# wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 07:03 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 6P5U |
| Title | : | Structure of an enoyl-CoA hydratase/aldolase isolated from a lignin-degrading consortium |
| Authors | : | Liberato, M.V.; Squina, F.M. |
| Deposited on | : | 2019-05-31 |
| Resolution | : | 2.10 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 (i) 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 (i)) were used in the production of this report:

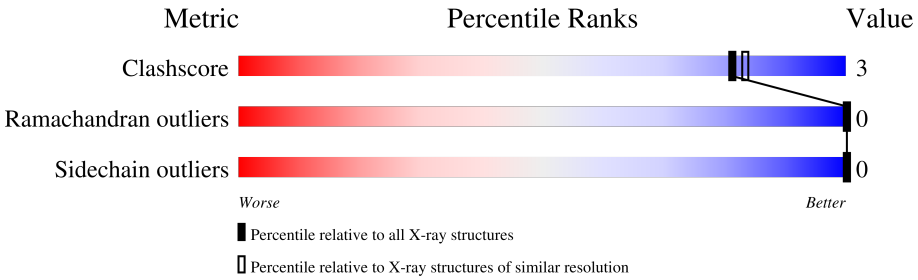
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | FAILED |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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)) |
|---|---|---|
| Clashscore | 141614 | 5710 (2.10-2.10) |
| Ramachandran outliers | 138981 | 5647 (2.10-2.10) |
| Sidechain outliers | 138945 | 5648 (2.10-2.10) |

## 2 Entry composition (i)

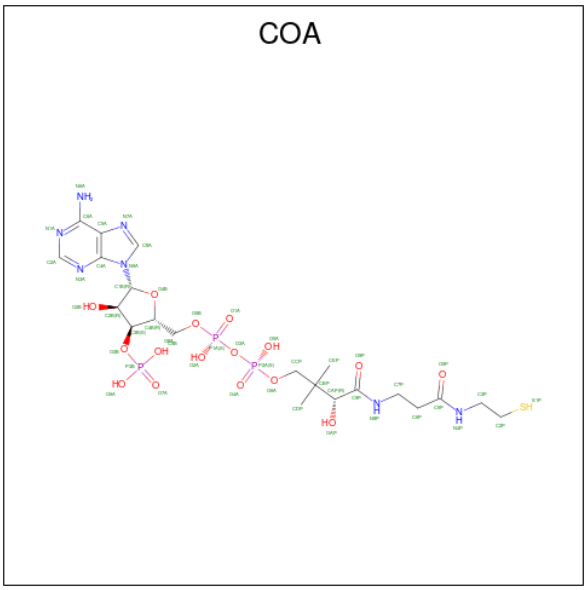
There are 4 unique types of molecules in this entry. The entry contains 12510 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Enoyl-CoA hydratase.

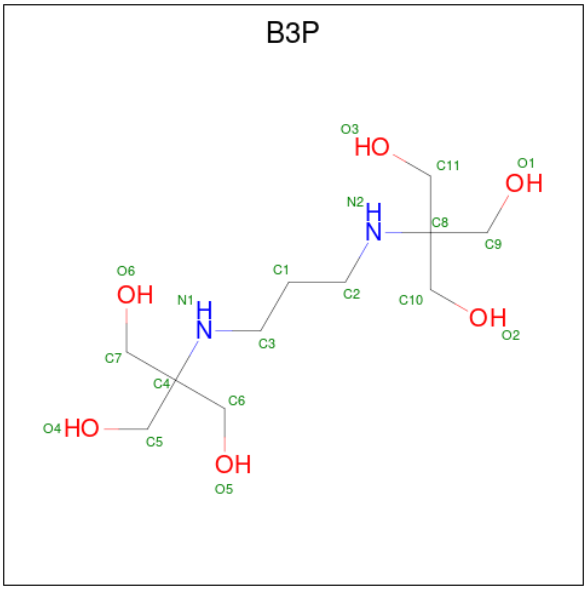
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 239 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1817 | 1155 | 315 | 337 | 10 | | | |
| 1 | B | 239 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1159 | 315 | 340 | 10 | | | |
| 1 | C | 239 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1159 | 318 | 337 | 10 | | | |
| 1 | D | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1835 | 1165 | 320 | 340 | 10 | | | |
| 1 | E | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1872 | 1189 | 331 | 342 | 10 | | | |
| 1 | F | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1840 | 1169 | 319 | 342 | 10 | | | |

