



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:29 am BST

PDB ID : 6CMZ
Title : 2.3 Angstrom Resolution Crystal Structure of Dihydrolipoamide Dehydrogenase from Burkholderia cenocepacia in Complex with FAD and NAD
Authors : Minasov, G.; Shuvalova, L.; Dubrovskaya, I.; Kiryukhina, O.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2018-03-06
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

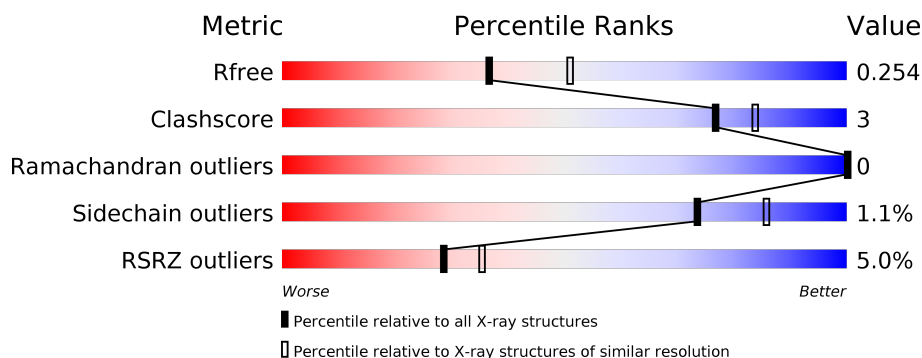
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 5042 (2.30-2.30) |
| Clashscore | 141614 | 5643 (2.30-2.30) |
| Ramachandran outliers | 138981 | 5575 (2.30-2.30) |
| Sidechain outliers | 138945 | 5575 (2.30-2.30) |
| RSRZ outliers | 127900 | 4938 (2.30-2.30) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 | 466 | <div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div> |
| 1 | B | 466 | <div> <div>6%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div> |
| 1 | C | 466 | <div> <div>4%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> </div> |
| 1 | D | 466 | <div> <div>8%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | FMN | A | 505 | - | - | - | X |

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14440 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 Dihydrolipoyl dehydrogenase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 462 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 3442 | 2155 | 641 | 630 | 16 | | | |
| 1 | B | 459 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 3390 | 2122 | 633 | 619 | 16 | | | |
| 1 | C | 462 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 3416 | 2139 | 639 | 622 | 16 | | | |
| 1 | D | 459 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 3389 | 2122 | 633 | 617 | 17 | | | |

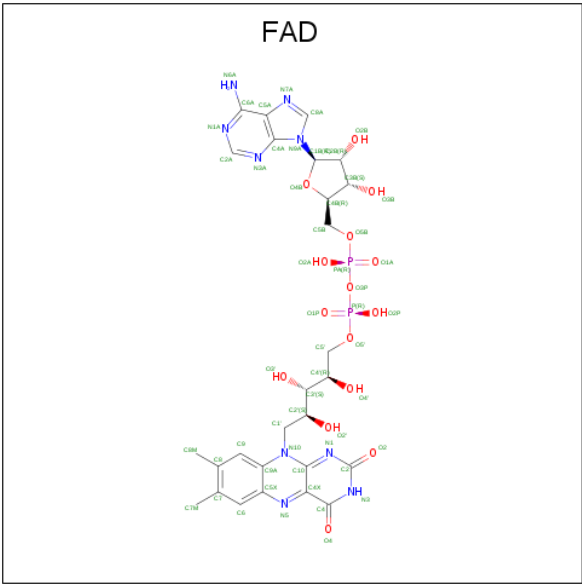
There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -2 | SER | - | expression tag | UNP B4EEF2 |
| A | -1 | ASN | - | expression tag | UNP B4EEF2 |
| A | 0 | ALA | - | expression tag | UNP B4EEF2 |
| B | -2 | SER | - | expression tag | UNP B4EEF2 |
| B | -1 | ASN | - | expression tag | UNP B4EEF2 |
| B | 0 | ALA | - | expression tag | UNP B4EEF2 |
| C | -2 | SER | - | expression tag | UNP B4EEF2 |
| C | -1 | ASN | - | expression tag | UNP B4EEF2 |
| C | 0 | ALA | - | expression tag | UNP B4EEF2 |
| D | -2 | SER | - | expression tag | UNP B4EEF2 |
| D | -1 | ASN | - | expression tag | UNP B4EEF2 |
| D | 0 | ALA | - | expression tag | UNP B4EEF2 |

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

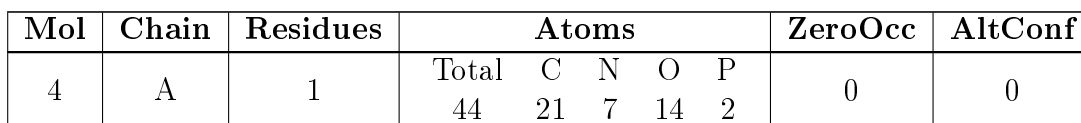
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | A | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | C | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by author).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |

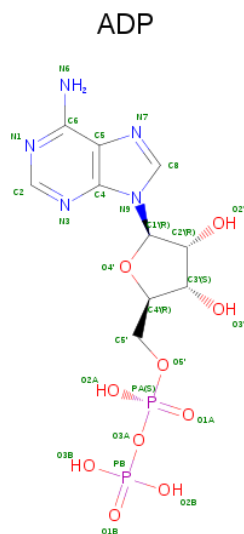
- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system (rings 1, 2, and 4) with atoms N1, N3, N5, N9, C2, C4, C6, C8, C9, C10, C12, and C14. The ring is substituted with a ribitol chain at position 10 (C10) and a phosphate group at position 2 (C2). The ribitol chain consists of a ribose ring (C1, C2, C3, C4, C5) with a hydroxyl group at C1 (O1), a phosphate group at C2 (O2), and a hydroxyl group at C3 (O3). The phosphate group is linked to a ribitol chain (C4, C5, C6, C7, C8) which is further linked to a phosphate group (O9). The ribitol chain has a hydroxyl group at C4 (O4), a phosphate group at C5 (O5), and a hydroxyl group at C6 (O6). The phosphate group is linked to a ribitol chain (C7, C8, C9, C10, C11) which is further linked to a phosphate group (O12). The ribitol chain has a hydroxyl group at C7 (O7), a phosphate group at C8 (O8), and a hydroxyl group at C9 (O9). The phosphate group is linked to a ribitol chain (C10, C11, C12, C13, C14) which is further linked to a phosphate group (O15). The ribitol chain has a hydroxyl group at C10 (O10), a phosphate group at C11 (O11), and a hydroxyl group at C12 (O12). The phosphate group is linked to a ribitol chain (C13, C14, C15, C16, C17) which is further linked to a phosphate group (O18). The ribitol chain has a hydroxyl group at C13 (O13), a phosphate group at C14 (O14), and a hydroxyl group at C15 (O15). The phosphate group is linked to a ribitol chain (C16, C17, C18, C19, C20) which is further linked to a phosphate group (O21). The ribitol chain has a hydroxyl group at C16 (O16), a phosphate group at C17 (O17), and a hydroxyl group at C18 (O18). The phosphate group is linked to a ribitol chain (C19, C20, C21, C22, C23) which is further linked to a phosphate group (O24). The ribitol chain has a hydroxyl group at C19 (O19), a phosphate group at C20 (O20), and a hydroxyl group at C21 (O21). The phosphate group is linked to a ribitol chain (C22, C23, C24, C25, C26) which is further linked to a phosphate group (O27). The ribitol chain has a hydroxyl group at C22 (O22), a phosphate group at C23 (O23), and a hydroxyl group at C24 (O24). The phosphate group is linked to a ribitol chain (C25, C26, C27, C28, C29) which is further linked to a phosphate group (O30). The ribitol chain has a hydroxyl group at C25 (O25), a phosphate group at C26 (O26), and a hydroxyl group at C27 (O27). The phosphate group is linked to a ribitol chain (C28, C29, C30, C31, C32) which is further linked to a phosphate group (O33). The ribitol chain has a hydroxyl group at C28 (O28), a phosphate group at C29 (O29), and a hydroxyl group at C30 (O30). The phosphate group is linked to a ribitol chain (C31, C32, C33, C34, C35) which is further linked to a phosphate group (O36). The ribitol chain has a hydroxyl group at C31 (O31), a phosphate group at C32 (O32), and a hydroxyl group at C33 (O33). The phosphate group is linked to a ribitol chain (C34, C35, C36, C37, C38) which is further linked to a phosphate group (O39). The ribitol chain has a hydroxyl group at C34 (O34), a phosphate group at C35 (O35), and a hydroxyl group at C36 (O36). The phosphate group is linked to a ribitol chain (C37, C38, C39, C40, C41) which is further linked to a phosphate group (O42). The ribitol chain has a hydroxyl group at C37 (O37), a phosphate group at C38 (O38), and a hydroxyl group at C39 (O39). The phosphate group is linked to a ribitol chain (C40, C41, C42, C43, C44) which is further linked to a phosphate group (O45). The ribitol chain has a hydroxyl group at C40 (O40), a phosphate group at C41 (O41), and a hydroxyl group at C42 (O42). The phosphate group is linked to a ribitol chain (C43, C44, C45, C46, C47) which is further linked to a phosphate group (O48). The ribitol chain has a hydroxyl group at C43 (O43), a phosphate group at C44 (O44), and a hydroxyl group at C45 (O45). The phosphate group is linked to a ribitol chain (C46, C47, C48, C49, C50) which is further linked to a phosphate group (O51). The ribitol chain has a hydroxyl group at C46 (O46), a phosphate group at C47 (O47), and a hydroxyl group at C48 (O48). The phosphate group is linked to a ribitol chain (C49, C50, C51, C52, C53) which is further linked to a phosphate group (O54). The ribitol chain has a hydroxyl group at C49 (O49), a phosphate group at C50 (O50), and a hydroxyl group at C51 (O51). The phosphate group is linked to a ribitol chain (C52, C53, C54, C55, C56) which is further linked to a phosphate group (O57). The ribitol chain has a hydroxyl group at C52 (O52), a phosphate group at C53 (O53), and a hydroxyl group at C54 (O54). The phosphate group is linked to a ribitol chain (C55, C56, C57, C58, C59) which is further linked to a phosphate group (O60). The ribitol chain has a hydroxyl group at C55 (O55), a phosphate group at C56 (O56), and a hydroxyl group at C57 (O57). The phosphate group is linked to a ribitol chain (C58, C59, C60, C61, C62) which is further linked to a phosphate group (O63). The ribitol chain has a hydroxyl group at C58 (O58), a phosphate group at C59 (O59), and a hydroxyl group at C60 (O60). The phosphate group is linked to a ribitol chain (C61, C62, C63, C64, C65) which is further linked to a phosphate group (O66). The ribitol chain has a hydroxyl group at C61 (O61), a phosphate group at C62 (O62), and a hydroxyl group at C63 (O63). The phosphate group is linked to a ribitol chain (C64, C65, C66, C67, C68) which is further linked to a phosphate group (O69). The ribitol chain has a hydroxyl group at C64 (O64), a phosphate group at C65 (O65), and a hydroxyl group at C66 (O66). The phosphate group is linked to a ribitol chain (C67, C68, C69, C70, C71) which is further linked to a phosphate group (O72). The ribitol chain has a hydroxyl group at C67 (O67), a phosphate group at C68 (O68), and a hydroxyl group at C69 (O69). The phosphate group is linked to a ribitol chain (C70, C71, C72, C73, C74) which is further linked to a phosphate group (O75). The ribitol chain has a hydroxyl group at C70 (O70), a phosphate group at C71 (O71), and a hydroxyl group at C72 (O72). The phosphate group is linked to a ribitol chain (C73, C74, C75, C76, C77) which is further linked to a phosphate group (O78). The ribitol chain has a hydroxyl group at C73 (O73), a phosphate group at C74 (O74), and a hydroxyl group at C75 (O75). The phosphate group is linked to a ribitol chain (C76, C77, C78, C79, C80) which is further linked to a phosphate group (O81). The ribitol chain has a hydroxyl group at C76 (O76), a phosphate group at C77 (O77), and a hydroxyl group at C78 (O78). The phosphate group is linked to a ribitol chain (C79, C80, C81, C82, C83) which is further linked to a phosphate group (O84). The ribitol chain has a hydroxyl group at C79 (O79), a phosphate group at C80 (O80), and a hydroxyl group at C81 (O81). The phosphate group is linked to a ribitol chain (C82, C83, C84, C85, C86) which is further linked to a phosphate group (O87). The ribitol chain has a hydroxyl group at C82 (O82), a phosphate group at C83 (O83), and a hydroxyl group at C84 (O84). The phosphate group is linked to a ribitol chain (C85, C86, C87, C88, C89) which is further linked to a phosphate group (O90). The ribitol chain has a hydroxyl group at C85 (O85), a phosphate group at C86 (O86), and a hydroxyl group at C87 (O87). The phosphate group is linked to a ribitol chain (C88, C89, C90, C91, C92) which is further linked to a phosphate group (O93). The ribitol chain has a hydroxyl group at C88 (O88), a phosphate group at C89 (O89), and a hydroxyl group at C90 (O90). The phosphate group is linked to a ribitol chain (C91, C92, C93, C94, C95) which is further linked to a phosphate group (O96). The ribitol chain has a hydroxyl group at C91 (O91), a phosphate group at C92 (O92), and a hydroxyl group at C93 (O93). The phosphate group is linked to a ribitol chain (C94, C95, C96, C97, C98) which is further linked to a phosphate group (O99). The ribitol chain has a hydroxyl group at C94 (O94), a phosphate group at C95 (O95), and a hydroxyl group at C96 (O96). The phosphate group is linked to a ribitol chain (C97, C98, C99, C100, C101) which is further linked to a phosphate group (O102). The ribitol chain has a hydroxyl group at C97 (O97), a phosphate group at C98 (O98), and a hydroxyl group at C99 (O99). The phosphate group is linked to a ribitol chain (C100, C101, C102, C103, C104) which is further linked to a phosphate group (O105). The ribitol chain has a hydroxyl group at C100 (O100), a phosphate group at C101 (O101), and a hydroxyl group at C102 (O102). The phosphate group is linked to a ribitol chain (C103, C104, C105, C106, C107) which is further linked to a phosphate group (O108). The ribitol chain has a hydroxyl group at C103 (O103), a phosphate group at C104 (O104), and a hydroxyl group at C105 (O105). The phosphate group is linked to a ribitol chain (C106, C107, C108, C109, C110) which is further linked to a phosphate group (O111). The ribitol chain has a hydroxyl group at C106 (O106), a phosphate group at C107 (O107), and a hydroxyl group at C108 (O108). The phosphate group is linked to a ribitol chain (C109, C110, C111, C112, C113) which is further linked to a phosphate group (O114). The ribitol chain has a hydroxyl group at C109 (O109), a phosphate group at C110 (O110), and a hydroxyl group at C111 (O111). The phosphate group is linked to a ribitol chain (C112, C113, C114, C115, C116) which is further linked to a phosphate group (O117). The ribitol chain has a hydroxyl group at C112 (O112), a phosphate group at C113 (O113), and a hydroxyl group at C114 (O114). The phosphate group is linked to a ribitol chain (C115, C116, C117, C118, C119) which is further linked to a phosphate group (O120). The ribitol chain has a hydroxyl group at C115 (O115), a phosphate group at C116 (O116), and a hydroxyl group at C117 (O117). The phosphate group is linked to a ribitol chain (C118, C119, C120, C121, C122) which is further linked to a phosphate group (O123). The ribitol chain has a hydroxyl group at C118 (O118), a phosphate group at C119 (O119), and a hydroxyl group at C120 (O120). The phosphate group is linked to a ribitol chain (C121, C122, C123, C124, C125) which is further linked to a phosphate group (O126). The ribitol chain has a hydroxyl group at C121 (O121), a phosphate group at C122 (O122), and a hydroxyl group at C123 (O123). The phosphate group is linked to a ribitol chain (C124, C125, C126, C127, C128) which is further linked to a phosphate group (O129). The ribitol chain has a hydroxyl group at C124 (O124), a phosphate group at C125 (O125), and a hydroxyl group at C126 (O126). The phosphate group is linked to a ribitol chain (C127, C128, C129, C130, C131) which is further linked to a phosphate group (O132). The ribitol chain has a hydroxyl group at C127 (O127), a phosphate group at C128 (O128), and a hydroxyl group at C129 (O129). The phosphate group

