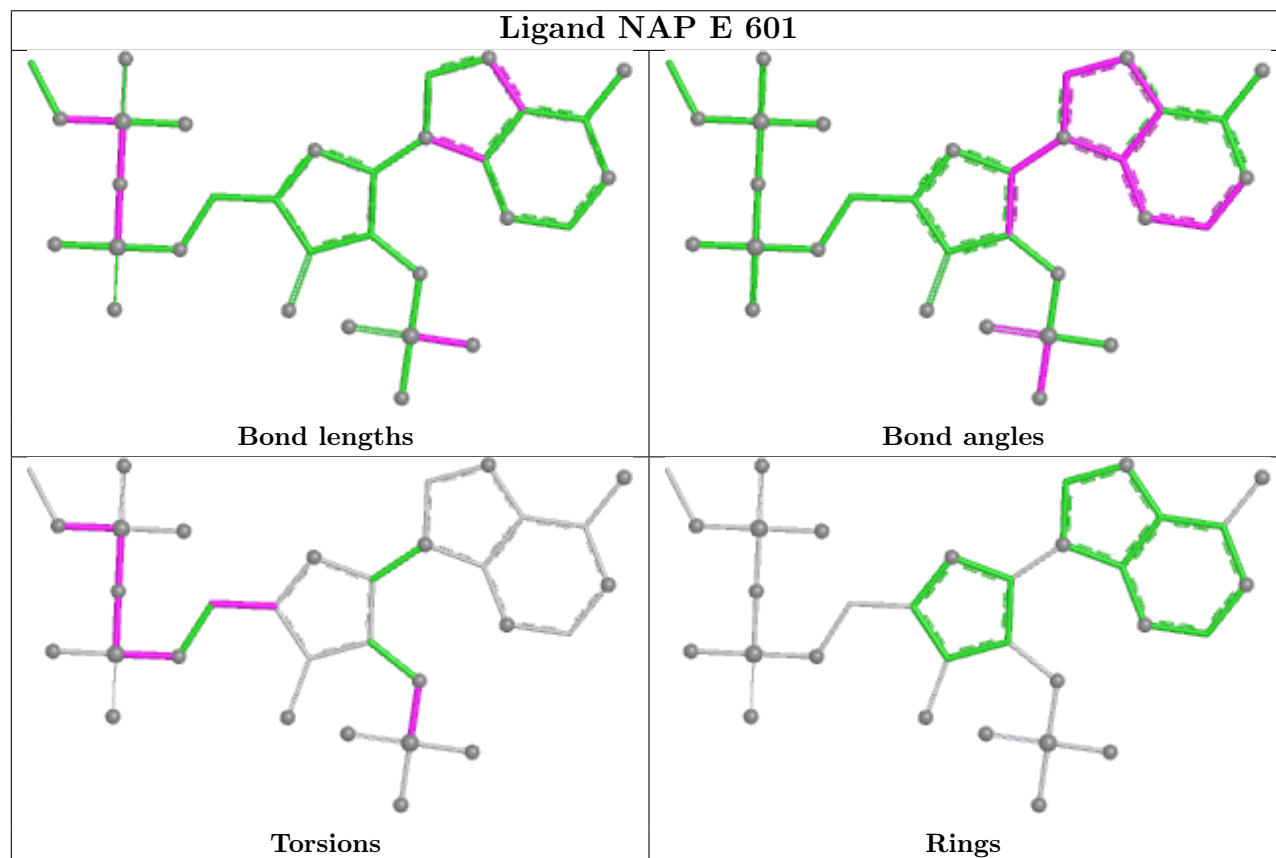


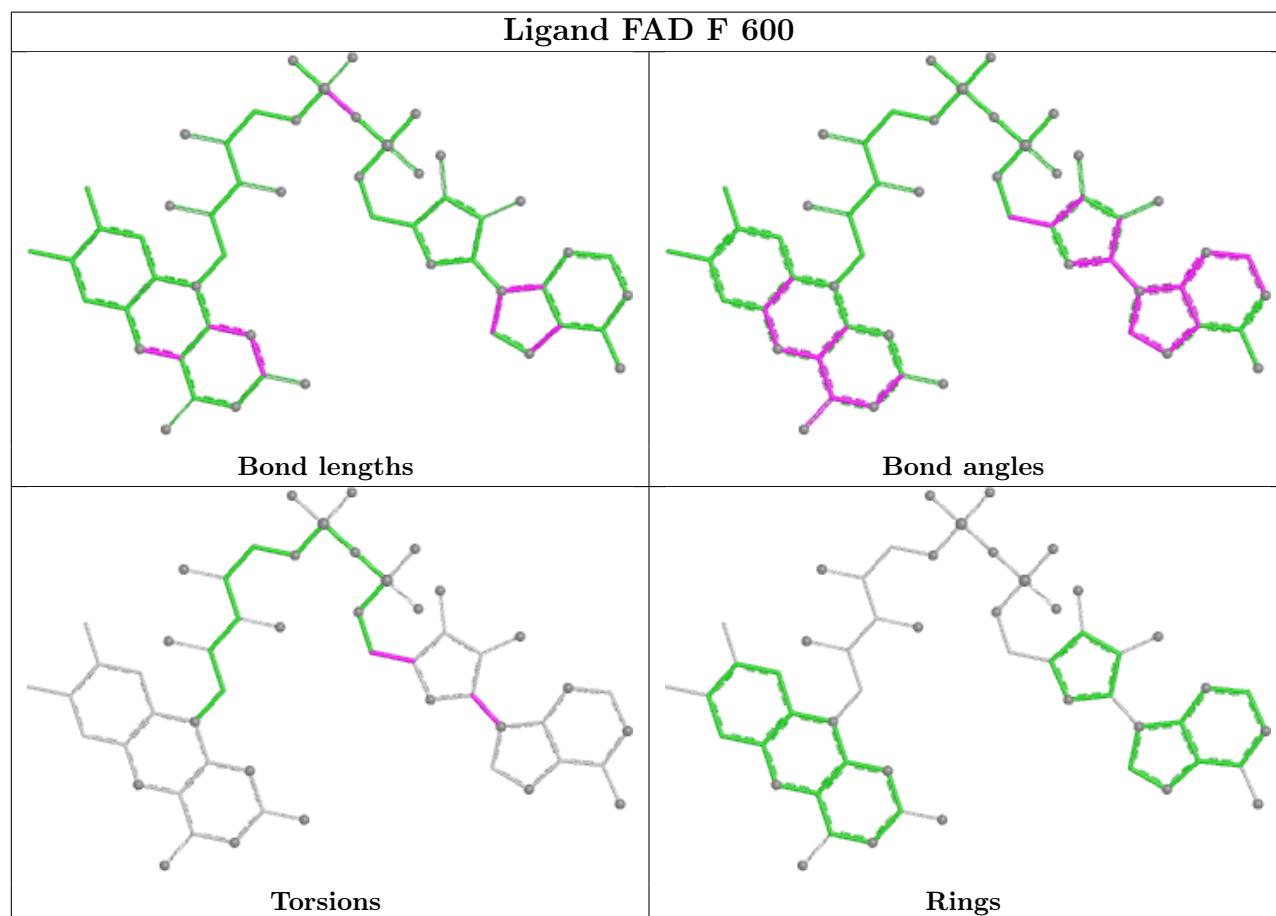
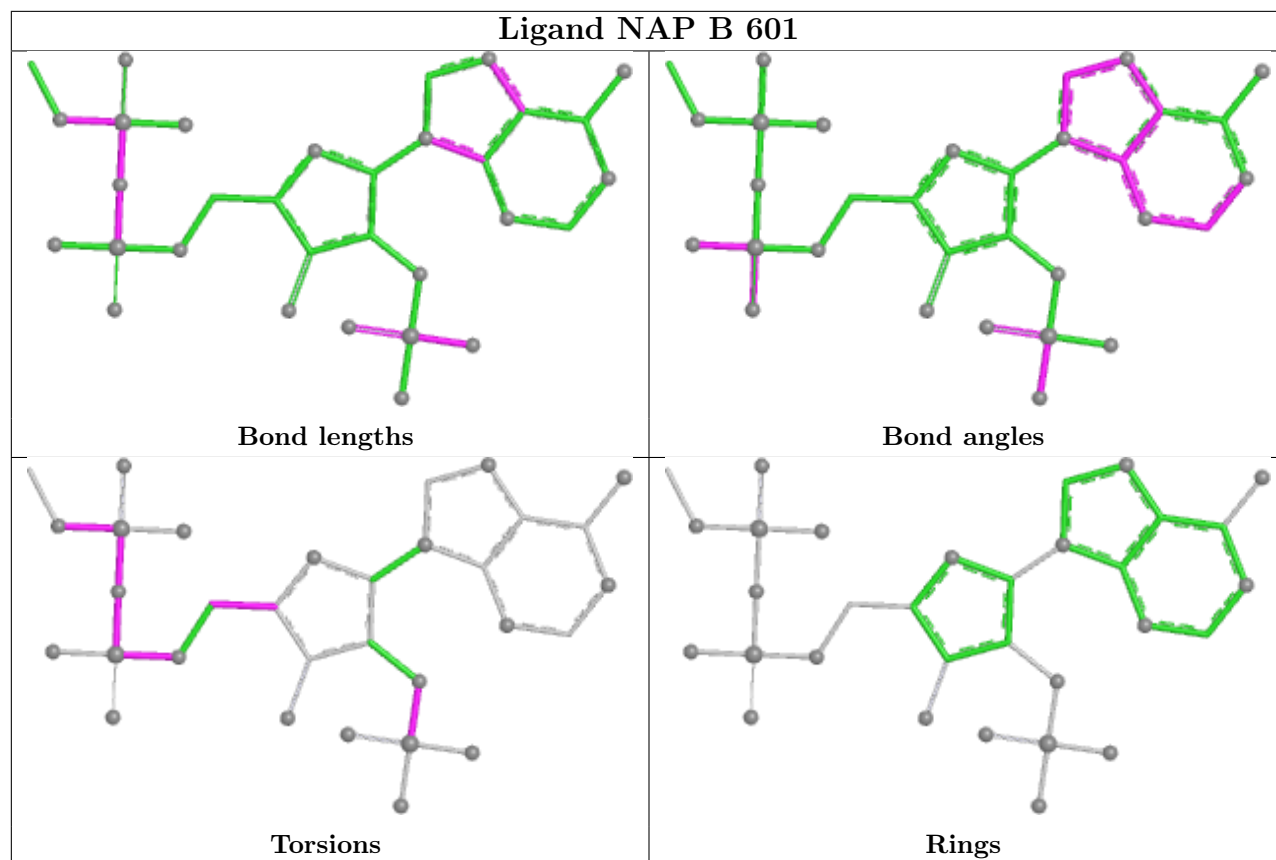