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 48 | 21 | 7 | 16 | 3 | 1 | | |
| 2 | B | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 48 | 21 | 7 | 16 | 3 | 1 | | |
| 2 | C | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 48 | 21 | 7 | 16 | 3 | 1 | | |
| 2 | D | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 48 | 21 | 7 | 16 | 3 | 1 | | |
| 2 | E | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 48 | 21 | 7 | 16 | 3 | 1 | | |
| 2 | F | 1 | Total | C | N | O | P | S | 0 | 0 |
| | | | 48 | 21 | 7 | 16 | 3 | 1 | | |

- Molecule 3 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 3 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 19 | 11 | 2 | 6 | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 4 | A | 189 | Total | O | 0 | 0 |
| | | | 189 | 189 | | |
| 4 | B | 221 | Total | O | 0 | 0 |
| | | | 221 | 221 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | C | 200 | Total O<br>200 200 | 0 | 0 |
| 4 | D | 188 | Total O<br>188 188 | 0 | 0 |
| 4 | E | 188 | Total O<br>188 188 | 0 | 0 |
| 4 | F | 205 | Total O<br>205 205 | 0 | 0 |

SEQUENCE-PLOTS INFOmissingINFO

# 3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 99.28Å 130.96Å 115.91Å<br>90.00° 90.68° 90.00° | Depositor |
| Resolution (Å) | 43.40 – 2.10 | Depositor |
| % Data completeness<br>(in resolution range) | 98.8 (43.40-2.10) | Depositor |
| $R_{merge}$ | 0.13 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.79 (at 2.10Å) | Xtriage |
| Refinement program | PHENIX 1.14 | Depositor |
| R, $R_{free}$ | 0.196 , 0.229 | Depositor |
| Wilson B-factor (Å$^2$) | 22.2 | Xtriage |
| Anisotropy | 0.345 | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Estimated twinning fraction | 0.024 for -h,-k,l | Xtriage |
| Total number of atoms | 12510 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 25.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, COA

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 | 0.29 | 0/1852 | 0.44 | 0/2512 |
| 1 | B | 0.27 | 0/1859 | 0.43 | 0/2522 |
| 1 | C | 0.31 | 0/1859 | 0.47 | 0/2521 |
| 1 | D | 0.28 | 0/1870 | 0.44 | 0/2537 |
| 1 | E | 0.30 | 0/1908 | 0.46 | 0/2588 |
| 1 | F | 0.31 | 0/1875 | 0.47 | 0/2544 |
| All | All | 0.29 | 0/11223 | 0.45 | 0/15224 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 4.2 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 | 1817 | 0 | 1795 | 8 | 0 |
| 1 | B | 1824 | 0 | 1802 | 10 | 0 |
| 1 | C | 1824 | 0 | 1810 | 9 | 0 |
| 1 | D | 1835 | 0 | 1812 | 8 | 0 |
| 1 | E | 1872 | 0 | 1865 | 11 | 0 |
| 1 | F | 1840 | 0 | 1819 | 10 | 0 |
| 2 | A | 48 | 0 | 32 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | B | 48 | 0 | 31 | 4 | 0 |
| 2 | C | 48 | 0 | 32 | 0 | 0 |
| 2 | D | 48 | 0 | 31 | 4 | 0 |
| 2 | E | 48 | 0 | 31 | 2 | 0 |
| 2 | F | 48 | 0 | 32 | 0 | 0 |
| 3 | B | 19 | 0 | 26 | 0 | 0 |
| 4 | A | 189 | 0 | 0 | 2 | 0 |
| 4 | B | 221 | 0 | 0 | 1 | 0 |
| 4 | C | 200 | 0 | 0 | 1 | 0 |
| 4 | D | 188 | 0 | 0 | 3 | 0 |
| 4 | E | 188 | 0 | 0 | 0 | 0 |
| 4 | F | 205 | 0 | 0 | 1 | 0 |
| All | All | 12510 | 0 | 11118 | 59 | 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 59 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:E:28:SER:HA | 1:E:65:THR:O | 1.94 | 0.67 |
| 2:B:501:COA:O5P | 2:B:501:COA:N8P | 2.27 | 0.65 |
| 1:E:46:MET:HG2 | 1:E:102:TRP:CE3 | 2.34 | 0.62 |
| 1:D:82:ARG:N | 4:D:602:HOH:O | 2.29 | 0.60 |
| 1:B:203:ARG:NH1 | 4:B:607:HOH:O | 2.34 | 0.60 |