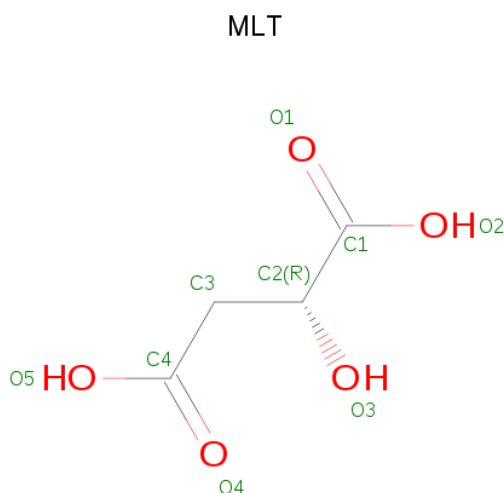
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 5 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 6 | B | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 6 | C | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 6 | D | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |

- Molecule 7 is D-MALATE (three-letter code: MLT) (formula: $\text{C}_4\text{H}_6\text{O}_5$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7 | D | 1 | Total | C | O | 0 | 0 |
| | | | 9 | 4 | 5 | | |

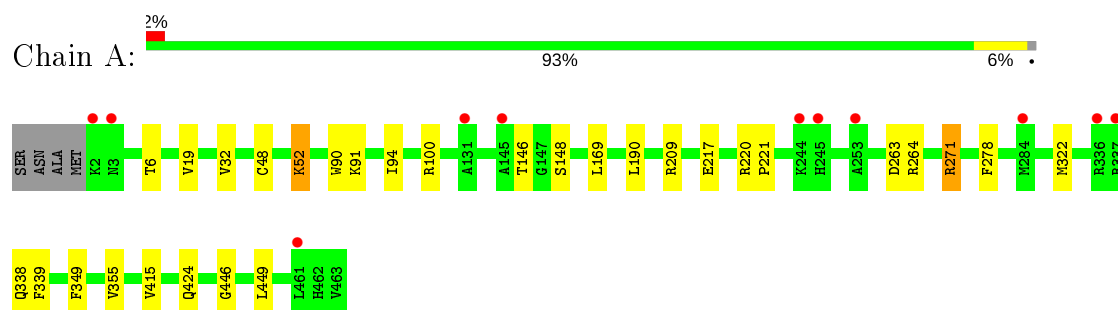
- Molecule 8 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 8 | A | 115 | Total 117 | O 117 | 0 | 2 |
| 8 | B | 90 | Total 92 | O 92 | 0 | 2 |
| 8 | C | 79 | Total 82 | O 82 | 0 | 3 |
| 8 | D | 76 | Total 80 | O 80 | 0 | 4 |

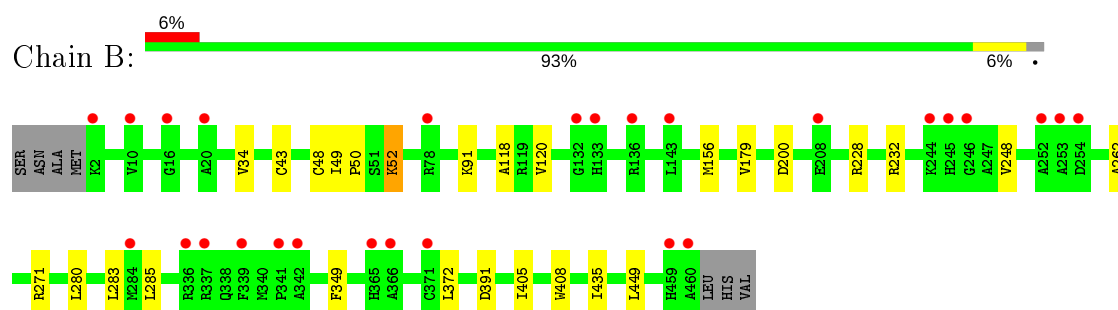
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

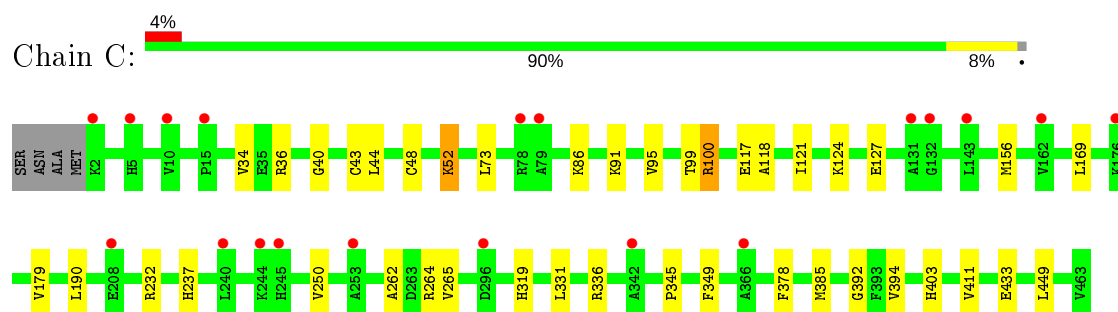
• Molecule 1: Dihydrolipoyl dehydrogenase



• Molecule 1: Dihydrolipoyl dehydrogenase

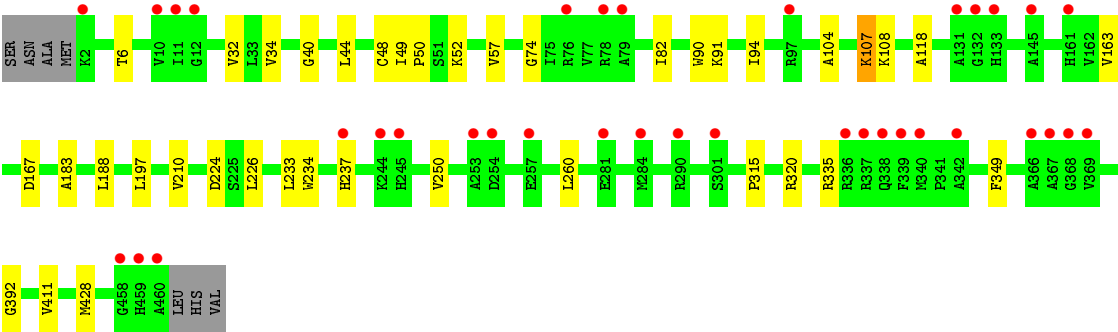


• Molecule 1: Dihydrolipoyl dehydrogenase



• Molecule 1: Dihydrolipoyl dehydrogenase





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 83.56Å 107.25Å 105.43Å 90.00° 106.09° 90.00° | Depositor |
| Resolution (Å) | 29.21 – 2.30 29.21 – 2.30 | Depositor EDS |
| % Data completeness (in resolution range) | 99.7 (29.21-2.30) 99.8 (29.21-2.30) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | 0.11 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.80 (at 2.31Å) | Xtriage |
| Refinement program | REFMAC 5.8.0189 | Depositor |
| R, R_{free} | 0.199 , 0.253 0.200 , 0.254 | Depositor DCC |
| R_{free} test set | 3962 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 42.0 | Xtriage |
| Anisotropy | 0.056 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 38.5 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 14440 | wwPDB-VP |
| Average B, all atoms (Å ²) | 51.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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.

