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

Aug 5, 2026 – 12:02 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 1TGU / pdb_00001tgu |
| Title | : | The crystal structure of bovine liver catalase without NADPH |
| Authors | : | Sugadev, R.; Balasundaresan, D.; Ponnuswamy, M.N.; Kumaran, D.; Swaminathan, S.; Sekar, K. |
| Deposited on | : | 2004-05-31 |
| Resolution | : | 2.80 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 (i)) were used in the production of this report:

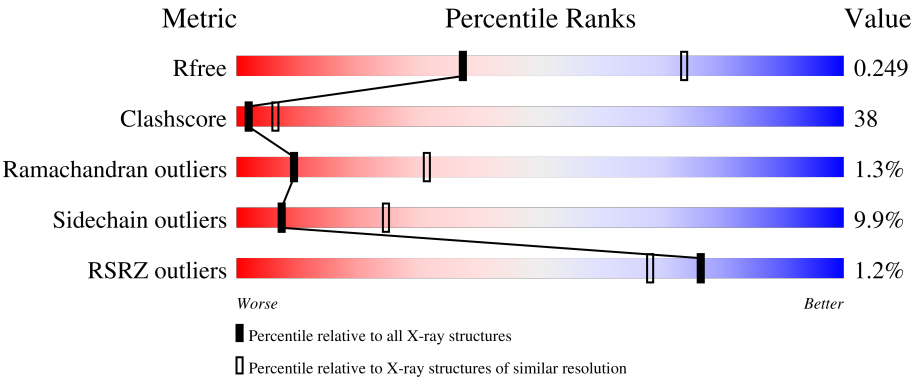
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4 | : | 9.0.015 (Gargrove) |
| Density-Fitness | : | 1.0.12 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

# 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 2.80 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)) |
|---|---|---|
| $R_{free}$ | 180053 | 3866 (2.80-2.80) |
| Clashscore | 190562 | 4276 (2.80-2.80) |
| Ramachandran outliers | 187476 | 4196 (2.80-2.80) |
| Sidechain outliers | 187428 | 4198 (2.80-2.80) |
| RSRZ outliers | 180081 | 3869 (2.80-2.80) |

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% 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 | 506 | 50% 40% 7% |
| 1 | B | 506 | 36% 52% 9% |
| 1 | C | 506 | 42% 45% 9% |
| 1 | D | 506 | 39% 53% 6% |

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 criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 2 | HEM | A | 2000 | - | - | X | - |
| 2 | HEM | B | 2001 | - | - | X | - |
| 2 | HEM | D | 2003 | - | - | X | - |

## 2 Entry composition (i)

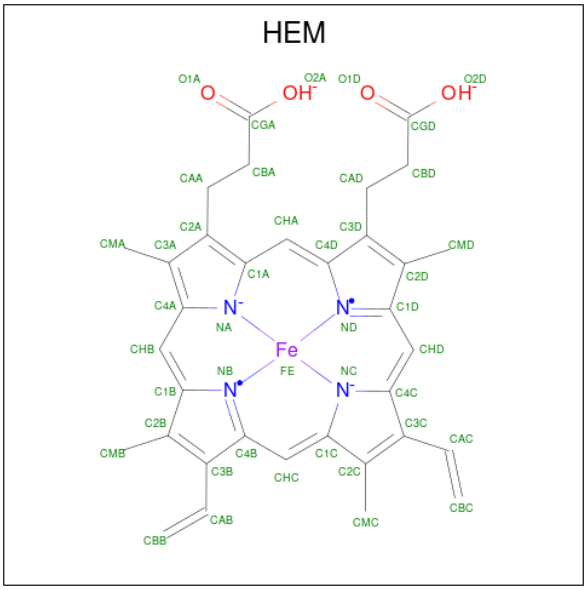
There are 3 unique types of molecules in this entry. The entry contains 17173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

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

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




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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | A | 229 | Total | O | 0 | 0 |
| | | | 229 | 229 | | |
| 3 | B | 236 | Total | O | 0 | 0 |
| | | | 236 | 236 | | |
| 3 | C | 236 | Total | O | 0 | 0 |
| | | | 236 | 236 | | |
| 3 | D | 232 | Total | O | 0 | 0 |
| | | | 232 | 232 | | |

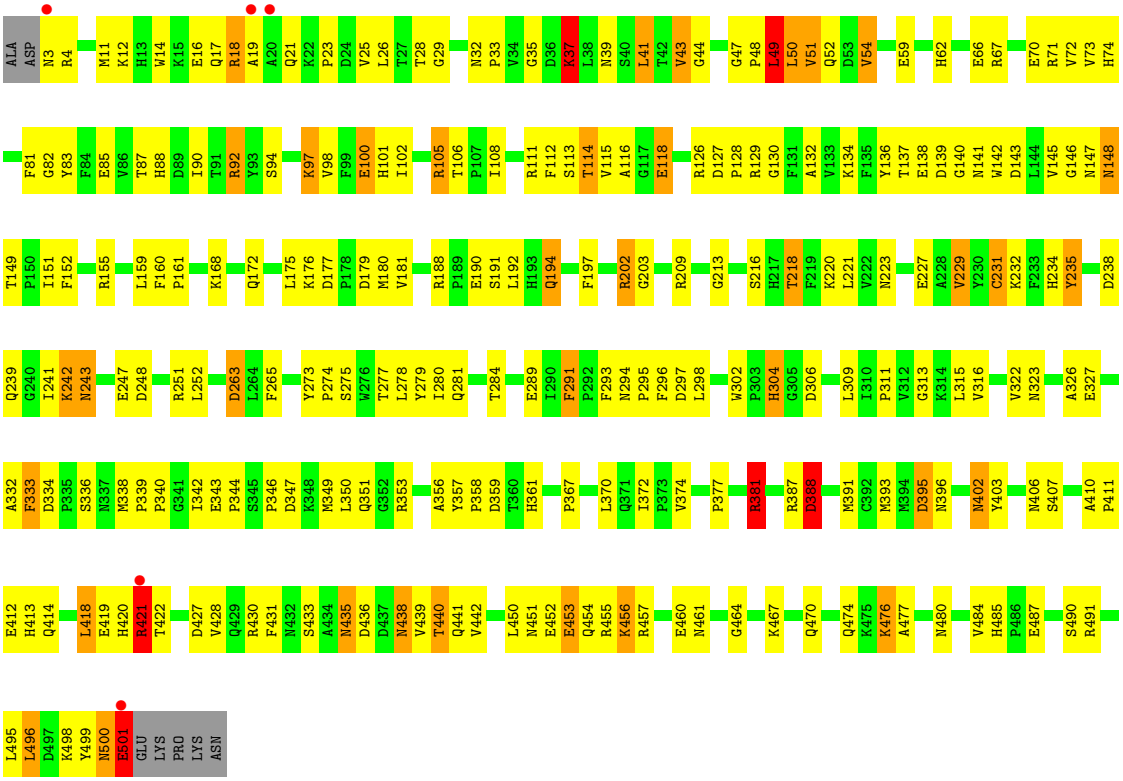
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Catalase

