



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:28 AM UTC

PDB ID : 2KIK / pdb\_00002kik  
Title : An artificial di-iron oxo-protein with phenol oxidase activity  
Authors : Maglio, O.; Lombardi, A.  
Deposited on : 2009-05-06

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | <b>FAILED</b>                                                    |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI                      | : | v_1n_11_5_13_A (Berjanski et al., 2005)                          |
| PANAV                          | : | Wang et al. (2010)                                               |
| wwPDB-ShiftChecker             | : | v1.2                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

## 2 Ensemble composition and analysis

This entry contains 30 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues |                         |                   |              |
|--------------------------------------|-------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)   | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:2-A:48, B:1-B:46 (93) | 0.63              | 16           |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

| Cluster number        | Models                           |
|-----------------------|----------------------------------|
| 1                     | 1, 8, 11, 18, 20, 21, 22, 23, 26 |
| 2                     | 3, 5, 6, 10, 12, 19, 24, 28      |
| 3                     | 13, 14, 15, 16, 17, 27, 29       |
| 4                     | 2, 30                            |
| Single-model clusters | 4; 7; 9; 25                      |

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1642 atoms, of which 822 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Artificial diiron protein.

| Mol | Chain | Residues | Atoms |     |     |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 1   | A     | 50       | Total | C   | H   | N  | O  | 1     |
|     |       |          | 820   | 263 | 411 | 67 | 79 |       |
| 1   | B     | 50       | Total | C   | H   | N  | O  | 1     |
|     |       |          | 820   | 263 | 411 | 67 | 79 |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

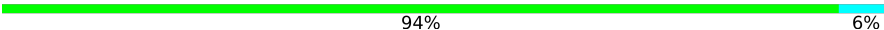
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 1        | Total | Zn |
|     |       |          | 1     | 1  |
| 2   | B     | 1        | Total | Zn |
|     |       |          | 1     | 1  |

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

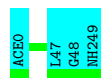
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



- Molecule 1: Artificial diiron protein

Chain B:  92% 8%

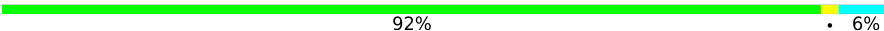


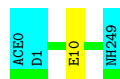
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

#### 4.2.1 Score per residue for model 1

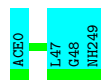
- Molecule 1: Artificial diiron protein

Chain A:  92% • 6%



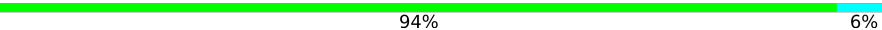
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



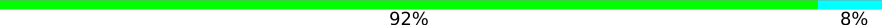
### 4.2.2 Score per residue for model 2

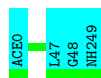
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



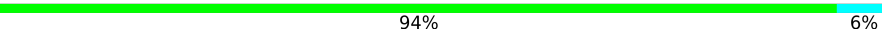
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



### 4.2.3 Score per residue for model 3

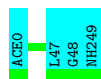
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



### 4.2.4 Score per residue for model 4

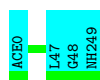
- Molecule 1: Artificial diiron protein

Chain A:  92% 6%



- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.5 Score per residue for model 5

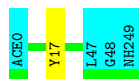
- Molecule 1: Artificial diiron protein

Chain A: 94% 6%



- Molecule 1: Artificial diiron protein

Chain B: 90% 8%



#### 4.2.6 Score per residue for model 6

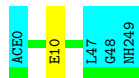
- Molecule 1: Artificial diiron protein

Chain A: 94% 6%



- Molecule 1: Artificial diiron protein

Chain B: 90% 8%



#### 4.2.7 Score per residue for model 7

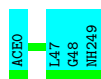
- Molecule 1: Artificial diiron protein

Chain A: 92% 6%



- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.8 Score per residue for model 8

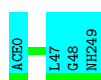
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



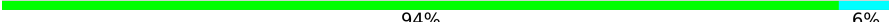
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.9 Score per residue for model 9

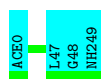
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



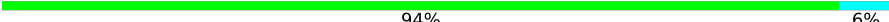
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.10 Score per residue for model 10

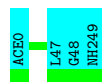
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



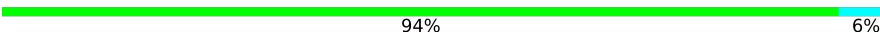
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.11 Score per residue for model 11

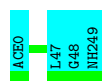
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



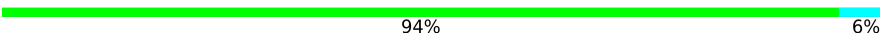
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



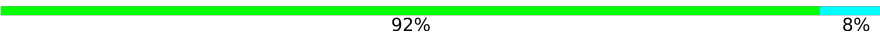
#### 4.2.12 Score per residue for model 12

