Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:19 PM GMT

PDB ID	:	1A88
Title	:	CHLOROPEROXIDASE L
Authors	:	Hofmann, B.; Toelzer, S.; Pelletier, I.; Altenbuchner, J.; Van Pee, K.-H.; Hecht, H.-J.
Deposited on	:	1998-04-03
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

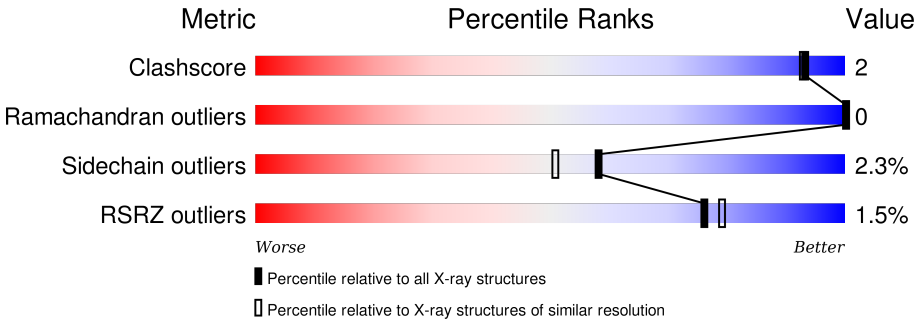
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 <=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.

Mol	Chain	Length	Quality of chain
1	A	275	89% 10%
1	B	275	3% 88% 12%
1	C	275	% 86% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6822 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 CHLOROPEROXIDASE L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2105	1331	366	401	7			
1	B	275	Total	C	N	O	S	0	0	0
			2105	1331	366	401	7			
1	C	275	Total	C	N	O	S	0	0	0
			2105	1331	366	401	7			

- Molecule 2 is water.

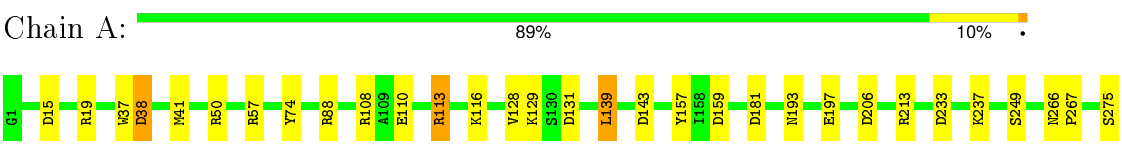
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	169	Total	O	0	0
			169	169		
2	B	154	Total	O	0	0
			154	154		
2	C	184	Total	O	0	0
			184	184		

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 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.

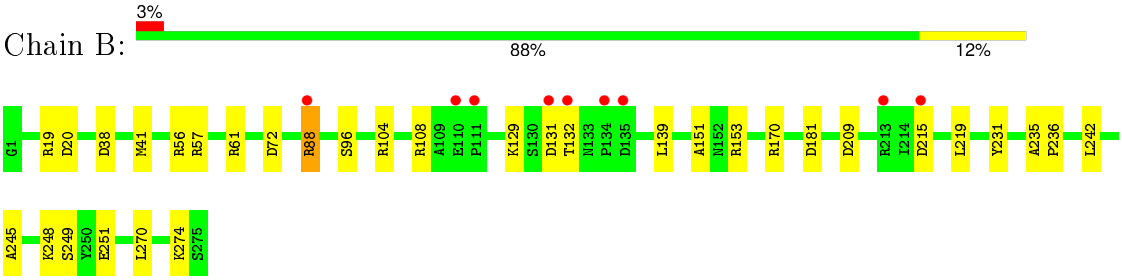
- Molecule 1: CHLOROPEROXIDASE L

Chain A:



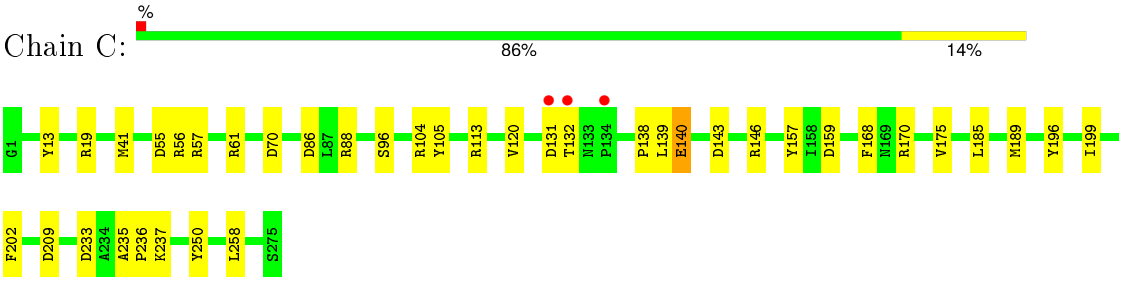
- Molecule 1: CHLOROPEROXIDASE L

Chain B:



- Molecule 1: CHLOROPEROXIDASE L

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	176.50Å 176.50Å 64.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.00 – 1.90 44.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.7 (130.00-1.90) 84.7 (44.12-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.89 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.160 , 0.193 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.8	EDS
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 65934 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6822	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.72	0/2165	1.38	24/2955 (0.8%)
1	B	0.66	0/2165	1.30	21/2955 (0.7%)
1	C	0.75	0/2165	1.40	29/2955 (1.0%)
All	All	0.71	0/6495	1.36	74/8865 (0.8%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	88	ARG	CD-NE-CZ	11.00	139.00	123.60
1	C	104	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	B	57	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	113	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	C	86	ASP	CB-CG-OD1	9.31	126.68	118.30
1	B	56	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	170	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	C	19	ARG	NE-CZ-NH1	-8.67	115.97	120.30
1	B	61	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	153	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	C	41	MET	CA-CB-CG	-8.29	99.20	113.30
1	B	88	ARG	CD-NE-CZ	8.25	135.15	123.60
1	A	113	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	C	70	ASP	CB-CG-OD1	8.03	125.53	118.30
1	C	196	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	88	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	213	ARG	CD-NE-CZ	7.20	133.68	123.60
1	C	157	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	B	41	MET	CA-CB-CG	-7.00	101.40	113.30
1	A	157	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	A	213	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	108	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	C	170	ARG	NE-CZ-NH2	6.79	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	19	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	C	105	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	A	108	ARG	CD-NE-CZ	6.61	132.85	123.60
1	A	206	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	56	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	C	143	ASP	CB-CG-OD1	6.55	124.19	118.30
1	C	250	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	C	146	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	143	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	70	ASP	OD1-CG-OD2	-6.48	110.98	123.30
1	A	181	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	56	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	C	105	TYR	CB-CG-CD1	6.21	124.73	121.00
1	B	153	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	181	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	41	MET	CA-CB-CG	-6.03	103.05	113.30
1	C	113	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	96	SER	N-CA-CB	-5.96	101.56	110.50
1	B	20	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	19	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	213	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	15	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	38	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	C	159	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	C	96	SER	N-CA-CB	-5.68	101.98	110.50
1	B	151	ALA	CB-CA-C	-5.67	101.59	110.10
1	B	61	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	143	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	C	57	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	209	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	70	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	57	ARG	CD-NE-CZ	5.58	131.42	123.60
1	B	88	ARG	CG-CD-NE	5.56	123.48	111.80
1	C	55	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	88	ARG	CD-NE-CZ	5.42	131.19	123.60
1	C	61	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	157	TYR	CB-CG-CD1	5.36	124.22	121.00
1	C	170	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	88	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	74	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	143	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	C	13	TYR	CB-CG-CD1	5.21	124.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	B	72	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	170	ARG	NH1-CZ-NH2	5.15	125.07	119.40
1	B	38	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	C	250	TYR	CB-CG-CD1	5.09	124.05	121.00
1	C	209	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	131	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	159	ASP	CB-CG-OD2	-5.02	113.78	118.30

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	2105	0	1998	8	0
1	B	2105	0	1998	6	0
1	C	2105	0	1998	9	0
2	A	169	0	0	0	0
2	B	154	0	0	1	0
2	C	184	0	0	0	0
All	All	6822	0	5994	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 2.