Chain A:

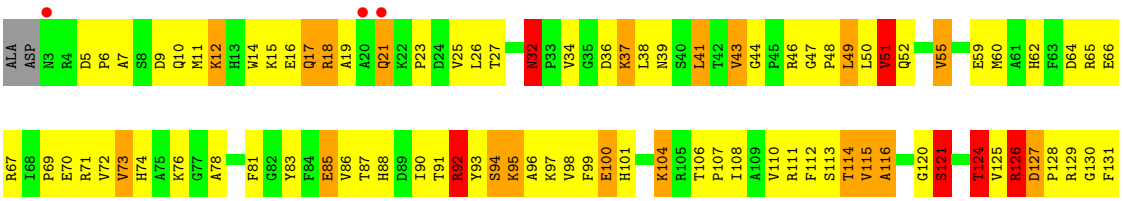


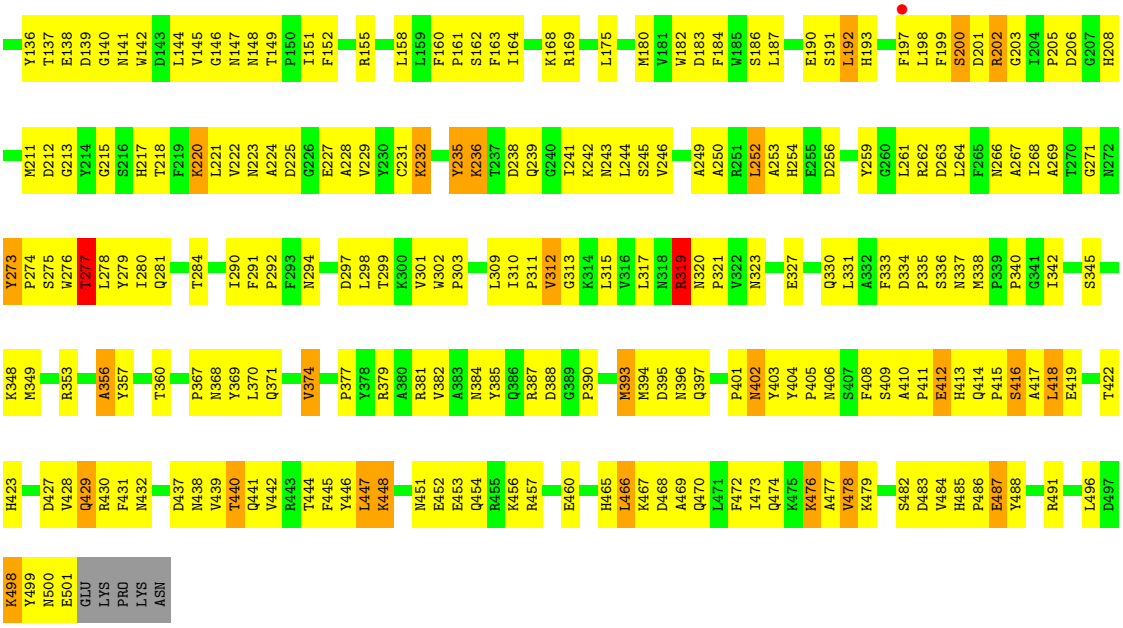




• Molecule 1: Catalase

Chain B:



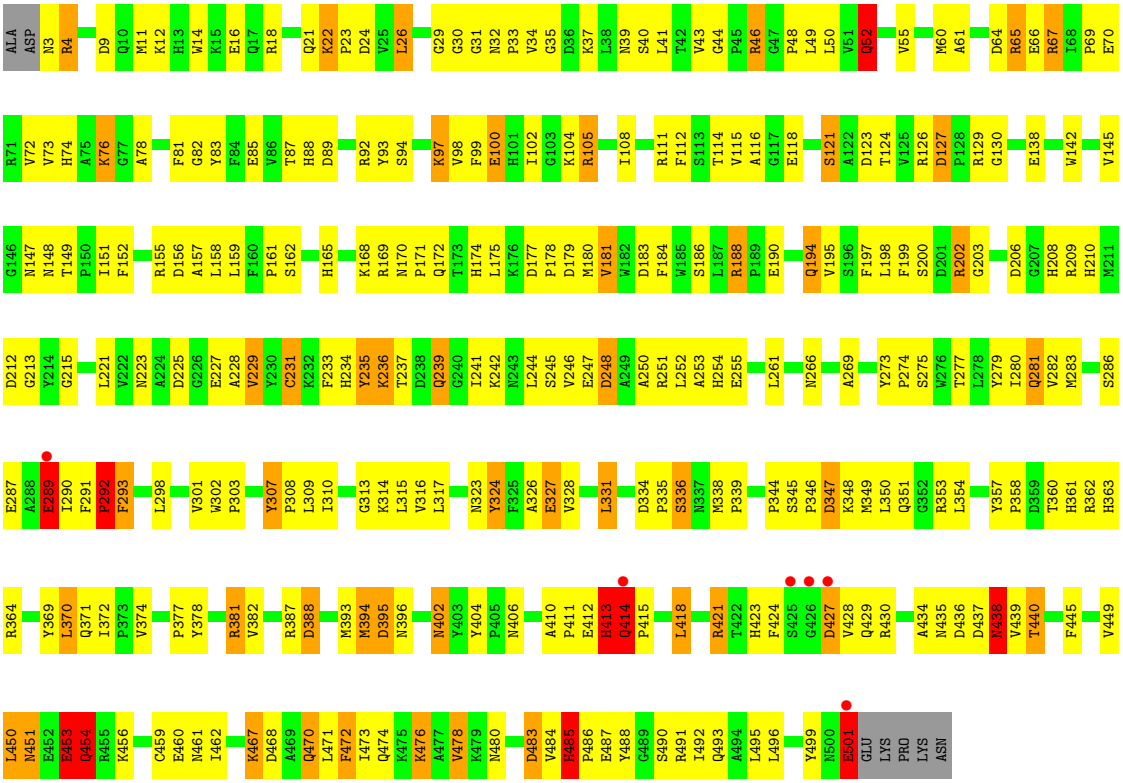





• Molecule 1: Catalase

Chain C:

