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

Sep 6, 2023 – 09:29 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 4BLC |
| Title | : | THE STRUCTURE OF ORTHORHOMBIC CRYSTALS OF BEEF LIVER CATALASE |
| Authors | : | Ko, T.P.; Day, J.; Malkin, A.; McPherson, A. |
| Deposited on | : | 1998-09-27 |
| 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 (i) 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 (1)) were used in the production of this report:

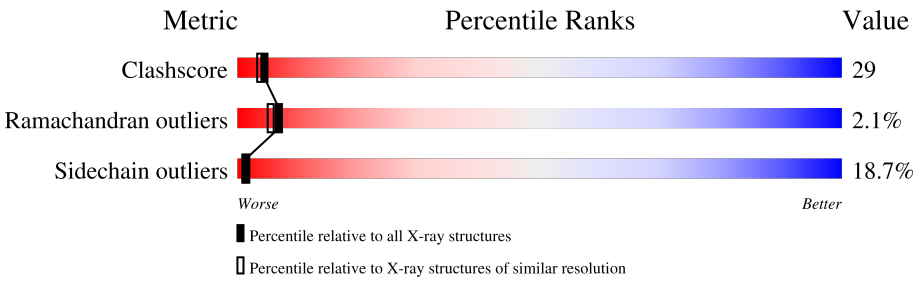
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 1 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 2.30 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)) |
|---|---|---|
| Clashscore | 141614 | 5643 (2.30-2.30) |
| Ramachandran outliers | 138981 | 5575 (2.30-2.30) |
| Sidechain outliers | 138945 | 5575 (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 of 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 <=5%

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 506 | 56% 36% 6% • |
| 1 | B | 506 | 38% 45% 15% •• |
| 1 | C | 506 | 44% 41% 13% •• |
| 1 | D | 506 | 47% 42% 10% • |

# 2 Entry composition (i)

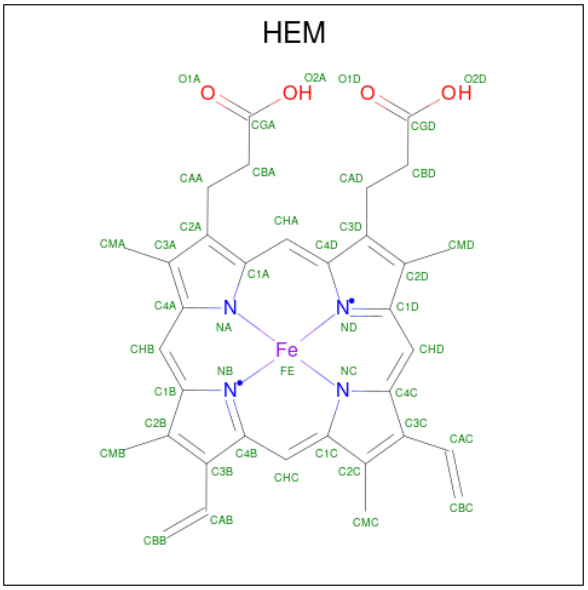
There are 4 unique types of molecules in this entry. The entry contains 16816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CATALASE).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 499 | 4017 | 2548 | 715 | 740 | 14 | 0 | 0 | 0 |
| 1 | B | 499 | 4017 | 2548 | 715 | 740 | 14 | 0 | 0 | 0 |
| 1 | C | 499 | 4017 | 2548 | 715 | 740 | 14 | 0 | 0 | 0 |
| 1 | D | 499 | 4017 | 2548 | 715 | 740 | 14 | 0 | 0 | 0 |

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Fe | N | O | | |
| 2 | A | 1 | 43 | 34 | 1 | 4 | 4 | 0 | 0 |
| 2 | B | 1 | 43 | 34 | 1 | 4 | 4 | 0 | 0 |

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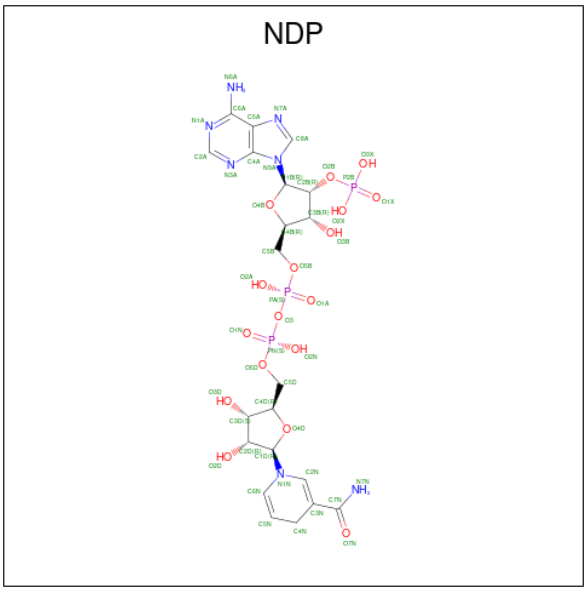
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Fe | N | O | | |
| 2 | C | 1 | 43 | 34 | 1 | 4 | 4 | 0 | 0 |
| | | | Total | C | Fe | N | O | | |
| 2 | D | 1 | 43 | 34 | 1 | 4 | 4 | 0 | 0 |

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).




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

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 4 | A | 119 | 119 | 119 | 0 | 0 |
| | | | Total | O | | |
| 4 | B | 89 | 89 | 89 | 0 | 0 |
| | | | Total | O | | |
| 4 | C | 83 | 83 | 83 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 4 | D | 93 | 93 | 93 | 0 | 0 |

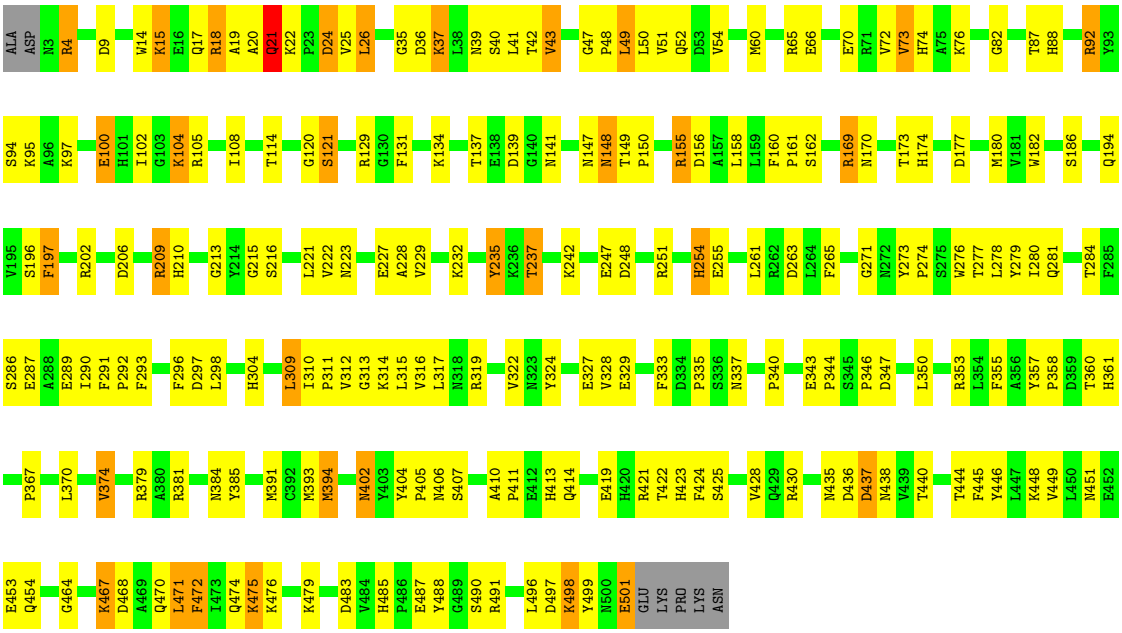
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

