



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:41 PM GMT

PDB ID : 3UKH  
Title : Crystal structure of udp-galactopyranose mutase from *Aspergillus fumigatus* in complex with UDPGALP (non-reduced)  
Authors : Van Straaten, K.E.; Sanders, D.A.R.  
Deposited on : 2011-11-09  
Resolution : 2.30 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

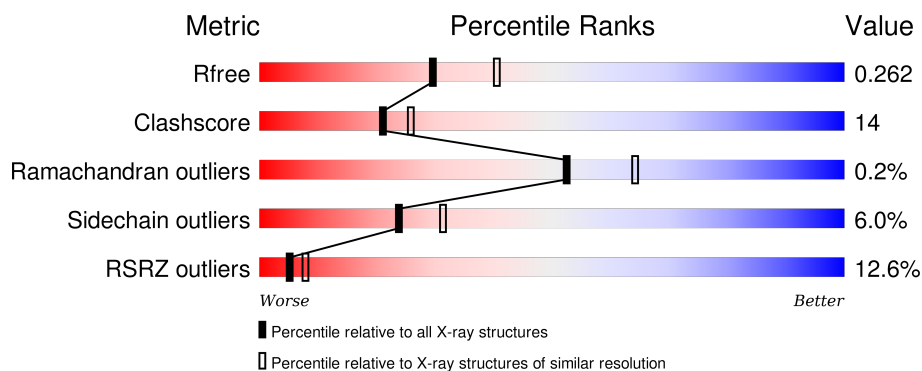
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	519	<div> <div>9%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	B	519	<div> <div>14%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	C	519	<div> <div>13%</div> <div>70%</div> <div>26%</div> <div>• •</div> </div>
1	D	519	<div> <div>12%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	E	519	<div> <div>18%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	
1	G	519	
1	H	519	

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
3	GDU	A	521	-	-	-	X
3	GDU	B	521	-	-	-	X
3	GDU	C	521	-	-	-	X
3	GDU	D	521	-	-	-	X
3	GDU	E	521	-	-	-	X
3	GDU	F	521	-	-	-	X
3	GDU	G	521	-	-	-	X
3	GDU	H	521	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34881 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	504	Total	C	N	O	S	0	15	0
			4080	2590	699	768	23			
1	B	510	Total	C	N	O	S	0	15	0
			4126	2619	711	774	22			
1	C	511	Total	C	N	O	S	0	42	0
			4270	2713	734	801	22			
1	D	510	Total	C	N	O	S	0	3	0
			4035	2560	694	759	22			
1	E	510	Total	C	N	O	S	0	9	0
			4074	2586	700	767	21			
1	F	504	Total	C	N	O	S	0	8	0
			4026	2554	689	761	22			
1	G	504	Total	C	N	O	S	0	1	0
			3977	2525	680	751	21			
1	H	511	Total	C	N	O	S	0	42	0
			4301	2733	740	807	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
A	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
A	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
A	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
A	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
B	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
B	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2

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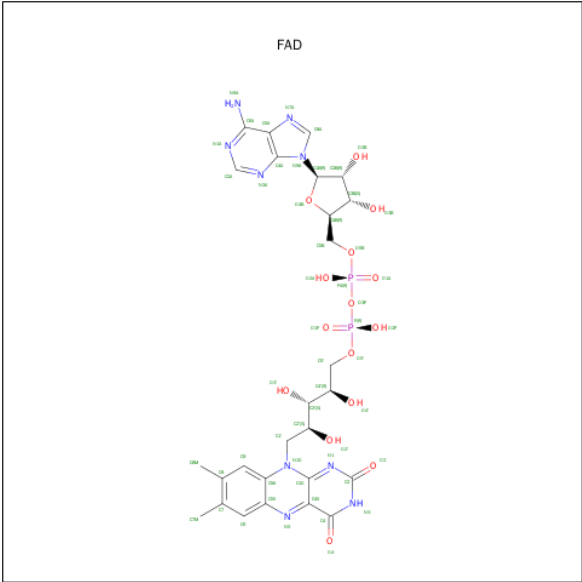
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
B	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
C	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
C	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
C	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
C	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
D	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
D	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
D	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
D	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
E	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
E	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
E	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
E	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
F	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
F	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
F	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
F	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2