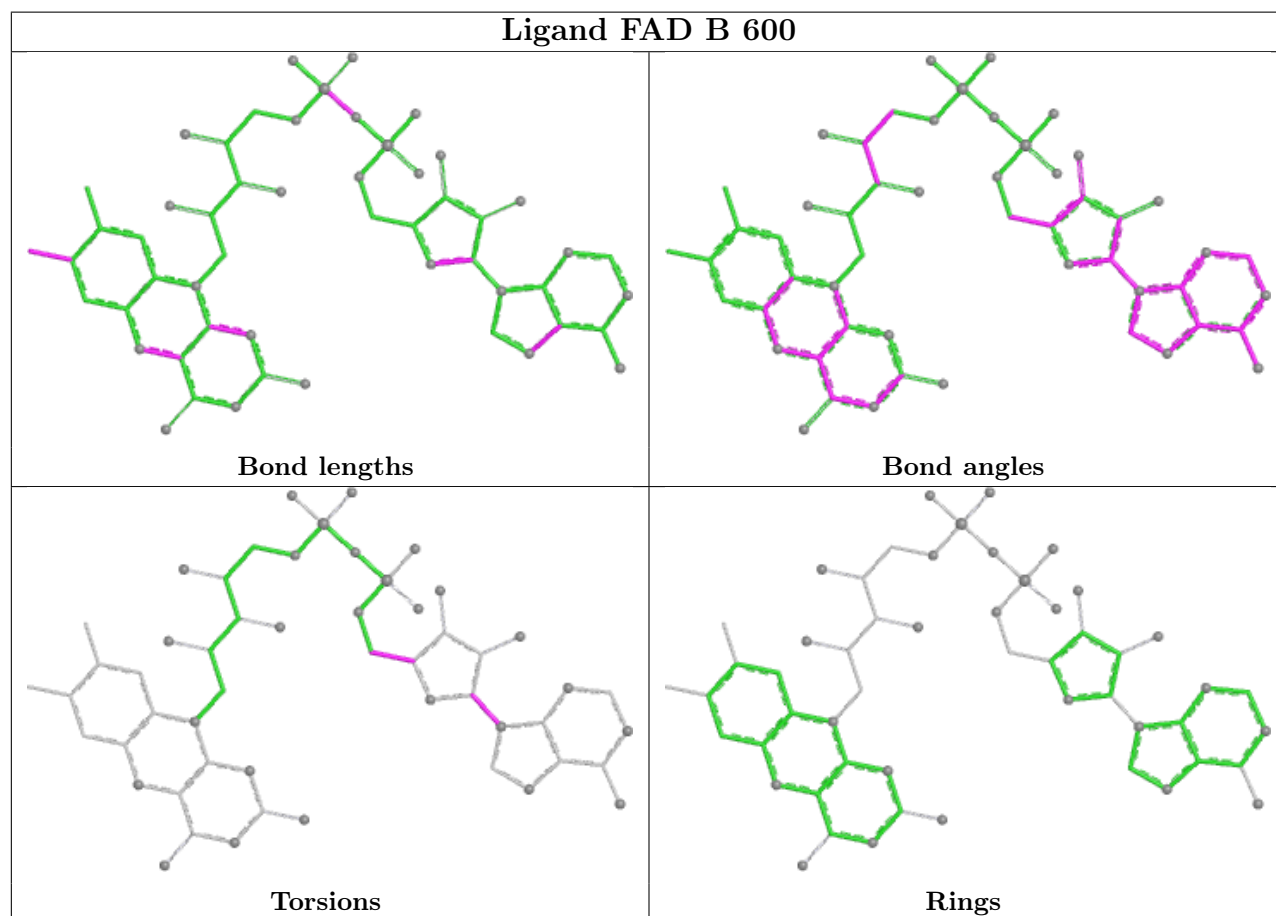
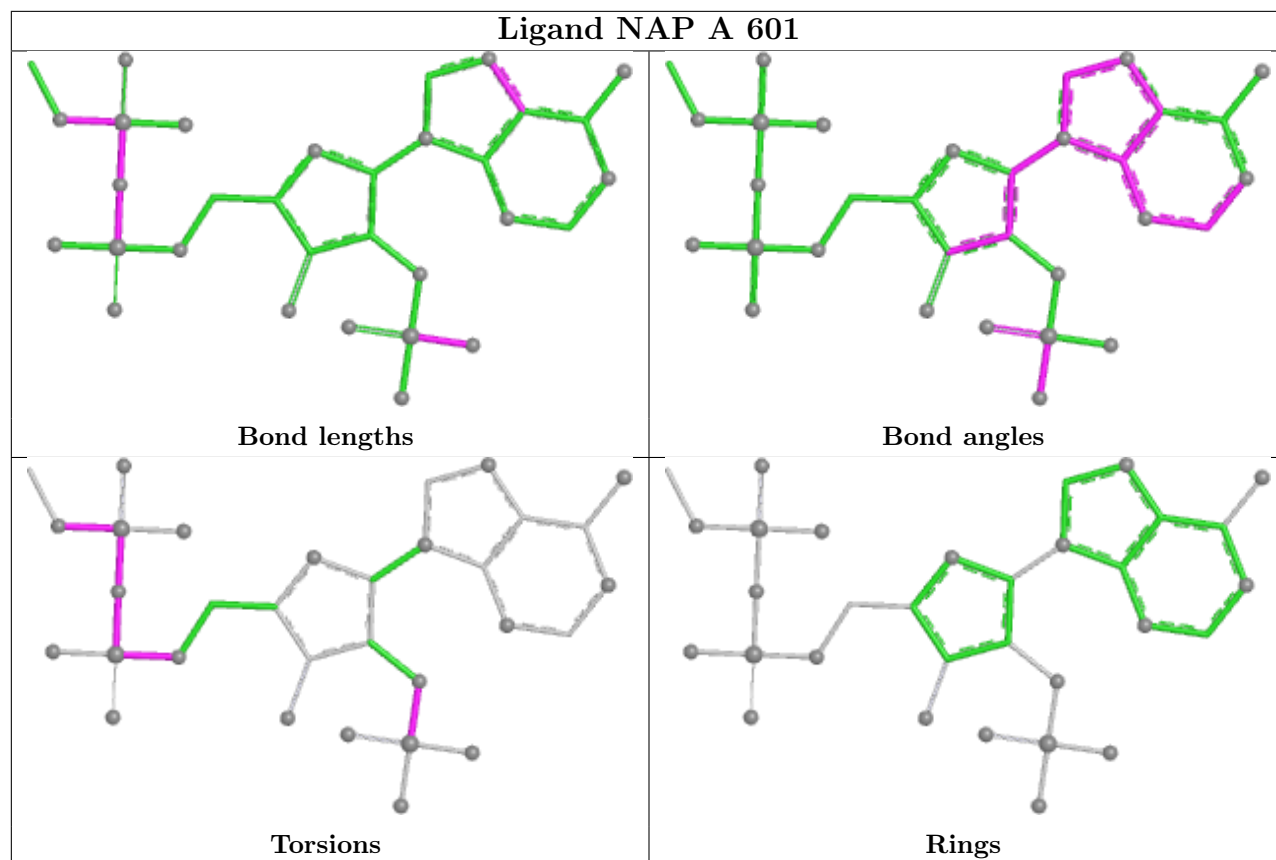
## Ligand FAD A 600



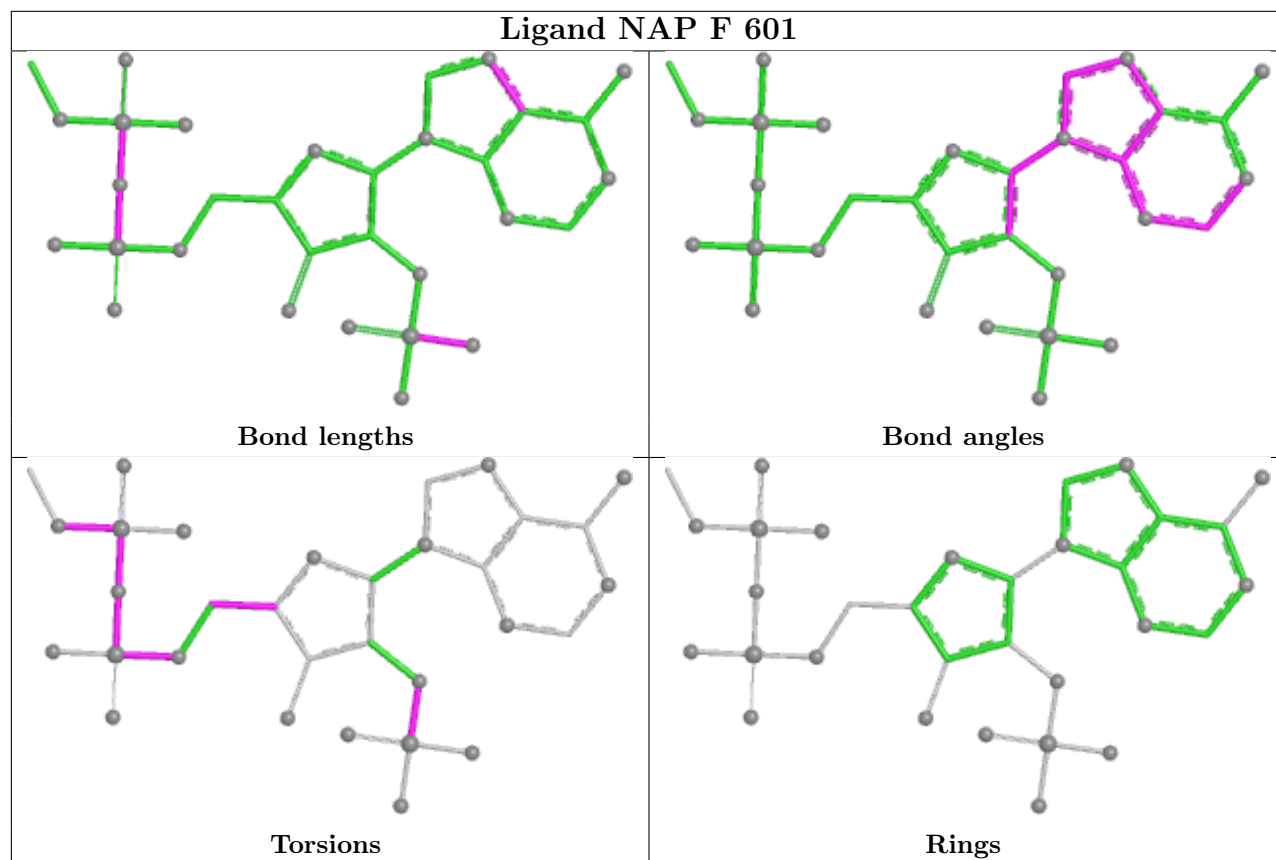
## Ligand NAP E 601











## 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     | 489/499 (97%)   | 1.17   | 66 (13%) 7 5   | 24, 63, 74, 102       | 0     |
| 1   | B     | 489/499 (97%)   | 1.20   | 52 (10%) 11 10 | 24, 63, 74, 102       | 0     |
| 1   | C     | 485/499 (97%)   | 2.05   | 225 (46%) 0 0  | 24, 63, 74, 103       | 0     |
| 1   | D     | 490/499 (98%)   | 1.65   | 127 (25%) 1 1  | 24, 63, 75, 102       | 0     |
| 1   | E     | 489/499 (97%)   | 1.48   | 110 (22%) 2 2  | 24, 63, 74, 101       | 0     |
| 1   | F     | 488/499 (97%)   | 2.04   | 238 (48%) 0 0  | 24, 63, 74, 101       | 0     |
| All | All   | 2930/2994 (97%) | 1.60   | 818 (27%) 1 1  | 24, 63, 74, 103       | 0     |

