

# wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 12:12 PM EDT

PDB ID : 1A9Y

Title : UDP-GALACTOSE 4-EPIMERASE MUTANT S124A/Y149F COM-

PLEXED WITH UDP-GLUCOSE

Authors: Thoden, J.B.; Holden, H.M.

Deposited on : 1998-04-14

Resolution : 1.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

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)

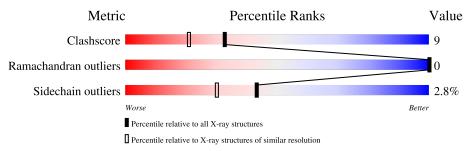
Validation Pipeline (wwPDB-VP) : 2.23.2

### 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 1.80 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 <=5%

Note EDS was not executed.

Mo	l Chain	Length	Quality of chain						
1	A	338	72%	22%	6% •				



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3249 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 UDP-GALACTOSE 4-EPIMERASE.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	Λ	338	Total	С	N	О	S	0	0	0
1	A	330	2624	1656	463	493	12	0	U	

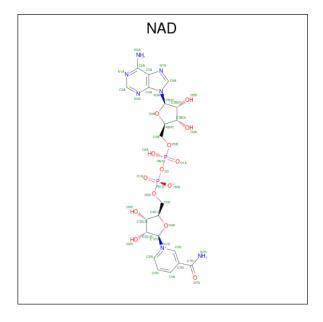
There are 2 discrepancies between the modelled and reference sequences:

Chain	hain Residue Modelled		Actual	Comment	Reference	
Α	124	ALA	SER	engineered mutation	UNP P09147	
A	149	PHE	TYR	engineered mutation	UNP P09147	

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Na 4 4	0	0

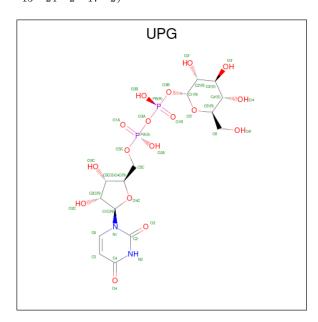
• Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Λ	1	Total	С	N	О	Р	0	0
3	А	1	44	21	7	14	2		

• Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula:  $C_{15}H_{24}N_2O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 36		_	O 17	P 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	541	Total O 541 541	0	0

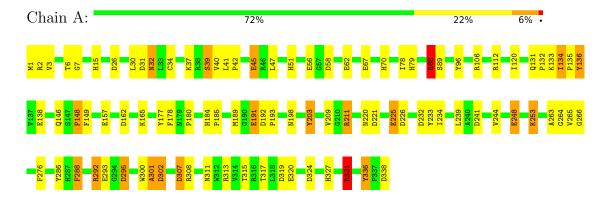


## 3 Residue-property plots (i)

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 was not executed.

• Molecule 1: UDP-GALACTOSE 4-EPIMERASE





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 32 2 1	Depositor	
Cell constants	85.00Å 85.00Å 106.70Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	30.00 - 1.80	Depositor	
% Data completeness	91.0 (30.00-1.80)	Depositor	
(in resolution range)	31.0 (80.00 1.00)		
$R_{merge}$	0.04	Depositor	
$R_{sym}$	0.04	Depositor	
Refinement program	TNT 5E	Depositor	
$R, R_{free}$	0.181 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3249	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	25.0	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: NAD, UPG, NA

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	Bo	nd lengths	Bond angles		
			RMSZ	# Z  > 5	RMSZ	# Z  > 5	
	1	A	1.21	25/2690~(0.9%)	1.75	61/3660 (1.7%)	

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
1	A	203	TYR	CG-CD2	21.09	1.66	1.39
1	A	203	TYR	CG-CD1	-18.61	1.15	1.39
1	A	203	TYR	CE1-CZ	15.95	1.59	1.38
1	A	276	PHE	CE1-CZ	8.64	1.53	1.37
1	A	253	LYS	CE-NZ	8.20	1.69	1.49

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	203	TYR	CG-CD1-CE1	23.00	139.70	121.30
1	A	203	TYR	CB-CG-CD1	20.84	133.51	121.00
1	A	203	TYR	CB-CG-CD2	-15.74	111.56	121.00
1	A	203	TYR	CD1-CE1-CZ	-15.71	105.66	119.80
1	A	203	TYR	CG-CD2-CE2	-13.80	110.26	121.30

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	2624	0	2557	46	0
2	A	4	0	0	0	0
3	A	44	0	26	0	0
4	A	36	0	22	0	0
5	A	541	0	0	10	3
All	All	3249	0	2605	46	3

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 9.