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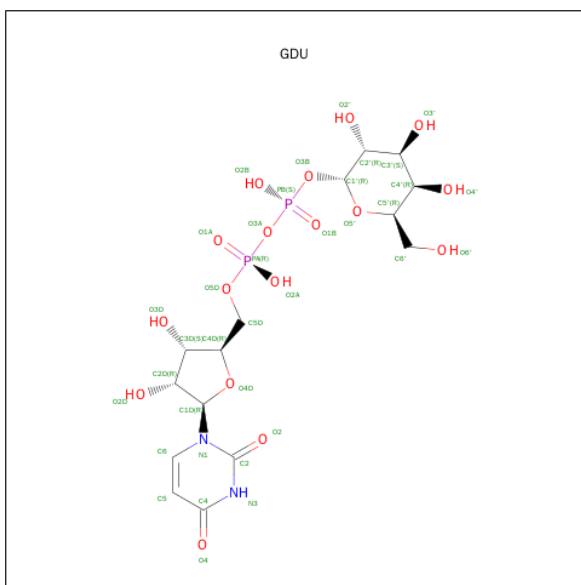
Chain	Residue	Modelled	Actual	Comment	Reference
F	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
G	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
G	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
G	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
G	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
H	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
H	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
H	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
H	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2

- 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	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		

- Molecule 3 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: C<sub>15</sub>H<sub>24</sub>N<sub>2</sub>O<sub>17</sub>P<sub>2</sub>).



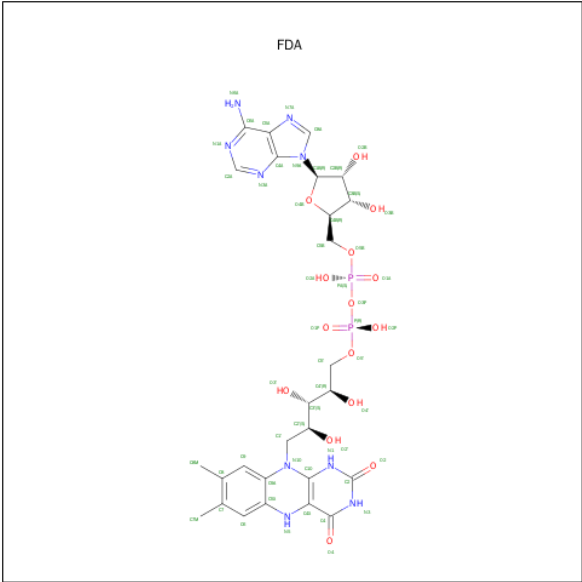
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	E	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	F	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	G	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	H	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

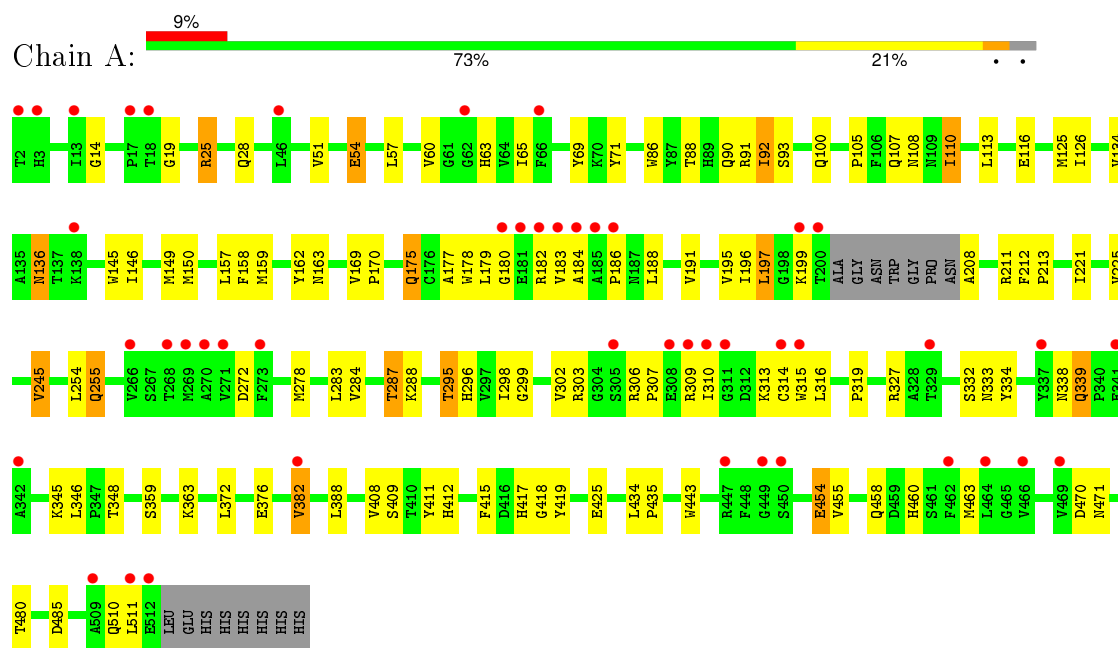
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	207	Total	O	0	0
			207	207		
6	B	180	Total	O	0	0
			180	180		
6	C	150	Total	O	0	0
			150	150		
6	D	172	Total	O	0	0
			172	172		
6	E	137	Total	O	0	0
			137	137		
6	F	126	Total	O	0	0
			126	126		
6	G	156	Total	O	0	0
			156	156		
6	H	150	Total	O	0	0
			150	150		

