WORLD WIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2024 – 10:06 AM EST

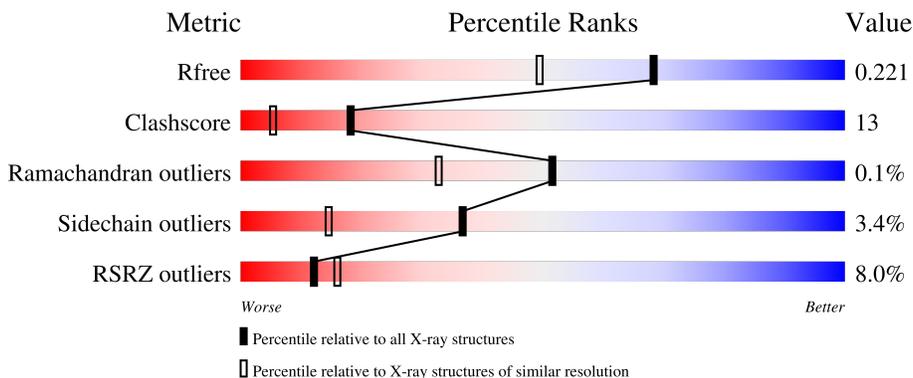|		
PDB ID	:	3U49
Title	:	Crystal structure of YwfH, NADPH dependent reductase involved in Bacilysin biosynthesis
Authors	:	Rajavel, M.; Gopal, B.
Deposited on	:	2011-10-07
Resolution	:	1.75 Å(reported)

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 1.75 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		0.221
Clashscore		13
Ramachandran outliers		0.1%
Sidechain outliers		3.4%
RSRZ outliers		8.0%

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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	281	6% / 75% 11% · 11%
1	B	281	7% / 72% 15% · 11%
1	C	281	9% / 70% 17% · 10%
1	D	281	6% / 74% 11% · 14%

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2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8008 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 Bacilysin biosynthesis oxidoreductase ywfH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1881	1174	330	364	13			
1	B	251	Total	C	N	O	S	0	4	0
			1941	1209	342	377	13			
1	C	252	Total	C	N	O	S	0	1	0
			1907	1186	338	370	13			
1	D	242	Total	C	N	O	S	0	4	0
			1869	1160	332	364	13			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P39644
A	-18	GLY	-	expression tag	UNP P39644
A	-17	SER	-	expression tag	UNP P39644
A	-16	SER	-	expression tag	UNP P39644
A	-15	HIS	-	expression tag	UNP P39644
A	-14	HIS	-	expression tag	UNP P39644
A	-13	HIS	-	expression tag	UNP P39644
A	-12	HIS	-	expression tag	UNP P39644
A	-11	HIS	-	expression tag	UNP P39644
A	-10	HIS	-	expression tag	UNP P39644
A	-9	SER	-	expression tag	UNP P39644
A	-8	SER	-	expression tag	UNP P39644
A	-7	GLY	-	expression tag	UNP P39644
A	-6	LEU	-	expression tag	UNP P39644
A	-5	VAL	-	expression tag	UNP P39644
A	-4	PRO	-	expression tag	UNP P39644
A	-3	ARG	-	expression tag	UNP P39644
A	-2	GLY	-	expression tag	UNP P39644
A	-1	SER	-	expression tag	UNP P39644
A	0	HIS	-	expression tag	UNP P39644
A	260	LEU	-	cloning artifact	UNP P39644

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Chain	Residue	Modelled	Actual	Comment	Reference
A	261	GLU	-	cloning artifact	UNP P39644
B	-19	MET	-	expression tag	UNP P39644
B	-18	GLY	-	expression tag	UNP P39644
B	-17	SER	-	expression tag	UNP P39644
B	-16	SER	-	expression tag	UNP P39644
B	-15	HIS	-	expression tag	UNP P39644
B	-14	HIS	-	expression tag	UNP P39644
B	-13	HIS	-	expression tag	UNP P39644
B	-12	HIS	-	expression tag	UNP P39644
B	-11	HIS	-	expression tag	UNP P39644
B	-10	HIS	-	expression tag	UNP P39644
B	-9	SER	-	expression tag	UNP P39644
B	-8	SER	-	expression tag	UNP P39644
B	-7	GLY	-	expression tag	UNP P39644
B	-6	LEU	-	expression tag	UNP P39644
B	-5	VAL	-	expression tag	UNP P39644
B	-4	PRO	-	expression tag	UNP P39644
B	-3	ARG	-	expression tag	UNP P39644
B	-2	GLY	-	expression tag	UNP P39644
B	-1	SER	-	expression tag	UNP P39644
B	0	HIS	-	expression tag	UNP P39644
B	260	LEU	-	cloning artifact	UNP P39644
B	261	GLU	-	cloning artifact	UNP P39644
C	-19	MET	-	expression tag	UNP P39644
C	-18	GLY	-	expression tag	UNP P39644
C	-17	SER	-	expression tag	UNP P39644
C	-16	SER	-	expression tag	UNP P39644
C	-15	HIS	-	expression tag	UNP P39644
C	-14	HIS	-	expression tag	UNP P39644
C	-13	HIS	-	expression tag	UNP P39644
C	-12	HIS	-	expression tag	UNP P39644
C	-11	HIS	-	expression tag	UNP P39644
C	-10	HIS	-	expression tag	UNP P39644
C	-9	SER	-	expression tag	UNP P39644
C	-8	SER	-	expression tag	UNP P39644
C	-7	GLY	-	expression tag	UNP P39644
C	-6	LEU	-	expression tag	UNP P39644
C	-5	VAL	-	expression tag	UNP P39644
C	-4	PRO	-	expression tag	UNP P39644
C	-3	ARG	-	expression tag	UNP P39644
C	-2	GLY	-	expression tag	UNP P39644
C	-1	SER	-	expression tag	UNP P39644