There are no symmetry-related clashes.

## 4.3 Torsion angles (i)

### 4.3.1 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 | 235/283 (83%) | 225 (96%) | 10 (4%) | 0 | 100 | 100 |
| 1 | B | 235/283 (83%) | 228 (97%) | 7 (3%) | 0 | 100 | 100 |
| 1 | C | 235/283 (83%) | 226 (96%) | 9 (4%) | 0 | 100 | 100 |
| 1 | D | 237/283 (84%) | 228 (96%) | 9 (4%) | 0 | 100 | 100 |
| 1 | E | 244/283 (86%) | 235 (96%) | 9 (4%) | 0 | 100 | 100 |
| 1 | F | 238/283 (84%) | 229 (96%) | 9 (4%) | 0 | 100 | 100 |
| All | All | 1424/1698 (84%) | 1371 (96%) | 53 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 4.3.2 Protein sidechains (i)

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 | 181/225 (80%) | 181 (100%) | 0 | 100 | 100 |
| 1 | B | 182/225 (81%) | 182 (100%) | 0 | 100 | 100 |
| 1 | C | 182/225 (81%) | 182 (100%) | 0 | 100 | 100 |
| 1 | D | 183/225 (81%) | 183 (100%) | 0 | 100 | 100 |
| 1 | E | 185/225 (82%) | 185 (100%) | 0 | 100 | 100 |
| 1 | F | 184/225 (82%) | 184 (100%) | 0 | 100 | 100 |
| All | All | 1097/1350 (81%) | 1097 (100%) | 0 | 100 | 100 |

There are no protein residues with a non-rotameric sidechain to report.

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

### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

## 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 monosaccharides in this entry.

## 4.6 Ligand geometry (i)

7 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

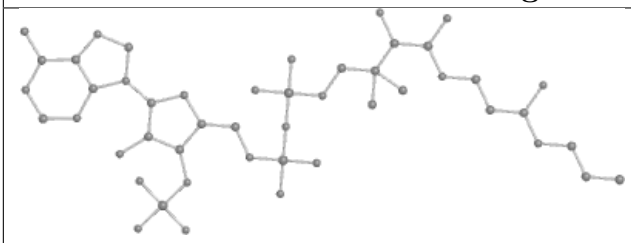
There are no torsion outliers.

There are no ring outliers.

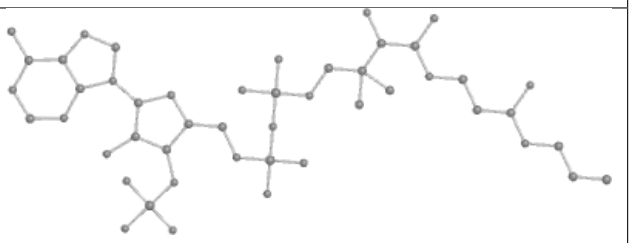
No monomer is involved in short contacts.

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 then 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.

