



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:43 PM GMT

PDB ID : 3UKP
Title : Crystal structure of R327A UDP-galactopyranose mutase from *Aspergillus fumigatus* in complex with UDPgalp
Authors : Van Straaten, K.E.; Sanders, D.A.R.
Deposited on : 2011-11-09
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

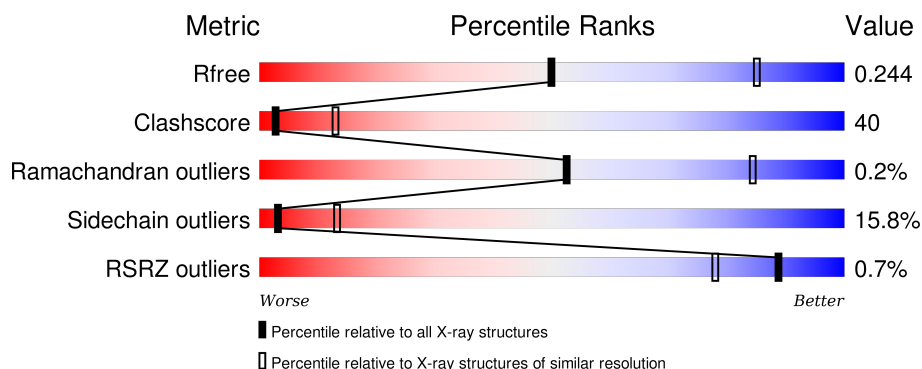
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	509	<div> <div></div> <div> <div></div> <div>50%</div> <div>43%</div> <div>7%</div> </div> </div>
1	B	509	<div> <div></div> <div> <div></div> <div>48%</div> <div>44%</div> <div>8%</div> </div> </div>
1	C	509	<div> <div></div> <div> <div></div> <div>49%</div> <div>45%</div> <div>6%</div> </div> </div>
1	D	509	<div> <div></div> <div> <div></div> <div>50%</div> <div>43%</div> <div>7%</div> </div> </div>
1	E	509	<div> <div></div> <div> <div></div> <div>37%</div> <div>55%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	509	
1	G	509	
1	H	509	

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
2	FAD	A	601	X	-	-	-
2	FAD	D	601	-	-	X	-
2	FAD	F	601	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32560 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	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	B	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	C	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	D	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	E	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	F	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	G	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	H	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			

There are 8 discrepancies between the modelled and reference sequences:

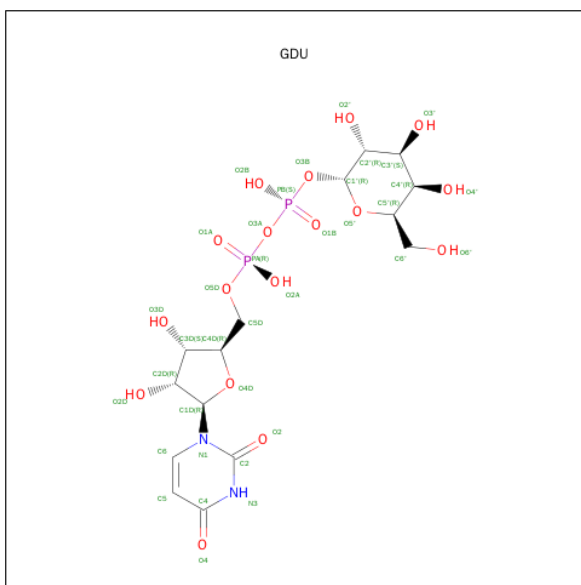
Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
B	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
C	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
D	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
E	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
F	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
G	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
H	327	ALA	ARG	ENGINEERED MUTATION	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	D	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	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	A	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		

- Molecule 3 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂).

