



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:30 pm GMT

PDB ID : 3N74
Title : Crystal structure of 3-ketoacyl-(acyl-carrier-protein) reductase from *Brucella melitensis*
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2010-05-26
Resolution : 2.20 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

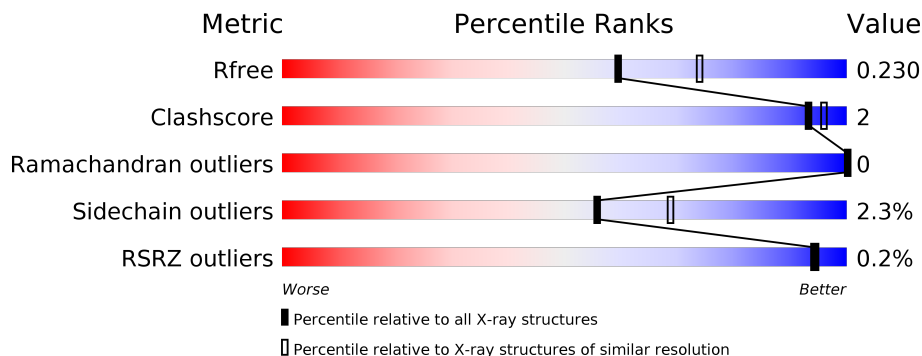
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	
1	C	261	
1	D	261	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7154 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 3-ketoacyl-(acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1617	1022	282	307	6			
1	B	227	Total	C	N	O	S	0	4	0
			1642	1037	285	314	6			
1	C	235	Total	C	N	O	S	0	1	0
			1683	1061	293	322	7			
1	D	227	Total	C	N	O	S	0	0	0
			1619	1024	280	309	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q2YJS1
A	-2	PRO	-	EXPRESSION TAG	UNP Q2YJS1
A	-1	GLY	-	EXPRESSION TAG	UNP Q2YJS1
A	0	SER	-	EXPRESSION TAG	UNP Q2YJS1
A	120	SER	ARG	ENGINEERED MUTATION	UNP Q2YJS1
A	253	GLY	-	EXPRESSION TAG	UNP Q2YJS1
A	254	GLY	-	EXPRESSION TAG	UNP Q2YJS1
A	255	ARG	-	EXPRESSION TAG	UNP Q2YJS1
A	256	SER	-	EXPRESSION TAG	UNP Q2YJS1
A	257	ILE	-	EXPRESSION TAG	UNP Q2YJS1
B	-3	GLY	-	EXPRESSION TAG	UNP Q2YJS1
B	-2	PRO	-	EXPRESSION TAG	UNP Q2YJS1
B	-1	GLY	-	EXPRESSION TAG	UNP Q2YJS1
B	0	SER	-	EXPRESSION TAG	UNP Q2YJS1
B	120	SER	ARG	ENGINEERED MUTATION	UNP Q2YJS1
B	253	GLY	-	EXPRESSION TAG	UNP Q2YJS1
B	254	GLY	-	EXPRESSION TAG	UNP Q2YJS1
B	255	ARG	-	EXPRESSION TAG	UNP Q2YJS1
B	256	SER	-	EXPRESSION TAG	UNP Q2YJS1
B	257	ILE	-	EXPRESSION TAG	UNP Q2YJS1
C	-3	GLY	-	EXPRESSION TAG	UNP Q2YJS1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PRO	-	EXPRESSION TAG	UNP Q2YJS1
C	-1	GLY	-	EXPRESSION TAG	UNP Q2YJS1
C	0	SER	-	EXPRESSION TAG	UNP Q2YJS1
C	120	SER	ARG	ENGINEERED MUTATION	UNP Q2YJS1
C	253	GLY	-	EXPRESSION TAG	UNP Q2YJS1
C	254	GLY	-	EXPRESSION TAG	UNP Q2YJS1
C	255	ARG	-	EXPRESSION TAG	UNP Q2YJS1
C	256	SER	-	EXPRESSION TAG	UNP Q2YJS1
C	257	ILE	-	EXPRESSION TAG	UNP Q2YJS1
D	-3	GLY	-	EXPRESSION TAG	UNP Q2YJS1
D	-2	PRO	-	EXPRESSION TAG	UNP Q2YJS1
D	-1	GLY	-	EXPRESSION TAG	UNP Q2YJS1
D	0	SER	-	EXPRESSION TAG	UNP Q2YJS1
D	120	SER	ARG	ENGINEERED MUTATION	UNP Q2YJS1
D	253	GLY	-	EXPRESSION TAG	UNP Q2YJS1
D	254	GLY	-	EXPRESSION TAG	UNP Q2YJS1
D	255	ARG	-	EXPRESSION TAG	UNP Q2YJS1
D	256	SER	-	EXPRESSION TAG	UNP Q2YJS1
D	257	ILE	-	EXPRESSION TAG	UNP Q2YJS1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	150	Total O 150 150	0	0
2	B	159	Total O 159 159	0	0
2	C	153	Total O 153 153	0	0
2	D	131	Total O 131 131	0	0