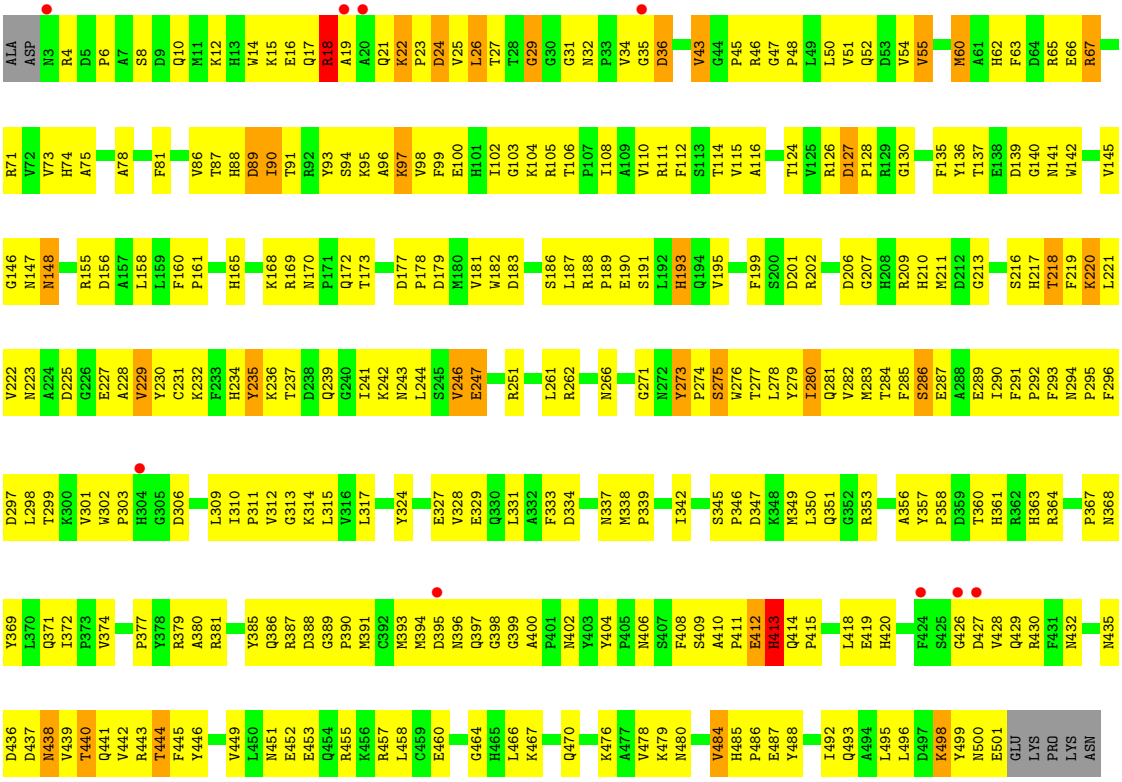


• Molecule 1: Catalase

Chain D:




ALA ASP N3 R4 D5 P6 A7 S8 D9 Q10 M11 K12 H13 W14 K15 E16 Q17 R18 A19 A20 Q21 K22 P23 D24 V25 L26 T27 T28 G29 G30 G31 N32 P33 V34 G35 D36 V43 G44 P45 R46 G47 P48 L49 L50 V51 Q52 D53 V54 V55 M60 A61 H62 F63 D64 R65 E66 R67
R71 V72 V73 H74 A75 A78 F81 V86 T87 H88 D89 I90 T91 R92 Y93 S94 K95 A96 K97 V98 F99 E100 H101 I102 G103 K104 R105 T106 P107 I108 A109 V110 R111 F112 S113 T114 V115 A116 T124 V125 R126 D127 P128 R129 G130 F135 Y136 T137 E138 D139 G140 N141 W142 V145
G146 N147 N148 R155 D156 A157 L158 L159 F160 P161 H165 K168 R169 N170 P171 Q172 T173 D177 P178 D179 M180 V181 W182 D183 S186 L187 R188 P189 E190 S191 L192 H193 Q194 V195 F199 S200 D201 R202 D206 G207 H208 R209 H210 M211 D212 G213 S216 H217 T218 F219 K220 L221
V222 N223 A224 D225 G226 E227 A228 V229 Y230 C231 K232 F233 H234 Y235 K236 T237 D238 Q239 G240 I241 K242 N243 L244 S245 V246 E247 R251 L261 R262 N266 G271 N272 Y273 P274 S275 W276 T277 L278 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 A288 E289 I290 F291 P292 F293 N294 P295 F296
D297 L298 T299 K300 V301 W302 P303 H304 G305 D306 L309 I310 P311 V312 G313 K314 L315 V316 L317 Y324 E327 V328 E329 Q330 L331 A332 F333 D334 N337 M338 P339 I342 S345 P346 D347 K348 M349 L350 Q351 G352 R353 A356 Y357 P358 D359 T360 H361 R362 H363 R364 P367 N368
Y369 L370 Q371 I372 P373 V374 P377 Y378 R379 A380 R381 Y385 Q386 R387 D388 G389 P390 M391 G392 M393 M394 D395 N396 Q397 G398 G399 A400 P401 N402 Y403 Y404 P405 N406 S407 F408 S409 A410 P411 E412 H413 Q414 P415 L418 E419 H420 F424 S425 G426 D427 V428 Q429 R430 F431 N432 N435
D436 D437 N438 V439 T440 Q441 V442 R443 T444 F445 Y446 V449 L450 N451 E452 E453 G454 R455 K456 R457 L458 C459 E460 G464 H465 L466 K467 Q470 K476 A477 V478 K479 N480 V484 H485 P486 E487 Y488 I492 Q493 A494 L495 L496 D497 K498 Y499 N500 E501 GLU LYS PRO LYS ASN

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 85.53Å 139.67Å 225.14Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 2.80<br>40.00 – 2.80 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 89.9 (40.00-2.80)<br>89.9 (40.00-2.80) | Depositor<br>EDS |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | 0.11 | Depositor |
| $< I/\sigma(I) >$ [1] | 2.47 (at 2.77Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.200 , 0.249<br>0.198 , 0.249 | Depositor<br>DCC |
| $R_{free}$ test set | 1822 reflections (3.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 29.9 | Xtriage |
| Anisotropy | 0.532 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 51.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 17173 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 31.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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.

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.73 | 6/4137 (0.1%) | 1.83 | 64/5619 (1.1%) |
| 1 | B | 1.20 | 4/4137 (0.1%) | 1.72 | 38/5619 (0.7%) |
| 1 | C | 0.89 | 10/4137 (0.2%) | 1.73 | 56/5619 (1.0%) |
| 1 | D | 0.76 | 1/4137 (0.0%) | 1.25 | 18/5619 (0.3%) |
| All | All | 0.91 | 21/16548 (0.1%) | 1.65 | 176/22476 (0.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 1 | 1 |
| 1 | B | 0 | 2 |
| 1 | C | 2 | 2 |
| All | All | 3 | 5 |

The worst 5 of 21 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 319 | ARG | CD-NE | 60.36 | 2.30 | 1.46 |
| 1 | D | 413 | HIS | CA-CB | -26.33 | 1.08 | 1.53 |
| 1 | C | 202 | ARG | NE-CZ | 20.07 | 1.55 | 1.33 |
| 1 | B | 319 | ARG | NE-CZ | 18.99 | 1.53 | 1.33 |
| 1 | C | 292 | PRO | C-N | 16.18 | 1.56 | 1.33 |

