



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:06 AM GMT

PDB ID : 1ZQ1
Title : Structure of GatDE tRNA-Dependent Amidotransferase from *Pyrococcus abyssi*
Authors : Schmitt, E.; Panvert, M.; Blanquet, S.; Mechulam, Y.
Deposited on : 2005-05-18
Resolution : 3.00 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

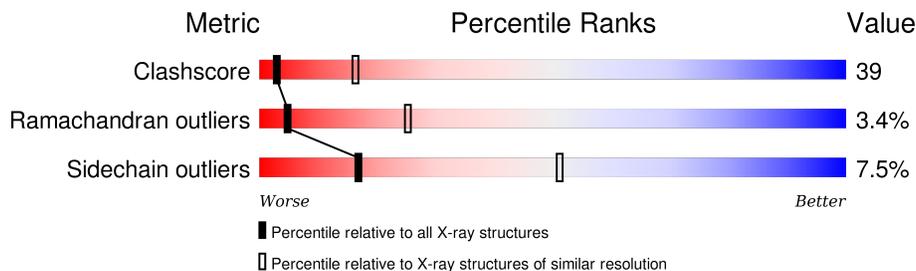
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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	438	
1	B	438	
2	C	633	
2	D	633	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ASP	A	1000	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14869 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(Gln) amidotransferase subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	437	3406	2159	578	650	5	14	0	0	0
1	B	437	3406	2162	575	650	5	14	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	36	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	127	LEU	VAL	CONFLICT	UNP Q9V0T9
A	149	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	181	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	191	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	217	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	225	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	234	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	237	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	257	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	362	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	393	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	403	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	418	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
A	419	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	36	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	127	LEU	VAL	CONFLICT	UNP Q9V0T9
B	149	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	181	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	191	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	217	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	225	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	234	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9

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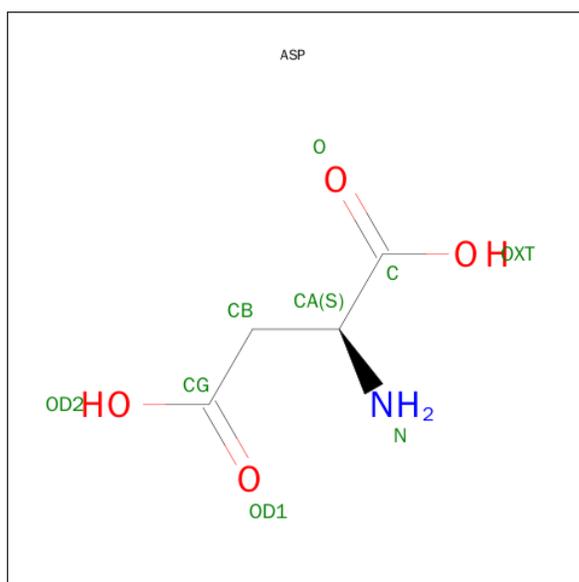
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Chain	Residue	Modelled	Actual	Comment	Reference
B	237	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	257	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	362	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	393	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	403	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	418	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9
B	419	MSE	MET	MODIFIED RESIDUE	UNP Q9V0T9

- Molecule 2 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	508	Total	C	N	O	S	0	0	0
			4005	2543	700	755	7			
2	D	508	Total	C	N	O	S	0	0	0
			3966	2523	693	743	7			

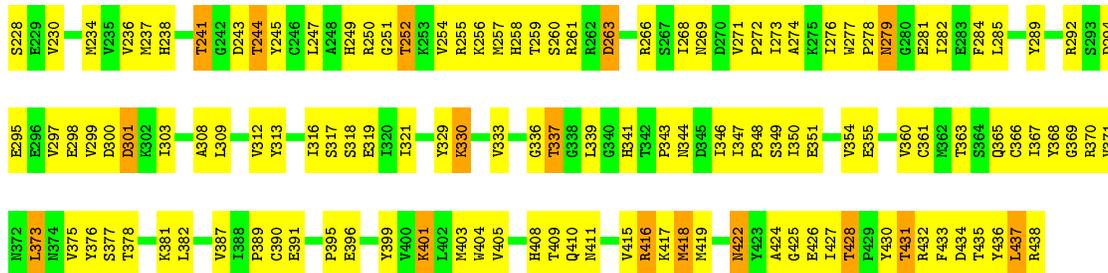
- Molecule 3 is ASPARTIC ACID (three-letter code: ASP) (formula: C₄H₇NO₄).