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: ADP, NAD, CL, FMN, MLT, FAD

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 | 0.44 | 0/3500 | 0.75 | 2/4750 (0.0%) |
| 1 | B | 0.42 | 0/3447 | 0.71 | 0/4679 |
| 1 | C | 0.42 | 0/3474 | 0.70 | 0/4714 |
| 1 | D | 0.43 | 0/3446 | 0.72 | 0/4676 |
| All | All | 0.43 | 0/13867 | 0.72 | 2/18819 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 271 | ARG | NE-CZ-NH1 | 6.06 | 123.33 | 120.30 |
| 1 | A | 271 | ARG | NE-CZ-NH2 | -5.13 | 117.73 | 120.30 |

There are no chirality outliers.

There are no planarity outliers.

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 | 3442 | 0 | 3496 | 17 | 0 |
| 1 | B | 3390 | 0 | 3451 | 20 | 0 |
| 1 | C | 3416 | 0 | 3479 | 25 | 0 |
| 1 | D | 3389 | 0 | 3451 | 26 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 106 | 0 | 62 | 0 | 0 |
| 3 | B | 53 | 0 | 31 | 0 | 0 |
| 3 | C | 53 | 0 | 31 | 0 | 0 |
| 3 | D | 53 | 0 | 31 | 0 | 0 |
| 4 | A | 44 | 0 | 26 | 0 | 0 |
| 5 | A | 31 | 0 | 19 | 0 | 0 |
| 6 | B | 27 | 0 | 12 | 0 | 0 |
| 6 | C | 27 | 0 | 12 | 0 | 0 |
| 6 | D | 27 | 0 | 12 | 0 | 0 |
| 7 | D | 9 | 0 | 4 | 0 | 0 |
| 8 | A | 117 | 0 | 0 | 1 | 0 |
| 8 | B | 92 | 0 | 0 | 1 | 0 |
| 8 | C | 82 | 0 | 0 | 1 | 0 |
| 8 | D | 80 | 0 | 0 | 0 | 0 |
| All | All | 14440 | 0 | 14117 | 83 | 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 3.

The worst 5 of 83 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:A:6:THR:HG21 | 1:A:32:VAL:HG23 | 1.57 | 0.84 |
| 1:B:43:CYS:HG | 1:B:48:CYS:HG | 0.83 | 0.82 |
| 1:D:6:THR:HG21 | 1:D:32:VAL:HG23 | 1.66 | 0.77 |
| 1:C:43:CYS:HG | 1:C:48:CYS:HG | 1.38 | 0.71 |
| 1:B:52:LYS:HD2 | 1:B:349:PHE:CD1 | 2.30 | 0.66 |

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 | 464/466 (100%) | 448 (97%) | 16 (3%) | 0 | 100 | 100 |
| 1 | B | 458/466 (98%) | 437 (95%) | 21 (5%) | 0 | 100 | 100 |
| 1 | C | 461/466 (99%) | 446 (97%) | 15 (3%) | 0 | 100 | 100 |
| 1 | D | 458/466 (98%) | 440 (96%) | 18 (4%) | 0 | 100 | 100 |
| All | All | 1841/1864 (99%) | 1771 (96%) | 70 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

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 | 347/346 (100%) | 343 (99%) | 4 (1%) | 71 | 84 |
| 1 | B | 341/346 (99%) | 339 (99%) | 2 (1%) | 86 | 94 |
| 1 | C | 344/346 (99%) | 338 (98%) | 6 (2%) | 60 | 76 |
| 1 | D | 341/346 (99%) | 338 (99%) | 3 (1%) | 78 | 89 |
| All | All | 1373/1384 (99%) | 1358 (99%) | 15 (1%) | 73 | 86 |

5 of 15 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 52 | LYS |
| 1 | C | 91 | LYS |
| 1 | D | 91 | LYS |
| 1 | B | 91 | LYS |
| 1 | C | 264 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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 | FAD | B | 501 | - | 51,58,58 | 2.01 | 7 (13%) | 60,89,89 | 2.03 | 10 (16%) |
| 6 | ADP | D | 503 | - | 24,29,29 | 1.03 | 2 (8%) | 29,45,45 | 1.41 | 4 (13%) |
| 3 | FAD | C | 502 | - | 51,58,58 | 1.93 | 8 (15%) | 60,89,89 | 1.93 | 9 (15%) |
| 3 | FAD | A | 502 | - | 51,58,58 | 1.91 | 7 (13%) | 60,89,89 | 2.02 | 9 (15%) |
| 4 | NAD | A | 504 | - | 42,48,48 | 0.92 | 4 (9%) | 50,73,73 | 1.28 | 5 (10%) |
| 5 | FMN | A | 505 | - | 31,33,33 | 2.64 | 6 (19%) | 40,50,50 | 2.13 | 8 (20%) |
| 6 | ADP | B | 502 | - | 24,29,29 | 1.06 | 2 (8%) | 29,45,45 | 1.33 | 3 (10%) |
| 7 | MLT | D | 501 | - | 2,8,8 | 0.91 | 0 | 3,10,10 | 1.70 | 1 (33%) |
| 3 | FAD | A | 503 | - | 51,58,58 | 2.05 | 8 (15%) | 60,89,89 | 1.94 | 10 (16%) |
| 3 | FAD | D | 502 | - | 51,58,58 | 1.85 | 6 (11%) | 60,89,89 | 2.05 | 9 (15%) |
| 6 | ADP | C | 503 | - | 24,29,29 | 1.06 | 2 (8%) | 29,45,45 | 1.38 | 3 (10%) |

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 | FAD | B | 501 | - | - | 2/30/50/50 | 0/6/6/6 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 6 | ADP | D | 503 | - | - | 3/12/32/32 | 0/3/3/3 |
| 3 | FAD | C | 502 | - | - | 2/30/50/50 | 0/6/6/6 |
| 3 | FAD | A | 502 | - | - | 2/30/50/50 | 0/6/6/6 |
| 4 | NAD | A | 504 | - | - | 11/26/62/62 | 0/5/5/5 |
| 5 | FMN | A | 505 | - | - | 4/18/18/18 | 0/3/3/3 |
| 6 | ADP | B | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 7 | MLT | D | 501 | - | - | 2/2/8/8 | - |
| 3 | FAD | A | 503 | - | - | 5/30/50/50 | 0/6/6/6 |
| 3 | FAD | D | 502 | - | - | 3/30/50/50 | 0/6/6/6 |
| 6 | ADP | C | 503 | - | - | 6/12/32/32 | 0/3/3/3 |

The worst 5 of 52 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | A | 505 | FMN | C4A-C10 | 10.95 | 1.49 | 1.38 |
| 3 | B | 501 | FAD | C4X-C10 | 10.25 | 1.49 | 1.38 |
| 3 | A | 503 | FAD | C4X-C10 | 10.22 | 1.49 | 1.38 |
| 3 | A | 502 | FAD | C4X-C10 | 9.58 | 1.48 | 1.38 |
| 3 | C | 502 | FAD | C4X-C10 | 9.48 | 1.48 | 1.38 |

The worst 5 of 71 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3 | B | 501 | FAD | C4-N3-C2 | 8.07 | 121.95 | 115.14 |
| 5 | A | 505 | FMN | C4-N3-C2 | 8.05 | 121.94 | 115.14 |
| 3 | D | 502 | FAD | C4-N3-C2 | 7.93 | 121.83 | 115.14 |
| 3 | A | 503 | FAD | C4-N3-C2 | 7.90 | 121.81 | 115.14 |
| 3 | C | 502 | FAD | C4-N3-C2 | 7.85 | 121.77 | 115.14 |

There are no chirality outliers.

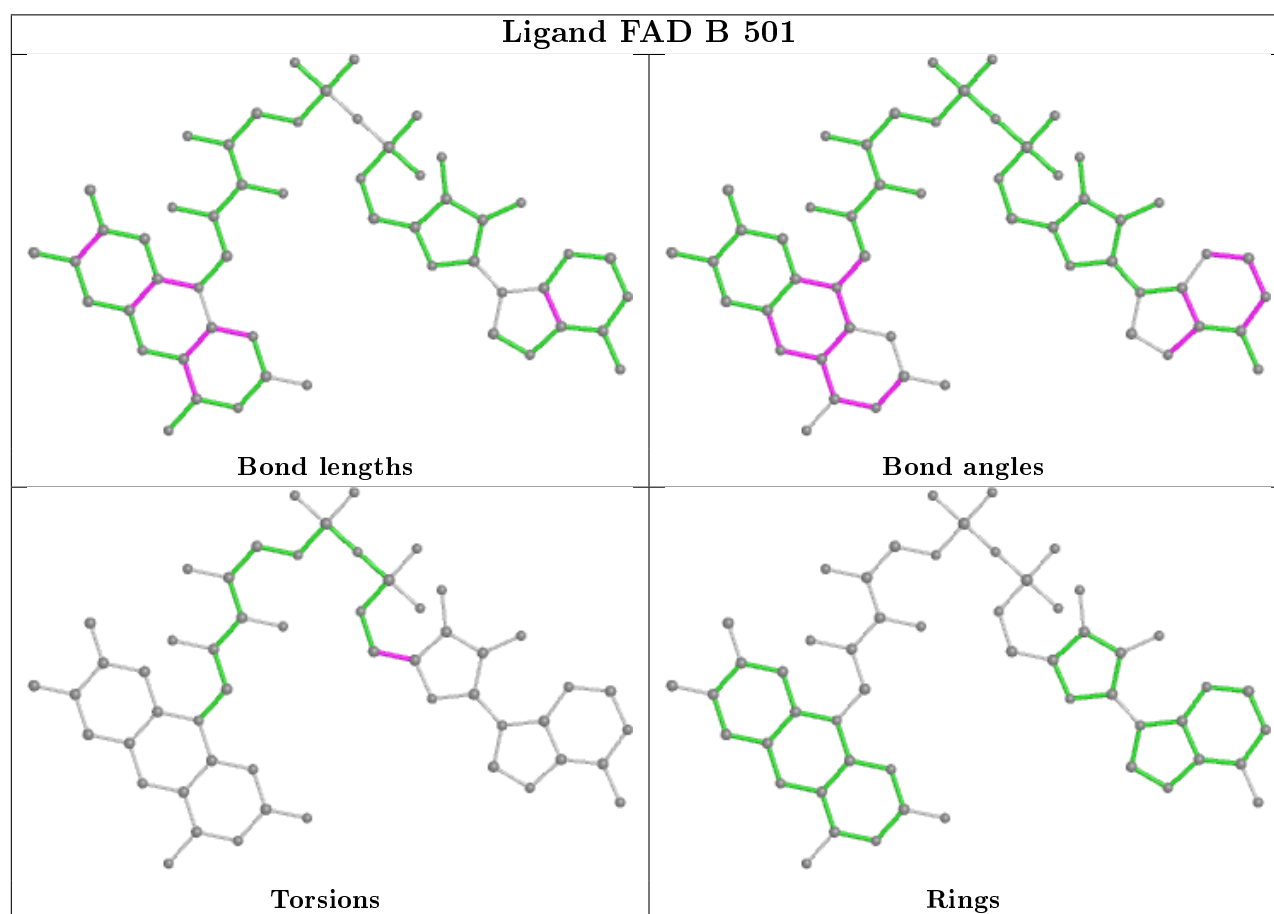
5 of 40 torsion outliers are listed below:

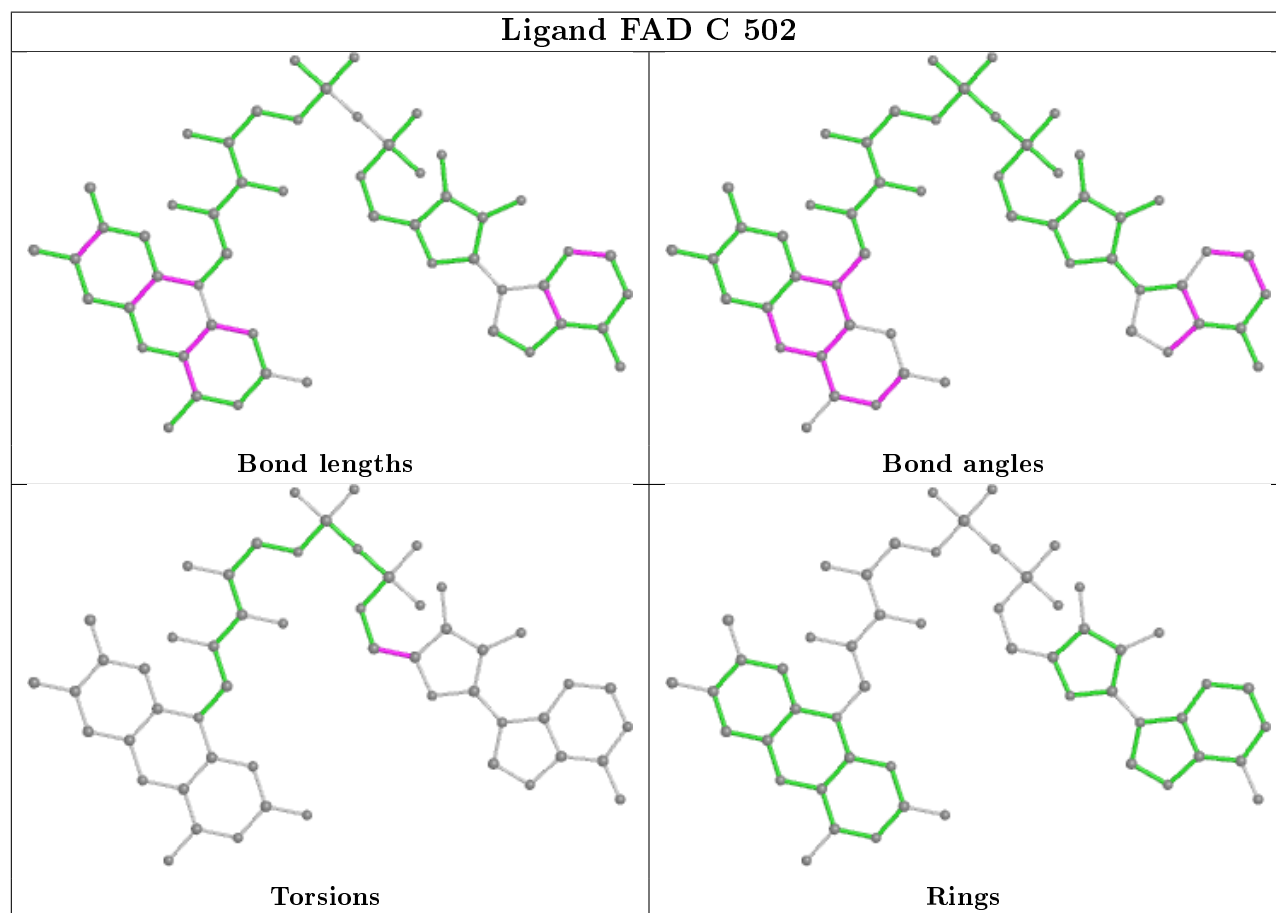
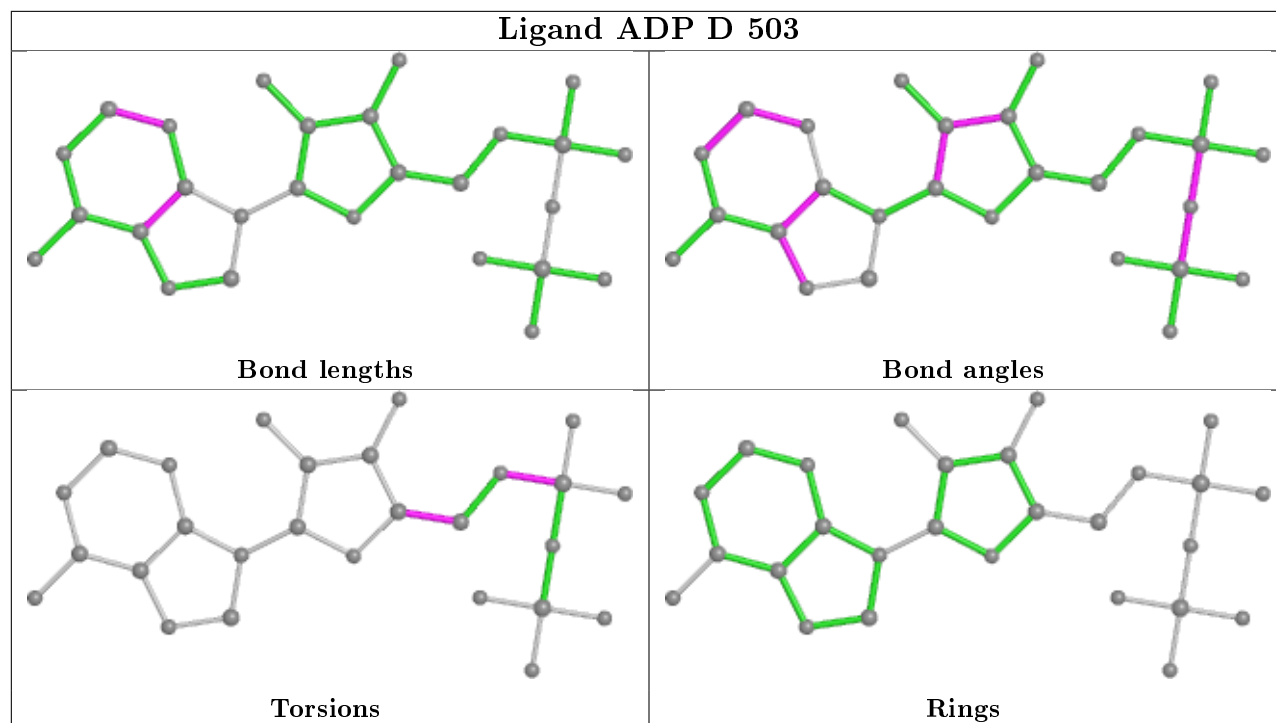
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | A | 502 | FAD | PA-O3P-P-O5' |
| 4 | A | 504 | NAD | C5B-O5B-PA-O2A |
| 4 | A | 504 | NAD | C5B-O5B-PA-O3 |
| 5 | A | 505 | FMN | C2'-C1'-N10-C9A |
| 5 | A | 505 | FMN | C2'-C1'-N10-C10 |

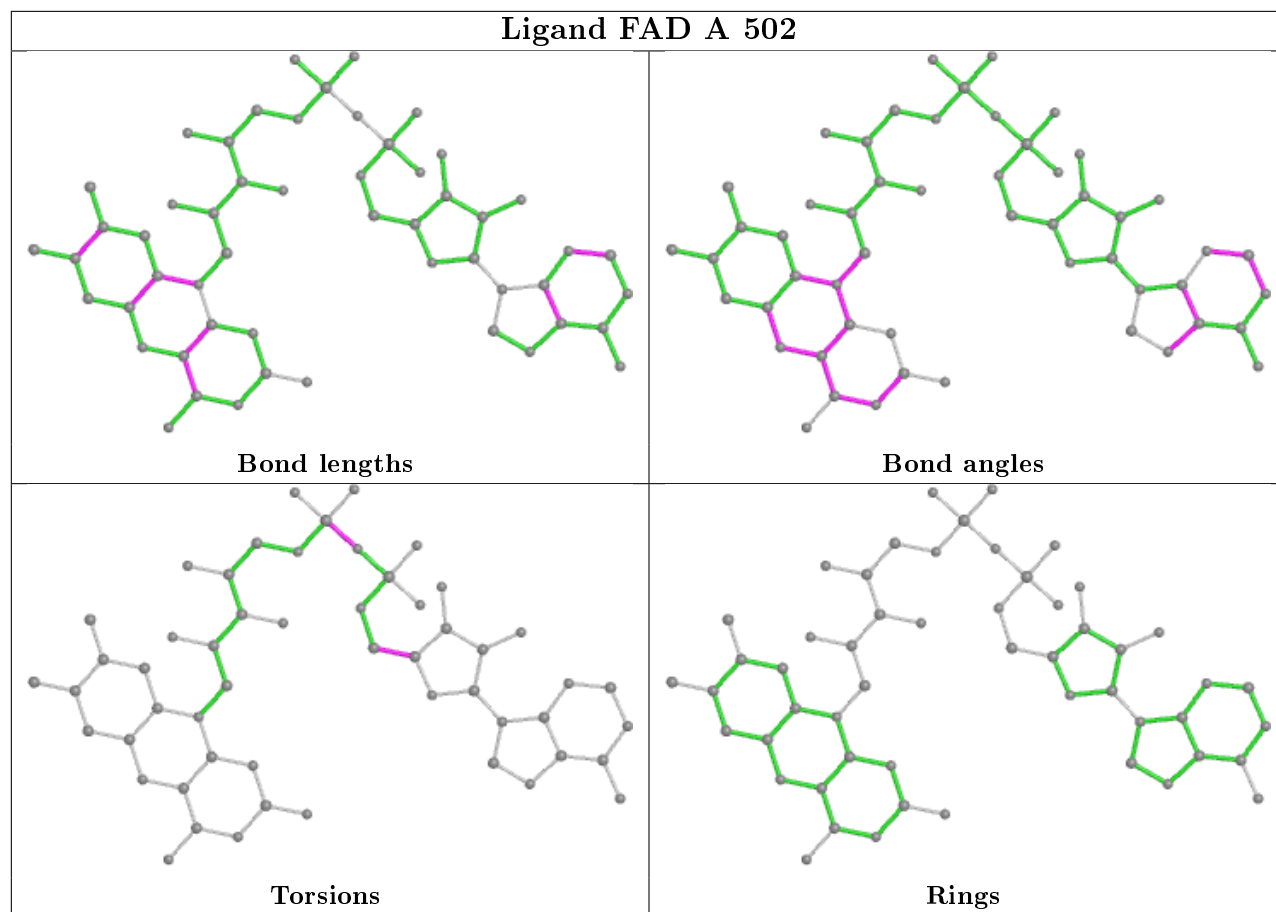
There are no ring outliers.

