



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:09 AM UTC

PDB ID : 2N18 / pdb_00002n18
BMRB ID : 25551
Title : Dominant form of the low-affinity complex of yeast cytochrome c and cytochrome c peroxidase
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Deposited on : 2015-03-24

This is a Full wwPDB NMR Structure Validation 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/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>.

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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 is 7%.

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 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:1-A:294, B:-5-B:-1, B:1-B:103 (402)	0.00	1
2	C:-5-C:-1, C:1-C:103 (108)	0.00	2

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

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

NmrClust was unable to cluster the ensemble.

Error message: 1 Unexpected character

3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8241 atoms, of which 4046 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytochrome c peroxidase, mitochondrial.

Mol	Chain	Residues	Atoms						Trace
1	A	294	Total	C	H	N	O	S	0
			4621	1512	2249	395	459	6	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	CYS	engineered mutation	UNP P00431
A	197	CYS	VAL	engineered mutation	UNP P00431

- Molecule 2 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms						Trace
2	B	108	Total	C	H	N	O	S	0
			1698	534	851	151	157	5	

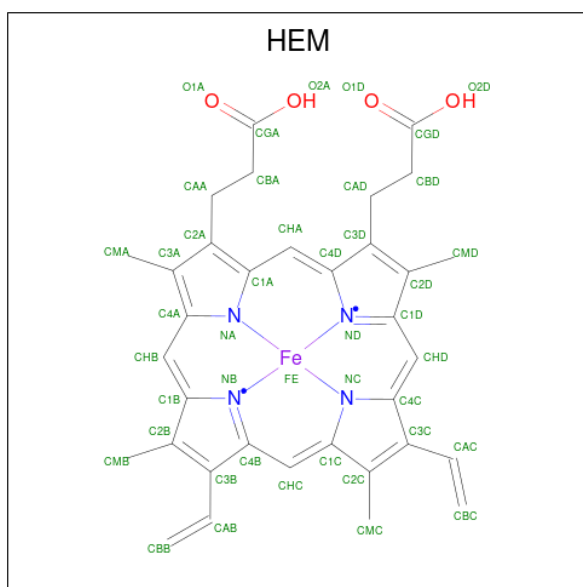
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	ALA	-	expression tag	UNP P00044
B	81	CYS	ALA	engineered mutation	UNP P00044
B	102	THR	CYS	engineered mutation	UNP P00044

- Molecule 3 is a protein called Cytochrome c iso-1.

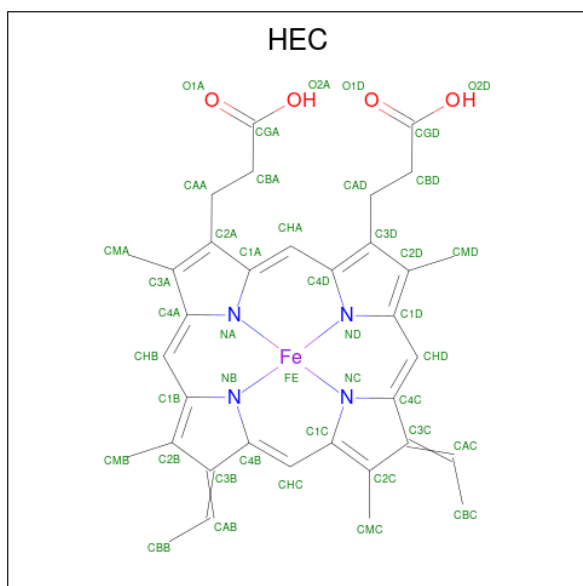
Mol	Chain	Residues	Atoms						Trace
3	C	108	Total	C	H	N	O	S	0
			1699	534	852	151	157	5	

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
4	A	1	Total	C	Fe	H	N	O
			73	34	1	30	4	4

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					
5	B	1	Total 75	C 34	Fe 1	H 32	N 4	O 4
5	C	1	Total 75	C 34	Fe 1	H 32	N 4	O 4

4 Residue-property plots

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: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

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 (medoid)

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.2 Score per residue for model 2

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

4.2.15 Score per residue for model 15

- Molecule 1: Cytochrome c peroxidase, mitochondrial

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: Cytochrome c iso-1

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 3: Cytochrome c iso-1

Chain C:  100%

There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 15 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	458
Number of shifts mapped to atoms	458
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	7%

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 7% for the well-defined parts and 7% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	458
Number of shifts mapped to atoms	458
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	229	0.34 ± 0.17	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 7%, i.e. 458 atoms were assigned a chemical shift out of a possible 6863. 0 out of 60 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	458/2550 (18%)	229/1044 (22%)	0/1020 (0%)	229/486 (47%)
Sidechain	0/3620 (0%)	0/2324 (0%)	0/1146 (0%)	0/150 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/693 (0%)	0/336 (0%)	0/323 (0%)	0/34 (0%)
Overall	458/6863 (7%)	229/3704 (6%)	0/2489 (0%)	229/670 (34%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 458 atoms were assigned a chemical shift out of a possible 6863. 0 out of 60 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	458/2550 (18%)	229/1044 (22%)	0/1020 (0%)	229/486 (47%)
Sidechain	0/3620 (0%)	0/2324 (0%)	0/1146 (0%)	0/150 (0%)
Aromatic	0/693 (0%)	0/336 (0%)	0/323 (0%)	0/34 (0%)
Overall	458/6863 (7%)	229/3704 (6%)	0/2489 (0%)	229/670 (34%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

