



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:36 AM GMT

PDB ID : 2RE8
Title : Glutaminyl-tRNA synthetase mutant C229R with bound analog 5'-O-[N-(L-GLUTAMYL)-SULFAMOYL]ADENOSINE
Authors : Bullock, T.L.; Perona, J.J.
Deposited on : 2007-09-25
Resolution : 2.60 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

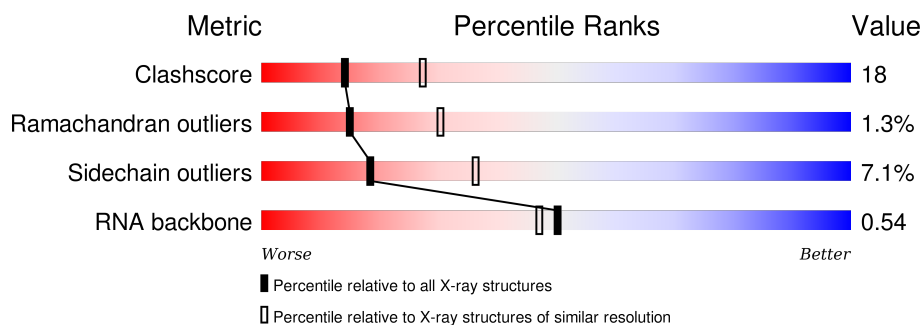
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RNA backbone	2183	1022 (3.00-2.20)

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	B	75	 43% 36% 17% ..
2	A	556	 64% 26% . 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6033 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 RNA chain called Glutamine tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	74	Total	C	N	O	P	0	0	0
			1570	702	279	516	73			

- Molecule 2 is a protein called Glutaminyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	529	Total	C	N	O	S	0	0	0
			4284	2707	755	802	20			

There are 9 discrepancies between the modelled and reference sequences:

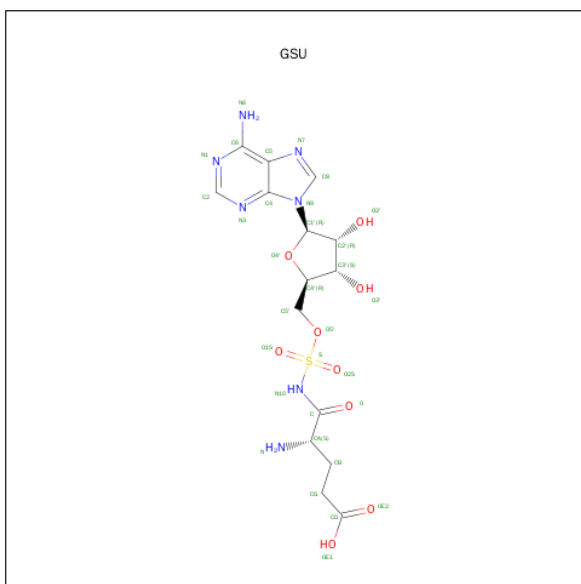
Chain	Residue	Modelled	Actual	Comment	Reference
A	229	ARG	CYS	ENGINEERED	UNP P00962
A	548	LEU	-	EXPRESSION TAG	UNP P00962
A	549	GLU	-	EXPRESSION TAG	UNP P00962
A	550	HIS	-	EXPRESSION TAG	UNP P00962
A	551	HIS	-	EXPRESSION TAG	UNP P00962
A	552	HIS	-	EXPRESSION TAG	UNP P00962
A	553	HIS	-	EXPRESSION TAG	UNP P00962
A	554	HIS	-	EXPRESSION TAG	UNP P00962
A	555	HIS	-	EXPRESSION TAG	UNP P00962

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is O5'-(L-GLUTAMYL-SULFAMOYL)-ADENOSINE (three-letter code: GSU) (formula: $C_{15}H_{21}N_7O_9S$).



- Molecule 5 is water.

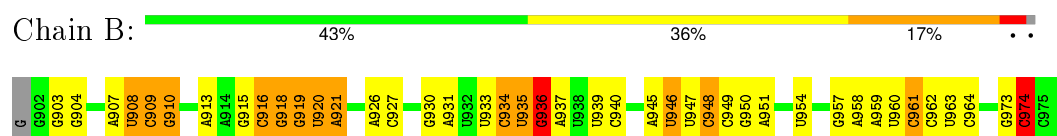
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total 108	O 108	0	0
5	B	29	Total 29	O 29	0	0