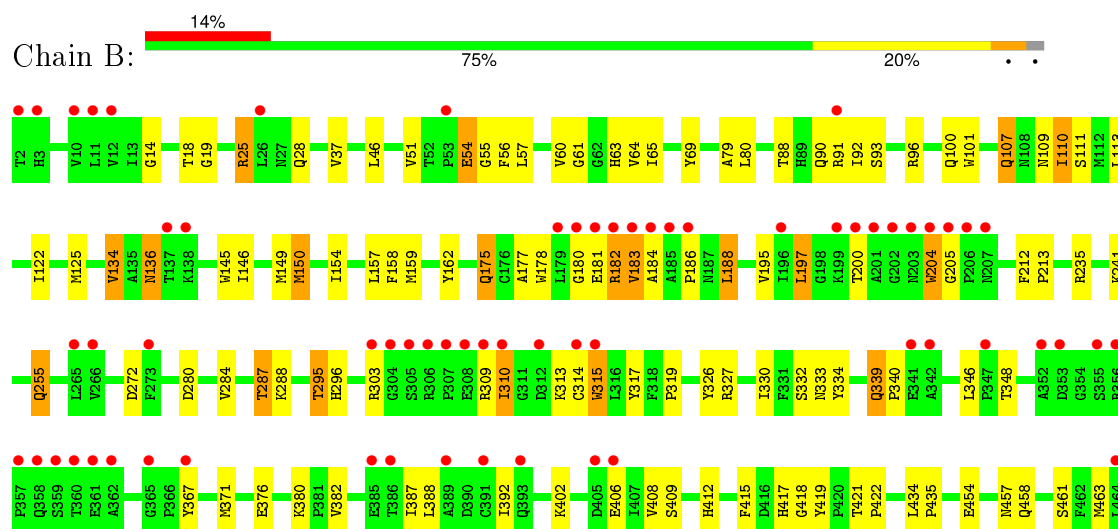
### 3 Residue-property plots [i](#)

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.