All (818) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 499 | GLY  | 8.7  |
| 1   | D     | 497 | CYS  | 7.0  |
| 1   | B     | 499 | GLY  | 6.5  |
| 1   | E     | 499 | GLY  | 6.2  |
| 1   | C     | 302 | LEU  | 6.1  |
| 1   | F     | 331 | ALA  | 6.0  |
| 1   | D     | 496 | GLY  | 5.7  |
| 1   | E     | 495 | SER  | 5.7  |
| 1   | C     | 157 | PHE  | 5.7  |
| 1   | E     | 427 | CYS  | 5.5  |
| 1   | C     | 154 | ALA  | 5.4  |
| 1   | F     | 140 | ILE  | 5.4  |
| 1   | C     | 335 | ILE  | 5.4  |
| 1   | E     | 429 | LEU  | 5.4  |
| 1   | E     | 428 | ASN  | 5.3  |
| 1   | F     | 134 | PHE  | 5.1  |
| 1   | E     | 362 | THR  | 5.0  |
| 1   | C     | 168 | LEU  | 5.0  |
| 1   | D     | 429 | LEU  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 398 | ASN  | 4.9  |
| 1   | F     | 305 | VAL  | 4.9  |
| 1   | C     | 295 | SER  | 4.9  |
| 1   | C     | 297 | THR  | 4.9  |
| 1   | D     | 394 | PHE  | 4.9  |
| 1   | C     | 296 | CYS  | 4.9  |
| 1   | C     | 132 | GLY  | 4.8  |
| 1   | F     | 306 | GLY  | 4.8  |
| 1   | C     | 140 | ILE  | 4.7  |
| 1   | F     | 297 | THR  | 4.7  |
| 1   | E     | 497 | CYS  | 4.6  |
| 1   | F     | 269 | VAL  | 4.6  |
| 1   | C     | 256 | ILE  | 4.6  |
| 1   | A     | 499 | GLY  | 4.6  |
| 1   | C     | 158 | LEU  | 4.6  |
| 1   | F     | 15  | LEU  | 4.5  |
| 1   | F     | 135 | ILE  | 4.5  |
| 1   | C     | 152 | TYR  | 4.5  |
| 1   | F     | 328 | TYR  | 4.4  |
| 1   | F     | 358 | TYR  | 4.4  |
| 1   | C     | 15  | LEU  | 4.4  |
| 1   | C     | 354 | ALA  | 4.4  |
| 1   | C     | 365 | CYS  | 4.4  |
| 1   | E     | 433 | GLU  | 4.4  |
| 1   | C     | 153 | SER  | 4.4  |
| 1   | F     | 427 | CYS  | 4.4  |
| 1   | C     | 253 | PRO  | 4.3  |
| 1   | E     | 490 | GLY  | 4.3  |
| 1   | C     | 135 | ILE  | 4.3  |
| 1   | F     | 132 | GLY  | 4.3  |
| 1   | C     | 255 | LYS  | 4.3  |
| 1   | C     | 163 | GLU  | 4.2  |
| 1   | C     | 324 | THR  | 4.2  |
| 1   | F     | 399 | ILE  | 4.2  |
| 1   | A     | 10  | SER  | 4.2  |
| 1   | C     | 271 | ALA  | 4.2  |
| 1   | C     | 329 | ILE  | 4.1  |
| 1   | B     | 154 | ALA  | 4.1  |
| 1   | C     | 334 | ASP  | 4.1  |
| 1   | B     | 497 | CYS  | 4.1  |
| 1   | F     | 137 | PRO  | 4.1  |
| 1   | F     | 160 | ALA  | 4.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 131 | TYR  | 4.1  |
| 1   | B     | 169 | GLY  | 4.1  |
| 1   | C     | 316 | ILE  | 4.1  |
| 1   | D     | 186 | LEU  | 4.1  |
| 1   | C     | 305 | VAL  | 4.1  |
| 1   | C     | 495 | SER  | 4.1  |
| 1   | E     | 461 | THR  | 4.1  |
| 1   | F     | 158 | LEU  | 4.0  |
| 1   | F     | 324 | THR  | 4.0  |
| 1   | C     | 299 | THR  | 4.0  |
| 1   | F     | 130 | ALA  | 4.0  |
| 1   | D     | 402 | TYR  | 4.0  |
| 1   | B     | 334 | ASP  | 4.0  |
| 1   | D     | 251 | PHE  | 4.0  |
| 1   | D     | 334 | ASP  | 4.0  |
| 1   | E     | 432 | ASN  | 4.0  |
| 1   | F     | 318 | VAL  | 3.9  |
| 1   | F     | 279 | THR  | 3.9  |
| 1   | C     | 151 | VAL  | 3.9  |
| 1   | F     | 52  | ARG  | 3.9  |
| 1   | E     | 400 | GLU  | 3.9  |
| 1   | E     | 402 | TYR  | 3.9  |
| 1   | C     | 281 | GLU  | 3.9  |
| 1   | E     | 469 | ILE  | 3.9  |
| 1   | F     | 391 | VAL  | 3.9  |
| 1   | C     | 330 | TYR  | 3.8  |
| 1   | C     | 16  | ILE  | 3.8  |
| 1   | C     | 328 | TYR  | 3.8  |
| 1   | E     | 396 | GLU  | 3.8  |
| 1   | D     | 354 | ALA  | 3.8  |
| 1   | F     | 142 | ALA  | 3.8  |
| 1   | C     | 304 | THR  | 3.8  |
| 1   | C     | 169 | GLY  | 3.8  |
| 1   | C     | 496 | GLY  | 3.8  |
| 1   | C     | 282 | ASP  | 3.8  |
| 1   | F     | 131 | TYR  | 3.8  |
| 1   | F     | 141 | MET  | 3.8  |
| 1   | C     | 307 | VAL  | 3.8  |
| 1   | C     | 188 | TYR  | 3.7  |
| 1   | C     | 332 | ILE  | 3.7  |
| 1   | D     | 332 | ILE  | 3.7  |
| 1   | F     | 157 | PHE  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 300 | ILE  | 3.7  |
| 1   | D     | 495 | SER  | 3.7  |
| 1   | E     | 425 | VAL  | 3.7  |
| 1   | C     | 322 | GLU  | 3.7  |
| 1   | C     | 284 | PHE  | 3.7  |
| 1   | F     | 228 | PHE  | 3.7  |
| 1   | C     | 44  | VAL  | 3.7  |
| 1   | C     | 137 | PRO  | 3.7  |
| 1   | C     | 252 | VAL  | 3.7  |
| 1   | B     | 493 | LEU  | 3.6  |
| 1   | E     | 482 | LEU  | 3.6  |
| 1   | F     | 152 | TYR  | 3.6  |
| 1   | C     | 134 | PHE  | 3.6  |
| 1   | C     | 56  | GLY  | 3.6  |
| 1   | B     | 92  | ASP  | 3.6  |
| 1   | C     | 130 | ALA  | 3.6  |
| 1   | C     | 306 | GLY  | 3.6  |
| 1   | F     | 438 | PHE  | 3.6  |
| 1   | B     | 52  | ARG  | 3.6  |
| 1   | F     | 143 | THR  | 3.6  |
| 1   | C     | 303 | GLU  | 3.6  |
| 1   | D     | 494 | GLN  | 3.6  |
| 1   | F     | 304 | THR  | 3.5  |
| 1   | D     | 459 | GLY  | 3.5  |
| 1   | F     | 278 | GLU  | 3.5  |
| 1   | E     | 463 | GLN  | 3.5  |
| 1   | F     | 22  | SER  | 3.5  |
| 1   | F     | 398 | ASN  | 3.5  |
| 1   | D     | 57  | GLY  | 3.5  |
| 1   | C     | 116 | TYR  | 3.5  |
| 1   | C     | 143 | THR  | 3.5  |
| 1   | A     | 244 | GLY  | 3.5  |
| 1   | F     | 335 | ILE  | 3.5  |
| 1   | D     | 427 | CYS  | 3.5  |
| 1   | D     | 272 | LYS  | 3.5  |
| 1   | C     | 260 | GLU  | 3.5  |
| 1   | F     | 283 | GLU  | 3.5  |
| 1   | F     | 307 | VAL  | 3.5  |
| 1   | C     | 65  | ILE  | 3.4  |
| 1   | C     | 270 | THR  | 3.4  |
| 1   | B     | 496 | GLY  | 3.4  |
| 1   | C     | 35  | ASP  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 352 | LEU  | 3.4  |
| 1   | F     | 436 | VAL  | 3.4  |
| 1   | C     | 139 | LYS  | 3.4  |
| 1   | F     | 21  | GLY  | 3.4  |
| 1   | F     | 387 | GLU  | 3.4  |
| 1   | F     | 428 | ASN  | 3.4  |
| 1   | F     | 38  | VAL  | 3.4  |
| 1   | E     | 468 | THR  | 3.4  |
| 1   | D     | 31  | ALA  | 3.4  |
| 1   | F     | 171 | PRO  | 3.4  |
| 1   | F     | 284 | PHE  | 3.4  |
| 1   | C     | 142 | ALA  | 3.3  |
| 1   | E     | 496 | GLY  | 3.3  |
| 1   | F     | 323 | GLN  | 3.3  |
| 1   | F     | 196 | VAL  | 3.3  |
| 1   | D     | 259 | ILE  | 3.3  |
| 1   | F     | 256 | ILE  | 3.3  |
| 1   | C     | 161 | THR  | 3.3  |
| 1   | E     | 279 | THR  | 3.3  |
| 1   | C     | 219 | MET  | 3.3  |
| 1   | C     | 261 | ALA  | 3.3  |
| 1   | E     | 418 | ASN  | 3.3  |
| 1   | F     | 247 | PHE  | 3.3  |
| 1   | D     | 169 | GLY  | 3.3  |
| 1   | F     | 20  | GLY  | 3.3  |
| 1   | C     | 125 | VAL  | 3.3  |
| 1   | F     | 294 | ASP  | 3.3  |
| 1   | B     | 396 | GLU  | 3.3  |
| 1   | C     | 45  | THR  | 3.3  |
| 1   | C     | 63  | GLY  | 3.3  |
| 1   | C     | 40  | VAL  | 3.3  |
| 1   | C     | 318 | VAL  | 3.3  |
| 1   | F     | 13  | PHE  | 3.3  |
| 1   | F     | 497 | CYS  | 3.2  |
| 1   | D     | 166 | ARG  | 3.2  |
| 1   | C     | 19  | GLY  | 3.2  |
| 1   | E     | 394 | PHE  | 3.2  |
| 1   | F     | 184 | PHE  | 3.2  |
| 1   | F     | 326 | VAL  | 3.2  |
| 1   | C     | 336 | LEU  | 3.2  |
| 1   | C     | 58  | THR  | 3.2  |
| 1   | F     | 499 | GLY  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 390 | ALA  | 3.2  |
| 1   | C     | 220 | VAL  | 3.2  |
| 1   | F     | 394 | PHE  | 3.2  |
| 1   | F     | 400 | GLU  | 3.2  |
| 1   | C     | 338 | GLY  | 3.2  |
| 1   | F     | 19  | GLY  | 3.2  |
| 1   | C     | 331 | ALA  | 3.2  |
| 1   | F     | 60  | VAL  | 3.2  |
| 1   | C     | 320 | ASP  | 3.2  |
| 1   | F     | 64  | CYS  | 3.2  |
| 1   | C     | 21  | GLY  | 3.2  |
| 1   | D     | 56  | GLY  | 3.2  |
| 1   | D     | 198 | ALA  | 3.2  |
| 1   | D     | 273 | SER  | 3.2  |
| 1   | F     | 295 | SER  | 3.2  |
| 1   | F     | 334 | ASP  | 3.1  |
| 1   | F     | 39  | MET  | 3.1  |
| 1   | B     | 447 | GLU  | 3.1  |
| 1   | A     | 365 | CYS  | 3.1  |
| 1   | C     | 20  | GLY  | 3.1  |
| 1   | C     | 280 | ILE  | 3.1  |
| 1   | C     | 361 | SER  | 3.1  |
| 1   | E     | 431 | ASP  | 3.1  |
| 1   | C     | 250 | GLN  | 3.1  |
| 1   | E     | 360 | GLY  | 3.1  |
| 1   | D     | 114 | TRP  | 3.1  |
| 1   | F     | 276 | SER  | 3.1  |
| 1   | C     | 141 | MET  | 3.1  |
| 1   | C     | 176 | TYR  | 3.1  |
| 1   | F     | 225 | LEU  | 3.1  |
| 1   | F     | 138 | HIS  | 3.1  |
| 1   | C     | 170 | ILE  | 3.1  |
| 1   | D     | 426 | ILE  | 3.1  |
| 1   | F     | 280 | ILE  | 3.1  |
| 1   | C     | 312 | LYS  | 3.1  |
| 1   | F     | 34  | PHE  | 3.1  |
| 1   | C     | 460 | LEU  | 3.1  |
| 1   | D     | 168 | LEU  | 3.1  |
| 1   | F     | 41  | LEU  | 3.1  |
| 1   | C     | 323 | GLN  | 3.1  |
| 1   | F     | 254 | THR  | 3.1  |
| 1   | E     | 455 | ALA  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 493 | LEU  | 3.0  |
| 1   | F     | 176 | TYR  | 3.0  |
| 1   | C     | 317 | PRO  | 3.0  |
| 1   | E     | 491 | ASP  | 3.0  |
| 1   | F     | 268 | LYS  | 3.0  |
| 1   | C     | 314 | GLY  | 3.0  |
| 1   | C     | 43  | PHE  | 3.0  |
| 1   | F     | 342 | LEU  | 3.0  |
| 1   | E     | 294 | ASP  | 3.0  |
| 1   | E     | 399 | ILE  | 3.0  |
| 1   | E     | 434 | ARG  | 3.0  |
| 1   | F     | 172 | GLY  | 3.0  |
| 1   | F     | 300 | ILE  | 3.0  |
| 1   | C     | 269 | VAL  | 3.0  |
| 1   | C     | 345 | VAL  | 3.0  |
| 1   | F     | 208 | PHE  | 3.0  |
| 1   | D     | 482 | LEU  | 3.0  |
| 1   | C     | 39  | MET  | 3.0  |
| 1   | C     | 178 | ILE  | 3.0  |
| 1   | F     | 356 | ARG  | 3.0  |
| 1   | F     | 270 | THR  | 3.0  |
| 1   | F     | 354 | ALA  | 3.0  |
| 1   | D     | 436 | VAL  | 3.0  |
| 1   | C     | 49  | LEU  | 3.0  |
| 1   | C     | 267 | LEU  | 3.0  |
| 1   | C     | 456 | LEU  | 3.0  |
| 1   | F     | 267 | LEU  | 3.0  |
| 1   | F     | 357 | LEU  | 3.0  |
| 1   | A     | 59  | CYS  | 3.0  |
| 1   | C     | 497 | CYS  | 3.0  |
| 1   | C     | 144 | ASN  | 3.0  |
| 1   | F     | 200 | TYR  | 3.0  |
| 1   | C     | 356 | ARG  | 3.0  |
| 1   | F     | 329 | ILE  | 3.0  |
| 1   | C     | 279 | THR  | 3.0  |
| 1   | E     | 345 | VAL  | 3.0  |
| 1   | E     | 435 | VAL  | 3.0  |
| 1   | E     | 493 | LEU  | 2.9  |
| 1   | E     | 277 | GLU  | 2.9  |
| 1   | F     | 303 | GLU  | 2.9  |
| 1   | C     | 180 | SER  | 2.9  |
| 1   | A     | 39  | MET  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 92  | ASP  | 2.9  |
| 1   | D     | 58  | THR  | 2.9  |
| 1   | C     | 122 | GLU  | 2.9  |
| 1   | C     | 278 | GLU  | 2.9  |
| 1   | F     | 311 | GLU  | 2.9  |
| 1   | C     | 259 | ILE  | 2.9  |
| 1   | D     | 291 | VAL  | 2.9  |
| 1   | E     | 278 | GLU  | 2.9  |
| 1   | E     | 397 | GLU  | 2.9  |
| 1   | F     | 139 | LYS  | 2.9  |
| 1   | C     | 165 | PRO  | 2.9  |
| 1   | F     | 144 | ASN  | 2.9  |
| 1   | C     | 18  | ILE  | 2.9  |
| 1   | D     | 92  | ASP  | 2.9  |
| 1   | E     | 422 | TYR  | 2.9  |
| 1   | F     | 248 | ILE  | 2.9  |
| 1   | F     | 282 | ASP  | 2.9  |
| 1   | F     | 332 | ILE  | 2.9  |
| 1   | D     | 157 | PHE  | 2.9  |
| 1   | D     | 257 | GLU  | 2.9  |
| 1   | A     | 334 | ASP  | 2.9  |
| 1   | E     | 92  | ASP  | 2.9  |
| 1   | C     | 286 | THR  | 2.9  |
| 1   | F     | 58  | THR  | 2.9  |
| 1   | F     | 313 | THR  | 2.9  |
| 1   | F     | 154 | ALA  | 2.9  |
| 1   | C     | 283 | GLU  | 2.8  |
| 1   | D     | 397 | GLU  | 2.8  |
| 1   | B     | 172 | GLY  | 2.8  |
| 1   | C     | 360 | GLY  | 2.8  |
| 1   | F     | 136 | GLY  | 2.8  |
| 1   | F     | 314 | GLY  | 2.8  |
| 1   | F     | 359 | GLY  | 2.8  |
| 1   | A     | 497 | CYS  | 2.8  |
| 1   | F     | 423 | ALA  | 2.8  |
| 1   | F     | 178 | ILE  | 2.8  |
| 1   | C     | 268 | LYS  | 2.8  |
| 1   | F     | 45  | THR  | 2.8  |
| 1   | F     | 167 | TYR  | 2.8  |
| 1   | F     | 271 | ALA  | 2.8  |
| 1   | F     | 372 | THR  | 2.8  |
| 1   | E     | 391 | VAL  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 91  | GLU  | 2.8  |
| 1   | D     | 430 | LYS  | 2.8  |
| 1   | E     | 430 | LYS  | 2.8  |
| 1   | E     | 492 | ILE  | 2.8  |
| 1   | F     | 153 | SER  | 2.8  |
| 1   | D     | 261 | ALA  | 2.8  |
| 1   | D     | 379 | GLU  | 2.8  |
| 1   | F     | 195 | VAL  | 2.8  |
| 1   | E     | 59  | CYS  | 2.8  |
| 1   | C     | 121 | ARG  | 2.8  |
| 1   | E     | 258 | GLN  | 2.8  |
| 1   | A     | 56  | GLY  | 2.8  |
| 1   | C     | 384 | GLY  | 2.8  |
| 1   | D     | 472 | HIS  | 2.8  |
| 1   | C     | 290 | ALA  | 2.8  |
| 1   | C     | 374 | VAL  | 2.8  |
| 1   | C     | 383 | CYS  | 2.7  |
| 1   | C     | 123 | LYS  | 2.7  |
| 1   | F     | 272 | LYS  | 2.7  |
| 1   | A     | 276 | SER  | 2.7  |
| 1   | E     | 19  | GLY  | 2.7  |
| 1   | E     | 437 | GLY  | 2.7  |
| 1   | C     | 138 | HIS  | 2.7  |
| 1   | C     | 149 | GLU  | 2.7  |
| 1   | E     | 436 | VAL  | 2.7  |
| 1   | F     | 40  | VAL  | 2.7  |
| 1   | F     | 161 | THR  | 2.7  |
| 1   | C     | 298 | ARG  | 2.7  |
| 1   | F     | 406 | PHE  | 2.7  |
| 1   | A     | 358 | TYR  | 2.7  |
| 1   | C     | 46  | PRO  | 2.7  |
| 1   | C     | 167 | TYR  | 2.7  |
| 1   | C     | 367 | TYR  | 2.7  |
| 1   | F     | 37  | LYS  | 2.7  |
| 1   | E     | 332 | ILE  | 2.7  |
| 1   | D     | 493 | LEU  | 2.7  |
| 1   | F     | 352 | LEU  | 2.7  |
| 1   | D     | 21  | GLY  | 2.7  |
| 1   | D     | 54  | GLY  | 2.7  |
| 1   | E     | 114 | TRP  | 2.7  |
| 1   | C     | 34  | PHE  | 2.7  |
| 1   | C     | 38  | VAL  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 126 | VAL  | 2.7  |
| 1   | C     | 274 | THR  | 2.7  |
| 1   | D     | 44  | VAL  | 2.7  |
| 1   | D     | 297 | THR  | 2.7  |
| 1   | D     | 346 | ALA  | 2.7  |
| 1   | C     | 327 | PRO  | 2.7  |
| 1   | F     | 253 | PRO  | 2.7  |
| 1   | B     | 494 | GLN  | 2.7  |
| 1   | C     | 59  | CYS  | 2.7  |
| 1   | C     | 159 | ILE  | 2.7  |
| 1   | C     | 409 | LEU  | 2.7  |
| 1   | A     | 147 | GLY  | 2.7  |
| 1   | A     | 311 | GLU  | 2.7  |
| 1   | C     | 175 | GLU  | 2.7  |
| 1   | F     | 293 | ARG  | 2.7  |
| 1   | F     | 218 | VAL  | 2.7  |
| 1   | F     | 42  | ASP  | 2.7  |
| 1   | E     | 464 | GLN  | 2.7  |
| 1   | E     | 176 | TYR  | 2.7  |
| 1   | B     | 399 | ILE  | 2.7  |
| 1   | E     | 383 | CYS  | 2.7  |
| 1   | D     | 115 | GLY  | 2.7  |
| 1   | F     | 197 | GLY  | 2.7  |
| 1   | A     | 199 | SER  | 2.7  |
| 1   | D     | 433 | GLU  | 2.7  |
| 1   | E     | 274 | THR  | 2.7  |
| 1   | F     | 315 | LYS  | 2.7  |
| 1   | F     | 349 | ALA  | 2.7  |
| 1   | E     | 366 | ASP  | 2.7  |
| 1   | F     | 231 | ASP  | 2.7  |
| 1   | D     | 399 | ILE  | 2.6  |
| 1   | A     | 69  | LEU  | 2.6  |
| 1   | C     | 357 | LEU  | 2.6  |
| 1   | F     | 183 | LEU  | 2.6  |
| 1   | F     | 340 | LEU  | 2.6  |
| 1   | C     | 266 | ARG  | 2.6  |
| 1   | A     | 40  | VAL  | 2.6  |
| 1   | F     | 484 | VAL  | 2.6  |
| 1   | C     | 187 | PRO  | 2.6  |
| 1   | B     | 11  | TYR  | 2.6  |
| 1   | D     | 471 | ILE  | 2.6  |
| 1   | E     | 426 | ILE  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 11  | TYR  | 2.6  |
| 1   | F     | 219 | MET  | 2.6  |
| 1   | D     | 117 | ARG  | 2.6  |
| 1   | D     | 28  | ALA  | 2.6  |
| 1   | D     | 432 | ASN  | 2.6  |
| 1   | F     | 199 | SER  | 2.6  |
| 1   | C     | 263 | THR  | 2.6  |
| 1   | C     | 376 | THR  | 2.6  |
| 1   | F     | 327 | PRO  | 2.6  |
| 1   | E     | 494 | GLN  | 2.6  |
| 1   | F     | 18  | ILE  | 2.6  |
| 1   | E     | 465 | LEU  | 2.6  |
| 1   | A     | 91  | GLU  | 2.6  |
| 1   | C     | 128 | GLU  | 2.6  |
| 1   | F     | 147 | GLY  | 2.6  |
| 1   | F     | 442 | GLY  | 2.6  |
| 1   | C     | 326 | VAL  | 2.6  |
| 1   | E     | 363 | VAL  | 2.6  |
| 1   | F     | 435 | VAL  | 2.6  |
| 1   | F     | 405 | PHE  | 2.6  |
| 1   | B     | 449 | THR  | 2.6  |
| 1   | C     | 258 | GLN  | 2.6  |
| 1   | D     | 143 | THR  | 2.6  |
| 1   | F     | 223 | ILE  | 2.6  |
| 1   | C     | 353 | LEU  | 2.6  |
| 1   | F     | 441 | LEU  | 2.6  |
| 1   | A     | 328 | TYR  | 2.6  |
| 1   | C     | 337 | GLU  | 2.6  |
| 1   | C     | 264 | PRO  | 2.6  |
| 1   | F     | 220 | VAL  | 2.6  |
| 1   | A     | 494 | GLN  | 2.6  |
| 1   | C     | 182 | ASP  | 2.5  |
| 1   | A     | 309 | ILE  | 2.5  |
| 1   | D     | 469 | ILE  | 2.5  |
| 1   | F     | 492 | ILE  | 2.5  |
| 1   | F     | 336 | LEU  | 2.5  |
| 1   | D     | 268 | LYS  | 2.5  |
| 1   | F     | 36  | LYS  | 2.5  |
| 1   | F     | 486 | LYS  | 2.5  |
| 1   | B     | 127 | TYR  | 2.5  |
| 1   | E     | 257 | GLU  | 2.5  |
| 1   | F     | 337 | GLU  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 265 | GLY  | 2.5  |
| 1   | B     | 137 | PRO  | 2.5  |
| 1   | F     | 251 | PHE  | 2.5  |
| 1   | D     | 35  | ASP  | 2.5  |
| 1   | D     | 466 | ASP  | 2.5  |
| 1   | D     | 140 | ILE  | 2.5  |
| 1   | A     | 278 | GLU  | 2.5  |
| 1   | D     | 91  | GLU  | 2.5  |
| 1   | D     | 337 | GLU  | 2.5  |
| 1   | F     | 322 | GLU  | 2.5  |
| 1   | F     | 48  | PRO  | 2.5  |
| 1   | C     | 105 | VAL  | 2.5  |
| 1   | A     | 455 | ALA  | 2.5  |
| 1   | C     | 177 | CYS  | 2.5  |
| 1   | F     | 325 | ASN  | 2.5  |
| 1   | D     | 22  | SER  | 2.5  |
| 1   | C     | 309 | ILE  | 2.5  |
| 1   | E     | 29  | LYS  | 2.5  |
| 1   | E     | 65  | ILE  | 2.5  |
| 1   | F     | 259 | ILE  | 2.5  |
| 1   | A     | 90  | LEU  | 2.5  |
| 1   | B     | 460 | LEU  | 2.5  |
| 1   | D     | 460 | LEU  | 2.5  |
| 1   | F     | 120 | LEU  | 2.5  |
| 1   | F     | 224 | LEU  | 2.5  |
| 1   | F     | 493 | LEU  | 2.5  |
| 1   | D     | 122 | GLU  | 2.5  |
| 1   | E     | 136 | GLY  | 2.5  |
| 1   | C     | 344 | PRO  | 2.5  |
| 1   | F     | 44  | VAL  | 2.5  |
| 1   | F     | 287 | VAL  | 2.5  |
| 1   | B     | 134 | PHE  | 2.5  |
| 1   | D     | 32  | ALA  | 2.5  |
| 1   | A     | 124 | LYS  | 2.5  |
| 1   | C     | 36  | LYS  | 2.5  |
| 1   | D     | 419 | ASN  | 2.5  |
| 1   | B     | 135 | ILE  | 2.5  |
| 1   | D     | 55  | LEU  | 2.5  |
| 1   | F     | 156 | ARG  | 2.5  |
| 1   | F     | 298 | ARG  | 2.5  |
| 1   | F     | 302 | LEU  | 2.5  |
| 1   | F     | 460 | LEU  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 162 | GLY  | 2.5  |
| 1   | C     | 48  | PRO  | 2.5  |
| 1   | C     | 425 | VAL  | 2.5  |
| 1   | E     | 44  | VAL  | 2.5  |
| 1   | D     | 119 | ALA  | 2.5  |
| 1   | E     | 32  | ALA  | 2.5  |
| 1   | A     | 52  | ARG  | 2.4  |
| 1   | C     | 145 | ASN  | 2.4  |
| 1   | E     | 121 | ARG  | 2.4  |
| 1   | E     | 159 | ILE  | 2.4  |
| 1   | F     | 426 | ILE  | 2.4  |
| 1   | B     | 495 | SER  | 2.4  |
| 1   | E     | 334 | ASP  | 2.4  |
| 1   | E     | 403 | HIS  | 2.4  |
| 1   | A     | 306 | GLY  | 2.4  |
| 1   | D     | 162 | GLY  | 2.4  |
| 1   | F     | 244 | GLY  | 2.4  |
| 1   | F     | 116 | TYR  | 2.4  |
| 1   | A     | 420 | LYS  | 2.4  |
| 1   | C     | 150 | LYS  | 2.4  |
| 1   | C     | 233 | ALA  | 2.4  |
| 1   | D     | 228 | PHE  | 2.4  |
| 1   | A     | 93  | THR  | 2.4  |
| 1   | F     | 49  | LEU  | 2.4  |
| 1   | F     | 180 | SER  | 2.4  |
| 1   | C     | 155 | GLU  | 2.4  |
| 1   | D     | 400 | GLU  | 2.4  |
| 1   | A     | 317 | PRO  | 2.4  |
| 1   | C     | 395 | GLY  | 2.4  |
| 1   | F     | 24  | GLY  | 2.4  |
| 1   | F     | 133 | LYS  | 2.4  |
| 1   | A     | 11  | TYR  | 2.4  |
| 1   | B     | 328 | TYR  | 2.4  |
| 1   | B     | 422 | TYR  | 2.4  |
| 1   | E     | 200 | TYR  | 2.4  |
| 1   | E     | 374 | VAL  | 2.4  |
| 1   | C     | 160 | ALA  | 2.4  |
| 1   | A     | 225 | LEU  | 2.4  |
| 1   | C     | 426 | ILE  | 2.4  |
| 1   | D     | 313 | THR  | 2.4  |
| 1   | E     | 90  | LEU  | 2.4  |
| 1   | A     | 275 | ASN  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 83  | SER  | 2.4  |
| 1   | F     | 361 | SER  | 2.4  |
| 1   | D     | 320 | ASP  | 2.4  |
| 1   | C     | 189 | CYS  | 2.4  |
| 1   | D     | 296 | CYS  | 2.4  |
| 1   | C     | 364 | LYS  | 2.4  |
| 1   | F     | 169 | GLY  | 2.4  |
| 1   | F     | 437 | GLY  | 2.4  |
| 1   | B     | 318 | VAL  | 2.4  |
| 1   | D     | 401 | VAL  | 2.4  |
| 1   | F     | 62  | VAL  | 2.4  |
| 1   | F     | 203 | LEU  | 2.4  |
| 1   | A     | 324 | THR  | 2.4  |
| 1   | D     | 161 | THR  | 2.4  |
| 1   | D     | 285 | ASN  | 2.4  |
| 1   | B     | 10  | SER  | 2.4  |
| 1   | C     | 386 | SER  | 2.4  |
| 1   | F     | 277 | GLU  | 2.4  |
| 1   | A     | 294 | ASP  | 2.4  |
| 1   | B     | 466 | ASP  | 2.4  |
| 1   | C     | 97  | ASP  | 2.4  |
| 1   | D     | 491 | ASP  | 2.4  |
| 1   | F     | 317 | PRO  | 2.4  |
| 1   | B     | 206 | ALA  | 2.4  |
| 1   | B     | 155 | GLU  | 2.3  |
| 1   | F     | 175 | GLU  | 2.3  |
| 1   | A     | 182 | ASP  | 2.3  |
| 1   | A     | 495 | SER  | 2.3  |
| 1   | E     | 36  | LYS  | 2.3  |
| 1   | F     | 222 | SER  | 2.3  |
| 1   | B     | 338 | GLY  | 2.3  |
| 1   | D     | 23  | GLY  | 2.3  |
| 1   | F     | 191 | GLY  | 2.3  |
| 1   | C     | 52  | ARG  | 2.3  |
| 1   | F     | 463 | GLN  | 2.3  |
| 1   | A     | 62  | VAL  | 2.3  |
| 1   | C     | 60  | VAL  | 2.3  |
| 1   | C     | 196 | VAL  | 2.3  |
| 1   | C     | 291 | VAL  | 2.3  |
| 1   | D     | 118 | VAL  | 2.3  |
| 1   | C     | 251 | PHE  | 2.3  |
| 1   | C     | 41  | LEU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 352 | LEU  | 2.3  |
| 1   | E     | 460 | LEU  | 2.3  |
| 1   | F     | 289 | LEU  | 2.3  |
| 1   | E     | 480 | THR  | 2.3  |
| 1   | F     | 343 | THR  | 2.3  |
| 1   | C     | 99  | GLU  | 2.3  |
| 1   | C     | 133 | LYS  | 2.3  |
| 1   | D     | 277 | GLU  | 2.3  |
| 1   | D     | 341 | GLU  | 2.3  |
| 1   | F     | 388 | GLU  | 2.3  |
| 1   | F     | 165 | PRO  | 2.3  |
| 1   | A     | 54  | GLY  | 2.3  |
| 1   | F     | 207 | GLY  | 2.3  |
| 1   | B     | 60  | VAL  | 2.3  |
| 1   | C     | 202 | ALA  | 2.3  |
| 1   | F     | 378 | LEU  | 2.3  |
| 1   | B     | 316 | ILE  | 2.3  |
| 1   | D     | 245 | ILE  | 2.3  |
| 1   | F     | 316 | ILE  | 2.3  |
| 1   | A     | 127 | TYR  | 2.3  |
| 1   | C     | 313 | THR  | 2.3  |
| 1   | D     | 176 | TYR  | 2.3  |
| 1   | F     | 274 | THR  | 2.3  |
| 1   | B     | 37  | LYS  | 2.3  |
| 1   | B     | 392 | GLU  | 2.3  |
| 1   | F     | 155 | GLU  | 2.3  |
| 1   | F     | 386 | SER  | 2.3  |
| 1   | D     | 84  | ARG  | 2.3  |
| 1   | D     | 121 | ARG  | 2.3  |
| 1   | E     | 407 | TRP  | 2.3  |
| 1   | E     | 350 | GLY  | 2.3  |
| 1   | F     | 227 | GLY  | 2.3  |
| 1   | A     | 305 | VAL  | 2.3  |
| 1   | C     | 436 | VAL  | 2.3  |
| 1   | F     | 374 | VAL  | 2.3  |
| 1   | B     | 340 | LEU  | 2.3  |
| 1   | D     | 284 | PHE  | 2.3  |
| 1   | C     | 212 | ILE  | 2.3  |
| 1   | E     | 16  | ILE  | 2.3  |
| 1   | E     | 140 | ILE  | 2.3  |
| 1   | F     | 31  | ALA  | 2.3  |
| 1   | A     | 312 | LYS  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 150 | LYS  | 2.3  |
| 1   | D     | 428 | ASN  | 2.3  |
| 1   | F     | 351 | ARG  | 2.3  |
| 1   | C     | 25  | LEU  | 2.3  |
| 1   | C     | 75  | LEU  | 2.3  |
| 1   | E     | 401 | VAL  | 2.3  |
| 1   | C     | 248 | ILE  | 2.2  |
| 1   | D     | 492 | ILE  | 2.2  |
| 1   | E     | 335 | ILE  | 2.2  |
| 1   | E     | 346 | ALA  | 2.2  |
| 1   | E     | 365 | CYS  | 2.2  |
| 1   | F     | 177 | CYS  | 2.2  |
| 1   | F     | 445 | ALA  | 2.2  |
| 1   | F     | 255 | LYS  | 2.2  |
| 1   | A     | 313 | THR  | 2.2  |
| 1   | B     | 128 | GLU  | 2.2  |
| 1   | F     | 260 | GLU  | 2.2  |
| 1   | D     | 358 | TYR  | 2.2  |
| 1   | C     | 129 | ASN  | 2.2  |
| 1   | E     | 419 | ASN  | 2.2  |
| 1   | F     | 121 | ARG  | 2.2  |
| 1   | A     | 320 | ASP  | 2.2  |
| 1   | C     | 147 | GLY  | 2.2  |
| 1   | C     | 197 | GLY  | 2.2  |
| 1   | E     | 20  | GLY  | 2.2  |
| 1   | E     | 23  | GLY  | 2.2  |
| 1   | F     | 87  | GLY  | 2.2  |
| 1   | B     | 220 | VAL  | 2.2  |
| 1   | C     | 289 | LEU  | 2.2  |
| 1   | D     | 38  | VAL  | 2.2  |
| 1   | D     | 62  | VAL  | 2.2  |
| 1   | D     | 391 | VAL  | 2.2  |
| 1   | F     | 69  | LEU  | 2.2  |
| 1   | F     | 353 | LEU  | 2.2  |
| 1   | D     | 16  | ILE  | 2.2  |
| 1   | D     | 27  | ALA  | 2.2  |
| 1   | E     | 471 | ILE  | 2.2  |
| 1   | C     | 382 | CYS  | 2.2  |
| 1   | C     | 257 | GLU  | 2.2  |
| 1   | E     | 387 | GLU  | 2.2  |
| 1   | D     | 61  | ASN  | 2.2  |
| 1   | F     | 275 | ASN  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 23  | GLY  | 2.2  |
| 1   | C     | 181 | ASP  | 2.2  |
| 1   | C     | 276 | SER  | 2.2  |
| 1   | C     | 301 | GLY  | 2.2  |
| 1   | F     | 14  | ASP  | 2.2  |
| 1   | F     | 496 | GLY  | 2.2  |
| 1   | C     | 225 | LEU  | 2.2  |
| 1   | D     | 90  | LEU  | 2.2  |
| 1   | F     | 456 | LEU  | 2.2  |
| 1   | F     | 345 | VAL  | 2.2  |
| 1   | D     | 280 | ILE  | 2.2  |
| 1   | E     | 453 | ALA  | 2.2  |
| 1   | F     | 290 | ALA  | 2.2  |
| 1   | C     | 362 | THR  | 2.2  |
| 1   | F     | 296 | CYS  | 2.2  |
| 1   | F     | 348 | GLN  | 2.2  |
| 1   | F     | 450 | GLN  | 2.2  |
| 1   | A     | 207 | GLY  | 2.2  |
| 1   | C     | 172 | GLY  | 2.2  |
| 1   | A     | 22  | SER  | 2.2  |
| 1   | A     | 120 | LEU  | 2.2  |
| 1   | A     | 338 | GLY  | 2.2  |
| 1   | A     | 153 | SER  | 2.2  |
| 1   | C     | 378 | LEU  | 2.2  |
| 1   | C     | 389 | LYS  | 2.2  |
| 1   | E     | 146 | LYS  | 2.2  |
| 1   | F     | 82  | ASP  | 2.2  |
| 1   | F     | 429 | LEU  | 2.2  |
| 1   | D     | 60  | VAL  | 2.2  |
| 1   | D     | 109 | ILE  | 2.2  |
| 1   | F     | 261 | ALA  | 2.2  |
| 1   | F     | 454 | ALA  | 2.2  |
| 1   | B     | 311 | GLU  | 2.2  |
| 1   | F     | 241 | GLU  | 2.2  |
| 1   | D     | 167 | TYR  | 2.2  |
| 1   | B     | 463 | GLN  | 2.2  |
| 1   | C     | 224 | LEU  | 2.2  |
| 1   | D     | 267 | LEU  | 2.2  |
| 1   | F     | 214 | LEU  | 2.2  |
| 1   | F     | 182 | ASP  | 2.2  |
| 1   | C     | 22  | SER  | 2.2  |
| 1   | D     | 222 | SER  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 179 | SER  | 2.2  |
| 1   | B     | 426 | ILE  | 2.2  |
| 1   | D     | 178 | ILE  | 2.2  |
| 1   | F     | 252 | VAL  | 2.2  |
| 1   | F     | 309 | ILE  | 2.2  |
| 1   | E     | 479 | PHE  | 2.2  |
| 1   | A     | 31  | ALA  | 2.1  |
| 1   | A     | 271 | ALA  | 2.1  |
| 1   | C     | 397 | GLU  | 2.1  |
| 1   | D     | 163 | GLU  | 2.1  |
| 1   | C     | 254 | THR  | 2.1  |
| 1   | D     | 434 | ARG  | 2.1  |
| 1   | E     | 487 | ARG  | 2.1  |
| 1   | C     | 457 | LYS  | 2.1  |
| 1   | E     | 11  | TYR  | 2.1  |
| 1   | C     | 120 | LEU  | 2.1  |
| 1   | C     | 499 | GLY  | 2.1  |
| 1   | F     | 350 | GLY  | 2.1  |
| 1   | A     | 243 | HIS  | 2.1  |
| 1   | B     | 280 | ILE  | 2.1  |
| 1   | D     | 425 | VAL  | 2.1  |
| 1   | F     | 12  | ASP  | 2.1  |
| 1   | E     | 404 | SER  | 2.1  |
| 1   | E     | 228 | PHE  | 2.1  |
| 1   | F     | 53  | TRP  | 2.1  |
| 1   | F     | 84  | ARG  | 2.1  |
| 1   | B     | 143 | THR  | 2.1  |
| 1   | F     | 376 | THR  | 2.1  |
| 1   | E     | 327 | PRO  | 2.1  |
| 1   | F     | 364 | LYS  | 2.1  |
| 1   | F     | 355 | GLN  | 2.1  |
| 1   | F     | 383 | CYS  | 2.1  |
| 1   | C     | 232 | MET  | 2.1  |
| 1   | D     | 127 | TYR  | 2.1  |
| 1   | F     | 422 | TYR  | 2.1  |
| 1   | B     | 20  | GLY  | 2.1  |
| 1   | C     | 136 | GLY  | 2.1  |
| 1   | C     | 359 | GLY  | 2.1  |
| 1   | F     | 57  | GLY  | 2.1  |
| 1   | F     | 63  | GLY  | 2.1  |
| 1   | A     | 245 | ILE  | 2.1  |
| 1   | A     | 252 | VAL  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 326 | VAL  | 2.1  |
| 1   | D     | 126 | VAL  | 2.1  |
| 1   | B     | 251 | PHE  | 2.1  |
| 1   | E     | 34  | PHE  | 2.1  |
| 1   | D     | 455 | ALA  | 2.1  |
| 1   | B     | 163 | GLU  | 2.1  |
| 1   | D     | 53  | TRP  | 2.1  |
| 1   | D     | 164 | ARG  | 2.1  |
| 1   | E     | 117 | ARG  | 2.1  |
| 1   | E     | 58  | THR  | 2.1  |
| 1   | D     | 174 | LYS  | 2.1  |
| 1   | E     | 268 | LYS  | 2.1  |
| 1   | A     | 340 | LEU  | 2.1  |
| 1   | E     | 385 | LEU  | 2.1  |
| 1   | D     | 145 | ASN  | 2.1  |
| 1   | A     | 176 | TYR  | 2.1  |
| 1   | C     | 24  | GLY  | 2.1  |
| 1   | C     | 50  | GLY  | 2.1  |
| 1   | C     | 358 | TYR  | 2.1  |
| 1   | C     | 459 | GLY  | 2.1  |
| 1   | F     | 265 | GLY  | 2.1  |
| 1   | F     | 459 | GLY  | 2.1  |
| 1   | F     | 448 | VAL  | 2.1  |
| 1   | A     | 228 | PHE  | 2.1  |
| 1   | C     | 293 | ARG  | 2.1  |
| 1   | D     | 271 | ALA  | 2.1  |
| 1   | D     | 283 | GLU  | 2.1  |
| 1   | D     | 331 | ALA  | 2.1  |
| 1   | F     | 166 | ARG  | 2.1  |
| 1   | F     | 455 | ALA  | 2.1  |
| 1   | D     | 29  | LYS  | 2.1  |
| 1   | D     | 37  | LYS  | 2.1  |
| 1   | C     | 371 | PRO  | 2.1  |
| 1   | D     | 317 | PRO  | 2.1  |
| 1   | A     | 342 | LEU  | 2.1  |
| 1   | B     | 69  | LEU  | 2.1  |
| 1   | F     | 385 | LEU  | 2.1  |
| 1   | A     | 325 | ASN  | 2.1  |
| 1   | B     | 432 | ASN  | 2.1  |
| 1   | C     | 325 | ASN  | 2.1  |
| 1   | D     | 338 | GLY  | 2.1  |
| 1   | D     | 458 | CYS  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 395 | GLY  | 2.1  |
| 1   | F     | 365 | CYS  | 2.1  |
| 1   | B     | 176 | TYR  | 2.1  |
| 1   | C     | 380 | TYR  | 2.1  |
| 1   | E     | 256 | ILE  | 2.1  |
| 1   | C     | 173 | ASP  | 2.0  |
| 1   | C     | 184 | PHE  | 2.1  |
| 1   | C     | 346 | ALA  | 2.0  |
| 1   | C     | 37  | LYS  | 2.0  |
| 1   | D     | 89  | LYS  | 2.0  |
| 1   | A     | 279 | THR  | 2.0  |
| 1   | C     | 186 | LEU  | 2.0  |
| 1   | D     | 120 | LEU  | 2.0  |
| 1   | F     | 168 | LEU  | 2.0  |
| 1   | E     | 145 | ASN  | 2.0  |
| 1   | A     | 211 | GLY  | 2.0  |
| 1   | A     | 496 | GLY  | 2.0  |
| 1   | B     | 471 | ILE  | 2.0  |
| 1   | E     | 24  | GLY  | 2.0  |
| 1   | B     | 188 | TYR  | 2.0  |
| 1   | C     | 200 | TYR  | 2.0  |
| 1   | D     | 59  | CYS  | 2.0  |
| 1   | F     | 163 | GLU  | 2.0  |
| 1   | C     | 119 | ALA  | 2.0  |
| 1   | C     | 420 | LYS  | 2.0  |
| 1   | E     | 139 | LYS  | 2.0  |
| 1   | E     | 154 | ALA  | 2.0  |
| 1   | D     | 276 | SER  | 2.0  |
| 1   | F     | 495 | SER  | 2.0  |
| 1   | C     | 98  | TRP  | 2.0  |
| 1   | B     | 55  | LEU  | 2.0  |
| 1   | C     | 55  | LEU  | 2.0  |
| 1   | C     | 333 | GLY  | 2.0  |
| 1   | C     | 398 | ASN  | 2.0  |
| 1   | D     | 135 | ILE  | 2.0  |
| 1   | D     | 360 | GLY  | 2.0  |
| 1   | F     | 50  | GLY  | 2.0  |
| 1   | A     | 121 | ARG  | 2.0  |
| 1   | B     | 370 | VAL  | 2.0  |
| 1   | C     | 363 | VAL  | 2.0  |
| 1   | E     | 196 | VAL  | 2.0  |
| 1   | F     | 249 | ARG  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 266 | ARG  | 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](#)