The worst 5 of 176 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 413 | HIS | CA-CB-CG | 43.35 | 157.15 | 113.80 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 395 | ASP | CA-CB-CG | 43.13 | 155.73 | 112.60 |
| 1 | B | 319 | ARG | CG-CD-NE | -39.44 | 25.24 | 112.00 |
| 1 | B | 395 | ASP | N-CA-CB | -38.75 | 53.99 | 110.56 |
| 1 | A | 402 | ASN | CA-CB-CG | 34.82 | 147.42 | 112.60 |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | A | 395 | ASP | CA |
| 1 | C | 453 | GLU | CA |
| 1 | C | 501 | GLU | CA |

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 421 | ARG | Sidechain |
| 1 | B | 126 | ARG | Sidechain |
| 1 | B | 319 | ARG | Sidechain |
| 1 | C | 289 | GLU | Sidechain |
| 1 | C | 292 | PRO | Peptide |

## 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 | 3840 | 303 | 0 |
| 1 | B | 4017 | 0 | 3840 | 417 | 0 |
| 1 | C | 4017 | 0 | 3839 | 341 | 2 |
| 1 | D | 4017 | 0 | 3839 | 331 | 0 |
| 2 | A | 43 | 0 | 30 | 36 | 0 |
| 2 | B | 43 | 0 | 30 | 28 | 0 |
| 2 | C | 43 | 0 | 30 | 18 | 0 |
| 2 | D | 43 | 0 | 30 | 29 | 0 |
| 3 | A | 229 | 0 | 0 | 22 | 0 |
| 3 | B | 236 | 0 | 0 | 29 | 2 |
| 3 | C | 236 | 0 | 0 | 21 | 2 |
| 3 | D | 232 | 0 | 0 | 18 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 17173 | 0 | 15478 | 1218 | 3 |

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 38.

The worst 5 of 1218 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:421:ARG:HD2 | 1:B:429:GLN:CG | 1.19 | 1.58 |
| 1:B:353:ARG:HG3 | 2:B:2001:HEM:CBB | 1.34 | 1.57 |
| 1:D:147:ASN:ND2 | 2:D:2003:HEM:CAC | 1.74 | 1.50 |
| 1:B:353:ARG:CG | 2:B:2001:HEM:HBB2 | 1.02 | 1.49 |
| 1:D:147:ASN:ND2 | 2:D:2003:HEM:HAC | 1.27 | 1.44 |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:2109:HOH:O | 3:C:2220:HOH:O[3_655] | 2.15 | 0.05 |
| 1:C:85:GLU:OE2 | 3:C:2084:HOH:O[3_645] | 2.15 | 0.05 |
| 1:C:102:ILE:O | 3:B:2221:HOH:O[3_645] | 2.16 | 0.04 |

## 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%) | 452 (91%) | 42 (8%) | 3 (1%) | 21 51 |
| 1 | B | 497/506 (98%) | 419 (84%) | 70 (14%) | 8 (2%) | 7 27 |
| 1 | C | 497/506 (98%) | 434 (87%) | 55 (11%) | 8 (2%) | 7 27 |
| 1 | D | 497/506 (98%) | 435 (88%) | 55 (11%) | 7 (1%) | 9 30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 1988/2024 (98%) | 1740 (88%) | 222 (11%) | 26 (1%) | 9 31 |

5 of 26 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 19 | ALA |
| 1 | B | 100 | GLU |
| 1 | B | 124 | THR |
| 1 | D | 36 | ASP |
| 1 | A | 440 | THR |

### 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%) | 390 (90%) | 41 (10%) | 8 26 |
| 1 | B | 431/437 (99%) | 378 (88%) | 53 (12%) | 4 16 |
| 1 | C | 431/437 (99%) | 384 (89%) | 47 (11%) | 6 21 |
| 1 | D | 431/437 (99%) | 401 (93%) | 30 (7%) | 14 40 |
| All | All | 1724/1748 (99%) | 1553 (90%) | 171 (10%) | 7 24 |

5 of 171 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 286 | SER |
| 1 | D | 26 | LEU |
| 1 | C | 331 | LEU |
| 1 | C | 438 | ASN |
| 1 | D | 193 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 74 | HIS |
| 1 | D | 480 | ASN |
| 1 | D | 148 | ASN |
| 1 | D | 363 | HIS |
| 1 | B | 402 | ASN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry (i)

4 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 | B | 2001 | - | 50,50,50 | 1.73 | 6 (12%) | 67,82,82 | 2.50 | 4 (5%) |
| 2 | HEM | A | 2000 | - | 50,50,50 | 1.39 | 6 (12%) | 67,82,82 | 0.97 | 3 (4%) |
| 2 | HEM | C | 2002 | 1 | 50,50,50 | 1.48 | 6 (12%) | 67,82,82 | 0.94 | 2 (2%) |
| 2 | HEM | D | 2003 | 1 | 50,50,50 | 3.13 | 7 (14%) | 67,82,82 | 0.94 | 2 (2%) |

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 | B | 2001 | - | - | 5/14/54/54 | - |
| 2 | HEM | A | 2000 | - | - | 3/14/54/54 | - |
| 2 | HEM | C | 2002 | 1 | - | 5/14/54/54 | - |
| 2 | HEM | D | 2003 | 1 | - | 5/14/54/54 | - |

The worst 5 of 25 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | D | 2003 | HEM | FE-ND | 18.21 | 2.51 | 1.94 |
| 2 | B | 2001 | HEM | CHB-C4A | 8.41 | 1.58 | 1.39 |
| 2 | D | 2003 | HEM | FE-NA | 7.85 | 2.21 | 1.95 |
| 2 | A | 2000 | HEM | CMC-C2C | -5.88 | 1.38 | 1.50 |
| 2 | C | 2002 | HEM | FE-ND | 5.88 | 2.13 | 1.94 |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 2001 | HEM | CHC-C1C-NC | -15.79 | 107.27 | 124.45 |
| 2 | B | 2001 | HEM | CHC-C1C-C2C | -10.14 | 104.39 | 125.49 |
| 2 | B | 2001 | HEM | CHB-C4A-NA | -2.56 | 119.21 | 123.86 |
| 2 | C | 2002 | HEM | CMB-C2B-C1B | 2.46 | 128.88 | 125.03 |
| 2 | D | 2003 | HEM | CMB-C2B-C1B | 2.46 | 128.88 | 125.03 |

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 2000 | HEM | C2B-C3B-CAB-CBB |
| 2 | A | 2000 | HEM | C4B-C3B-CAB-CBB |
| 2 | B | 2001 | HEM | C2B-C3B-CAB-CBB |
| 2 | B | 2001 | HEM | C4B-C3B-CAB-CBB |
| 2 | B | 2001 | HEM | C2C-C3C-CAC-CBC |

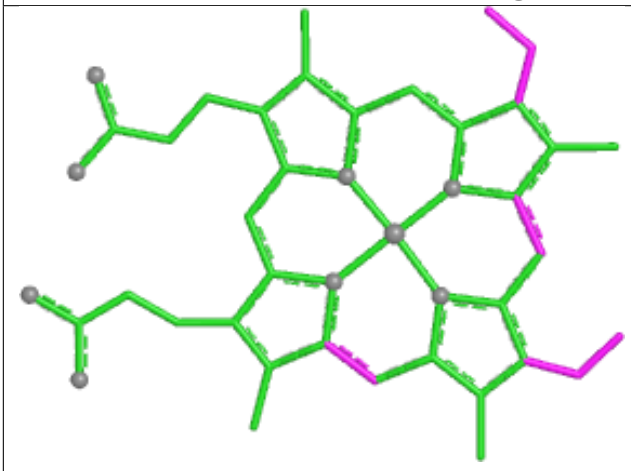
There are no ring outliers.