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

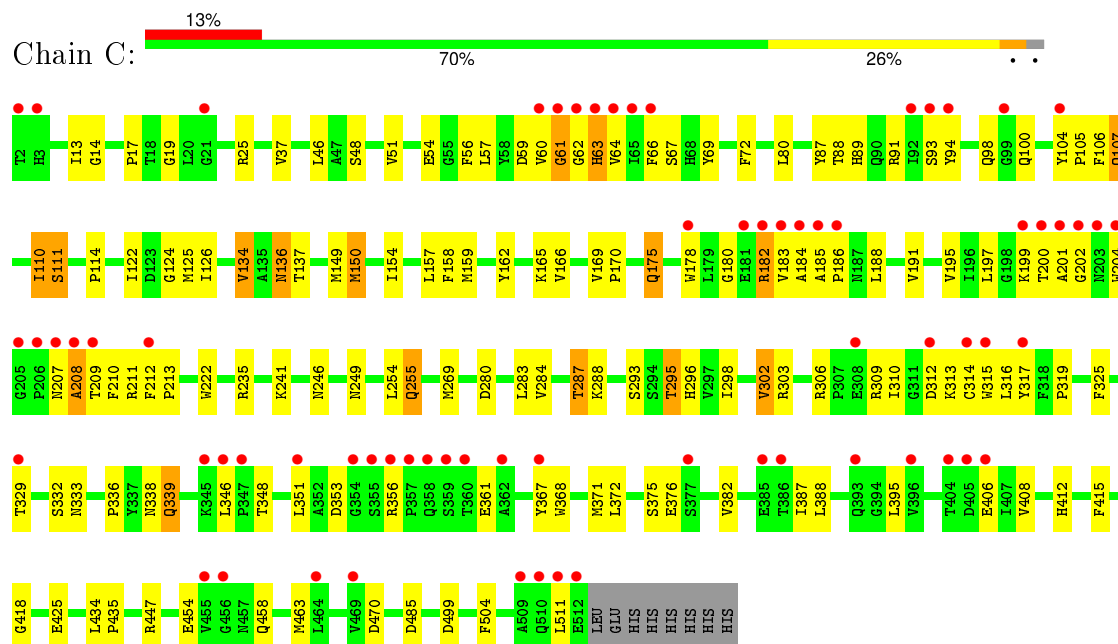


#### • Molecule 1: UDP-galactopyranose mutase

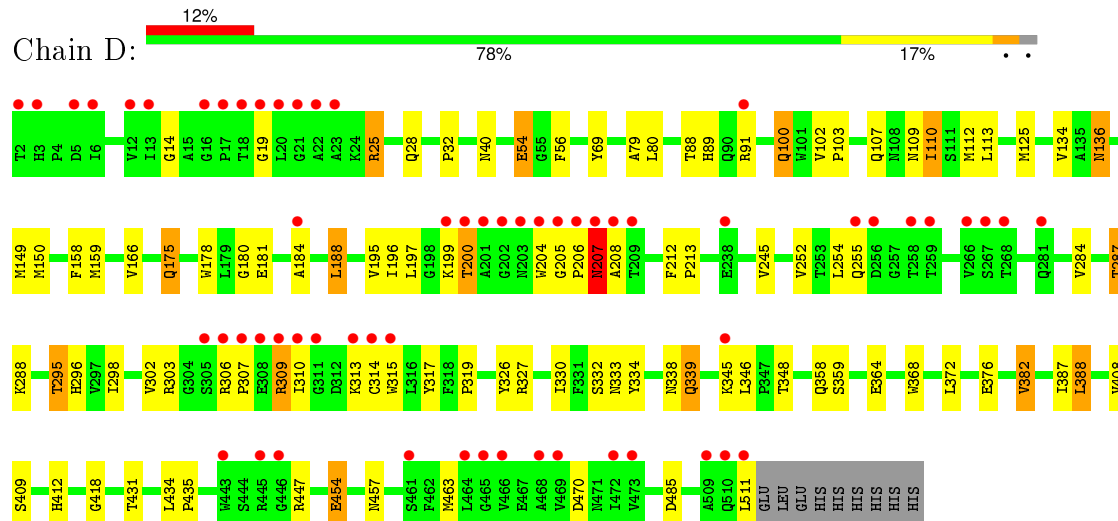




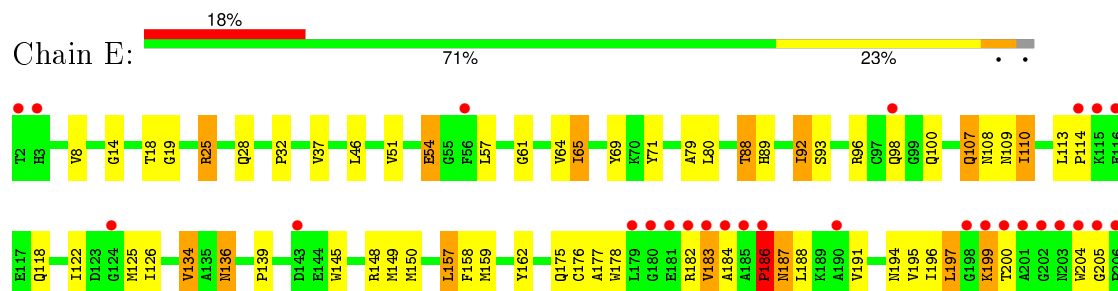
• Molecule 1: UDP-galactopyranose mutase

