



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2022 – 01:14 pm BST

PDB ID : 7QCF
Title : X-ray crystallographic structure of E. coli K-12 glycyl-tRNA synthetase alpha subunit (glyQ)
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Deposited on : 2021-11-23
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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

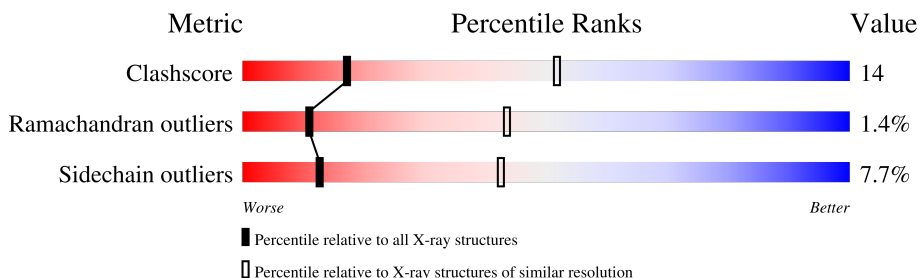
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	
1	C	305	
1	D	305	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9032 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 Glycine-tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2244	1448	363	421	12			
1	B	285	Total	C	N	O	S	0	0	0
			2263	1455	369	427	12			
1	C	282	Total	C	N	O	S	0	0	0
			2246	1444	367	423	12			
1	D	287	Total	C	N	O	S	0	0	0
			2279	1465	374	428	12			

There are 12 discrepancies between the modelled and reference sequences:

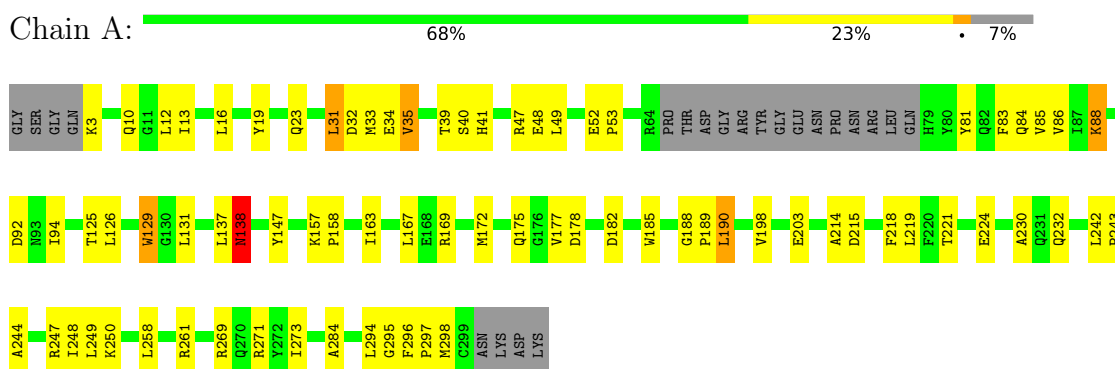
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P00960
A	0	SER	-	expression tag	UNP P00960
A	1	GLY	-	expression tag	UNP P00960
B	-1	GLY	-	expression tag	UNP P00960
B	0	SER	-	expression tag	UNP P00960
B	1	GLY	-	expression tag	UNP P00960
C	-1	GLY	-	expression tag	UNP P00960
C	0	SER	-	expression tag	UNP P00960
C	1	GLY	-	expression tag	UNP P00960
D	-1	GLY	-	expression tag	UNP P00960
D	0	SER	-	expression tag	UNP P00960
D	1	GLY	-	expression tag	UNP P00960

