



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 11:30 AM UTC

PDB ID : 3CF2 / pdb_00003cf2
Title : Structure of P97/vcp in complex with ADP/AMP-PNP
Authors : Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.
Deposited on : 2008-03-01
Resolution : 3.50 Å(reported)

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

We welcome your comments at 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>.

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

2 Entry composition [i](#)

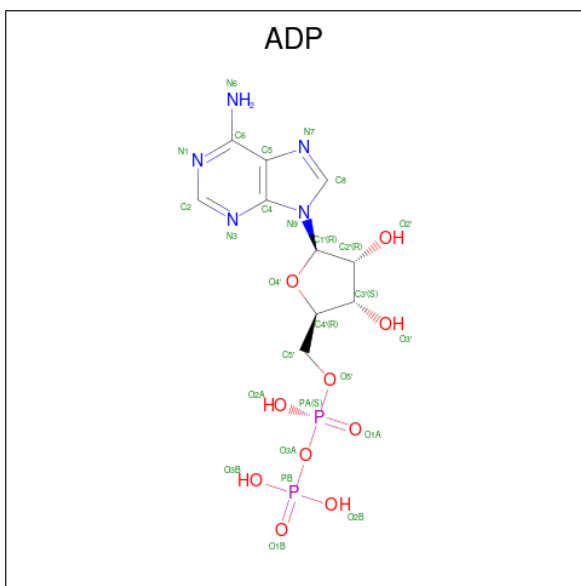
There are 3 unique types of molecules in this entry. The entry contains 20917 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transitional endoplasmic reticulum ATPase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 659 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5172 | 3263 | 903 | 977 | 29 | | | |
| 1 | B | 659 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5172 | 3263 | 903 | 977 | 29 | | | |
| 1 | C | 659 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5172 | 3263 | 903 | 977 | 29 | | | |
| 1 | D | 659 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5169 | 3260 | 903 | 977 | 29 | | | |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



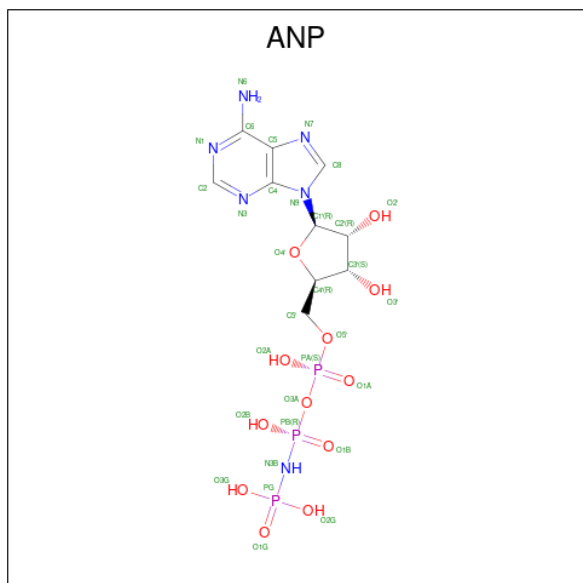
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| | | | Total | C | N | O | P | | |
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|---|----|---------|---------|---|
| | | | Total | C | N | O | | | P |
| 2 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|---|----|---------|---------|---|
| | | | Total | C | N | O | | | P |
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 6 | 12 | 3 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 6 | 12 | 3 | | |
| 3 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 6 | 12 | 3 | | |
| 3 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 6 | 12 | 3 | | |

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 3 | Depositor |
| Cell constants a, b, c, α , β , γ | 144.90Å 144.90Å 164.40Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 23.00 – 3.50 23.00 – 3.50 | Depositor EDS |
| % Data completeness (in resolution range) | 99.6 (23.00-3.50) 99.5 (23.00-3.50) | Depositor EDS |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.22 (at 3.23Å) | Xtrriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.271 , 0.285 0.289 , 0.291 | Depositor DCC |
| R_{free} test set | 6358 reflections (5.03%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 75.9 | Xtrriage |
| Anisotropy | 0.841 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.25 , 89.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$ | Xtrriage |
| Estimated twinning fraction | 0.369 for -h,-k,l 0.377 for h,-h-k,-l 0.369 for -k,-h,-l | Xtrriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 20917 | wwPDB-VP |
| Average B, all atoms (Å ²) | 148.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

8 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 |
| 3 | ANP | A | 901 | - | 33,33,33 | 2.06 | 12 (36%) | 45,52,52 | 2.06 | 10 (22%) |
| 2 | ADP | B | 807 | - | 28,29,29 | 1.89 | 4 (14%) | 43,45,45 | 2.05 | 8 (18%) |
| 2 | ADP | C | 807 | - | 28,29,29 | 1.89 | 4 (14%) | 43,45,45 | 2.06 | 8 (18%) |
| 2 | ADP | D | 807 | - | 28,29,29 | 1.89 | 4 (14%) | 43,45,45 | 2.06 | 8 (18%) |
| 3 | ANP | B | 901 | - | 33,33,33 | 2.06 | 12 (36%) | 45,52,52 | 2.06 | 10 (22%) |
| 3 | ANP | D | 901 | - | 33,33,33 | 2.06 | 12 (36%) | 45,52,52 | 2.07 | 10 (22%) |
| 2 | ADP | A | 807 | - | 28,29,29 | 1.89 | 4 (14%) | 43,45,45 | 2.06 | 8 (18%) |
| 3 | ANP | C | 901 | - | 33,33,33 | 2.05 | 12 (36%) | 45,52,52 | 2.06 | 10 (22%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | ANP | A | 901 | - | - | 7/18/38/38 | 0/3/3/3 |
| 2 | ADP | B | 807 | - | - | 6/16/32/32 | 0/3/3/3 |
| 2 | ADP | C | 807 | - | - | 6/16/32/32 | 0/3/3/3 |
| 2 | ADP | D | 807 | - | - | 6/16/32/32 | 0/3/3/3 |
| 3 | ANP | B | 901 | - | - | 7/18/38/38 | 0/3/3/3 |
| 3 | ANP | D | 901 | - | - | 7/18/38/38 | 0/3/3/3 |
| 2 | ADP | A | 807 | - | - | 6/16/32/32 | 0/3/3/3 |
| 3 | ANP | C | 901 | - | - | 7/18/38/38 | 0/3/3/3 |

The worst 5 of 64 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | A | 807 | ADP | PA-O3A | -5.34 | 1.53 | 1.59 |
| 2 | C | 807 | ADP | PA-O3A | -5.33 | 1.53 | 1.59 |
| 2 | D | 807 | ADP | PA-O3A | -5.33 | 1.53 | 1.59 |
| 2 | B | 807 | ADP | PA-O3A | -5.33 | 1.53 | 1.59 |
| 2 | B | 807 | ADP | C5-N7 | -5.13 | 1.29 | 1.39 |

The worst 5 of 72 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | C | 807 | ADP | N3-C2-N1 | -6.95 | 118.06 | 128.58 |
| 2 | A | 807 | ADP | N3-C2-N1 | -6.94 | 118.07 | 128.58 |
| 2 | D | 807 | ADP | N3-C2-N1 | -6.93 | 118.08 | 128.58 |
| 2 | B | 807 | ADP | N3-C2-N1 | -6.92 | 118.11 | 128.58 |
| 3 | B | 901 | ANP | N3-C2-N1 | -6.90 | 118.14 | 128.58 |

There are no chirality outliers.

