



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:40 AM GMT

PDB ID : 3MJ4  
Title : Crystal structure of UDP-galactopyranose mutase in complex with phosphonate analog of UDP-galactopyranose  
Authors : Karunan Partha, S.; Sadeghi-Khomami, A.; Slowski, K.; Kotake, T.; Thomas, N.R.; Jakeman, D.L.; Sanders, D.A.R.  
Deposited on : 2010-04-12  
Resolution : 2.65 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

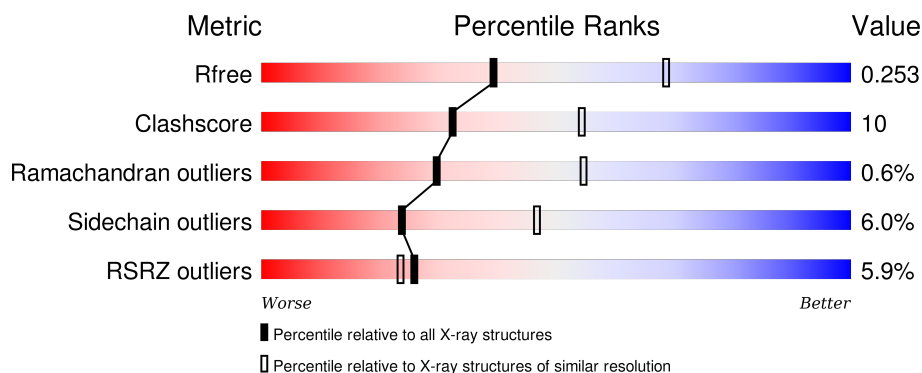
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	397	<div> <div>2%</div> <div>70% 20% 8%</div> </div>
1	B	397	<div> <div>12%</div> <div>66% 22% 9%</div> </div>
1	C	397	<div> <div>3%</div> <div>70% 20% 9%</div> </div>
1	D	397	<div> <div>12%</div> <div>68% 20% 10%</div> </div>
1	E	397	<div> <div>8%</div> <div>66% 23% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	397	
1	G	397	
1	H	397	
1	I	397	
1	J	397	

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
4	GOL	A	398	-	-	-	X
4	GOL	B	398	-	-	-	X
4	GOL	C	398	-	-	-	X
4	GOL	E	398	-	-	-	X
4	GOL	F	398	-	-	-	X
4	GOL	F	400	-	-	-	X
4	GOL	G	399	-	-	-	X
4	GOL	H	398	-	-	-	X
4	GOL	I	398	-	-	-	X
4	GOL	J	399	-	-	-	X
4	GOL	J	400	-	-	-	X
6	XYL	F	399	-	-	-	X
6	XYL	I	401	-	-	-	X

## 2 Entry composition

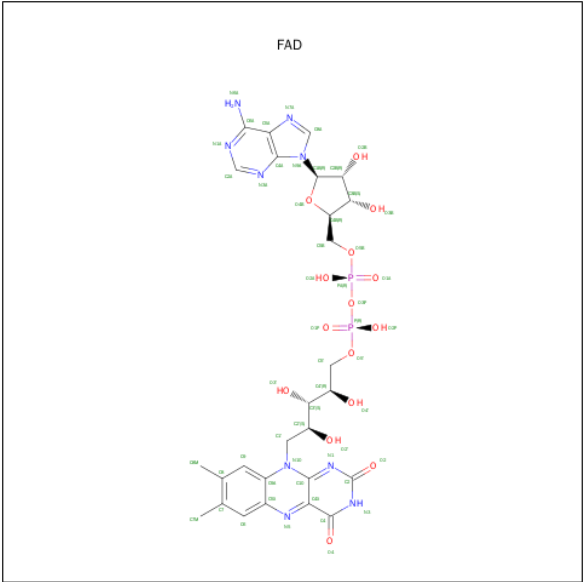
There are 7 unique types of molecules in this entry. The entry contains 31256 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-galactopyranose mutase.

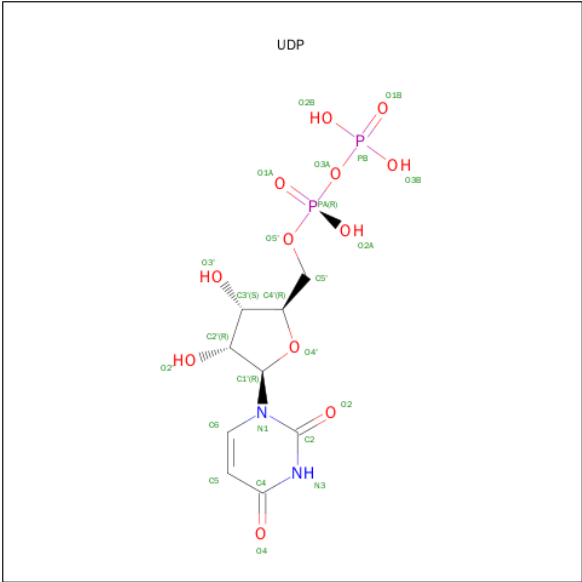
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	1	1	0
			2992	1909	521	554	8			
1	B	363	Total	C	N	O	S	1	0	0
			2969	1896	516	549	8			
1	C	363	Total	C	N	O	S	1	0	0
			2969	1896	516	549	8			
1	D	359	Total	C	N	O	S	0	0	0
			2943	1881	510	544	8			
1	E	361	Total	C	N	O	S	2	0	0
			2951	1885	512	546	8			
1	F	364	Total	C	N	O	S	1	1	0
			2984	1906	520	550	8			
1	G	363	Total	C	N	O	S	1	0	0
			2966	1894	515	549	8			
1	H	364	Total	C	N	O	S	0	0	0
			2975	1899	517	551	8			
1	I	364	Total	C	N	O	S	1	0	0
			2975	1899	516	552	8			
1	J	363	Total	C	N	O	S	2	0	0
			2966	1894	515	549	8			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	J	1	Total	C	N	O	P	0	0
			53	27	9	15	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	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	E	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
3	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	G	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	H	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	I	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
3	J	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

