



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:57 PM GMT

PDB ID : 3HTZ
Title : Crystal Structure of the catalytic fragment of alanyl-tRNA synthetase in complex with L-serine: Re-refined
Authors : Guo, M.; Swairjo, M.A.; Schimmel, P.
Deposited on : 2009-06-12
Resolution : 2.50 Å(reported)

This is a full wwPDB validation 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>

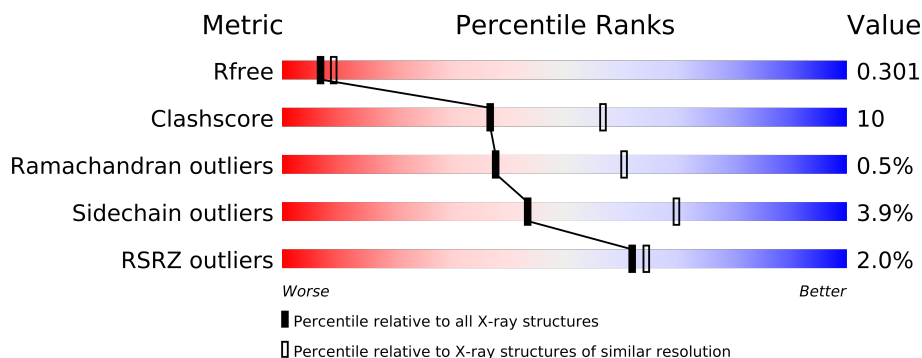
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	464	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3690 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 Alanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3631	2333	612	674	12	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	ALA	-	EXPRESSION TAG	UNP O67323
A	455	ALA	-	EXPRESSION TAG	UNP O67323
A	456	ALA	-	EXPRESSION TAG	UNP O67323
A	457	LEU	-	EXPRESSION TAG	UNP O67323
A	458	GLU	-	EXPRESSION TAG	UNP O67323
A	459	HIS	-	EXPRESSION TAG	UNP O67323
A	460	HIS	-	EXPRESSION TAG	UNP O67323
A	461	HIS	-	EXPRESSION TAG	UNP O67323
A	462	HIS	-	EXPRESSION TAG	UNP O67323
A	463	HIS	-	EXPRESSION TAG	UNP O67323
A	464	HIS	-	EXPRESSION TAG	UNP O67323

- Molecule 2 is water.

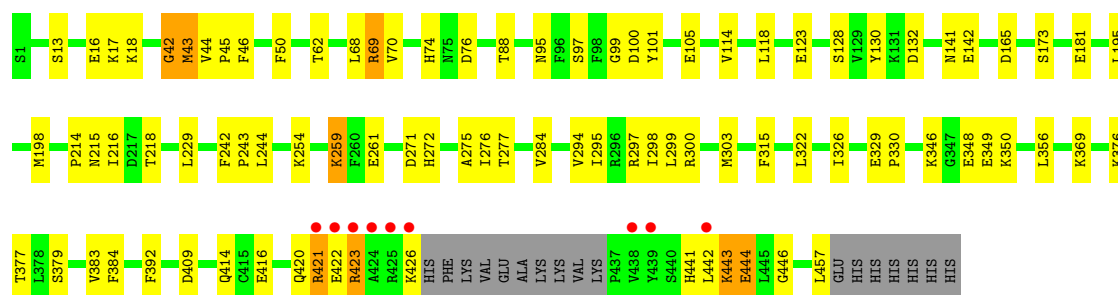
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total	O	0	0
			59	59		

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 ($\text{RSRZ} > 2$). 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: Alanyl-tRNA synthetase

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.09Å 74.09Å 173.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.05 – 2.50 37.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.05-2.50) 98.7 (37.05-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.250 , 0.315 0.241 , 0.301	Depositor DCC
R_{free} test set	882 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 11.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 17259 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3690	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.25	0/3714	0.43	0/5001

There are no bond length outliers.

There are no bond angle outliers.

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	A	3631	0	3594	74	0
2	A	59	0	0	7	0
All	All	3690	0	3594	74	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 10.

