



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:50 pm GMT

PDB ID : 2C1U  
Title : CRYSTAL STRUCTURE OF THE DI-HAEM CYTOCHROME C PEROXIDASE FROM PARACOCCLUS PANTOTROPHUS - OXIDISED FORM  
Authors : Echalier, A.; Fulop, V.  
Deposited on : 2005-09-21  
Resolution : 1.95 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

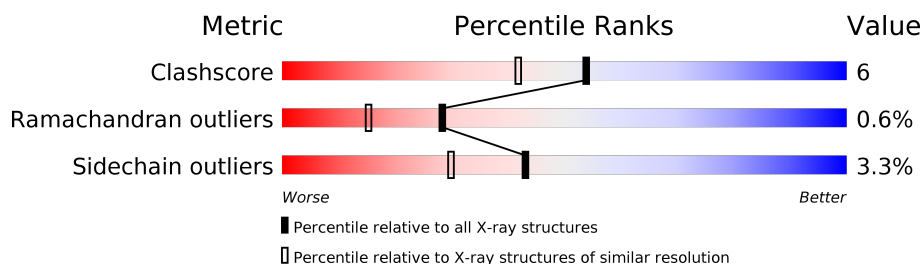
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)

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. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	
1	B	338	
1	C	338	
1	D	338	

## 2 Entry composition [i](#)

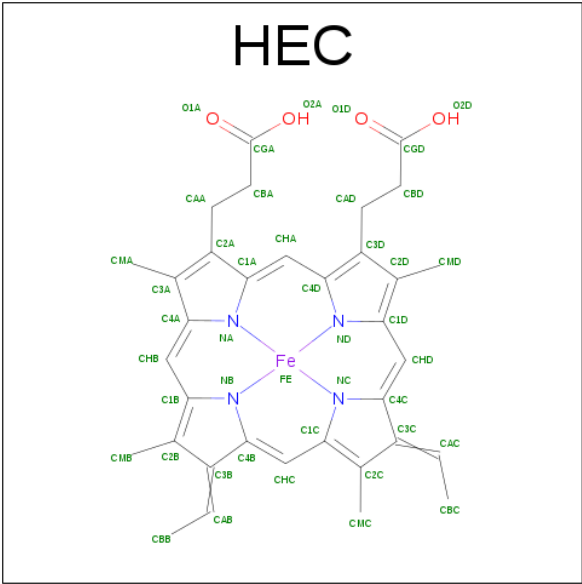
There are 4 unique types of molecules in this entry. The entry contains 11016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DI-HAEM CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2479	1566	415	486	12			
1	B	324	Total	C	N	O	S	0	0	0
			2446	1545	410	479	12			
1	C	329	Total	C	N	O	S	0	0	0
			2479	1567	415	485	12			
1	D	322	Total	C	N	O	S	0	0	0
			2431	1537	408	474	12			

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

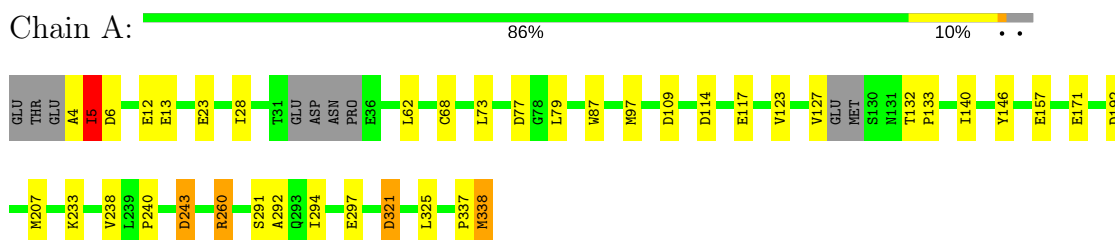
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total 208	O 208	0	0
4	B	199	Total 199	O 199	0	0
4	C	221	Total 221	O 221	0	0
4	D	205	Total 205	O 205	0	0