4 monomers are involved in 111 short contacts:

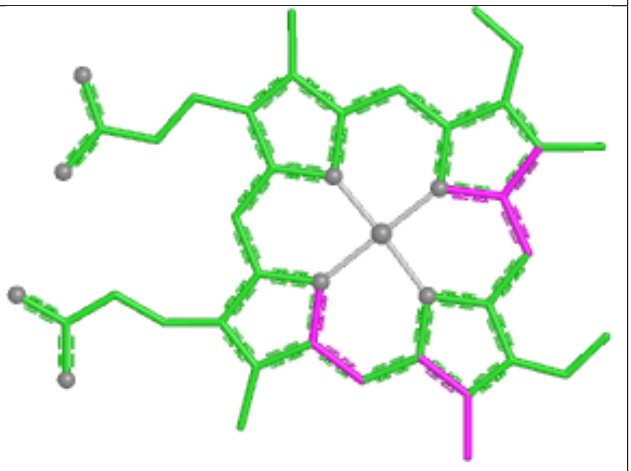
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 2001 | HEM | 28 | 0 |
| 2 | A | 2000 | HEM | 36 | 0 |
| 2 | C | 2002 | HEM | 18 | 0 |
| 2 | D | 2003 | HEM | 29 | 0 |

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.

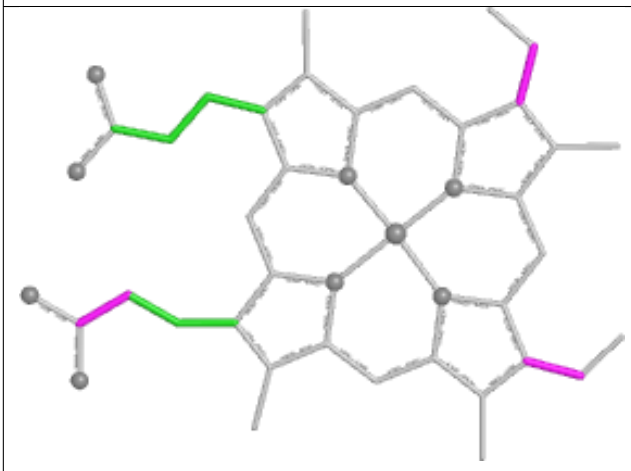
**Ligand HEM B 2001**



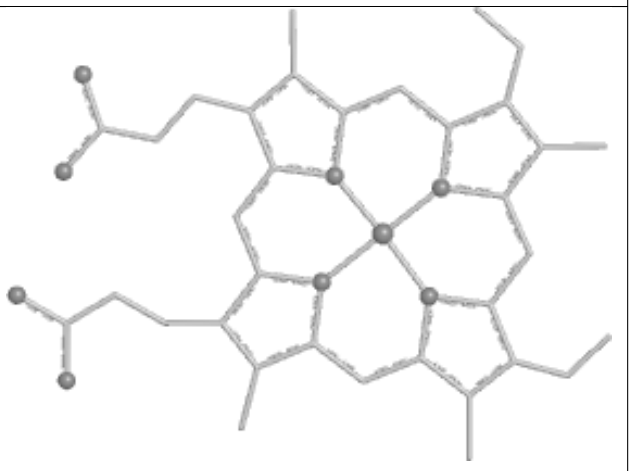
**Bond lengths**



**Bond angles**

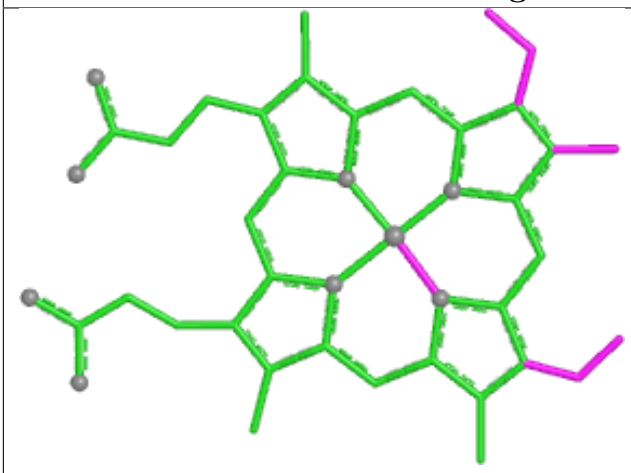


**Torsions**

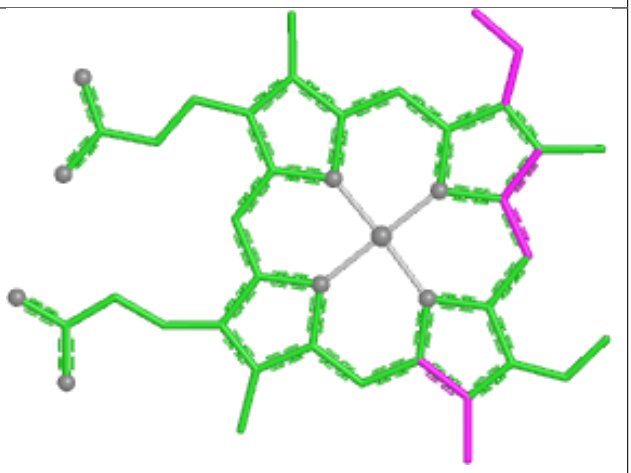


**Rings**

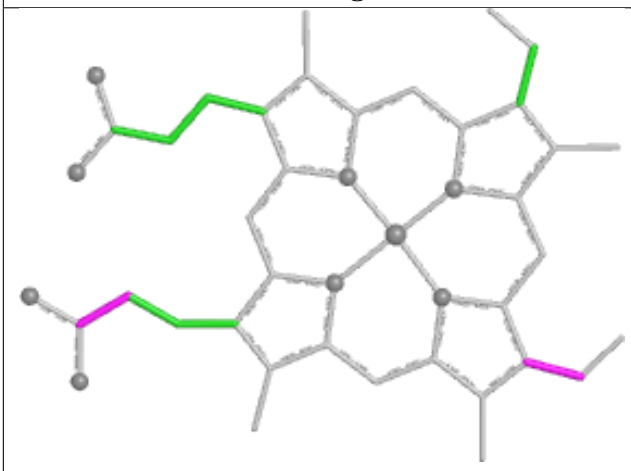
**Ligand HEM A 2000**



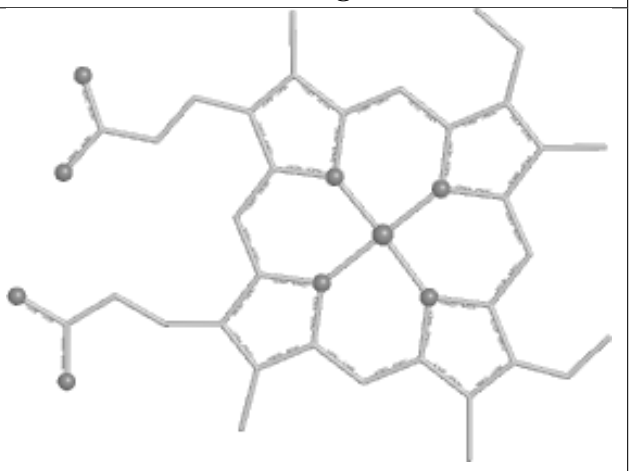
**Bond lengths**



**Bond angles**

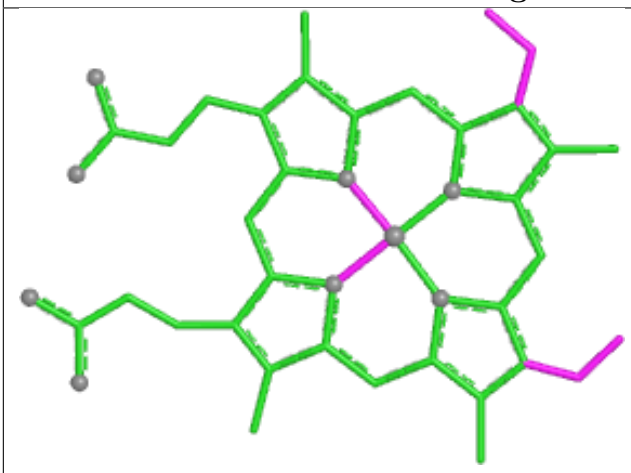


**Torsions**

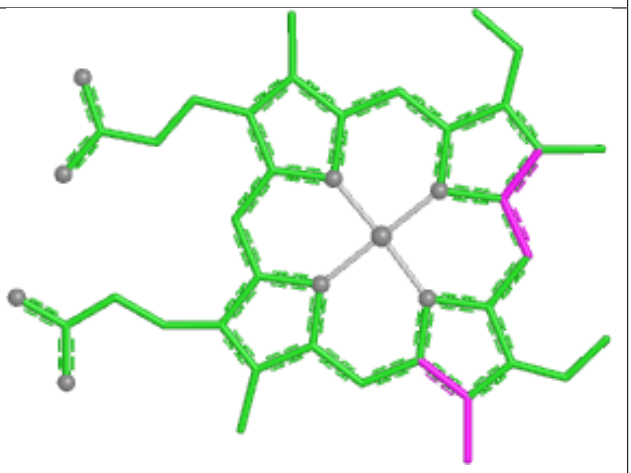


**Rings**

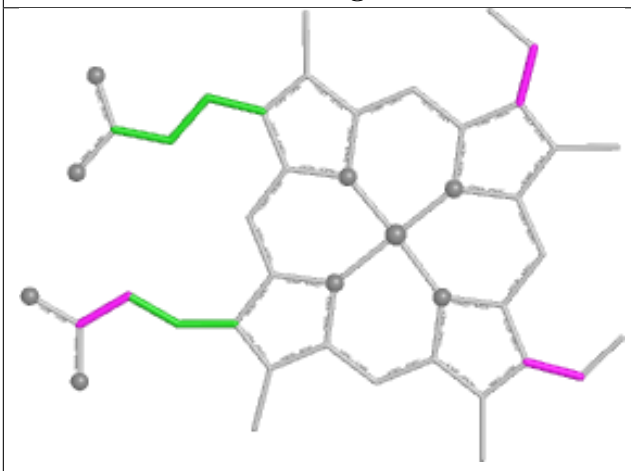