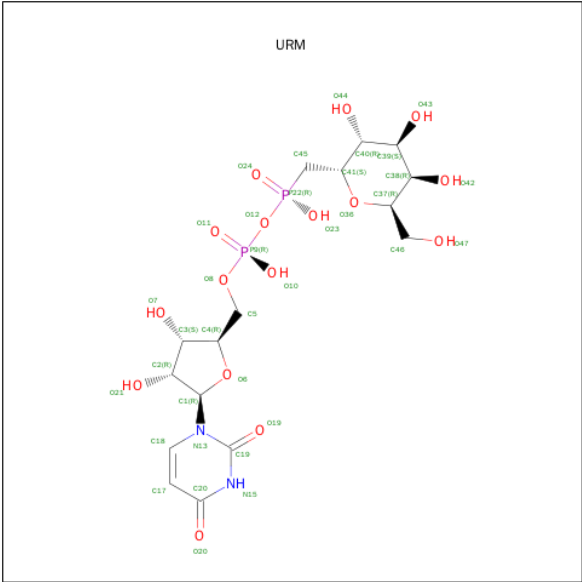
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

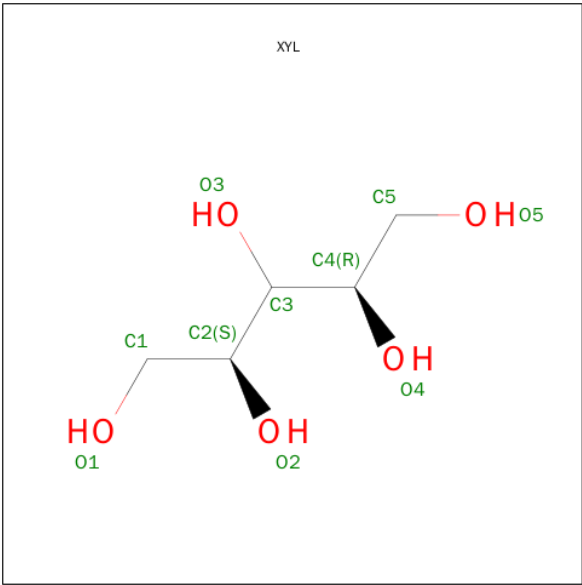
- Molecule 5 is (((2S,3R,4S,5R,6R)-3,4,5-TRIHIDROXY-6-(HYDROXYMETHYL)TETRAHYDRO-2H-PYRAN-2-YL)METHYL)PHOSPHONIC (((2R,3S,4R,5R)-5-(2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL)METHYL PHOSPHORIC) ANHYDRIDE (three-letter code: URM) (formula: C<sub>16</sub>H<sub>26</sub>N<sub>2</sub>O<sub>16</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

- Molecule 6 is SUGAR (D-XYLITOL) (three-letter code: XYL) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			10	5	5		
6	I	1	Total	C	O	0	0
			10	5	5		

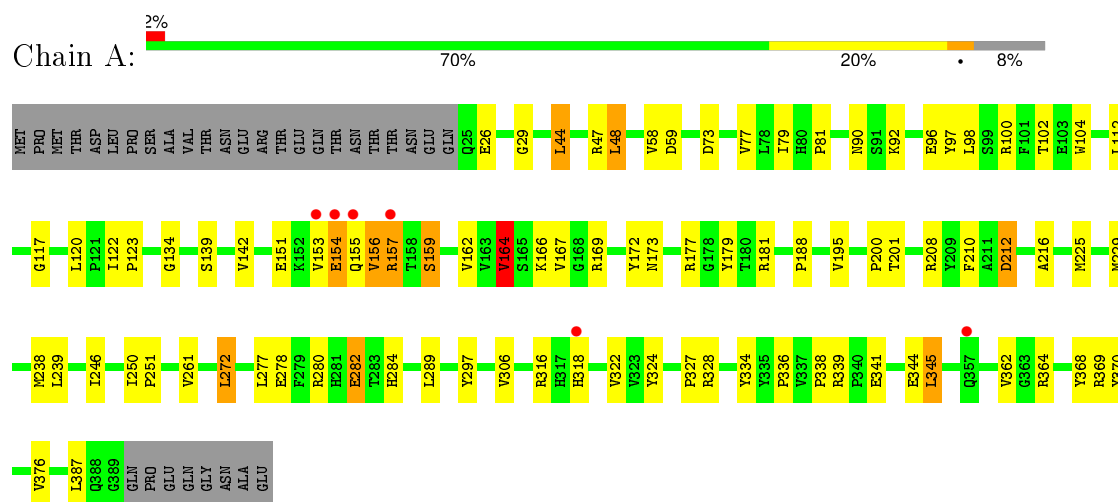
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	89	Total 89	O 89	0	0
7	B	68	Total 68	O 68	0	0
7	C	60	Total 60	O 60	0	0
7	D	46	Total 46	O 46	0	0
7	E	51	Total 51	O 51	0	0
7	F	60	Total 60	O 60	0	0
7	G	53	Total 53	O 53	0	0
7	H	75	Total 75	O 75	0	0
7	I	65	Total 65	O 65	0	0
7	J	46	Total 46	O 46	0	0