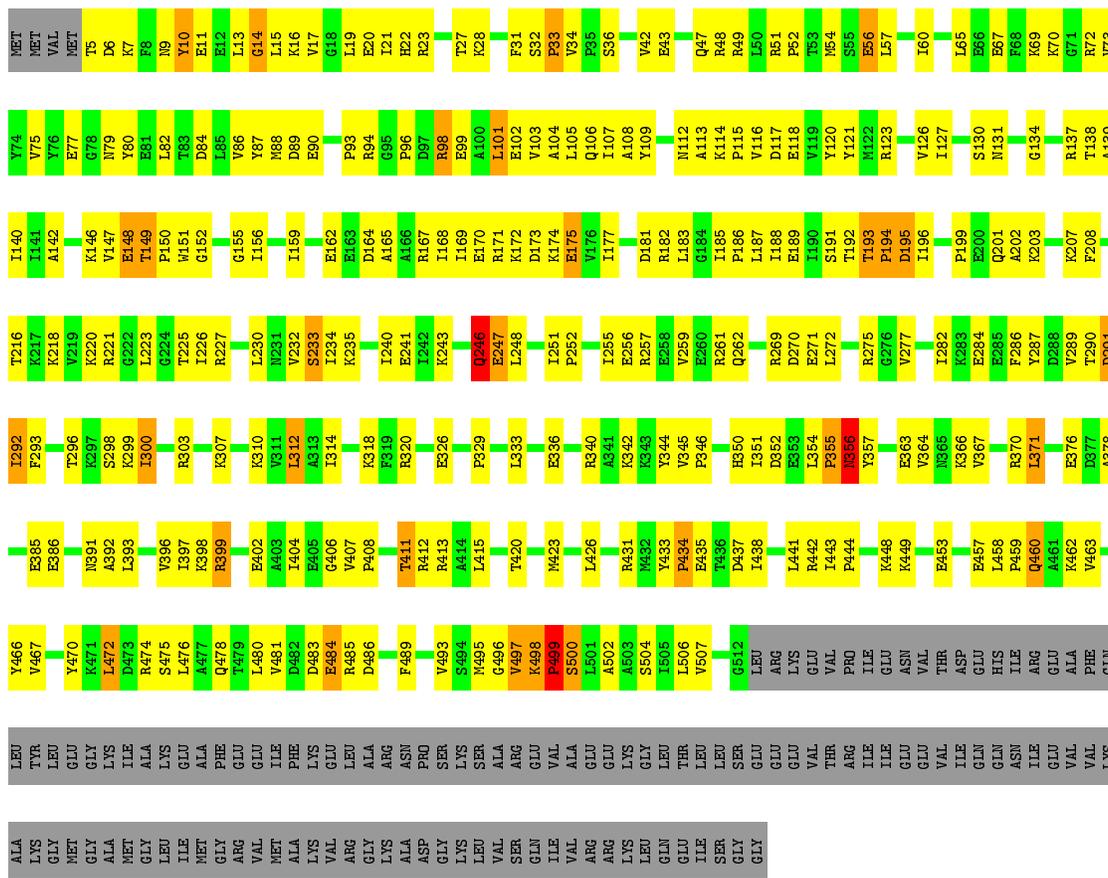
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		
3	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 4 is water.

