wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:35 PM GMT

PDB ID	:	1GAR
Title	:	TOWARDS STRUCTURE-BASED DRUG DESIGN: CRYSTAL STRUCTURE OF A MULTISUBSTRATE ADDUCT COMPLEX OF GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE AT 1.96 ANGSTROMS RESOLUTION
Authors	:	Wilson, I.A.; Klein, C.; Chen, P.; Arevalo, J.H.
Deposited on	:	1994-12-08
Resolution	:	1.96 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 (i) symbol.

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

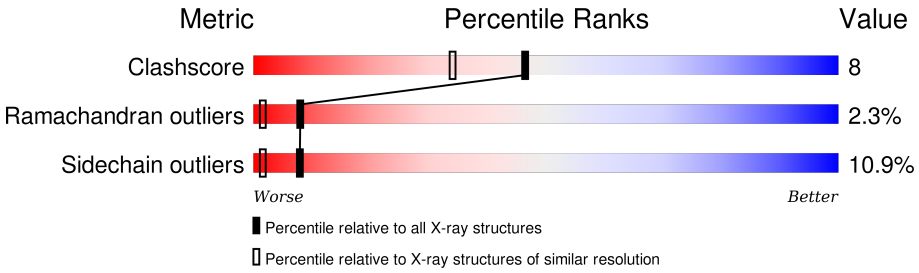
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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 <=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	212	74% 20%
1	B	212	67% 20% 8%

2 Entry composition

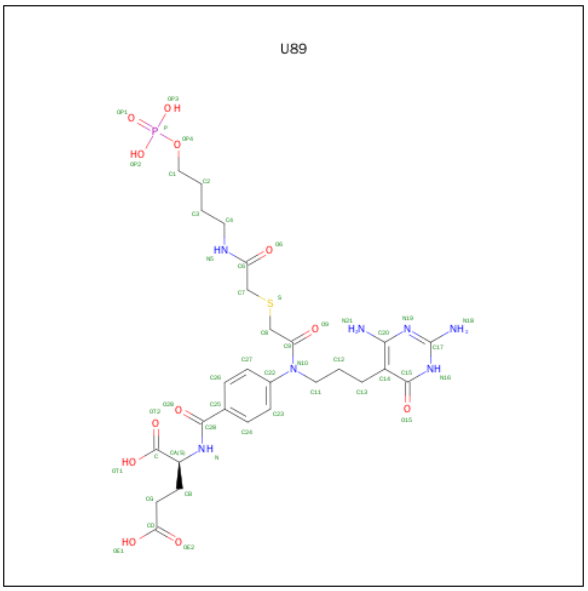
There are 3 unique types of molecules in this entry. The entry contains 3567 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	3	1
			1553	978	279	291	5			
1	B	194	Total	C	N	O	S	0	1	1
			1496	948	264	279	5			

- Molecule 2 is N-[4-[[3-(2,4-DIAMINO-1,6-DIHYDRO-6-OXO-4-PYRIMIDINYL)-PROPYL]-[2-((2-OXO-2-((4-PHOSPHORIBOXY)-BUTYL)-AMINO)-ETHYL)-THIO-ACETYL]-AMINO]BENZOYL]-1-GLUTAMIC ACID (three-letter code: U89) (formula: $C_{27}H_{38}N_7O_{12}PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	1
			96	54	14	24	2	2		
2	B	1	Total	C	N	O	P	S	0	1
			96	54	14	24	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	B	163	Total 163	O 163	0	0

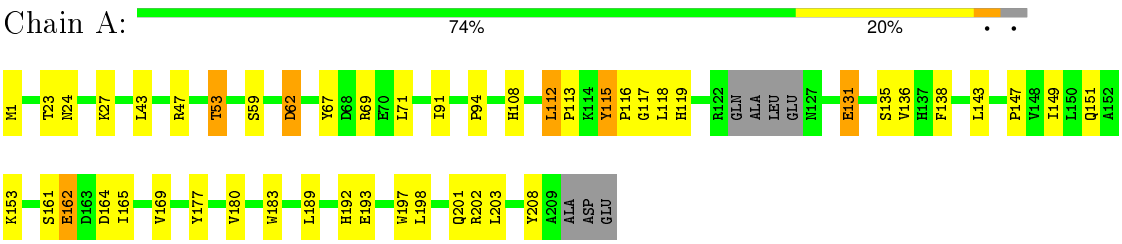
3 Residue-property plots (i)

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 (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.

