



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:56 am GMT

PDB ID : 4LK3  
Title : Crystal structure of Human UDP-xylose synthase R236A substitution  
Authors : Walsh Jr., R.M.; Polizzi, S.J.; Wood, Z.A.  
Deposited on : 2013-07-05  
Resolution : 2.64 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](mailto: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.

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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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

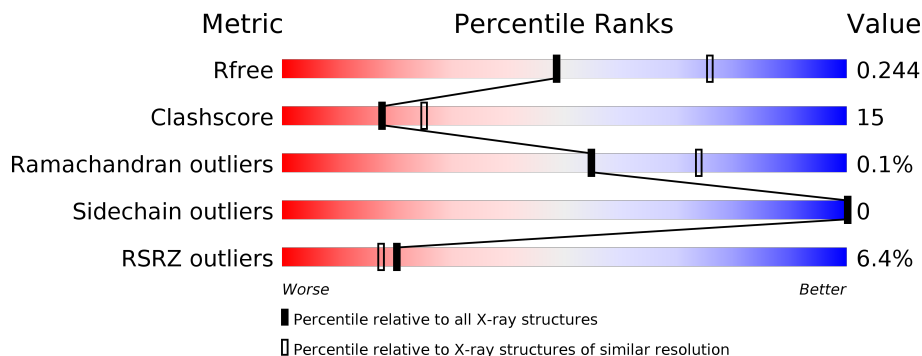
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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))
$R_{free}$	100719	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	336	<div> <div>11%</div> <div> <div></div> <div>53%</div> <div>26%</div> <div>21%</div> </div> </div>
1	B	336	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>16%</div> <div>18%</div> </div> </div>
1	C	336	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>14%</div> <div>19%</div> </div> </div>
1	D	336	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>20%</div> <div>19%</div> </div> </div>
1	E	336	<div> <div>7%</div> <div> <div></div> <div>61%</div> <div>19%</div> <div>20%</div> </div> </div>
1	F	336	<div> <div>8%</div> <div> <div></div> <div>47%</div> <div>31%</div> <div>22%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	505	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13434 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.

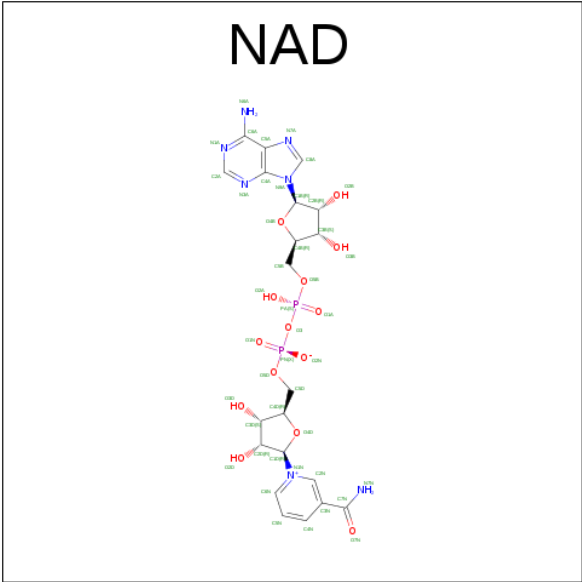
- Molecule 1 is a protein called UDP-glucuronic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2113	1349	367	387	10			
1	B	274	Total	C	N	O	S	0	0	0
			2156	1375	374	396	11			
1	C	271	Total	C	N	O	S	0	0	0
			2130	1359	368	393	10			
1	D	273	Total	C	N	O	S	0	0	0
			2148	1370	373	395	10			
1	E	269	Total	C	N	O	S	0	0	0
			2118	1350	369	389	10			
1	F	261	Total	C	N	O	S	0	0	0
			2062	1314	360	378	10			

There are 6 discrepancies between the modelled and reference sequences:

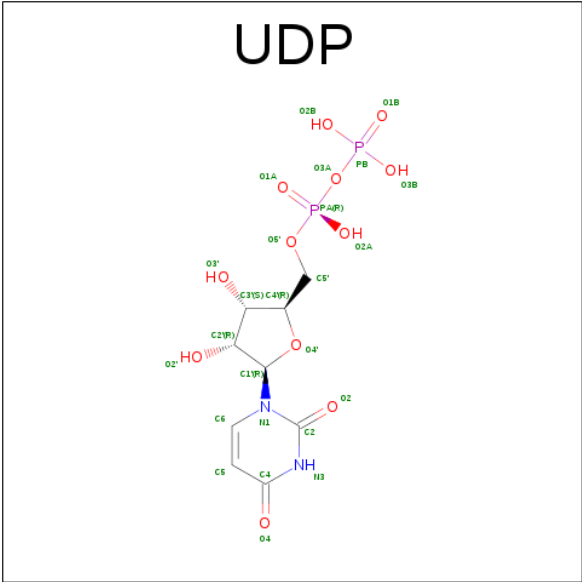
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
B	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
C	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
D	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
E	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
F	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



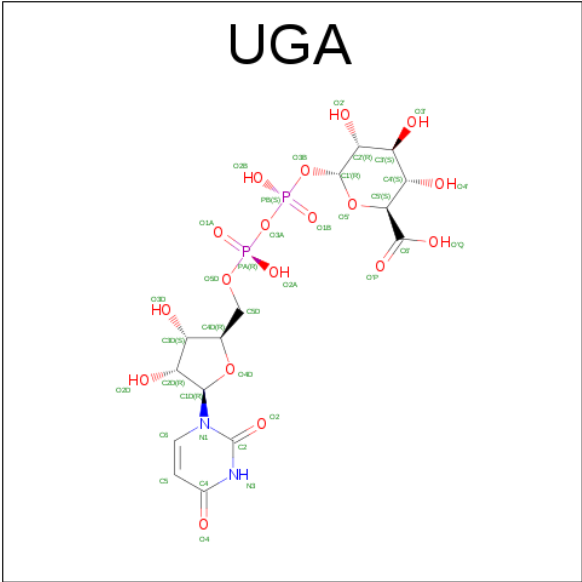
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



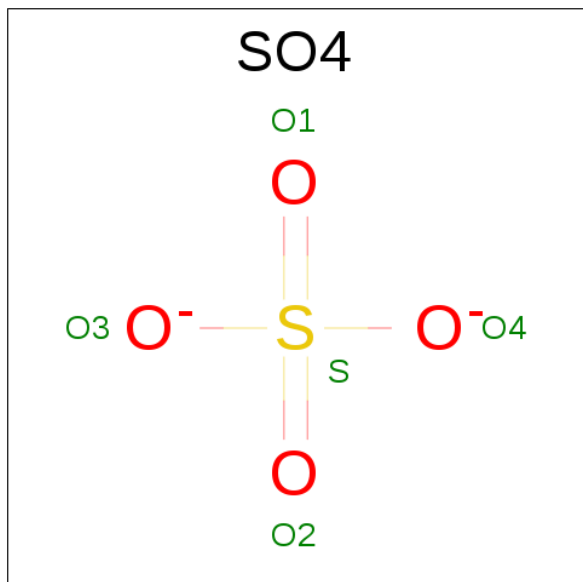
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O<sub>18</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	E	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	F	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



