WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 10:18 AM GMT

PDB ID	:	3HQ6
Title	:	Cytochrome c peroxidase from G. sulfurreducens, wild type
Authors	:	Hoffmann, M.; Seidel, J.; Einsle, O.
Deposited on	:	2009-06-05
Resolution	:	2.00 Å(reported)

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)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.00 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		12
Ramachandran outliers		0.8%
Sidechain outliers		4.3%
RSRZ outliers		1.2%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
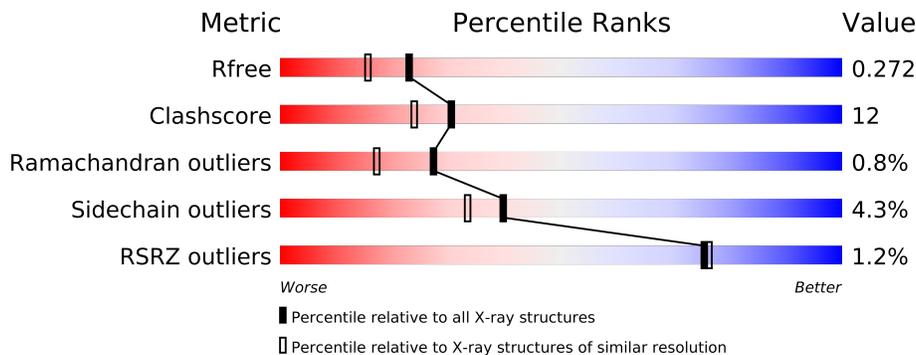
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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.

| Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5716 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 Cytochrome c551 peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2451	1566	418	458	9			
1	B	313	Total	C	N	O	S	0	0	0
			2370	1514	405	442	9			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
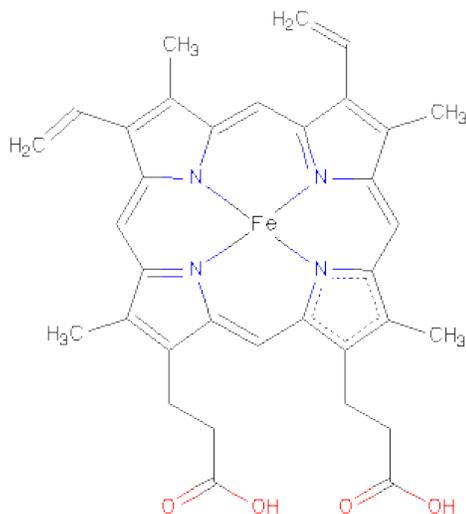
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	342	Total 342	O 342	0	0
4	B	379	Total 379	O 379	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 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.

• Molecule 1: Cytochrome c551 peroxidase

Chain A:
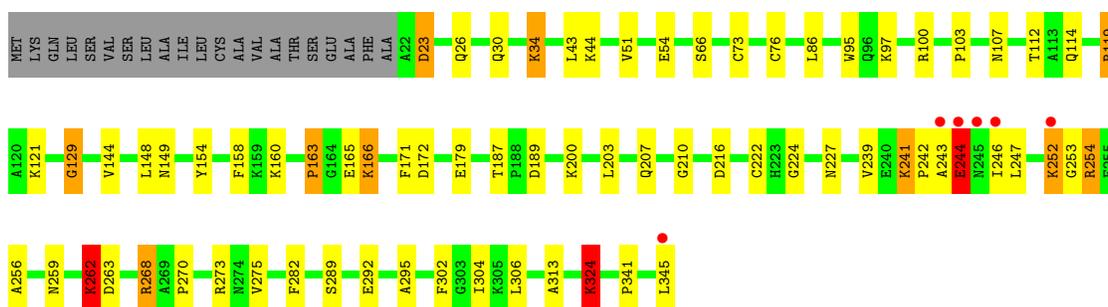
• Molecule 1: Cytochrome c551 peroxidase

Chain B:
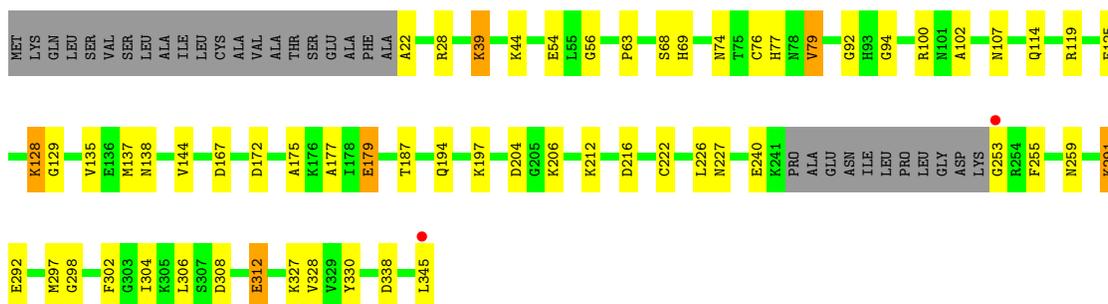
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.24Å 55.78Å 78.64Å 68.69° 71.84° 57.76°	Depositor
Resolution (Å)	70.00 – 2.00 36.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.6 (70.00-2.00) 94.7 (36.22-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.266 0.192 , 0.272	Depositor DCC
R_{free} test set	2319 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 26.3	EDS
Estimated twinning fraction	0.010 for -h+k,k,k-l	Xtriage
L-test for twinning	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Outliers	0 of 45908 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5716	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CA