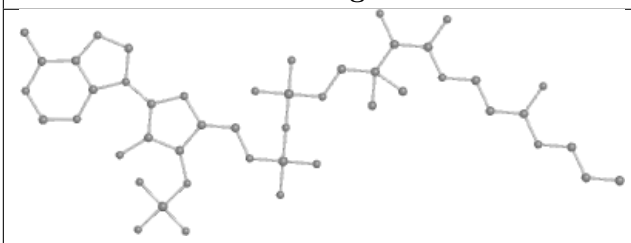
## Ligand COA A 501



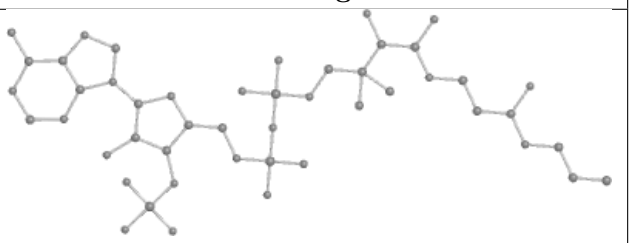
Bond lengths



Bond angles

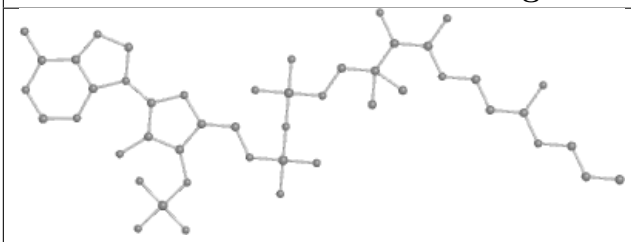


Torsions

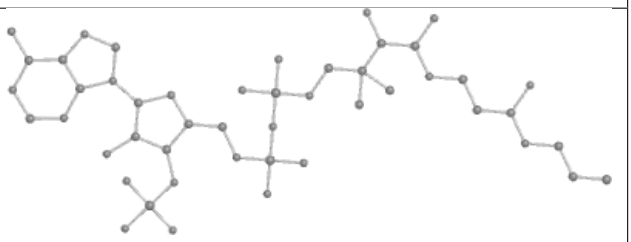


Rings

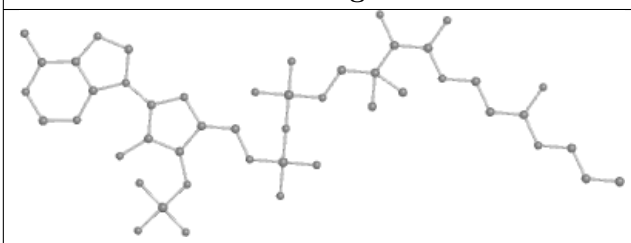
## Ligand COA B 501



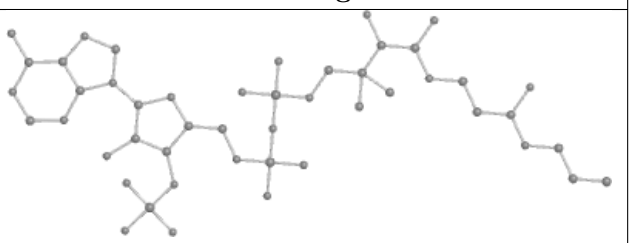
Bond lengths



Bond angles

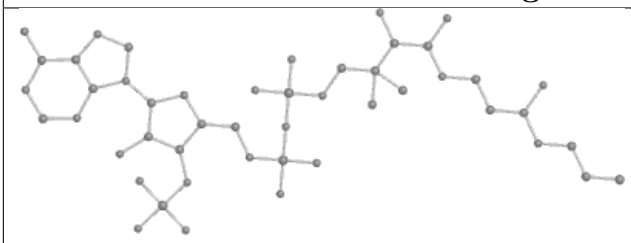


Torsions

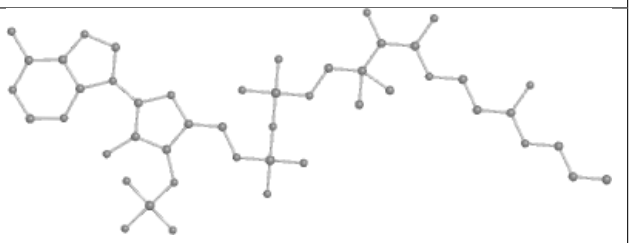


Rings

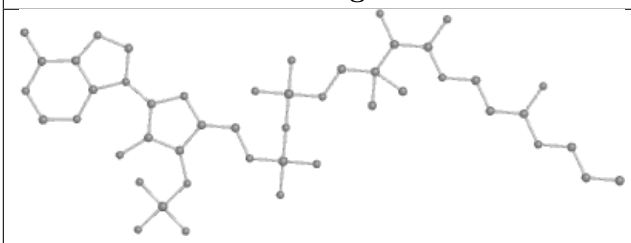