The worst 5 of 46 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:A:253:LYS:CE	1:A:253:LYS:NZ	1.69	1.54
1:A:327:HIS:O	1:A:331:ARG:HG3	1.89	0.72
1:A:88:GLU:HG3	5:A:884:HOH:O	1.89	0.71
1:A:131:GLN:NE2	1:A:132:PRO:HD2	2.06	0.70
1:A:146:GLN:HG3	5:A:880:HOH:O	1.96	0.65

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
5:A:922:HOH:O	5:A:922:HOH:O[5_675]	1.83	0.37	
5:A:624:HOH:O	5:A:624:HOH:O[6_554]	2.02	0.18	
5:A:572:HOH:O	5:A:709:HOH:O[6_554]	2.17	0.03	

### 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	336/338 (99%)	327 (97%)	9 (3%)	0	100	100



There are no Ramachandran outliers to report.

#### 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	281/281 (100%)	273 (97%)	8 (3%)	43 30	

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	ARG
1	A	225	GLU
1	A	209	VAL
1	A	203	TYR
1	A	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	131	GLN
1	A	158	GLN
1	A	274	ASN
1	A	285	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	Trus	Chain	Res	Link	Bo	Bond lengths			Bond angles		
MOI	Type	Chain			Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
3	NAD	A	340	-	42,48,48	2.06	8 (19%)	50,73,73	2.19	10 (20%)	
4	UPG	A	341	-	31,38,38	1.43	2 (6%)	41,58,58	1.71	7 (17%)	

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	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
3	NAD	A	340	-	-	5/26/62/62	0/5/5/5
4	UPG	A	341	-	-	1/21/59/59	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
3	A	340	NAD	C5N-C4N	7.57	1.54	1.38
3	A	340	NAD	C4N-C3N	5.69	1.49	1.39
3	A	340	NAD	C2N-C3N	5.02	1.46	1.39
4	A	341	UPG	C4-N3	4.23	1.40	1.33
3	A	340	NAD	C2D-C1D	-4.20	1.47	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
3	A	340	NAD	C3N-C7N-N7N	7.45	126.69	117.75

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	340	NAD	C5N-C4N-C3N	-6.40	112.77	120.34
3	A	340	NAD	O7N-C7N-C3N	-5.90	112.57	119.63
3	A	340	NAD	C6N-N1N-C2N	-4.71	117.68	121.97
4	A	341	UPG	O4C-C1C-C2C	-4.55	100.27	106.93

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

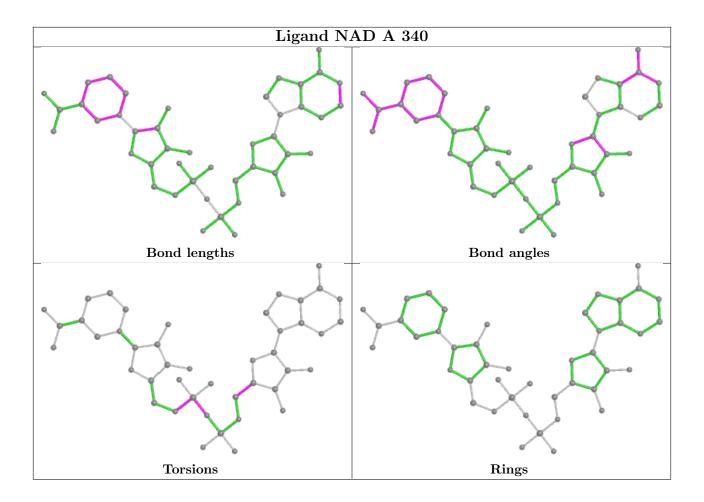
Mol	Chain	Res	Type	Atoms
4	A	341	UPG	PA-O3A-PB-O1B
3	A	340	NAD	C5D-O5D-PN-O2N
3	A	340	NAD	PA-O3-PN-O2N
3	A	340	NAD	O4B-C4B-C5B-O5B
3	A	340	NAD	C5D-O5D-PN-O3

There are no ring outliers.

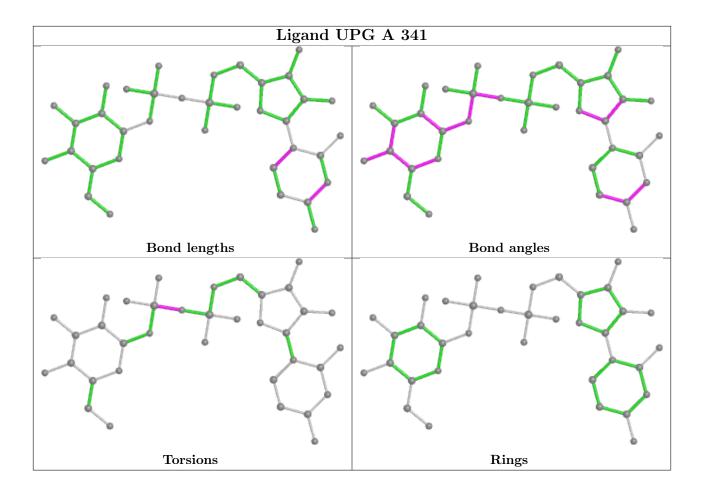
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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.