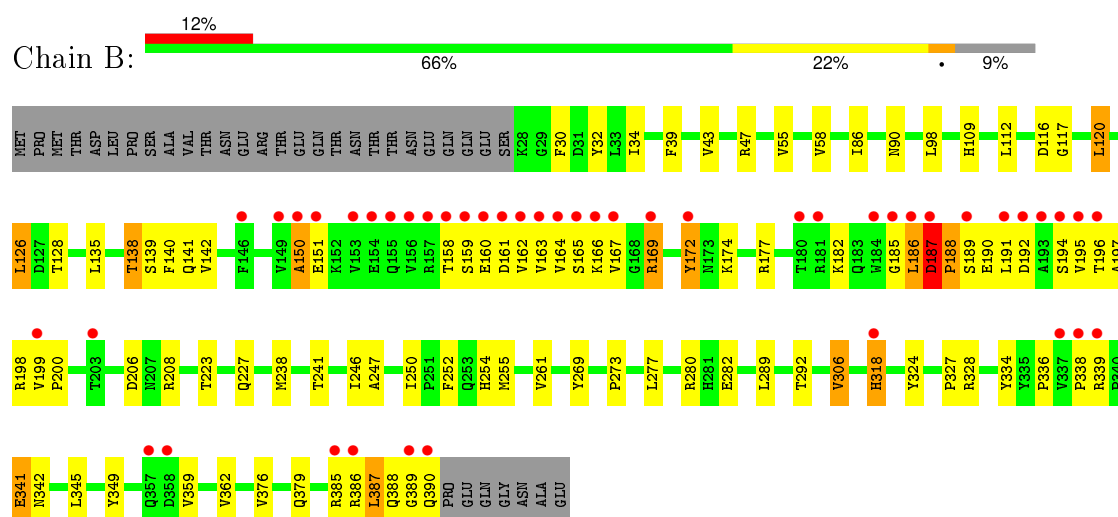
### 3 Residue-property plots

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.

