



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:12 AM GMT

PDB ID : 3HDQ
Title : Crystal structure of UDP-galactopyranose mutase (oxidized form) in complex with substrate
Authors : Partha, S.K.; van Straaten, K.E.; Sanders, D.A.
Deposited on : 2009-05-07
Resolution : 2.36 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

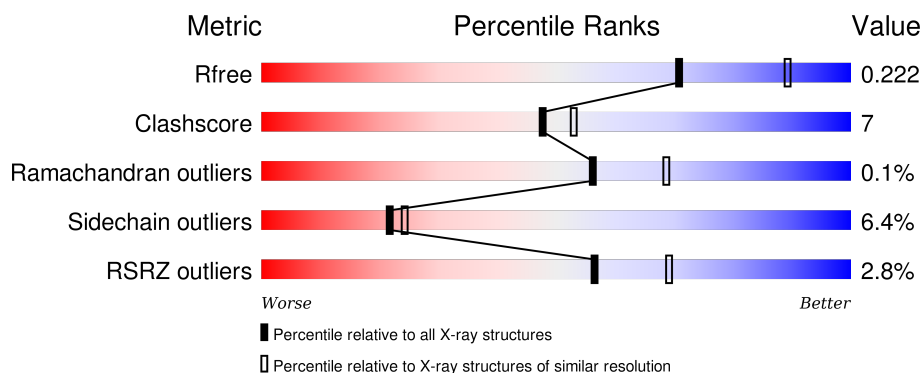
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	397	<div> <div>2%</div> <div>76%</div> <div>14%</div> <div>8%</div> </div>
1	B	397	<div> <div>3%</div> <div>76%</div> <div>14%</div> <div>8%</div> </div>
1	C	397	<div> <div>3%</div> <div>72%</div> <div>18%</div> <div>9%</div> </div>
1	D	397	<div> <div>3%</div> <div>74%</div> <div>15%</div> <div>9%</div> </div>
1	E	397	<div> <div>3%</div> <div>77%</div> <div>13%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	397	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>76%</div><div>15%</div><div>•</div><div>9%</div></div></div>
1	G	397	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>77%</div><div>13%</div><div>•</div><div>9%</div></div></div>
1	H	397	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>78%</div><div>13%</div><div>•</div><div>8%</div></div></div>
1	I	397	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>75%</div><div>14%</div><div>•</div><div>9%</div></div></div>
1	J	397	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>72%</div><div>18%</div><div>•</div><div>9%</div></div></div>

2 Entry composition

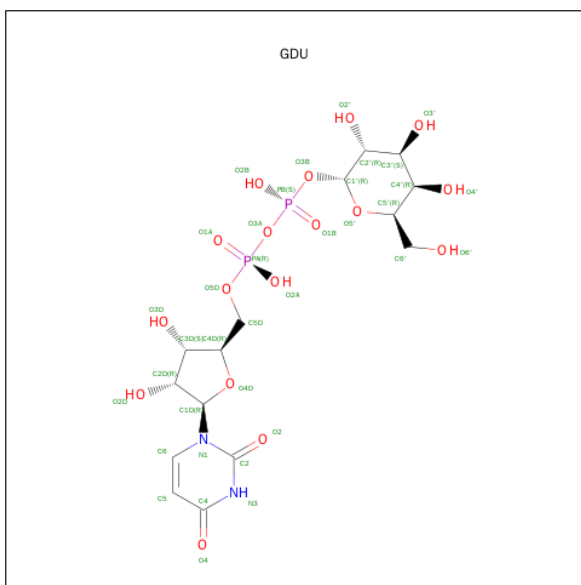
There are 4 unique types of molecules in this entry. The entry contains 31875 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	1	0
			2992	1909	521	554	8			
1	B	364	Total	C	N	O	S	4	2	0
			2990	1909	522	551	8			
1	C	361	Total	C	N	O	S	23	1	0
			2964	1894	516	546	8			
1	D	360	Total	C	N	O	S	0	1	0
			2955	1888	514	545	8			
1	E	364	Total	C	N	O	S	8	0	0
			2975	1899	516	552	8			
1	F	363	Total	C	N	O	S	4	1	0
			2977	1901	519	549	8			
1	G	363	Total	C	N	O	S	4	1	0
			2974	1899	518	549	8			
1	H	364	Total	C	N	O	S	0	1	0
			2983	1904	520	551	8			
1	I	363	Total	C	N	O	S	4	1	0
			2975	1899	517	551	8			
1	J	361	Total	C	N	O	S	4	1	0
			2959	1890	515	546	8			

