



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:35 PM GMT

PDB ID : 1QU3
Title : INSIGHTS INTO EDITING FROM AN ILE-TRNA SYNTHETASE STRUCTURE WITH TRNA(ILE) AND MUPIROCIN
Authors : Silvian, L.F.; Wang, J.; Steitz, T.A.
Deposited on : 1999-07-06
Resolution : 2.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

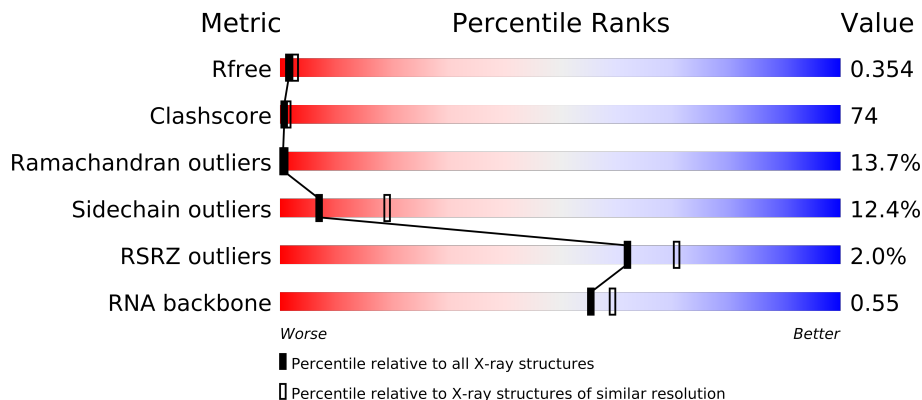
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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	T	75	
2	A	917	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	MRC	A	993	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8870 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 RNA chain called ISOLEUCYL-TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	75	Total	C	N	O	P	24	0	0
			1603	715	289	525	74			

- Molecule 2 is a protein called ISOLEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	880	Total	C	N	O	S	0	0	0
			7113	4537	1198	1358	20			

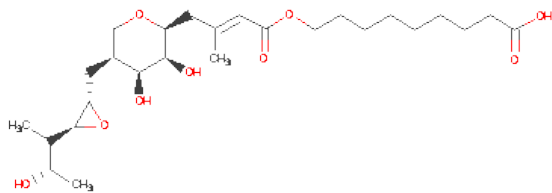
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	LYS	CONFLICT	UNP P41972
A	5	LYS	GLU	CONFLICT	UNP P41972
A	295	TRP	TYR	CONFLICT	UNP P41972
A	340	GLN	LYS	CONFLICT	UNP P41972
A	644	ASP	VAL	CONFLICT	UNP P41972

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MUPIROCIN (three-letter code: MRC) (formula: C₂₆H₄₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	26	9		

- Molecule 5 is water.

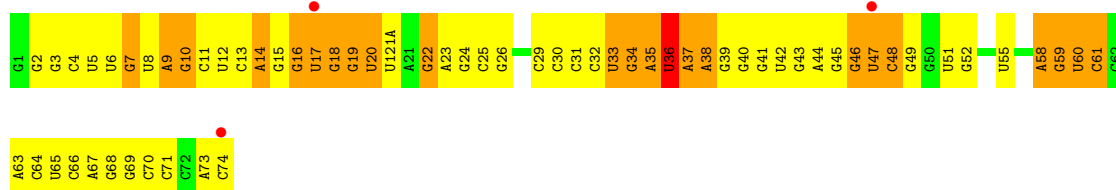
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total	O	0	0
			82	82		
5	T	36	Total	O	0	0
			36	36		

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.