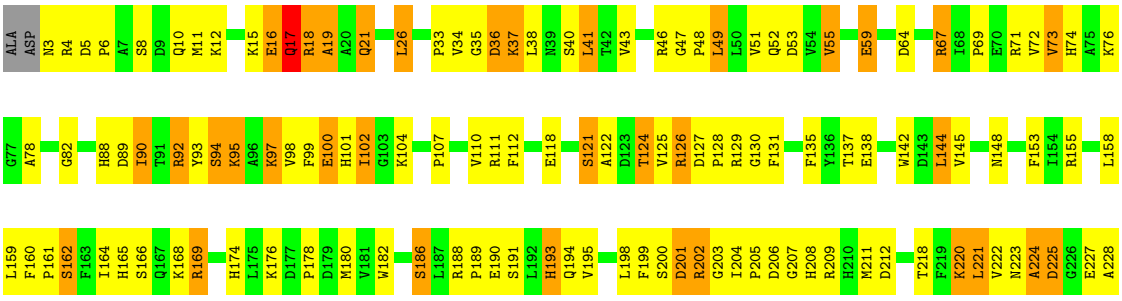
• Molecule 1: PROTEIN (CATALASE)

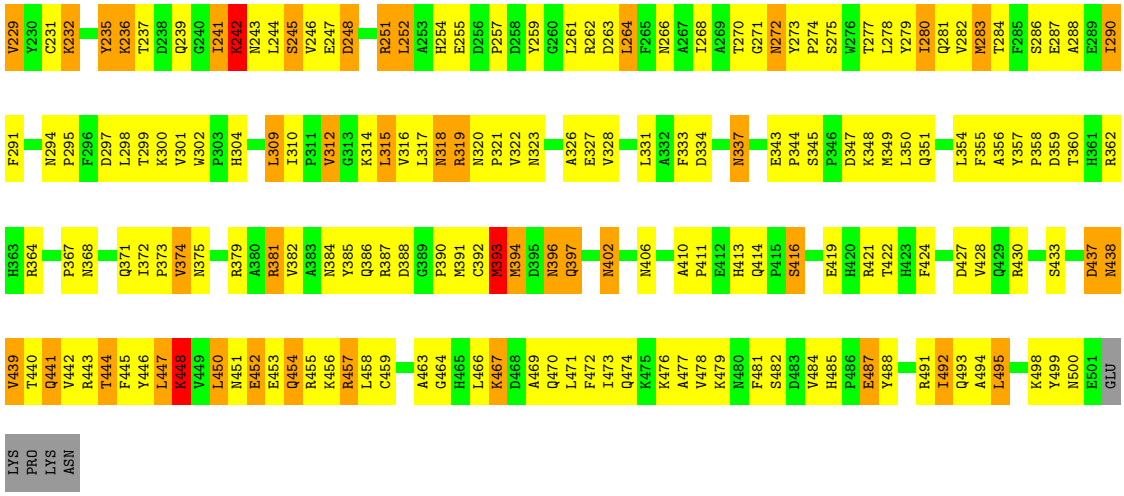
Chain A: 56% 36% 6% •




• Molecule 1: PROTEIN (CATALASE)

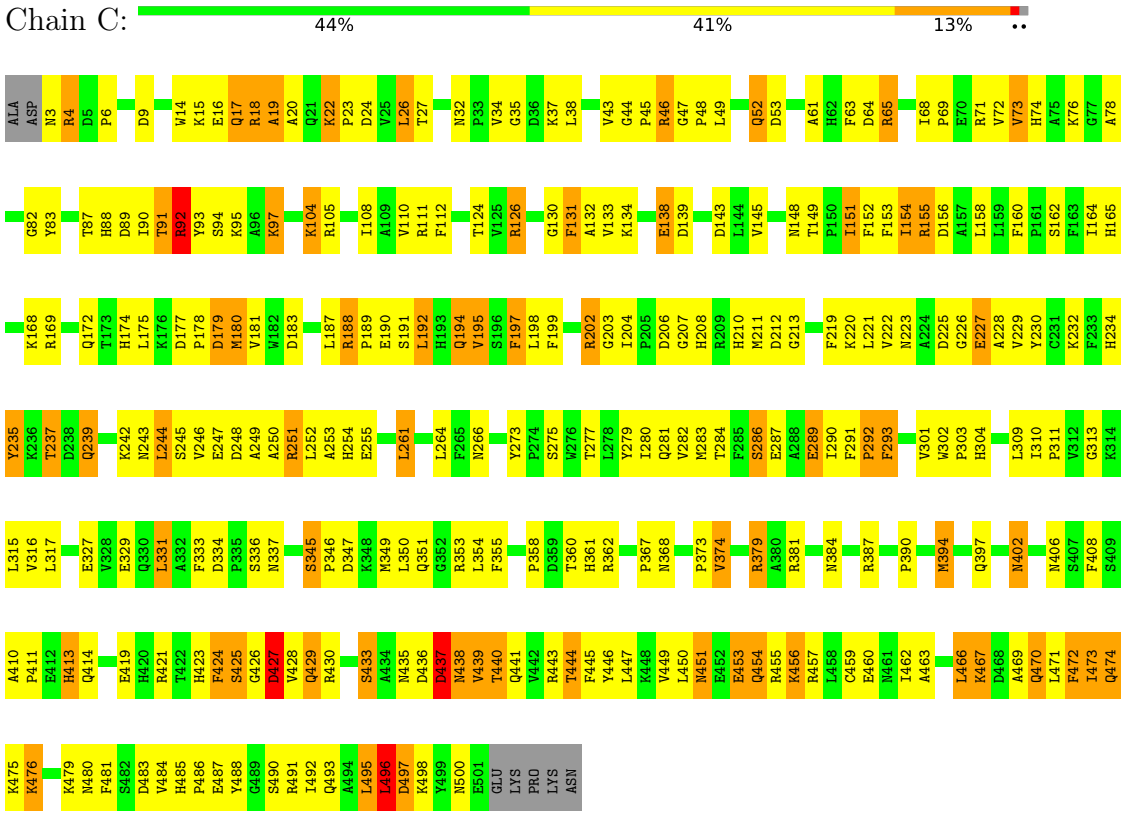
Chain B: 38% 45% 15% ••





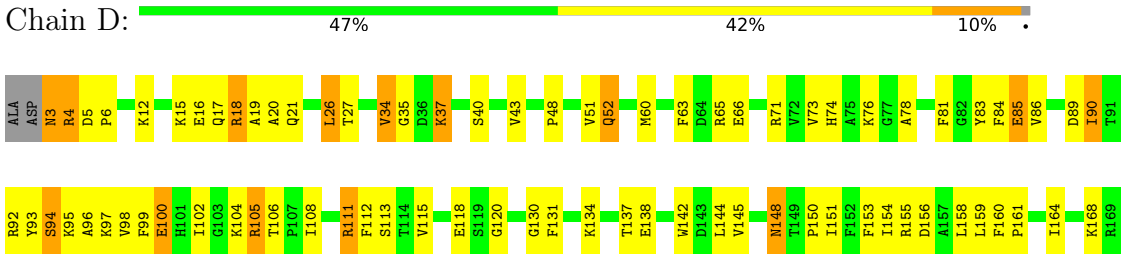
- Molecule 1: PROTEIN (CATALASE)