- Molecule 2 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

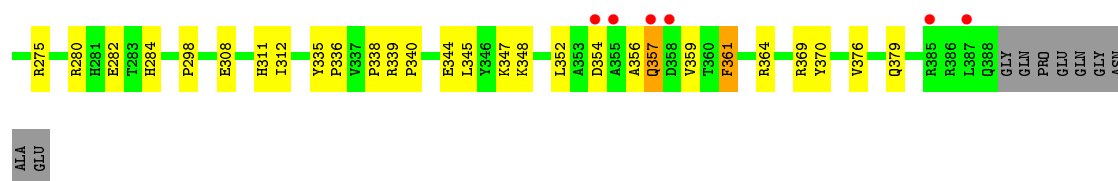
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	164	Total	O	0	0
			164	164		
4	B	104	Total	O	0	0
			104	104		

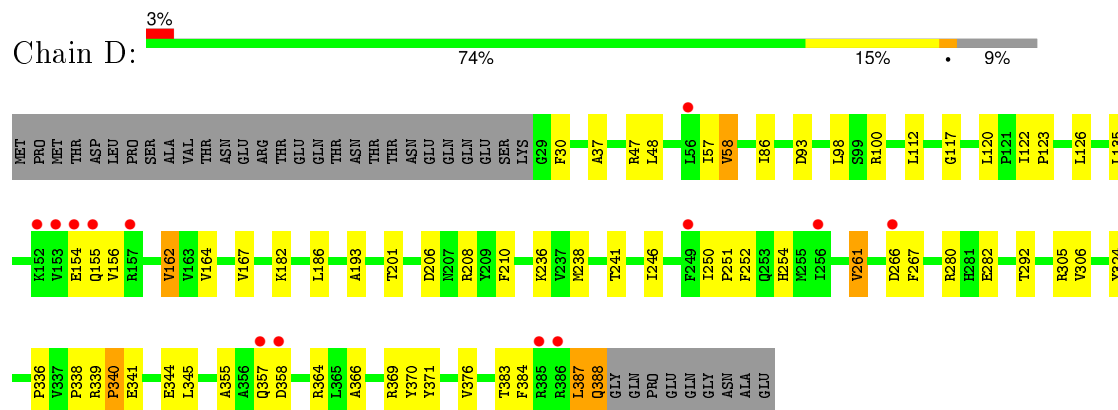
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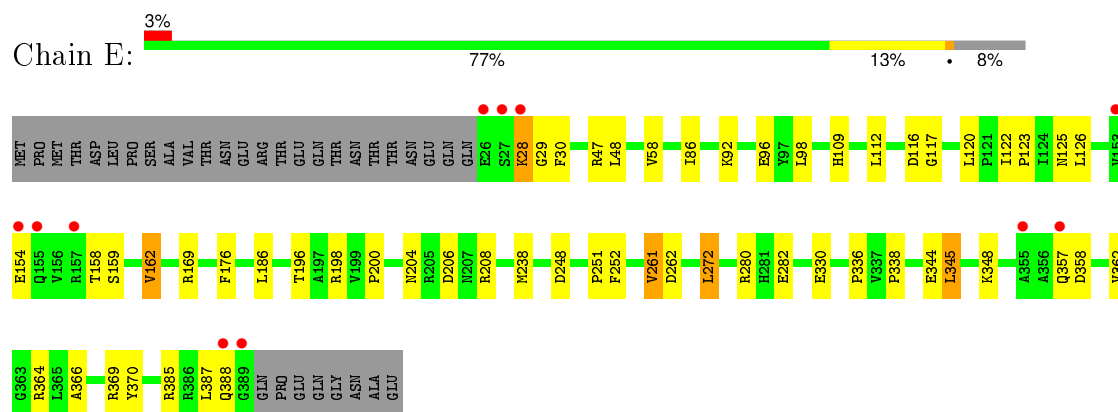
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	88	Total 88	O 88	0	0
4	D	86	Total 86	O 86	0	0
4	E	110	Total 110	O 110	0	0
4	F	143	Total 143	O 143	0	0
4	G	116	Total 116	O 116	0	0
4	H	143	Total 143	O 143	0	0
4	I	160	Total 160	O 160	0	0
4	J	127	Total 127	O 127	0	0