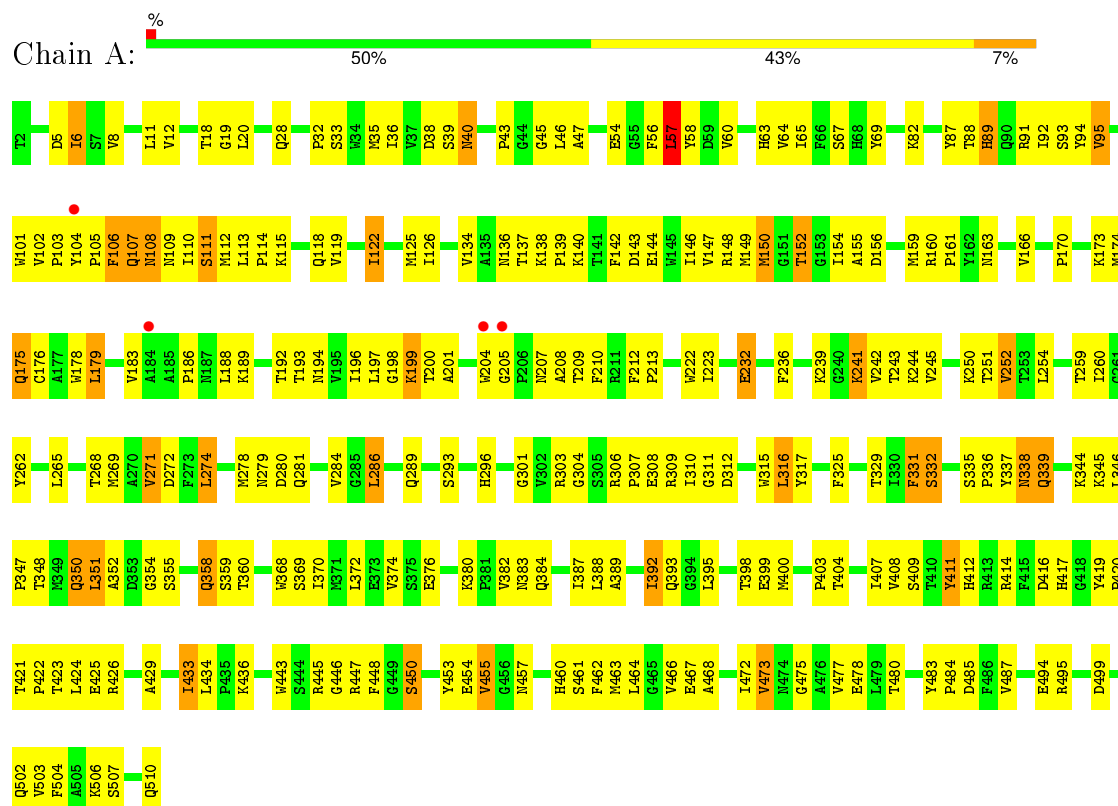


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	B	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	D	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	C	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	E	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	F	1	Total 36	C 15	N 2	O 17	P 2	0	0

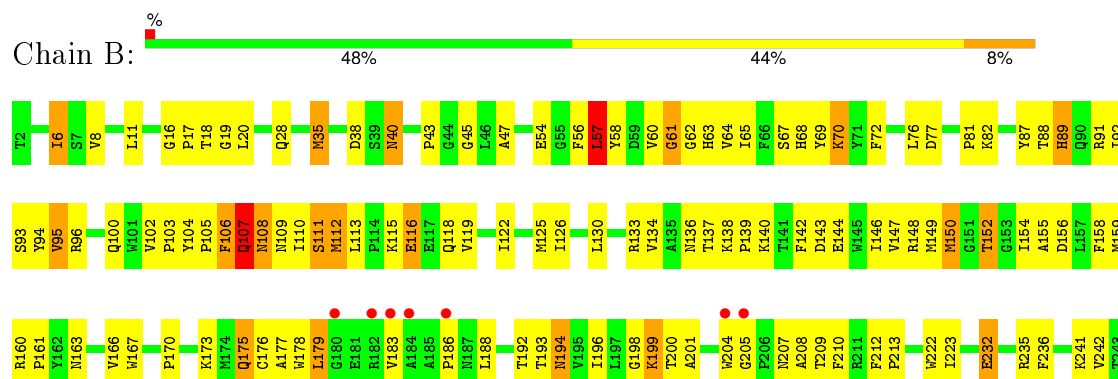
3 Residue-property plots

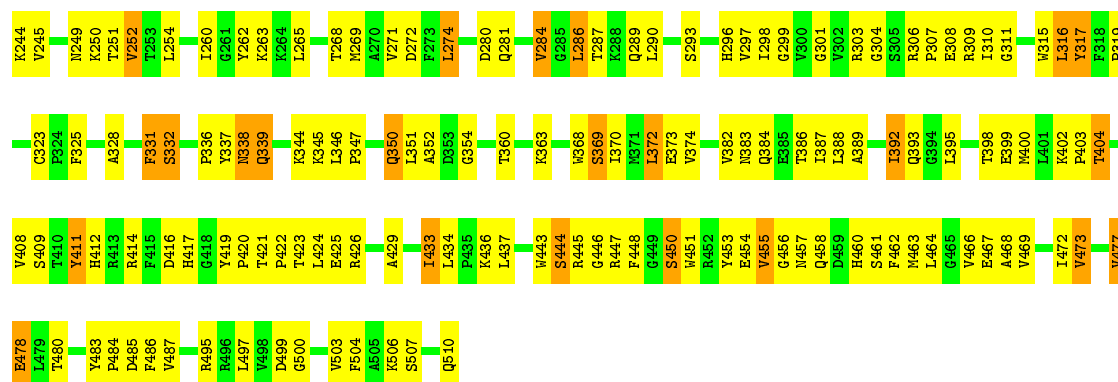
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

