



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2016 – 02:53 PM EDT

PDB ID : 5KNN  
Title : Evolutionary gain of alanine mischarging to non-cognate tRNAs with a G4:U69 base pair  
Authors : Sun, L.; He, W.; Yang, X.-L.  
Deposited on : 2016-06-28  
Resolution : 2.68 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

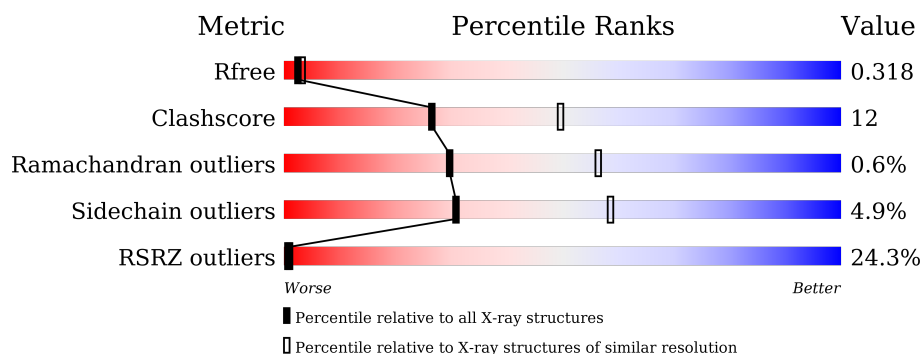
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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))
$R_{free}$	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	450	<div> <div>18%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	B	450	<div> <div>23%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>
1	C	450	<div> <div>28%</div> <div>66%</div> <div>26%</div> <div>5% ..</div> </div>
1	D	450	<div> <div>29%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	E	450	<div> <div>19%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	F	450	<div> <div>20%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	450	<div><div></div><div>27%</div><div></div><div>73%</div><div></div><div>24%</div><div></div><div>..</div></div>
1	H	450	<div><div></div><div>29%</div><div></div><div>69%</div><div></div><div>25%</div><div></div><div>..</div></div>

## 2 Entry composition

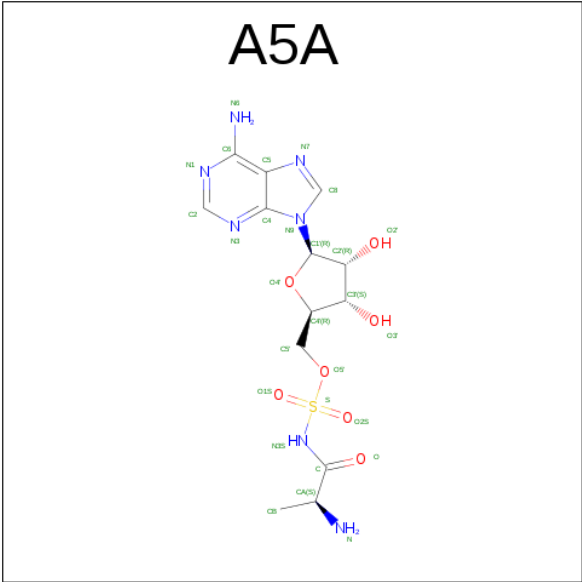
There are 2 unique types of molecules in this entry. The entry contains 28584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alanine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	B	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	C	444	Total	C	N	O	S	0	0	0
			3514	2227	604	667	16			
1	D	447	Total	C	N	O	S	0	0	0
			3536	2241	608	671	16			
1	E	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	F	449	Total	C	N	O	S	0	0	0
			3551	2250	611	674	16			
1	G	449	Total	C	N	O	S	0	0	0
			3551	2250	611	674	16			
1	H	446	Total	C	N	O	S	0	0	0
			3528	2235	607	670	16			

- Molecule 2 is '5'-O-(N-(L-ALANYL)-SULFAMOYL)ADENOSINE (three-letter code: A5A) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>7</sub>O<sub>7</sub>S).