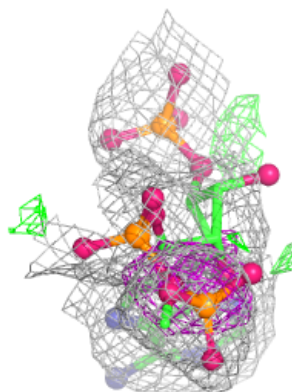
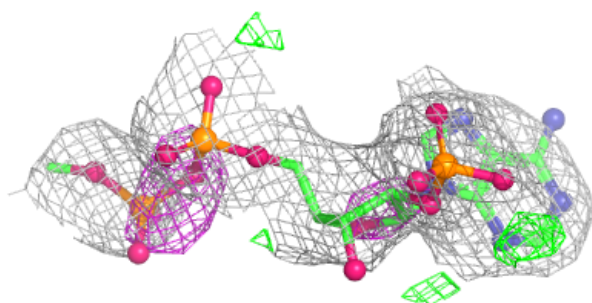
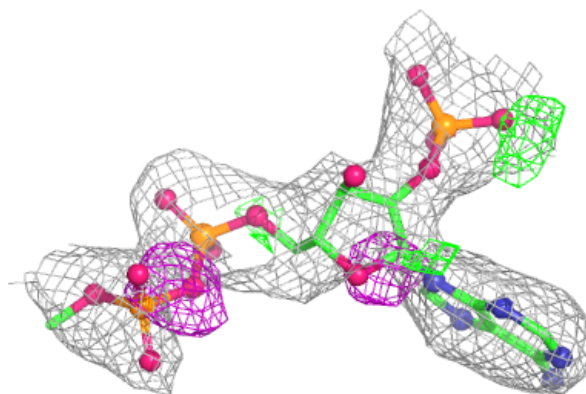
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | NAP  | F     | 601 | 32/48 | 0.67 | 0.19 | 64,74,99,100               | 0     |
| 2   | FAD  | F     | 600 | 53/53 | 0.68 | 0.20 | 60,64,70,71                | 0     |
| 3   | NAP  | C     | 601 | 32/48 | 0.74 | 0.18 | 64,74,99,100               | 0     |
| 2   | FAD  | C     | 600 | 53/53 | 0.79 | 0.18 | 60,64,70,71                | 0     |
| 3   | NAP  | E     | 601 | 32/48 | 0.82 | 0.17 | 64,74,99,100               | 0     |
| 3   | NAP  | D     | 601 | 32/48 | 0.85 | 0.17 | 64,74,99,100               | 0     |
| 3   | NAP  | B     | 601 | 32/48 | 0.86 | 0.16 | 64,74,99,100               | 0     |
| 3   | NAP  | A     | 601 | 32/48 | 0.87 | 0.13 | 64,74,99,99                | 0     |
| 2   | FAD  | E     | 600 | 53/53 | 0.93 | 0.15 | 60,64,70,71                | 0     |
| 2   | FAD  | B     | 600 | 53/53 | 0.94 | 0.12 | 60,64,70,72                | 0     |
| 2   | FAD  | A     | 600 | 53/53 | 0.94 | 0.11 | 60,64,70,71                | 0     |
| 2   | FAD  | D     | 600 | 53/53 | 0.95 | 0.16 | 60,64,70,72                | 0     |