**Ligand HEM C 2002**



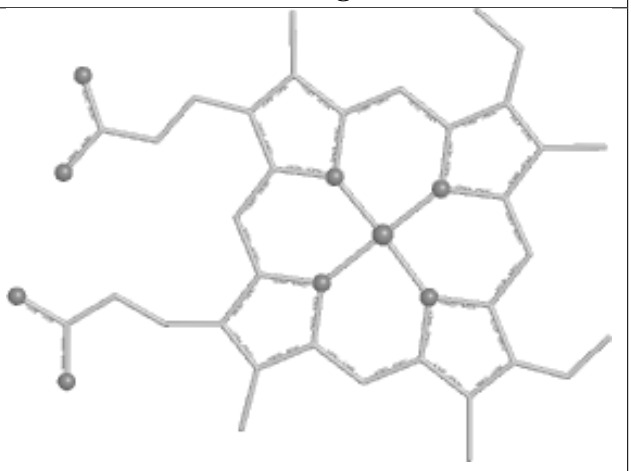
**Bond lengths**



**Bond angles**

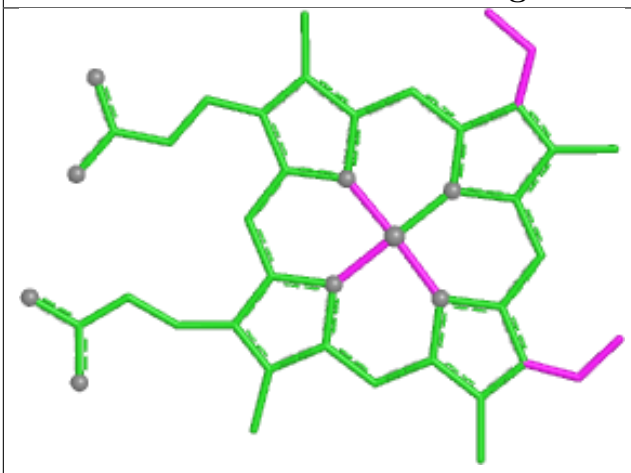


**Torsions**

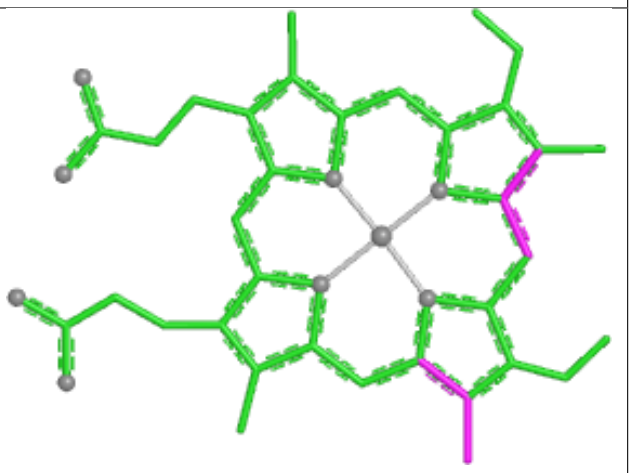


**Rings**

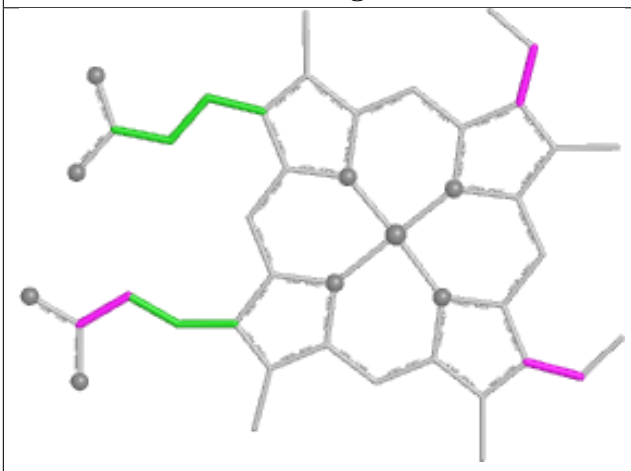
**Ligand HEM D 2003**



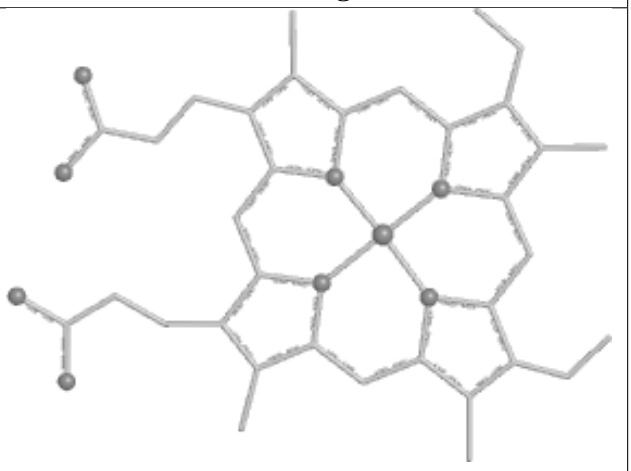
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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 | 499/506 (98%) | -0.28 | 5 (1%) | 79 | 72 | 8, 24, 48, 89 | 0 |
| 1 | B | 499/506 (98%) | 0.03 | 4 (0%) | 82 | 75 | 10, 31, 56, 88 | 0 |
| 1 | C | 499/506 (98%) | -0.09 | 6 (1%) | 76 | 68 | 6, 27, 56, 81 | 1 (0%) |
| 1 | D | 499/506 (98%) | -0.04 | 9 (1%) | 67 | 58 | 10, 30, 60, 87 | 0 |
| All | All | 1996/2024 (98%) | -0.10 | 24 (1%) | 76 | 68 | 6, 28, 55, 89 | 1 (0%) |

The worst 5 of 24 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 20 | ALA | 3.8 |