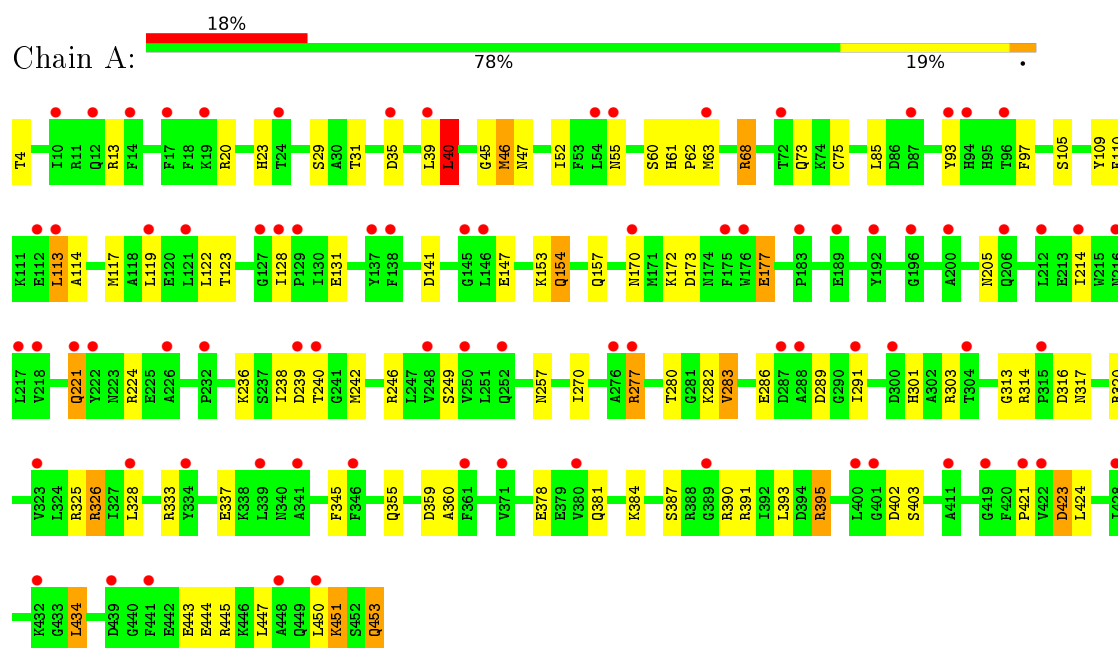


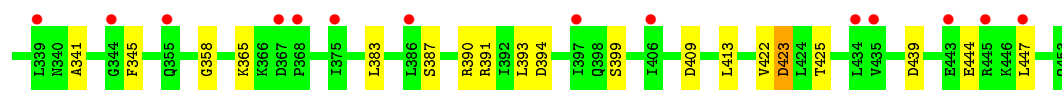
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	B	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	C	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	D	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	E	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	F	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	G	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	H	1	Total	C	N	O	S	0	0
			28	13	7	7	1		

### 3 Residue-property plots

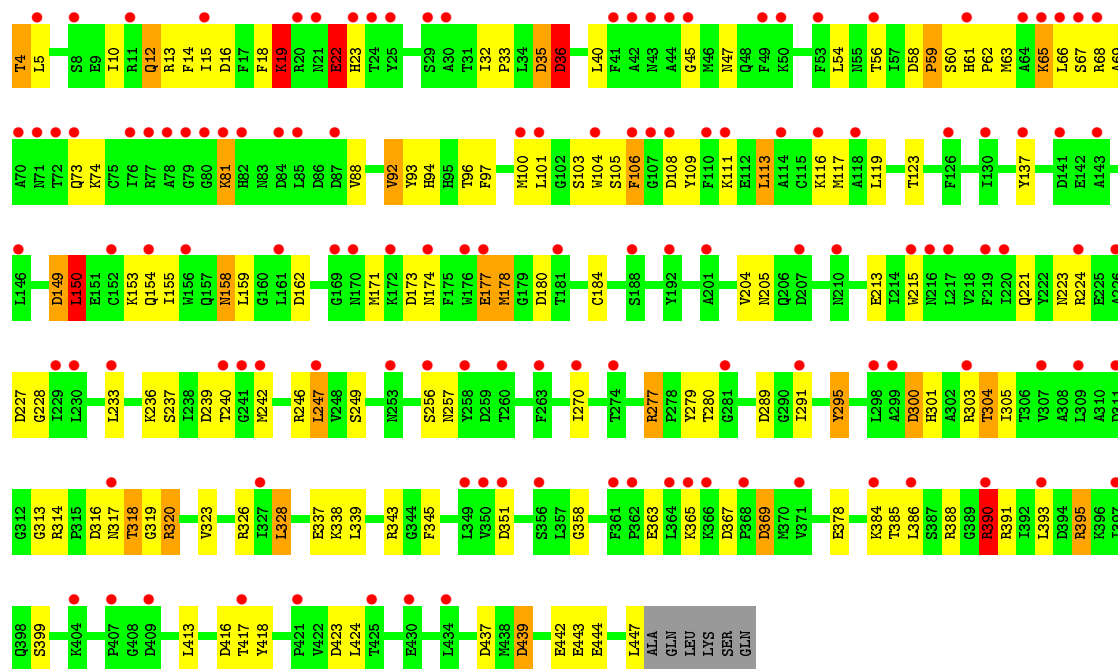
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