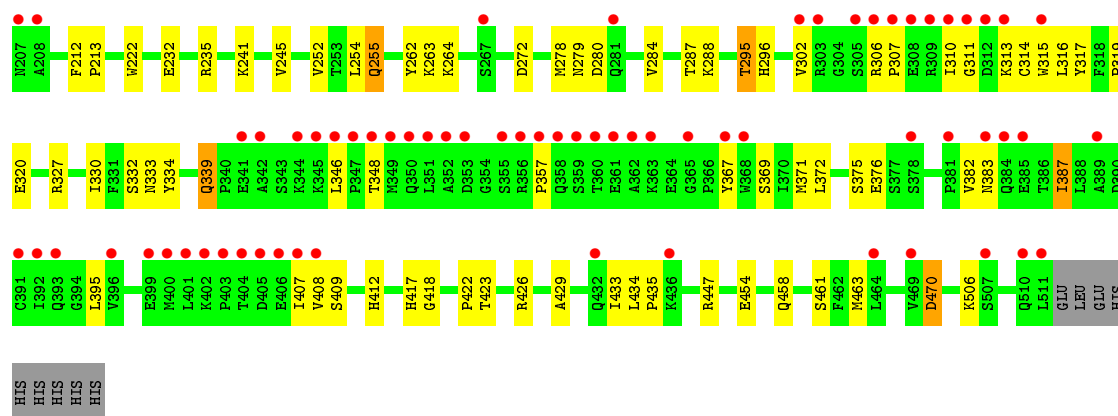


• Molecule 1: UDP-galactopyranose mutase

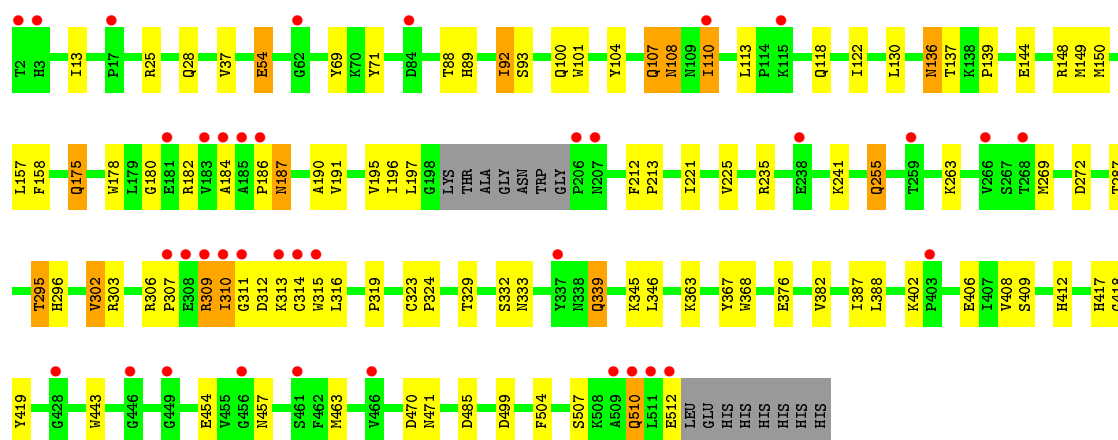
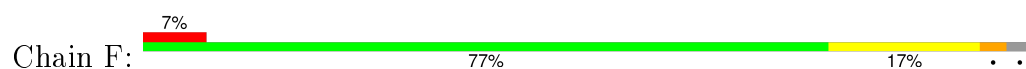


• Molecule 1: UDP-galactopyranose mutase

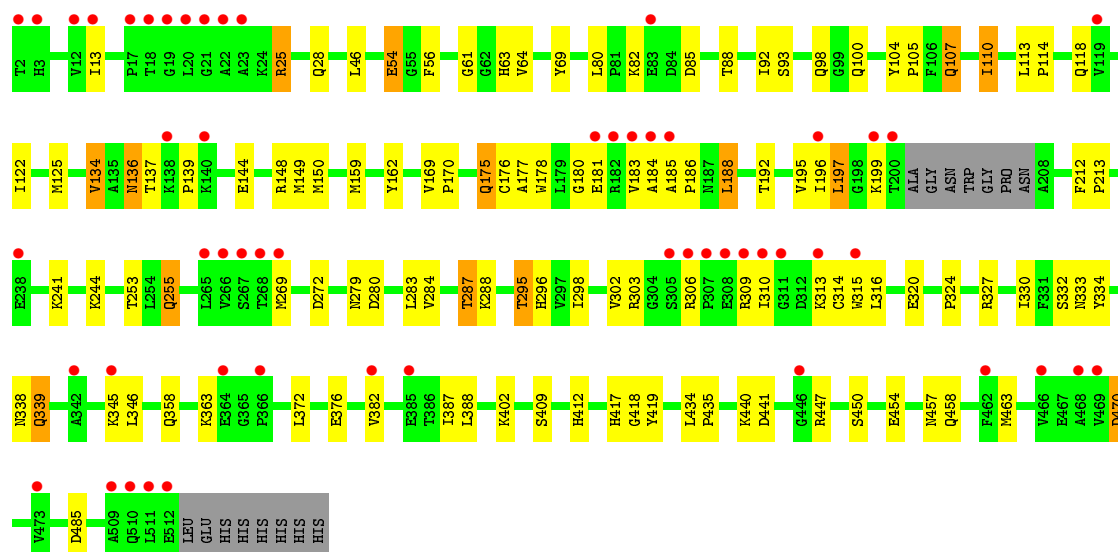
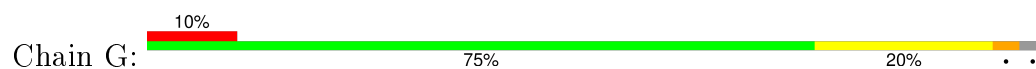