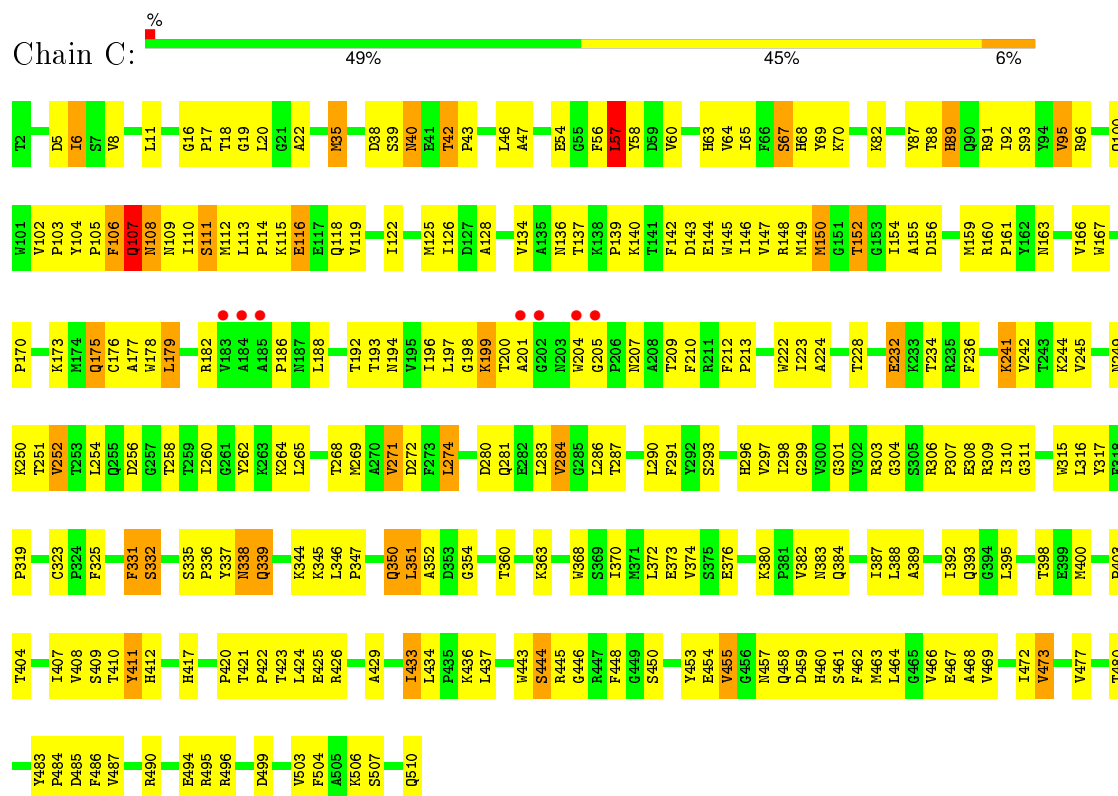


• Molecule 1: UDP-galactopyranose mutase

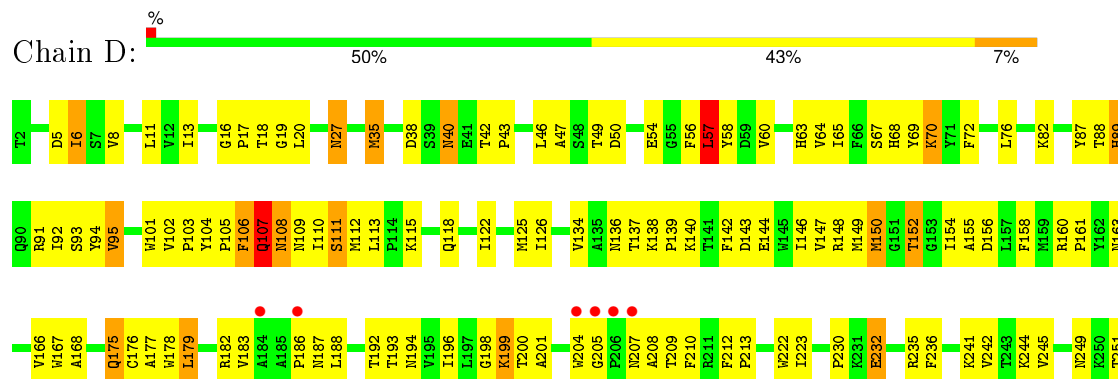


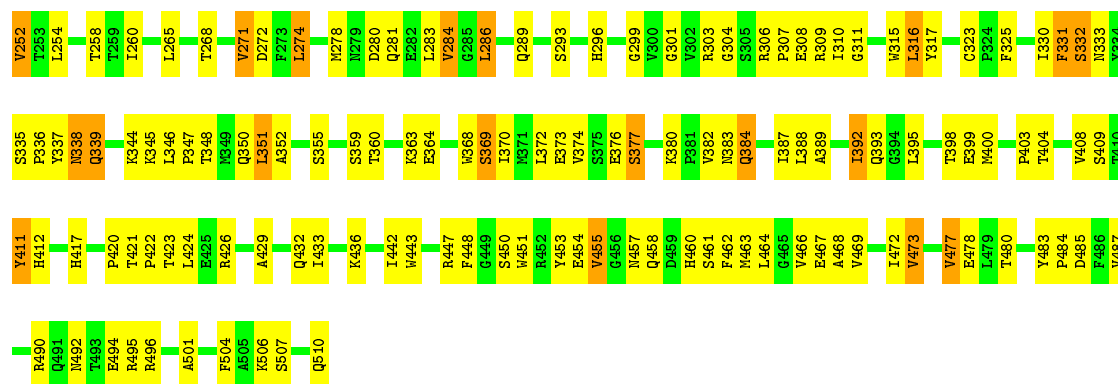


• Molecule 1: UDP-galactopyranose mutase

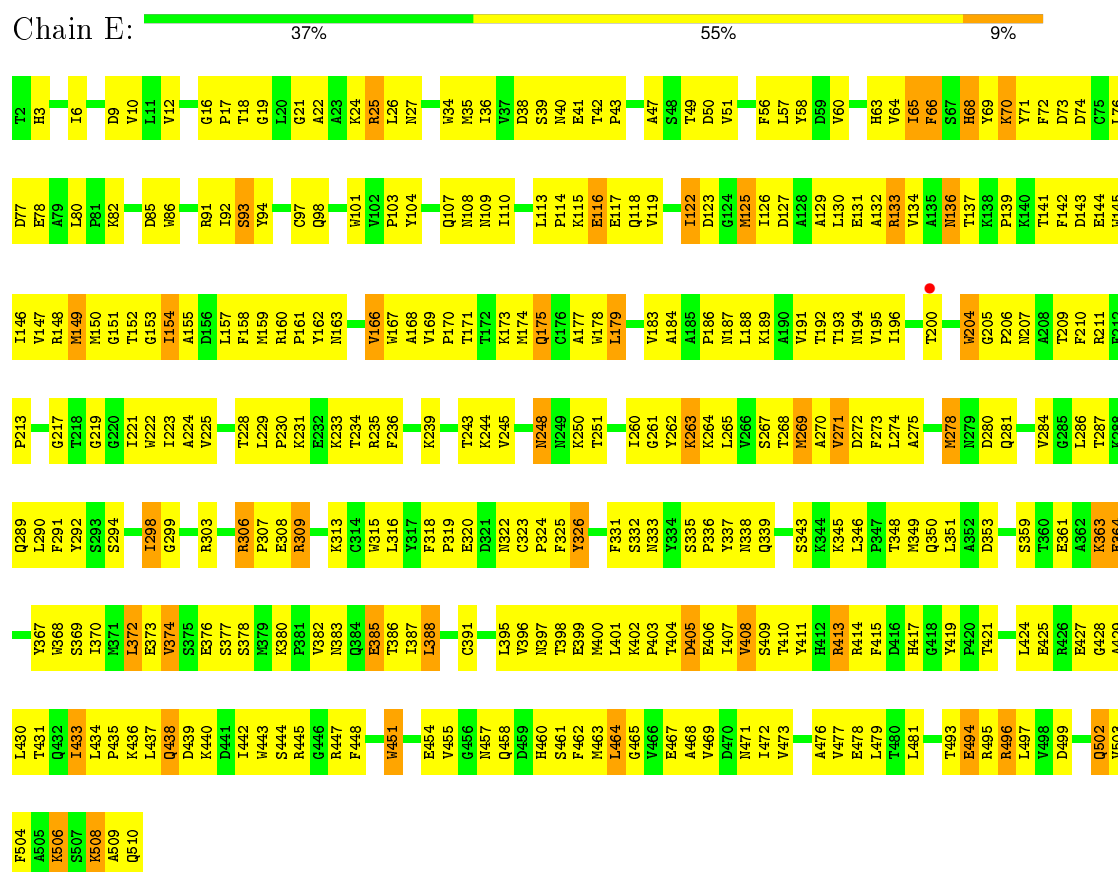


• Molecule 1: UDP-galactopyranose mutase

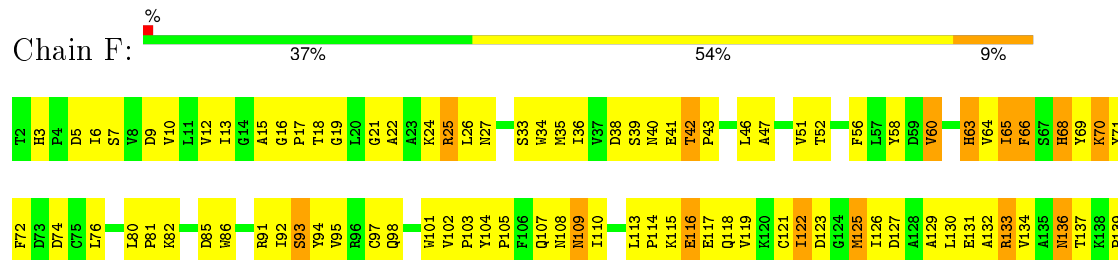


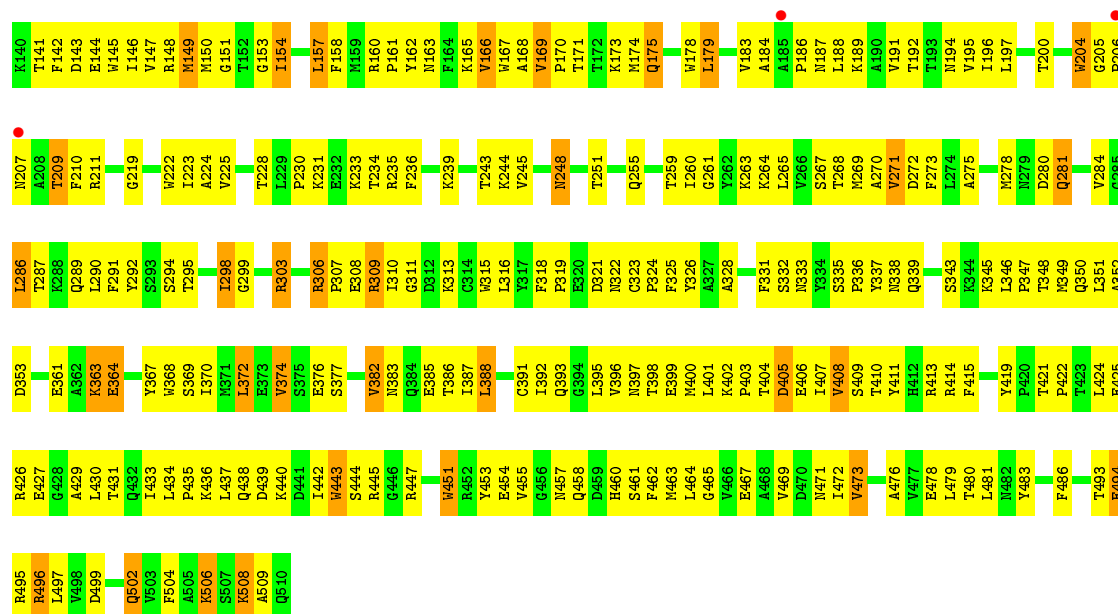


- Molecule 1: UDP-galactopyranose mutase

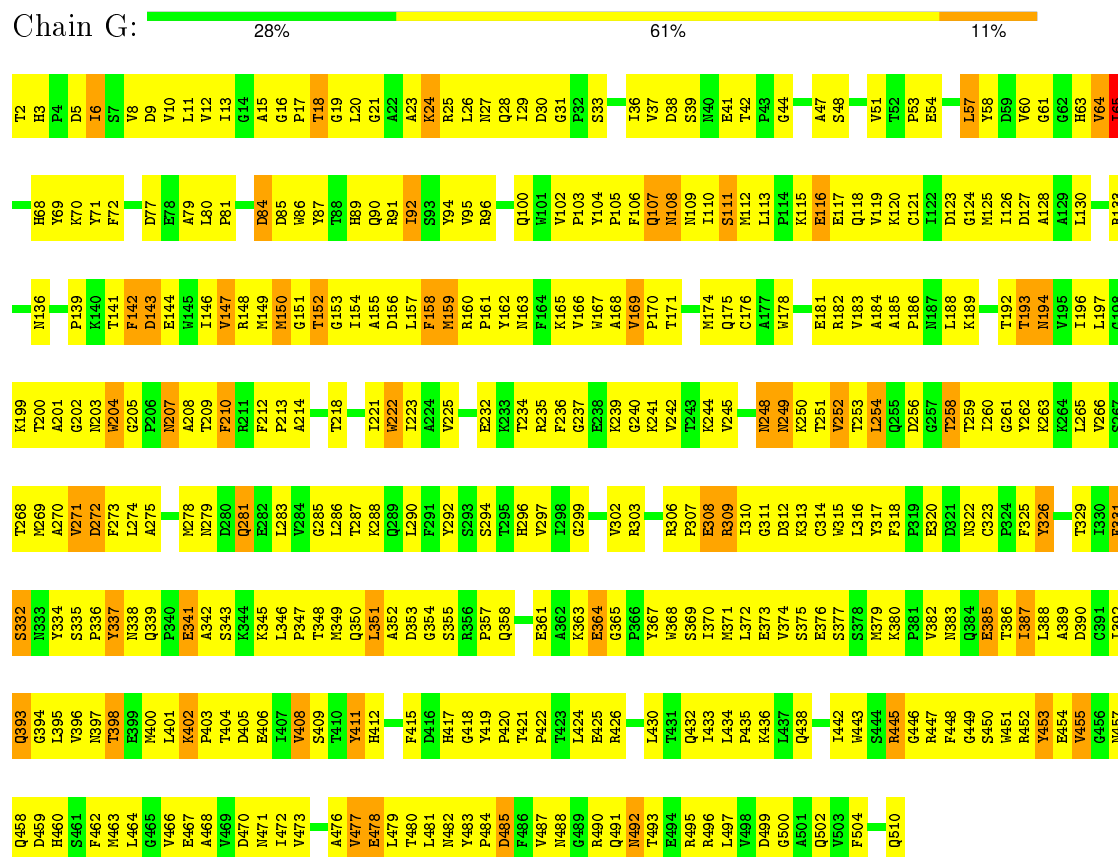


- Molecule 1: UDP-galactopyranose mutase





• Molecule 1: UDP-galactopyranose mutase



• Molecule 1: UDP-galactopyranose mutase



Q458	L395	Y334	T268	K199	R133	S67	T2
D459	V396	S336	T269	T200	V134	H68	H3
H460	N397	P336	A270	A201	P139	Y69	P4
S461	T398	T337	V271	G202	K140	K70	D5
F462	E399	N338	D272	N203	T141	S7	I6
H463	M400	D339	T273	G205	F142	Y71	S7
L464	L401	P340	L274	P206	D143	V8	V8
G465	K402	E341	A275	E144	E145	D77	D9
V466	P403	A342	E276	A207	H146	E78	V10
E467	T404	S343	A277	A208	H147	A79	L11