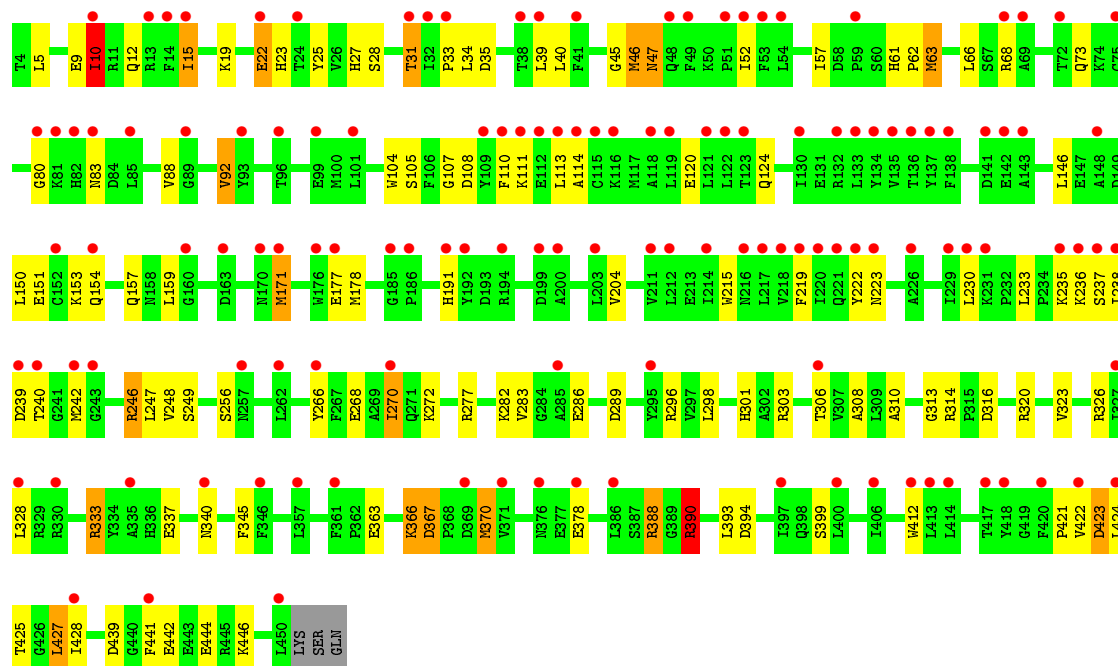
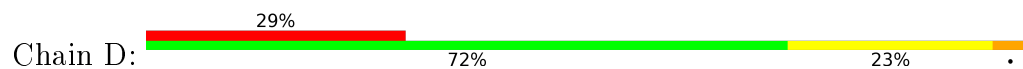




