



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:43 PM GMT

PDB ID : 1GZA
Title : PEROXIDASE
Authors : Fukuyama, K.; Itakura, H.
Deposited on : 1996-11-13
Resolution : 2.06 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

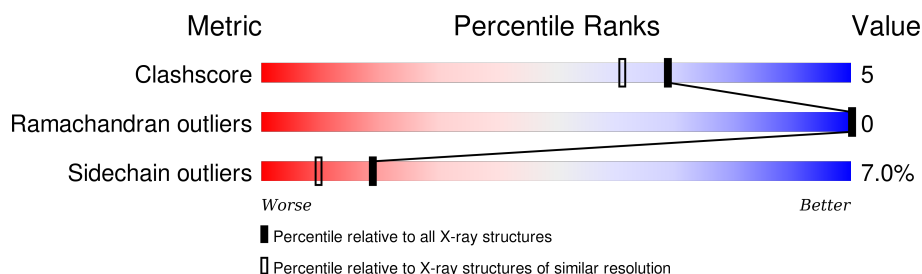
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)

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	344	<div>82% 13% ...</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	A	702	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2786 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 PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2465	1537	421	492	15			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

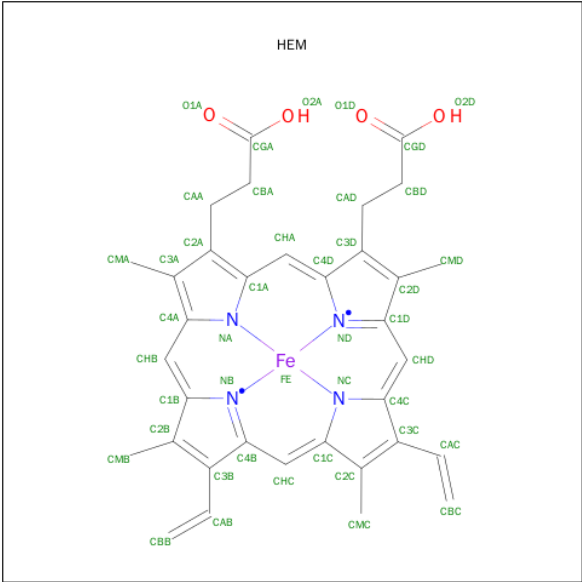
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	I	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



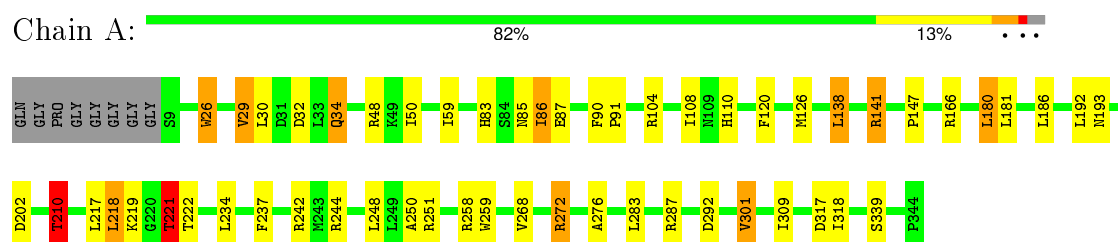
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	247	Total	O	0	0
			247	247		

Note EDS was not executed.

- Molecule 1: PEROXIDASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.57Å 74.57Å 117.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.06	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.06)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2786	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: HEM, CA, IOD, NAG

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	0.75	0/2521	1.58	34/3436 (1.0%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ARG	NE-CZ-NH2	-21.86	109.37	120.30
1	A	141	ARG	NE-CZ-NH2	-17.57	111.52	120.30
1	A	141	ARG	NE-CZ-NH1	16.41	128.50	120.30
1	A	48	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	A	272	ARG	NE-CZ-NH1	10.89	125.74	120.30
1	A	287	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	287	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	A	244	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	210	THR	N-CA-CB	-7.88	95.32	110.30
1	A	126	MET	CA-CB-CG	-7.56	100.45	113.30
1	A	30	LEU	CA-CB-CG	7.49	132.53	115.30
1	A	242	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	259	TRP	CD1-CG-CD2	6.89	111.81	106.30
1	A	301	VAL	CG1-CB-CG2	-6.80	100.01	110.90
1	A	166	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	244	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	26	TRP	CD1-CG-CD2	6.60	111.58	106.30
1	A	26	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	A	272	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	141	ARG	CG-CD-NE	-6.41	98.35	111.80
1	A	242	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	83	HIS	CA-CB-CG	-6.01	103.39	113.60
1	A	259	TRP	CE2-CD2-CG	-5.96	102.53	107.30
1	A	309	ILE	N-CA-C	-5.90	95.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASP	CA-CB-CG	5.89	126.36	113.40
1	A	221	THR	N-CA-CB	-5.70	99.47	110.30
1	A	218	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	272	ARG	CB-CG-CD	5.49	125.87	111.60
1	A	104	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	258	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	48	ARG	CB-CG-CD	-5.32	97.77	111.60
1	A	251	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	339	SER	N-CA-C	-5.17	97.04	111.00
1	A	26	TRP	CG-CD2-CE3	5.03	138.43	133.90

There are no chirality outliers.