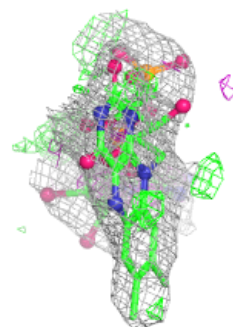
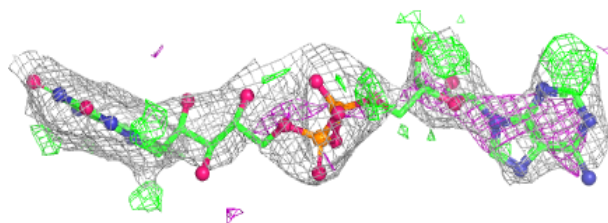
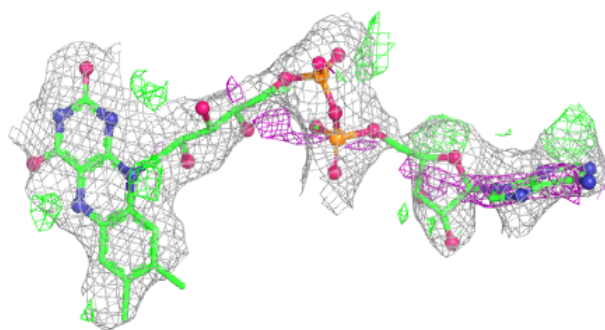
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP 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)