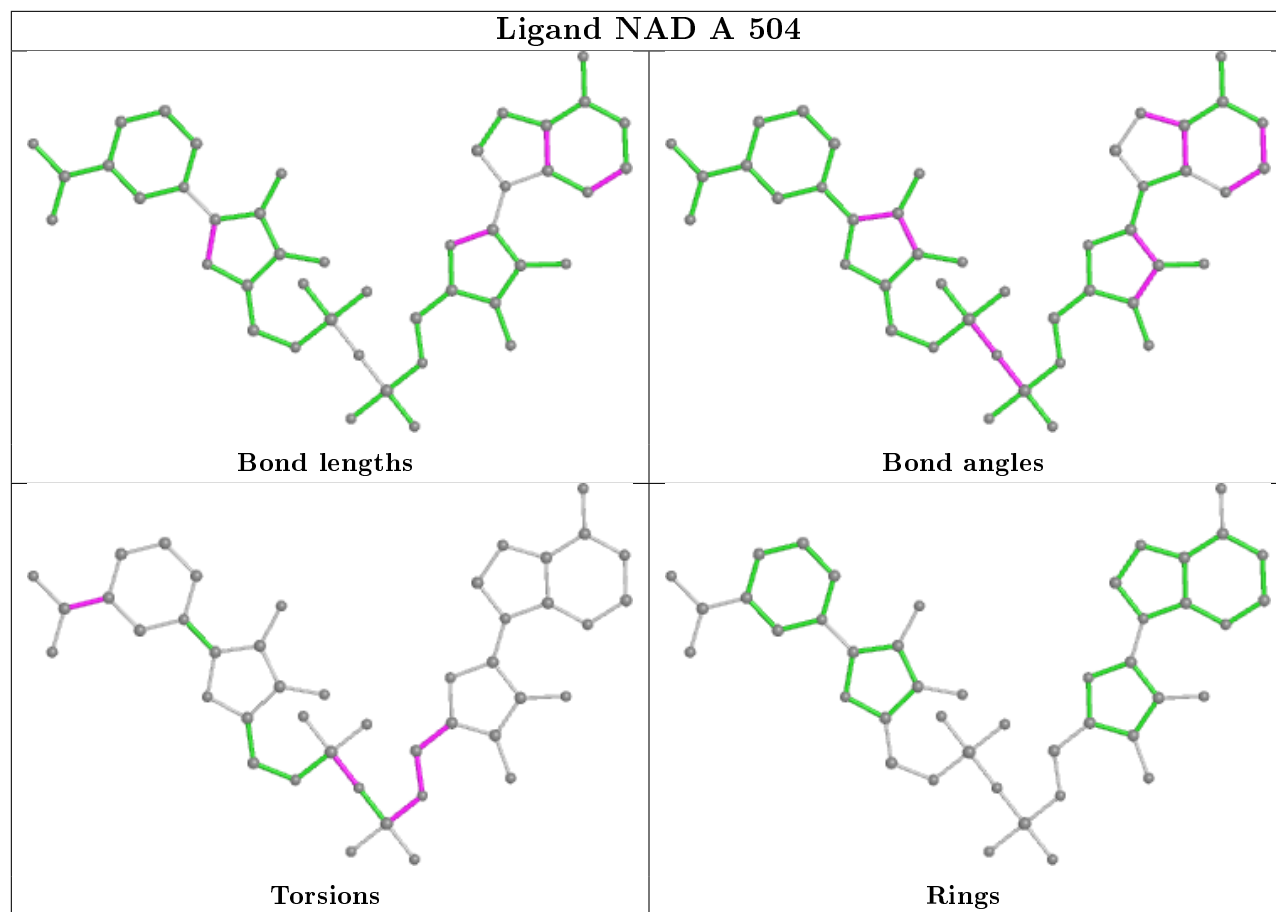
No monomer is involved in short contacts.

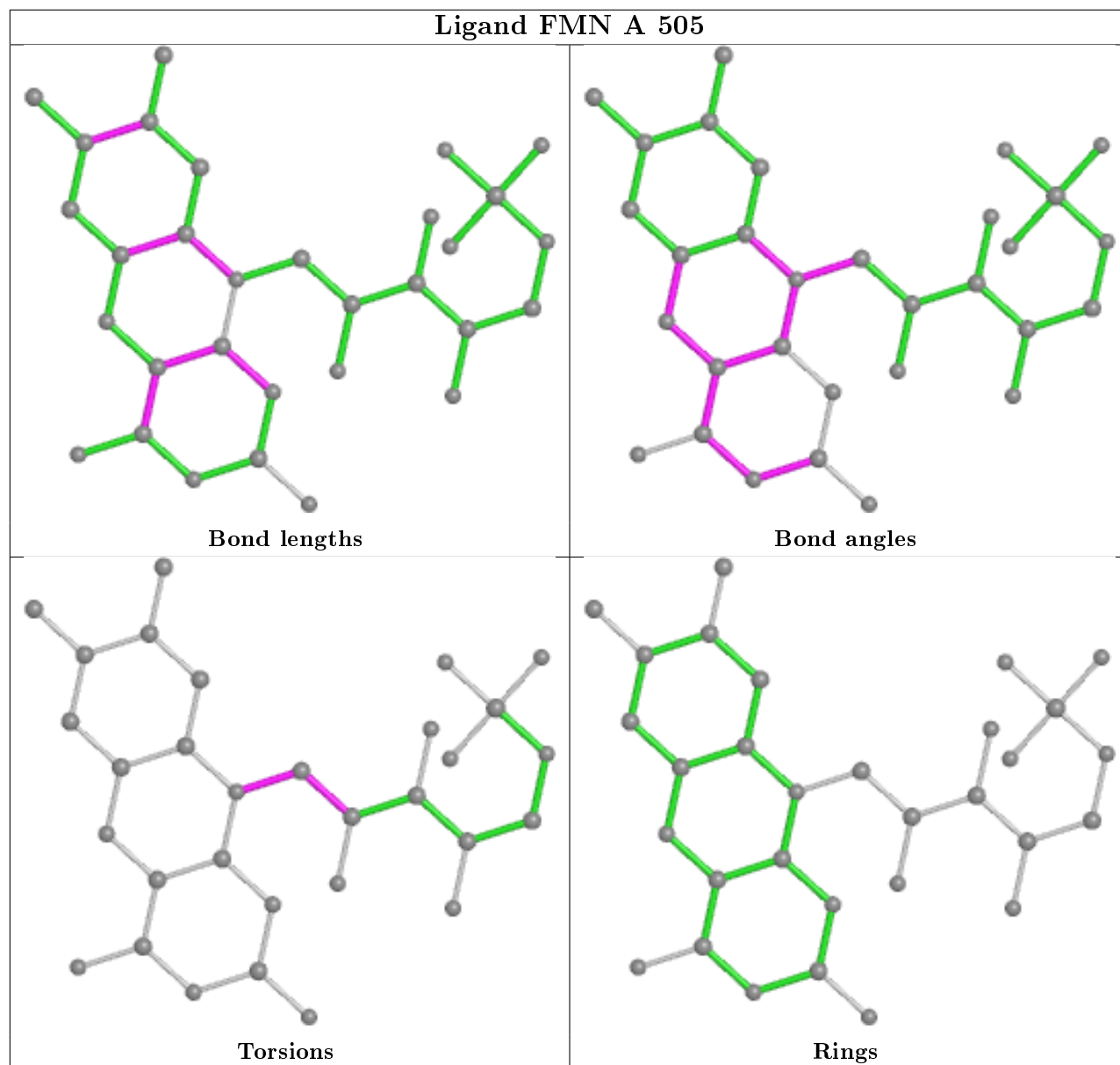
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