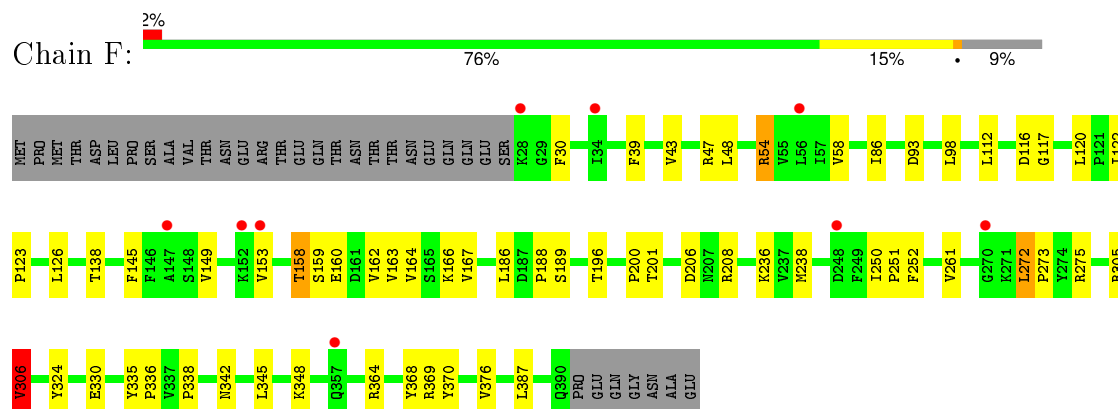
- Molecule 1: UDP-galactopyranose mutase



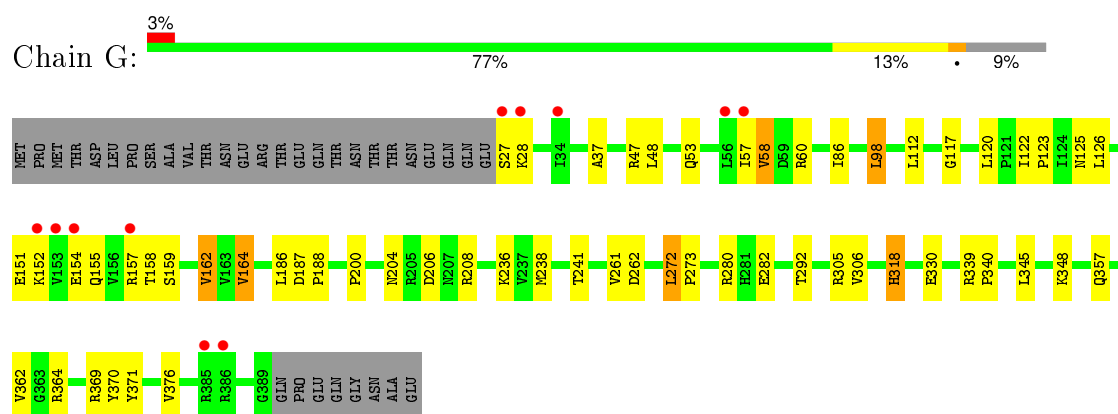
- Molecule 1: UDP-galactopyranose mutase



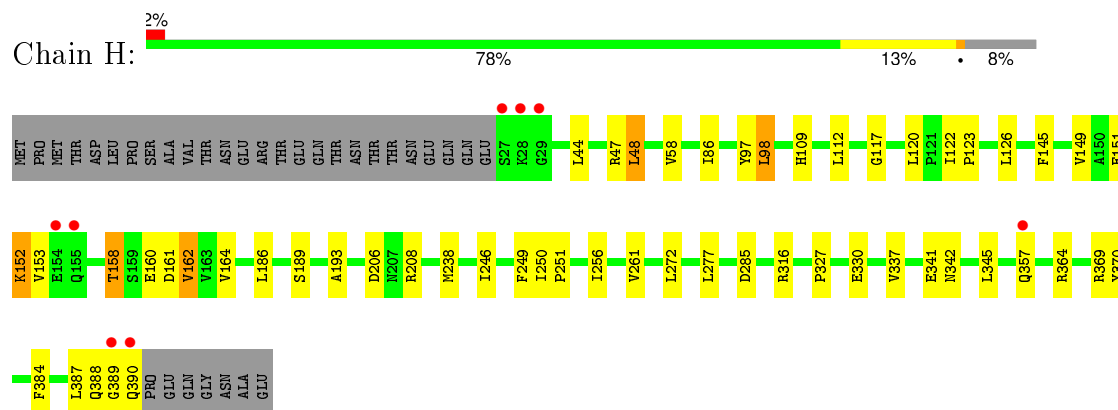
- Molecule 1: UDP-galactopyranose mutase