#### • Molecule 1: UDP-galactopyranose mutase

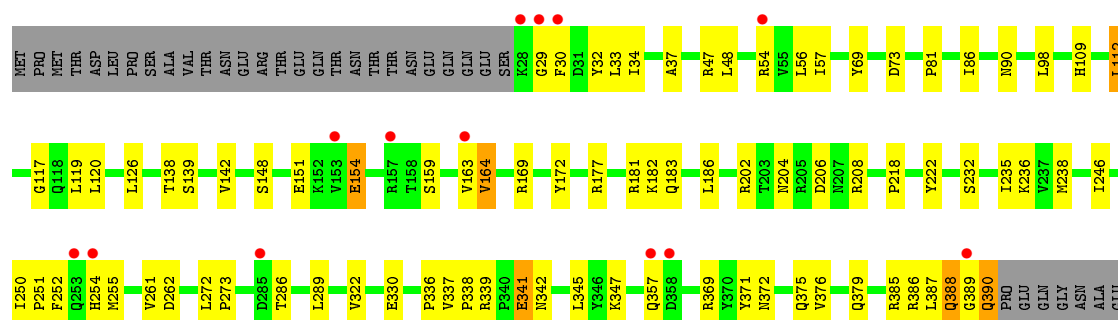


#### • Molecule 1: UDP-galactopyranose mutase

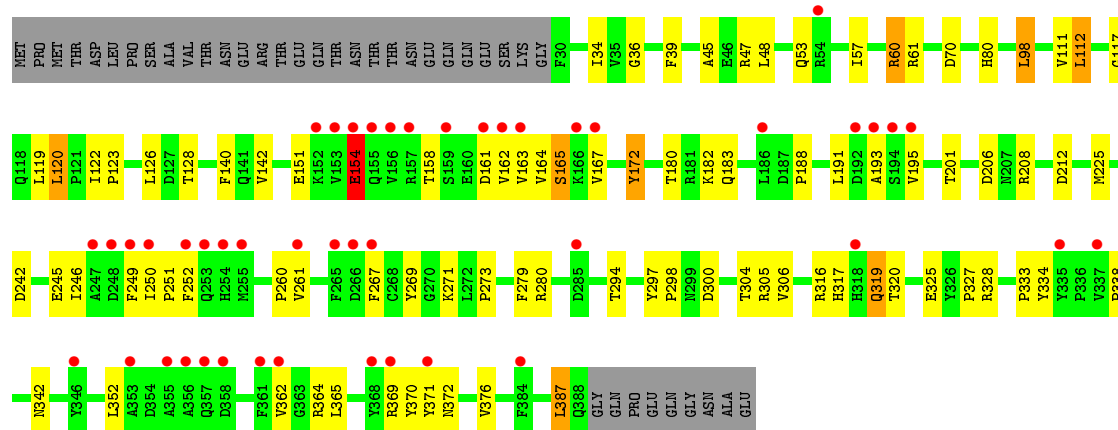


#### • Molecule 1: UDP-galactopyranose mutase

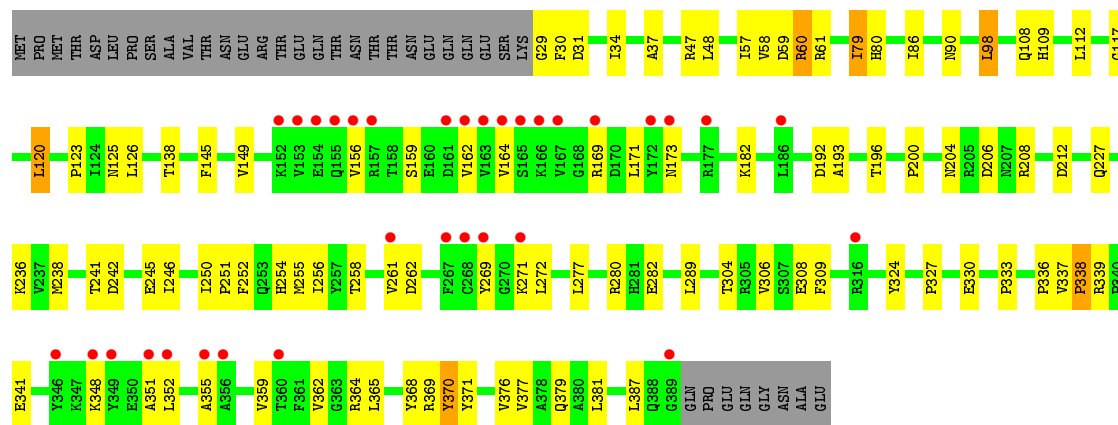




• Molecule 1: UDP-galactopyranose mutase



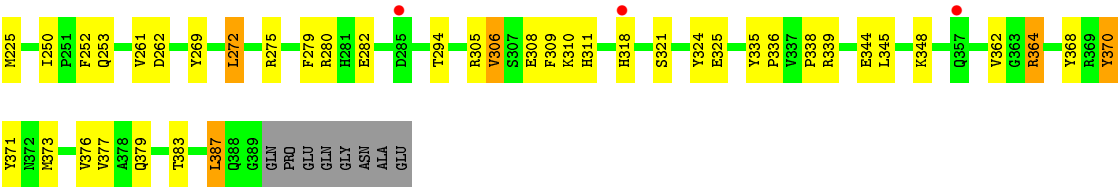
• Molecule 1: UDP-galactopyranose mutase



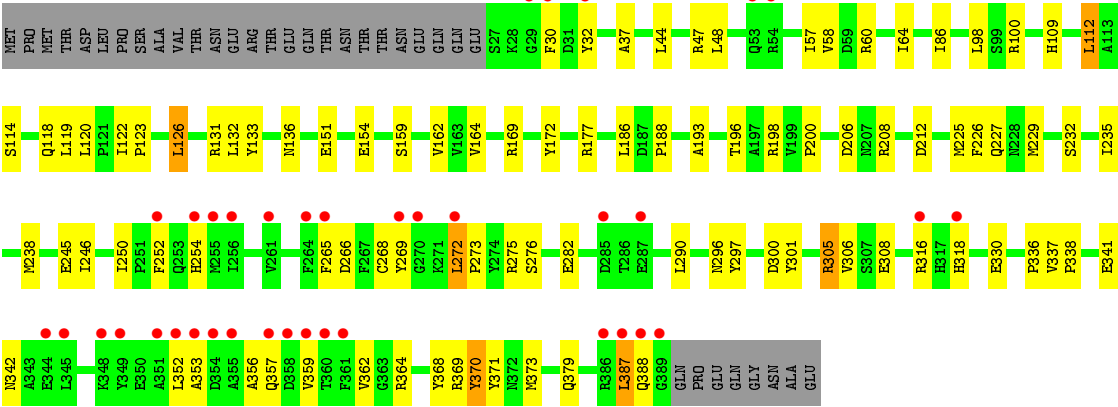
• Molecule 1: UDP-galactopyranose mutase







● Molecule 1: UDP-galactopyranose mutase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.15Å 175.72Å 223.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.54 – 2.65 44.54 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.54-2.65) 99.5 (44.54-2.65)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.207 , 0.262 0.205 , 0.253	Depositor DCC
$R_{free}$ test set	7713 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 153569 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	31256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, UDP, XYL, FAD, URM

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	0.50	0/3079	0.65	0/4185
1	B	0.46	0/3053	0.62	0/4151
1	C	0.45	0/3053	0.62	0/4151
1	D	0.41	0/3027	0.57	0/4118
1	E	0.39	0/3035	0.55	0/4128
1	F	0.44	0/3072	0.62	0/4177
1	G	0.44	0/3050	0.59	0/4147
1	H	0.46	0/3059	0.60	0/4159
1	I	0.47	0/3059	0.62	0/4159
1	J	0.43	0/3050	0.58	0/4147
All	All	0.45	0/30537	0.60	0/41522

There are no bond length outliers.