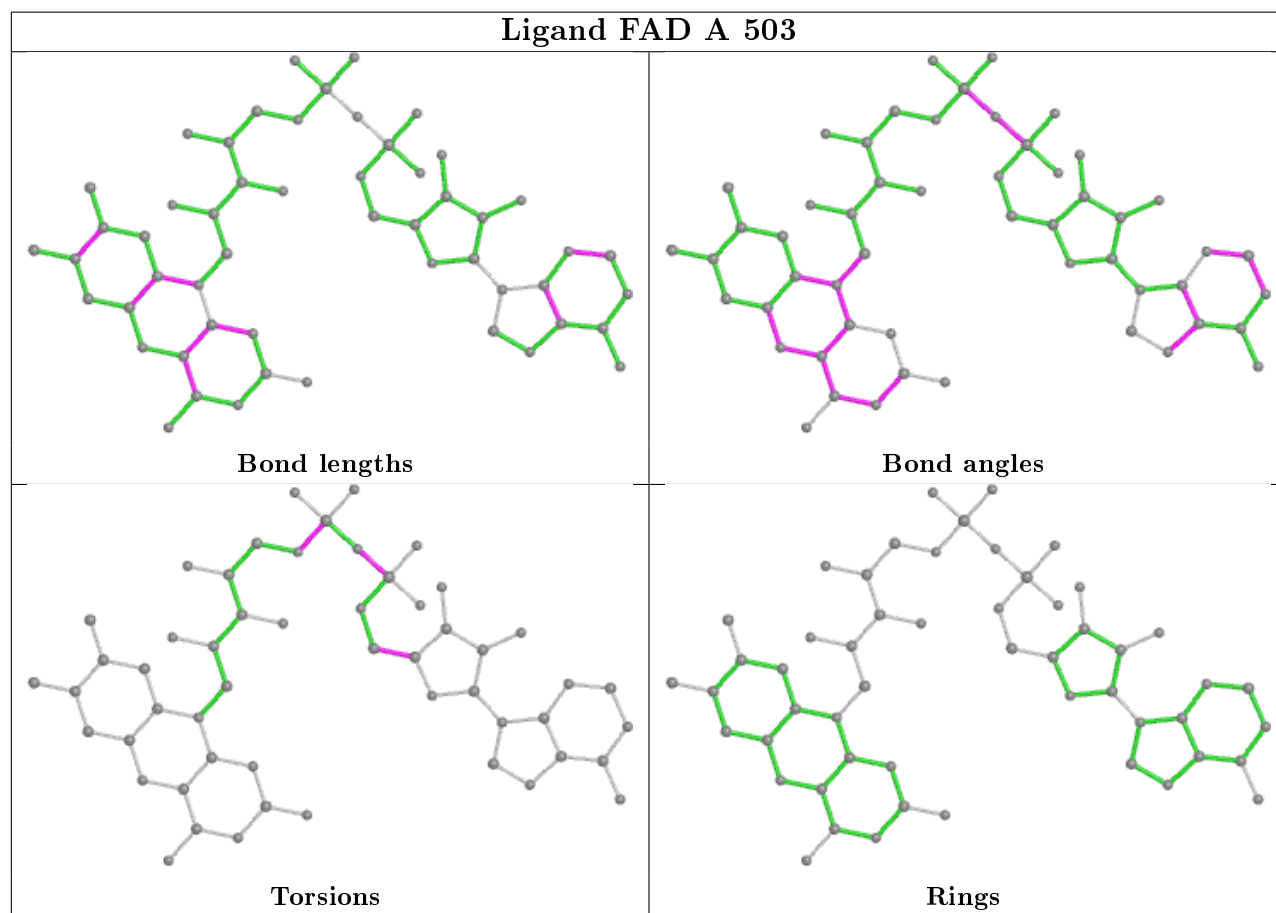
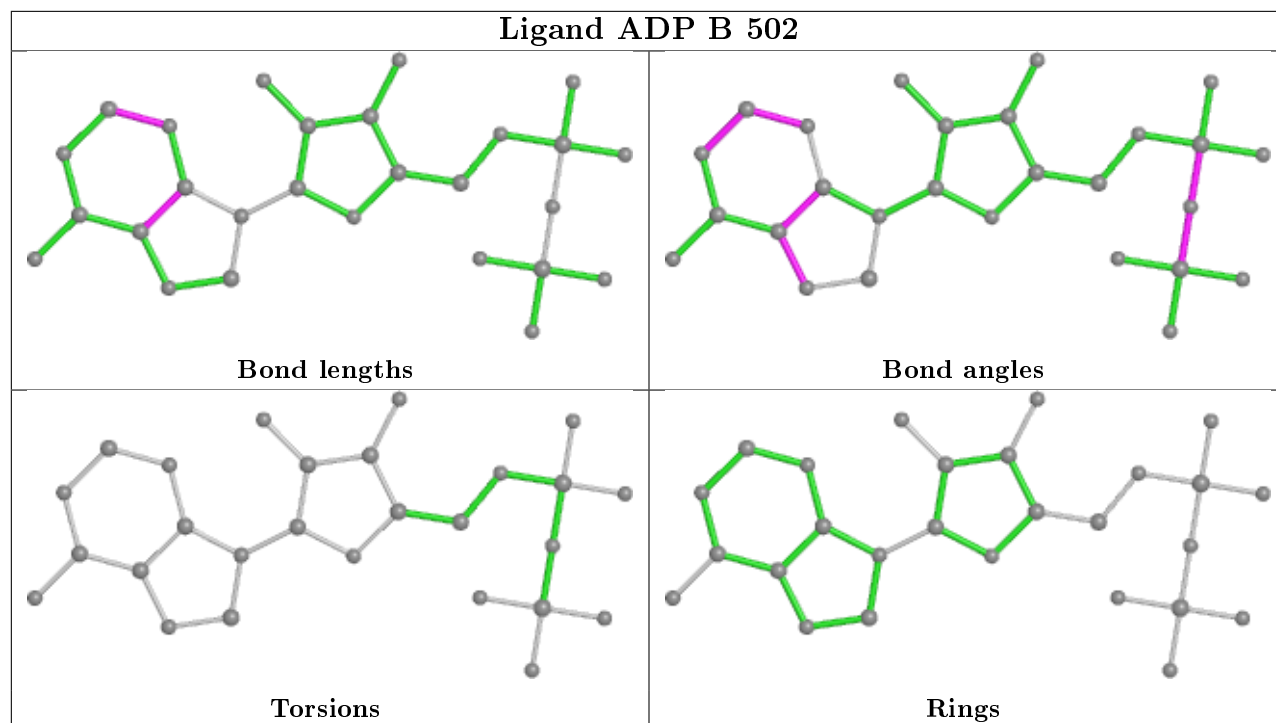


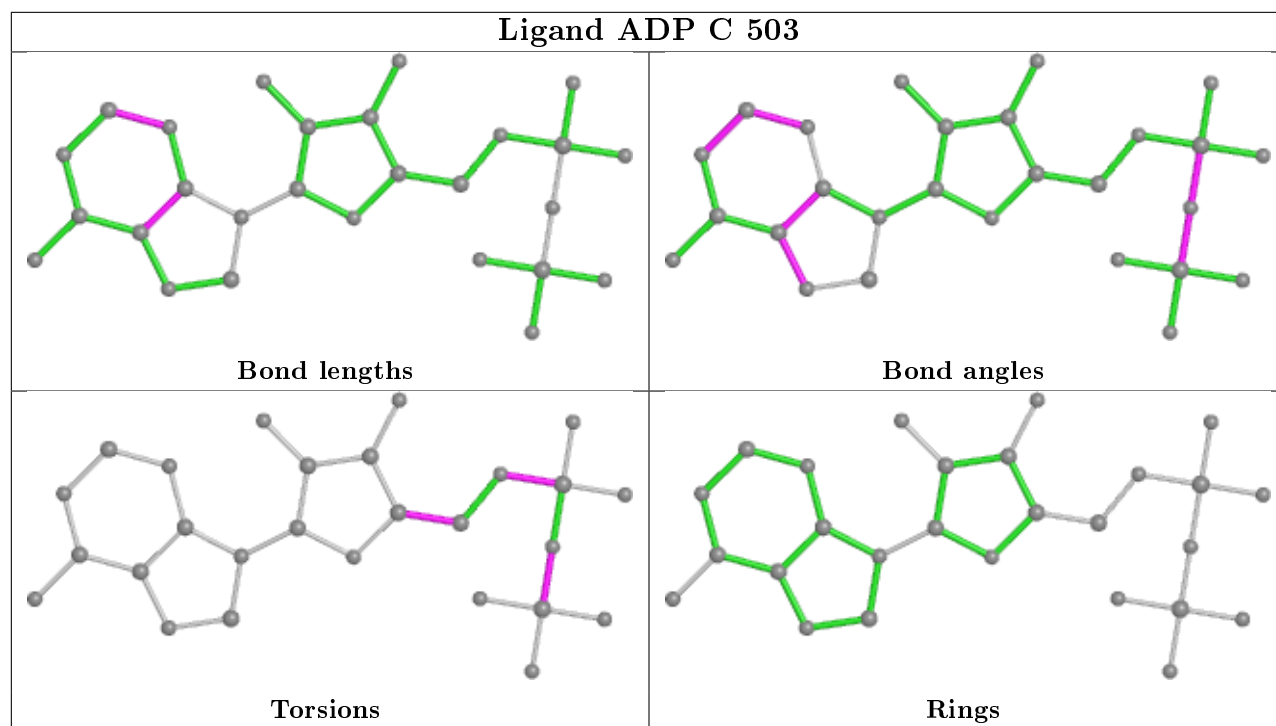
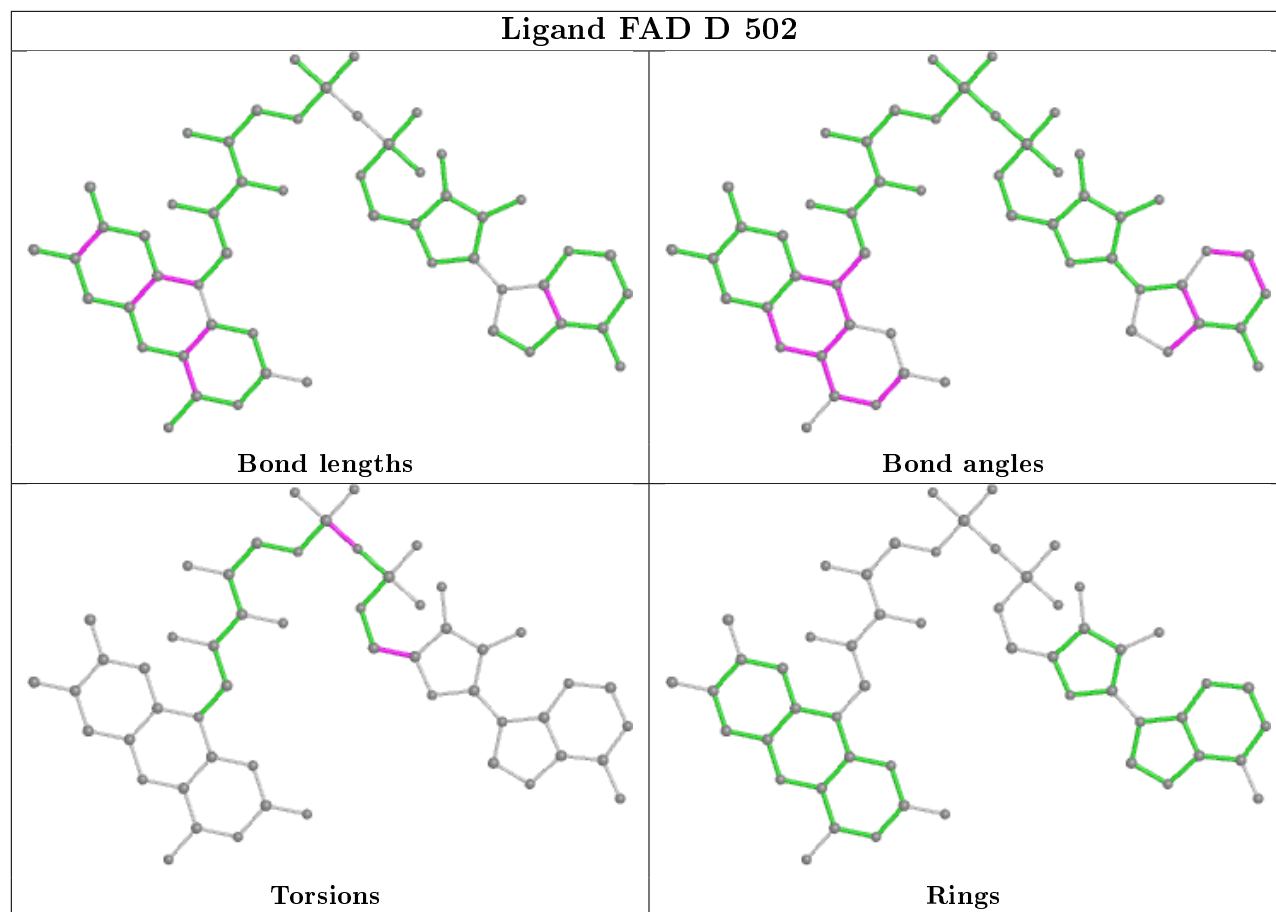












5.7 Other polymers [i](#)

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 [i](#)

6.1 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 | 462/466 (99%) | 0.05 | 11 (2%) 59 66 | 27, 42, 71, 103 | 0 |
| 1 | B | 459/466 (98%) | 0.24 | 27 (5%) 22 28 | 27, 45, 85, 116 | 0 |
| 1 | C | 462/466 (99%) | 0.11 | 19 (4%) 37 44 | 32, 49, 77, 120 | 0 |
| 1 | D | 459/466 (98%) | 0.29 | 36 (7%) 13 17 | 30, 49, 93, 123 | 0 |
| All | All | 1842/1864 (98%) | 0.17 | 93 (5%) 28 35 | 27, 47, 81, 123 | 0 |

The worst 5 of 93 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 342 | ALA | 8.2 |
| 1 | D | 254 | ASP | 6.9 |
| 1 | B | 253 | ALA | 6.8 |
| 1 | B | 460 | ALA | 6.7 |
| 1 | B | 337 | ARG | 6.2 |

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 carbohydrates in this entry.

