wwPDB X-ray Structure Validation Summary Report (i)

Mar 14, 2018 – 10:56 am GMT

PDB ID	:	3V1U
Title	:	Crystal structure of a beta-ketoacyl reductase FabG4 from Mycobacterium tuberculosis H37Rv complexed with NAD+ and Hexanoyl-CoA at 2.5 Angstrom resolution
Authors	:	Dutta, D.; Bhattacharyya, S.; Das, A.K.
Deposited on	:	2011-12-10
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

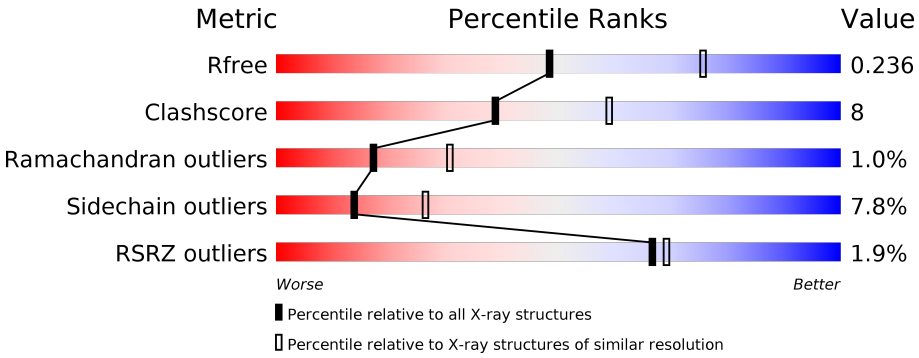
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

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 2.50 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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	462	2% 73% 14% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3224 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.

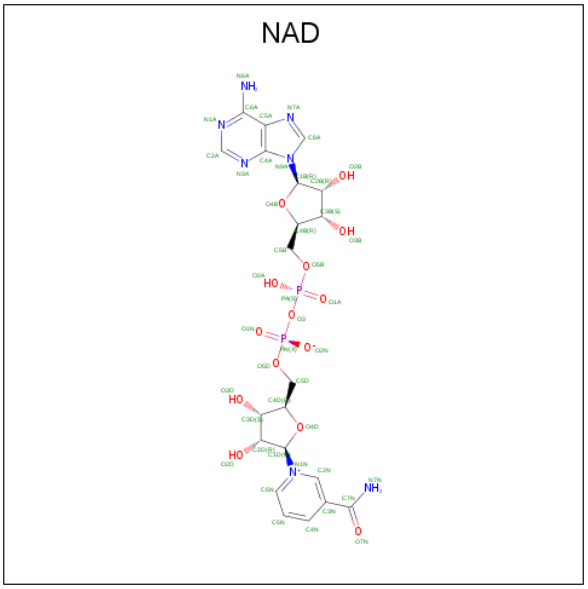
- Molecule 1 is a protein called 3-oxoacyl-(Acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	416	2994	1870	536	581	7	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

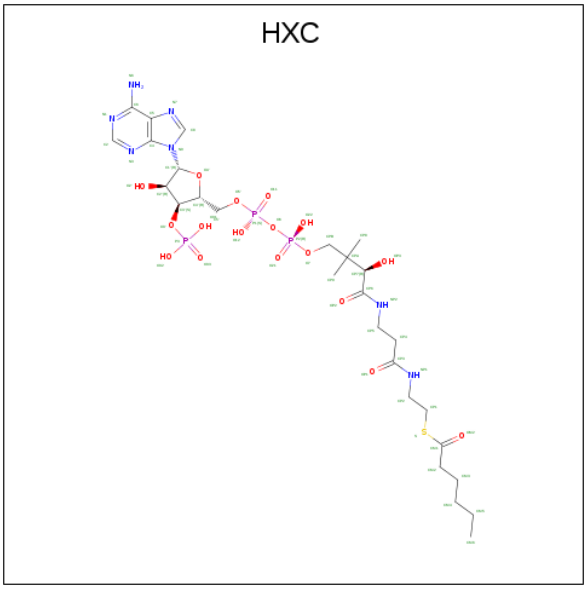
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	EXPRESSION TAG	UNP O53665
A	-6	HIS	-	EXPRESSION TAG	UNP O53665
A	-5	HIS	-	EXPRESSION TAG	UNP O53665
A	-4	HIS	-	EXPRESSION TAG	UNP O53665
A	-3	HIS	-	EXPRESSION TAG	UNP O53665
A	-2	HIS	-	EXPRESSION TAG	UNP O53665
A	-1	GLY	-	EXPRESSION TAG	UNP O53665
A	0	SER	-	EXPRESSION TAG	UNP O53665

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



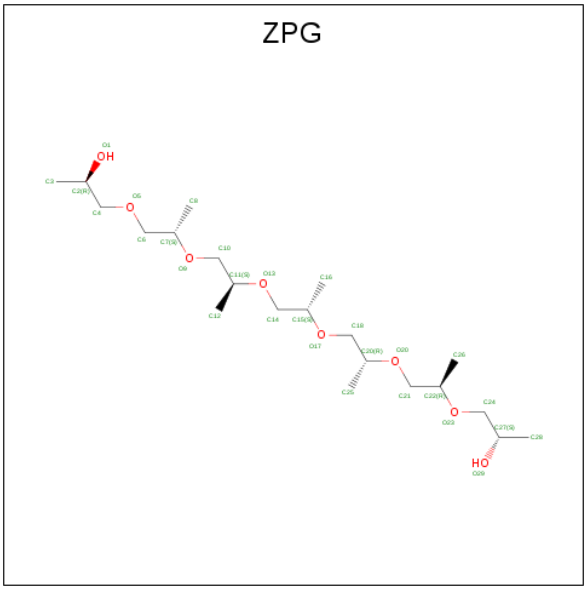
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is HEXANOYL-COENZYME A (three-letter code: HXC) (formula: $C_{27}H_{46}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			51	27	7	14	2	1		

- Molecule 4 is (2S,5R,8R,11S,14S,17S,21R)-5,8,11,14,17-PENTAMETHYL-4,7,10,13,16,19-HEXAOXADOCOSANE-2,21-DIOL (three-letter code: ZPG) (formula: $C_{21}H_{44}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 9 4	0	0

- Molecule 5 is water.

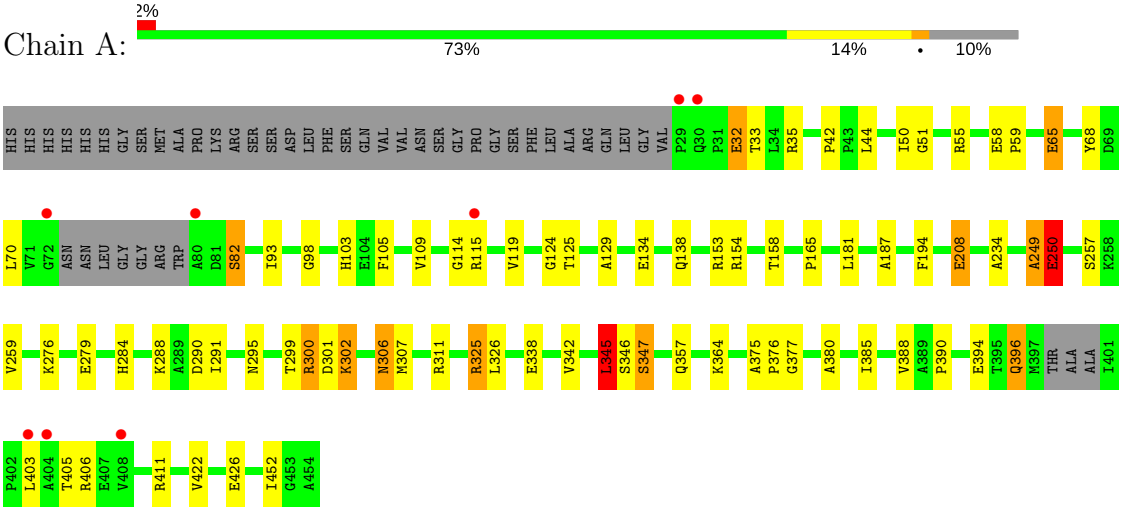
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	122	Total O 122 122	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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: 3-oxoacyl-(Acyl-carrier-protein) reductase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.06Å 103.06Å 76.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	89.25 – 2.50 19.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (89.25-2.50) 98.8 (19.77-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0095	Depositor
R, R_{free}	0.190 , 0.240 0.188 , 0.236	Depositor DCC
R_{free} test set	825 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3224	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HXC, NAD, ZPG