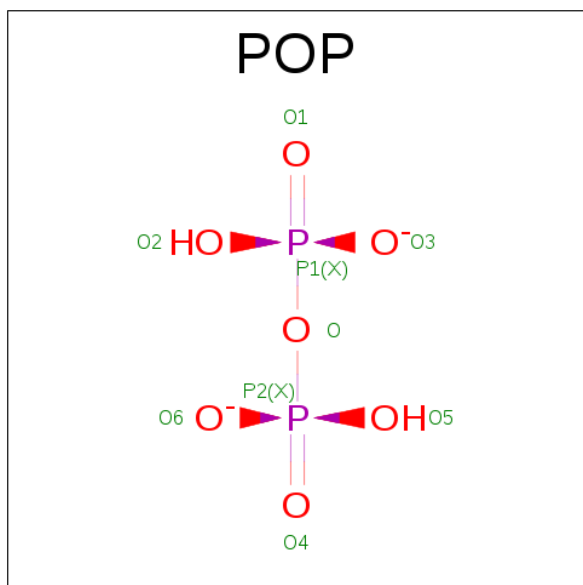
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5 4 1			
5	A	1	Total	O S	0	0
			5 4 1			
5	B	1	Total	O S	0	0
			5 4 1			
5	B	1	Total	O S	0	0
			5 4 1			
5	C	1	Total	O S	0	0
			5 4 1			
5	D	1	Total	O S	0	0
			5 4 1			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			9	7	2		
6	E	1	Total	O	P	0	0
			9	7	2		
6	F	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	32	Total	O	0	0
			32	32		
7	C	31	Total	O	0	0
			31	31		
7	D	9	Total	O	0	0
			9	9		

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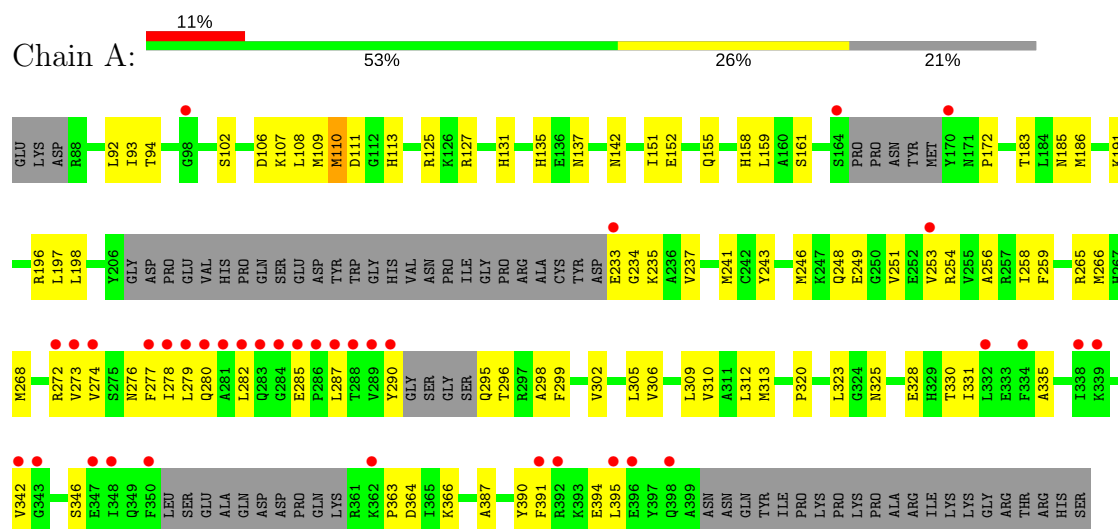
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	2	Total	O	0	0
			2	2		

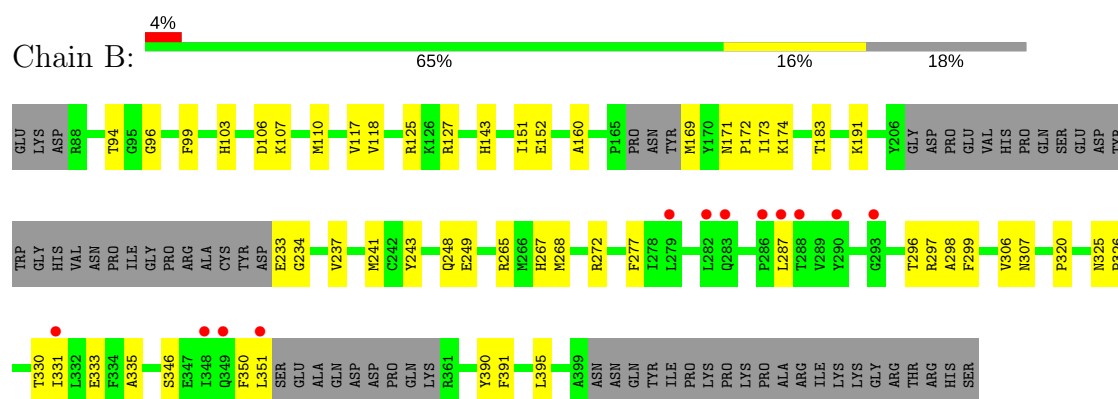
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