A468	D405	S344	M278	T209	R148	L80	V12
V469	E406	K345	D280	P210	M149	P81	I13
D470	L407	L346	Q281	R211	M150	K82	G14
N471	V408	P347	Q282	F212	D84	E83	A15
L472	S409	T348	E282	P213	D85	G16	G16
V473	T410	P349	L283	A214	W86	P17	P17
A476	Y411	Q350	V284	T218	T152		L20
V477	H412	L351	G285	G219	G153	Y87	G21
E478		A352	L286	G220	I154	T88	A22
L479	F415	D353	T287	I221	A155	H89	A23
T480	D416	G354	K288	W222	L157	Q90	K24
L481	H417	S355	Q289	I223	F158	R91	R25
N482	G418	K356	L290	A224	M159	S93	L26
Y483	Y419	P357	F291	V225	R160	Y94	N27
P484	P420	O358	Y292	A226	P161	V95	Q28
D485	T421	S359	S293		Y162	R96	I29
F486	P422	T360	S294	L229	M163	D90	G31
Y487	T423	E361	T295	T234	F164	Q100	P32
N488	L424	A362	H296	R235	K165	W101	S33
G489	E425	K363	V297	F236	V166	V103	H34
R490	R426	E364	L298	G237	W167	P103	P35
Q491	L430	P366	V302	E238	A168	Y104	N36
N492	T431	Y367	R303	K241	V169	P105	I36
T493	Q432	N368		V242	P170	F106	V37
E494	I433	S369		T243	T171	Q107	D38