- Molecule 1: 3-ketoacyl-(acyl-carrier-protein) reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.52Å 96.50Å 130.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 45.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.20) 99.5 (45.25-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.68 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.170 , 0.230 0.171 , 0.230	Depositor DCC
R_{free} test set	2301 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7154	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.64	0/1639	0.64	0/2224
1	B	0.63	0/1676	0.65	0/2274
1	C	0.67	0/1708	0.66	0/2314
1	D	0.64	0/1641	0.63	0/2226
All	All	0.64	0/6664	0.65	0/9038

There are no bond length outliers.

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	1617	0	1638	9	0
1	B	1642	0	1662	3	0
1	C	1683	0	1696	4	0
1	D	1619	0	1642	8	0
2	A	150	0	0	0	0
2	B	159	0	0	1	0
2	C	153	0	0	0	0
2	D	131	0	0	1	0
All	All	7154	0	6638	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:D:79:LYS:HE3	2:D:263:HOH:O	1.94	0.66
1:A:117:LEU:O	1:A:121:LYS:HG2	1.98	0.63
1:C:37:ARG:HD2	1:C:59:ASP:HB2	1.81	0.62
1:A:187:VAL:HG21	1:A:250:ARG:HD3	1.80	0.62
1:A:112:VAL:HG13	1:A:162:TRP:CE2	2.40	0.57
1:D:79:LYS:HE2	1:D:81:ASP:OD2	2.11	0.50
1:A:142:ALA:HA	1:A:160:LYS:HD2	1.95	0.48
1:B:139:LEU:HD11	1:B:184:LEU:HG	1.96	0.46
1:D:5:GLY:O	1:D:79:LYS:NZ	2.50	0.45
1:A:2:SER:OG	1:A:235:GLN:OE1	2.37	0.43
1:C:119:THR:O	1:C:123:ILE:HG13	2.19	0.42
1:D:143:SER:HB3	1:D:160:LYS:HG3	2.01	0.42
1:B:160:LYS:HD3	1:B:160:LYS:HA	1.84	0.41
1:C:151:PRO:O	1:C:152:ASN:HB2	2.21	0.41
1:D:144:THR:HB	1:D:251:SER:OG	2.19	0.41
1:C:142:ALA:HB3	1:C:185:ASN:OD1	2.21	0.41
1:A:172:ILE:HB	1:D:252:ILE:HG21	2.02	0.41
1:D:142:ALA:HB3	1:D:185:ASN:OD1	2.21	0.41
1:B:31:LYS:HE3	2:B:317:HOH:O	2.21	0.41
1:A:11:THR:O	1:A:86:ASN:HB3	2.21	0.41
1:D:92:LYS:O	1:D:93:PRO:C	2.57	0.41
1:A:213:ILE:HG12	1:A:250:ARG:HD2	2.03	0.41
1:A:151:PRO:O	1:A:152:ASN:HB2	2.20	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	223/261 (85%)	218 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	227/261 (87%)	221 (97%)	6 (3%)	0	100	100
1	C	230/261 (88%)	223 (97%)	7 (3%)	0	100	100
1	D	223/261 (85%)	214 (96%)	9 (4%)	0	100	100
All	All	903/1044 (86%)	876 (97%)	27 (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	159/193 (82%)	156 (98%)	3 (2%)	62	76
1	B	163/193 (84%)	158 (97%)	5 (3%)	45	57
1	C	167/193 (86%)	162 (97%)	5 (3%)	46	58
1	D	160/193 (83%)	157 (98%)	3 (2%)	62	76
All	All	649/772 (84%)	633 (98%)	16 (2%)	56	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	71	GLU
1	A	166	VAL
1	B	2	SER
1	B	37	ARG
1	B	71[A]	GLU
1	B	71[B]	GLU
1	B	166	VAL
1	C	2	SER
1	C	106	ARG
1	C	166	VAL
1	C	187	VAL
1	C	218	LEU

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Mol	Chain	Res	Type
1	D	79	LYS
1	D	166	VAL
1	D	222	ASP

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	227/261 (86%)	-0.79	0 100 100	9, 16, 26, 35	0
1	B	227/261 (86%)	-0.77	0 100 100	8, 15, 25, 36	0
1	C	235/261 (90%)	-0.71	2 (0%) 84 83	7, 15, 37, 53	0
1	D	227/261 (86%)	-0.77	0 100 100	8, 14, 26, 36	0
All	All	916/1044 (87%)	-0.76	2 (0%) 94 94	7, 15, 28, 53	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	202	SER	2.4
1	C	213	ILE	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.