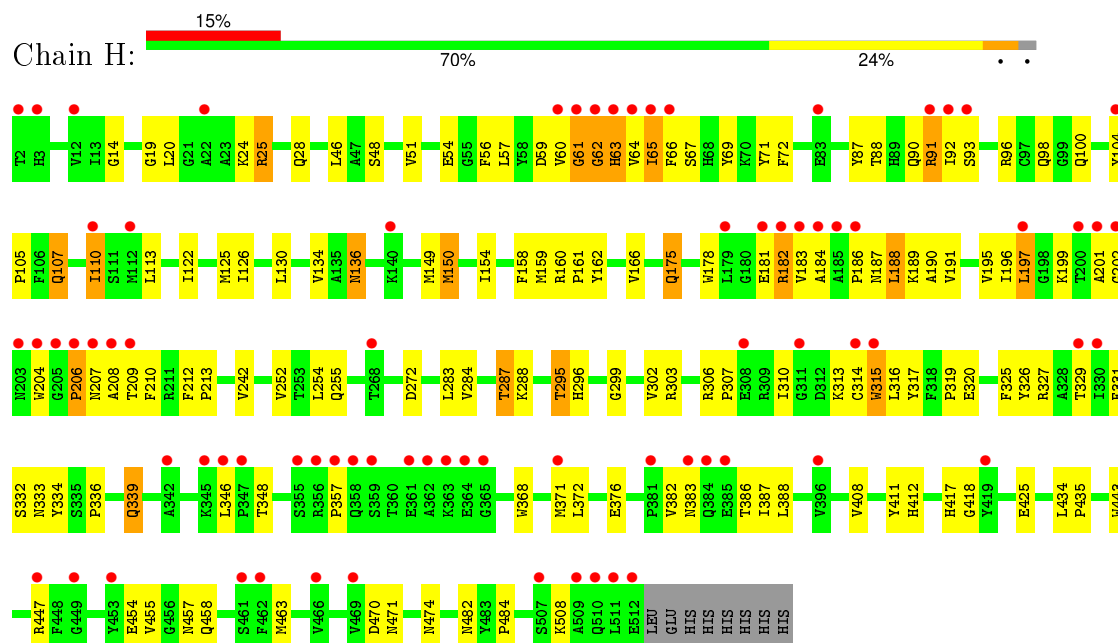
• Molecule 1: UDP-galactopyranose mutase



• Molecule 1: UDP-galactopyranose mutase



• Molecule 1: UDP-galactopyranose mutase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.97 Å   129.26 Å   173.88 Å 89.87°   84.64°   81.21°	Depositor
Resolution (Å)	35.55 – 2.30 35.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (35.55-2.30) 97.1 (35.55-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.222   ,   0.264 0.220   ,   0.262	Depositor DCC
$R_{free}$ test set	13334 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 266579 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: FDA, GDU, FAD, CL

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	0.25	0/4180	0.43	0/5680
1	B	0.25	0/4230	0.43	0/5751
1	C	0.25	0/4378	0.43	0/5951
1	D	0.25	0/4136	0.43	0/5621
1	E	0.25	0/4176	0.43	0/5677
1	F	0.24	0/4125	0.42	0/5603
1	G	0.25	0/4074	0.43	0/5534
1	H	0.26	0/4413	0.44	0/6000
All	All	0.25	0/33712	0.43	0/45817

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	E	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	186[B]	PRO	Peptide
1	H	206[A]	PRO	Peptide

## 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	4080	0	3999	120	0
1	B	4126	0	4041	123	0
1	C	4270	0	4171	135	0
1	D	4035	0	3951	91	0
1	E	4074	0	3992	130	0
1	F	4026	0	3941	88	0
1	G	3977	0	3899	88	0
1	H	4301	0	4193	154	0
2	A	53	0	30	6	0
2	B	53	0	30	4	0
2	D	53	0	30	2	0
2	E	53	0	30	2	0
2	F	53	0	30	6	0
2	G	53	0	30	4	0
3	A	36	0	22	10	0
3	B	36	0	22	10	0
3	C	36	0	22	7	0
3	D	36	0	22	4	0
3	E	36	0	22	12	0
3	F	36	0	22	3	0
3	G	36	0	22	8	0
3	H	36	0	22	11	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
5	C	53	0	32	6	0
5	H	53	0	32	6	0
6	A	207	0	0	4	0
6	B	180	0	0	13	0
6	C	150	0	0	12	0
6	D	172	0	0	8	0
6	E	137	0	0	7	0
6	F	126	0	0	5	0
6	G	156	0	0	4	0
6	H	150	0	0	4	0
All	All	34881	0	32607	949	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 14.