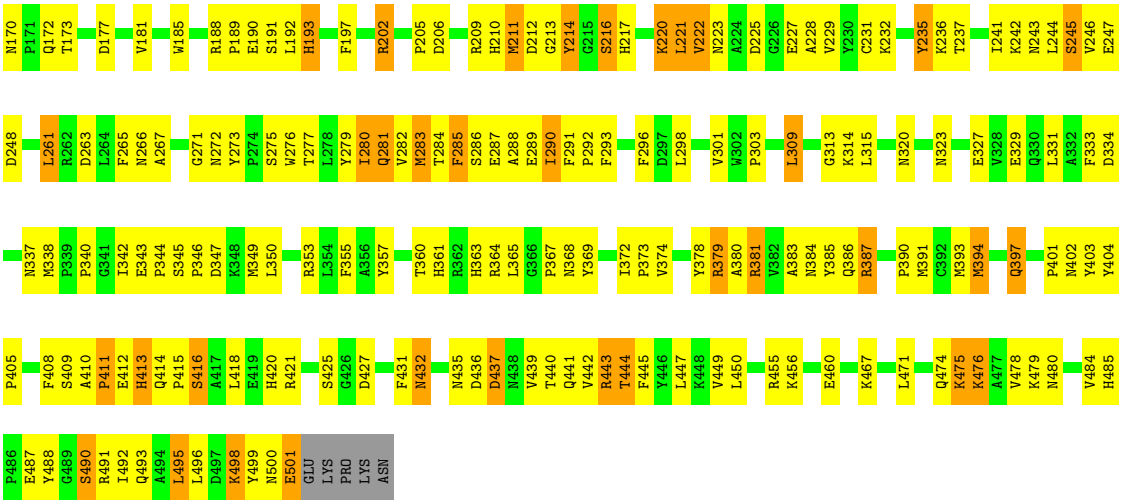
Chain C:




- Molecule 1: PROTEIN (CATALASE)

Chain D:




N170 P171 Q172 T173 D177 V181 W185 R188 P189 E190 S191 L192 H193 F197 R202 P205 D206 R209 H210 M211 D212 G213 Y214 G215 S216 H217 K220 L221 V222 N223 A224 D225 G226 E227 A228 V229 Y230 C231 K232 Y235 K236 T237 I241 K242 N243 L244 S245 V246 E247
D248 L261 R262 D263 L264 F265 N266 A267 G271 N272 Y273 P274 S275 W276 T277 L278 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 A288 E289 I290 F291 P292 F293 F296 D297 L298 V301 W302 P303 L309 G313 K314 L315 N320 N323 E327 V328 E329 Q330 L331 A332 F333 D334
N337 M338 P339 P340 G341 I342 E343 P344 S345 P346 D347 K348 M349 L350 R353 L354 F355 A356 Y357 T360 H361 R362 H363 R364 L365 G366 P367 M368 Y369 I372 P373 V374 Y378 R379 A380 R381 V382 A383 N384 Y385 Q386 R387 P390 M391 C392 M393 M394 Q397 P401 N402 Y403 Y404
P405 F408 S409 A410 P411 E412 H413 Q414 P415 S416 A417 L418 E419 H420 R421 S425 G426 D427 F431 N432 N435 D436 D437 N438 V439 T440 Q441 V442 R443 T444 F445 Y446 L447 K448 V449 L450 R455 K456 E460 K467 L471 Q474 K475 K476 A477 V478 K479 N480 V484 H485
P486 E487 Y488 G489 S490 R491 I492 Q493 A494 L495 L496 D497 K498 Y499 N500 E501 GLU LYS PRO LYS ASN

# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 87.80Å 140.60Å 232.40Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 2.30 | Depositor |
| % Data completeness<br>(in resolution range) | 87.5 (20.00-2.30) | Depositor |
| $R_{merge}$ | 0.12 | Depositor |
| $R_{sym}$ | 0.12 | Depositor |
| Refinement program | X-PLOR 3.851 | Depositor |
| R, $R_{free}$ | 0.205 , 0.273 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 16816 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 47.0 | wwPDB-VP |

# 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: HEM, NDP

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 | 0.41 | 0/4137 | 0.62 | 0/5619 |
| 1 | B | 0.39 | 0/4137 | 0.59 | 0/5619 |
| 1 | C | 0.39 | 0/4137 | 0.60 | 0/5619 |
| 1 | D | 0.41 | 0/4137 | 0.60 | 0/5619 |
| All | All | 0.40 | 0/16548 | 0.60 | 0/22476 |

There are no bond length outliers.

There are no bond angle outliers.

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 | 4017 | 0 | 3839 | 171 | 0 |
| 1 | B | 4017 | 0 | 3839 | 305 | 0 |
| 1 | C | 4017 | 0 | 3839 | 273 | 0 |
| 1 | D | 4017 | 0 | 3839 | 253 | 0 |
| 2 | A | 43 | 0 | 30 | 5 | 0 |
| 2 | B | 43 | 0 | 30 | 0 | 0 |
| 2 | C | 43 | 0 | 30 | 4 | 0 |
| 2 | D | 43 | 0 | 30 | 2 | 0 |
| 3 | A | 48 | 0 | 26 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | B | 48 | 0 | 26 | 4 | 0 |
| 3 | C | 48 | 0 | 26 | 2 | 0 |
| 3 | D | 48 | 0 | 26 | 1 | 0 |
| 4 | A | 119 | 0 | 0 | 8 | 0 |
| 4 | B | 89 | 0 | 0 | 16 | 0 |
| 4 | C | 83 | 0 | 0 | 8 | 0 |
| 4 | D | 93 | 0 | 0 | 10 | 0 |
| All | All | 16816 | 0 | 15580 | 917 | 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 29.

The worst 5 of 917 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:D:223:ASN:HD21 | 1:D:227:GLU:HB3 | 0.98 | 1.12 |
| 1:A:451:ASN:H | 1:A:454:GLN:HE21 | 1.06 | 1.01 |
| 1:D:223:ASN:ND2 | 1:D:227:GLU:HB3 | 1.79 | 0.98 |
| 1:B:169:ARG:HG2 | 1:B:169:ARG:HH11 | 1.30 | 0.95 |
| 1:B:457:ARG:HH11 | 1:B:457:ARG:HB2 | 1.28 | 0.95 |

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 | 497/506 (98%) | 442 (89%) | 50 (10%) | 5 (1%) | 15 17 |
| 1 | B | 497/506 (98%) | 423 (85%) | 58 (12%) | 16 (3%) | 4 2 |
| 1 | C | 497/506 (98%) | 417 (84%) | 65 (13%) | 15 (3%) | 4 2 |
| 1 | D | 497/506 (98%) | 442 (89%) | 49 (10%) | 6 (1%) | 13 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 1988/2024 (98%) | 1724 (87%) | 222 (11%) | 42 (2%) | 7 5 |

5 of 42 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 19 | ALA |
| 1 | A | 437 | ASP |
| 1 | B | 124 | THR |
| 1 | B | 242 | LYS |
| 1 | B | 394 | MET |

### 5.3.2 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 | 431/437 (99%) | 365 (85%) | 66 (15%) | 2 2 |
| 1 | B | 431/437 (99%) | 332 (77%) | 99 (23%) | 1 0 |
| 1 | C | 431/437 (99%) | 349 (81%) | 82 (19%) | 1 1 |
| 1 | D | 431/437 (99%) | 356 (83%) | 75 (17%) | 2 2 |
| All | All | 1724/1748 (99%) | 1402 (81%) | 322 (19%) | 1 1 |

5 of 322 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 439 | VAL |
| 1 | D | 261 | LEU |
| 1 | C | 467 | LYS |
| 1 | D | 90 | ILE |
| 1 | D | 381 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 3 | ASN |
| 1 | C | 402 | ASN |
| 1 | D | 500 | ASN |
| 1 | D | 363 | HIS |
| 1 | C | 17 | 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 monosaccharides in this entry.