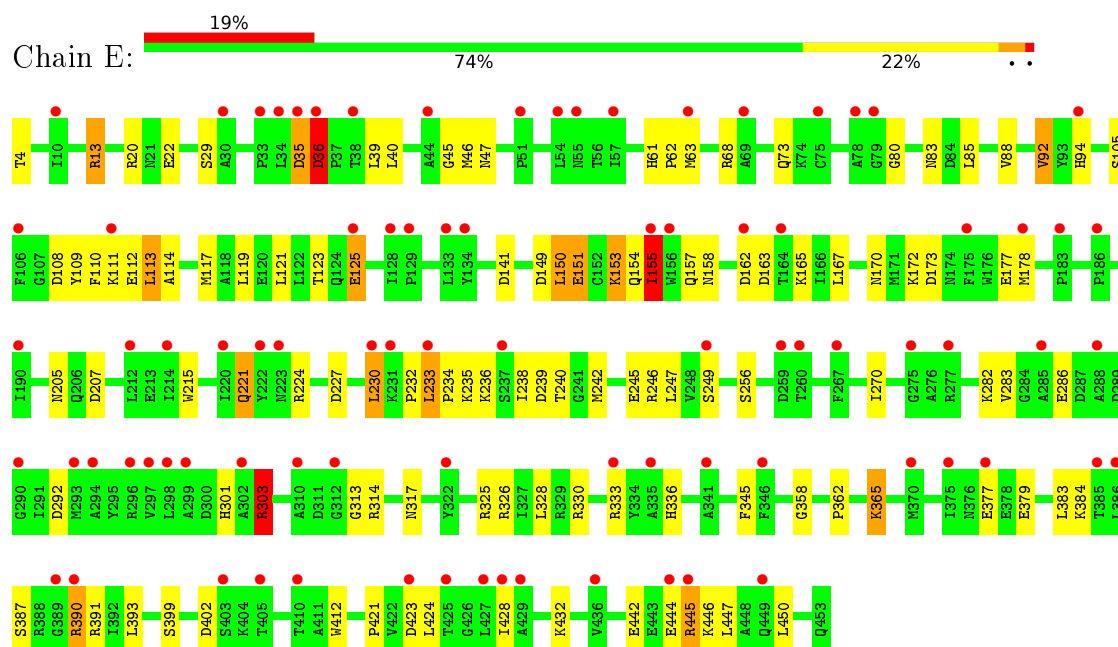
• Molecule 1: Alanine-tRNA ligase, cytoplasmic



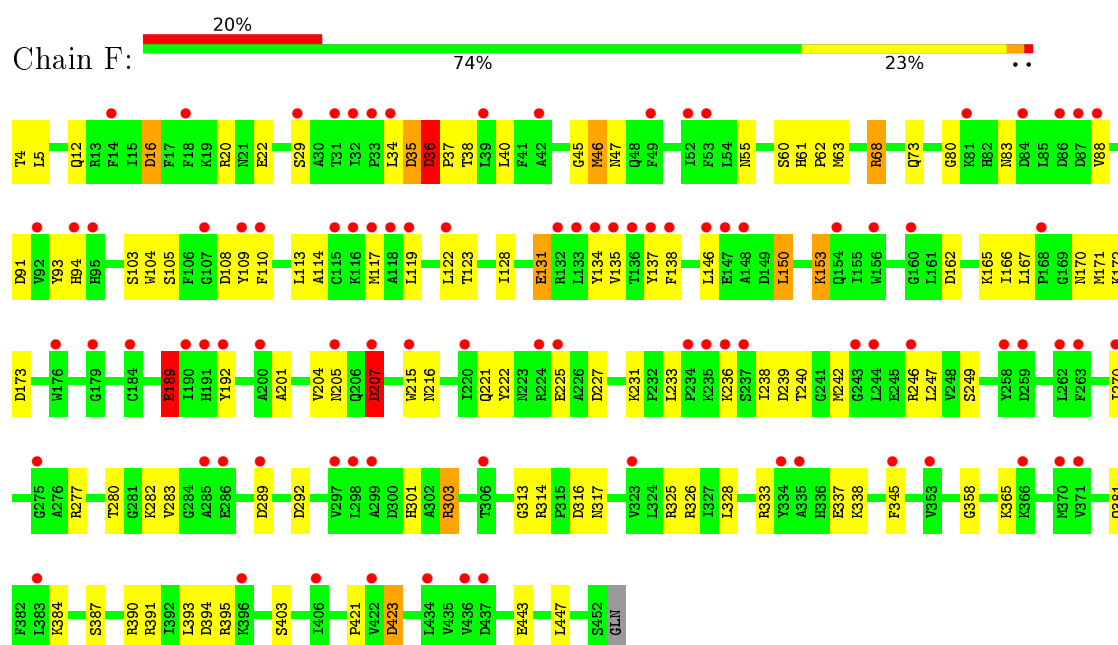
• Molecule 1: Alanine-tRNA ligase, cytoplasmic