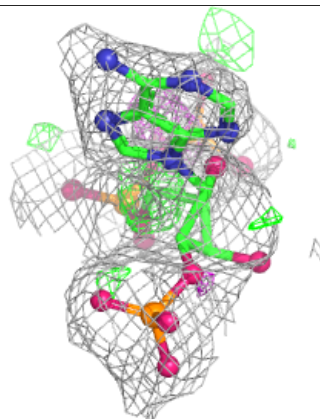
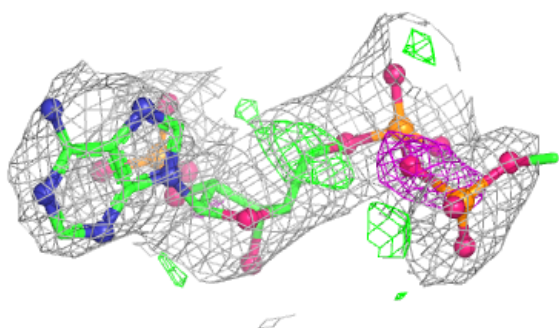
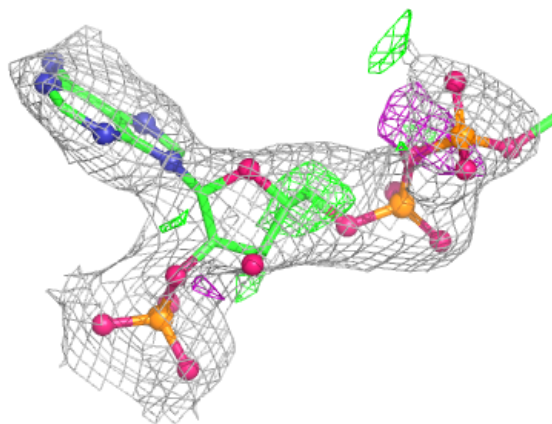
**Electron density around FAD F 600:**