The worst 5 of 949 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:H:104[A]:TYR:O	1:H:202[A]:GLY:HA2	1.68	0.92
1:E:175:GLN:HG2	6:E:820:HOH:O	1.67	0.92
3:B:521:GDU:O1A	6:B:1234:HOH:O	1.88	0.89
1:B:109:ASN:OD1	1:B:200:THR:HG21	1.74	0.88
1:F:296:HIS:HD2	1:F:412:HIS:HE1	1.22	0.87

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	515/519 (99%)	501 (97%)	14 (3%)	0	100	100
1	B	523/519 (101%)	501 (96%)	22 (4%)	0	100	100
1	C	541/519 (104%)	509 (94%)	28 (5%)	4 (1%)	26	31
1	D	511/519 (98%)	494 (97%)	16 (3%)	1 (0%)	52	64
1	E	517/519 (100%)	487 (94%)	27 (5%)	3 (1%)	30	36
1	F	508/519 (98%)	490 (96%)	15 (3%)	3 (1%)	30	36
1	G	501/519 (96%)	481 (96%)	20 (4%)	0	100	100
1	H	545/519 (105%)	515 (94%)	26 (5%)	4 (1%)	26	31
All	All	4161/4152 (100%)	3978 (96%)	168 (4%)	15 (0%)	52	48

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	186[A]	PRO
1	E	186[B]	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	187	ASN
1	C	208[B]	ALA
1	H	61[A]	GLY

### 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	440/441 (100%)	415 (94%)	25 (6%)	25	34
1	B	443/441 (100%)	413 (93%)	30 (7%)	20	25
1	C	459/441 (104%)	428 (93%)	31 (7%)	20	25
1	D	435/441 (99%)	406 (93%)	29 (7%)	20	26
1	E	438/441 (99%)	412 (94%)	26 (6%)	24	32
1	F	436/441 (99%)	413 (95%)	23 (5%)	28	37
1	G	430/441 (98%)	406 (94%)	24 (6%)	26	35
1	H	461/441 (104%)	427 (93%)	34 (7%)	17	21
All	All	3542/3528 (100%)	3320 (94%)	222 (6%)	24	29

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	207	ASN
1	E	136	ASN
1	H	182[A]	ARG
1	D	287	THR
1	D	454	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	339	GLN
1	E	333	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	H	175	GLN
1	D	393	GLN
1	E	98	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](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GDU	A	521	-	29,38,38	1.79	7 (24%)	43,58,58	1.64	5 (11%)
2	FAD	A	600	-	48,58,58	2.21	12 (25%)	54,89,89	2.28	15 (27%)
3	GDU	B	521	-	29,38,38	1.81	8 (27%)	43,58,58	1.64	4 (9%)
2	FAD	B	600	-	48,58,58	2.29	15 (31%)	54,89,89	2.29	16 (29%)
3	GDU	C	521	-	29,38,38	1.82	7 (24%)	43,58,58	1.62	5 (11%)
5	FDA	C	600	-	48,58,58	2.24	12 (25%)	54,89,89	2.26	15 (27%)
3	GDU	D	521	-	29,38,38	1.78	8 (27%)	43,58,58	1.71	5 (11%)
2	FAD	D	600	-	48,58,58	2.32	14 (29%)	54,89,89	2.24	16 (29%)
3	GDU	E	521	-	29,38,38	1.75	7 (24%)	43,58,58	2.00	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	E	600	-	48,58,58	2.31	14 (29%)	54,89,89	2.27	17 (31%)
3	GDU	F	521	-	29,38,38	1.78	8 (27%)	43,58,58	1.72	5 (11%)
2	FAD	F	600	-	48,58,58	2.28	13 (27%)	54,89,89	2.42	17 (31%)
3	GDU	G	521	-	29,38,38	1.80	8 (27%)	43,58,58	1.70	5 (11%)
2	FAD	G	600	-	48,58,58	2.35	14 (29%)	54,89,89	2.36	21 (38%)
3	GDU	H	521	-	29,38,38	1.81	7 (24%)	43,58,58	1.69	6 (13%)
5	FDA	H	600	-	48,58,58	2.32	14 (29%)	54,89,89	2.39	14 (25%)

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	GDU	A	521	-	-	0/19/59/59	0/3/3/3
2	FAD	A	600	-	-	0/30/50/50	0/6/6/6
3	GDU	B	521	-	-	0/19/59/59	0/3/3/3
2	FAD	B	600	-	-	0/30/50/50	0/6/6/6
3	GDU	C	521	-	-	0/19/59/59	0/3/3/3
5	FDA	C	600	-	-	0/30/50/50	0/6/6/6
3	GDU	D	521	-	-	0/19/59/59	0/3/3/3
2	FAD	D	600	-	-	0/30/50/50	0/6/6/6
3	GDU	E	521	-	-	0/19/59/59	0/3/3/3
2	FAD	E	600	-	-	0/30/50/50	0/6/6/6
3	GDU	F	521	-	-	0/19/59/59	0/3/3/3
2	FAD	F	600	-	-	0/30/50/50	0/6/6/6
3	GDU	G	521	-	-	0/19/59/59	0/3/3/3
2	FAD	G	600	-	-	0/30/50/50	0/6/6/6
3	GDU	H	521	-	-	0/19/59/59	0/3/3/3
5	FDA	H	600	-	-	0/30/50/50	0/6/6/6