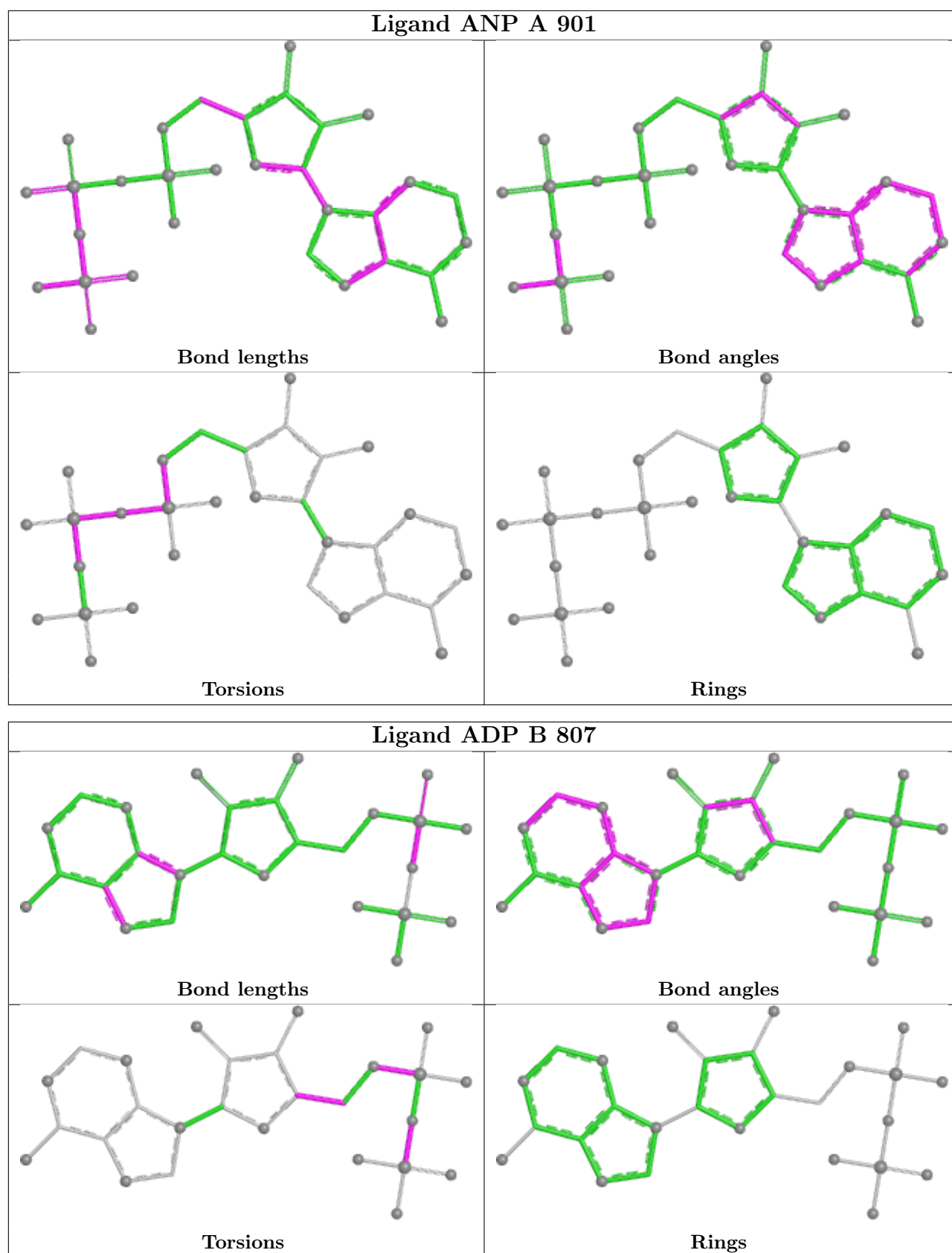
5 of 52 torsion outliers are listed below:

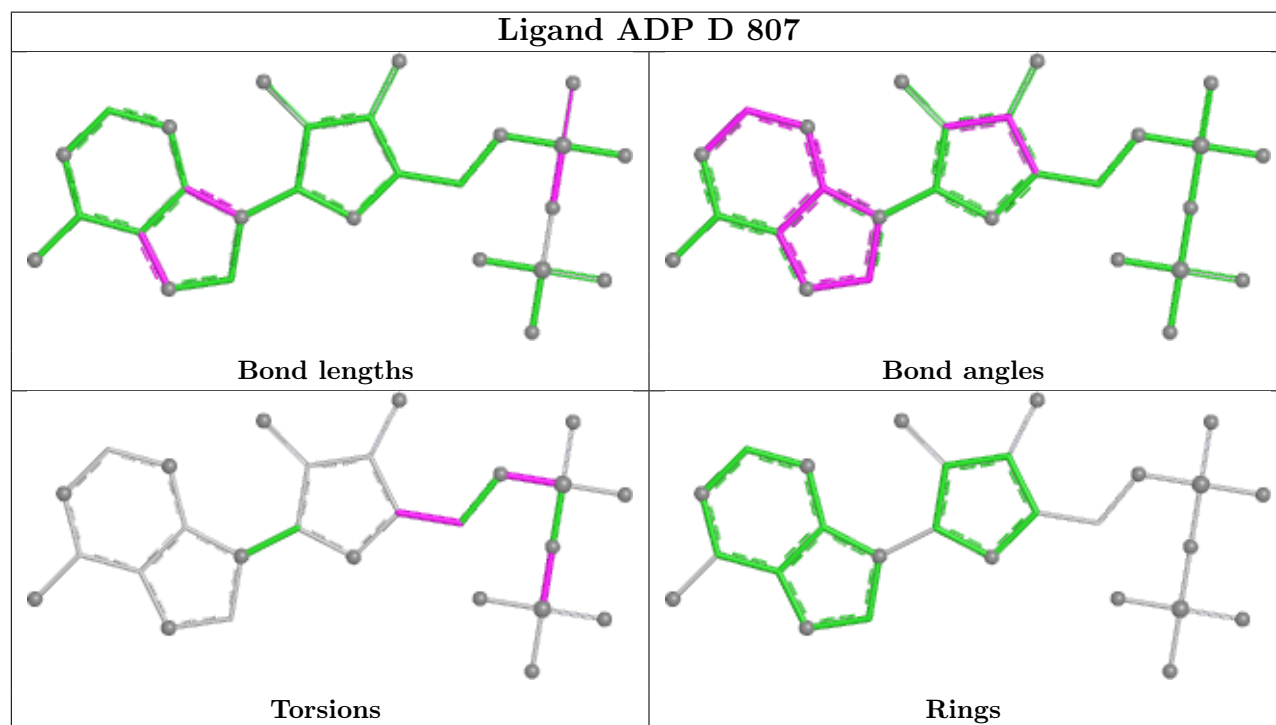
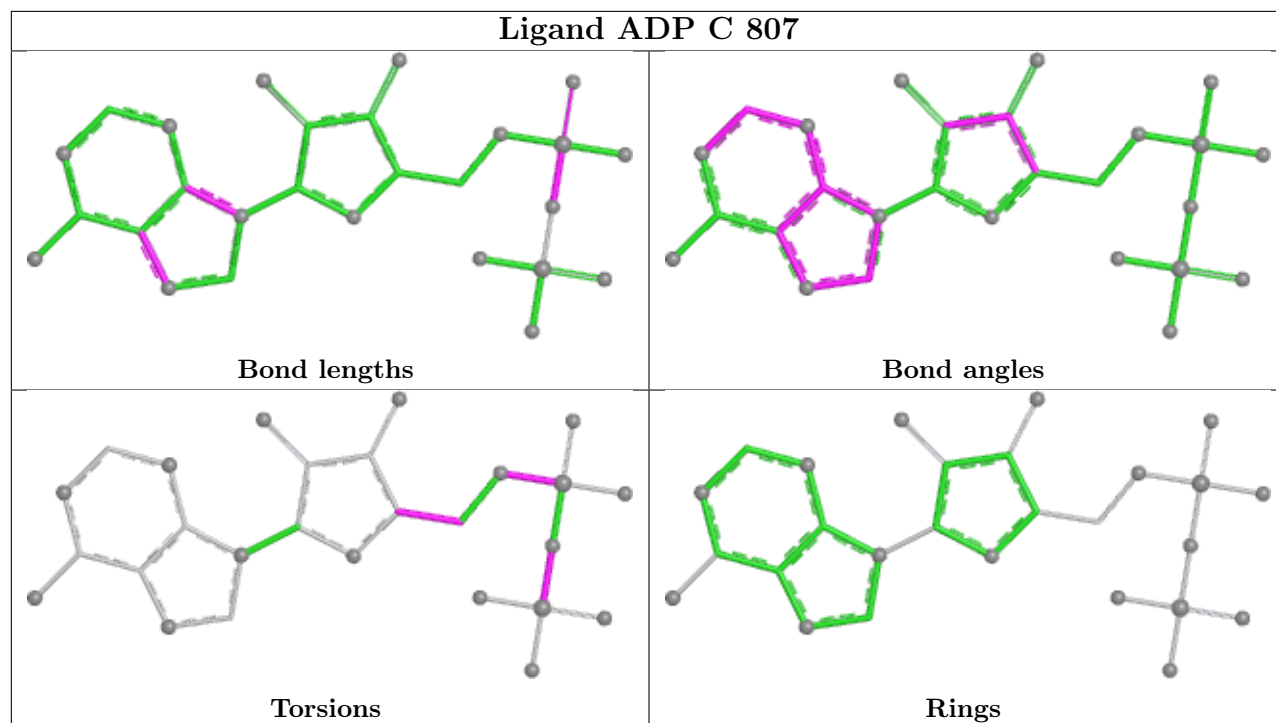
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | A | 807 | ADP | C5'-O5'-PA-O1A |
| 2 | A | 807 | ADP | C5'-O5'-PA-O2A |
| 2 | A | 807 | ADP | C5'-O5'-PA-O3A |
| 2 | A | 807 | ADP | O4'-C4'-C5'-O5' |
| 2 | B | 807 | ADP | C5'-O5'-PA-O1A |

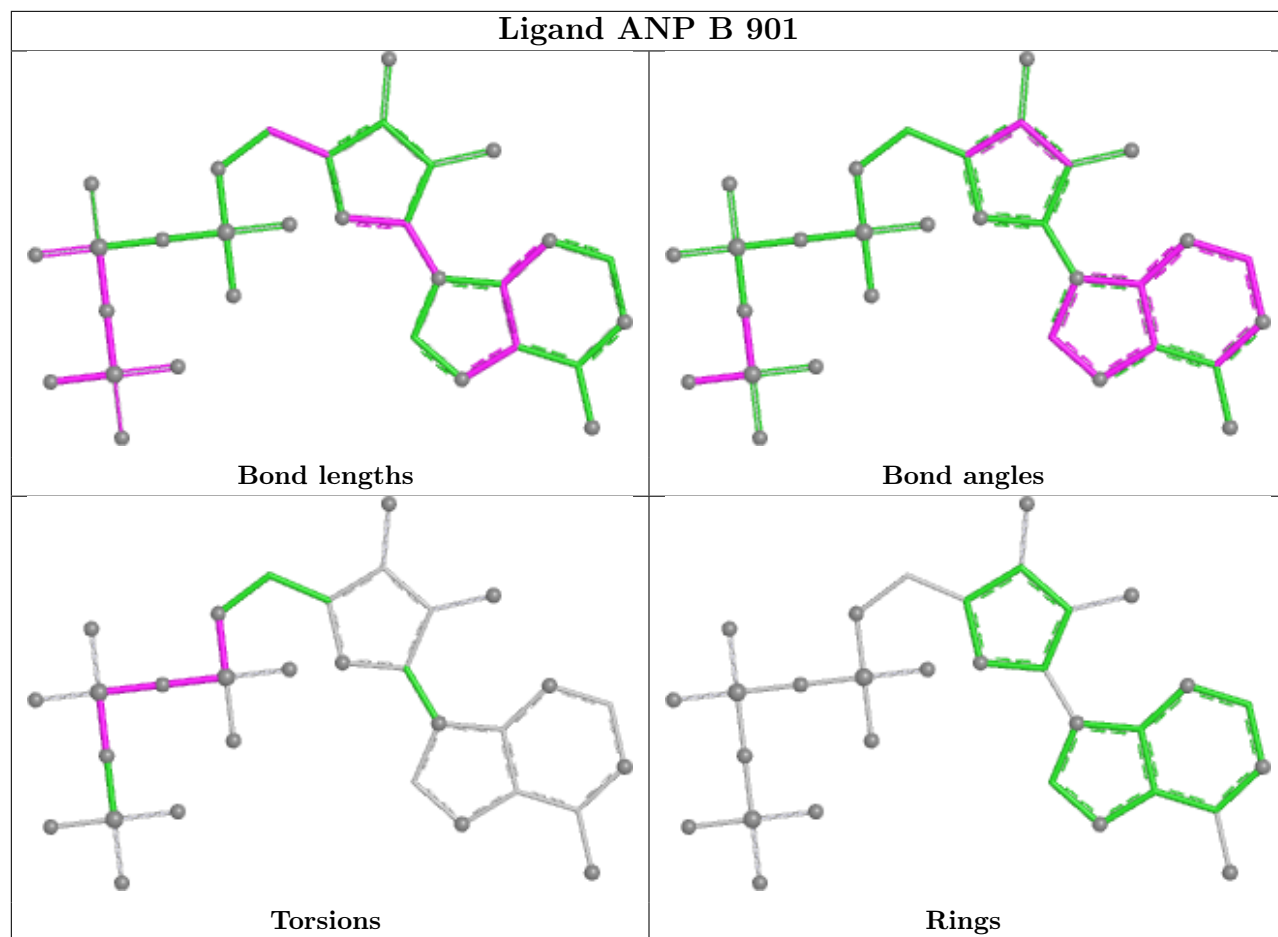
There are no ring outliers.