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	0.81	0/3037	0.83	2/4127 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	345	LEU	CA-CB-CG	-6.72	99.85	115.30
1	A	300	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	GLY	Peptide

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	2994	0	2992	50	0
2	A	44	0	26	2	0
3	A	51	0	42	1	0
4	A	13	0	19	0	0
5	A	122	0	0	3	0
All	All	3224	0	3079	50	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 8.

The worst 5 of 50 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:394:GLU:O	1:A:396:GLN:HA	1.67	0.95
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.38	0.85
1:A:325:ARG:CG	1:A:325:ARG:HH11	1.89	0.83
1:A:58:GLU:HB3	1:A:59:PRO:HD3	1.70	0.74
1:A:249:ALA:O	1:A:250:GLU:HB3	1.90	0.71

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	411/462 (89%)	377 (92%)	30 (7%)	4 (1%)	17 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ALA
1	A	82	SER
1	A	250	GLU

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Mol	Chain	Res	Type
1	A	187	ALA

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	295/338 (87%)	272 (92%)	23 (8%)	14 26

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	GLU
1	A	306	ASN
1	A	411	ARG
1	A	302	LYS
1	A	307	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN

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)

3 ligands 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	NAD	A	501	-	40,48,48	2.24	7 (17%)	44,73,73	2.62	7 (15%)
3	HXC	A	502	-	45,53,57	1.92	7 (15%)	53,76,83	2.20	4 (7%)
4	ZPG	A	503	-	12,12,28	1.14	1 (8%)	11,14,34	0.86	0

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	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	HXC	A	502	-	-	0/47/67/72	0/3/3/3
4	ZPG	A	503	-	-	0/12/12/31	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C2D-C3D	-4.09	1.42	1.53
2	A	501	NAD	C8A-N9A	-3.92	1.32	1.36
2	A	501	NAD	C3D-C4D	-2.59	1.46	1.53
2	A	501	NAD	C3B-C4B	-2.48	1.46	1.53
2	A	501	NAD	O2D-C2D	-2.30	1.37	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	HXC	N3-C2-N1	-13.90	116.97	128.86
2	A	501	NAD	N3A-C2A-N1A	-11.85	118.72	128.86
2	A	501	NAD	O7N-C7N-C3N	-6.49	111.50	119.62
2	A	501	NAD	C4B-O4B-C1B	-5.46	104.13	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAD	O7N-C7N-N7N	-4.65	115.84	122.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	2	0
3	A	502	HXC	1	0

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

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	416/462 (90%)	-0.37	8 (1%) 66 69	23, 40, 69, 94	1 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	ALA	5.5
1	A	72	GLY	4.0
1	A	404	ALA	3.3
1	A	403	LEU	3.0
1	A	408	VAL	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HXC	A	502	51/55	0.80	0.27	74,88,98,98	1
4	ZPG	A	503	13/29	0.80	0.31	86,91,92,92	0
2	NAD	A	501	44/44	0.97	0.11	34,44,69,71	0

6.5 Other polymers (i)

There are no such residues in this entry.