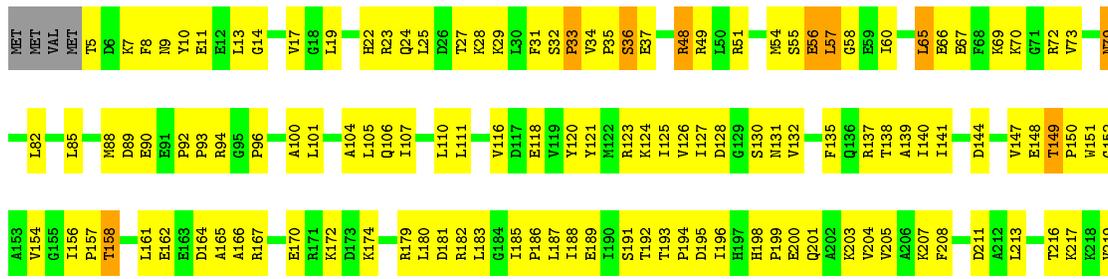
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	24	Total 24	O 24	0	0
4	C	22	Total 22	O 22	0	0
4	D	10	Total 10	O 10	0	0



• Molecule 2: Glutanyl-tRNA(Gln) amidotransferase subunit E



• Molecule 2: Glutanyl-tRNA(Gln) amidotransferase subunit E



4 Data and refinement statistics

Xtrriage (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	102.70Å 138.20Å 134.40Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.9 (50.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14869	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/3455	0.72	2/4651 (0.0%)
1	B	0.42	0/3455	0.73	0/4652
2	C	0.39	0/4070	0.69	0/5497
2	D	0.33	0/4031	0.62	0/5450
All	All	0.39	0/15011	0.69	2/20250 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	PRO	N-CA-C	5.26	125.78	112.10
1	A	45	ASP	N-CA-C	-5.25	96.82	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3406	0	3410	355	0
1	B	3406	0	3417	335	0
2	C	4005	0	4058	287	0
2	D	3966	0	4003	279	0
3	A	9	0	3	4	0
3	B	9	0	3	1	0
4	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	0	0
4	C	22	0	0	0	0
4	D	10	0	0	0	0
All	All	14869	0	14894	1160	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 39.

The worst 5 of 1160 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)
2:C:192:THR:HG22	2:C:193:THR:H	1.02	1.12
2:D:192:THR:HG22	2:D:193:THR:H	1.00	1.11
1:B:276:ILE:HG22	1:B:282:ILE:HG12	1.27	1.09
1:A:266:ARG:HD2	1:B:437:LEU:HD21	1.36	1.07
1:A:409:THR:HG22	1:A:411:ASN:H	1.18	1.05

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	435/438 (99%)	374 (86%)	49 (11%)	12 (3%)	6	30
1	B	435/438 (99%)	366 (84%)	56 (13%)	13 (3%)	5	29
2	C	506/633 (80%)	434 (86%)	54 (11%)	18 (4%)	4	24
2	D	506/633 (80%)	428 (85%)	57 (11%)	21 (4%)	3	20
All	All	1882/2142 (88%)	1602 (85%)	216 (12%)	64 (3%)	5	25

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	77	PRO
1	A	78	GLU
1	A	163	LYS
1	A	251	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	366/357 (102%)	338 (92%)	28 (8%)	16	50
1	B	367/357 (103%)	331 (90%)	36 (10%)	10	36
2	C	421/548 (77%)	395 (94%)	26 (6%)	23	60
2	D	412/548 (75%)	384 (93%)	28 (7%)	20	56
All	All	1566/1810 (86%)	1448 (92%)	118 (8%)	17	51

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	366	CYS
2	C	98	ARG
2	D	399	ARG
1	B	371	VAL
1	B	422	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	344	ASN
2	C	47	GLN
2	D	356	ASN
1	B	408	HIS
1	B	422	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	ASP	A	1000	-	2,8,8	0.52	0	0,10,10	0.00	-
3	ASP	B	5000	-	2,8,8	0.62	0	0,10,10	0.00	-

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
3	ASP	A	1000	-	-	0/2/8/8	0/0/0/0
3	ASP	B	5000	-	-	0/2/8/8	0/0/0/0

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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	ASP	4	0
3	B	5000	ASP	1	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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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