



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 06:57 pm GMT

PDB ID : 2RD2
Title : Glutaminyl-tRNA synthetase mutant C229R with bound analog 5'-O-[N-(L-GLUTAMINYL)-SULFAMOYL]ADENOSINE
Authors : Bullock, T.L.; Perona, J.J.
Deposited on : 2007-09-20
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

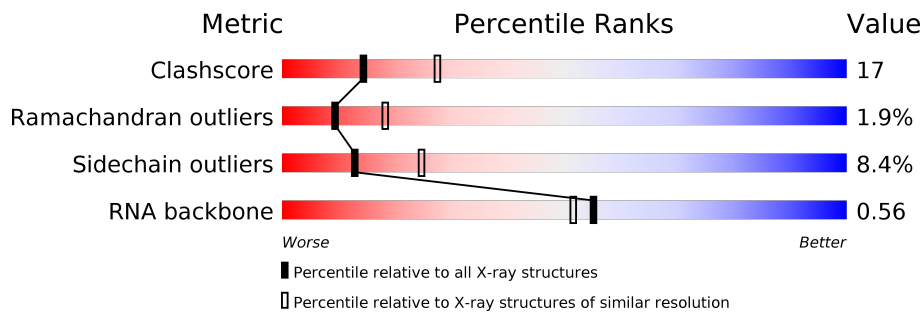
1 Overall quality at a glance

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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RNA backbone	2435	1140 (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	 41% 40% 16% ..
2	A	556	 63% 27% 5% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6032 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:

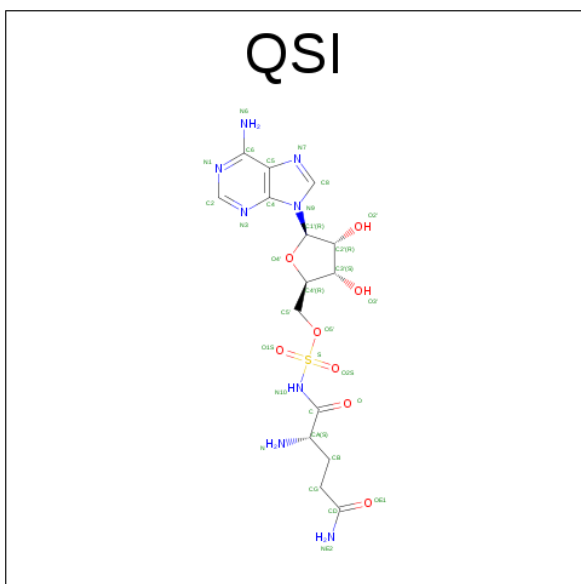
Chain	Residue	Modelled	Actual	Comment	Reference
A	229	ARG	CYS	ENGINEERED	UNP P00962
A	548	LEU	-	EXPRESSION TAG	UNP P00962
A	549	GLU	-	EXPRESSION TAG	UNP P00962
A	550	HIS	-	EXPRESSION TAG	UNP P00962
A	551	HIS	-	EXPRESSION TAG	UNP P00962
A	552	HIS	-	EXPRESSION TAG	UNP P00962
A	553	HIS	-	EXPRESSION TAG	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 5'-O-[N-(L-GLUTAMINYL)-SULFAMOYL]ADENOSINE (three-letter code: QSI) (formula: C₁₅H₂₂N₈O₈S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0
			32	15	8	8	1	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total 110	O 110	0	0
5	B	26	Total 26	O 26	0	0

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	237.66Å 93.34Å 114.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.50 – 2.60	Depositor
% Data completeness (in resolution range)	94.0 (119.50-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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: QSI, 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	0.77	2/2730 (0.1%)
2	A	0.40	0/4384	0.62	0/5934
All	All	0.39	0/6137	0.67	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(°)	Ideal(°)
1	B	974	C	N1-C1'-C2'	6.16	122.01	114.00
1	B	936	G	N9-C1'-C2'	5.85	121.60	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	960	U	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	43	0
2	A	4284	0	4180	151	0
3	A	10	0	0	0	0
4	A	32	0	22	3	0
5	A	110	0	0	13	0
5	B	26	0	0	0	0
All	All	6032	0	5003	188	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 17.

The worst 5 of 188 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	1.31	0.93
1:B:950:G:H1	1:B:964:C:H42	1.23	0.87
2:A:136:LEU:HD23	2:A:183:ILE:HD11	1.58	0.83
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.63	0.80
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.64	0.79

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%)	487 (93%)	28 (5%)	10 (2%)	9 18

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	405	LEU
2	A	370	ASN
2	A	397	ASN
2	A	396	ALA
2	A	32	PRO

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
2	A	463/486 (95%)	424 (92%)	39 (8%)	13 25

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	232	GLU
2	A	322	ILE
2	A	506	SER
2	A	234	GLN
2	A	263	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	234	GLN
2	A	236	ASN
2	A	429	ASN
2	A	226	HIS
2	A	368	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/75 (97%)	18 (24%)	0

5 of 18 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	908	U
1	B	910	G
1	B	916	C
1	B	918	G
1	B	919	G

There are no RNA pucker outliers to report.

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	0.22	0	6,6,6	0.09	0
3	SO4	A	1395	-	4,4,4	0.36	0	6,6,6	0.10	0
4	QSI	A	998	-	30,34,34	1.49	5 (16%)	32,50,50	2.04	6 (18%)

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	QSI	A	998	-	-	0/19/40/40	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	998	QSI	O5'-S	-3.23	1.54	1.59
4	A	998	QSI	C8-N7	-3.15	1.28	1.34
4	A	998	QSI	O1S-S	-2.55	1.40	1.42
4	A	998	QSI	O4'-C1'	2.04	1.44	1.41
4	A	998	QSI	S-N10	5.17	1.65	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	QSI	N3-C2-N1	-8.71	121.27	128.86
4	A	998	QSI	C5'-O5'-S	-3.52	111.18	118.03
4	A	998	QSI	O2S-S-N10	-2.93	104.37	108.47
4	A	998	QSI	CG-CB-CA	-2.00	109.17	113.84
4	A	998	QSI	O4'-C4'-C3'	2.00	109.14	105.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	998	QSI	3	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.