### 3 Residue-property plots

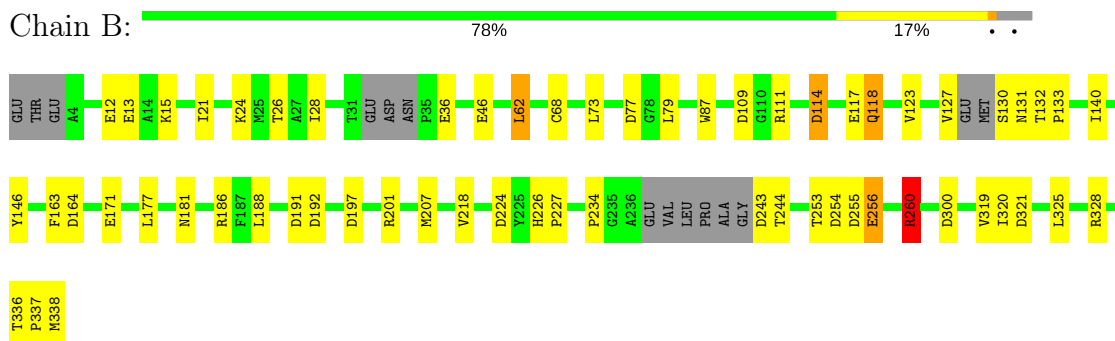
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

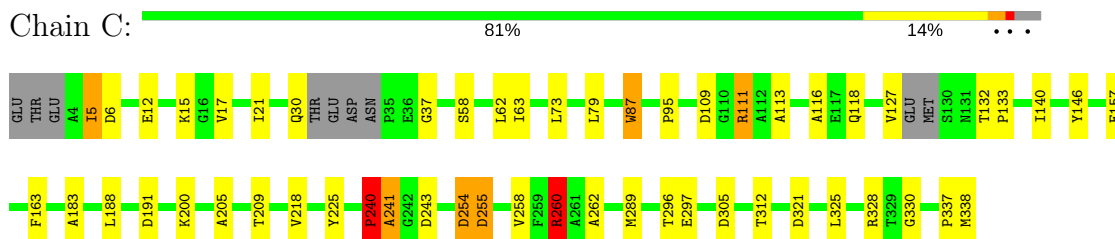
#### • Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE



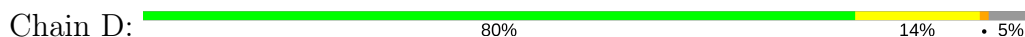
#### • Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE

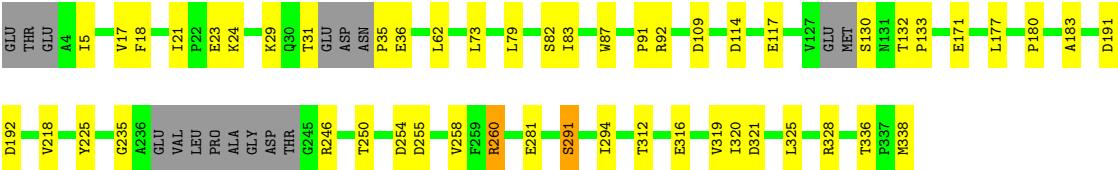


#### • Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE



#### • Molecule 1: DI-HAEM CYTOCHROME C PEROXIDASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.80Å 51.10Å 167.90Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	29.88 – 1.95	Depositor
% Data completeness (in resolution range)	88.6 (29.88-1.95)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.169 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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: CA, HEC

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	0.74	0/2535	0.89	8/3449 (0.2%)
1	B	0.72	0/2501	0.89	10/3400 (0.3%)
1	C	0.80	2/2536 (0.1%)	0.89	10/3450 (0.3%)
1	D	0.71	0/2486	0.87	10/3379 (0.3%)
All	All	0.74	2/10058 (0.0%)	0.88	38/13678 (0.3%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12	GLU	CD-OE2	11.62	1.38	1.25
1	C	12	GLU	CD-OE1	5.39	1.31	1.25

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	B	328	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	B	328	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	C	328	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	321	ASP	CB-CG-OD2	7.02	124.61	118.30

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	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	2479	0	2392	24	0
1	B	2446	0	2358	33	0
1	C	2479	0	2393	38	0
1	D	2431	0	2347	31	0
2	A	86	0	60	5	0
2	B	86	0	60	6	0
2	C	86	0	60	7	0
2	D	86	0	60	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	208	0	0	2	0
4	B	199	0	0	4	0
4	C	221	0	0	3	0
4	D	205	0	0	3	0
All	All	11016	0	9730	122	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 6.