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

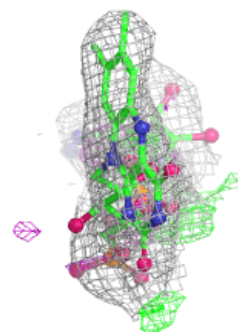
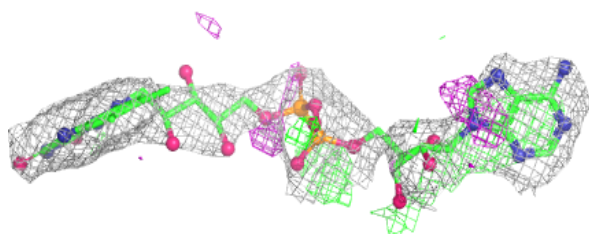
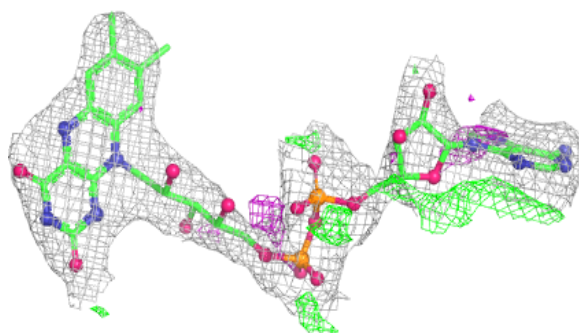


**Electron density around NAP C 601:**

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

**Electron density around FAD C 600:**

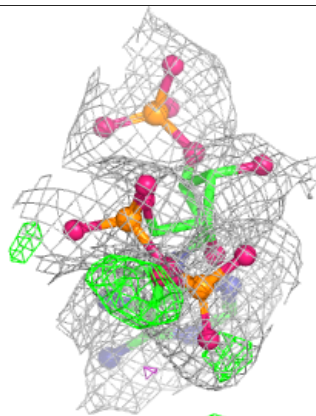
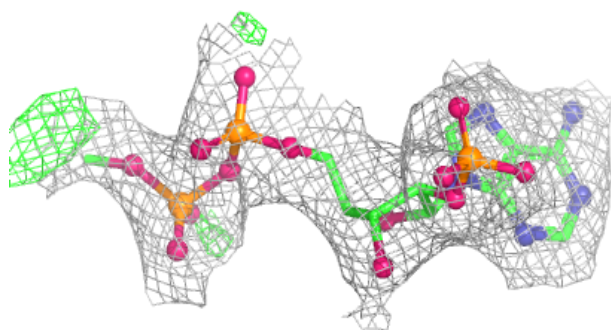
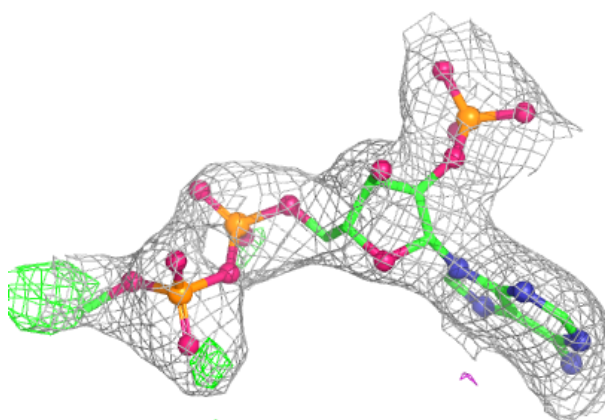
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





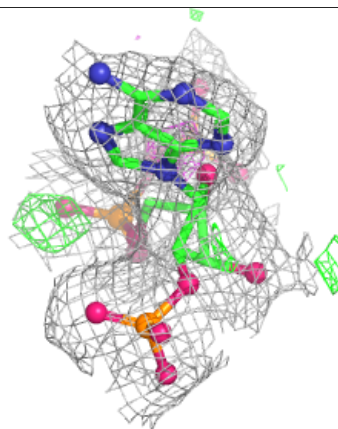
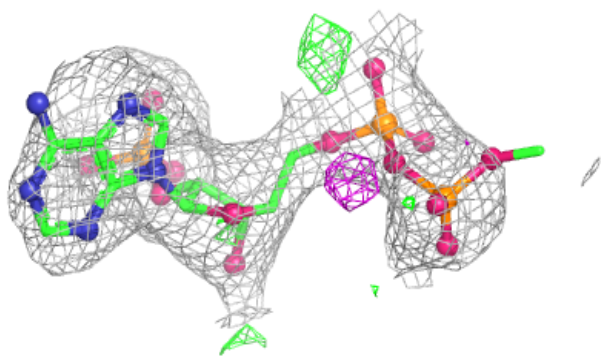
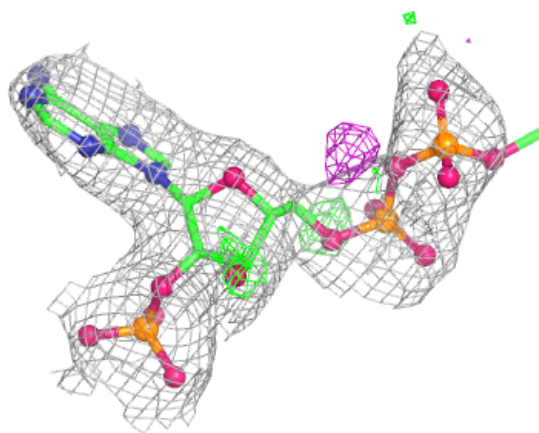
**Electron density around NAP E 601:**