## Ligand COA C 501



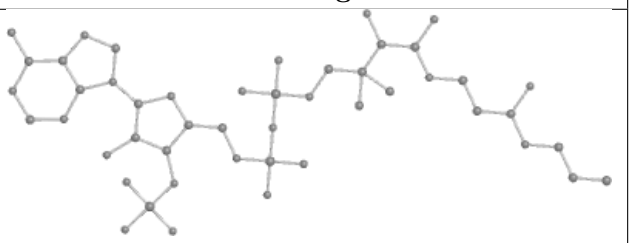
Bond lengths



Bond angles

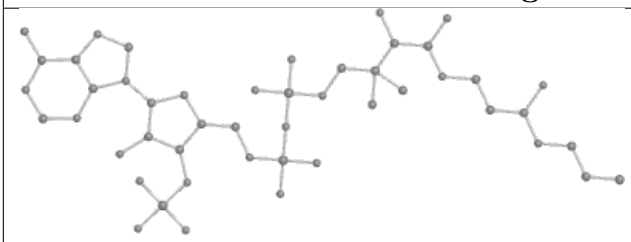


Torsions

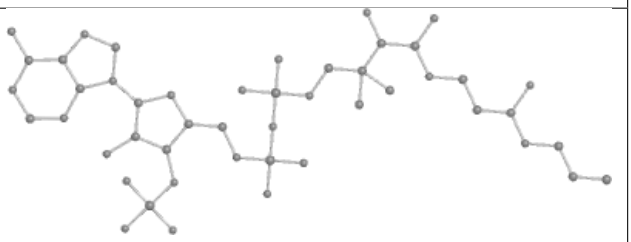


Rings

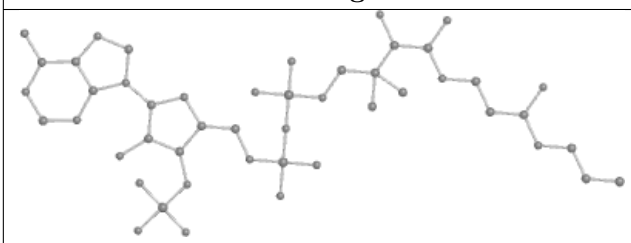
## Ligand COA D 501



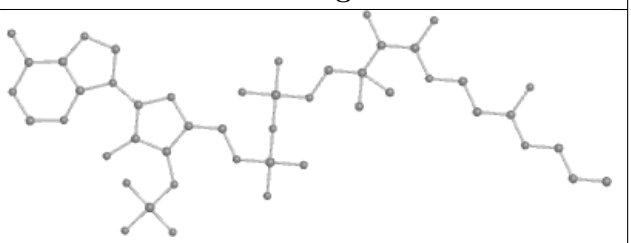
Bond lengths



Bond angles

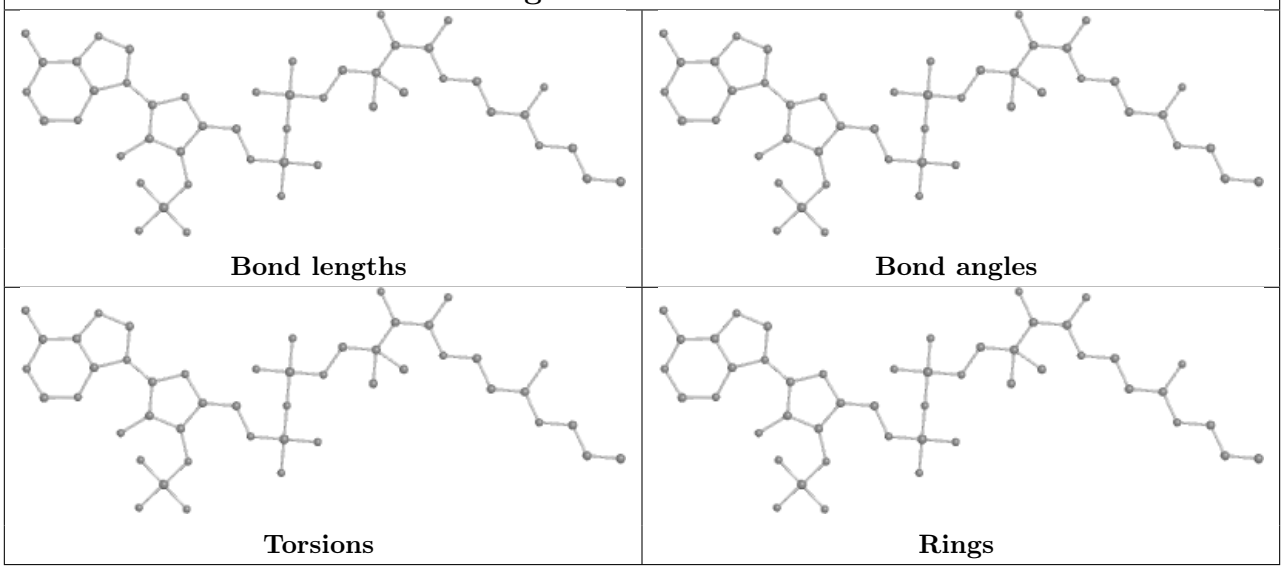


Torsions

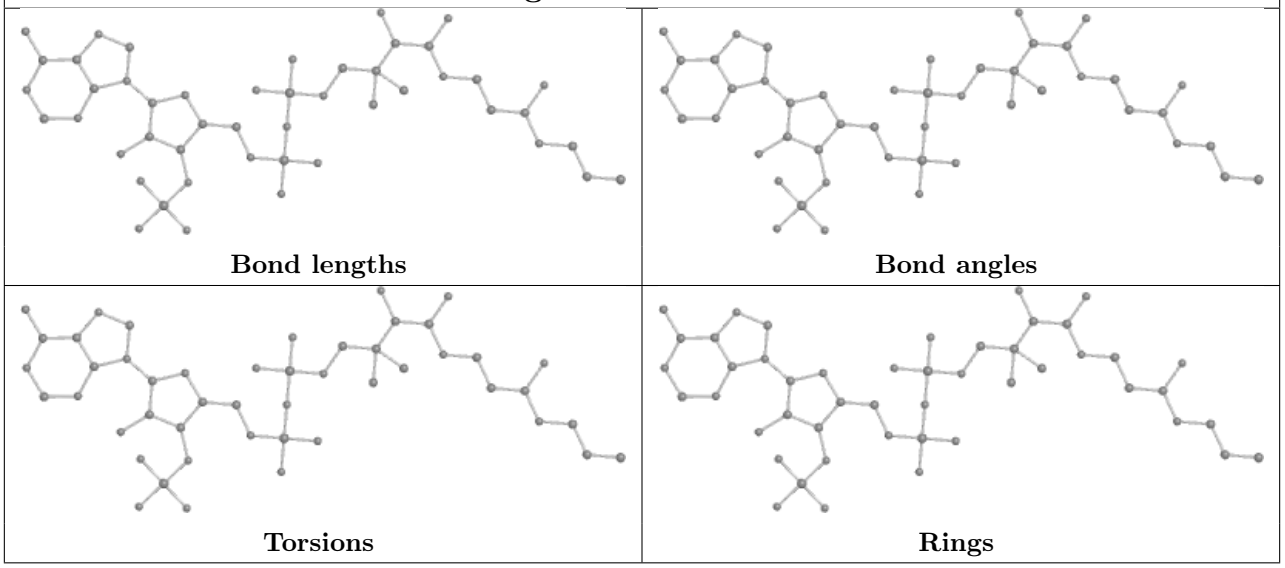


Rings

**Ligand COA E 501**




**Ligand COA F 501**




## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 5 Fit of model and data

## 5.1 Protein, DNA and RNA chains

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

## 5.2 Non-standard residues in protein, DNA, RNA chains

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

## 5.3 Carbohydrates

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

## 5.4 Ligands

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

## 5.5 Other polymers

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