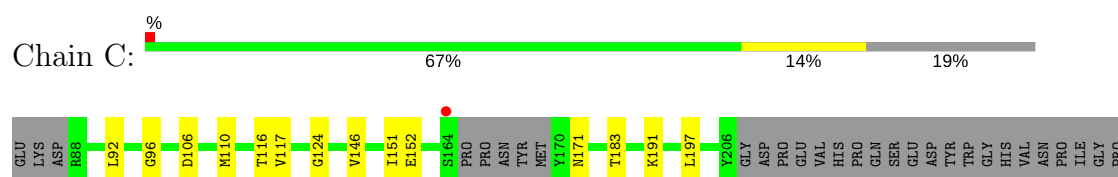
#### • Molecule 1: UDP-glucuronic acid decarboxylase 1

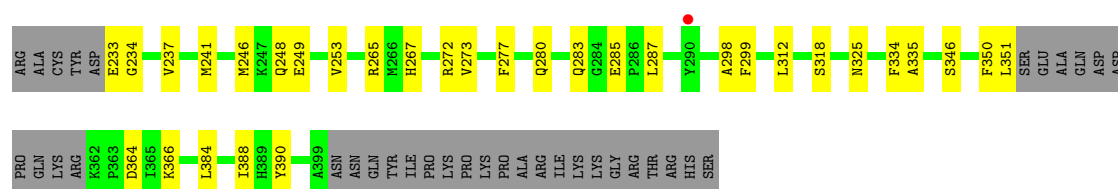


#### • Molecule 1: UDP-glucuronic acid decarboxylase 1

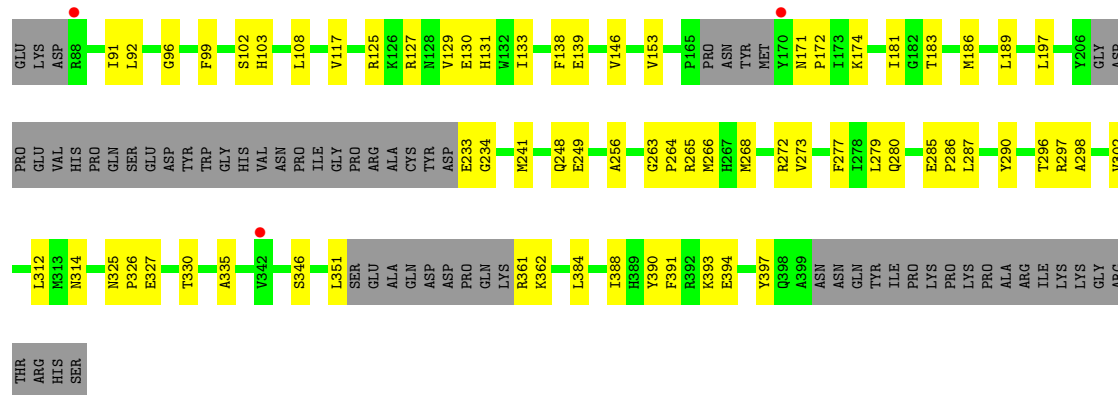


#### • Molecule 1: UDP-glucuronic acid decarboxylase 1

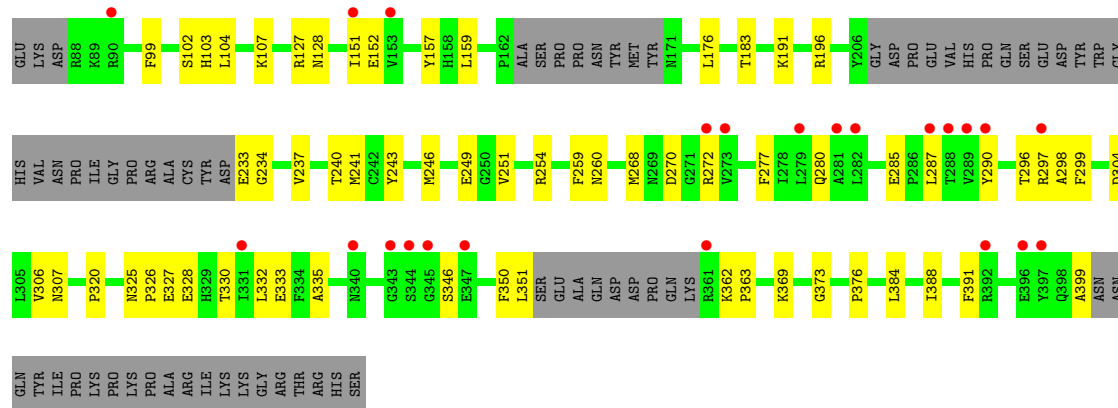




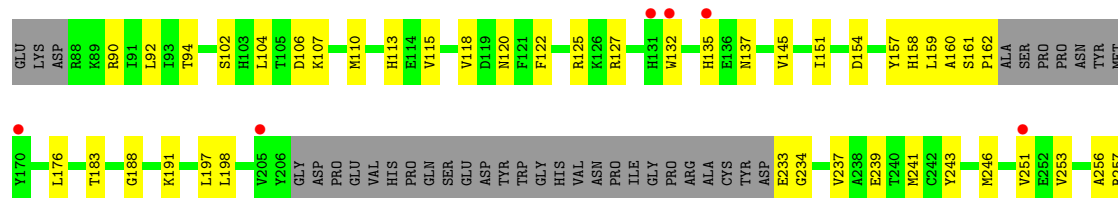
• Molecule 1: UDP-glucuronic acid decarboxylase 1



• Molecule 1: UDP-glucuronic acid decarboxylase 1



• Molecule 1: UDP-glucuronic acid decarboxylase 1



I331	T258
I332	F259
E333	N260
F334	T261
A335	F262
I338	R265
K339	M266
R340	H267
L341	M268
V342	R272
G343	V273
S344	V274
G345	
S346	
E347	F277
I348	I278
	L279
GLN	Q280
PHE	A281
LEU	L282
SER	
GLU	Q283
ALA	G284
GLN	E285
ASP	P286
ASP	L287
PRO	THR
GLN	VAL
LYS	TYR
	GLY
R361	SER
K362	GLY
P363	
D364	S294
I365	Q295
K366	T296
	R297
K369	A298
L370	F299
	Q300
G373	Y301
	V302
L380	S303
E381	D304
F382	L305
G383	V306
L384	N307
N385	
K386	L312
A387	
I388	V317
H389	S318
Y390	S319
F391	P320
R392	N325
K393	P326
E394	E327
L395	E328
E396	H329
Y397	T330
Q398	

A399
ASN
ASN
GLN
TYR
ILE
PRO
LYS
PRO
LYS
PRO
ALA
ARG
ILE
LYS
LYS
GLY
ARG
THR
ARG
HIS
SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.57Å 92.07Å 290.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.37 – 2.64 38.90 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.37-2.64) 95.6 (38.90-2.64)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.198 , 0.245 0.197 , 0.244	Depositor DCC
$R_{free}$ test set	3331 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, UDP, UGA, NAD, POP

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	0.48	0/2152	0.67	0/2905
1	B	0.57	0/2197	0.73	0/2967
1	C	0.56	0/2170	0.72	0/2931
1	D	0.50	0/2189	0.67	1/2957 (0.0%)
1	E	0.48	0/2157	0.66	0/2912
1	F	0.47	0/2099	0.70	0/2832
All	All	0.51	0/12964	0.69	1/17504 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	314	ASN	O-C-N	-5.18	114.41	122.70