6.4 Ligands [i](#)

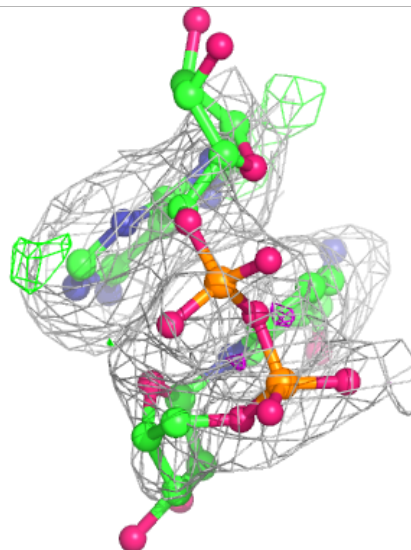
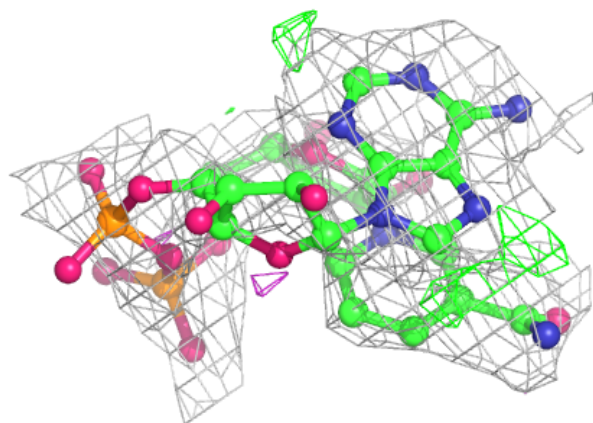
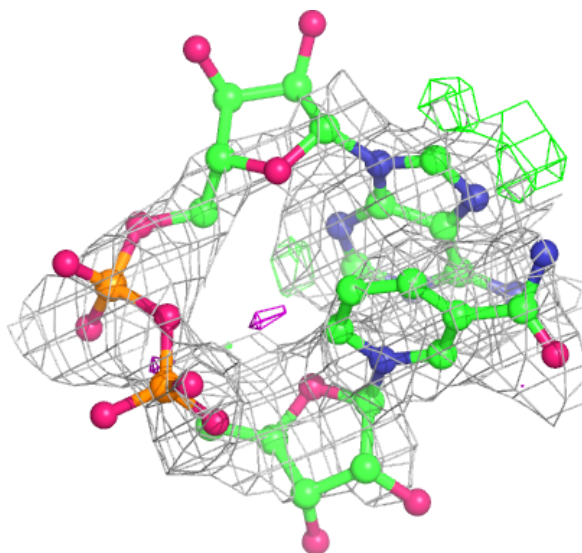
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | NAD | A | 504 | 44/44 | 0.63 | 0.31 | 85,122,155,161 | 0 |
| 5 | FMN | A | 505 | 31/31 | 0.68 | 0.48 | 82,101,136,141 | 0 |
| 6 | ADP | B | 502 | 27/27 | 0.69 | 0.34 | 98,117,130,138 | 0 |
| 2 | CL | C | 501 | 1/1 | 0.76 | 0.09 | 81,81,81,81 | 0 |
| 7 | MLT | D | 501 | 9/9 | 0.85 | 0.20 | 61,69,77,79 | 0 |
| 6 | ADP | D | 503 | 27/27 | 0.89 | 0.22 | 60,68,85,91 | 0 |
| 3 | FAD | A | 503 | 53/53 | 0.90 | 0.19 | 48,64,85,86 | 0 |
| 6 | ADP | C | 503 | 27/27 | 0.90 | 0.15 | 56,60,89,94 | 0 |
| 2 | CL | A | 501 | 1/1 | 0.94 | 0.12 | 64,64,64,64 | 0 |
| 3 | FAD | D | 502 | 53/53 | 0.95 | 0.15 | 31,36,53,57 | 0 |
| 3 | FAD | A | 502 | 53/53 | 0.96 | 0.15 | 28,33,40,45 | 0 |
| 3 | FAD | C | 502 | 53/53 | 0.96 | 0.12 | 36,41,47,47 | 0 |
| 3 | FAD | B | 501 | 53/53 | 0.97 | 0.12 | 31,38,42,43 | 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.

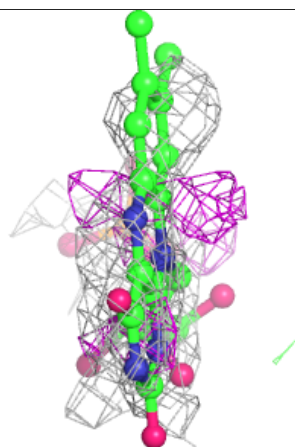
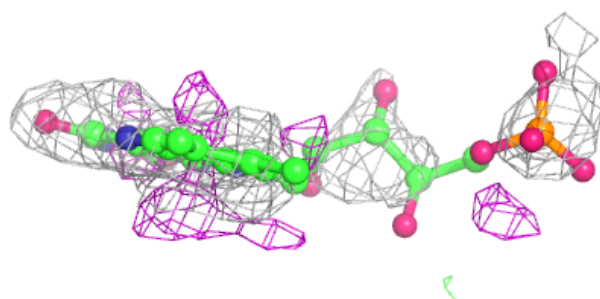
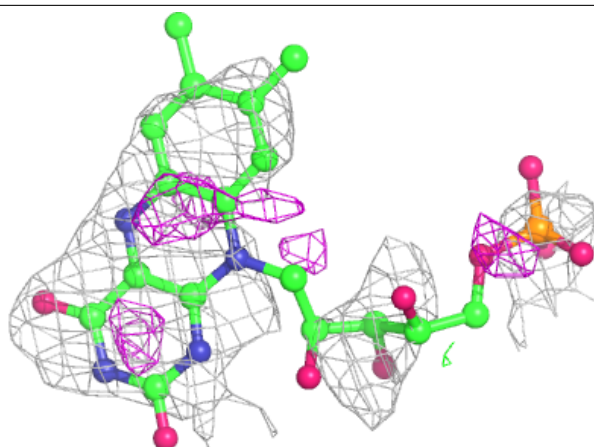
Electron density around NAD A 504:

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

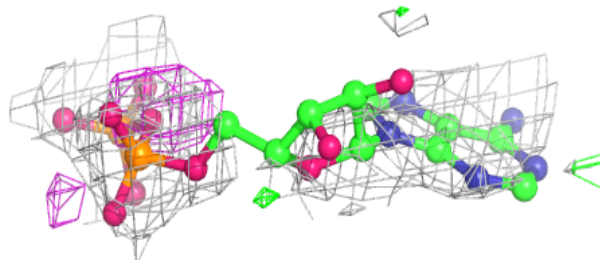
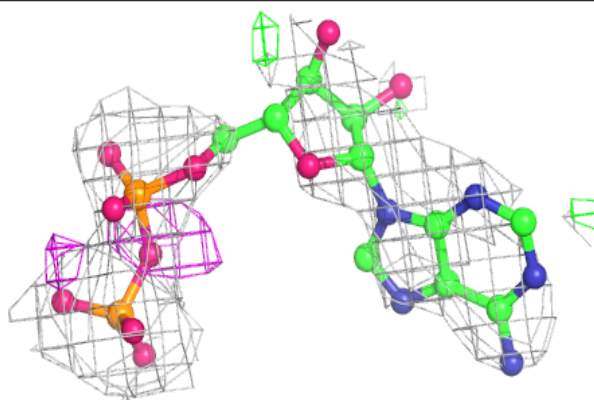


Electron density around FMN A 505:

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

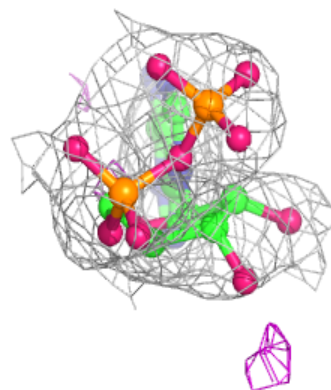
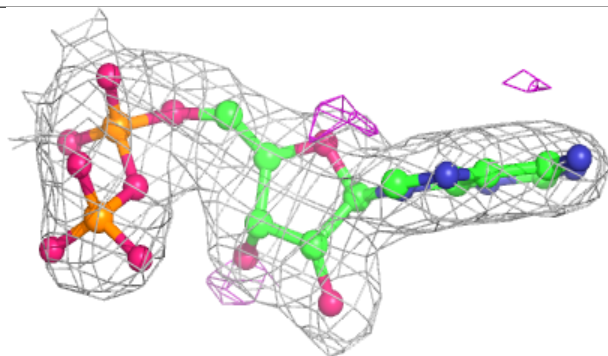
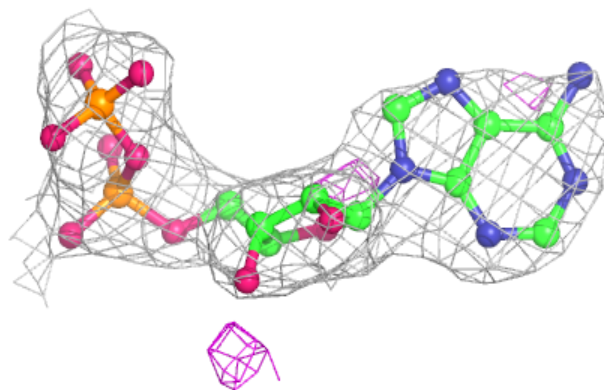
**Electron density around ADP B 502:**

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

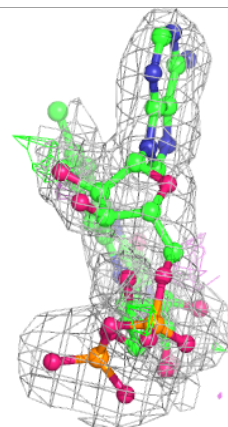
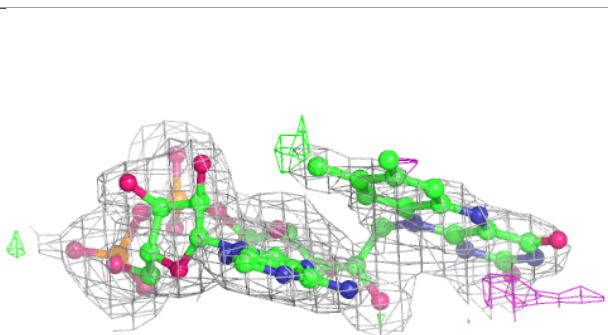
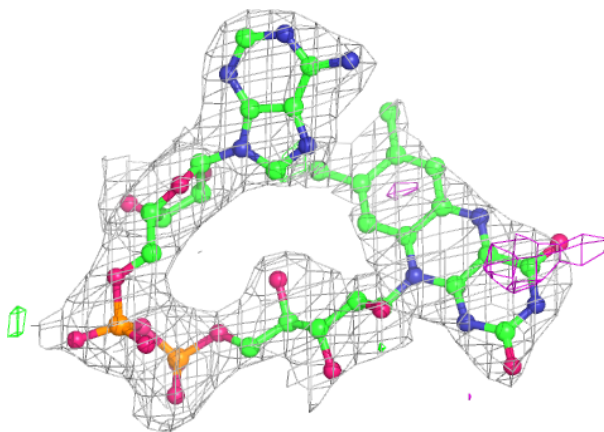