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	600	FAD	C1'-N10	-8.39	1.39	1.48
5	H	600	FDA	C1'-N10	-8.31	1.39	1.48
2	D	600	FAD	C1'-N10	-8.24	1.39	1.48
2	E	600	FAD	C1'-N10	-8.23	1.39	1.48
2	B	600	FAD	C1'-N10	-7.98	1.40	1.48

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	600	FDA	N3A-C2A-N1A	-9.42	121.68	128.89
2	A	600	FAD	N3A-C2A-N1A	-9.34	121.75	128.89
2	F	600	FAD	N3A-C2A-N1A	-9.19	121.86	128.89
2	E	600	FAD	N3A-C2A-N1A	-9.13	121.90	128.89
2	B	600	FAD	N3A-C2A-N1A	-9.11	121.92	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	521	GDU	10	0
2	A	600	FAD	6	0
3	B	521	GDU	10	0
2	B	600	FAD	4	0
3	C	521	GDU	7	0
5	C	600	FDA	6	0
3	D	521	GDU	4	0
2	D	600	FAD	2	0
3	E	521	GDU	12	0
2	E	600	FAD	2	0
3	F	521	GDU	3	0
2	F	600	FAD	6	0
3	G	521	GDU	8	0
2	G	600	FAD	4	0
3	H	521	GDU	11	0
5	H	600	FDA	6	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	504/519 (97%)	0.58	46 (9%) 11 17	27, 50, 80, 137	0
1	B	510/519 (98%)	0.85	75 (14%) 3 5	28, 53, 88, 163	0
1	C	511/519 (98%)	0.89	69 (13%) 4 6	28, 54, 84, 138	10 (1%)
1	D	510/519 (98%)	0.63	61 (11%) 6 9	30, 52, 87, 150	0
1	E	510/519 (98%)	1.06	94 (18%) 2 2	30, 56, 89, 147	2 (0%)
1	F	504/519 (97%)	0.50	38 (7%) 17 24	31, 53, 85, 137	0
1	G	504/519 (97%)	0.66	54 (10%) 8 12	28, 53, 85, 140	0
1	H	511/519 (98%)	0.93	77 (15%) 3 5	27, 54, 82, 137	6 (1%)
All	All	4064/4152 (97%)	0.76	514 (12%) 5 8	27, 53, 85, 163	18 (0%)

The worst 5 of 514 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	GLY	16.7
1	C	204[B]	TRP	15.3
1	E	202	GLY	13.6
1	H	204[A]	TRP	12.8
1	E	201	ALA	12.6

### 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
3	GDU	F	521	36/36	0.55	0.71	7.05	41,69,87,93	36
3	GDU	D	521	36/36	0.67	0.54	5.07	49,70,84,88	36
3	GDU	G	521	36/36	0.73	0.41	4.17	56,75,90,90	36
3	GDU	A	521	36/36	0.67	0.67	2.89	48,67,79,83	36
3	GDU	B	521	36/36	0.64	0.58	2.78	43,62,81,86	36
3	GDU	E	521	36/36	0.62	0.58	2.41	48,69,78,84	36
3	GDU	H	521	36/36	0.82	0.57	1.83	45,67,85,85	36
3	GDU	C	521	36/36	0.85	0.47	1.73	31,57,76,85	36
2	FAD	F	600	53/53	0.93	0.19	-0.11	34,50,63,69	0
2	FAD	E	600	53/53	0.95	0.16	-0.12	36,55,64,69	0
2	FAD	B	600	53/53	0.94	0.17	-0.21	36,48,62,70	0
2	FAD	G	600	53/53	0.95	0.17	-0.31	34,48,60,63	0
2	FAD	D	600	53/53	0.94	0.19	-0.32	30,47,56,60	0
2	FAD	A	600	53/53	0.95	0.19	-0.37	30,42,57,66	0
5	FDA	C	600	53/53	0.93	0.17	-0.57	33,51,64,82	0
5	FDA	H	600	53/53	0.94	0.19	-0.62	28,53,65,76	0
4	CL	A	522	1/1	0.53	0.18	-	103,103,103,103	0
4	CL	B	1	1/1	0.60	0.15	-	99,99,99,99	0

## 6.5 Other polymers

There are no such residues in this entry.