| 1 | B | 197 | PHE | 3.8 |
| 1 | B | 20 | ALA | 3.4 |
| 1 | D | 20 | ALA | 3.2 |
| 1 | C | 427 | ASP | 3.0 |

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

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

## 6.3 Carbohydrates

There are no oligosaccharides in this entry.

## 6.4 Ligands

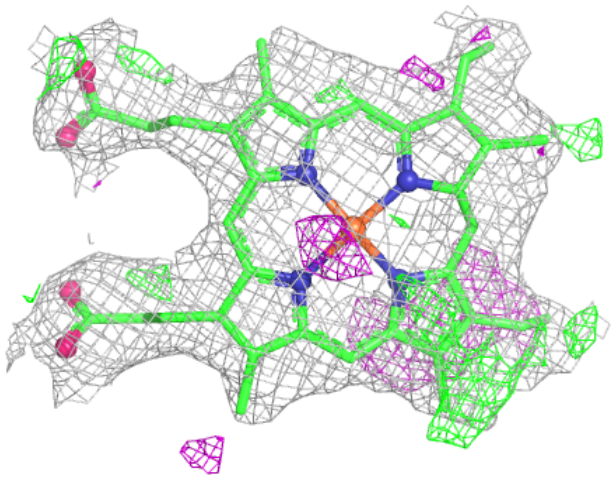
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

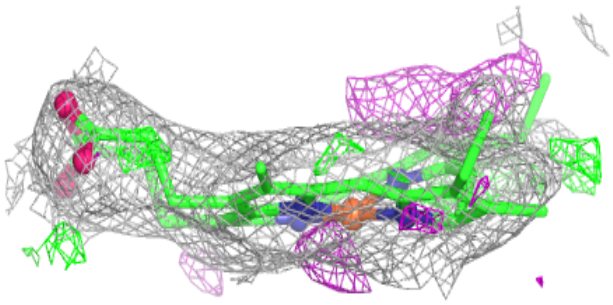
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | HEM | B | 2001 | 43/43 | 0.90 | 0.17 | 16,35,50,71 | 0 |
| 2 | HEM | D | 2003 | 43/43 | 0.91 | 0.13 | 17,33,49,60 | 0 |
| 2 | HEM | A | 2000 | 43/43 | 0.94 | 0.12 | 4,30,44,49 | 0 |
| 2 | HEM | C | 2002 | 43/43 | 0.95 | 0.10 | 15,31,42,91 | 0 |

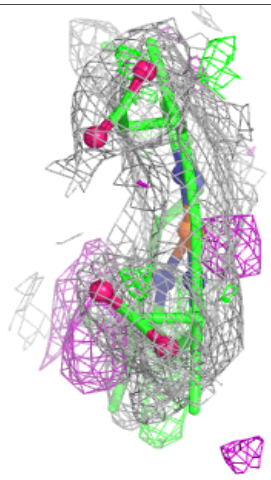
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HEM B 2001:**