The worst 5 of 122 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:C:296:THR:O	1:C:297:GLU:HG2	1.48	1.12
1:D:83:ILE:CD1	1:D:91:PRO:HA	1.96	0.96
1:D:83:ILE:HD13	1:D:91:PRO:HA	1.59	0.83
1:D:83:ILE:HD11	1:D:91:PRO:CA	2.13	0.79
1:C:79:LEU:HD11	1:D:62:LEU:HG	1.69	0.74

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	323/338 (96%)	309 (96%)	12 (4%)	2 (1%)	28	15
1	B	316/338 (94%)	299 (95%)	15 (5%)	2 (1%)	28	15
1	C	323/338 (96%)	312 (97%)	8 (2%)	3 (1%)	20	9
1	D	314/338 (93%)	300 (96%)	13 (4%)	1 (0%)	44	33
All	All	1276/1352 (94%)	1220 (96%)	48 (4%)	8 (1%)	28	15

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	C	5	ILE
1	C	240	PRO
1	C	241	ALA
1	B	244	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	258/267 (97%)	251 (97%)	7 (3%)	50	39
1	B	255/267 (96%)	242 (95%)	13 (5%)	28	13
1	C	258/267 (97%)	251 (97%)	7 (3%)	50	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	253/267 (95%)	246 (97%)	7 (3%)	49 37
All	All	1024/1068 (96%)	990 (97%)	34 (3%)	43 30

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	ASN
1	B	319	VAL
1	D	250	THR
1	B	256	GLU
1	A	338	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	GLN
1	B	106	GLN
1	B	131	ASN
1	C	118	GLN
1	D	181	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	HEC	A	401	1	28,50,50	2.28	7 (25%)	16,82,82	2.26	4 (25%)
2	HEC	A	402	1	28,50,50	2.42	5 (17%)	16,82,82	1.69	4 (25%)
2	HEC	B	401	1	28,50,50	2.20	7 (25%)	16,82,82	2.76	7 (43%)
2	HEC	B	402	1	28,50,50	2.17	8 (28%)	16,82,82	2.08	6 (37%)
2	HEC	C	401	1	28,50,50	2.64	10 (35%)	16,82,82	2.03	4 (25%)
2	HEC	C	402	1	28,50,50	2.35	10 (35%)	16,82,82	2.17	6 (37%)
2	HEC	D	401	1	28,50,50	2.32	7 (25%)	16,82,82	2.60	7 (43%)
2	HEC	D	402	1	28,50,50	2.05	5 (17%)	16,82,82	1.55	2 (12%)

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	HEC	A	401	1	-	0/6/54/54	0/0/8/8
2	HEC	A	402	1	-	0/6/54/54	0/0/8/8
2	HEC	B	401	1	-	0/6/54/54	0/0/8/8
2	HEC	B	402	1	-	0/6/54/54	0/0/8/8
2	HEC	C	401	1	-	0/6/54/54	0/0/8/8
2	HEC	C	402	1	-	0/6/54/54	0/0/8/8
2	HEC	D	401	1	-	0/6/54/54	0/0/8/8
2	HEC	D	402	1	-	0/6/54/54	0/0/8/8

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	HEC	C3B-C2B	-7.86	1.32	1.40
2	A	402	HEC	C3B-C2B	-7.14	1.33	1.40
2	A	401	HEC	C3B-C2B	-7.07	1.33	1.40
2	C	401	HEC	C3C-C2C	-6.44	1.34	1.40
2	C	402	HEC	C3B-C2B	-6.36	1.34	1.40

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEC	CMC-C2C-C1C	-6.84	117.96	128.46
2	A	401	HEC	CMB-C2B-C1B	-5.51	120.00	128.46
2	B	401	HEC	CMC-C2C-C1C	-5.43	120.12	128.46
2	B	401	HEC	CBD-CAD-C3D	-4.72	103.46	112.48
2	B	402	HEC	C1D-C2D-C3D	-4.35	103.97	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEC	4	0
2	A	402	HEC	1	0
2	B	401	HEC	5	0
2	B	402	HEC	1	0
2	C	401	HEC	3	0
2	C	402	HEC	4	0
2	D	401	HEC	2	0

## 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

### 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.