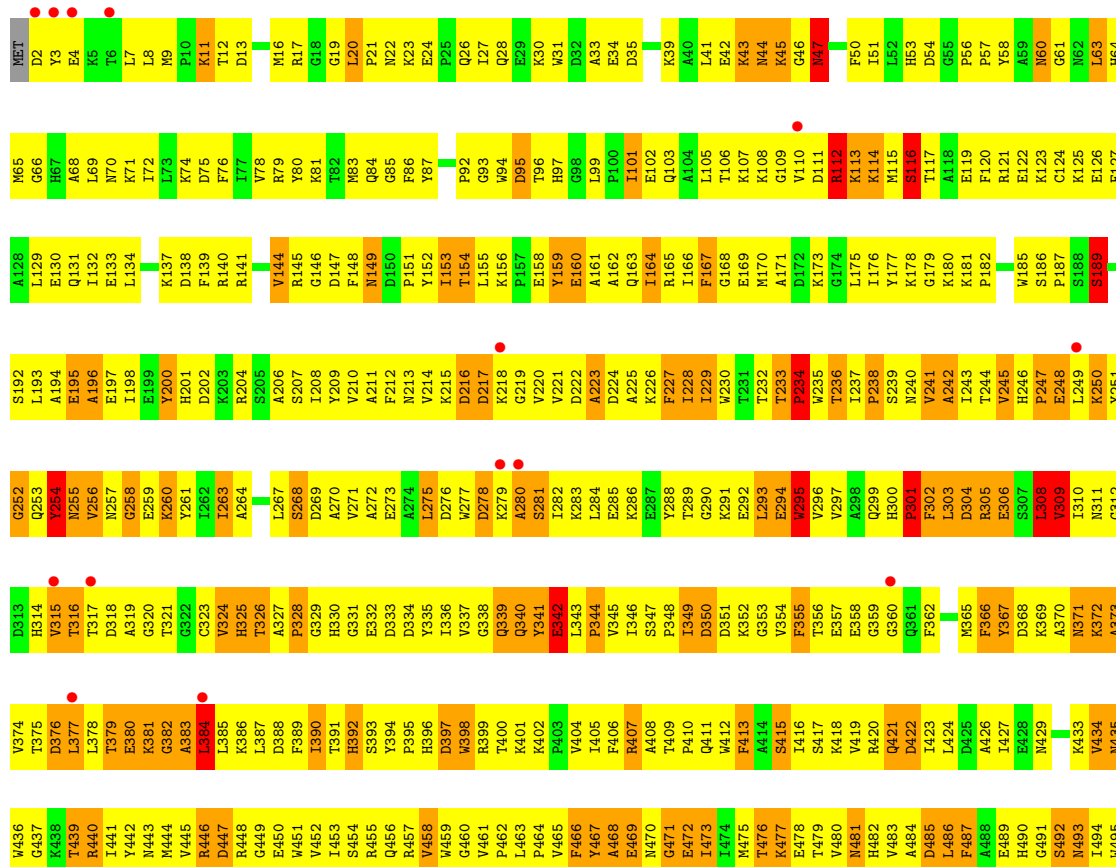
• Molecule 1: ISOLEUCYL-TRNA

Chain T: 



• Molecule 2: ISOLEUCYL-TRNA SYNTHETASE

Chain A: 



ARG	K823	R686	W621	G560	F496
CYS	S824	A757	V622	G561	E497
TRP	L825	P758	S623	W562	R498
ASN	E826	I759	S624	F563	E499
TYR	A827	L760	T625	N564	A500
SER	K828	V761	D626	K501	K501
GLU	V829	H762	Y627	I567	D502
ASP	T830		L628	T568	L503
LEU	I831	E765	A629	T569	L504
GLY	A832	E766	D630	P570	P505
ALA	S833	V767	V631	V571	E506
VAL	N834	V768	R632	A572	G507
ASP	D835	S769	L633	T573	F508
GLU	K836	H770	S634	R574	T509
LEU	F837	I771	D635	G576	H510
THR	N838	P772	E636	S577	P511
HIS	A839	H773	I637	P578	G512
LEU	S840	V774	L638	Y579	S513
CYS	F841	K775		K580	P514
PRO	F842	E776	S642	F581	N515
ARG	L843	E777	D643	L582	F518
GLN	T844	S778	D644	L583	T519
GLN	A848	V779	Y645	S584	K520
VAL	L849	H780	R646	H585	E521
VAL	H850	L781	K647	G586	
LYS	Q851	W784	I648	F587	L624
LEU	F853	D791	N649	V588	M525
LEU	V854	Q792	N650	M589	D526
	V855	A793	L652	D590	V527
	S856	L794	R653	G591	K528
	Q857	L795	F654	E592	F529
	V858	D796	M655	G593	D530
	K859	K797	L656	K594	
	V860	W798	G657	K595	S533
	V861	R799	N658	M596	S534
	D862	T800	I659	S597	H535
	D865	F801	N660	K598	R536
	D866	M802	D661	S599	G537
	Q867	L804	P664	L600	V538
	A868	R805	D665	G601	L539
	T869	D806	T666	V603	
	A870	D807	D667	I604	R542
	Y871	N808	S668	V605	P543
	H873	R809	I669	P606	E544
	G874	A810	P670	D607	L545
	D875	A811	S671	Q608	S546
	I876	L812	E672	F547	P548
	V877	E813	E673	V609	A549
	A881	T814	E676	V610	D550
	ASP	R815		Q612	M551
GLY	GLY	R816	L745	K613	Y552
GLU	GLU	N817	Y746	G614	L553
LYS	LYS	E818	Q747	A615	E554
CYS	CYS	K819	I748	D616	G555
GLU	GLU	V820	L749	I617	S556
		I821	D550	A618	D557
		G822	R683	R619	Q558
			L685	L620	Y559