3 Residue-property plots

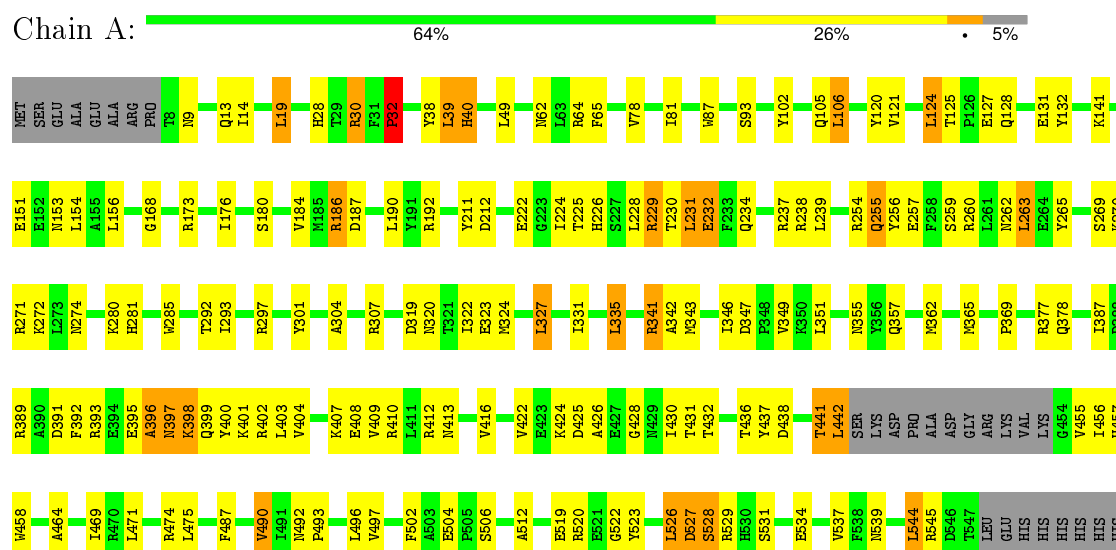
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: Glutamine tRNA



• Molecule 2: Glutaminyl-tRNA synthetase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	237.14Å 92.91Å 115.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.60 – 2.60	Depositor
% Data completeness (in resolution range)	93.5 (118.60-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6033	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GSU, SO4

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	B	0.35	0/1753	0.79	2/2730 (0.1%)
2	A	0.41	0/4384	0.63	0/5934
All	All	0.40	0/6137	0.68	2/8664 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	974	C	N1-C1'-C2'	6.25	122.13	114.00
1	B	936	G	N9-C1'-C2'	6.13	121.97	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	948	C	Sidechain

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	B	1570	0	801	41	0
2	A	4284	0	4180	158	0
3	A	10	0	0	2	0
4	A	32	0	20	3	0
5	A	108	0	0	8	0
5	B	29	0	0	1	0
All	All	6033	0	5001	194	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 18.

The worst 5 of 194 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:A:526:LEU:HG	2:A:527:ASP:H	1.34	0.92
2:A:393:ARG:HG2	2:A:396:ALA:HB2	1.53	0.88
2:A:529:ARG:HA	2:A:529:ARG:HE	1.39	0.87
2:A:255:GLN:HE21	2:A:255:GLN:N	1.72	0.85
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.59	0.85

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	
2	A	525/556 (94%)	493 (94%)	25 (5%)	7 (1%)	15	30

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	397	ASN
2	A	526	LEU
2	A	527	ASP
2	A	176	ILE

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	463/486 (95%)	430 (93%)	33 (7%)	18	36

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	192	ARG
2	A	255	GLN
2	A	490	VAL
2	A	229	ARG
2	A	231	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	226	HIS
2	A	236	ASN
2	A	368	HIS
2	A	153	ASN
2	A	355	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/75 (97%)	17 (23%)	8 (10%)

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	908	U
1	B	909	C
1	B	910	G
1	B	916	C
1	B	918	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	934	C
1	B	974	C
1	B	936	G
1	B	919	G
1	B	935	U

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](#)

3 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	SO4	A	1394	-	4,4,4	0.04	0	6,6,6	0.14	0
3	SO4	A	1395	-	4,4,4	0.45	0	6,6,6	0.21	0
4	GSU	A	998	-	24,34,34	1.02	2 (8%)	30,50,50	2.25	6 (20%)

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	SO4	A	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
4	GSU	A	998	-	-	0/16/40/40	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	998	GSU	C8-N7	-2.58	1.29	1.34
4	A	998	GSU	O4'-C1'	2.56	1.44	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	GSU	N3-C2-N1	-9.44	121.67	128.89
4	A	998	GSU	C5'-O5'-S	-3.87	110.61	118.02
4	A	998	GSU	O2S-S-N10	-3.33	104.05	108.50
4	A	998	GSU	C4-C5-N7	-2.63	107.06	109.48
4	A	998	GSU	O4'-C4'-C3'	2.10	109.37	105.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1394	SO4	1	0
3	A	1395	SO4	1	0
4	A	998	GSU	3	0

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

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.