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	2113	0	2123	88	0
1	B	2156	0	2167	47	0
1	C	2130	0	2138	46	0
1	D	2148	0	2158	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2118	0	2132	57	0
1	F	2062	0	2076	108	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	3	0
3	A	25	0	11	1	0
3	B	25	0	11	0	0
3	D	25	0	11	2	0
4	A	37	0	19	2	0
4	B	37	0	19	2	0
4	C	37	0	19	0	0
4	D	37	0	19	1	0
4	E	37	0	19	0	0
4	F	37	0	19	2	0
5	A	10	0	0	3	0
5	B	10	0	0	1	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	C	9	0	0	2	0
6	E	9	0	0	0	0
6	F	9	0	0	3	0
7	B	32	0	0	2	0
7	C	31	0	0	3	0
7	D	9	0	0	0	0
7	E	2	0	0	0	0
All	All	13434	0	13097	404	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 15.

The worst 5 of 404 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:F:262:PHE:HE2	1:F:299:PHE:CD1	1.43	1.37
1:F:262:PHE:CE2	1:F:299:PHE:CD1	2.34	1.15
1:B:233:GLU:HG2	1:B:234:GLY:H	1.05	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:GLU:HG2	1:F:234:GLY:H	0.94	1.06
1:F:262:PHE:CZ	1:F:272:ARG:HD3	1.90	1.06

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	257/336 (76%)	249 (97%)	7 (3%)	1 (0%)	38	54
1	B	266/336 (79%)	260 (98%)	6 (2%)	0	100	100
1	C	263/336 (78%)	254 (97%)	9 (3%)	0	100	100
1	D	265/336 (79%)	252 (95%)	13 (5%)	0	100	100
1	E	261/336 (78%)	255 (98%)	6 (2%)	0	100	100
1	F	251/336 (75%)	242 (96%)	9 (4%)	0	100	100
All	All	1563/2016 (78%)	1512 (97%)	50 (3%)	1 (0%)	55	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	MET

### 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	229/289 (79%)	229 (100%)	0	100	100
1	B	234/289 (81%)	234 (100%)	0	100	100
1	C	231/289 (80%)	231 (100%)	0	100	100
1	D	233/289 (81%)	233 (100%)	0	100	100
1	E	230/289 (80%)	230 (100%)	0	100	100
1	F	224/289 (78%)	224 (100%)	0	100	100
All	All	1381/1734 (80%)	1381 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	135	HIS
1	A	295	GLN
1	F	135	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

