



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2014 – 04:33 PM EDT

PDB ID : 3PIM
Title : Crystal structure of Mxr1 from *Saccharomyces cerevisiae* in unusual oxidized form
Authors : Ma, X.X.; Guo, P.C.; Shi, W.W.; Luo, M.; Tan, X.F.; Chen, Y.; Zhou, C.Z.
Deposited on : 2010-11-07
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>

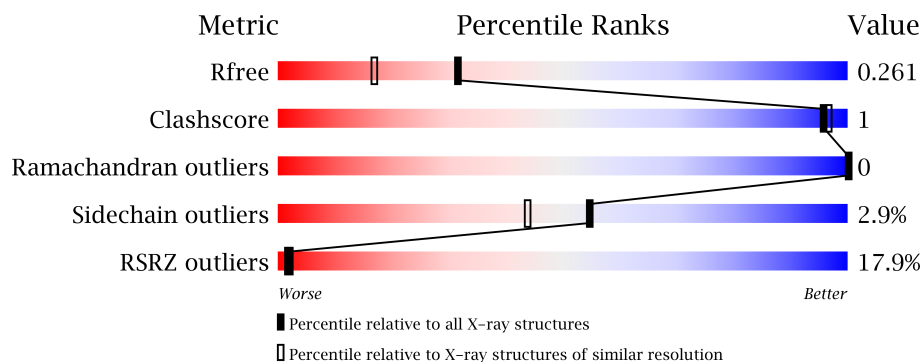
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
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) : stable22978

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))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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.

Mol	Chain	Length	Quality of chain
1	A	187	
1	B	187	
1	C	187	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4421 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 Peptide methionine sulfoxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1414	901	240	266	7			
1	B	177	Total	C	N	O	S	0	0	0
			1443	919	246	271	7			
1	C	163	Total	C	N	O	S	0	0	0
			1330	851	219	253	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	EXPRESSION TAG	UNP P40029
A	-1	HIS	-	EXPRESSION TAG	UNP P40029
A	0	HIS	-	EXPRESSION TAG	UNP P40029
A	1	GLY	-	EXPRESSION TAG	UNP P40029
B	-2	HIS	-	EXPRESSION TAG	UNP P40029
B	-1	HIS	-	EXPRESSION TAG	UNP P40029
B	0	HIS	-	EXPRESSION TAG	UNP P40029
B	1	GLY	-	EXPRESSION TAG	UNP P40029
C	-2	HIS	-	EXPRESSION TAG	UNP P40029
C	-1	HIS	-	EXPRESSION TAG	UNP P40029
C	0	HIS	-	EXPRESSION TAG	UNP P40029
C	1	GLY	-	EXPRESSION TAG	UNP P40029

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	102	Total	O	0	0
			102	102		
2	B	119	Total	O	0	0
			119	119		
2	C	13	Total	O	0	0
			13	13		

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.

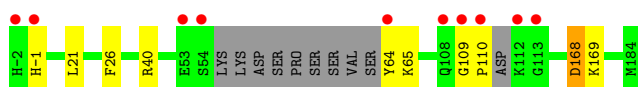
- Molecule 1: Peptide methionine sulfoxide reductase

Chain A: 



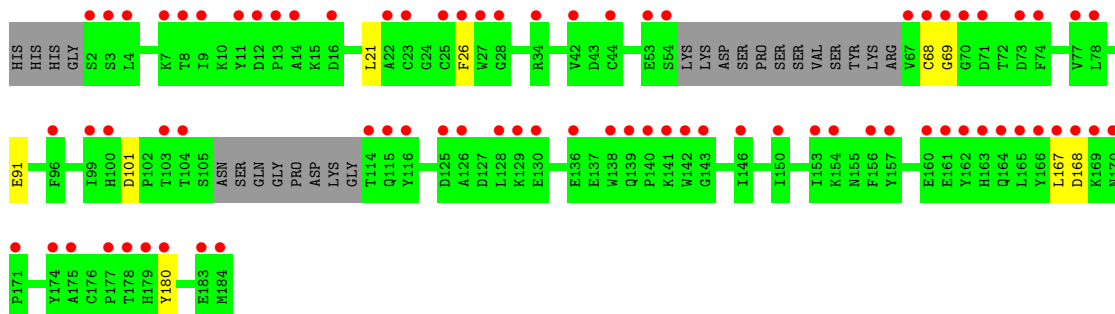
- Molecule 1: Peptide methionine sulfoxide reductase

Chain B: 



- Molecule 1: Peptide methionine sulfoxide reductase

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.89Å 111.89Å 108.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 38.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-1.90) 95.3 (38.88-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.236 , 0.264 0.237 , 0.261	Depositor DCC
R_{free} test set	2999 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.3	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58924 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4421	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.39 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1157e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.59	0/1451	0.62	0/1958
1	B	0.61	0/1481	0.64	0/1998
1	C	0.36	0/1363	0.52	1/1841 (0.1%)
All	All	0.53	0/4295	0.60	1/5797 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1414	0	0	0	0
1	B	1443	0	0	4	0
1	C	1330	0	0	2	0
2	A	102	0	0	0	0
2	B	119	0	0	0	0
2	C	13	0	0	0	0
All	All	4421	0	0	5	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 1.