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



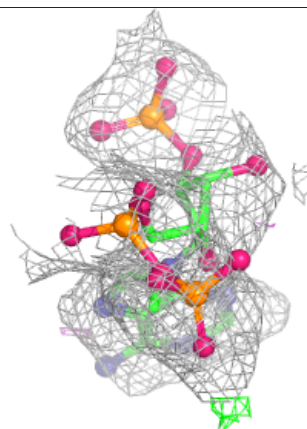
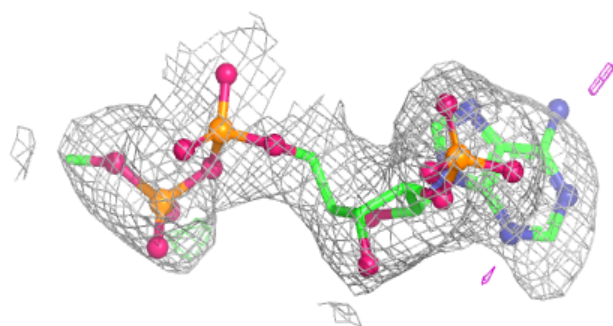
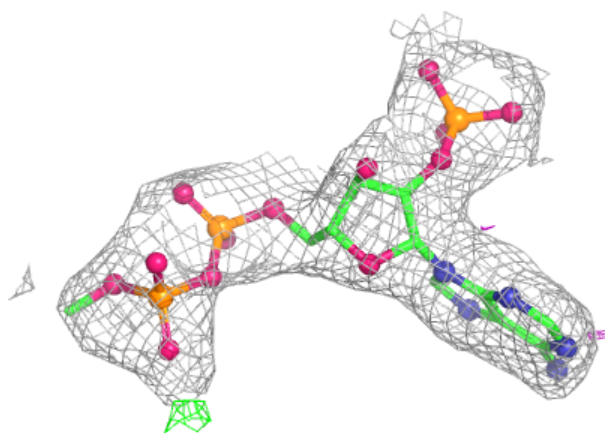
**Electron density around NAP D 601:**

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



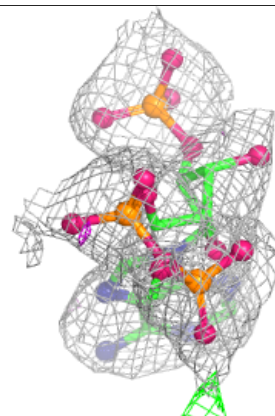
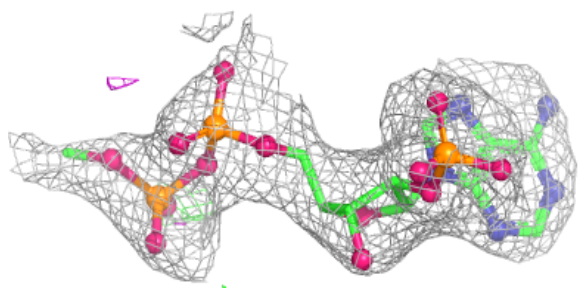
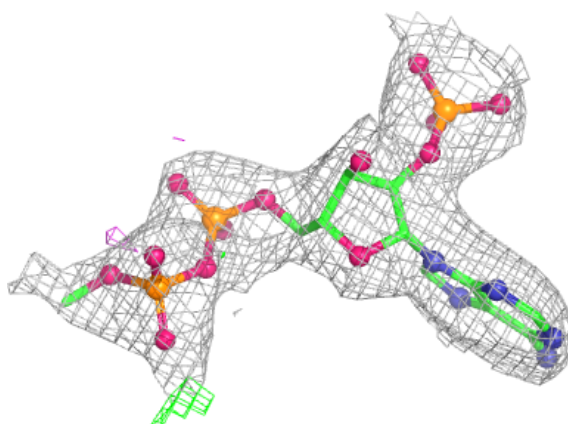
**Electron density around NAP B 601:**

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

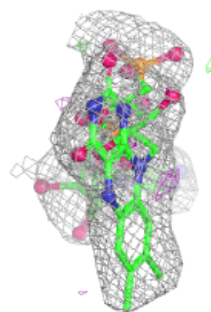
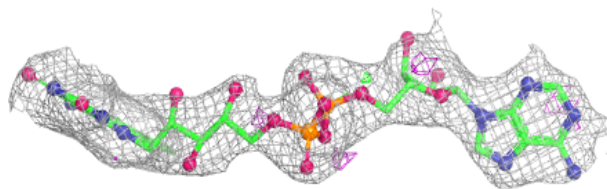
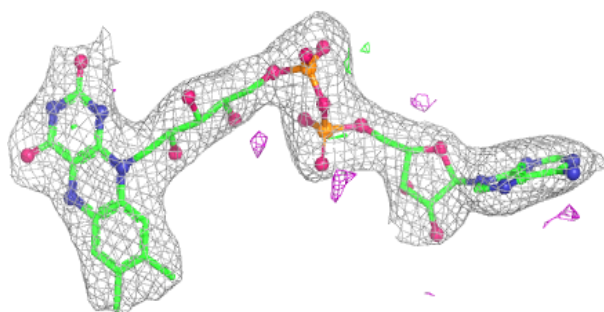


**Electron density around NAP A 601:**

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

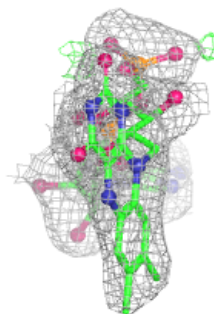
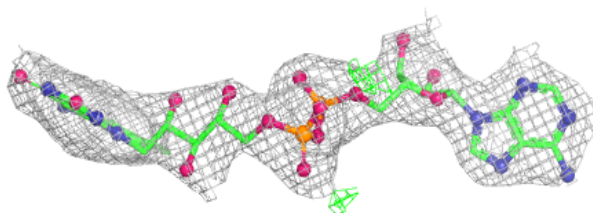
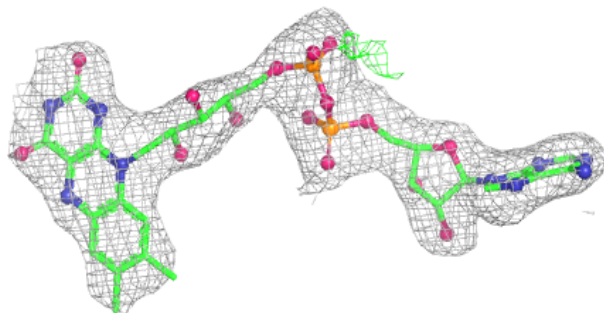
**Electron density around FAD E 600:**

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

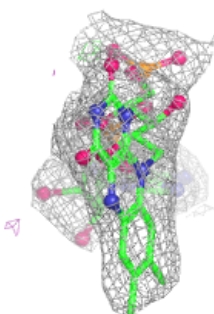
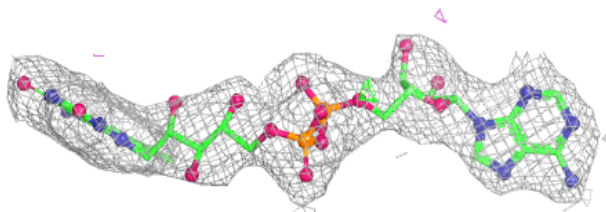
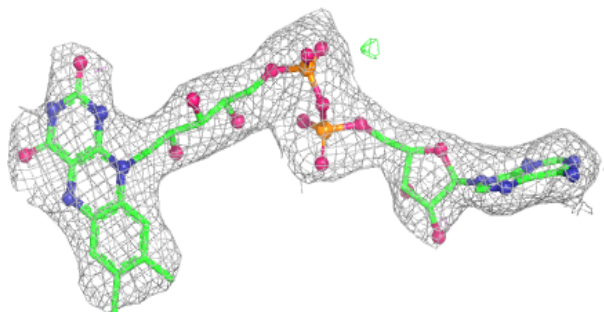


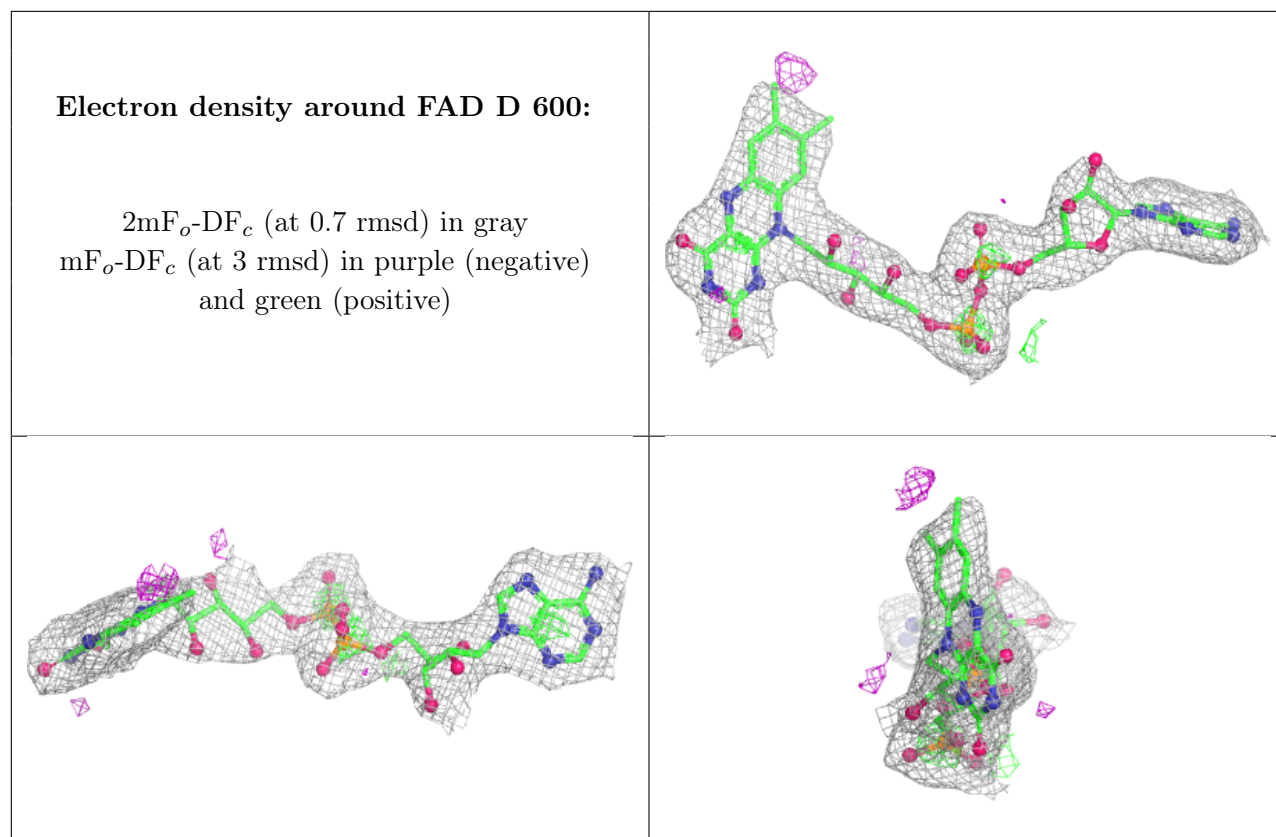
**Electron density around FAD B 600:**

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

**Electron density around FAD A 600:**

$2mF_o-DF_c$  (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.