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	1.28	10/2511 (0.4%)	1.06	6/3408 (0.2%)
1	B	1.33	8/2427 (0.3%)	1.08	8/3291 (0.2%)
All	All	1.30	18/4938 (0.4%)	1.07	14/6699 (0.2%)

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

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	GLU	CG-CD	7.84	1.63	1.51
1	A	275	VAL	CB-CG2	6.25	1.66	1.52
1	B	94	GLY	N-CA	6.06	1.55	1.46
1	A	282	PHE	CE2-CZ	5.86	1.48	1.37
1	A	66	SER	CB-OG	5.83	1.49	1.42

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	338	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	298	GLY	N-CA-C	-6.33	97.28	113.10
1	A	216	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	306	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	B	119	ARG	NE-CZ-NH2	5.65	123.12	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ASP	Peptide

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	2451	0	2454	68	0
1	B	2370	0	2369	50	0
2	A	86	0	60	18	0
2	B	86	0	60	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	342	0	0	10	4
4	B	379	0	0	13	4
All	All	5716	0	4943	118	4

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 12.

The worst 5 of 118 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:73:CYS:SG	2:A:400:HEM:CAB	2.03	1.47
1:A:73:CYS:SG	2:A:400:HEM:HAB	1.62	1.40
1:A:76:CYS:SG	2:A:400:HEM:CAC	2.10	1.39
1:A:222:CYS:HG	2:A:401:HEM:CAC	1.47	1.26
1:B:222:CYS:SG	2:B:401:HEM:CAC	2.25	1.25

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:669:HOH:O	4:B:414:HOH:O[1_655]	1.76	0.44
4:A:669:HOH:O	4:B:416:HOH:O[1_655]	1.94	0.26

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:463:HOH:O	4:B:690:HOH:O[1_556]	2.15	0.05
4:A:462:HOH:O	4:B:380:HOH:O[1_556]	2.16	0.04

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	322/345 (93%)	304 (94%)	13 (4%)	5 (2%)	14	5
1	B	309/345 (90%)	294 (95%)	15 (5%)	0	100	100
All	All	631/690 (91%)	598 (95%)	28 (4%)	5 (1%)	27	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
1	A	242	PRO
1	A	253	GLY
1	A	129	GLY
1	A	262	LYS

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	260/276 (94%)	245 (94%)	15 (6%)	28	21
1	B	251/276 (91%)	244 (97%)	7 (3%)	56	54
All	All	511/552 (93%)	489 (96%)	22 (4%)	40	33

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	ARG
1	A	324	LYS
1	B	308	ASP
1	A	262	LYS
1	A	268	ARG

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

Mol	Chain	Res	Type
1	A	107	ASN
1	A	114	GLN
1	A	149	ASN
1	B	107	ASN
1	B	114	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   ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	HEM	A	400	1	49,50,50	2.30	17 (34%)	46,82,82	2.33	17 (36%)
2	HEM	A	401	1	49,50,50	2.41	19 (38%)	46,82,82	2.26	15 (32%)
2	HEM	B	400	1	49,50,50	2.43	20 (40%)	46,82,82	2.52	17 (36%)
2	HEM	B	401	1	49,50,50	3.76	16 (32%)	46,82,82	2.27	16 (34%)

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	HEM	A	400	1	-	0/14/114/114	0/0/8/8
2	HEM	A	401	1	-	0/14/114/114	0/0/8/8
2	HEM	B	400	1	-	0/14/114/114	0/0/8/8
2	HEM	B	401	1	-	0/14/114/114	0/0/8/8

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C3D-C4D	16.75	1.48	1.44
2	B	401	HEM	C2B-C1B	11.88	1.47	1.44
2	A	401	HEM	C2D-C1D	-8.22	1.42	1.44
2	B	401	HEM	C2D-C1D	6.84	1.46	1.44
2	A	400	HEM	C2B-C1B	6.16	1.46	1.44

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	HEM	C3B-C4B-NB	-7.63	108.54	114.00
2	B	401	HEM	C3B-C4B-NB	-7.33	108.75	114.00
2	B	400	HEM	C3B-C4B-NB	-6.67	109.22	114.00
2	B	401	HEM	C4D-ND-C1D	6.15	111.46	105.16
2	B	400	HEM	C4D-ND-C1D	6.08	111.38	105.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	\<RSRZ\>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	324/345 (93%)	-0.24	6 (1%)	64	64	12, 21, 44, 66	0
1	B	313/345 (90%)	-0.31	2 (0%)	86	88	12, 20, 35, 52	0
All	All	637/690 (92%)	-0.27	8 (1%)	75	74	12, 21, 40, 66	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	LEU	7.0
1	A	244	GLU	3.9
1	A	243	ALA	3.4
1	A	345	LEU	3.4
1	A	245	ASN	3.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	A	400	43/43	0.12	1.12	8,14,19,28	0
3	CA	A	402	1/1	0.10	0.80	17,17,17,17	0
3	CA	B	402	1/1	0.11	0.64	18,18,18,18	0
2	HEM	B	400	43/43	0.11	0.36	4,12,19,26	0
2	HEM	A	401	43/43	0.10	0.26	12,19,23,24	0
2	HEM	B	401	43/43	0.10	0.12	11,18,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.