W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 11:38 AM EDT

PDB ID	:	3PNY
Title	:	Structure of Glutamyl-tRNA synthetase from Mycobacterium tuberculosis in space group P21
Authors	:	Kachalova, G.S.; Laurinavichiute, D.; Bartunik, H.D.
Deposited on	:	2010-11-20
Resolution	:	1.70 Å(reported)

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

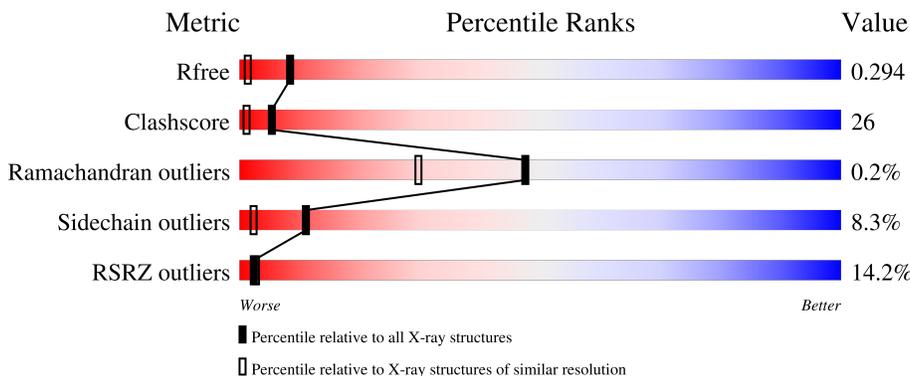|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.70 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		0.294
Clashscore		26
Ramachandran outliers		0.2%
Sidechain outliers		8.3%
RSRZ outliers		14.2%

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	505	16% / 62% / 29% / 5%
1	B	505	11% / 66% / 26% / · / ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 7841 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 Glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total 3822	C 2419	N 689	O 707	S 7	0	10	0
1	B	485	Total 3849	C 2432	N 699	O 710	S 8	0	8	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P0A636
A	-13	HIS	-	expression tag	UNP P0A636
A	-12	HIS	-	expression tag	UNP P0A636
A	-11	HIS	-	expression tag	UNP P0A636
A	-10	HIS	-	expression tag	UNP P0A636
A	-9	HIS	-	expression tag	UNP P0A636
A	-8	SER	-	expression tag	UNP P0A636
A	-7	SER	-	expression tag	UNP P0A636
A	-6	GLY	-	expression tag	UNP P0A636
A	-5	LEU	-	expression tag	UNP P0A636
A	-4	VAL	-	expression tag	UNP P0A636
A	-3	PRO	-	expression tag	UNP P0A636
A	-2	ARG	-	expression tag	UNP P0A636
A	-1	GLY	-	expression tag	UNP P0A636
A	0	SER	-	expression tag	UNP P0A636
B	-14	HIS	-	expression tag	UNP P0A636
B	-13	HIS	-	expression tag	UNP P0A636
B	-12	HIS	-	expression tag	UNP P0A636
B	-11	HIS	-	expression tag	UNP P0A636
B	-10	HIS	-	expression tag	UNP P0A636
B	-9	HIS	-	expression tag	UNP P0A636
B	-8	SER	-	expression tag	UNP P0A636
B	-7	SER	-	expression tag	UNP P0A636
B	-6	GLY	-	expression tag	UNP P0A636
B	-5	LEU	-	expression tag	UNP P0A636

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	VAL	-	expression tag	UNP P0A636
B	-3	PRO	-	expression tag	UNP P0A636
B	-2	ARG	-	expression tag	UNP P0A636
B	-1	GLY	-	expression tag	UNP P0A636
B	0	SER	-	expression tag	UNP P0A636

- Molecule 2 is water.