There are no bond angle outliers.

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	2992	0	2867	69	0
1	B	2969	0	2843	109	0
1	C	2969	0	2843	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2943	0	2816	65	0
1	E	2951	0	2822	66	0
1	F	2984	0	2863	52	0
1	G	2966	0	2840	60	0
1	H	2975	0	2848	44	0
1	I	2975	0	2846	70	0
1	J	2966	0	2840	64	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	5	0
2	E	53	0	31	3	0
2	F	53	0	31	0	0
2	G	53	0	31	1	0
2	H	53	0	31	0	0
2	I	53	0	31	3	0
2	J	53	0	31	1	0
3	A	25	0	11	1	0
3	B	25	0	11	4	0
3	C	25	0	11	0	0
3	E	21	0	11	0	0
3	F	25	0	11	0	0
3	G	25	0	11	1	0
3	H	25	0	11	0	0
3	I	21	0	11	0	0
3	J	25	0	11	1	0
4	A	18	0	24	1	0
4	B	6	0	8	2	0
4	C	12	0	16	2	0
4	D	12	0	16	1	0
4	E	24	0	32	2	0
4	F	12	0	16	2	0
4	G	18	0	24	0	0
4	H	12	0	16	2	0
4	I	24	0	32	5	0
4	J	12	0	16	0	0
5	D	36	0	24	1	0
6	F	10	0	11	0	0
6	I	10	0	12	1	0
7	A	89	0	0	3	0
7	B	68	0	0	2	0
7	C	60	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	46	0	0	3	0
7	E	51	0	0	0	0
7	F	60	0	0	1	0
7	G	53	0	0	1	0
7	H	75	0	0	0	0
7	I	65	0	0	2	0
7	J	46	0	0	3	0
All	All	31256	0	29084	624	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 10.

The worst 5 of 624 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:C:388:GLN:HA	1:C:388:GLN:NE2	1.45	1.12
1:A:153:VAL:HA	1:A:154:GLU:HB3	1.31	1.11
1:C:388:GLN:HE21	1:C:388:GLN:CA	1.66	1.08
1:C:389:GLY:C	1:C:390:GLN:HG2	1.74	1.02
1:G:58:VAL:HG23	1:G:238:MET:HB3	1.41	0.99

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	364/397 (92%)	349 (96%)	12 (3%)	3 (1%)	24 47
1	B	361/397 (91%)	331 (92%)	24 (7%)	6 (2%)	11 25
1	C	361/397 (91%)	341 (94%)	17 (5%)	3 (1%)	24 47
1	D	357/397 (90%)	333 (93%)	22 (6%)	2 (1%)	30 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	359/397 (90%)	329 (92%)	27 (8%)	3 (1%)	24	47
1	F	363/397 (91%)	351 (97%)	12 (3%)	0	100	100
1	G	361/397 (91%)	345 (96%)	15 (4%)	1 (0%)	46	72
1	H	362/397 (91%)	342 (94%)	20 (6%)	0	100	100
1	I	362/397 (91%)	342 (94%)	20 (6%)	0	100	100
1	J	361/397 (91%)	340 (94%)	17 (5%)	4 (1%)	17	38
All	All	3611/3970 (91%)	3403 (94%)	186 (5%)	22 (1%)	30	54

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
1	B	150	ALA
1	B	188	PRO
1	C	357	GLN
1	B	186	LEU

### 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	
1	A	318/346 (92%)	295 (93%)	23 (7%)	18	37
1	B	315/346 (91%)	300 (95%)	15 (5%)	31	59
1	C	315/346 (91%)	293 (93%)	22 (7%)	19	38
1	D	313/346 (90%)	297 (95%)	16 (5%)	29	55
1	E	313/346 (90%)	293 (94%)	20 (6%)	22	43
1	F	317/346 (92%)	297 (94%)	20 (6%)	22	44
1	G	315/346 (91%)	302 (96%)	13 (4%)	37	66
1	H	316/346 (91%)	294 (93%)	22 (7%)	19	38
1	I	316/346 (91%)	295 (93%)	21 (7%)	21	42
1	J	315/346 (91%)	296 (94%)	19 (6%)	24	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3153/3460 (91%)	2962 (94%)	191 (6%)	24 46

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	212	ASP
1	F	182	LYS
1	J	120	LEU
1	E	254	HIS
1	F	44	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	90	ASN
1	E	173	ASN
1	H	311	HIS
1	D	311	HIS
1	D	319	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](#)