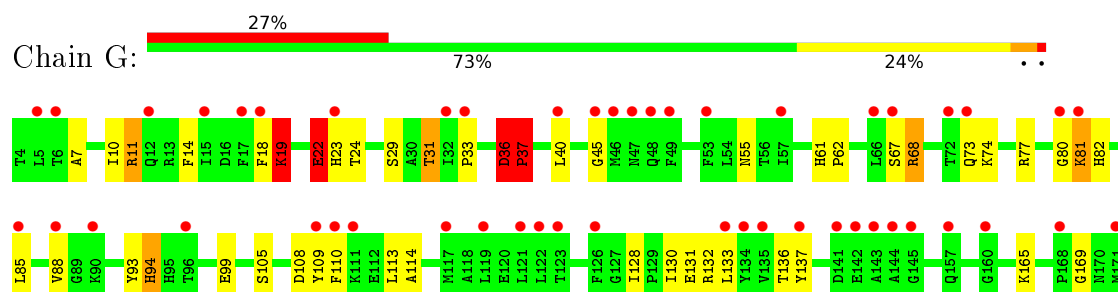
• Molecule 1: Alanine-tRNA ligase, cytoplasmic



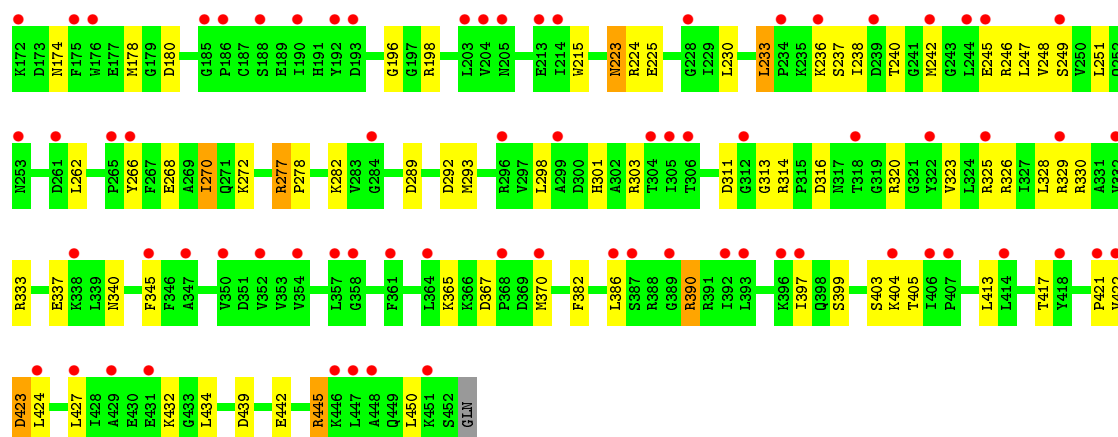
• Molecule 1: Alanine-tRNA ligase, cytoplasmic