27 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	NAD	A	501	-	41,48,48	0.80	1 (2%)	43,73,73	1.32	2 (4%)
3	UDP	A	502	-	21,26,26	0.76	0	22,40,40	1.99	1 (4%)
4	UGA	A	503	-	32,39,39	2.51	6 (18%)	44,60,60	1.88	6 (13%)
5	SO4	A	504	-	4,4,4	0.21	0	6,6,6	0.27	0
5	SO4	A	505	-	4,4,4	0.12	0	6,6,6	0.18	0
2	NAD	B	501	-	41,48,48	0.90	3 (7%)	43,73,73	1.34	2 (4%)
3	UDP	B	502	-	21,26,26	0.76	0	22,40,40	1.98	2 (9%)
4	UGA	B	503	-	32,39,39	2.62	6 (18%)	44,60,60	1.93	5 (11%)
5	SO4	B	504	-	4,4,4	0.16	0	6,6,6	0.60	0
5	SO4	B	505	-	4,4,4	0.23	0	6,6,6	0.40	0
2	NAD	C	501	-	41,48,48	0.91	1 (2%)	43,73,73	1.43	4 (9%)
4	UGA	C	502	-	32,39,39	2.61	6 (18%)	44,60,60	2.08	7 (15%)
6	POP	C	503	-	8,8,8	0.80	0	8,13,13	1.27	0
5	SO4	C	504	-	4,4,4	0.15	0	6,6,6	0.37	0
2	NAD	D	501	-	41,48,48	0.79	1 (2%)	43,73,73	1.40	2 (4%)
3	UDP	D	502	-	21,26,26	0.85	0	22,40,40	1.75	1 (4%)
4	UGA	D	503	-	32,39,39	2.66	6 (18%)	44,60,60	1.95	6 (13%)
5	SO4	D	504	-	4,4,4	0.20	0	6,6,6	0.48	0
5	SO4	D	505	-	4,4,4	0.27	0	6,6,6	0.47	0
2	NAD	E	501	-	41,48,48	0.80	1 (2%)	43,73,73	1.38	3 (6%)
6	POP	E	502	-	8,8,8	1.14	0	8,13,13	1.57	2 (25%)
4	UGA	E	503	-	32,39,39	2.66	5 (15%)	44,60,60	1.99	5 (11%)
5	SO4	E	504	-	4,4,4	0.07	0	6,6,6	0.31	0
2	NAD	F	501	-	41,48,48	0.84	1 (2%)	43,73,73	1.49	2 (4%)
4	UGA	F	502	-	32,39,39	2.55	6 (18%)	44,60,60	2.19	8 (18%)
6	POP	F	503	-	8,8,8	0.79	0	8,13,13	1.27	0
5	SO4	F	504	-	4,4,4	0.21	0	6,6,6	0.16	0

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	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	UDP	A	502	-	-	0/12/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UGA	A	503	-	-	0/21/61/61	0/3/3/3
5	SO4	A	504	-	-	0/0/0/0	0/0/0/0
5	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
3	UDP	B	502	-	-	0/12/32/32	0/2/2/2
4	UGA	B	503	-	-	0/21/61/61	0/3/3/3
5	SO4	B	504	-	-	0/0/0/0	0/0/0/0
5	SO4	B	505	-	-	0/0/0/0	0/0/0/0
2	NAD	C	501	-	-	0/22/62/62	0/5/5/5
4	UGA	C	502	-	-	0/21/61/61	0/3/3/3
6	POP	C	503	-	-	0/6/6/6	0/0/0/0
5	SO4	C	504	-	-	0/0/0/0	0/0/0/0
2	NAD	D	501	-	-	0/22/62/62	0/5/5/5
3	UDP	D	502	-	-	0/12/32/32	0/2/2/2
4	UGA	D	503	-	-	0/21/61/61	0/3/3/3
5	SO4	D	504	-	-	0/0/0/0	0/0/0/0
5	SO4	D	505	-	-	0/0/0/0	0/0/0/0
2	NAD	E	501	-	-	0/22/62/62	0/5/5/5
6	POP	E	502	-	-	0/6/6/6	0/0/0/0
4	UGA	E	503	-	-	0/21/61/61	0/3/3/3
5	SO4	E	504	-	-	0/0/0/0	0/0/0/0
2	NAD	F	501	-	-	0/22/62/62	0/5/5/5
4	UGA	F	502	-	-	0/21/61/61	0/3/3/3
6	POP	F	503	-	-	0/6/6/6	0/0/0/0
5	SO4	F	504	-	-	0/0/0/0	0/0/0/0

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	503	UGA	C6-N1	-10.64	1.33	1.47
4	D	503	UGA	C6-N1	-10.56	1.33	1.47
4	B	503	UGA	C6-N1	-10.49	1.33	1.47
4	F	502	UGA	C6-N1	-10.44	1.33	1.47
4	A	503	UGA	C6-N1	-9.89	1.34	1.47