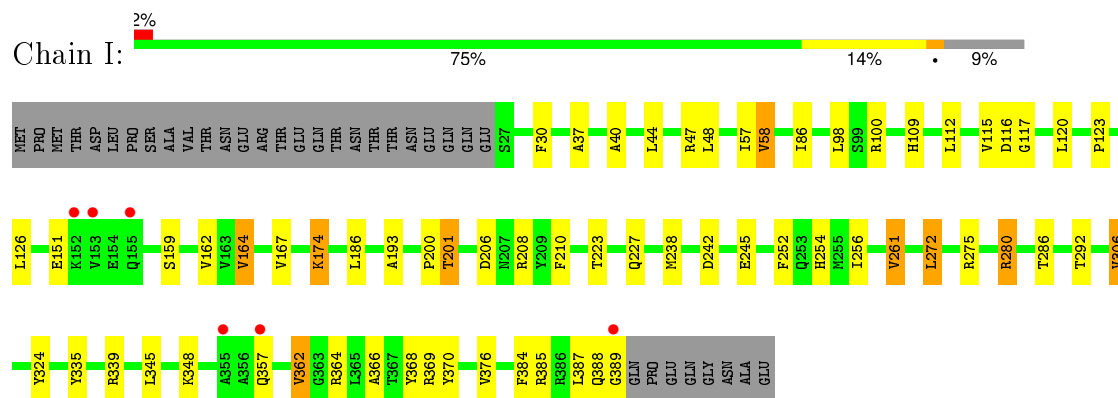
- Molecule 1: UDP-galactopyranose mutase



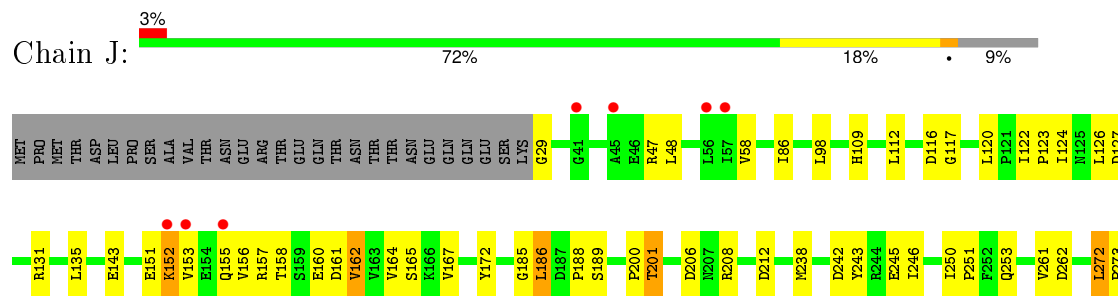
- Molecule 1: UDP-galactopyranose mutase