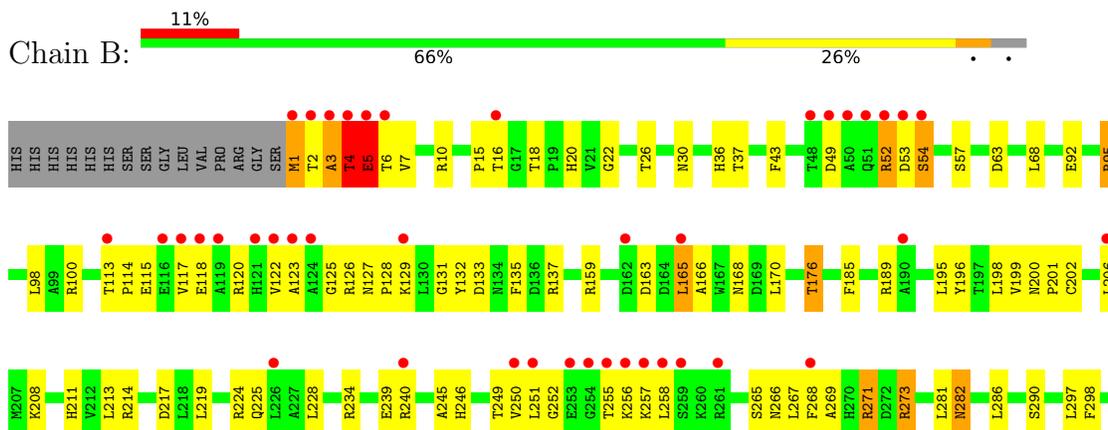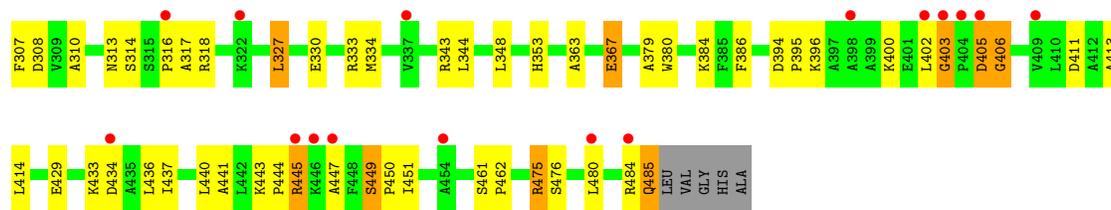| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total 73	O 73	0	11
2	B	97	Total 97	O 97	0	7

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: Glutamyl-tRNA synthetase

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F307 D308 V309 A310 N313 S314 S315 P316 A317 R318 K322 L327 E330 R333 M334 V337 R343 L344 L348 H353 A363 E367 A379 W380 K384 F385 F386 D394 P395 K396 A397 A398 A399 K400 E401 L402 G403 P404 D405 G406 V409 L410 D411 A412 A413

L414 E429 K433 D434 A435 L436 I437 L440 A441 L442 K443 P444 R445 K446 A447 F448 S449 P450 I451 A454 S461 P462 R475 S476 L480 R484 Q485 LEU VAL GLY HIS ALA
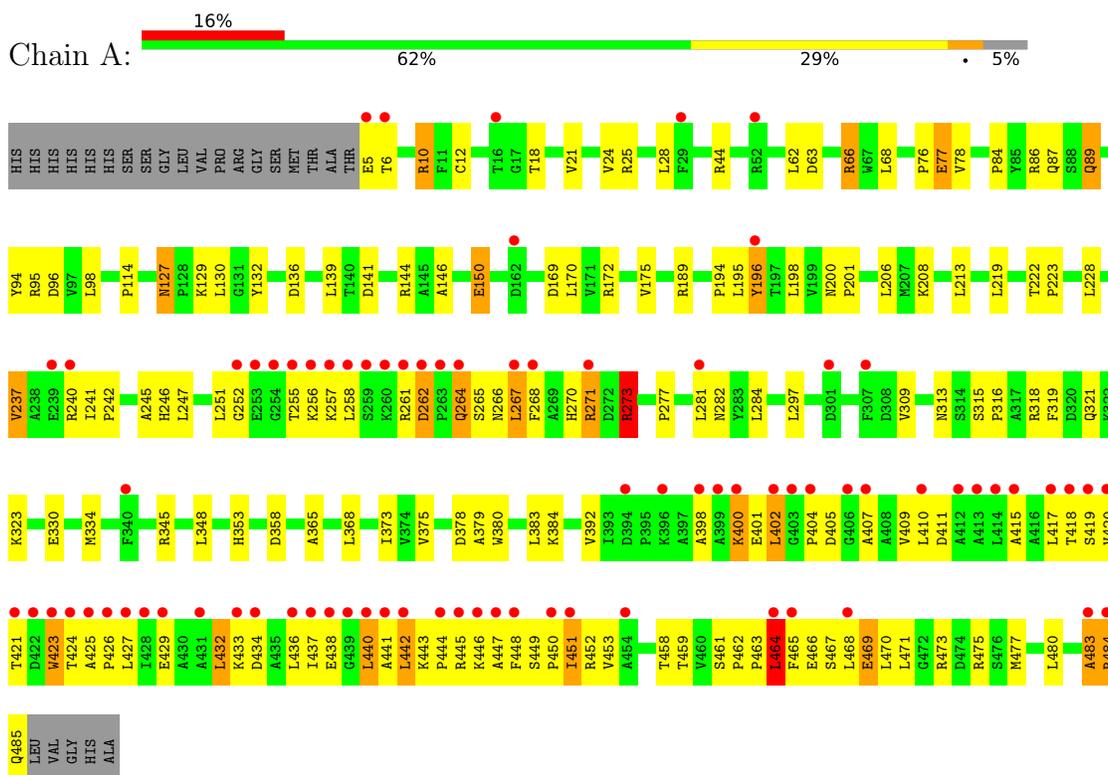
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.16Å 210.55Å 58.15Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	10.41 – 1.70 19.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.7 (10.41-1.70) 90.7 (19.98-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.285 0.266 , 0.294	Depositor DCC
R_{free} test set	5179 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.6	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7841	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.57% 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 ⓘ