Electron density around ADP D 503:

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

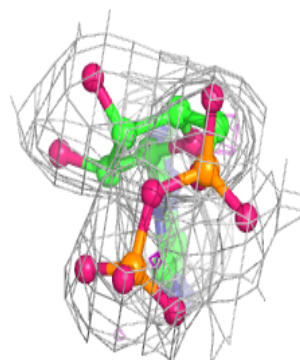
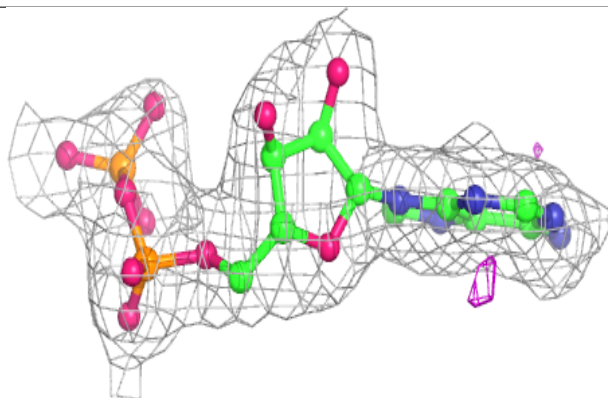
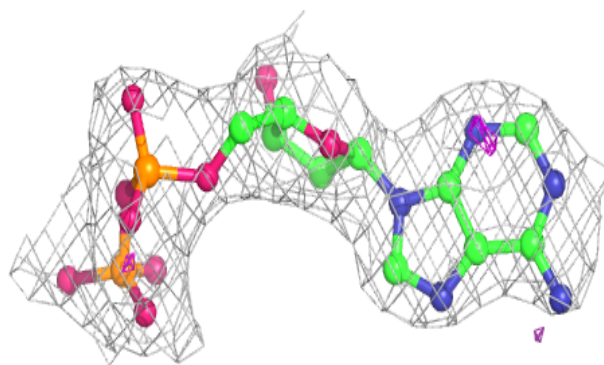
**Electron density around FAD A 503:**

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

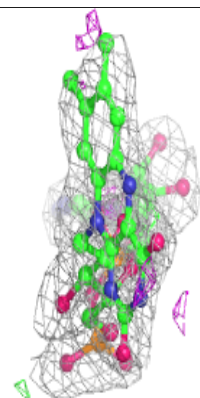
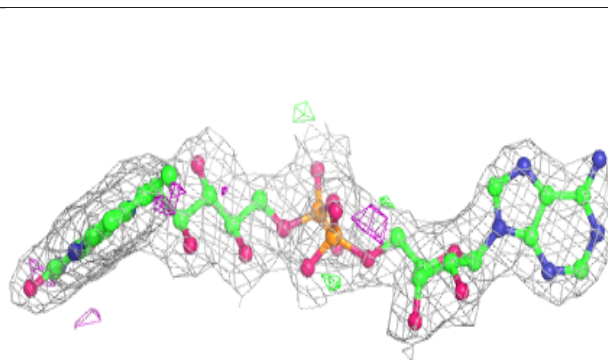
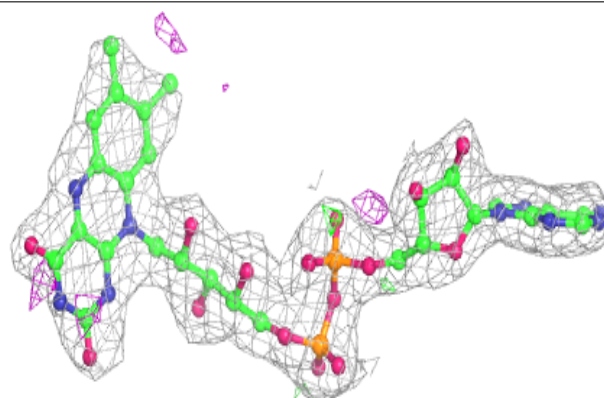


Electron density around ADP C 503:

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

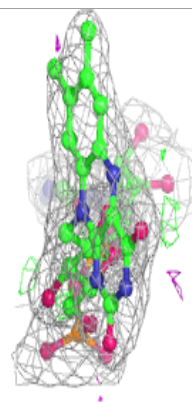
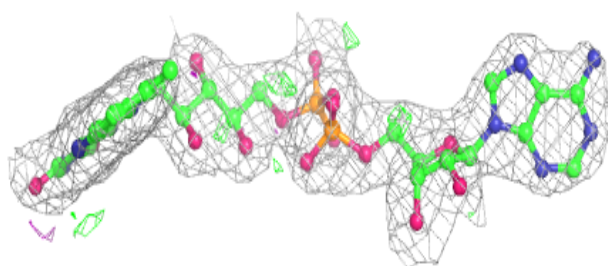
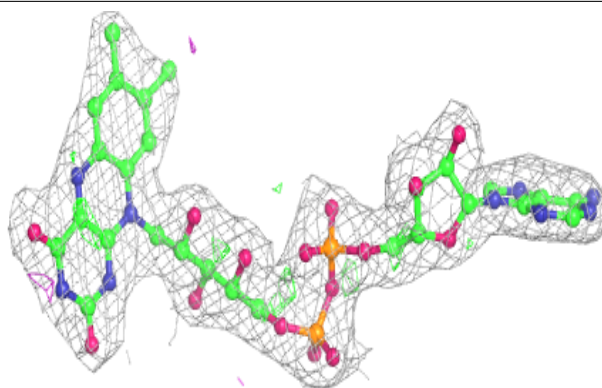
**Electron density around FAD D 502:**

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

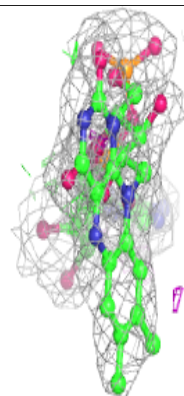
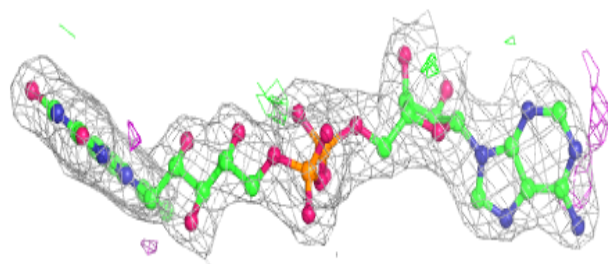
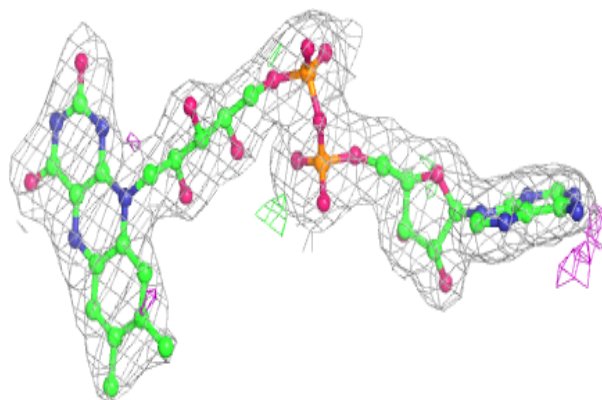


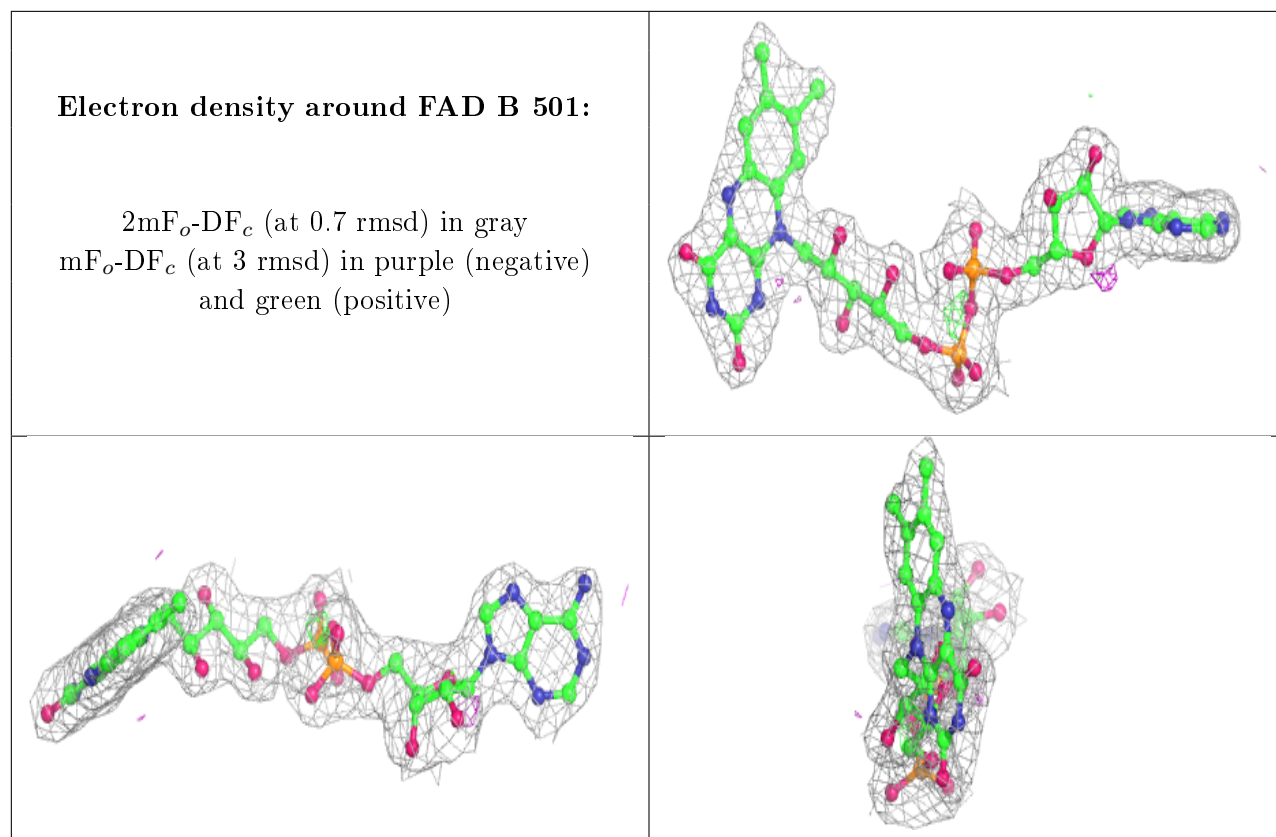
Electron density around FAD A 502:

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

**Electron density around FAD C 502:**

$2mF_o-DF_c$ (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.