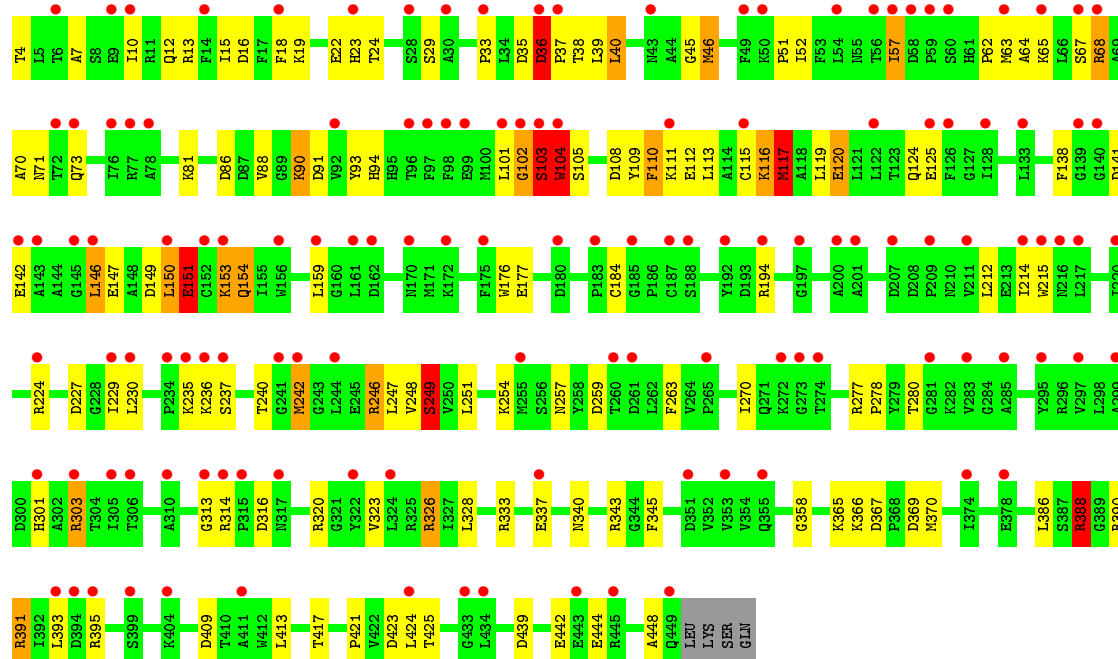
• Molecule 1: Alanine-tRNA ligase, cytoplasmic







● Molecule 1: Alanine-tRNA ligase, cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.17Å 98.26Å 201.38Å 90.07° 89.95° 90.11°	Depositor
Resolution (Å)	49.13 – 2.68 49.13 – 2.68	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.13-2.68) 99.4 (49.13-2.68)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.254 0.282 , 0.318	Depositor DCC
$R_{free}$ test set	5431 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l 0.079 for -h,k,-l 0.146 for -h,-k,l	Xtriage
Reported twinning fraction	0.441 for H, K, L 0.076 for -H, -K, L 0.275 for H, -K, -L 0.209 for -H, K, -L	Depositor
Outliers	0 of 112184 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	28584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: A5A

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	1/3635 (0.0%)	1.01	22/4915 (0.4%)
1	B	0.78	4/3635 (0.1%)	1.01	26/4915 (0.5%)
1	C	0.86	6/3589 (0.2%)	1.16	39/4854 (0.8%)
1	D	0.81	2/3611 (0.1%)	1.11	29/4884 (0.6%)
1	E	0.79	2/3635 (0.1%)	1.04	26/4915 (0.5%)
1	F	0.80	1/3626 (0.0%)	0.99	22/4903 (0.4%)
1	G	0.81	0/3626	1.08	28/4903 (0.6%)
1	H	0.87	5/3603 (0.1%)	1.16	36/4873 (0.7%)
All	All	0.81	21/28960 (0.1%)	1.07	228/39162 (0.6%)

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
1	B	0	2
1	C	0	2
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	4
All	All	0	12

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	151	GLU	C-O	-7.96	1.08	1.23
1	C	149	ASP	CG-OD2	-7.35	1.08	1.25
1	C	442	GLU	CD-OE1	7.21	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	GLU	CD-OE1	6.73	1.33	1.25
1	B	177	GLU	CD-OE1	-6.72	1.18	1.25