There are no planarity outliers.

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	2465	0	2373	23	0
2	A	28	0	25	1	0
3	A	2	0	0	0	0
4	A	1	0	0	2	0
5	A	43	0	30	0	0
6	A	247	0	0	4	0
All	All	2786	0	2428	23	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 5.

All (23) 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:219:LYS:HE2	1:A:317:ASP:HA	1.75	0.69
1:A:34:GLN:HE21	1:A:34:GLN:HA	1.58	0.68
1:A:86:ILE:HG12	1:A:147:PRO:HB3	1.84	0.58
1:A:210:THR:HG22	6:A:530:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ILE:HG13	1:A:87:GLU:N	2.22	0.53
1:A:301:VAL:HG12	6:A:482:HOH:O	2.09	0.52
1:A:26:TRP:HA	1:A:29:VAL:HG13	1.91	0.52
1:A:217:LEU:HD13	1:A:250:ALA:HB1	1.92	0.51
1:A:219:LYS:HE3	6:A:611:HOH:O	2.10	0.51
1:A:180:LEU:HD13	1:A:276:ALA:HB1	1.92	0.51
1:A:221:THR:HG21	6:A:538:HOH:O	2.11	0.51
1:A:90:PHE:HB3	4:A:702:IOD:I	2.82	0.49
1:A:268:VAL:O	1:A:272:ARG:HG3	2.13	0.49
1:A:32:ASP:OD2	1:A:110:HIS:HE1	1.97	0.47
1:A:138:LEU:HD12	1:A:292:ASP:HA	1.95	0.47
1:A:108:ILE:HD11	2:A:349:NAG:H2	1.97	0.47
1:A:219:LYS:HG3	1:A:317:ASP:O	2.15	0.46
1:A:34:GLN:NE2	1:A:34:GLN:HA	2.29	0.46
1:A:91:PRO:HD2	4:A:702:IOD:I	2.86	0.46
1:A:138:LEU:O	1:A:141:ARG:NH2	2.49	0.45
1:A:29:VAL:HG22	1:A:120:PHE:CE2	2.51	0.45
1:A:221:THR:HG22	1:A:222:THR:OG1	2.18	0.43
1:A:59:ILE:HA	1:A:59:ILE:HD12	1.92	0.42

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	334/344 (97%)	325 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	271/273 (99%)	252 (93%)	19 (7%)	19	10

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	34	GLN
1	A	50	ILE
1	A	85	ASN
1	A	86	ILE
1	A	138	LEU
1	A	180	LEU
1	A	181	LEU
1	A	186	LEU
1	A	192	LEU
1	A	193	ASN
1	A	210	THR
1	A	218	LEU
1	A	221	THR
1	A	234	LEU
1	A	237	PHE
1	A	248	LEU
1	A	283	LEU
1	A	318	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	39	GLN
1	A	70	GLN
1	A	85	ASN
1	A	110	HIS
1	A	128	ASN

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Mol	Chain	Res	Type
1	A	193	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

2 carbohydrates 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	NAG	A	348	1,2	14,14,15	0.69	0	15,19,21	1.21	2 (13%)
2	NAG	A	349	2	14,14,15	0.57	0	15,19,21	1.33	3 (20%)

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	NAG	A	348	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	349	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	349	NAG	C3-C4-C5	-2.29	106.20	110.20
2	A	349	NAG	O4-C4-C5	2.01	114.57	109.24
2	A	348	NAG	C1-O5-C5	2.34	115.22	112.25
2	A	348	NAG	C3-C4-C5	2.42	114.41	110.20
2	A	349	NAG	C6-C5-C4	3.06	120.57	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	349	NAG	1	0

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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
5	HEM	A	345	1	30,50,50	2.98	9 (30%)	24,82,82	2.27	8 (33%)

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
5	HEM	A	345	1	-	0/10/54/54	0/0/8/8

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	345	HEM	C3D-C4D	-7.26	1.42	1.51
5	A	345	HEM	C3B-C4B	-6.64	1.45	1.51
5	A	345	HEM	C2D-C3D	-6.55	1.34	1.54
5	A	345	HEM	C3C-CAC	-6.32	1.39	1.51
5	A	345	HEM	C3B-CAB	-5.66	1.40	1.51
5	A	345	HEM	C2C-C1C	-4.44	1.44	1.52
5	A	345	HEM	C2D-C1D	-2.34	1.44	1.51
5	A	345	HEM	CBC-CAC	2.81	1.45	1.29
5	A	345	HEM	CBB-CAB	2.94	1.46	1.29

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	345	HEM	CAA-C2A-C1A	-3.09	123.65	127.01
5	A	345	HEM	C3C-CAC-CBC	2.16	127.77	124.46
5	A	345	HEM	CMD-C2D-C3D	3.06	127.89	114.35
5	A	345	HEM	CAD-C3D-C4D	3.47	124.72	112.47
5	A	345	HEM	C2D-C3D-C4D	3.84	108.01	101.50
5	A	345	HEM	CMC-C2C-C3C	4.45	127.65	116.53
5	A	345	HEM	CMB-C2B-C3B	4.69	128.23	116.53
5	A	345	HEM	CAD-C3D-C2D	4.85	127.16	113.22

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 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.