All (74) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:421:ARG:HH11	1:A:421:ARG:HG2	1.09	1.10
1:A:442:LEU:O	1:A:443:LYS:HB2	1.64	0.95
1:A:95:ASN:OD1	1:A:218:THR:OG1	1.85	0.94
1:A:444:GLU:HA	1:A:444:GLU:OE2	1.68	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:416:GLU:O	1:A:420:GLN:HG2	1.70	0.90
1:A:421:ARG:HG2	1:A:421:ARG:NH1	1.80	0.86
1:A:284:VAL:HG11	1:A:295:ILE:HD12	1.60	0.83
1:A:300:ARG:HD3	1:A:303:MET:HE3	1.61	0.83
1:A:422:GLU:O	1:A:426:LYS:N	2.13	0.81
1:A:384:PHE:CZ	1:A:420:GLN:HG3	2.16	0.79
1:A:329:GLU:HB2	1:A:330:PRO:HD3	1.66	0.76
1:A:254:LYS:HE2	2:A:504:HOH:O	1.85	0.75
1:A:423:ARG:CG	1:A:423:ARG:HH11	1.99	0.74
1:A:384:PHE:CE1	1:A:420:GLN:HG3	2.23	0.74
1:A:195:LEU:HA	1:A:218:THR:HG22	1.71	0.72
1:A:416:GLU:HG3	1:A:420:GLN:HE21	1.57	0.70
1:A:421:ARG:HH11	1:A:421:ARG:CG	1.96	0.68
1:A:414:GLN:OE1	1:A:446:GLY:N	2.29	0.65
1:A:329:GLU:HB2	1:A:330:PRO:CD	2.25	0.65
1:A:198:MET:HB3	1:A:215:ASN:HB2	1.78	0.65
1:A:141:ASN:HB3	2:A:503:HOH:O	1.96	0.64
1:A:181:GLU:CD	1:A:181:GLU:H	2.02	0.62
1:A:329:GLU:HG3	2:A:486:HOH:O	1.99	0.62
1:A:284:VAL:HG11	1:A:295:ILE:CD1	2.29	0.61
1:A:97:SER:HB3	1:A:216:ILE:HB	1.83	0.60
1:A:13:SER:O	1:A:17:LYS:HG3	2.03	0.58
1:A:409:ASP:HA	2:A:477:HOH:O	2.02	0.58
1:A:44:VAL:HB	1:A:45:PRO:CD	2.35	0.57
1:A:441:HIS:HB2	1:A:444:GLU:HG2	1.86	0.57
1:A:444:GLU:CA	1:A:444:GLU:OE2	2.50	0.56
1:A:423:ARG:NH1	1:A:423:ARG:HG3	2.19	0.56
1:A:276:ILE:HG13	1:A:277:THR:N	2.22	0.55
1:A:423:ARG:HG3	1:A:423:ARG:HH11	1.72	0.55
1:A:130:TYR:CE2	1:A:132:ASP:HB2	2.44	0.53
1:A:70:VAL:HG11	1:A:298:ILE:HD11	1.90	0.52
1:A:423:ARG:HG2	1:A:423:ARG:HH11	1.73	0.51
1:A:377:THR:HG21	2:A:477:HOH:O	2.10	0.51
1:A:315:PHE:N	1:A:315:PHE:CD2	2.78	0.51
1:A:294:VAL:HG22	1:A:297:ARG:HH21	1.76	0.51
1:A:42:GLY:HA3	2:A:473:HOH:O	2.10	0.50
1:A:259:LYS:HD2	1:A:261:GLU:HG2	1.92	0.50
1:A:50:PHE:HB3	1:A:198:MET:HE1	1.94	0.49
1:A:198:MET:CE	1:A:215:ASN:HD22	2.26	0.49
1:A:118:LEU:HD22	1:A:229:LEU:HD11	1.94	0.49
1:A:100:ASP:HB3	1:A:101:TYR:H	1.49	0.48
1:A:69:ARG:HH21	1:A:76:ASP:CG	2.16	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:303:MET:SD	1:A:349:GLU:HA	2.54	0.47
1:A:294:VAL:HG22	1:A:297:ARG:NH2	2.29	0.47
1:A:43:MET:O	1:A:46:PHE:N	2.47	0.46
1:A:99:GLY:HA3	1:A:214:PRO:O	2.16	0.46
1:A:88:THR:OG1	1:A:275:ALA:HB2	2.16	0.45
1:A:69:ARG:NH2	1:A:76:ASP:CG	2.70	0.45
1:A:68:LEU:HA	1:A:88:THR:O	2.17	0.45
1:A:128:SER:O	1:A:173:SER:HA	2.17	0.45
1:A:50:PHE:HB3	1:A:198:MET:CE	2.47	0.45
1:A:346:LYS:O	1:A:350:LYS:HB2	2.17	0.45
1:A:244:LEU:HD23	1:A:322:LEU:HD23	2.00	0.45
1:A:379:SER:O	1:A:383:VAL:HG23	2.17	0.44
1:A:322:LEU:O	1:A:326:ILE:HG13	2.17	0.44
1:A:423:ARG:NH1	1:A:423:ARG:CG	2.63	0.44
1:A:69:ARG:NH2	1:A:76:ASP:OD2	2.51	0.43
1:A:44:VAL:HB	1:A:45:PRO:HD3	2.01	0.43
1:A:195:LEU:HD22	1:A:218:THR:HG21	2.01	0.43
1:A:242:PHE:N	1:A:243:PRO:CD	2.83	0.42
1:A:181:GLU:CD	1:A:181:GLU:N	2.70	0.42
1:A:356:LEU:HD12	1:A:392:PHE:CZ	2.54	0.42
1:A:421:ARG:CG	1:A:421:ARG:NH1	2.60	0.42
1:A:441:HIS:O	1:A:444:GLU:HB2	2.20	0.42
1:A:101:TYR:HB2	1:A:105:GLU:HB2	2.01	0.42
1:A:299:LEU:HD13	1:A:348:GLU:HG2	2.02	0.41
1:A:114:VAL:HA	1:A:118:LEU:HD12	2.02	0.41
1:A:16:GLU:C	1:A:18:LYS:H	2.24	0.40
1:A:44:VAL:N	1:A:45:PRO:HD2	2.35	0.40
1:A:142:GLU:HG3	2:A:503:HOH:O	2.22	0.40

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	443/464 (96%)	424 (96%)	17 (4%)	2 (0%)	38 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLY
1	A	443	LYS

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	387/403 (96%)	372 (96%)	15 (4%)	43	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET
1	A	62	THR
1	A	69	ARG
1	A	74	HIS
1	A	123	GLU
1	A	165	ASP
1	A	259	LYS
1	A	271	ASP
1	A	272	HIS
1	A	369	LYS
1	A	376	LYS
1	A	421	ARG
1	A	423	ARG
1	A	444	GLU
1	A	457	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN

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 ⓘ

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(Å ²)	Q<0.9
1	A	447/464 (96%)	-0.00	9 (2%) 62 64	26, 39, 56, 86	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	ARG	4.5
1	A	424	ALA	4.0
1	A	426	LYS	3.9
1	A	439	TYR	2.9
1	A	423	ARG	2.8
1	A	438	VAL	2.5
1	A	422	GLU	2.4
1	A	421	ARG	2.3
1	A	442	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.