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.00Å 100.00Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 19.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	85.9 (10.00-2.90) 55.5 (19.93-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.75Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.234 , 0.345 0.239 , 0.354	Depositor DCC
R_{free} test set	902 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 11.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19777 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8870	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	T	0.53	0/1792	0.80	1/2794 (0.0%)
2	A	0.44	0/7287	0.72	3/9879 (0.0%)
All	All	0.46	0/9079	0.74	4/12673 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	471	GLY	N-CA-C	-6.82	96.06	113.10
2	A	681	LEU	CA-CB-CG	-5.37	102.94	115.30
1	T	36	U	N1-C1'-C2'	5.28	120.86	114.00
2	A	255	ASN	N-CA-C	5.25	125.18	111.00

There are no chirality outliers.

There are no planarity outliers.

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	T	1603	0	811	99	1
2	A	7113	0	6935	1135	1
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	40	5	0
5	A	82	0	0	15	0
5	T	36	0	0	2	0
All	All	8870	0	7786	1212	1

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 74.

The worst 5 of 1212 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:13:C:H2'	1:T:14:A:H5''	1.32	1.10
2:A:366:PHE:H	2:A:370:ALA:HB3	1.18	1.07
2:A:53:HIS:NE2	2:A:534:SER:HB3	1.73	1.02
2:A:250:LYS:HG2	2:A:290:GLY:N	1.77	1.00
2:A:302:PHE:HA	2:A:378:LEU:HD13	1.43	0.99

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	Distance(Å)	Clash(Å)
1:T:19:G:O2'	2:A:672:SER:O[4_576]	2.19	0.01

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
2	A	878/917 (96%)	572 (65%)	186 (21%)	120 (14%)	0 1

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	45	LYS
2	A	47	ASN
2	A	112	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	114	LYS
2	A	195	GLU

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
2	A	772/806 (96%)	676 (88%)	96 (12%)	7 19

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	371	ASN
2	A	450	GLU
2	A	813	GLU
2	A	384	LEU
2	A	398	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	456	GLN
2	A	493	ASN
2	A	851	GLN
2	A	481	ASN
2	A	482	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	T	74/75 (98%)	21 (28%)	12 (16%)

5 of 21 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	T	8	U
1	T	9	A
1	T	10	G
1	T	14	A
1	T	16	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	T	34	G
1	T	36	U
1	T	48	C
1	T	33	U
1	T	47	U

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	MRC	A	993	-	36,36,36	2.20	10 (27%)	48,48,48	2.14	11 (22%)

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
4	MRC	A	993	-	1/1/11/12	0/32/54/54	0/1/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	993	MRC	C11-C10	-7.40	1.36	1.46
4	A	993	MRC	C8-C7	4.56	1.59	1.53
4	A	993	MRC	O1A-C1	3.82	1.43	1.34
4	A	993	MRC	C9-C8	3.22	1.60	1.53
4	A	993	MRC	C4-C5	2.97	1.58	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	993	MRC	C16-C8-C7	-6.48	102.91	108.72
4	A	993	MRC	C11-O10-C10	-5.34	57.39	60.59
4	A	993	MRC	C9-C8-C7	4.40	119.33	113.19
4	A	993	MRC	C11-C12-C13	4.30	120.59	110.71
4	A	993	MRC	O1A-C1-C2	3.97	118.98	110.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	993	MRC	C12

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(Å ²)	Q<0.9
1	T	75/75 (100%)	-0.01	3 (4%) 36 43	5, 30, 78, 100	2 (2%)
2	A	880/917 (95%)	-0.30	16 (1%) 65 74	3, 32, 70, 83	0
All	All	955/992 (96%)	-0.27	19 (1%) 62 71	3, 32, 70, 100	2 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	2	ASP	5.3
2	A	3	TYR	5.1
2	A	4	GLU	5.1
1	T	74	C	4.7
2	A	280	ALA	4.0

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 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(\AA^2)	Q<0.9
4	MRC	A	993	35/35	0.20	2.32	22,29,57,58	0
3	ZN	A	992	1/1	0.03	-1.48	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.