



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:06 PM GMT

PDB ID : 1IRX
Title : Crystal structure of class I lysyl-tRNA synthetase
Authors : Nureki, O.; Terada, T.; Ishitani, R.; Ambrogelly, A.; Ibba, M.; Soll, D.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2001-10-25
Resolution : 2.60 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

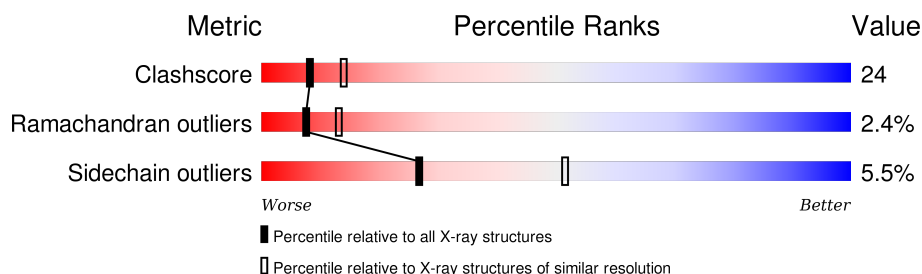
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	523	 58% 36% . .
1	B	523	 51% 41% 5% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8754 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 lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4247	2738	733	764	12			
1	B	508	Total	C	N	O	S	0	0	0
			4255	2742	734	767	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	LEU	PHE	CONFLICT	UNP O57963
A	331	GLU	ASP	CONFLICT	UNP O57963
B	124	LEU	PHE	CONFLICT	UNP O57963
B	331	GLU	ASP	CONFLICT	UNP O57963

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

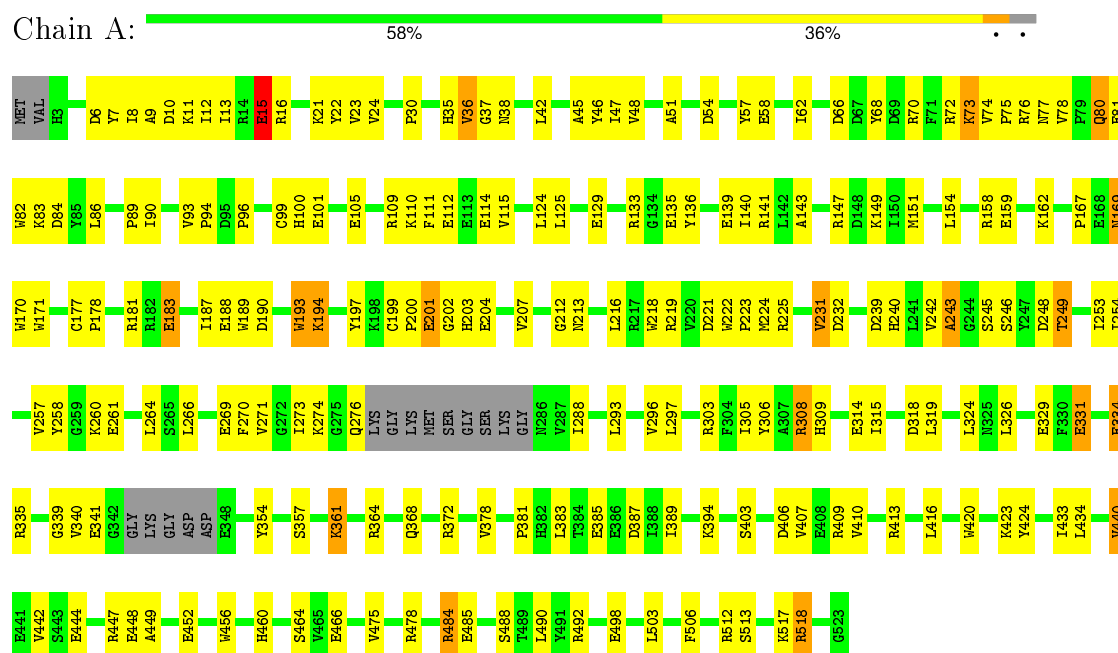
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	102	Total	O	0	0
			102	102		