R495	L434	I370		K244		M108	S39
R496	P435	N371		V245	M174	N109	N40
L497	K436	L372		R306	Q175	I110	E41
V498	L437	E373		E307	C176	S111	T42
D499	Q438	V374		E308	A177	M112	P43
G500	D439	S375		R309	W178	L113	Q44
A501	K440	E376		I310		P114	
Q502	D441	S377		G311	E181	K115	A47
F503	L442	S378		D312	N182	E116	S48
F504	W443	P379		K313	V183	E117	
S507	S444			W315	A184	Q118	V51
Q510	R445	V382		L316		V119	
	G446	N383		Y317	M187	K120	E54
	R447	Q384		F318	L188	C121	
	F448	E386		N322	K189	I122	L57
	G449	T386		G257	A190	D123	Y58
	S450	I387		T258	V191	G124	D59
	W451	L388		T259	T192	M125	V60
	R452	A389		I260	T193	I126	G61
	Y453	D390		G261	N194	D127	G62
	E454	C391		Y326	V195	A128	H63
	V455	I392		F331	I196	V64	V64
	G456	Q393		S332	L197	L130	L65
	N457	G394		N333	G198		F66

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.60Å 175.71Å 135.35Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	34.77 – 3.10 34.77 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (34.77-3.10) 96.2 (34.77-3.10)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.202 , 0.260 0.201 , 0.244	Depositor DCC
R_{free} test set	5331 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.479 for H,-K,-L 0.000 for l,k,-h 0.327 for h,-k,-l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.479 for H,-K,-L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 105627 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32560	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.04 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.6278e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: GDU, FAD

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	0.30	0/4089	0.55	1/5558 (0.0%)
1	B	0.30	0/4089	0.55	1/5558 (0.0%)
1	C	0.30	0/4089	0.55	1/5558 (0.0%)
1	D	0.30	0/4089	0.55	1/5558 (0.0%)
1	E	0.32	0/4089	0.57	0/5558
1	F	0.32	0/4089	0.58	0/5558
1	G	0.32	0/4089	0.61	2/5558 (0.0%)
1	H	0.31	0/4089	0.59	1/5558 (0.0%)
All	All	0.31	0/32712	0.57	7/44464 (0.0%)