## 5.6 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 | $\#\|Z\| > 2$ |
| 2 | HEM | C | 507 | 1 | 41,50,50 | 1.37 | 5 (12%) | 45,82,82 | 1.08 | 1 (2%) |
| 3 | NDP | D | 1402 | - | 45,52,52 | 1.55 | 9 (20%) | 53,80,80 | 1.42 | 7 (13%) |
| 2 | HEM | B | 507 | 1 | 41,50,50 | 1.27 | 5 (12%) | 45,82,82 | 1.04 | 3 (6%) |
| 2 | HEM | A | 507 | 1 | 41,50,50 | 1.41 | 6 (14%) | 45,82,82 | 0.99 | 2 (4%) |
| 3 | NDP | B | 1202 | - | 45,52,52 | 1.55 | 7 (15%) | 53,80,80 | 1.81 | 10 (18%) |
| 3 | NDP | C | 1302 | - | 45,52,52 | 1.55 | 7 (15%) | 53,80,80 | 1.78 | 10 (18%) |
| 3 | NDP | A | 1102 | - | 45,52,52 | 1.53 | 7 (15%) | 53,80,80 | 1.53 | 8 (15%) |
| 2 | HEM | D | 507 | 1 | 41,50,50 | 1.29 | 6 (14%) | 45,82,82 | 1.25 | 5 (11%) |

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 | HEM | C | 507 | 1 | - | 4/12/54/54 | - |
| 3 | NDP | D | 1402 | - | - | 11/30/77/77 | 0/5/5/5 |
| 2 | HEM | B | 507 | 1 | - | 6/12/54/54 | - |
| 2 | HEM | A | 507 | 1 | - | 3/12/54/54 | - |
| 3 | NDP | B | 1202 | - | - | 10/30/77/77 | 0/5/5/5 |
| 3 | NDP | C | 1302 | - | - | 7/30/77/77 | 0/5/5/5 |
| 3 | NDP | A | 1102 | - | - | 6/30/77/77 | 0/5/5/5 |
| 2 | HEM | D | 507 | 1 | - | 4/12/54/54 | - |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 1302 | NDP | C6N-C5N | 4.91 | 1.42 | 1.33 |
| 3 | D | 1402 | NDP | C6N-C5N | 4.71 | 1.41 | 1.33 |
| 3 | A | 1102 | NDP | C6N-C5N | 4.69 | 1.41 | 1.33 |
| 3 | B | 1202 | NDP | C6N-C5N | 4.61 | 1.41 | 1.33 |
| 2 | A | 507 | HEM | C3C-CAC | -4.15 | 1.39 | 1.47 |

The worst 5 of 46 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 1302 | NDP | O4D-C1D-N1N | 6.07 | 119.91 | 108.06 |
| 3 | B | 1202 | NDP | N3A-C2A-N1A | -5.63 | 119.88 | 128.68 |
| 3 | B | 1202 | NDP | O4D-C1D-N1N | 5.39 | 118.60 | 108.06 |
| 3 | C | 1302 | NDP | N3A-C2A-N1A | -4.95 | 120.94 | 128.68 |
| 3 | D | 1402 | NDP | N3A-C2A-N1A | -4.36 | 121.86 | 128.68 |

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 507 | HEM | C2B-C3B-CAB-CBB |
| 2 | A | 507 | HEM | C4B-C3B-CAB-CBB |
| 2 | B | 507 | HEM | C2B-C3B-CAB-CBB |
| 2 | D | 507 | HEM | C2B-C3B-CAB-CBB |
| 2 | D | 507 | HEM | C4B-C3B-CAB-CBB |

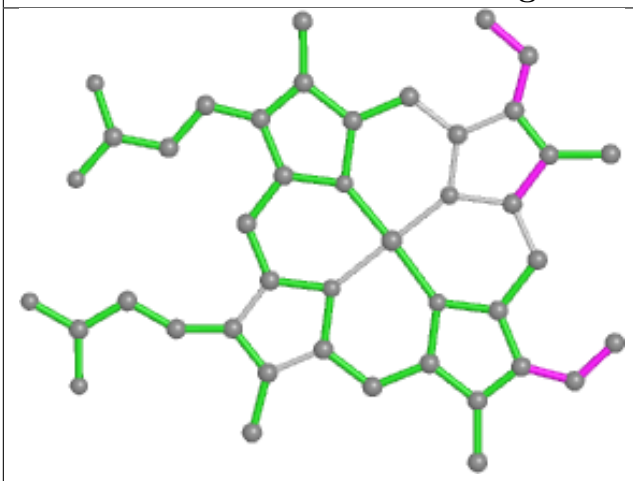
There are no ring outliers.

7 monomers are involved in 21 short contacts:

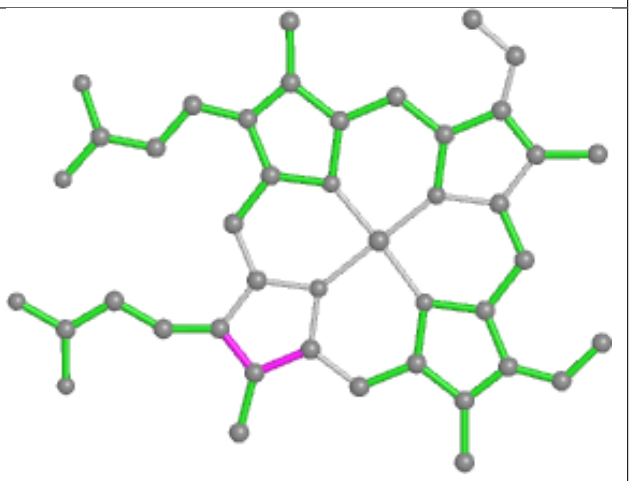
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | C | 507 | HEM | 4 | 0 |
| 3 | D | 1402 | NDP | 1 | 0 |
| 2 | A | 507 | HEM | 5 | 0 |
| 3 | B | 1202 | NDP | 4 | 0 |
| 3 | C | 1302 | NDP | 2 | 0 |
| 3 | A | 1102 | NDP | 3 | 0 |
| 2 | D | 507 | HEM | 2 | 0 |

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 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.