3 Residue-property plots [i](#)

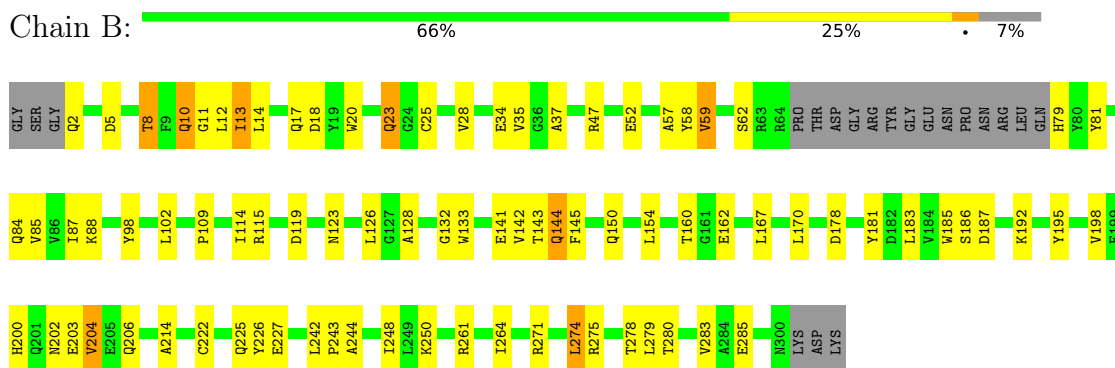
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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 failed to run properly.

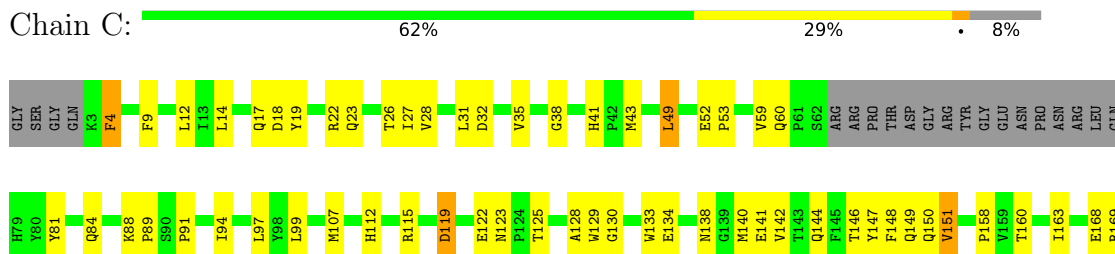
- Molecule 1: Glycine-tRNA ligase alpha subunit



- Molecule 1: Glycine-tRNA ligase alpha subunit



- Molecule 1: Glycine-tRNA ligase alpha subunit



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	232.41Å 232.41Å 123.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (49.43-3.00)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.219 , 0.258	Depositor
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.310	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9032	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	0.31	0/2304	0.67	0/3141
1	B	0.33	0/2323	0.70	0/3167
1	C	0.34	0/2306	0.73	0/3144
1	D	0.37	0/2339	0.77	0/3189
All	All	0.34	0/9272	0.72	0/12641

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 [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	2244	0	2139	56	0
1	B	2263	0	2146	69	0
1	C	2246	0	2134	68	0
1	D	2279	0	2163	66	0
All	All	9032	0	8582	245	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 14.

The worst 5 of 245 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:35:VAL:HG21	1:A:249:LEU:HB3	1.40	1.03
1:D:248:ILE:CD1	1:D:283:VAL:HG21	1.90	1.02
1:D:169:ARG:HG3	1:D:169:ARG:HH11	1.23	0.99
1:C:123:ASN:HD21	1:C:125:THR:HG22	1.36	0.91
1:C:130:GLY:HA2	1:C:149:GLN:HG3	1.54	0.88

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	279/305 (92%)	257 (92%)	17 (6%)	5 (2%)	8	37
1	B	281/305 (92%)	255 (91%)	25 (9%)	1 (0%)	34	72
1	C	278/305 (91%)	253 (91%)	23 (8%)	2 (1%)	22	60
1	D	283/305 (93%)	249 (88%)	26 (9%)	8 (3%)	5	25
All	All	1121/1220 (92%)	1014 (90%)	91 (8%)	16 (1%)	11	43

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	D	34	GLU
1	D	35	VAL
1	D	39	THR
1	A	40	SER

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	234/261 (90%)	219 (94%)	15 (6%)	17	51
1	B	236/261 (90%)	219 (93%)	17 (7%)	14	45
1	C	235/261 (90%)	217 (92%)	18 (8%)	13	42
1	D	237/261 (91%)	214 (90%)	23 (10%)	8	31
All	All	942/1044 (90%)	869 (92%)	73 (8%)	13	42

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	111	ILE
1	D	254	SER
1	D	141	GLU
1	D	186	SER
1	B	144	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	200	HIS
1	D	29	GLN
1	D	149	GLN
1	C	270	GLN
1	C	10	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.