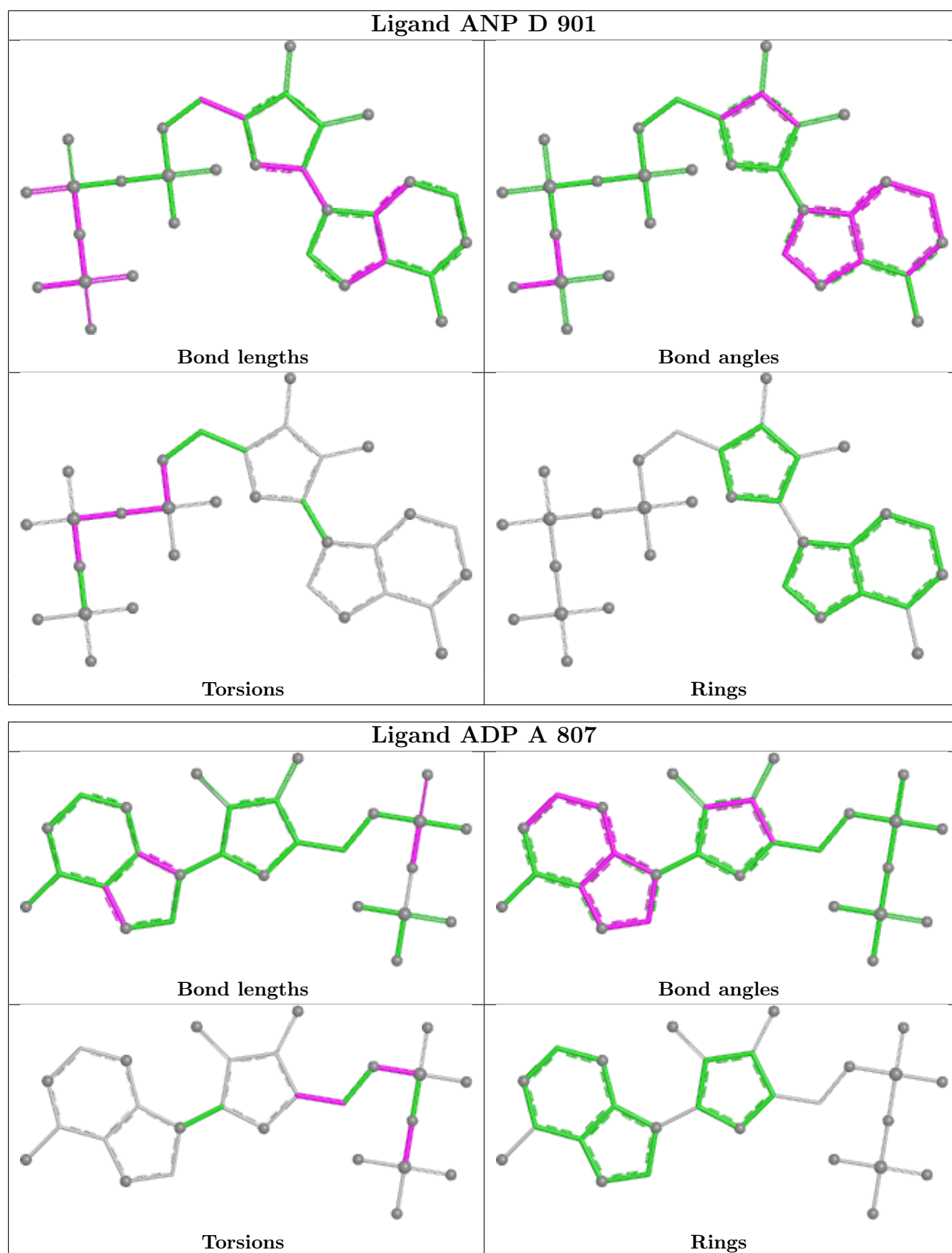
No monomer is involved in short contacts.