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	NAD	N3A-C2A-N1A	-7.15	122.63	128.86
4	C	502	UGA	C4-N3-C2	-6.67	120.09	125.81
4	F	502	UGA	C4-N3-C2	-6.60	120.16	125.81
4	A	503	UGA	C4-N3-C2	-6.43	120.30	125.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	N3A-C2A-N1A	-6.41	123.28	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	UDP	1	0
4	A	503	UGA	2	0
5	A	505	SO4	3	0
4	B	503	UGA	2	0
5	B	504	SO4	1	0
2	C	501	NAD	1	0
6	C	503	POP	2	0
3	D	502	UDP	2	0
4	D	503	UGA	1	0
2	F	501	NAD	3	0
4	F	502	UGA	2	0
6	F	503	POP	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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	267/336 (79%)	0.55	37 (13%) <b>3</b> <b>1</b>	45, 83, 138, 167	0
1	B	274/336 (81%)	0.16	12 (4%) <b>35</b> <b>31</b>	33, 54, 104, 131	0
1	C	271/336 (80%)	-0.20	2 (0%) <b>87</b> <b>86</b>	38, 59, 95, 130	0
1	D	273/336 (81%)	-0.01	3 (1%) <b>80</b> <b>78</b>	40, 65, 111, 126	0
1	E	269/336 (80%)	0.45	23 (8%) <b>11</b> <b>9</b>	57, 89, 127, 152	0
1	F	261/336 (77%)	0.55	27 (10%) <b>7</b> <b>5</b>	63, 105, 136, 168	0
All	All	1615/2016 (80%)	0.24	104 (6%) <b>20</b> <b>17</b>	33, 75, 126, 168	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	282	LEU	6.2
1	B	290	TYR	5.7
1	F	131	HIS	5.6
1	A	338	ILE	5.3
1	A	395	LEU	5.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	C	504	5/5	0.92	0.23	1.47	79,90,95,100	0
3	UDP	D	502	25/25	0.82	0.23	0.80	84,100,120,147	0
3	UDP	B	502	25/25	0.82	0.35	0.75	81,108,119,173	0
5	SO4	D	504	5/5	0.96	0.33	0.74	75,83,84,87	0
5	SO4	E	504	5/5	0.86	0.24	0.40	109,118,119,123	0
4	UGA	A	503	37/37	0.94	0.18	0.40	70,87,112,114	0
5	SO4	D	505	5/5	0.92	0.22	0.24	88,96,98,107	0
2	NAD	A	501	44/44	0.97	0.22	0.10	47,67,76,84	0
4	UGA	E	503	37/37	0.95	0.19	0.06	60,81,112,120	0
6	POP	F	503	9/9	0.85	0.26	0.04	86,91,184,186	3
2	NAD	B	501	44/44	0.98	0.19	0.04	23,40,51,63	0
2	NAD	E	501	44/44	0.96	0.19	-0.02	51,67,89,94	0
2	NAD	C	501	44/44	0.98	0.18	-0.05	25,42,58,77	0
2	NAD	F	501	44/44	0.96	0.19	-0.10	54,76,103,105	0
2	NAD	D	501	44/44	0.97	0.19	-0.22	36,51,71,88	0
4	UGA	C	502	37/37	0.97	0.15	-0.26	45,63,114,118	0
4	UGA	B	503	37/37	0.96	0.16	-0.43	36,69,115,120	0
5	SO4	B	504	5/5	0.94	0.16	-0.53	77,78,85,97	0
4	UGA	F	502	37/37	0.93	0.17	-0.59	90,98,139,142	0
5	SO4	F	504	5/5	0.84	0.18	-0.68	121,123,127,128	0
4	UGA	D	503	37/37	0.96	0.13	-0.77	40,59,90,93	0
3	UDP	A	502	25/25	0.82	0.23	-0.88	100,124,141,142	0
6	POP	C	503	9/9	0.87	0.17	-0.89	64,95,130,200	1
6	POP	E	502	9/9	0.85	0.14	-1.35	71,81,135,148	3
5	SO4	A	505	5/5	0.95	0.17	-1.76	95,96,100,102	0
5	SO4	B	505	5/5	0.98	0.16	-2.06	56,62,73,75	0
5	SO4	A	504	5/5	0.86	0.14	-	132,135,137,140	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.