



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 10:33 PM EST

PDB ID : 1CMP
Title : SMALL MOLECULE BINDING TO AN ARTIFICIALLY CREATED CAVITY AT THE ACTIVE SITE OF CYTOCHROME C PEROXIDASE
Authors : Fitzgerald, M.M.; Mcree, D.E.; Churchill, M.J.; Goodin, D.B.
Deposited on : unknown
Resolution : 1.90 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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)	:	rb-20030345

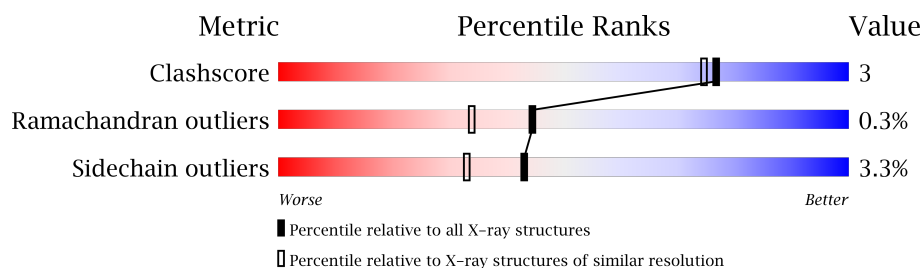
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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 ≥ 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	294	 84% 13% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2942 atoms, of which 504 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.

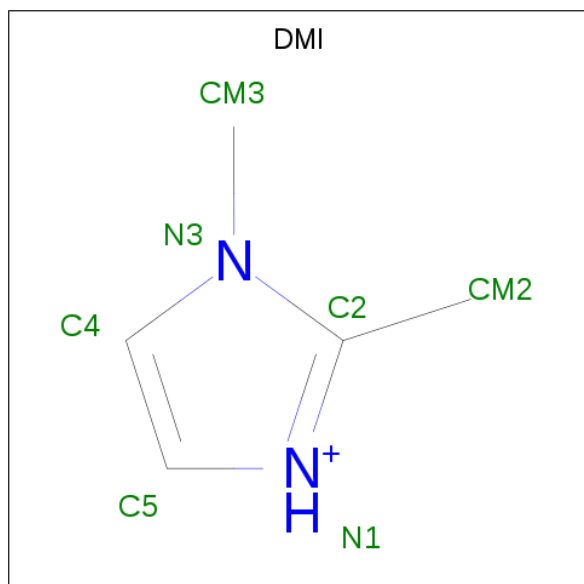
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	H	N	O	S	0	0	0
			2841	1492	503	389	451	6			

There are 3 discrepancies between the modelled and reference sequences:

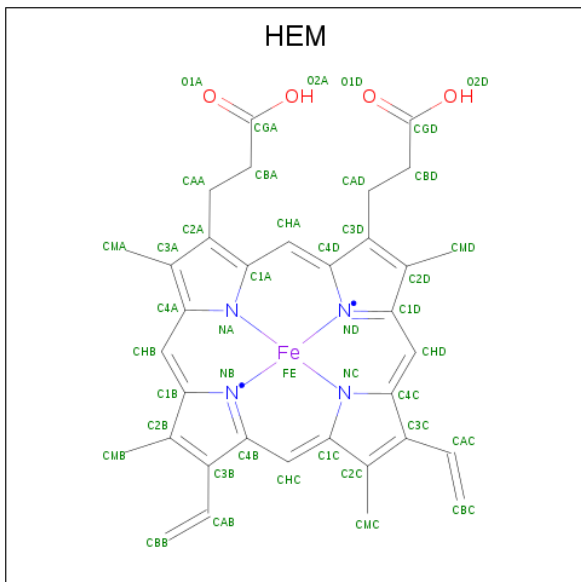
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	CONFLICT	UNP P00431
A	152	GLY	ASP	CONFLICT	UNP P00431
A	191	GLY	TRP	CONFLICT	UNP P00431

- Molecule 2 is 2,3-DIMETHYLIMIDAZOLIUM ION (three-letter code: DMI) (formula: $C_5H_9N_2^+$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	N	0	0
			8	5	1	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is water.

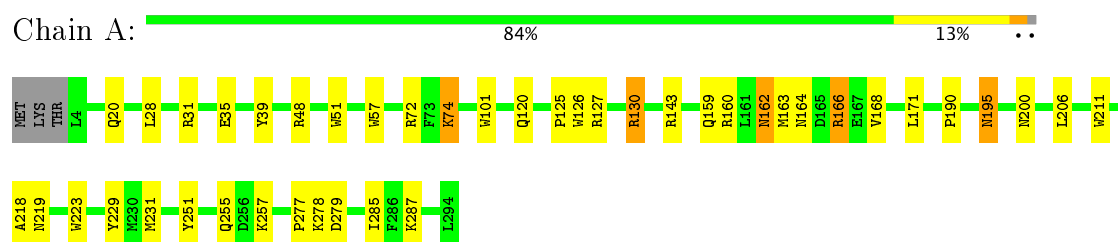
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		

3 Residue-property plots [i](#)

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: 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.20 Å 74.30 Å 45.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2942	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMI, 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	0.83	0/2402	1.56	37/3250 (1.1%)

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	0	1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	A	127	ARG	NE-CZ-NH2	-12.64	113.98	120.30
1	A	127	ARG	NE-CZ-NH1	12.63	126.61	120.30
1	A	31	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	51	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	101	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	A	223	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	A	51	TRP	CE2-CD2-CG	-8.18	100.76	107.30
1	A	143	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	126	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	A	223	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	126	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	A	51	TRP	CB-CG-CD1	-7.45	117.32	127.00
1	A	163	MET	CG-SD-CE	-7.34	88.45	100.20
1	A	162	ASN	CA-C-N	-7.34	101.06	117.20
1	A	229	TYR	CB-CG-CD2	-7.31	116.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	278	LYS	CA-CB-CG	-7.24	97.48	113.40
1	A	101	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	A	211	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	A	51	TRP	CG-CD2-CE3	6.59	139.83	133.90
1	A	130	ARG	CG-CD-NE	-6.38	98.40	111.80
1	A	211	TRP	CE2-CD2-CG	-6.21	102.33	107.30
1	A	48	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	57	TRP	CE2-CD2-CG	-6.07	102.44	107.30
1	A	39	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	57	TRP	CD1-CG-CD2	5.97	111.08	106.30
1	A	277	PRO	CA-C-N	5.85	130.08	117.20
1	A	166	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	101	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	A	51	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	A	162	ASN	N-CA-C	5.63	126.19	111.00
1	A	160	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	251	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	166	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	223	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	120	GLN	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	2338	503	2211	16	0
2	A	7	1	9	0	0
3	A	43	0	30	0	0
4	A	50	0	0	3	0
All	All	2438	504	2250	16	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 3.

All (16) 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:74:LYS:H	1:A:74:LYS:HD2	1.53	0.71
1:A:20:GLN:HE22	1:A:287:LYS:H	1.41	0.68
1:A:200:ASN:H	1:A:255:GLN:HE21	1.51	0.59
1:A:195:ASN:HD22	1:A:195:ASN:H	1.55	0.55
1:A:130:ARG:NE	4:A:326:HOH:O	2.39	0.54
1:A:20:GLN:HE22	1:A:287:LYS:N	2.04	0.53
1:A:166:ARG:HH21	1:A:257:LYS:HZ2	1.57	0.51
1:A:125:PRO:HG3	1:A:285:ILE:CD1	2.42	0.50
1:A:206:LEU:HD13	1:A:231:MET:SD	2.53	0.49
1:A:218:ALA:O	1:A:219:ASN:HB2	2.15	0.46
1:A:164:ASN:O	1:A:168:VAL:HG23	2.15	0.46
1:A:166:ARG:HH21	1:A:257:LYS:NZ	2.12	0.46
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.98	0.44
1:A:130:ARG:CZ	4:A:326:HOH:O	2.66	0.44
1:A:130:ARG:NH2	4:A:326:HOH:O	2.53	0.41
1:A:20:GLN:NE2	1:A:287:LYS:H	2.13	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	289/294 (98%)	283 (98%)	5 (2%)	1 (0%)	44	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN

5.3.2 Protein sidechains ⓘ

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	246/251 (98%)	238 (97%)	8 (3%)	43 33

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	35	GLU
1	A	74	LYS
1	A	159	GLN
1	A	171	LEU
1	A	190	PRO
1	A	195	ASN
1	A	279	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	87	ASN
1	A	195	ASN
1	A	208	ASN
1	A	220	ASN
1	A	240	GLN
1	A	255	GLN
1	A	292	GLN

5.3.3 RNA ⓘ

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](#)

2 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	DMI	A	295	-	6,7,7	2.52	3 (50%)	5,9,9	2.72	2 (40%)
3	HEM	A	296	1,4	28,50,50	1.62	7 (25%)	17,82,82	1.67	5 (29%)

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	DMI	A	295	-	-	0/0/0/0	0/1/1/1
3	HEM	A	296	1,4	-	0/6/54/54	0/0/8/8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	296	HEM	C3B-CAB	-4.20	1.39	1.47
2	A	295	DMI	C4-N3	-4.14	1.30	1.37
3	A	296	HEM	C4C-NC	-3.51	1.32	1.36
2	A	295	DMI	CM2-C2	-3.51	1.45	1.49
3	A	296	HEM	C3C-CAC	-3.49	1.40	1.47
3	A	296	HEM	C4D-ND	-2.70	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	296	HEM	C1C-NC	-2.09	1.34	1.36
2	A	295	DMI	C5-N1	-2.08	1.30	1.37
3	A	296	HEM	CBC-CAC	2.07	1.43	1.28
3	A	296	HEM	CBB-CAB	2.23	1.44	1.28

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	296	HEM	C4A-C3A-C2A	-2.79	105.05	107.00
3	A	296	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
3	A	296	HEM	CMC-C2C-C3C	2.35	129.26	124.89
3	A	296	HEM	CAD-CBD-CGD	2.53	116.98	112.66
3	A	296	HEM	CMB-C2B-C3B	3.41	131.23	124.89
2	A	295	DMI	C5-N1-C2	3.44	112.71	109.08
2	A	295	DMI	CM2-C2-N3	4.62	128.97	124.88

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 [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.