All (5) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:168:ASP:CG	1:B:169:LYS:N	2.32	0.82
1:B:168:ASP:OD2	1:B:169:LYS:N	2.23	0.72
1:B:109:GLY:N	1:B:110:PRO:CD	2.74	0.50
1:B:40:ARG:NH2	1:C:91:GLU:CD	2.66	0.48
1:C:68:CYS:N	1:C:69:GLY:CA	2.83	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	167/187 (89%)	165 (99%)	2 (1%)	0	100	100
1	B	171/187 (91%)	166 (97%)	5 (3%)	0	100	100
1	C	157/187 (84%)	147 (94%)	10 (6%)	0	100	100
All	All	495/561 (88%)	478 (97%)	17 (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	152/165 (92%)	150 (99%)	2 (1%)	80	77
1	B	155/165 (94%)	149 (96%)	6 (4%)	43	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	144/165 (87%)	139 (96%)	5 (4%)	48	34
All	All	451/495 (91%)	438 (97%)	13 (3%)	55	44

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	53	GLU
1	B	-1	HIS
1	B	21	LEU
1	B	26	PHE
1	B	64	TYR
1	B	65	LYS
1	B	168	ASP
1	C	21	LEU
1	C	26	PHE
1	C	101	ASP
1	C	168	ASP
1	C	180	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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, 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(Å ²)	Q<0.9
1	A	173/187 (92%)	0.14	5 (2%) 49 50	12, 21, 34, 48	0
1	B	177/187 (94%)	0.35	10 (5%) 24 24	11, 19, 39, 48	0
1	C	163/187 (87%)	2.41	77 (47%) 1 0	54, 80, 112, 125	0
All	All	513/561 (91%)	0.93	92 (17%) 2 2	11, 24, 102, 125	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	GLY	15.7
1	C	116	TYR	8.2
1	C	165	LEU	8.1
1	C	54	SER	7.5
1	B	64	TYR	7.1
1	C	180	TYR	7.1
1	C	168	ASP	6.9
1	B	54	SER	6.2
1	C	143	GLY	6.0
1	C	69	GLY	6.0
1	C	178	THR	5.9
1	C	14	ALA	5.7
1	C	167	LEU	5.6
1	C	8	THR	5.4
1	C	164	GLN	5.3
1	C	183	GLU	5.2
1	B	113	GLY	5.1
1	B	-1	HIS	5.1
1	C	157	TYR	4.9
1	C	34	ARG	4.9
1	C	74	PHE	4.8
1	C	27	TRP	4.7
1	C	7	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	136	GLU	4.5
1	C	166	TYR	4.5
1	A	-1	HIS	4.4
1	A	-2	HIS	4.4
1	C	140	PRO	4.4
1	C	9	ILE	4.4
1	C	170	ASN	4.3
1	C	53	GLU	3.9
1	C	12	ASP	3.9
1	C	142	TRP	3.8
1	C	68	CYS	3.8
1	B	-2	HIS	3.8
1	B	108	GLN	3.7
1	C	73	ASP	3.6
1	C	169	LYS	3.6
1	C	16	ASP	3.5
1	C	44	CYS	3.5
1	C	99	ILE	3.4
1	C	154	LYS	3.4
1	C	104	THR	3.4
1	C	103	THR	3.3
1	C	77	VAL	3.2
1	C	162	TYR	3.1
1	C	2	SER	3.1
1	A	105	SER	3.1
1	C	114	THR	3.0
1	C	160	GLU	3.0
1	C	126	ALA	3.0
1	C	175	ALA	3.0
1	C	13	PRO	3.0
1	C	67	VAL	3.0
1	C	115	GLN	2.9
1	C	179	HIS	2.9
1	C	125	ASP	2.9
1	A	107	SER	2.8
1	C	42	VAL	2.8
1	C	177	PRO	2.8
1	C	138	TRP	2.8
1	B	110	PRO	2.7
1	C	71	ASP	2.7
1	C	139	GLN	2.7
1	C	174	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	78	LEU	2.6
1	C	141	LYS	2.6
1	C	171	PRO	2.5
1	B	53	GLU	2.5
1	C	156	PHE	2.5
1	C	4	LEU	2.5
1	C	146	ILE	2.4
1	C	150	ILE	2.4
1	C	129	LYS	2.4
1	C	163	HIS	2.4
1	C	22	ALA	2.4
1	C	26	PHE	2.4
1	C	11	TYR	2.3
1	C	184	MET	2.3
1	C	23	CYS	2.3
1	C	25	CYS	2.3
1	C	153	ILE	2.3
1	C	3	SER	2.2
1	C	130	GLU	2.2
1	C	28	GLY	2.2
1	A	164	GLN	2.2
1	C	128	LEU	2.1
1	C	96	PHE	2.1
1	B	109	GLY	2.1
1	C	161	GLU	2.0
1	C	100	HIS	2.0
1	B	112	LYS	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.