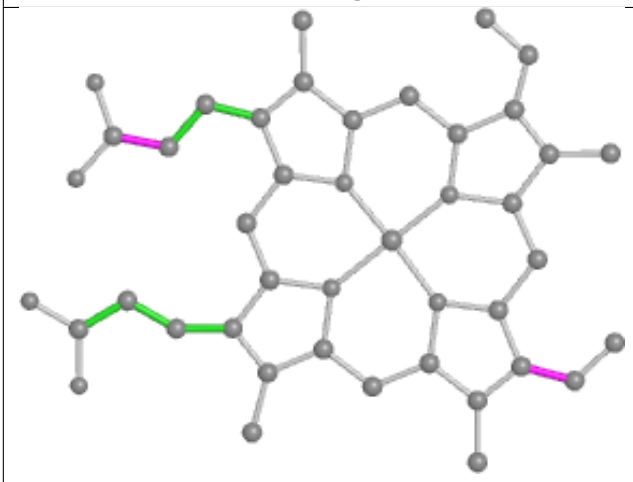
**Ligand HEM C 507**



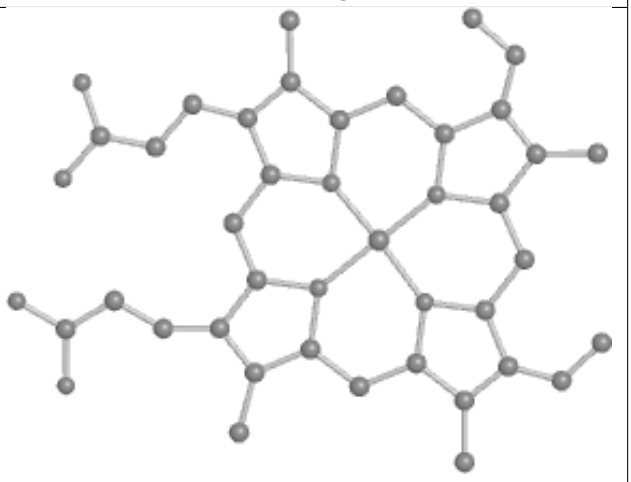
**Bond lengths**



**Bond angles**

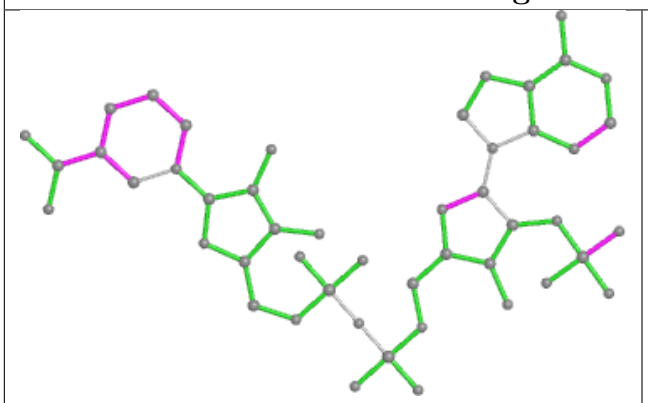


**Torsions**

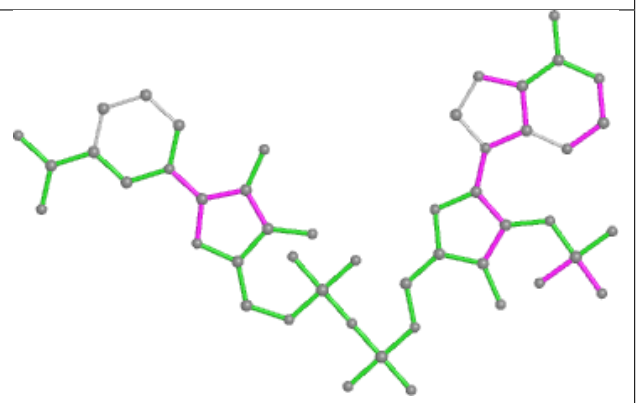


**Rings**

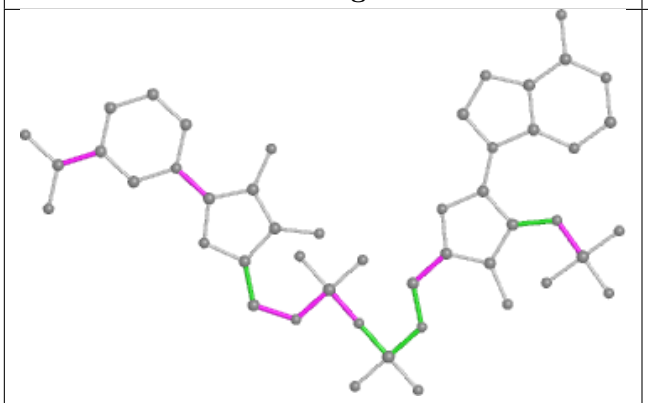
**Ligand NDP D 1402**



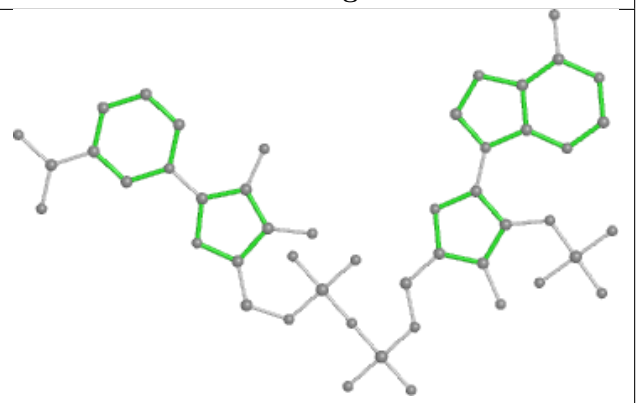
**Bond lengths**



**Bond angles**

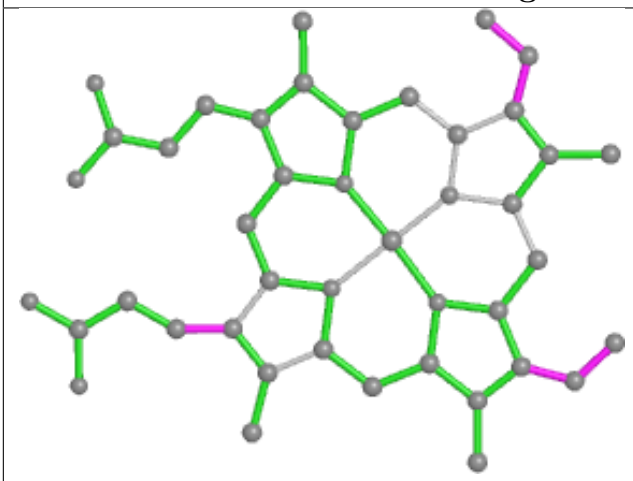


**Torsions**

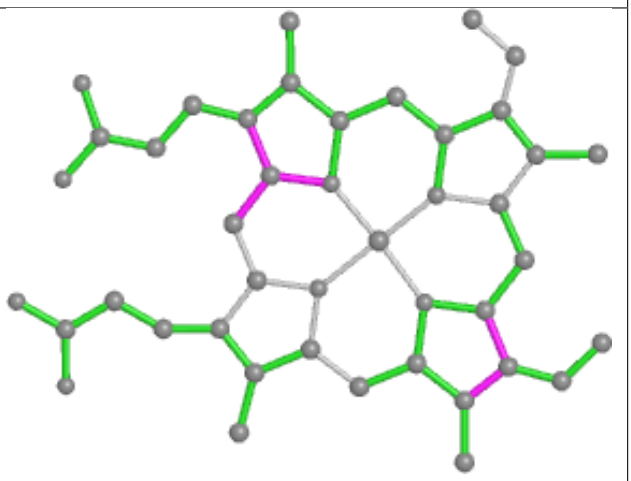


