



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:35 pm BST

PDB ID : 1HRB  
Title : ATOMIC MODELS FOR THE POLYPEPTIDE BACKBONES OF MYOHE-  
MERYTHRIN AND HEMERYTHRIN  
Authors : Hendrickson, W.A.; Ward, K.B.  
Deposited on : 1976-06-23  
Resolution : 5.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.11

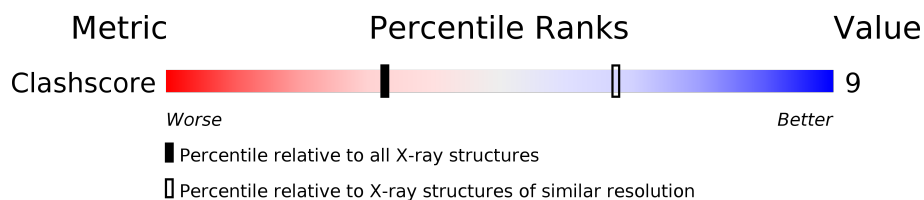
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 Å.

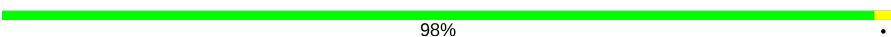
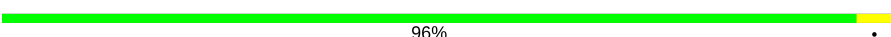
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric     | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|------------|-----------------------------|---|
| Clashscore | 141614                      | 1010 (7.10-3.90)                                      |

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 113    |  98% . |
| 1   | B     | 113    |  96% . |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 230 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 HEMERYTHRIN B.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 1   | A     | 113      | Total C<br>113 113 | 0       | 0       | 113   |
| 1   | B     | 113      | Total C<br>113 113 | 0       | 0       | 113   |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 58      | GLN      | GLU    | CONFLICT | UNP P02244 |
| A     | 59      | GLU      | GLN    | CONFLICT | UNP P02244 |
| A     | 63      | GLU      | GLN    | CONFLICT | UNP P02244 |
| A     | 78      | ASP      | GLU    | CONFLICT | UNP P02244 |
| A     | 82      | ASN      | HIS    | CONFLICT | UNP P02244 |
| A     | 96      | ALA      | SER    | CONFLICT | UNP P02244 |
| B     | 58      | GLN      | GLU    | CONFLICT | UNP P02244 |
| B     | 59      | GLU      | GLN    | CONFLICT | UNP P02244 |
| B     | 63      | GLU      | GLN    | CONFLICT | UNP P02244 |
| B     | 78      | ASP      | GLU    | CONFLICT | UNP P02244 |
| B     | 82      | ASN      | HIS    | CONFLICT | UNP P02244 |
| B     | 96      | ALA      | SER    | CONFLICT | UNP P02244 |

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | B     | 2        | Total Fe<br>2 2 | 0       | 0       |
| 2   | A     | 2        | Total Fe<br>2 2 | 0       | 0       |

### 3 Residue-property plots

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. 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.

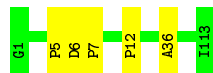
- Molecule 1: HEMERYTHRIN B

Chain A:  98% .



- Molecule 1: HEMERYTHRIN B

Chain B:  96% .



## 4 Data and refinement statistics

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

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | P 4 2 2  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 104.82Å 104.82Å 54.08Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | (Not available) – 5.50                         | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-5.50)         | Depositor |
| $R_{merge}$  | (Not available)                                | Depositor |
| $R_{sym}$  | (Not available)                                | Depositor |
| Refinement program                                       | unknown  | Depositor |
| R, $R_{free}$  | (Not available) , (Not available)              | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 230  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 0.0  | 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: FE

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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     | 113   | 0        | 0        | 1       | 0            |
| 1   | B     | 113   | 0        | 0        | 1       | 2            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 230   | 0        | 0        | 2       | 2            |

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 9.

All (2) 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:B:6:ASP:CA | 1:B:7:PRO:CA | 2.91                     | 0.49              |
| 1:A:6:ASP:CA | 1:A:7:PRO:CA | 2.91                     | 0.48              |

All (2) 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) |
|---------------|----------------------|--------------------------|-------------------|
| 1:B:12:PRO:CA | 1:B:12:PRO:CA[8_667] | 1.77                     | 0.43              |
| 1:B:5:PRO:CA  | 1:B:36:ALA:CA[4_665] | 1.79                     | 0.41              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.