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	0.77	2/3923 (0.1%)	0.82	9/5340 (0.2%)
1	B	0.84	4/3944 (0.1%)	0.85	9/5366 (0.2%)
All	All	0.81	6/7867 (0.1%)	0.83	18/10706 (0.2%)

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	3
1	B	0	3
All	All	0	6

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	PHE	CE1-CZ	5.75	1.48	1.37
1	B	298	PHE	CE2-CZ	5.30	1.47	1.37
1	A	89[A]	GLN	C-N	5.14	1.45	1.34
1	A	89[B]	GLN	C-N	5.14	1.45	1.34
1	B	95[A]	ARG	CA-C	-5.02	1.40	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4	THR	CB-CA-C	-7.08	92.47	111.60
1	B	43	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	A	25	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	273	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	B	343	ARG	NE-CZ-NH2	-5.80	117.40	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	LYS	Peptide
1	A	464	LEU	Peptide
1	A	483	ALA	Peptide
1	B	3	ALA	Peptide
1	B	402	LEU	Peptide

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	3822	0	3775	228	0
1	B	3849	0	3804	175	1
2	A	73	0	0	8	0
2	B	97	0	0	9	0
All	All	7841	0	7579	401	1

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 26.

The worst 5 of 401 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:B:249:THR:CG2	1:B:257:LYS:HG2	1.63	1.26
1:A:434:ASP:O	1:A:438:GLU:HB2	1.26	1.23
1:A:63:ASP:OD2	1:A:268[A]:PHE:HZ	1.21	1.18
1:B:117:VAL:HG22	1:B:132:TYR:OH	1.41	1.18
1:B:266:ASN:OD1	2:B:571[A]:HOH:O	1.57	1.17

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:NH2	1:B:125:GLY:O[1_655]	2.00	0.20

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	489/505 (97%)	475 (97%)	14 (3%)	0	100	100
1	B	491/505 (97%)	475 (97%)	14 (3%)	2 (0%)	34	18
All	All	980/1010 (97%)	950 (97%)	28 (3%)	2 (0%)	47	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	GLY
1	B	252	GLY

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	393/402 (98%)	356 (91%)	37 (9%)	8	1
1	B	394/402 (98%)	363 (92%)	31 (8%)	12	2
All	All	787/804 (98%)	719 (91%)	68 (9%)	11	2

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	313	ASN
1	B	367	GLU
1	B	449	SER
1	A	345	ARG

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Mol	Chain	Res	Type
1	A	330	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	313	ASN
1	B	353	HIS
1	A	313	ASN
1	B	225	GLN
1	B	264	GLN

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(Å²)	Q<0.9
1	A	481/505 (95%)	1.16	80 (16%)	1	1	13, 26, 52, 68	9 (1%)
1	B	485/505 (96%)	0.94	57 (11%)	4	5	12, 23, 46, 66	2 (0%)
All	All	966/1010 (95%)	1.05	137 (14%)	2	3	12, 25, 49, 68	11 (1%)

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	THR	13.3
1	B	4	THR	13.0
1	A	257	LYS	11.9
1	B	3	ALA	11.1
1	B	51	GLN	11.0

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 monosaccharides 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.

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PROTEIN DATA BANK