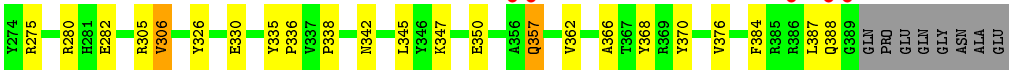


- Molecule 1: UDP-galactopyranose mutase



- 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, α , β , γ	134.02Å 176.65Å 220.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.36 19.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.88-2.36) 97.8 (19.88-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.177 , 0.226 0.178 , 0.222	Depositor DCC
R_{free} test set	10671 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 225489 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31875	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/3079	0.58	0/4185
1	B	0.39	0/3081	0.56	0/4188
1	C	0.35	0/3051	0.54	0/4148
1	D	0.40	0/3042	0.54	0/4137
1	E	0.34	0/3059	0.52	0/4159
1	F	0.38	0/3064	0.56	1/4165 (0.0%)
1	G	0.41	0/3061	0.54	0/4161
1	H	0.39	0/3070	0.54	0/4173
1	I	0.41	0/3059	0.57	1/4159 (0.0%)
1	J	0.39	0/3046	0.55	1/4142 (0.0%)
All	All	0.39	0/30612	0.55	3/41617 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	306	VAL	CB-CA-C	-5.47	101.01	111.40
1	F	306	VAL	CB-CA-C	-5.33	101.27	111.40
1	J	306	VAL	CB-CA-C	-5.05	101.81	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2992	0	2867	50	0
1	B	2990	0	2868	44	0
1	C	2964	0	2845	56	0
1	D	2955	0	2832	45	0
1	E	2975	0	2846	36	0
1	F	2977	0	2856	41	0
1	G	2974	0	2853	36	0
1	H	2983	0	2861	47	0
1	I	2975	0	2847	50	0
1	J	2959	0	2835	67	0
2	A	36	0	22	0	0
2	B	36	0	22	3	0
2	C	36	0	22	1	0
2	D	36	0	22	3	0
2	E	36	0	22	1	0
2	F	36	0	22	2	0
2	G	36	0	22	3	0
2	H	36	0	22	1	0
2	I	36	0	22	4	0
2	J	36	0	22	2	0
3	A	53	0	30	1	0
3	B	53	0	31	2	0
3	C	53	0	30	1	0
3	D	53	0	31	0	0
3	E	53	0	31	0	0
3	F	53	0	29	1	0
3	G	53	0	31	3	0
3	H	53	0	31	0	0
3	I	53	0	31	1	0
3	J	53	0	30	1	0
4	A	164	0	0	2	0
4	B	104	0	0	3	0
4	C	88	0	0	2	0
4	D	86	0	0	1	0
4	E	110	0	0	3	0
4	F	143	0	0	0	0
4	G	116	0	0	1	0
4	H	143	0	0	0	0
4	I	160	0	0	2	0
4	J	127	0	0	0	0
All	All	31875	0	29035	438	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 7.

The worst 5 of 438 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:A:152:LYS:CD	1:A:153:VAL:H	1.54	1.18
1:J:357:GLN:HA	1:J:357:GLN:HE21	1.15	1.10
1:A:152:LYS:HD3	1:A:153:VAL:N	1.72	1.04
1:E:58:VAL:HG22	1:E:238:MET:HB3	1.42	1.01
1:H:152:LYS:HA	1:H:152:LYS:HE2	1.38	1.01

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%)	355 (98%)	9 (2%)	0	100	100
1	B	364/397 (92%)	352 (97%)	12 (3%)	0	100	100
1	C	360/397 (91%)	347 (96%)	13 (4%)	0	100	100
1	D	359/397 (90%)	345 (96%)	13 (4%)	1 (0%)	46	55
1	E	362/397 (91%)	353 (98%)	9 (2%)	0	100	100
1	F	362/397 (91%)	356 (98%)	6 (2%)	0	100	100
1	G	362/397 (91%)	355 (98%)	6 (2%)	1 (0%)	46	55
1	H	363/397 (91%)	353 (97%)	10 (3%)	0	100	100
1	I	362/397 (91%)	353 (98%)	9 (2%)	0	100	100
1	J	360/397 (91%)	353 (98%)	7 (2%)	0	100	100
All	All	3618/3970 (91%)	3522 (97%)	94 (3%)	2 (0%)	56	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	340	PRO
1	G	154	GLU

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	318/346 (92%)	292 (92%)	26 (8%)	14	15
1	B	318/346 (92%)	299 (94%)	19 (6%)	24	28
1	C	315/346 (91%)	294 (93%)	21 (7%)	20	22
1	D	314/346 (91%)	294 (94%)	20 (6%)	22	24
1	E	316/346 (91%)	298 (94%)	18 (6%)	25	30
1	F	316/346 (91%)	296 (94%)	20 (6%)	22	25
1	G	316/346 (91%)	294 (93%)	22 (7%)	19	20
1	H	317/346 (92%)	301 (95%)	16 (5%)	30	37
1	I	316/346 (91%)	294 (93%)	22 (7%)	19	20
1	J	314/346 (91%)	295 (94%)	19 (6%)	23	27
All	All	3160/3460 (91%)	2957 (94%)	203 (6%)	22	24

