wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2014 – 04:09 AM GMT

PDB ID	:	2I3A
Title	:	Crystal structure of N-Acetyl-gamma-Glutamyl-PhosphateReductase (Rv1652) from Mycobacterium tuberculosis
Authors	:	Cherney, L.T.; Cherney, M.M.; Garen, C.R.; Moraidin, F.; James, M.N.G.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on	:	2006-08-17
Resolution	:	2.15 Å(reported)

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.15 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		0.164
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		3.5%
RSRZ outliers		0.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
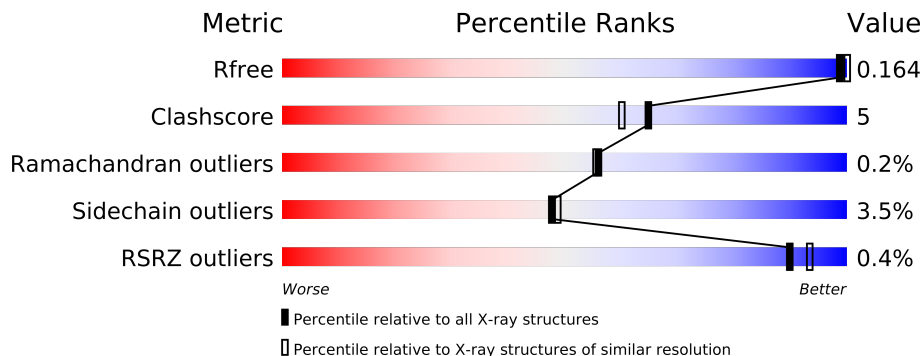
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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	352	
1	B	352	
1	C	352	
1	D	352	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Geometry	Electron density
2	BTB	A	1400	-	X
2	BTB	B	1500	-	X
2	BTB	C	1600	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10989 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 N-acetyl-gamma-glutamyl-phosphatereductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2496	1576	448	467	5			
1	B	346	Total	C	N	O	S	0	0	0
			2509	1583	451	470	5			
1	C	344	Total	C	N	O	S	0	0	0
			2496	1576	448	467	5			
1	D	347	Total	C	N	O	S	0	0	0
			2516	1588	452	471	5			

- Molecule 2 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).
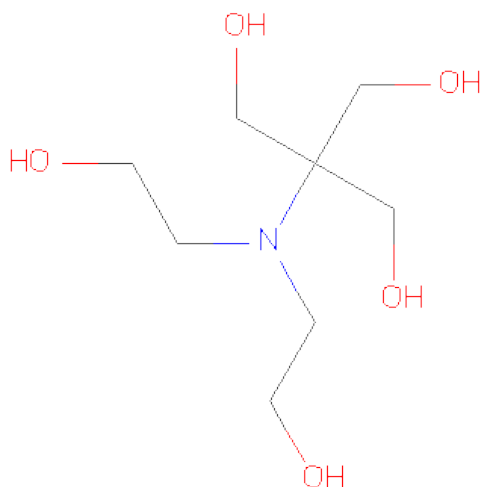
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total 203	O 203	0	0
3	B	230	Total 230	O 230	0	0
3	C	227	Total 227	O 227	0	0
3	D	256	Total 256	O 256	0	0

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: N-acetyl-gamma-glutamyl-phosphatereductase
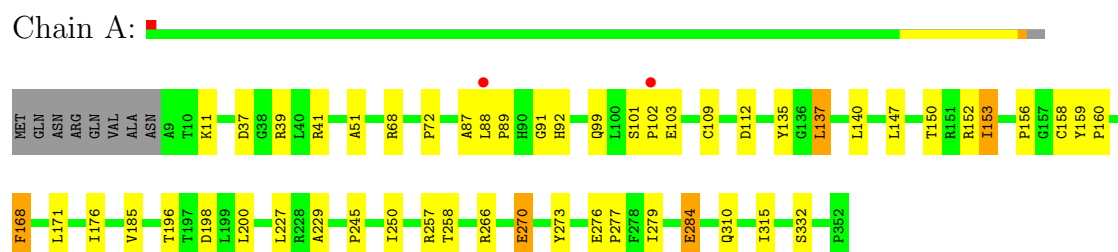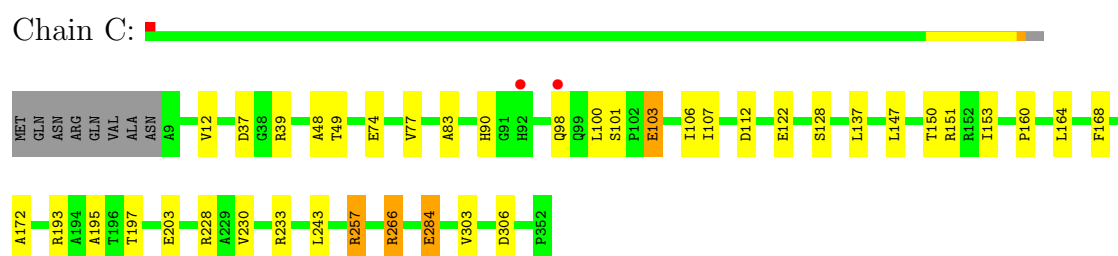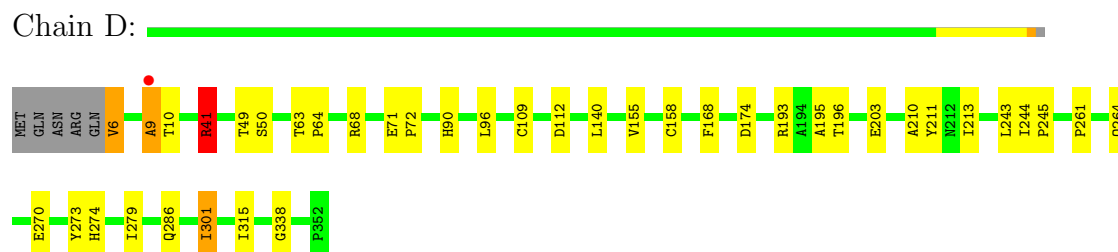
Chain A:

- Molecule 1: N-acetyl-gamma-glutamyl-phosphatereductase

Chain B:

- Molecule 1: N-acetyl-gamma-glutamyl-phosphatereductase

Chain C:

- Molecule 1: N-acetyl-gamma-glutamyl-phosphatereductase

Chain D:
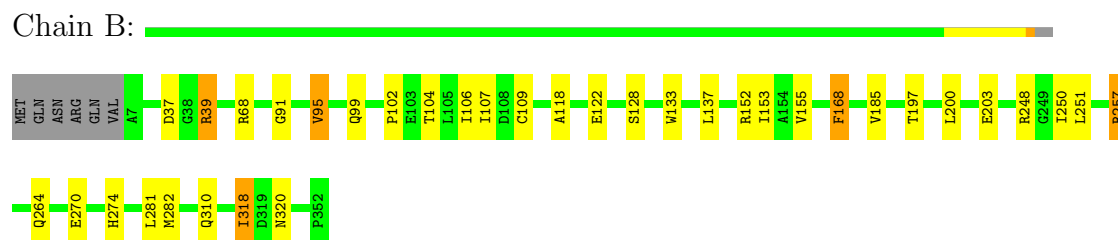
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.69Å　104.03Å　138.44Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	48.68　–　2.15 48.69　–　2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.68-2.15) 98.6 (48.69-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.161　,　0.225 0.161　,　0.164	Depositor DCC
R_{free} test set	3541 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 28.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 69806 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10989	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BTB

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	0.91	0/2552	0.85	1/3494 (0.0%)
1	B	0.92	0/2565	0.85	2/3512 (0.1%)
1	C	0.93	0/2552	0.88	4/3494 (0.1%)
1	D	0.95	1/2572 (0.0%)	0.87	2/3522 (0.1%)
All	All	0.92	1/10241 (0.0%)	0.86	9/14022 (0.1%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	158	CYS	CB-SG	5.37	1.91	1.82

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	248	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	228	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	41	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	C	243	LEU	CB-CG-CD1	-5.60	101.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	49	THR	Peptide

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	2496	0	2497	42	0
1	B	2509	0	2508	23	0
1	C	2496	0	2497	20	0
1	D	2516	0	2517	26	0
2	A	14	0	19	1	0
2	B	14	0	19	1	0
2	C	14	0	19	2	0
2	D	14	0	19	0	0
3	A	203	0	0	9	0
3	B	230	0	0	3	0
3	C	227	0	0	2	0
3	D	256	0	0	5	0
All	All	10989	0	10095	107	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 5.

The worst 5 of 107 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:310:GLN:HG3	3:A:1584:HOH:O	1.30	1.28
1:B:264:GLN:HG3	3:B:1710:HOH:O	1.37	1.22
1:C:101:SER:HB3	1:C:103:GLU:OE2	1.56	1.05
1:A:257:ARG:HD2	3:A:1541:HOH:O	1.55	1.04
1:B:39:ARG:HG3	2:B:1500:BTB:O1	1.84	0.76

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	342/352 (97%)	332 (97%)	9 (3%)	1 (0%)	50	47
1	B	344/352 (98%)	335 (97%)	9 (3%)	0	100	100
1	C	342/352 (97%)	332 (97%)	9 (3%)	1 (0%)	50	47
1	D	345/352 (98%)	336 (97%)	8 (2%)	1 (0%)	50	47
All	All	1373/1408 (98%)	1335 (97%)	35 (2%)	3 (0%)	56	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	ALA
1	A	284	GLU
1	D	9	ALA

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	247/254 (97%)	239 (97%)	8 (3%)	51	53
1	B	248/254 (98%)	240 (97%)	8 (3%)	51	53
1	C	247/254 (97%)	237 (96%)	10 (4%)	42	41
1	D	249/254 (98%)	240 (96%)	9 (4%)	47	47
All	All	991/1016 (98%)	956 (96%)	35 (4%)	48	49

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	318	ILE

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Mol	Chain	Res	Type
1	C	128	SER
1	D	196	THR
1	C	98	GLN
1	C	103	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	310	GLN
1	D	90	HIS
1	D	264	GLN

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 ⓘ

4 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	BTB	A	1400	-	13,13,13	1.17	1 (7%)	16,16,16	1.55	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
2	BTB	B	1500	-	13,13,13	0.99	1 (7%)	16,16,16	1.39	3 (18%)
2	BTB	C	1600	-	13,13,13	1.25	1 (7%)	16,16,16	1.91	2 (12%)
2	BTB	D	1700	-	13,13,13	1.45	2 (15%)	16,16,16	2.13	3 (18%)

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	BTB	A	1400	-	-	0/21/21/21	0/0/0/0
2	BTB	B	1500	-	-	0/21/21/21	0/0/0/0
2	BTB	C	1600	-	-	0/21/21/21	0/0/0/0
2	BTB	D	1700	-	-	0/21/21/21	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1700	BTB	C2-N	3.39	1.54	1.48
2	C	1600	BTB	C2-N	3.27	1.53	1.48
2	A	1400	BTB	C2-N	3.25	1.53	1.48
2	B	1500	BTB	C2-N	2.67	1.52	1.48
2	D	1700	BTB	C4-C2	2.48	1.56	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1700	BTB	C7-N-C5	-6.43	105.50	111.32
2	C	1600	BTB	C7-N-C5	-6.15	105.75	111.32
2	A	1400	BTB	C7-N-C5	-4.53	107.22	111.32
2	D	1700	BTB	C4-C2-C3	3.37	116.02	110.04
2	C	1600	BTB	C3-C2-C1	-3.17	104.41	110.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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(Å²)	Q<0.9
1	A	344/352 (97%)	-0.36	2 (0%)	86	90	17, 27, 46, 55	0
1	B	346/352 (98%)	-0.48	0	100	100	17, 27, 46, 56	0
1	C	344/352 (97%)	-0.39	2 (0%)	86	90	16, 26, 45, 54	0
1	D	347/352 (98%)	-0.41	1 (0%)	91	95	16, 25, 45, 53	0
All	All	1381/1408 (98%)	-0.41	5 (0%)	90	93	16, 26, 46, 56	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	HIS	3.7
1	A	102	PRO	2.9
1	C	98	GLN	2.5
1	D	9	ALA	2.4
1	A	88	LEU	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BTB	C	1600	14/14	0.26	3.15	44,52,55,57	0
2	BTB	B	1500	14/14	0.20	2.29	33,42,50,52	0
2	BTB	A	1400	14/14	0.21	2.23	52,58,59,61	0
2	BTB	D	1700	14/14	0.13	1.37	26,33,39,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.