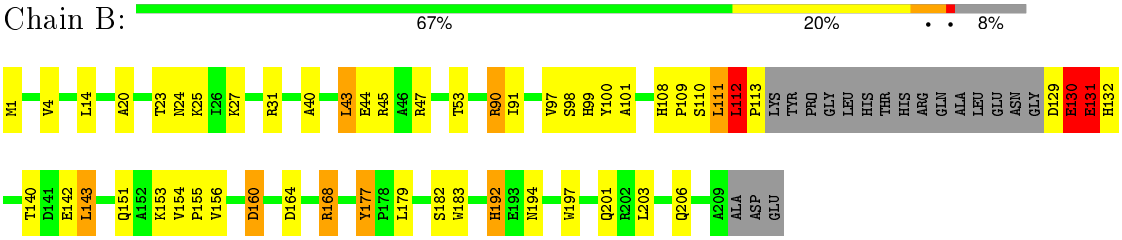
- Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE

Chain A:



- Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (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	75.70Å 73.30Å 35.50Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	6.00 – 1.96	Depositor
% Data completeness (in resolution range)	71.6 (6.00-1.96)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.168 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3567	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U89

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	0.81	0/1597	1.36	10/2165 (0.5%)
1	B	0.81	1/1532 (0.1%)	1.52	21/2082 (1.0%)
All	All	0.81	1/3129 (0.0%)	1.44	31/4247 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	LEU	C-N	-5.46	1.23	1.34

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	31	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	B	183	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	A	183	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	B	197	TRP	CE2-CD2-CG	-7.64	101.18	107.30
1	B	160	ASP	CA-C-N	-7.64	100.39	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1553	0	1498	20	0
1	B	1496	0	1471	28	0
2	A	96	0	68	4	0
2	B	96	0	68	3	0
3	A	163	0	0	3	0
3	B	163	0	0	4	0
All	All	3567	0	3105	48	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 8.

The worst 5 of 48 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:91:ILE:HG13	2:A:213[A]:U89:H26	1.66	0.78
1:A:135:SER:HB3	1:A:151:GLN:HG2	1.69	0.72
1:A:115:TYR:HA	1:A:131:GLU:HB3	1.73	0.71
1:B:111:LEU:HD12	1:B:151:GLN:HB3	1.83	0.60
1:B:40:ALA:HB3	1:B:43:LEU:HD22	1.84	0.58

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	204/212 (96%)	186 (91%)	10 (5%)	8 (4%)	4 0
1	B	191/212 (90%)	176 (92%)	14 (7%)	1 (0%)	34 21
All	All	395/424 (93%)	362 (92%)	24 (6%)	9 (2%)	8 1

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PRO
1	A	115	TYR
1	A	116	PRO
1	A	118	LEU
1	B	131	GLU

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	159/171 (93%)	143 (90%)	16 (10%)	9 2
1	B	157/171 (92%)	139 (88%)	18 (12%)	7 1
All	All	316/342 (92%)	282 (89%)	34 (11%)	8 2

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	LEU
1	B	43	LEU
1	B	201	GLN
1	B	14	LEU
1	A	94	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	B	99	HIS
1	B	151	GLN

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)

4 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	$\#\|Z\| > 2$
2	U89	A	213[A]	-	42,49,49	1.64	7 (16%)	42,66,66	1.74	8 (19%)
2	U89	A	213[B]	-	42,49,49	1.54	8 (19%)	42,66,66	1.94	10 (23%)
2	U89	B	213[A]	-	42,49,49	1.50	7 (16%)	42,66,66	1.61	7 (16%)
2	U89	B	213[B]	-	42,49,49	1.44	7 (16%)	42,66,66	1.66	7 (16%)

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
2	U89	A	213[A]	-	-	0/41/47/47	0/2/2/2
2	U89	A	213[B]	-	-	0/41/47/47	0/2/2/2
2	U89	B	213[A]	-	-	0/41/47/47	0/2/2/2
2	U89	B	213[B]	-	-	0/41/47/47	0/2/2/2

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	213[A]	U89	C25-C28	-4.90	1.39	1.50
2	A	213[B]	U89	C25-C28	-3.97	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	213[B]	U89	C25-C28	-3.94	1.41	1.50
2	B	213[A]	U89	C22-N10	-3.67	1.34	1.43
2	B	213[A]	U89	C25-C28	-3.30	1.43	1.50

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	213[B]	U89	C8-S-C7	-4.61	90.57	100.90
2	A	213[A]	U89	CG-CB-CA	-4.45	103.94	112.99
2	A	213[B]	U89	CG-CB-CA	-3.80	105.26	112.99
2	A	213[A]	U89	C11-N10-C22	-3.71	110.17	117.03
2	B	213[A]	U89	N16-C17-N19	-3.31	120.11	125.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	213[A]	U89	3	0
2	A	213[B]	U89	1	0
2	B	213[A]	U89	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

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.