47 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$
4	GOL	A	398	-	5,5,5	0.28	0	5,5,5	0.56	0
4	GOL	A	399	-	5,5,5	0.45	0	5,5,5	0.32	0
4	GOL	A	400	-	5,5,5	0.32	0	5,5,5	0.13	0
2	FAD	A	450	-	48,58,58	1.16	4 (8%)	54,89,89	2.09	8 (14%)
3	UDP	A	500	-	18,26,26	1.01	1 (5%)	26,40,40	1.45	2 (7%)
4	GOL	B	398	-	5,5,5	0.41	0	5,5,5	0.37	0
2	FAD	B	450	-	48,58,58	1.21	5 (10%)	54,89,89	2.19	8 (14%)
3	UDP	B	500	-	18,26,26	1.17	1 (5%)	26,40,40	1.68	3 (11%)
4	GOL	C	398	-	5,5,5	0.31	0	5,5,5	0.26	0
4	GOL	C	399	-	5,5,5	0.33	0	5,5,5	0.35	0
2	FAD	C	450	-	48,58,58	1.23	5 (10%)	54,89,89	2.08	6 (11%)
3	UDP	C	500	-	18,26,26	1.00	1 (5%)	26,40,40	1.57	2 (7%)
4	GOL	D	398	-	5,5,5	0.26	0	5,5,5	0.62	0
4	GOL	D	399	-	5,5,5	0.41	0	5,5,5	0.57	0
2	FAD	D	450	-	48,58,58	1.21	5 (10%)	54,89,89	2.17	7 (12%)
5	URM	D	600	-	30,38,38	3.42	4 (13%)	39,58,58	1.44	4 (10%)
4	GOL	E	398	-	5,5,5	0.35	0	5,5,5	0.53	0
4	GOL	E	399	-	5,5,5	0.33	0	5,5,5	0.22	0
4	GOL	E	400	-	5,5,5	0.24	0	5,5,5	0.45	0
4	GOL	E	401	-	5,5,5	0.32	0	5,5,5	0.36	0
2	FAD	E	450	-	48,58,58	1.19	4 (8%)	54,89,89	2.09	6 (11%)
3	UDP	E	500	-	16,22,26	1.15	1 (6%)	21,33,40	1.62	2 (9%)
4	GOL	F	398	-	5,5,5	0.24	0	5,5,5	0.70	0
6	XYL	F	399	-	9,9,9	1.63	2 (22%)	10,11,11	1.75	2 (20%)
4	GOL	F	400	-	5,5,5	0.37	0	5,5,5	0.40	0
2	FAD	F	450	-	48,58,58	1.23	5 (10%)	54,89,89	2.23	8 (14%)
3	UDP	F	500	-	18,26,26	1.14	1 (5%)	26,40,40	1.53	2 (7%)
4	GOL	G	398	-	5,5,5	0.37	0	5,5,5	0.33	0
4	GOL	G	399	-	5,5,5	0.34	0	5,5,5	0.57	0
4	GOL	G	400	-	5,5,5	0.34	0	5,5,5	0.36	0
2	FAD	G	450	-	48,58,58	1.21	5 (10%)	54,89,89	2.16	10 (18%)
3	UDP	G	500	-	18,26,26	1.11	1 (5%)	26,40,40	1.54	2 (7%)
4	GOL	H	398	-	5,5,5	0.30	0	5,5,5	0.40	0
4	GOL	H	399	-	5,5,5	0.41	0	5,5,5	0.30	0
2	FAD	H	450	-	48,58,58	1.23	5 (10%)	54,89,89	1.97	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	UDP	H	500	-	18,26,26	1.09	1 (5%)	26,40,40	1.38	3 (11%)
4	GOL	I	398	-	5,5,5	0.32	0	5,5,5	0.79	0
4	GOL	I	399	-	5,5,5	0.37	0	5,5,5	0.52	0
4	GOL	I	400	-	5,5,5	0.31	0	5,5,5	0.31	0
6	XYL	I	401	-	9,9,9	1.19	1 (11%)	10,11,11	2.52	4 (40%)
4	GOL	I	402	-	5,5,5	0.34	0	5,5,5	0.48	0
2	FAD	I	450	-	48,58,58	1.16	4 (8%)	54,89,89	2.03	7 (12%)
3	UDP	I	500	-	16,22,26	1.24	1 (6%)	21,33,40	1.44	1 (4%)
4	GOL	J	399	-	5,5,5	0.47	0	5,5,5	0.42	0
4	GOL	J	400	-	5,5,5	0.37	0	5,5,5	0.48	0
2	FAD	J	450	-	48,58,58	1.21	5 (10%)	54,89,89	2.10	7 (12%)
3	UDP	J	500	-	18,26,26	1.13	1 (5%)	26,40,40	1.34	2 (7%)