**Rings**

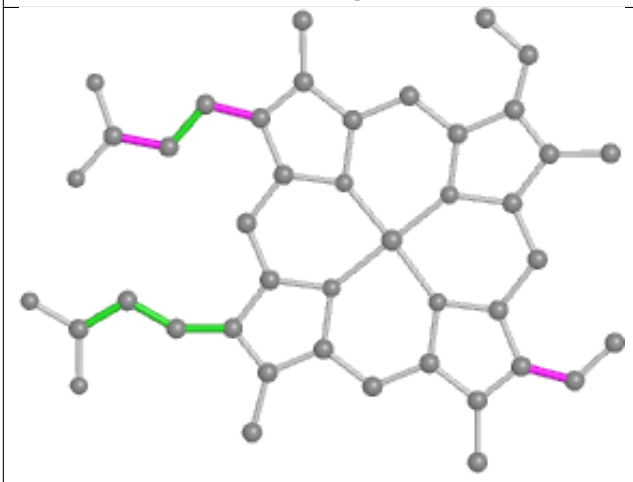
**Ligand HEM B 507**



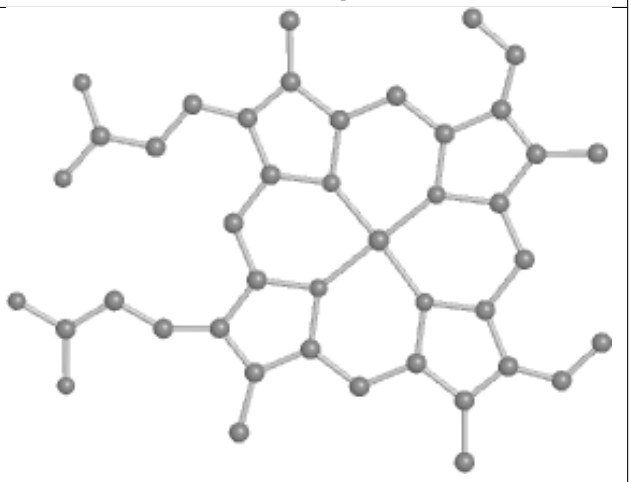
**Bond lengths**



**Bond angles**

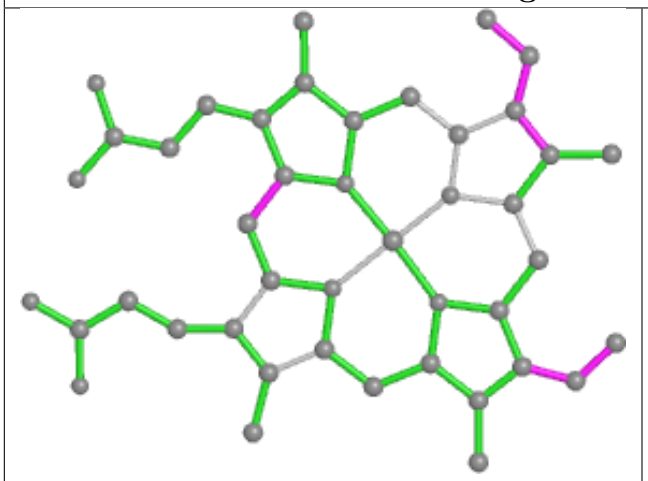


**Torsions**

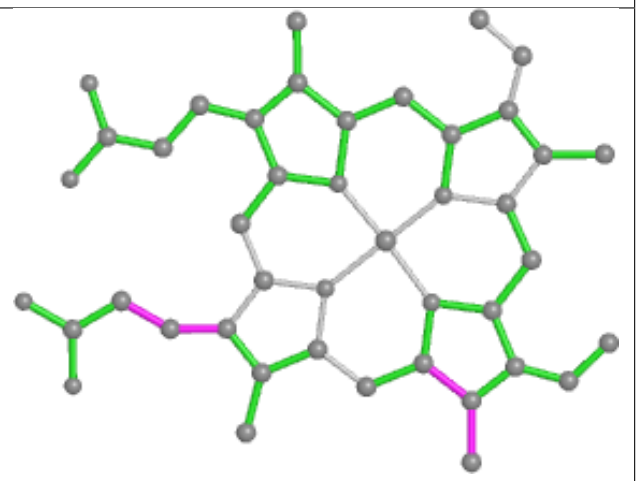


**Rings**

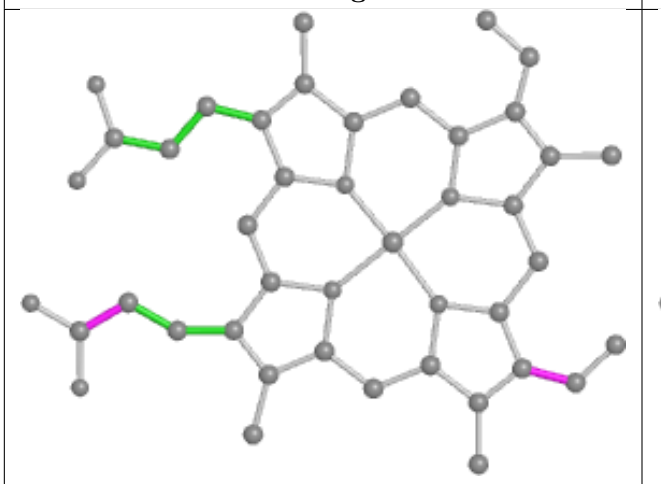
**Ligand HEM A 507**



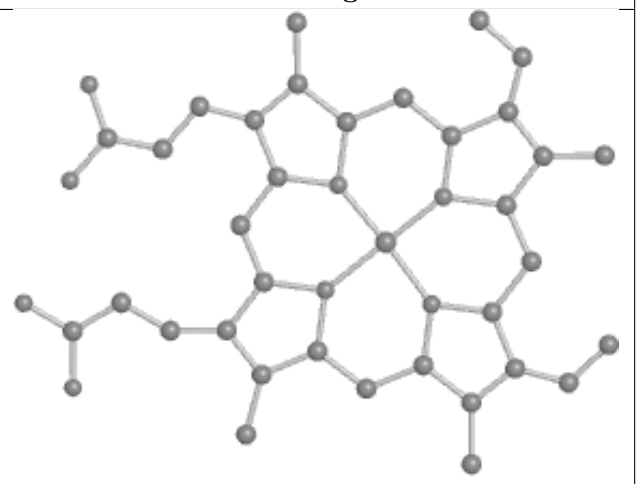
**Bond lengths**



**Bond angles**

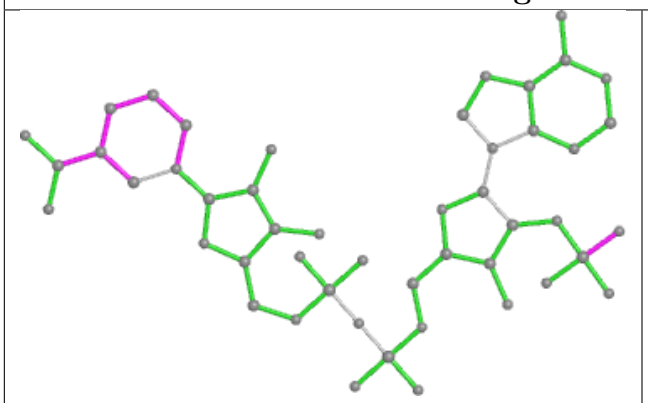