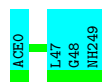
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



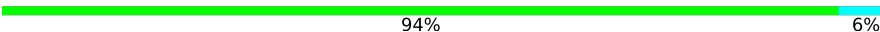
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.13 Score per residue for model 13

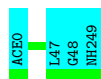
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



- Molecule 1: Artificial diiron protein

Chain B: 92% 8%



#### 4.2.14 Score per residue for model 14

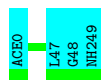
- Molecule 1: Artificial diiron protein

Chain A: 92% • 6%



- Molecule 1: Artificial diiron protein

Chain B: 92% 8%



#### 4.2.15 Score per residue for model 15

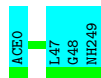
- Molecule 1: Artificial diiron protein

Chain A: 94% 6%



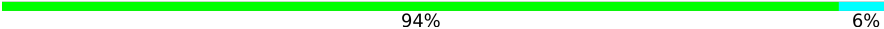
- Molecule 1: Artificial diiron protein

Chain B: 92% 8%



#### 4.2.16 Score per residue for model 16 (medoid)

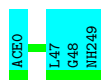
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.17 Score per residue for model 17

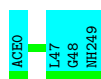
- Molecule 1: Artificial diiron protein

Chain A:  92% 6%



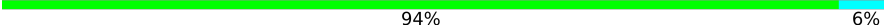
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.18 Score per residue for model 18

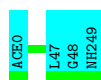
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



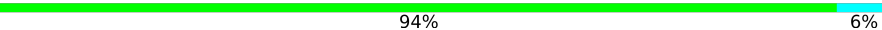
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.19 Score per residue for model 19

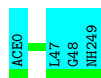
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



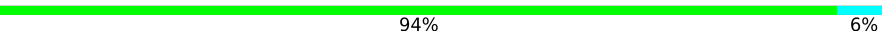
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.20 Score per residue for model 20

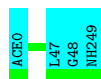
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



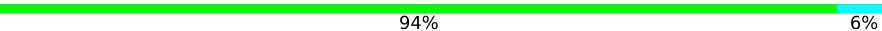
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.21 Score per residue for model 21

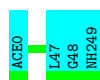
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



- Molecule 1: Artificial diiron protein

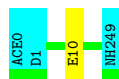
Chain B:  92% 8%



#### 4.2.22 Score per residue for model 22

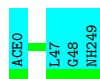
- Molecule 1: Artificial diiron protein

Chain A: 92% 6%



- Molecule 1: Artificial diiron protein

Chain B: 92% 8%



#### 4.2.23 Score per residue for model 23

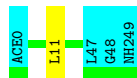
- Molecule 1: Artificial diiron protein

Chain A: 94% 6%



- Molecule 1: Artificial diiron protein

Chain B: 90% 8%



#### 4.2.24 Score per residue for model 24

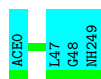
- Molecule 1: Artificial diiron protein

Chain A: 94% 6%



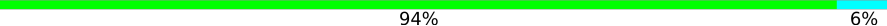
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.25 Score per residue for model 25

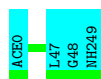
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



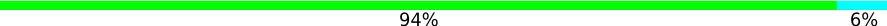
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.26 Score per residue for model 26

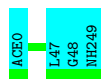
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



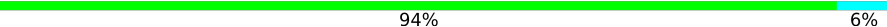
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.27 Score per residue for model 27

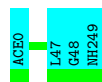
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



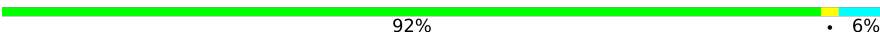
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.28 Score per residue for model 28

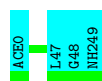
- Molecule 1: Artificial diiron protein

Chain A:  92% 6%



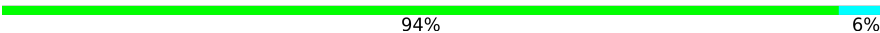
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



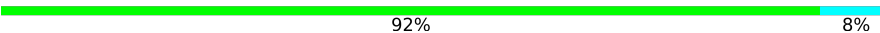
#### 4.2.29 Score per residue for model 29

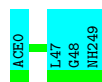
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



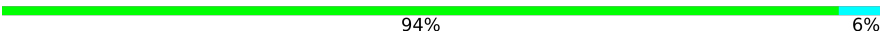
- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



#### 4.2.30 Score per residue for model 30

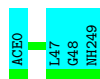
- Molecule 1: Artificial diiron protein

Chain A:  94% 6%



- Molecule 1: Artificial diiron protein

Chain B:  92% 8%



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *Energy restrained minimization*.

Of the 40 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 2.1     |
| Amber         | refinement         | 7.0     |

No chemical shift data was provided.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section will have to be empty.

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

MolProbity failed to run properly - this section will have to be empty.

#### 6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided