



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:28 PM GMT

PDB ID : 1IQC
Title : Crystal structure of Di-Heme Peroxidase from Nitrosomonas europaea
Authors : Shimizu, H.
Deposited on : 2001-07-20
Resolution : 1.80 Å(reported)

This is a wwPDB validation summary 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>

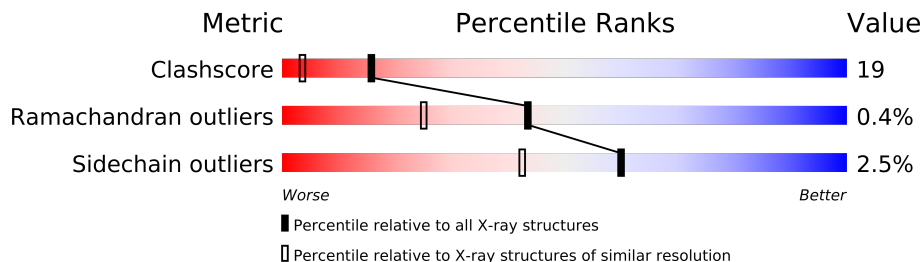
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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	308	
1	B	308	
1	C	308	
1	D	308	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10767 atoms, of which 0 are hydrogen 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 di-heme peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	B	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	C	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	D	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			

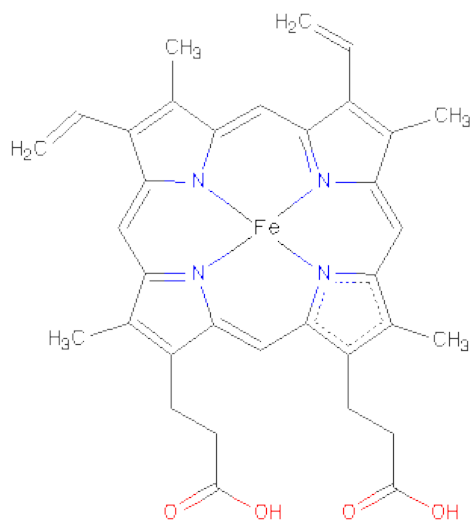
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	2	Total	Ca	0	0
			2	2		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

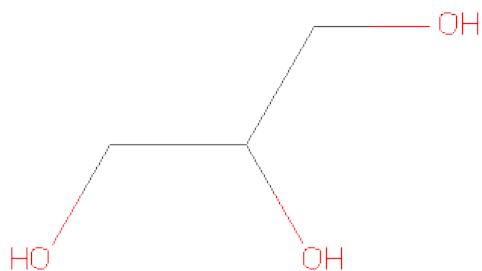
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

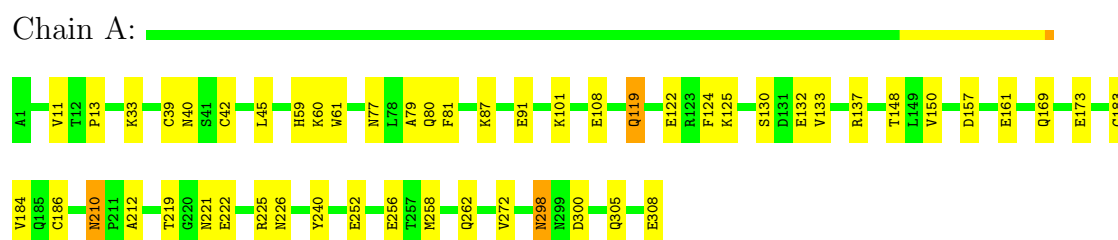
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	260	Total	O	0	0
			260	260		
6	B	199	Total	O	0	0
			199	199		
6	C	279	Total	O	0	0
			279	279		
6	D	120	Total	O	0	0
			120	120		

3 Residue-property plots

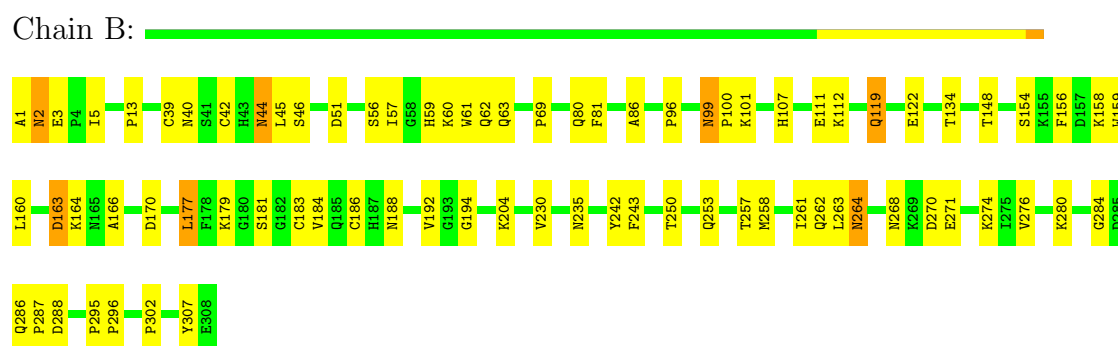
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

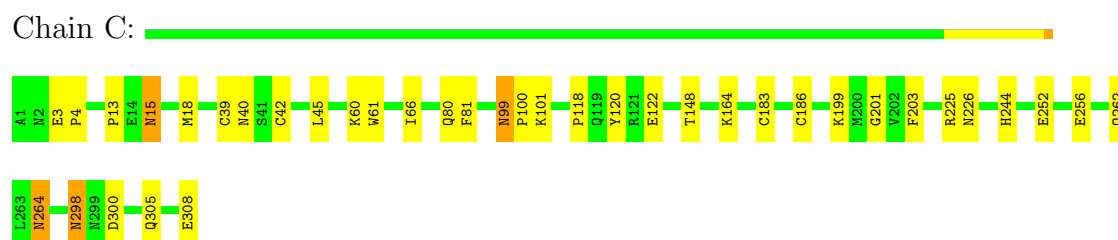
- Molecule 1: di-heme peroxidase



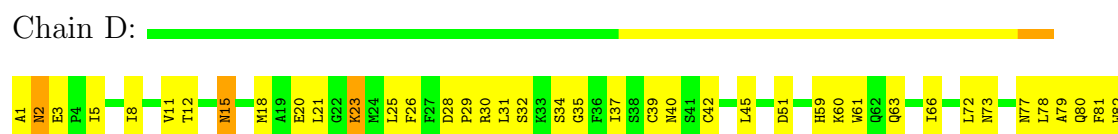
- Molecule 1: di-heme peroxidase



- Molecule 1: di-heme peroxidase



- Molecule 1: di-heme peroxidase



D83	G84	R85	A86	P96	P100	K101	E102	M103	A104	E108	I109	A110	V113	V114	A115	Q119	V120	R121	E122	R123	F124	K125	K126	V127	F128	G129	S130	D131	E132	V133	T134	I135	D136	R137	I138	T139	T140	A141	I142	A143	Q144	F145	E146	L149	V150	T151	P152	K155	F156	D157	E161	
K164	N165	A166	L167	N168	Q169	D170	E171	L172	E173	L177	C183	V184	Q185	C186	H187	N188	G189	V192	G193	G194	S195	S196	Y197	Q198	K199	W200	G201	K209	N210	E211	R215	M216	D217	V218	T219	G220	N221	E222	A223	D224	R225	N226	V227	F228	K229	V230	N235	L236	E237	L238	T239	Y240
P241	Y242	F243	H244	L251	E256	T257	M258	G259	R260	T261	Q262	L263	N264	N268	K269	D270	E271	K274	T281	K290	L291	P292	L293	L294	P295	P296	S297	N298	N299	D300	T301	P302	P306	Y307	E308																	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.13Å 55.11Å 144.00Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.9 (30.00-1.80)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10767	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: GOL, CA, MG, 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	0.32	0/2441	0.58	0/3304
1	B	0.29	0/2441	0.56	0/3304
1	C	0.32	0/2441	0.58	0/3304
1	D	0.29	0/2441	0.52	0/3304
All	All	0.30	0/9764	0.56	0/13216

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	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	2388	0	2331	59	0
1	B	2388	0	2331	85	0
1	C	2388	0	2331	43	0
1	D	2388	0	2331	185	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	86	0	60	18	0
4	B	86	0	60	18	0
4	C	86	0	60	15	0
4	D	86	0	60	22	0
5	B	6	0	8	0	0
6	A	260	0	0	4	0
6	B	199	0	0	4	0
6	C	279	0	0	0	0
6	D	120	0	0	6	0
All	All	10767	0	9572	360	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 19.

The worst 5 of 360 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:186:CYS:SG	4:B:402:HEM:HAC	1.50	1.50
1:A:39:CYS:SG	4:A:401:HEM:CAB	2.12	1.38
1:B:39:CYS:SG	4:B:401:HEM:CAB	2.13	1.37
1:A:42:CYS:SG	4:A:401:HEM:CAC	2.14	1.36
1:C:183:CYS:SG	4:C:402:HEM:CAB	2.13	1.36

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	306/308 (99%)	296 (97%)	10 (3%)	0	100	100
1	B	306/308 (99%)	287 (94%)	16 (5%)	3 (1%)	22	6
1	C	306/308 (99%)	298 (97%)	8 (3%)	0	100	100
1	D	306/308 (99%)	285 (93%)	19 (6%)	2 (1%)	30	13
All	All	1224/1232 (99%)	1166 (95%)	53 (4%)	5 (0%)	43	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASN
1	D	2	ASN
1	B	163	ASP
1	D	215	ARG
1	B	3	GLU

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	260/260 (100%)	255 (98%)	5 (2%)	69	56
1	B	260/260 (100%)	254 (98%)	6 (2%)	63	46
1	C	260/260 (100%)	255 (98%)	5 (2%)	69	56
1	D	260/260 (100%)	250 (96%)	10 (4%)	44	24
All	All	1040/1040 (100%)	1014 (98%)	26 (2%)	60	42

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ASN
1	C	264	ASN
1	D	268	ASN
1	C	99	ASN
1	C	120	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	268	ASN
1	C	62	GLN
1	D	226	ASN
1	B	299	ASN
1	C	15	ASN

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 ⓘ

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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$
4	HEM	A	401	1,6	49,50,50	2.39	16 (32%)	46,82,82	1.36	7 (15%)
4	HEM	A	402	1	49,50,50	1.93	11 (22%)	46,82,82	1.38	7 (15%)
5	GOL	B	1410	-	5,5,5	0.18	0	5,5,5	0.31	0
4	HEM	B	401	1,6	49,50,50	1.72	11 (22%)	46,82,82	1.11	4 (8%)
4	HEM	B	402	1	49,50,50	2.17	13 (26%)	46,82,82	1.12	3 (6%)
4	HEM	C	401	1,6	49,50,50	1.98	12 (24%)	46,82,82	1.27	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	C	402	1	49,50,50	2.13	12 (24%)	46,82,82	1.19	4 (8%)
4	HEM	D	401	1,6	49,50,50	2.07	13 (26%)	46,82,82	1.18	3 (6%)
4	HEM	D	402	1	49,50,50	2.14	11 (22%)	46,82,82	1.43	5 (10%)

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
4	HEM	A	401	1,6	-	0/14/114/114	0/0/8/8
4	HEM	A	402	1	-	0/14/114/114	0/0/8/8
5	GOL	B	1410	-	-	0/4/4/4	0/0/0/0
4	HEM	B	401	1,6	-	0/14/114/114	0/0/8/8
4	HEM	B	402	1	-	0/14/114/114	0/0/8/8
4	HEM	C	401	1,6	-	0/14/114/114	0/0/8/8
4	HEM	C	402	1	-	0/14/114/114	0/0/8/8
4	HEM	D	401	1,6	-	0/14/114/114	0/0/8/8
4	HEM	D	402	1	-	0/14/114/114	0/0/8/8

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	HEM	C2D-C1D	8.99	1.46	1.44
4	C	402	HEM	C2B-C1B	7.90	1.46	1.44
4	B	402	HEM	C2D-C1D	6.96	1.46	1.44
4	D	402	HEM	C2D-C1D	6.47	1.46	1.44
4	D	401	HEM	C3D-C4D	5.79	1.46	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	HEM	CBD-CAD-C3D	4.64	124.51	114.37
4	D	402	HEM	C3B-C4B-NB	-4.62	110.69	114.00
4	D	401	HEM	C3B-C4B-NB	-4.60	110.71	114.00
4	A	402	HEM	C3B-C4B-NB	-4.41	110.84	114.00
4	B	402	HEM	C3B-C4B-NB	-4.34	110.90	114.00

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.