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
4	GOL	A	398	-	-	0/4/4/4	0/0/0/0
4	GOL	A	399	-	-	0/4/4/4	0/0/0/0
4	GOL	A	400	-	-	0/4/4/4	0/0/0/0
2	FAD	A	450	-	-	0/30/50/50	0/6/6/6
3	UDP	A	500	-	-	0/12/32/32	0/2/2/2
4	GOL	B	398	-	-	0/4/4/4	0/0/0/0
2	FAD	B	450	-	-	0/30/50/50	0/6/6/6
3	UDP	B	500	-	-	0/12/32/32	0/2/2/2
4	GOL	C	398	-	-	0/4/4/4	0/0/0/0
4	GOL	C	399	-	-	0/4/4/4	0/0/0/0
2	FAD	C	450	-	-	0/30/50/50	0/6/6/6
3	UDP	C	500	-	-	0/12/32/32	0/2/2/2
4	GOL	D	398	-	-	0/4/4/4	0/0/0/0
4	GOL	D	399	-	-	0/4/4/4	0/0/0/0
2	FAD	D	450	-	-	0/30/50/50	0/6/6/6
5	URM	D	600	-	-	0/16/59/59	0/3/3/3
4	GOL	E	398	-	-	0/4/4/4	0/0/0/0
4	GOL	E	399	-	-	0/4/4/4	0/0/0/0
4	GOL	E	400	-	-	0/4/4/4	0/0/0/0
4	GOL	E	401	-	-	0/4/4/4	0/0/0/0
2	FAD	E	450	-	-	0/30/50/50	0/6/6/6
3	UDP	E	500	-	-	0/6/26/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	F	398	-	-	0/4/4/4	0/0/0/0
6	XYL	F	399	-	-	0/12/12/12	0/0/0/0
4	GOL	F	400	-	-	0/4/4/4	0/0/0/0
2	FAD	F	450	-	-	0/30/50/50	0/6/6/6
3	UDP	F	500	-	-	0/12/32/32	0/2/2/2
4	GOL	G	398	-	-	0/4/4/4	0/0/0/0
4	GOL	G	399	-	-	0/4/4/4	0/0/0/0
4	GOL	G	400	-	-	0/4/4/4	0/0/0/0
2	FAD	G	450	-	-	0/30/50/50	0/6/6/6
3	UDP	G	500	-	-	0/12/32/32	0/2/2/2
4	GOL	H	398	-	-	0/4/4/4	0/0/0/0
4	GOL	H	399	-	-	0/4/4/4	0/0/0/0
2	FAD	H	450	-	-	0/30/50/50	0/6/6/6
3	UDP	H	500	-	-	0/12/32/32	0/2/2/2
4	GOL	I	398	-	-	0/4/4/4	0/0/0/0
4	GOL	I	399	-	-	0/4/4/4	0/0/0/0
4	GOL	I	400	-	-	0/4/4/4	0/0/0/0
6	XYL	I	401	-	-	0/12/12/12	0/0/0/0
4	GOL	I	402	-	-	0/4/4/4	0/0/0/0
2	FAD	I	450	-	-	0/30/50/50	0/6/6/6
3	UDP	I	500	-	-	0/6/26/32	0/2/2/2
4	GOL	J	399	-	-	0/4/4/4	0/0/0/0
4	GOL	J	400	-	-	0/4/4/4	0/0/0/0
2	FAD	J	450	-	-	0/30/50/50	0/6/6/6
3	UDP	J	500	-	-	0/12/32/32	0/2/2/2

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	600	URM	P22-C45	-17.43	1.61	1.80
6	F	399	XYL	O2-C2	-3.48	1.35	1.43
5	D	600	URM	P22-O23	-2.55	1.50	1.56
6	F	399	XYL	O4-C4	-2.52	1.37	1.43
6	I	401	XYL	O2-C2	-2.35	1.38	1.43

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	FAD	N3A-C2A-N1A	-12.79	119.10	128.89
2	F	450	FAD	N3A-C2A-N1A	-12.15	119.59	128.89
2	D	450	FAD	N3A-C2A-N1A	-11.86	119.81	128.89
2	G	450	FAD	N3A-C2A-N1A	-11.84	119.83	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	450	FAD	N3A-C2A-N1A	-11.70	119.94	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	398	GOL	1	0
2	A	450	FAD	2	0
3	A	500	UDP	1	0
4	B	398	GOL	2	0
2	B	450	FAD	1	0
3	B	500	UDP	4	0
4	C	398	GOL	2	0
2	C	450	FAD	1	0
4	D	399	GOL	1	0
2	D	450	FAD	5	0
5	D	600	URM	1	0
4	E	398	GOL	1	0
4	E	400	GOL	1	0
2	E	450	FAD	3	0
4	F	398	GOL	1	0
4	F	400	GOL	1	0
2	G	450	FAD	1	0
3	G	500	UDP	1	0
4	H	398	GOL	2	0
4	I	398	GOL	3	0
6	I	401	XYL	1	0
4	I	402	GOL	2	0
2	I	450	FAD	3	0
2	J	450	FAD	1	0
3	J	500	UDP	1	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 ⓘ