3 Residue-property plots

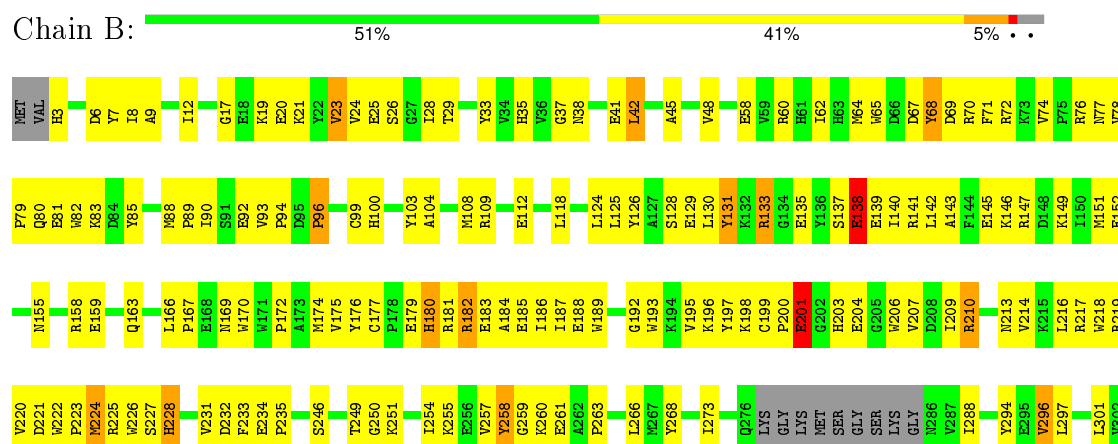
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: lysyl-tRNA synthetase



- Molecule 1: lysyl-tRNA synthetase



I389	I383
R390	F304
V391	I305
P399	R308
L402	P311
S403	I323
K404	L326
E405	E329
E408	R332
R409	V333
V410	E334
K411	R335
L412	I336
R413	Y337
I414	F338
R418	G339
R419	V340
W420	E341
K423	G342
D428	GLY
I433	LYS
L434	GLY
E435	ASP
K436	D347
E444	E348
A449	R351
E452	S357
V453	R358
W456	P359
L457	R360
H460	R361
E466	E363
E467	R364
F468	L365
I471	V366
I471	L374
E474	A375
R478	V376
R484	L377
F487	V378
S488	R379
Y491	L380
	P381
	R382
	L383
	T384
	E385
	E386
	D387
	I388
P501	
R502	
L503	
F506	
R512	
R518	
G523	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.95Å 74.77Å 156.94Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8754	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.40	0/4361	0.60	0/5886
1	B	0.38	0/4369	0.59	0/5897
All	All	0.39	0/8730	0.59	0/11783

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

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	4247	0	4181	173	0
1	B	4255	0	4187	239	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	146	0	0	8	0
3	B	102	0	0	10	0
All	All	8754	0	8368	412	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 24.

The worst 5 of 412 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:361:LYS:HD2	1:A:361:LYS:H	1.21	1.01
1:B:361:LYS:H	1:B:361:LYS:HE3	1.22	1.01
1:A:218:TRP:HZ3	1:A:246:SER:HG	0.99	0.98
1:B:209:ILE:HB	1:B:210:ARG:HH21	1.24	0.97
1:B:89:PRO:HB2	1:B:92:GLU:HG2	1.51	0.93

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	501/523 (96%)	457 (91%)	37 (7%)	7 (1%)	14	28
1	B	502/523 (96%)	443 (88%)	42 (8%)	17 (3%)	5	7
All	All	1003/1046 (96%)	900 (90%)	79 (8%)	24 (2%)	7	13

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	LYS
1	A	243	ALA
1	B	77	ASN
1	B	138	GLU
1	B	180	HIS

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	451/462 (98%)	429 (95%)	22 (5%)	31	57
1	B	452/462 (98%)	424 (94%)	28 (6%)	23	45
All	All	903/924 (98%)	853 (94%)	50 (6%)	27	51

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	VAL
1	B	99	CYS
1	B	474	GLU
1	B	42	LEU
1	B	69	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	ASN
1	B	3	HIS
1	B	169	ASN
1	A	460	HIS
1	B	203	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.