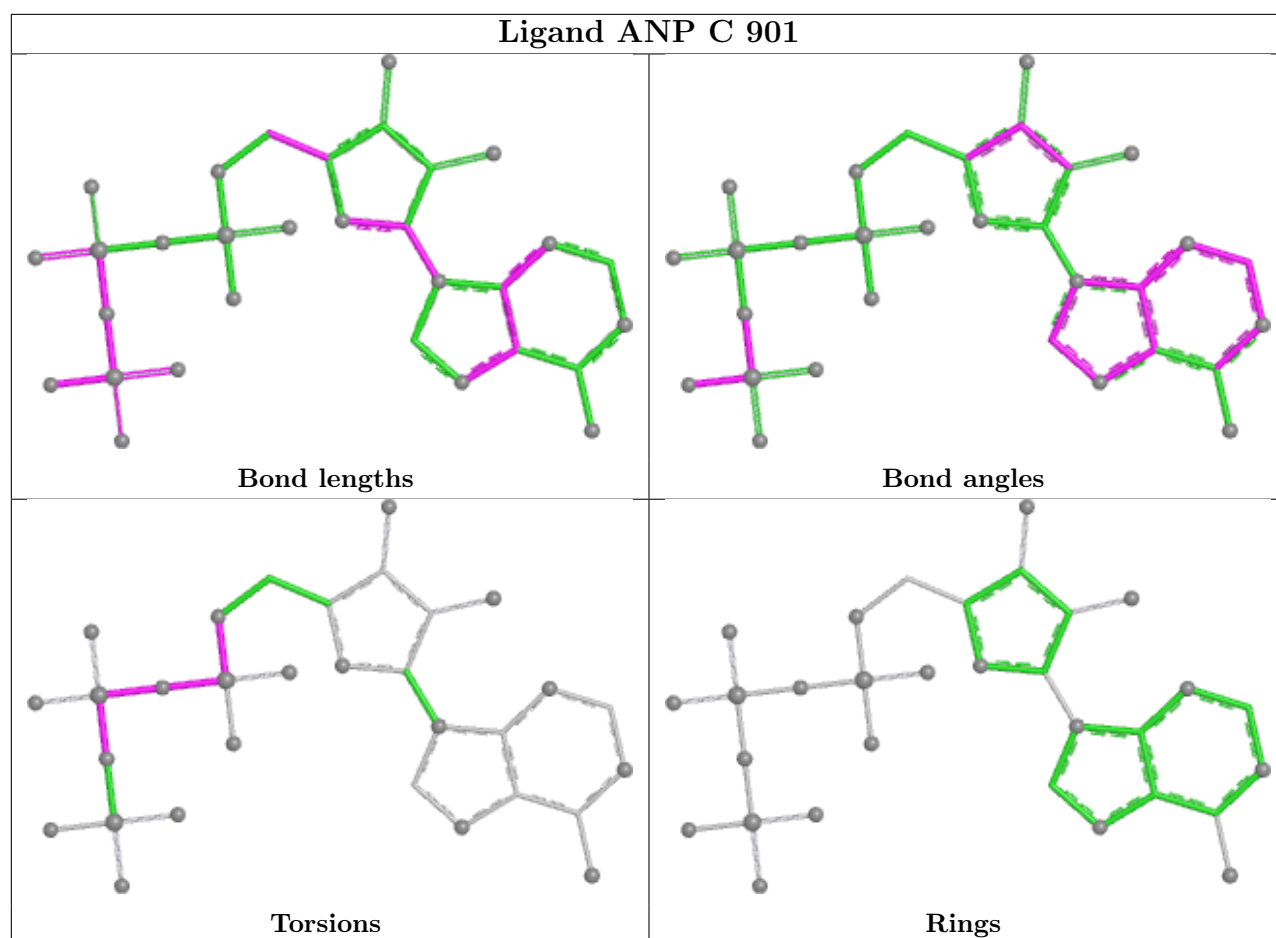
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | A | 2 |
| 1 | B | 2 |
| 1 | C | 2 |
| 1 | D | 2 |

The worst 5 of 8 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 438:ASP | C | 439:ALA | N | 1.17 |
| 1 | B | 438:ASP | C | 439:ALA | N | 1.17 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | C | 438:ASP | C | 439:ALA | N | 1.17 |
| 1 | D | 438:ASP | C | 439:ALA | N | 1.17 |
| 1 | A | 425:LYS | C | 426:LYS | N | 1.06 |

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----------------------|-------|
| 1 | A | 659/806 (81%) | -1.23 | 0 100 100 | 17, 128, 281, 412 | 0 |
| 1 | B | 659/806 (81%) | -1.22 | 0 100 100 | 17, 128, 281, 412 | 0 |
| 1 | C | 659/806 (81%) | -1.21 | 0 100 100 | 17, 128, 281, 412 | 0 |
| 1 | D | 659/806 (81%) | -1.24 | 0 100 100 | 17, 128, 281, 412 | 0 |
| All | All | 2636/3224 (81%) | -1.22 | 0 100 100 | 17, 128, 281, 412 | 0 |

There are no RSRZ outliers to report.

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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, 95th 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.

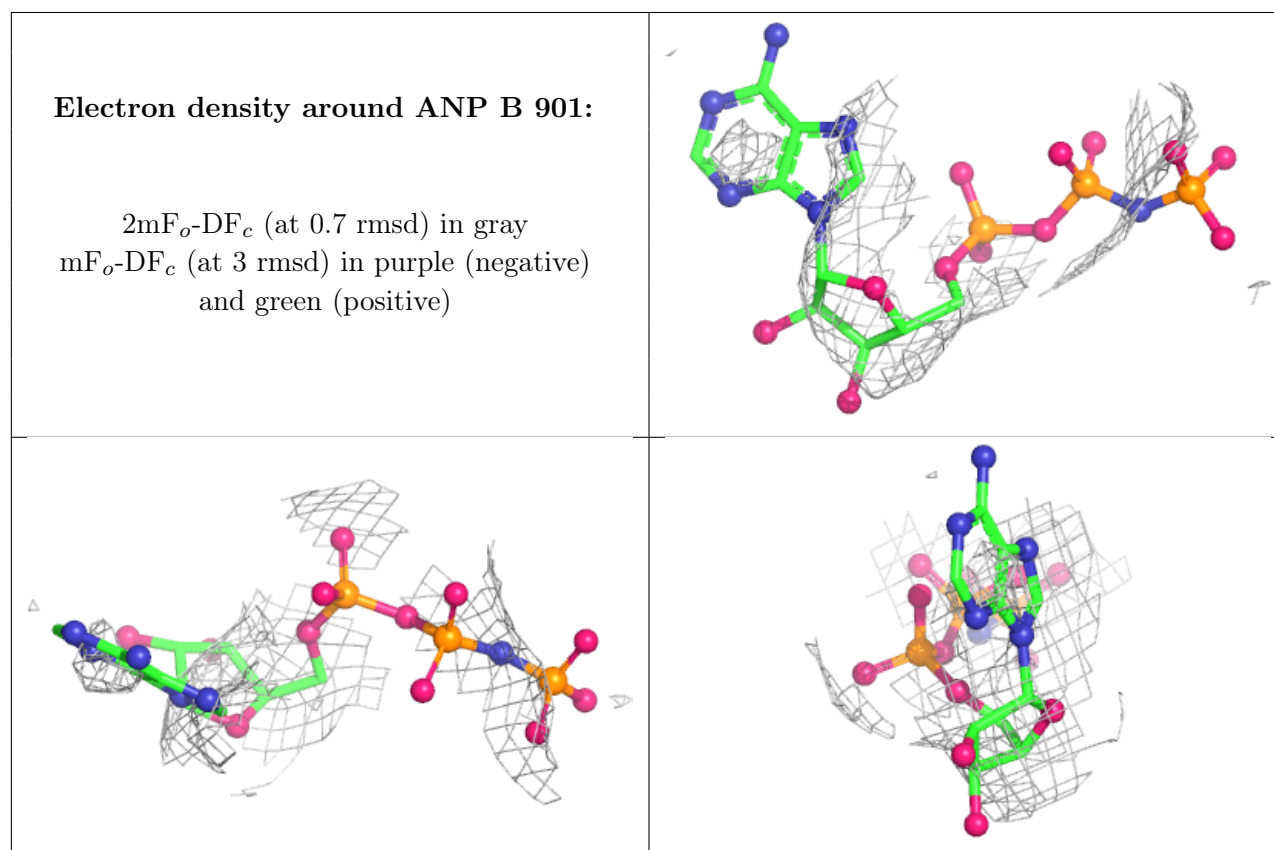
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3 | ANP | B | 901 | 31/31 | 0.98 | 0.03 | 150,150,150,150 | 0 |
| 3 | ANP | C | 901 | 31/31 | 0.98 | 0.04 | 150,150,150,150 | 0 |
| 2 | ADP | C | 807 | 27/27 | 0.99 | 0.04 | 163,163,163,163 | 0 |
| 2 | ADP | D | 807 | 27/27 | 0.99 | 0.04 | 163,163,163,163 | 0 |