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	365/397 (91%)	-0.09	6 (1%) 74 74	32, 43, 60, 93	1 (0%)
1	B	363/397 (91%)	0.47	46 (12%) 5 3	35, 47, 94, 152	1 (0%)
1	C	363/397 (91%)	0.06	13 (3%) 46 45	36, 49, 71, 104	1 (0%)
1	D	359/397 (90%)	0.60	46 (12%) 5 3	38, 55, 80, 120	2 (0%)
1	E	361/397 (90%)	0.44	33 (9%) 11 9	38, 59, 91, 122	2 (0%)
1	F	364/397 (91%)	0.11	12 (3%) 50 48	37, 49, 68, 95	2 (0%)
1	G	363/397 (91%)	-0.02	6 (1%) 73 72	34, 53, 78, 126	2 (0%)
1	H	364/397 (91%)	0.04	9 (2%) 61 59	35, 48, 69, 115	1 (0%)
1	I	364/397 (91%)	-0.11	7 (1%) 70 69	33, 46, 66, 113	1 (0%)
1	J	363/397 (91%)	0.34	37 (10%) 9 6	36, 53, 81, 109	3 (0%)
All	All	3629/3970 (91%)	0.18	215 (5%) 26 23	32, 49, 81, 152	16 (0%)

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	VAL	7.5
1	B	153	VAL	7.4
1	B	186	LEU	6.1
1	E	154	GLU	5.8
1	E	153	VAL	5.7

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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
4	GOL	I	398	6/6	0.92	0.23	11.78	41,50,55,56	0
4	GOL	E	398	6/6	0.80	0.37	9.23	61,64,71,72	0
4	GOL	B	398	6/6	0.64	0.28	7.69	52,58,59,59	0
6	XYL	F	399	10/10	0.66	0.47	7.46	20,20,20,20	0
4	GOL	H	398	6/6	0.83	0.19	7.28	50,55,61,62	0
4	GOL	G	399	6/6	0.83	0.21	5.82	54,57,63,64	0
4	GOL	J	400	6/6	0.54	0.33	5.02	56,62,70,72	0
6	XYL	I	401	10/10	0.71	0.25	4.03	62,67,73,76	0
4	GOL	F	400	6/6	0.75	0.27	3.74	59,65,67,69	0
4	GOL	F	398	6/6	0.75	0.28	3.37	48,55,60,62	0
4	GOL	C	398	6/6	0.87	0.23	3.14	51,55,57,60	0
4	GOL	J	399	6/6	0.77	0.28	2.89	46,60,64,69	0
4	GOL	A	398	6/6	0.82	0.26	2.17	51,56,64,66	0
4	GOL	I	399	6/6	0.86	0.20	1.68	55,64,67,73	0
4	GOL	E	400	6/6	0.75	0.21	1.28	61,66,73,76	0
4	GOL	D	398	6/6	0.87	0.15	0.77	47,52,61,65	0
3	UDP	E	500	21/25	0.90	0.18	0.33	57,63,72,76	0
3	UDP	B	500	25/25	0.92	0.32	0.33	60,80,102,117	0
3	UDP	A	500	25/25	0.95	0.17	0.26	39,46,72,90	0
4	GOL	G	398	6/6	0.91	0.14	0.22	51,52,57,61	0
2	FAD	C	450	53/53	0.97	0.17	-0.04	39,48,61,70	0
2	FAD	G	450	53/53	0.96	0.16	-0.06	46,54,65,67	0
3	UDP	J	500	25/25	0.95	0.15	-0.09	38,47,85,108	0
3	UDP	I	500	21/25	0.96	0.17	-0.12	48,50,63,69	0
5	URM	D	600	36/36	0.95	0.20	-0.14	54,63,76,85	0
3	UDP	H	500	25/25	0.95	0.16	-0.16	41,48,73,90	0
2	FAD	I	450	53/53	0.97	0.15	-0.18	38,45,56,62	0
2	FAD	B	450	53/53	0.97	0.17	-0.32	35,47,62,66	0
3	UDP	G	500	25/25	0.94	0.16	-0.40	52,59,87,108	0
2	FAD	F	450	53/53	0.96	0.17	-0.43	40,47,54,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	D	450	53/53	0.96	0.16	-0.56	50,57,65,66	0
2	FAD	E	450	53/53	0.96	0.16	-0.56	45,60,70,74	0
3	UDP	F	500	25/25	0.94	0.16	-0.57	47,52,90,107	0
2	FAD	A	450	53/53	0.97	0.14	-0.58	38,46,51,55	0
2	FAD	H	450	53/53	0.97	0.15	-0.77	38,48,52,56	0
3	UDP	C	500	25/25	0.96	0.14	-0.85	50,58,85,108	0
2	FAD	J	450	53/53	0.96	0.15	-0.91	44,57,64,65	0
4	GOL	H	399	6/6	0.76	0.26	-	60,72,75,81	0
4	GOL	G	400	6/6	0.75	0.32	-	63,68,72,76	0
4	GOL	C	399	6/6	0.82	0.18	-	65,72,77,78	0
4	GOL	D	399	6/6	0.81	0.38	-	73,75,76,77	0
4	GOL	E	401	6/6	0.77	0.27	-	67,73,74,78	0
4	GOL	I	402	6/6	0.64	0.32	-	61,62,68,74	0
4	GOL	A	400	6/6	0.87	0.43	-	58,63,69,70	0
4	GOL	I	400	6/6	0.71	0.39	-	67,76,80,80	0
4	GOL	E	399	6/6	0.78	0.21	-	60,65,74,76	0
4	GOL	A	399	6/6	0.74	0.22	-	58,62,75,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.