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ASP	CB-CG-OD1	13.34	130.31	118.30
1	E	402	ASP	CB-CG-OD2	-12.89	106.70	118.30
1	H	303	ARG	NE-CZ-NH1	11.53	126.07	120.30
1	D	367	ASP	CB-CG-OD1	11.23	128.41	118.30
1	D	367	ASP	CB-CG-OD2	-10.24	109.09	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	LYS	Peptide
1	B	277	ARG	Peptide
1	B	36	ASP	Peptide
1	C	22	GLU	Peptide
1	C	36	ASP	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	3560	0	3499	56	1
1	B	3560	0	3499	90	0
1	C	3514	0	3449	127	0
1	D	3536	0	3473	79	1
1	E	3560	0	3499	79	2
1	F	3551	0	3491	79	2
1	G	3551	0	3491	86	1
1	H	3528	0	3462	119	1
2	A	28	0	19	1	0
2	B	28	0	19	0	0
2	C	28	0	19	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	19	1	0
2	E	28	0	19	2	0
2	F	28	0	19	0	0
2	G	28	0	19	0	0
2	H	28	0	19	0	0
All	All	28584	0	28015	692	4

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 12.

The worst 5 of 692 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:277:ARG:NH2	1:A:289:ASP:OD2	1.76	1.18
1:H:40:LEU:O	1:H:320:ARG:NH1	1.84	1.10
1:H:10:ILE:HD11	1:H:251:LEU:HD12	1.16	1.09
1:F:153:LYS:CE	1:F:166:ILE:HG23	1.86	1.04
1:B:222:TYR:HB3	1:B:230:LEU:HD22	1.39	1.01

All (4) 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:E:377:GLU:OE1	1:F:395:ARG:NH1[1_546]	1.89	0.31
1:A:154:GLN:NE2	1:F:55:ASN:O[1_545]	2.10	0.10
1:E:445:ARG:NE	1:G:405:THR:OG1[1_655]	2.12	0.08
1:D:388:ARG:NH2	1:H:366:LYS:O[1_645]	2.15	0.05

## 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	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	52	79
1	B	448/450 (100%)	431 (96%)	12 (3%)	5 (1%)	17	40
1	C	442/450 (98%)	426 (96%)	12 (3%)	4 (1%)	21	46
1	D	445/450 (99%)	431 (97%)	14 (3%)	0	100	100
1	E	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	52	79
1	F	447/450 (99%)	434 (97%)	11 (2%)	2 (0%)	39	67
1	G	447/450 (99%)	429 (96%)	15 (3%)	3 (1%)	26	53
1	H	444/450 (99%)	421 (95%)	18 (4%)	5 (1%)	17	40
All	All	3569/3600 (99%)	3444 (96%)	104 (3%)	21 (1%)	30	56

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	B	37	PRO
1	C	22	GLU
1	F	37	PRO
1	H	37	PRO

### 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	379/379 (100%)	360 (95%)	19 (5%)	30	57
1	B	379/379 (100%)	358 (94%)	21 (6%)	27	52
1	C	374/379 (99%)	355 (95%)	19 (5%)	29	56
1	D	376/379 (99%)	357 (95%)	19 (5%)	29	56
1	E	379/379 (100%)	363 (96%)	16 (4%)	36	65
1	F	378/379 (100%)	362 (96%)	16 (4%)	36	65
1	G	378/379 (100%)	361 (96%)	17 (4%)	34	62
1	H	375/379 (99%)	353 (94%)	22 (6%)	24	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3018/3032 (100%)	2869 (95%)	149 (5%)	31 58

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	92	VAL
1	E	155	ILE
1	H	230	LEU
1	D	150	LEU
1	D	390	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	340	ASN
1	E	154	GLN
1	H	257	ASN
1	E	94	HIS
1	E	205	ASN