**Torsions**

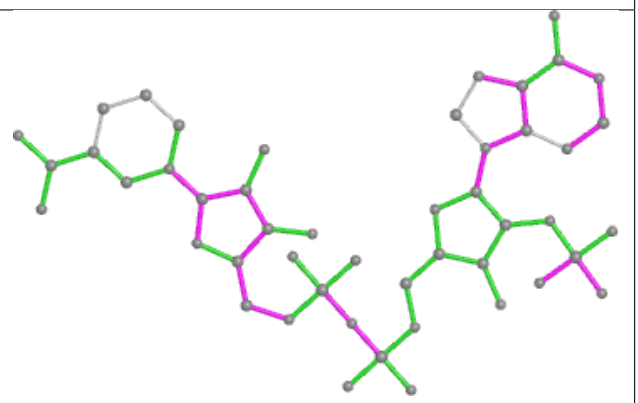


**Rings**

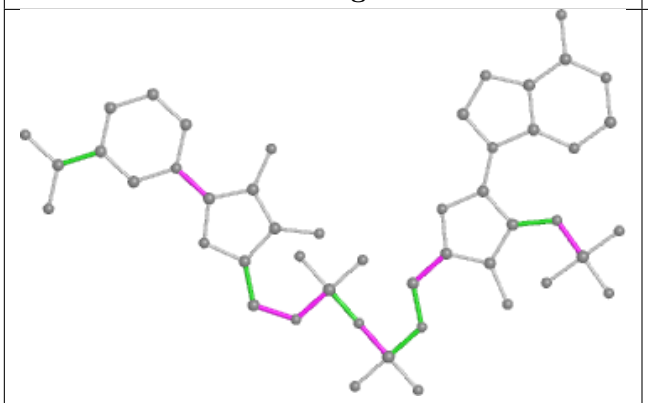
**Ligand NDP B 1202**



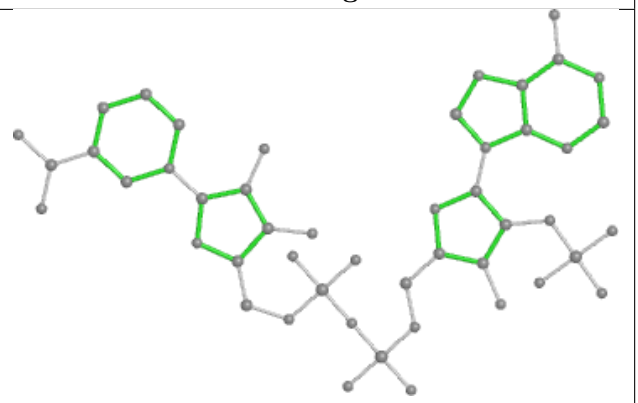
**Bond lengths**



**Bond angles**

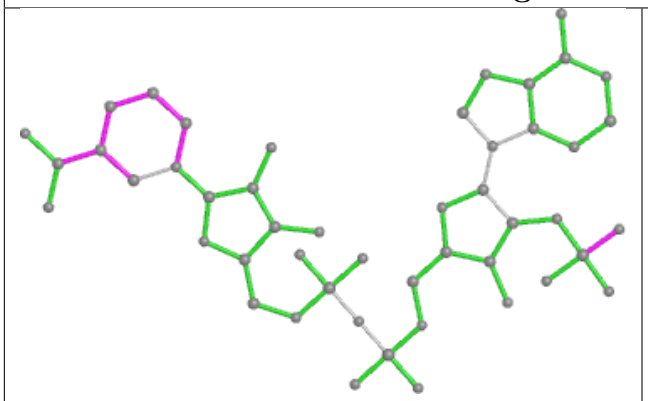


**Torsions**



**Rings**

**Ligand NDP C 1302**



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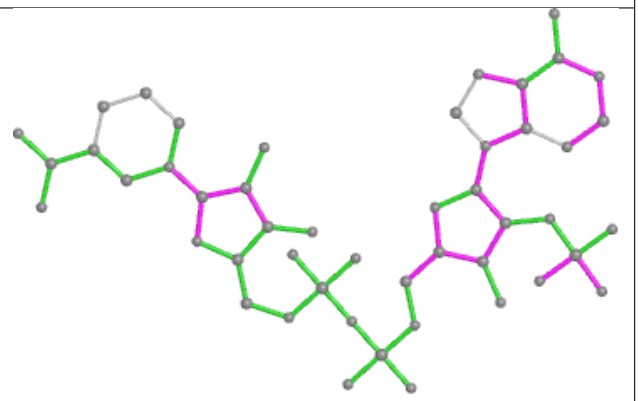
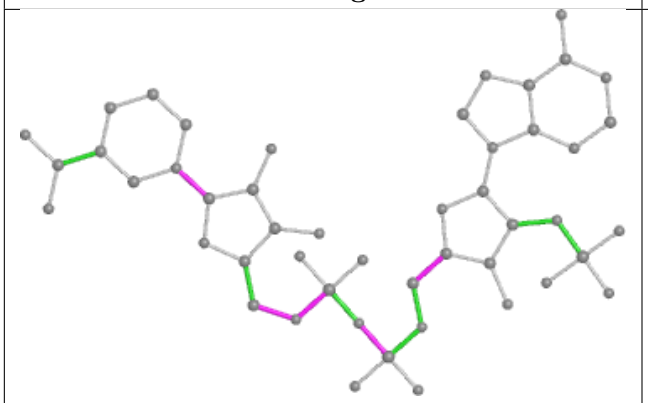
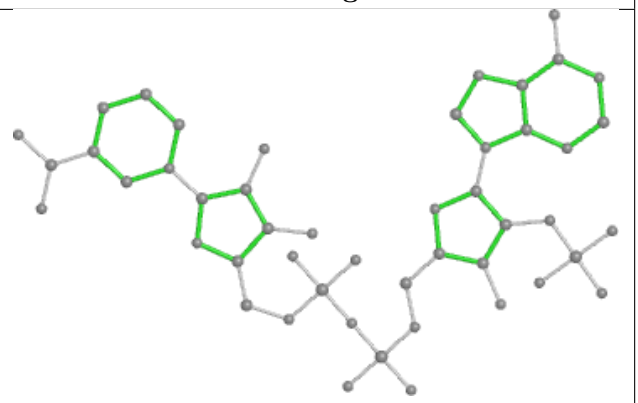


