



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:02 AM GMT

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 : 1993-11-23
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

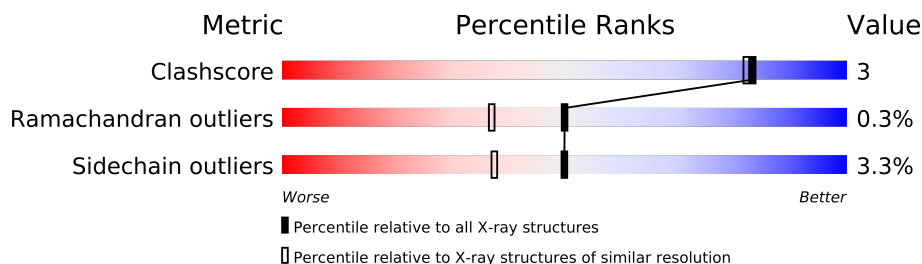
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	294	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	DMI	A	295	X	-

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 deuterium.

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.

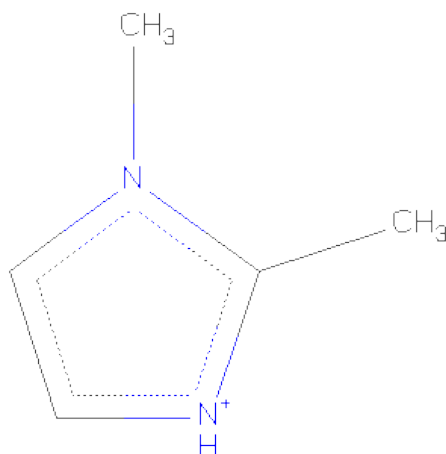
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

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-DIMETHYLIMIDAZOLIUMION (three-letter code: DMI) (formula: C₅H₉N₂).



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
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0

- Molecule 4 is water.

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

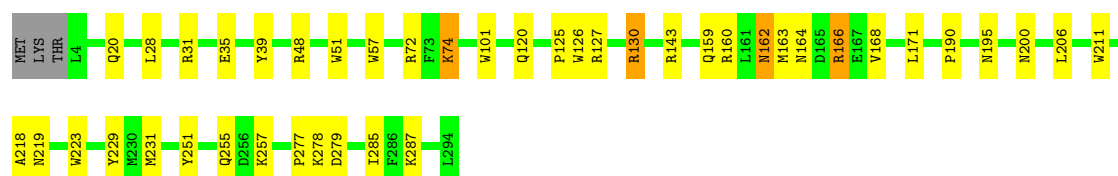
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.20Å 74.30Å 45.40Å 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2338	503	1709	14	0
2	A	7	1	8	0	0
3	A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	50	0	0	3	0
All	All	2438	504	1747	14	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (14) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:LYS:H	1:A:74:LYS:HD2	1.58	0.68
1:A:130:ARG:NE	4:A:326:HOH:O	2.39	0.54
1:A:166:ARG:HH21	1:A:257:LYS:HZ1	1.55	0.53
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:20:GLN:HE21	1:A:287:LYS:N	2.12	0.47
1:A:166:ARG:HH21	1:A:257:LYS:NZ	2.12	0.46
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:125:PRO:HG3	1:A:285:ILE:HD11	1.98	0.44
1:A:200:ASN:H	1:A:255:GLN:HE22	1.64	0.44
1:A:130:ARG:CZ	4:A:326:HOH:O	2.66	0.44
1:A:20:GLN:HE21	1:A:287:LYS:H	1.68	0.42
1:A:130:ARG:NH2	4:A:326:HOH:O	2.53	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%)	50 37

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%)	50 37

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 chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	7,7,7	2.49	5 (71%)	9,9,9	2.79	4 (44%)
3	HEM	A	296	1,4	49,50,50	5.00	25 (51%)	46,82,82	1.44	7 (15%)

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	-	0/14/114/114	0/0/8/8

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	296	HEM	C2D-C1D	-23.37	1.38	1.44
3	A	296	HEM	C3D-C4D	-18.22	1.40	1.44
3	A	296	HEM	C2B-C1B	-12.05	1.41	1.44
3	A	296	HEM	CHB-C1B	4.29	1.41	1.35
2	A	295	DMI	C4-N3	-4.11	1.30	1.37
3	A	296	HEM	C4C-NC	-3.81	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	296	HEM	CHA-C4D	3.72	1.41	1.35
3	A	296	HEM	FE-NA	3.68	2.08	1.92
3	A	296	HEM	FE-NB	3.26	2.09	1.97
2	A	295	DMI	CM2-C2	-3.13	1.45	1.48
3	A	296	HEM	CHD-C4C	2.91	1.41	1.36
3	A	296	HEM	C4D-ND	-2.91	1.33	1.39
3	A	296	HEM	C1A-C2A	-2.90	1.38	1.43
3	A	296	HEM	CHC-C1C	2.82	1.41	1.36
3	A	296	HEM	C3B-C4B	-2.78	1.41	1.44
3	A	296	HEM	CBB-CAB	2.70	1.44	1.28
3	A	296	HEM	C1C-NC	-2.63	1.34	1.38
3	A	296	HEM	C3C-C2C	-2.58	1.39	1.43
3	A	296	HEM	CBC-CAC	2.52	1.43	1.28
3	A	296	HEM	FE-ND	2.50	2.07	1.97
3	A	296	HEM	C3D-C2D	-2.46	1.39	1.43
2	A	295	DMI	C2-N1	-2.33	1.29	1.33
3	A	296	HEM	C3B-C2B	-2.33	1.39	1.43
2	A	295	DMI	C2-N3	-2.33	1.30	1.34
3	A	296	HEM	C1D-ND	-2.29	1.32	1.37
3	A	296	HEM	O2A-CGA	-2.23	1.22	1.30
2	A	295	DMI	C5-N1	-2.18	1.30	1.37
3	A	296	HEM	FE-NC	2.17	2.06	1.97
3	A	296	HEM	O2D-CGD	-2.10	1.22	1.30
3	A	296	HEM	C1B-NB	-2.05	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	296	HEM	C3B-C4B-NB	-4.78	110.58	114.00
2	A	295	DMI	CM2-C2-N3	4.62	128.97	124.88
2	A	295	DMI	C4-N3-C2	4.49	112.52	108.72
2	A	295	DMI	C5-N1-C2	3.44	112.71	109.08
2	A	295	DMI	N1-C2-N3	-3.09	104.77	109.41
3	A	296	HEM	C4A-C3A-C2A	-2.79	105.05	107.00
3	A	296	HEM	C3A-C4A-NA	2.47	111.28	109.41
3	A	296	HEM	CHC-C1C-NC	-2.25	122.78	124.73
3	A	296	HEM	CHD-C4C-NC	-2.23	122.79	124.73
3	A	296	HEM	CMB-C2B-C3B	2.15	131.23	126.16
3	A	296	HEM	C4D-ND-C1D	2.05	107.26	105.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.