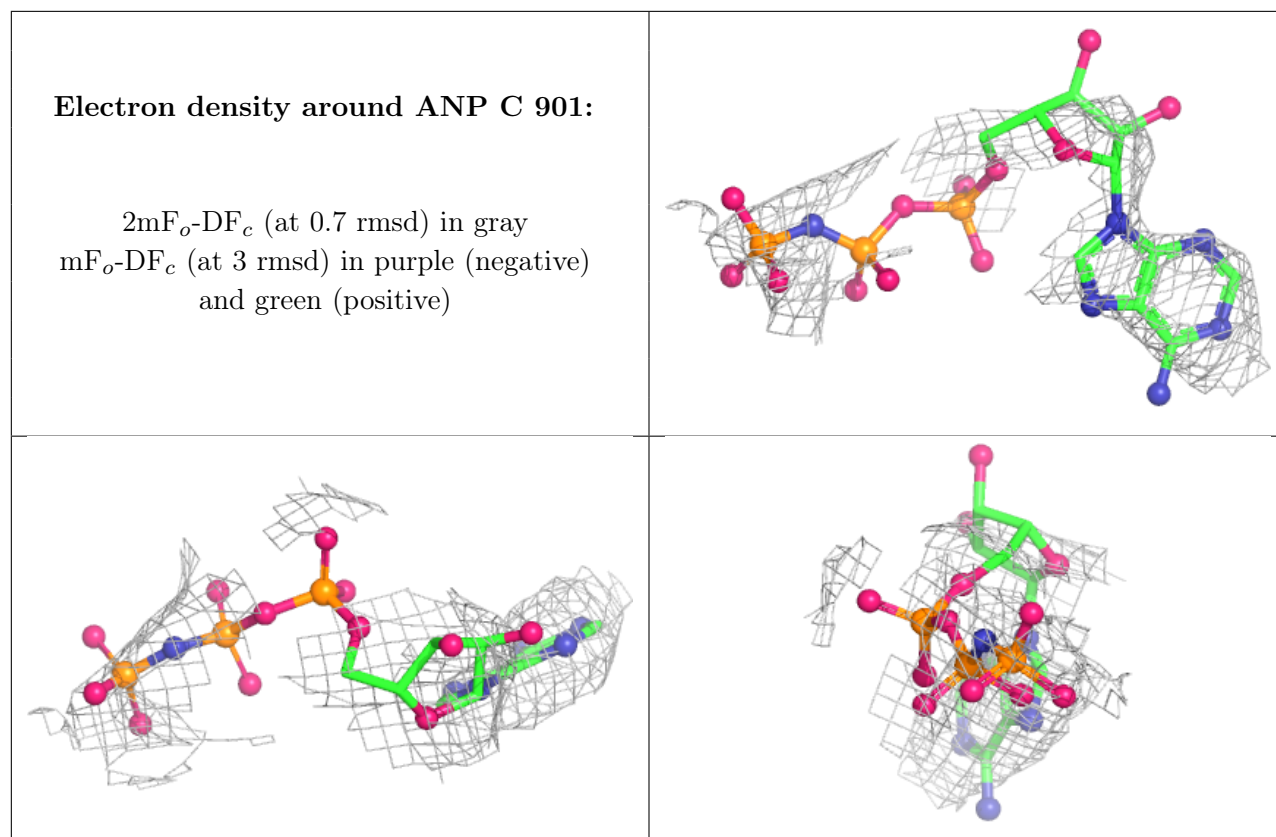
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3 | ANP | A | 901 | 31/31 | 0.99 | 0.03 | 150,150,150,150 | 0 |
| 2 | ADP | A | 807 | 27/27 | 0.99 | 0.04 | 163,163,163,163 | 0 |
| 2 | ADP | B | 807 | 27/27 | 0.99 | 0.04 | 163,163,163,163 | 0 |
| 3 | ANP | D | 901 | 31/31 | 0.99 | 0.03 | 150,150,150,150 | 0 |

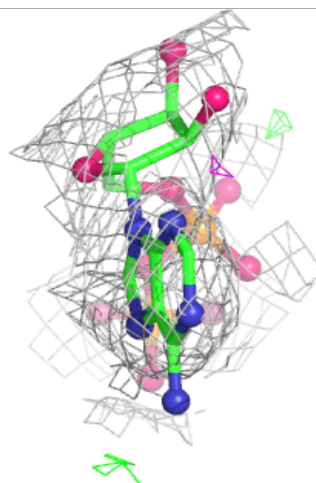
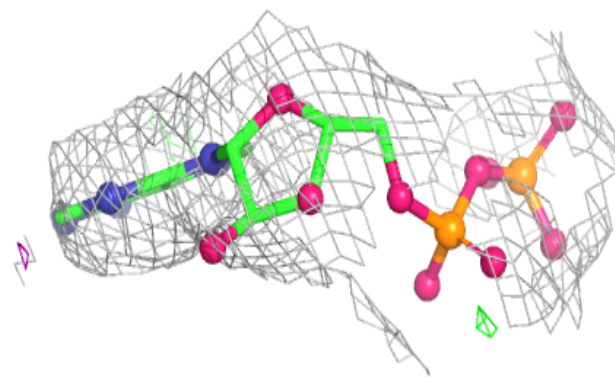
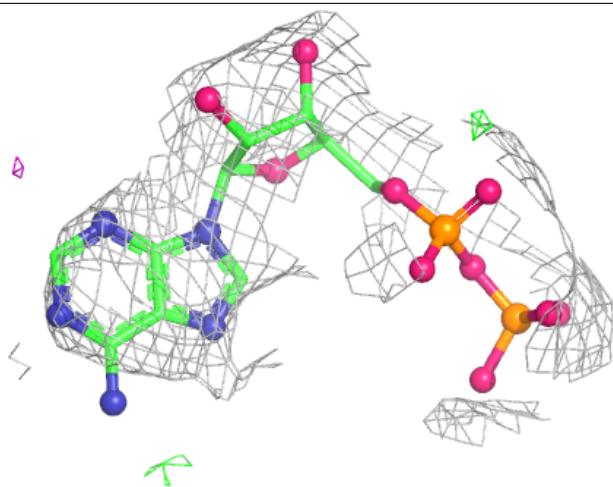
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