**Bond angles**

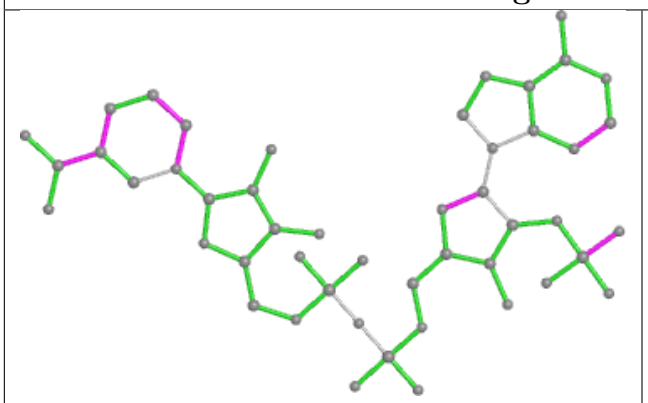


**Torsions**



**Rings**

**Ligand NDP A 1102**



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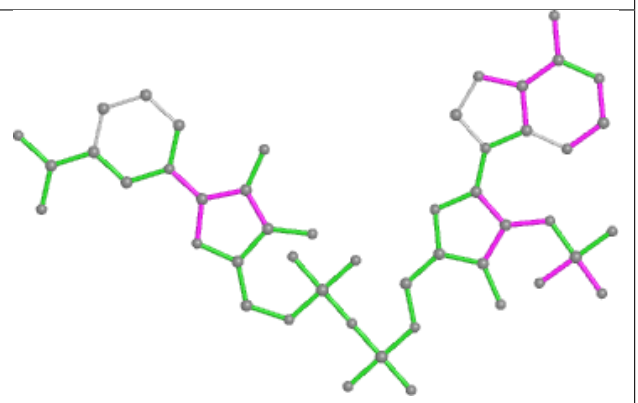
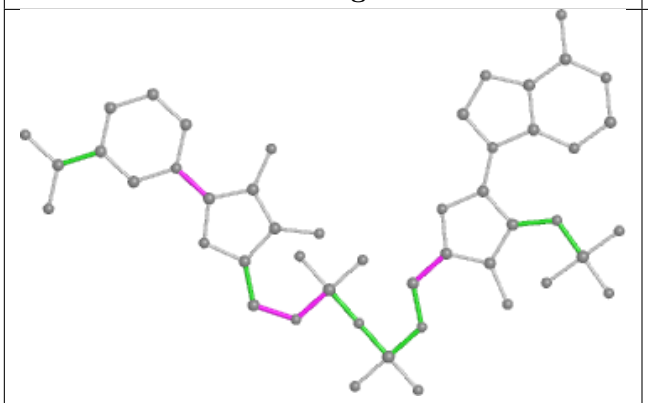
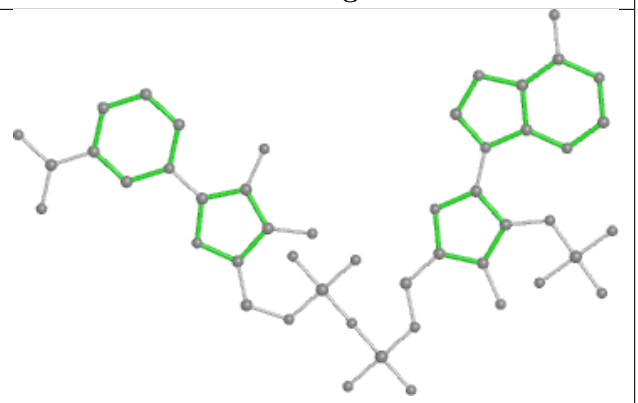


**Bond angles**

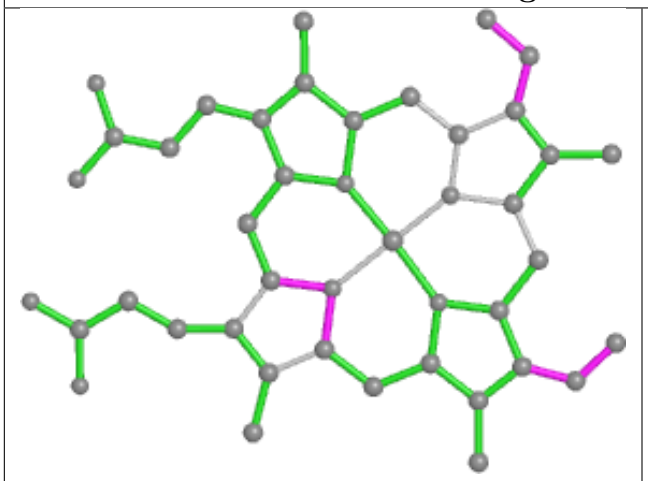


**Torsions**



**Rings**

**Ligand HEM D 507**



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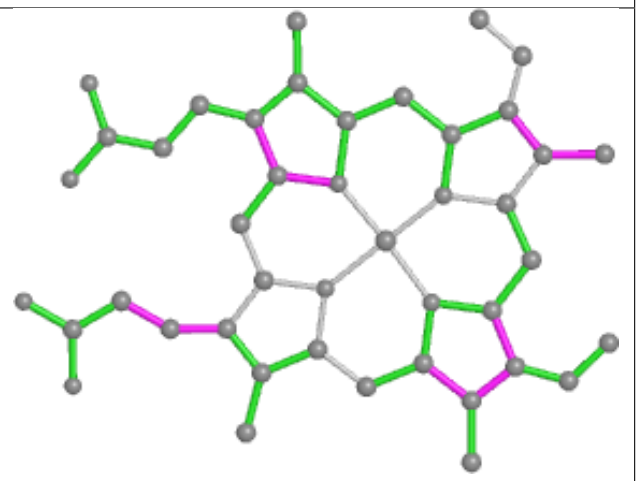
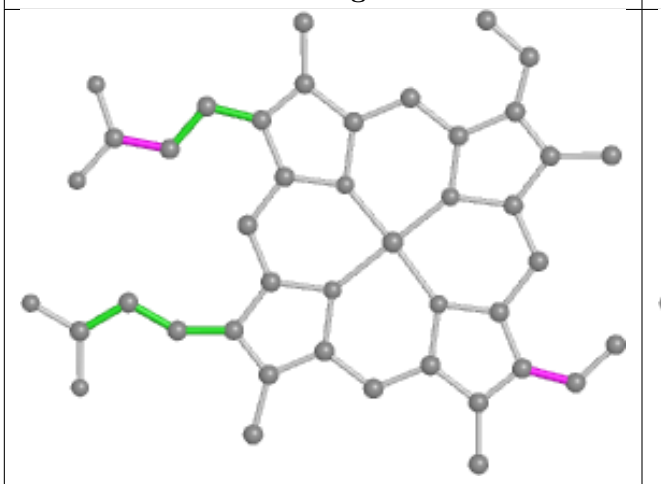
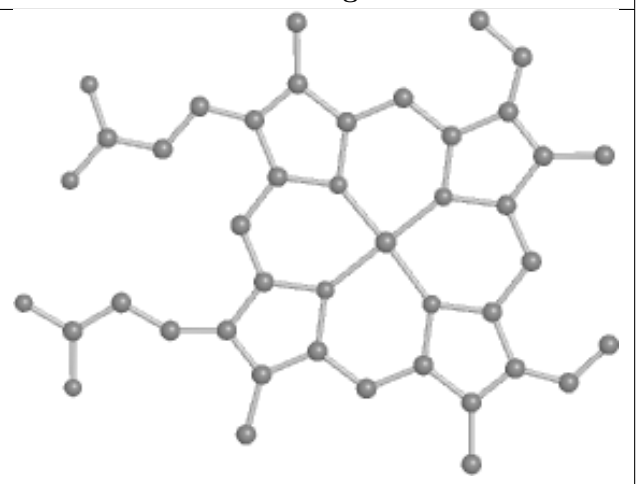


**Bond angles**



**Torsions**



**Rings**

## 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.