### 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 ⓘ

8 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	A5A	A	500	-	26,30,30	1.76	5 (19%)	27,45,45	2.60	10 (37%)
2	A5A	B	500	-	26,30,30	1.90	4 (15%)	27,45,45	2.51	6 (22%)
2	A5A	C	500	-	26,30,30	2.11	6 (23%)	27,45,45	2.34	8 (29%)
2	A5A	D	500	-	26,30,30	1.47	4 (15%)	27,45,45	2.56	7 (25%)
2	A5A	E	500	-	26,30,30	1.55	5 (19%)	27,45,45	2.22	7 (25%)
2	A5A	F	500	-	26,30,30	2.21	5 (19%)	27,45,45	2.43	7 (25%)
2	A5A	G	500	-	26,30,30	1.50	5 (19%)	27,45,45	1.88	5 (18%)
2	A5A	H	500	-	26,30,30	1.51	6 (23%)	27,45,45	1.72	4 (14%)

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	A5A	A	500	-	-	0/14/35/35	0/3/3/3
2	A5A	B	500	-	-	0/14/35/35	0/3/3/3
2	A5A	C	500	-	-	0/14/35/35	0/3/3/3
2	A5A	D	500	-	-	0/14/35/35	0/3/3/3
2	A5A	E	500	-	-	0/14/35/35	0/3/3/3
2	A5A	F	500	-	-	0/14/35/35	0/3/3/3
2	A5A	G	500	-	-	0/14/35/35	0/3/3/3
2	A5A	H	500	-	-	0/14/35/35	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	A5A	O5'-S	-6.12	1.50	1.59
2	B	500	A5A	O5'-S	-5.41	1.51	1.59
2	A	500	A5A	O5'-S	-5.18	1.51	1.59
2	F	500	A5A	O5'-S	-4.76	1.52	1.59
2	G	500	A5A	O5'-S	-3.26	1.54	1.59

The worst 5 of 54 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	500	A5A	N3-C2-N1	-10.17	120.88	128.87
2	D	500	A5A	N3-C2-N1	-9.59	121.34	128.87
2	B	500	A5A	N3-C2-N1	-9.16	121.67	128.87
2	F	500	A5A	N3-C2-N1	-7.45	123.02	128.87
2	H	500	A5A	N3-C2-N1	-6.75	123.56	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	A5A	1	0
2	C	500	A5A	3	0
2	D	500	A5A	1	0
2	E	500	A5A	2	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 [i](#)

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	450/450 (100%)	1.13	80 (17%) <b>2</b> <b>1</b>	19, 47, 69, 87	0
1	B	450/450 (100%)	1.43	105 (23%) <b>1</b> <b>1</b>	22, 48, 86, 113	0
1	C	444/450 (98%)	1.57	128 (28%) <b>1</b> <b>0</b>	34, 63, 92, 124	0
1	D	447/450 (99%)	1.70	131 (29%) <b>1</b> <b>0</b>	19, 61, 89, 127	0
1	E	450/450 (100%)	1.19	85 (18%) <b>2</b> <b>1</b>	21, 48, 75, 90	0
1	F	449/450 (99%)	1.23	91 (20%) <b>1</b> <b>1</b>	19, 46, 81, 100	0
1	G	449/450 (99%)	1.52	121 (26%) <b>1</b> <b>0</b>	31, 59, 85, 109	0
1	H	446/450 (99%)	1.54	131 (29%) <b>1</b> <b>0</b>	29, 60, 101, 122	0
All	All	3585/3600 (99%)	1.41	872 (24%) <b>1</b> <b>1</b>	19, 54, 88, 127	0

The worst 5 of 872 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	GLY	14.7
1	D	237	SER	13.8
1	E	288	ALA	11.0
1	G	122	LEU	10.3
1	H	237	SER	10.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	A5A	E	500	28/28	0.90	0.24	-0.18	20,24,46,63	0
2	A5A	D	500	28/28	0.89	0.29	-0.47	41,52,59,62	0
2	A5A	G	500	28/28	0.90	0.23	-0.58	22,53,68,75	0
2	A5A	B	500	28/28	0.91	0.23	-0.63	24,36,49,53	0
2	A5A	F	500	28/28	0.91	0.22	-0.86	26,32,35,39	0
2	A5A	A	500	28/28	0.87	0.21	-0.87	28,34,43,47	0
2	A5A	C	500	28/28	0.89	0.20	-1.12	43,52,63,65	0
2	A5A	H	500	28/28	0.88	0.21	-1.26	35,48,53,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.