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:C:233:ASP:HA	1:C:237:LYS:NZ	2.04	0.72
1:B:235:ALA:HB3	1:B:236:PRO:HD3	1.72	0.70
1:C:233:ASP:HA	1:C:237:LYS:HZ3	1.63	0.63
1:A:128:VAL:HG21	1:A:139:LEU:HD23	1.81	0.62
1:C:138:PRO:HB2	1:C:140:GLU:HG2	1.92	0.50
1:B:219:LEU:HD11	1:B:248:LYS:HG3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:O	1:A:139:LEU:HD13	2.13	0.49
1:B:231:TYR:HH	1:B:249:SER:HG	1.61	0.48
1:B:270:LEU:HG	1:B:274:LYS:HD2	1.96	0.47
1:B:242:LEU:HB2	1:B:245:ALA:HB2	1.99	0.45
1:C:233:ASP:HA	1:C:237:LYS:HZ2	1.80	0.45
1:A:193:ASN:O	1:A:197:GLU:HG3	2.17	0.44
1:C:185:LEU:O	1:C:189:MET:HG2	2.17	0.44
1:C:235:ALA:HB3	1:C:236:PRO:HD3	2.00	0.44
1:B:251:GLU:HG3	2:B:411:HOH:O	2.18	0.43
1:A:110:GLU:HB2	1:A:113:ARG:HG3	2.00	0.43
1:A:233:ASP:HA	1:A:237:LYS:HD2	2.00	0.42
1:A:116:LYS:NZ	1:A:275:SER:OG	2.52	0.42
1:A:266:ASN:N	1:A:267:PRO:CD	2.84	0.41
1:C:120:VAL:HG11	1:C:258:LEU:HD11	2.02	0.41
1:A:37:TRP:O	1:A:38:ASP:C	2.57	0.41
1:C:199:ILE:HA	1:C:202:PHE:CE2	2.57	0.40
1:C:168:PHE:HB3	1:C:175:VAL:HG22	2.03	0.40

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	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
1	B	273/275 (99%)	260 (95%)	13 (5%)	0	100	100
1	C	273/275 (99%)	262 (96%)	11 (4%)	0	100	100
All	All	819/825 (99%)	785 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	217/217 (100%)	214 (99%)	3 (1%)	74	71
1	B	217/217 (100%)	209 (96%)	8 (4%)	41	29
1	C	217/217 (100%)	213 (98%)	4 (2%)	66	61
All	All	651/651 (100%)	636 (98%)	15 (2%)	58	51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	139	LEU
1	A	249	SER
1	B	88	ARG
1	B	104	ARG
1	B	108	ARG
1	B	129	LYS
1	B	131	ASP
1	B	132	THR
1	B	139	LEU
1	B	215	ASP
1	C	131	ASP
1	C	132	THR
1	C	139	LEU
1	C	140	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	ASN
1	C	10	ASN
1	C	133	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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(Å^2)	Q<0.9
1	A	275/275 (100%)	-0.60	0 100 100	8, 18, 38, 52	0
1	B	275/275 (100%)	-0.33	9 (3%) 50 53	10, 23, 44, 60	0
1	C	275/275 (100%)	-0.52	3 (1%) 82 84	8, 18, 38, 59	0
All	All	825/825 (100%)	-0.48	12 (1%) 76 79	8, 19, 40, 60	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	ASP	5.5
1	B	131	ASP	4.7
1	B	132	THR	2.6
1	B	135	ASP	2.6
1	B	134	PRO	2.5
1	B	213	ARG	2.5
1	B	215	ASP	2.4
1	C	132	THR	2.4
1	B	111	PRO	2.3
1	B	88	ARG	2.1
1	B	110	GLU	2.1
1	C	134	PRO	2.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.