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

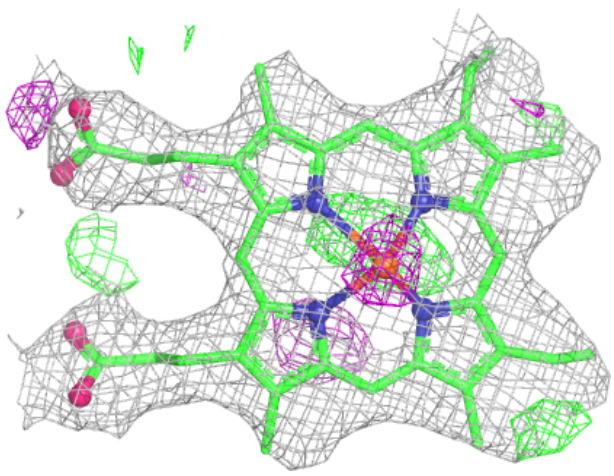


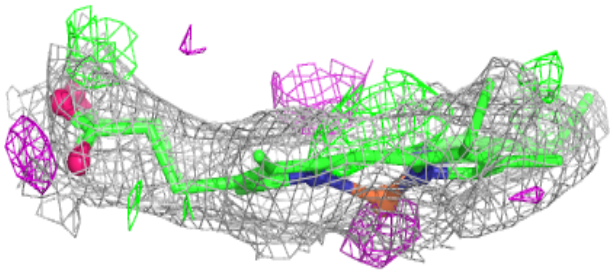


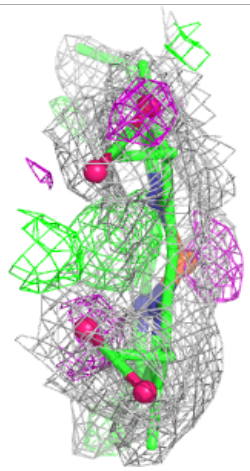


**Electron density around HEM D 2003:**

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

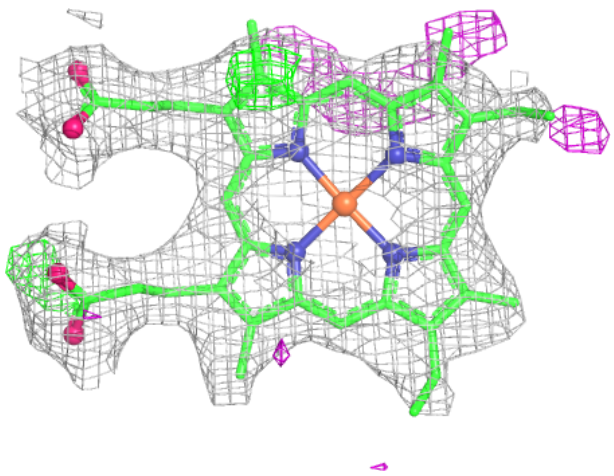


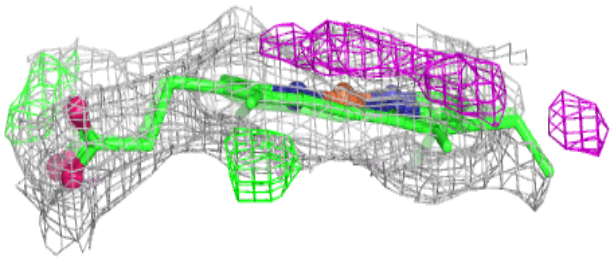


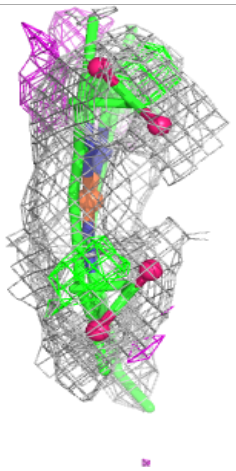


**Electron density around HEM A 2000:**

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

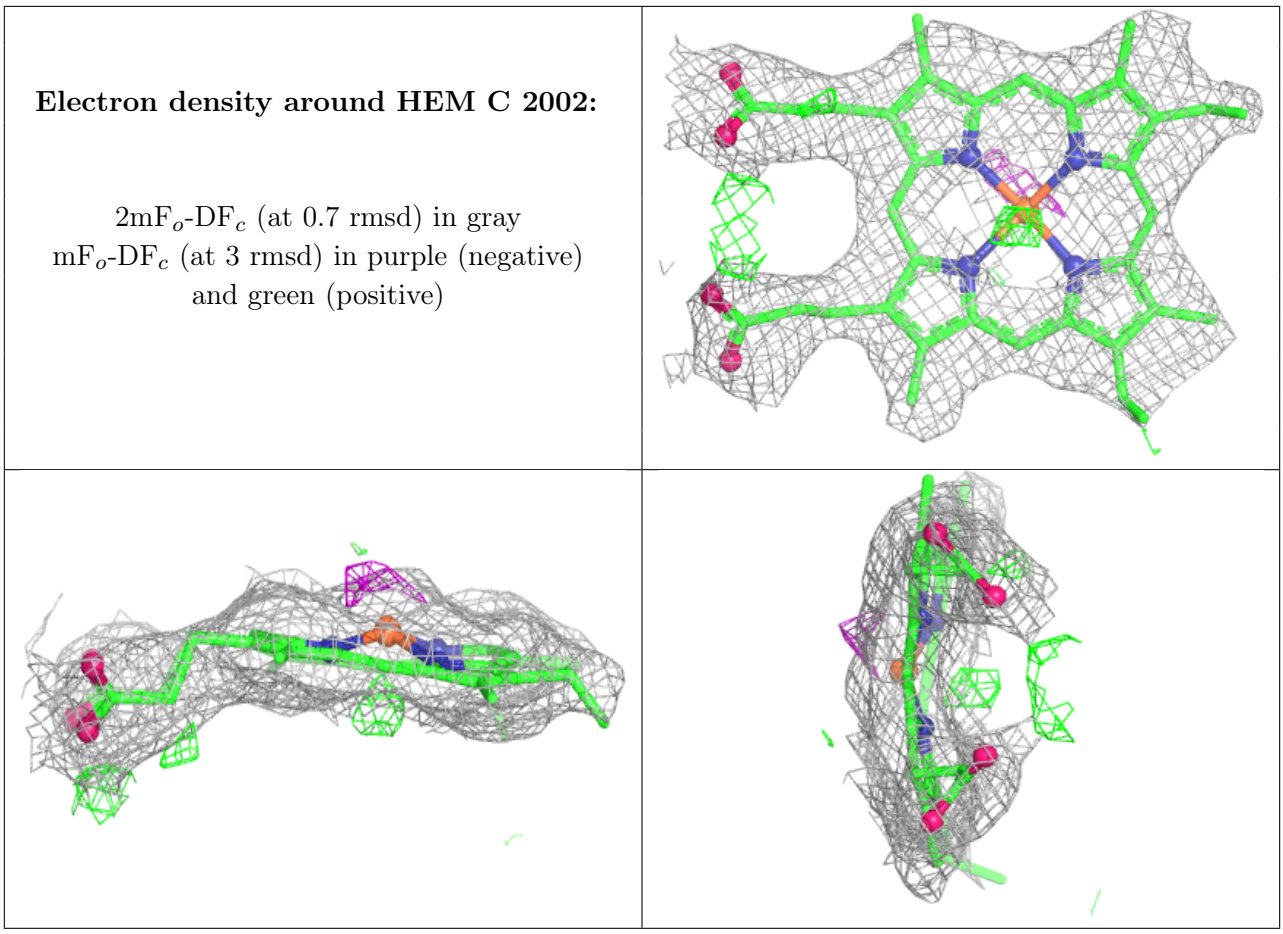






**Electron density around HEM C 2002:**

$2mF_o$-$DF_c$ (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.