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	G	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	LEU	CA-CB-CG	6.50	130.25	115.30
1	G	205	GLY	O-C-N	-6.40	108.95	121.10
1	B	57	LEU	CA-CB-CG	6.33	129.85	115.30
1	H	205	GLY	N-CA-C	-5.37	99.66	113.10
1	A	57	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	65	ILE	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	3990	0	3906	244	0
1	B	3990	0	3906	267	0
1	C	3990	0	3906	265	0
1	D	3990	0	3906	233	0
1	E	3990	0	3906	386	0
1	F	3990	0	3906	359	0
1	G	3990	0	3906	446	0
1	H	3990	0	3906	430	0
2	A	53	0	29	10	0
2	B	53	0	30	14	0
2	C	53	0	30	12	0
2	D	53	0	30	22	0
2	E	53	0	30	20	0
2	F	53	0	29	14	0
2	G	53	0	29	13	0
2	H	53	0	30	10	0
3	A	36	0	22	9	0
3	B	36	0	22	15	0
3	C	36	0	22	9	0
3	D	36	0	22	4	0
3	E	36	0	22	14	0
3	F	36	0	22	8	0
All	All	32560	0	31617	2587	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 40.

The worst 5 of 2587 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:E:70:LYS:HG3	1:E:496:ARG:HH22	0.96	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:LYS:HG3	1:F:496:ARG:HH22	1.12	1.10
1:F:461:SER:HA	1:F:464:LEU:HD12	1.37	1.06
1:D:303:ARG:NH2	1:D:346:LEU:O	1.90	1.05
1:E:461:SER:HA	1:E:464:LEU:HD12	1.38	1.05

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	507/509 (100%)	476 (94%)	30 (6%)	1 (0%)	52	84
1	B	507/509 (100%)	476 (94%)	29 (6%)	2 (0%)	39	75
1	C	507/509 (100%)	476 (94%)	30 (6%)	1 (0%)	52	84
1	D	507/509 (100%)	481 (95%)	25 (5%)	1 (0%)	52	84
1	E	507/509 (100%)	456 (90%)	51 (10%)	0	100	100
1	F	507/509 (100%)	457 (90%)	49 (10%)	1 (0%)	52	84
1	G	507/509 (100%)	462 (91%)	45 (9%)	0	100	100
1	H	507/509 (100%)	460 (91%)	46 (9%)	1 (0%)	52	84
All	All	4056/4072 (100%)	3744 (92%)	305 (8%)	7 (0%)	52	84

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	203	ASN
1	B	61	GLY
1	A	107	GLN
1	B	107	GLN
1	C	107	GLN

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	430/430 (100%)	372 (86%)	58 (14%)	5	20
1	B	430/430 (100%)	367 (85%)	63 (15%)	4	16
1	C	430/430 (100%)	370 (86%)	60 (14%)	4	18
1	D	430/430 (100%)	366 (85%)	64 (15%)	4	15
1	E	430/430 (100%)	363 (84%)	67 (16%)	3	14
1	F	430/430 (100%)	359 (84%)	71 (16%)	3	12
1	G	430/430 (100%)	347 (81%)	83 (19%)	2	8
1	H	430/430 (100%)	351 (82%)	79 (18%)	2	9
All	All	3440/3440 (100%)	2895 (84%)	545 (16%)	3	13

5 of 545 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	25	ARG
1	E	479	LEU
1	H	249	ASN
1	E	68	HIS
1	E	251	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	458	GLN
1	E	412	HIS
1	H	339	GLN
1	E	68	HIS
1	E	207	ASN

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 ⓘ

14 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	FAD	A	601	-	48,58,58	1.88	10 (20%)	54,89,89	2.82	19 (35%)
3	GDU	A	602	-	29,38,38	1.76	5 (17%)	43,58,58	1.72	7 (16%)
2	FAD	B	601	-	48,58,58	1.90	12 (25%)	54,89,89	2.52	15 (27%)
3	GDU	B	602	-	29,38,38	1.75	6 (20%)	43,58,58	2.11	10 (23%)
2	FAD	C	601	-	48,58,58	2.03	13 (27%)	54,89,89	2.90	17 (31%)
3	GDU	C	602	-	29,38,38	1.81	5 (17%)	43,58,58	1.75	8 (18%)
2	FAD	D	601	-	48,58,58	2.11	13 (27%)	54,89,89	2.75	15 (27%)
3	GDU	D	602	-	29,38,38	1.83	5 (17%)	43,58,58	1.93	9 (20%)
2	FAD	E	601	-	48,58,58	2.03	13 (27%)	54,89,89	2.35	17 (31%)
3	GDU	E	602	-	29,38,38	1.73	5 (17%)	43,58,58	1.74	7 (16%)
2	FAD	F	601	-	48,58,58	1.95	11 (22%)	54,89,89	2.53	18 (33%)
3	GDU	F	602	-	29,38,38	1.74	5 (17%)	43,58,58	1.89	10 (23%)
2	FAD	G	601	-	48,58,58	2.76	17 (35%)	54,89,89	2.65	17 (31%)
2	FAD	H	601	-	48,58,58	2.13	13 (27%)	54,89,89	2.58	20 (37%)