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP P39644
C	260	LEU	-	cloning artifact	UNP P39644
C	261	GLU	-	cloning artifact	UNP P39644
D	-19	MET	-	expression tag	UNP P39644
D	-18	GLY	-	expression tag	UNP P39644
D	-17	SER	-	expression tag	UNP P39644
D	-16	SER	-	expression tag	UNP P39644
D	-15	HIS	-	expression tag	UNP P39644
D	-14	HIS	-	expression tag	UNP P39644
D	-13	HIS	-	expression tag	UNP P39644
D	-12	HIS	-	expression tag	UNP P39644
D	-11	HIS	-	expression tag	UNP P39644
D	-10	HIS	-	expression tag	UNP P39644
D	-9	SER	-	expression tag	UNP P39644
D	-8	SER	-	expression tag	UNP P39644
D	-7	GLY	-	expression tag	UNP P39644
D	-6	LEU	-	expression tag	UNP P39644
D	-5	VAL	-	expression tag	UNP P39644
D	-4	PRO	-	expression tag	UNP P39644
D	-3	ARG	-	expression tag	UNP P39644
D	-2	GLY	-	expression tag	UNP P39644
D	-1	SER	-	expression tag	UNP P39644
D	0	HIS	-	expression tag	UNP P39644
D	260	LEU	-	cloning artifact	UNP P39644
D	261	GLU	-	cloning artifact	UNP P39644

- Molecule 2 is water.

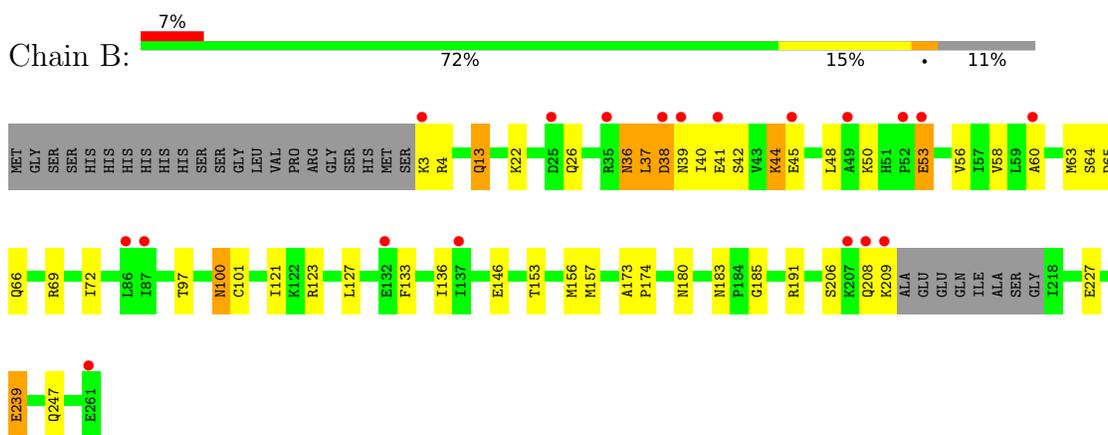| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total 122	O 122	0	0
2	B	77	Total 77	O 77	0	0
2	C	90	Total 90	O 90	0	0
2	D	121	Total 121	O 121	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.
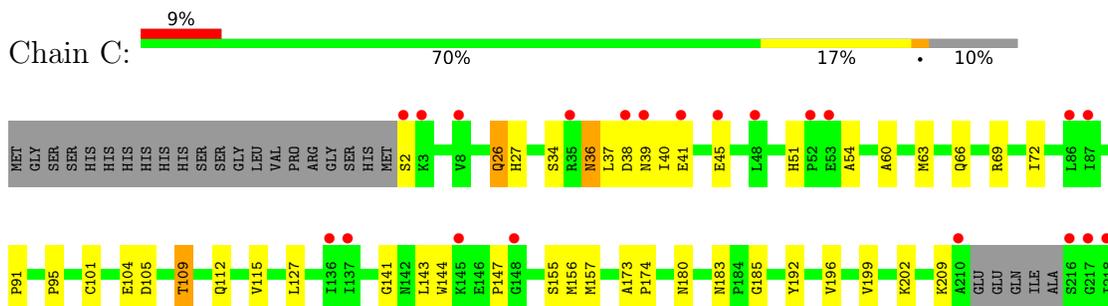
• Molecule 1: Bacilysin biosynthesis oxidoreductase ywfH
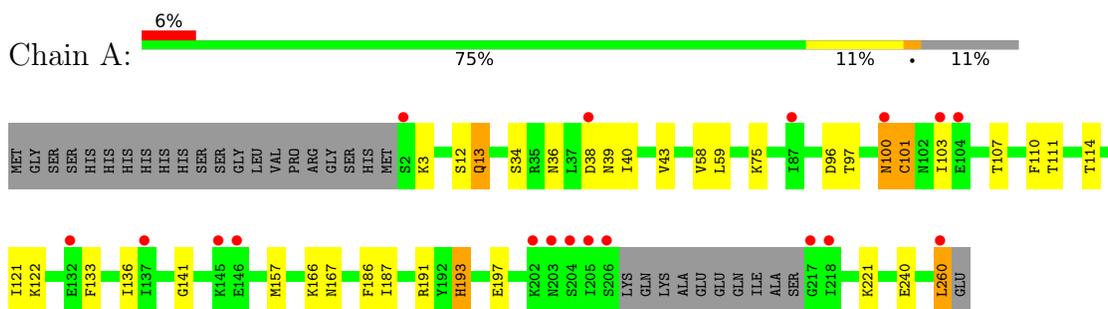
Chain A:

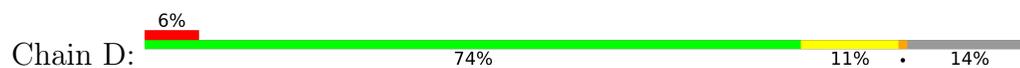• Molecule 1: Bacilysin biosynthesis oxidoreductase ywfH

Chain B:

• Molecule 1: Bacilysin biosynthesis oxidoreductase ywfH

Chain C:

• Molecule 1: Bacilysin biosynthesis oxidoreductase ywfH

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.85Å 136.99Å 66.70Å 90.00° 117.99° 90.00°	Depositor
Resolution (Å)	68.50 – 1.75 31.55 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (68.50-1.75) 99.0 (31.55-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.222 0.188 , 0.221	Depositor DCC
R_{free} test set	5116 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.014 for h,-k,-h-l 0.015 for -h-l,-k,l 0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8008	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.54	0/1906	0.52	0/2570
1	B	0.46	1/1966 (0.1%)	0.54	0/2649
1	C	0.54	0/1932	0.56	0/2603
1	D	0.48	0/1893	0.53	0/2550
All	All	0.51	1/7697 (0.0%)	0.54	0/10372

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	SER	CB-OG	-5.88	1.34	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1881	0	1891	39	0
1	B	1941	0	1945	56	0
1	C	1907	0	1906	68	0
1	D	1869	0	1861	49	0
2	A	122	0	0	4	0
2	B	77	0	0	3	0
2	C	90	0	0	5	0
2	D	121	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8008	0	7603	204	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 13.

The worst 5 of 204 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:95:PRO:HG2	1:C:199:VAL:HG21	1.21	1.16
1:C:63:MET:HE1	1:C:72:ILE:HG13	1.26	1.08
1:D:100:ASN:C	1:D:100:ASN:HD22	1.65	1.00
1:A:100:ASN:C	1:A:100:ASN:HD22	1.67	0.96
1:A:187:ILE:H	1:A:193:HIS:HD2	1.03	0.96

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	245/281 (87%)	241 (98%)	4 (2%)	0	100	100
1	B	251/281 (89%)	242 (96%)	8 (3%)	1 (0%)	34	17
1	C	249/281 (89%)	243 (98%)	6 (2%)	0	100	100
1	D	242/281 (86%)	236 (98%)	6 (2%)	0	100	100
All	All	987/1124 (88%)	962 (98%)	24 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	38	ASP

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	204/231 (88%)	199 (98%)	5 (2%)	47	25
1	B	211/231 (91%)	201 (95%)	10 (5%)	26	7
1	C	205/231 (89%)	195 (95%)	10 (5%)	25	7
1	D	202/231 (87%)	198 (98%)	4 (2%)	55	34
All	All	822/924 (89%)	793 (96%)	29 (4%)	37	13

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239[B]	GLU
1	D	127	LEU
1	C	66	GLN
1	C	257	LYS
1	C	36	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	171	GLN
1	D	167	ASN
1	C	180	ASN
1	D	66	GLN
1	D	203	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 monosaccharides 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	249/281 (88%)	0.31	18 (7%)	15	20	13, 23, 47, 69	0
1	B	251/281 (89%)	0.51	19 (7%)	13	18	13, 29, 63, 73	0
1	C	252/281 (89%)	0.53	26 (10%)	6	9	14, 25, 55, 82	0
1	D	242/281 (86%)	0.41	17 (7%)	16	21	12, 21, 50, 74	0
All	All	994/1124 (88%)	0.44	80 (8%)	12	16	12, 24, 55, 82	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	258	SER	9.4
1	D	256	MET	8.5
1	C	216	SER	8.0
1	C	217	GLY	7.8
1	A	2	SER	6.9

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

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6.5 Other polymers ⓘ

There are no such residues in this entry.