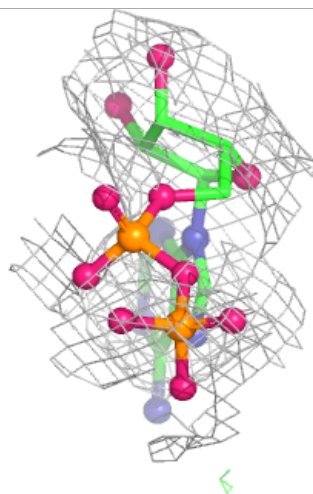
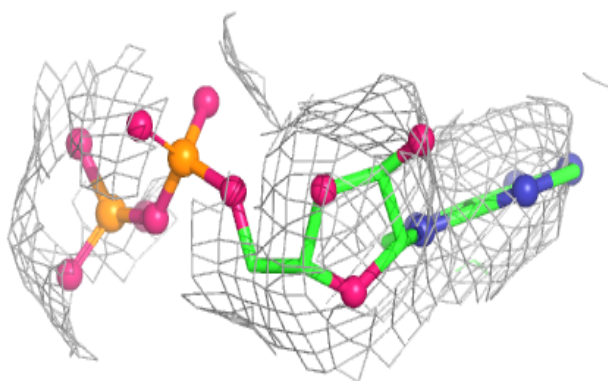
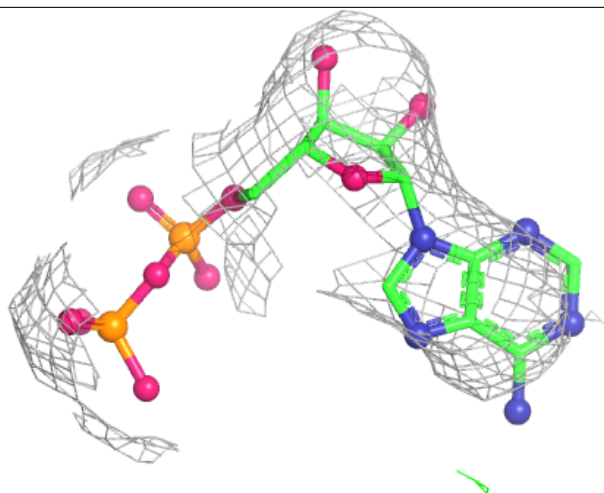
Electron density around ADP C 807:

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



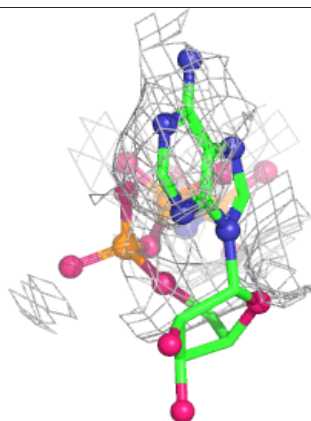
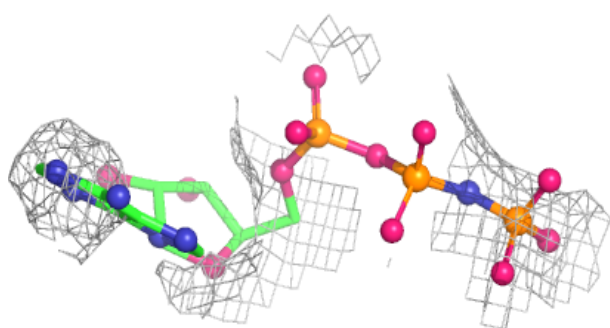
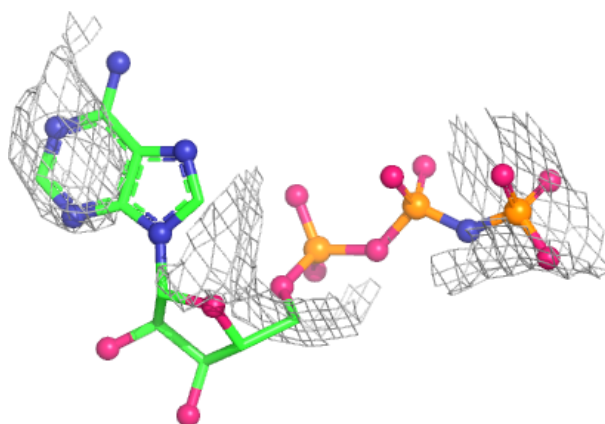
Electron density around ADP D 807:

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



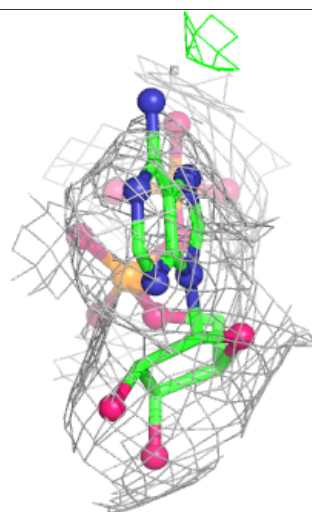
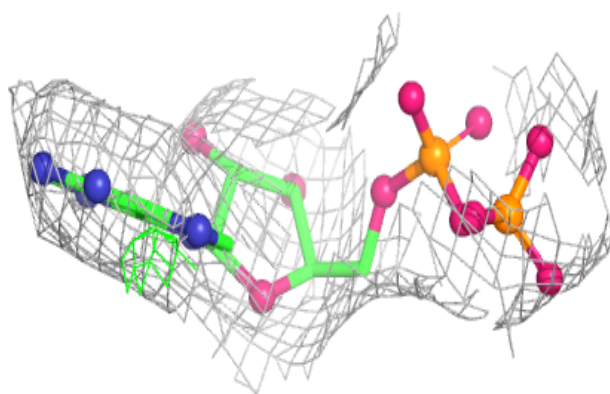
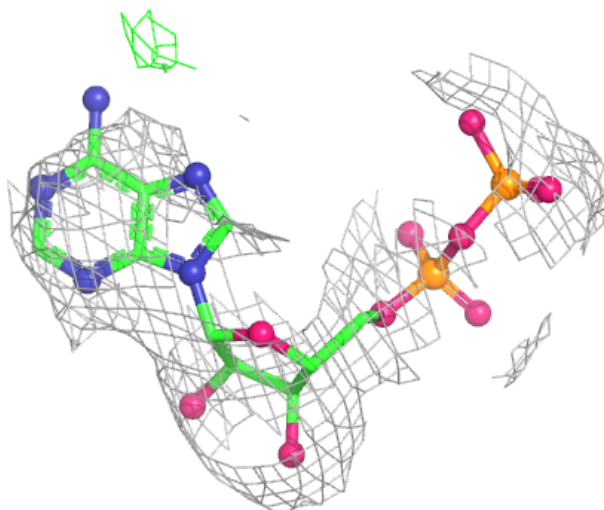
Electron density around ANP A 901:

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



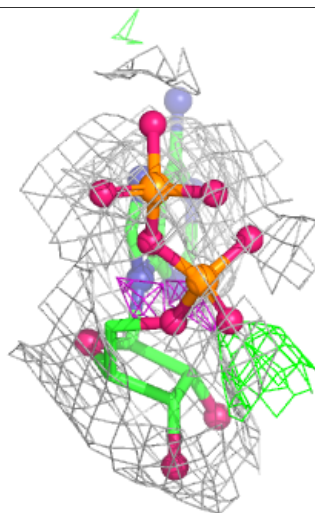
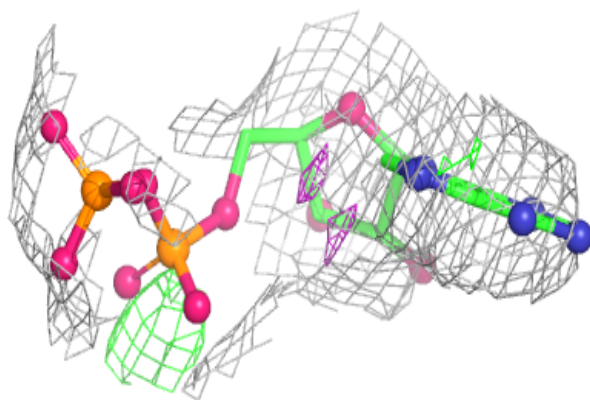
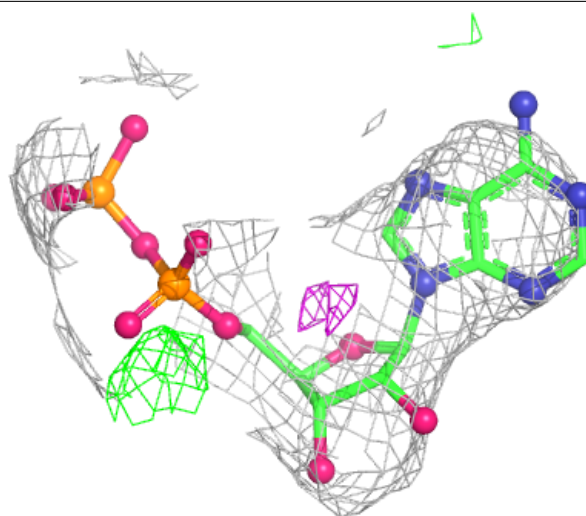
Electron density around ADP A 807:

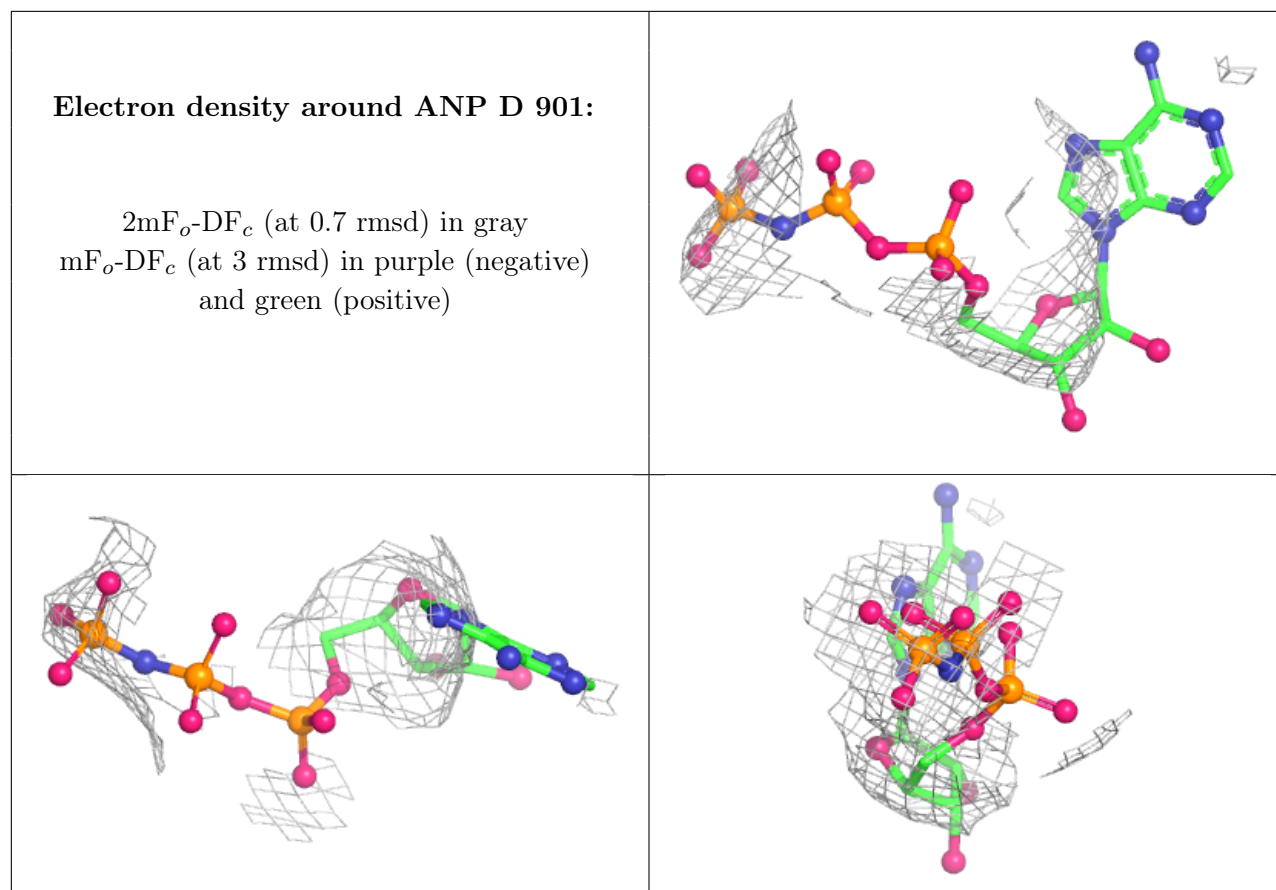
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP B 807:

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





5.5 Other polymers [i](#)

There are no such residues in this entry.