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	FAD	A	601	-	1/1/9/9	2/30/50/50	0/6/6/6
3	GDU	A	602	-	-	0/19/59/59	0/3/3/3
2	FAD	B	601	-	-	2/30/50/50	0/6/6/6
3	GDU	B	602	-	-	0/19/59/59	0/3/3/3
2	FAD	C	601	-	-	0/30/50/50	0/6/6/6
3	GDU	C	602	-	-	0/19/59/59	0/3/3/3
2	FAD	D	601	-	-	0/30/50/50	0/6/6/6
3	GDU	D	602	-	-	0/19/59/59	0/3/3/3
2	FAD	E	601	-	-	0/30/50/50	0/6/6/6
3	GDU	E	602	-	-	0/19/59/59	0/3/3/3
2	FAD	F	601	-	1/1/9/9	0/30/50/50	0/6/6/6
3	GDU	F	602	-	-	0/19/59/59	0/3/3/3
2	FAD	G	601	-	-	0/30/50/50	0/6/6/6
2	FAD	H	601	-	-	0/30/50/50	0/6/6/6

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FAD	C1'-N10	-9.53	1.38	1.48
2	G	601	FAD	C2B-C3B	-6.09	1.36	1.53
2	G	601	FAD	C10-N10	-5.53	1.32	1.39
2	G	601	FAD	C9A-C5X	-5.43	1.31	1.42
2	H	601	FAD	C2B-C3B	-5.04	1.39	1.53

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	FAD	N3A-C2A-N1A	-11.03	120.45	128.89
2	C	601	FAD	N3A-C2A-N1A	-10.00	121.24	128.89
2	C	601	FAD	C4B-O4B-C1B	-9.93	98.80	109.72
2	F	601	FAD	N3A-C2A-N1A	-9.91	121.31	128.89
2	A	601	FAD	N3A-C2A-N1A	-9.85	121.36	128.89

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	601	FAD	C2'
2	A	601	FAD	C2'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C2'-C1'-N10-C9A
2	B	601	FAD	C2'-C1'-N10-C10
2	A	601	FAD	C2'-C1'-N10-C10
2	B	601	FAD	C2'-C1'-N10-C9A

There are no ring outliers.

14 monomers are involved in 171 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	10	0
3	A	602	GDU	9	0
2	B	601	FAD	14	0
3	B	602	GDU	15	0
2	C	601	FAD	12	0
3	C	602	GDU	9	0
2	D	601	FAD	22	0
3	D	602	GDU	4	0
2	E	601	FAD	20	0
3	E	602	GDU	14	0
2	F	601	FAD	14	0
3	F	602	GDU	8	0
2	G	601	FAD	13	0
2	H	601	FAD	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	509/509 (100%)	-0.28	4 (0%) 87 75	22, 64, 110, 167	0
1	B	509/509 (100%)	-0.30	7 (1%) 78 60	24, 64, 106, 166	0
1	C	509/509 (100%)	-0.28	7 (1%) 78 60	29, 65, 108, 170	0
1	D	509/509 (100%)	-0.27	6 (1%) 81 64	27, 65, 109, 172	0
1	E	509/509 (100%)	-0.39	1 (0%) 95 91	22, 62, 99, 156	0
1	F	509/509 (100%)	-0.34	3 (0%) 90 80	23, 59, 99, 151	0
1	G	509/509 (100%)	-0.44	0 100 100	14, 61, 93, 126	0
1	H	509/509 (100%)	-0.42	1 (0%) 95 91	22, 63, 94, 132	1 (0%)
All	All	4072/4072 (100%)	-0.34	29 (0%) 89 78	14, 63, 104, 172	1 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	TRP	5.4
1	C	183	VAL	4.9
1	B	183	VAL	4.5
1	F	207	ASN	4.4
1	B	204	TRP	4.4

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 [i](#)

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, 95th 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 ²)	Q<0.9
2	FAD	B	601	53/53	0.97	0.20	-0.08	18,64,87,92	0
3	GDU	A	602	36/36	0.95	0.23	-0.37	30,108,162,203	0
2	FAD	F	601	53/53	0.98	0.18	-0.40	12,67,90,107	0
2	FAD	C	601	53/53	0.98	0.18	-0.42	0,49,83,94	0
3	GDU	B	602	36/36	0.96	0.21	-0.49	42,114,153,160	0
2	FAD	D	601	53/53	0.99	0.18	-0.52	0,57,88,102	0
2	FAD	E	601	53/53	0.98	0.17	-0.54	14,57,97,102	0
2	FAD	H	601	53/53	0.97	0.16	-0.60	20,79,102,111	0
2	FAD	A	601	53/53	0.98	0.17	-0.60	6,57,87,95	0
3	GDU	C	602	36/36	0.96	0.18	-0.68	25,103,142,180	0
3	GDU	E	602	36/36	0.94	0.18	-0.76	22,92,139,142	0
3	GDU	F	602	36/36	0.95	0.17	-0.77	28,101,153,194	0
2	FAD	G	601	53/53	0.98	0.15	-0.86	0,57,86,102	0
3	GDU	D	602	36/36	0.95	0.15	-1.18	35,99,135,179	0

6.5 Other polymers [i](#)

There are no such residues in this entry.