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	126	LEU
1	F	159	SER
1	J	120	LEU
1	E	186	LEU
1	E	387	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	388	GLN
1	F	390	GLN

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Mol	Chain	Res	Type
1	H	388	GLN
1	E	357	GLN
1	H	284	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 ⓘ

20 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	$\# Z > 2$
3	FAD	A	450	-	48,58,58	1.85	16 (33%)	54,89,89	2.33	10 (18%)
2	GDU	A	500	-	29,38,38	0.98	1 (3%)	43,58,58	1.82	12 (27%)
3	FAD	B	450	-	48,58,58	1.70	13 (27%)	54,89,89	2.57	13 (24%)
2	GDU	B	500	-	29,38,38	1.10	1 (3%)	43,58,58	1.94	12 (27%)
3	FAD	C	450	-	48,58,58	1.87	16 (33%)	54,89,89	2.37	14 (25%)
2	GDU	C	500	-	29,38,38	1.17	1 (3%)	43,58,58	1.92	12 (27%)
3	FAD	D	450	-	48,58,58	1.69	14 (29%)	54,89,89	2.38	14 (25%)
2	GDU	D	500	-	29,38,38	1.22	1 (3%)	43,58,58	2.08	13 (30%)
3	FAD	E	450	-	48,58,58	1.77	12 (25%)	54,89,89	2.06	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDU	E	500	-	29,38,38	1.10	1 (3%)	43,58,58	1.83	13 (30%)
3	FAD	F	450	-	48,58,58	1.82	17 (35%)	54,89,89	2.16	9 (16%)
2	GDU	F	500	-	29,38,38	1.13	1 (3%)	43,58,58	2.01	13 (30%)
3	FAD	G	450	-	48,58,58	1.65	9 (18%)	54,89,89	2.19	8 (14%)
2	GDU	G	500	-	29,38,38	1.00	1 (3%)	43,58,58	1.99	14 (32%)
3	FAD	H	450	-	48,58,58	1.86	16 (33%)	54,89,89	2.07	9 (16%)
2	GDU	H	500	-	29,38,38	1.14	2 (6%)	43,58,58	1.79	11 (25%)
3	FAD	I	450	-	48,58,58	1.76	15 (31%)	54,89,89	2.13	10 (18%)
2	GDU	I	500	-	29,38,38	1.04	1 (3%)	43,58,58	2.12	12 (27%)
3	FAD	J	450	-	48,58,58	1.85	14 (29%)	54,89,89	2.09	7 (12%)
2	GDU	J	500	-	29,38,38	1.20	1 (3%)	43,58,58	1.90	11 (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	FAD	A	450	-	-	0/30/50/50	0/6/6/6
2	GDU	A	500	-	-	0/19/59/59	0/3/3/3
3	FAD	B	450	-	-	0/30/50/50	0/6/6/6
2	GDU	B	500	-	-	0/19/59/59	0/3/3/3
3	FAD	C	450	-	-	0/30/50/50	0/6/6/6
2	GDU	C	500	-	-	0/19/59/59	0/3/3/3
3	FAD	D	450	-	-	0/30/50/50	0/6/6/6
2	GDU	D	500	-	-	0/19/59/59	0/3/3/3
3	FAD	E	450	-	-	0/30/50/50	0/6/6/6
2	GDU	E	500	-	-	0/19/59/59	0/3/3/3
3	FAD	F	450	-	-	0/30/50/50	0/6/6/6
2	GDU	F	500	-	-	0/19/59/59	0/3/3/3
3	FAD	G	450	-	-	0/30/50/50	0/6/6/6
2	GDU	G	500	-	-	0/19/59/59	0/3/3/3
3	FAD	H	450	-	-	0/30/50/50	0/6/6/6
2	GDU	H	500	-	-	0/19/59/59	0/3/3/3
3	FAD	I	450	-	-	0/30/50/50	0/6/6/6
2	GDU	I	500	-	-	0/19/59/59	0/3/3/3
3	FAD	J	450	-	-	0/30/50/50	0/6/6/6
2	GDU	J	500	-	-	0/19/59/59	0/3/3/3

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	450	FAD	C10-N10	-4.43	1.34	1.39
3	E	450	FAD	C10-N10	-4.37	1.34	1.39
3	H	450	FAD	C10-N10	-4.28	1.34	1.39
3	J	450	FAD	C6-C5X	-3.77	1.36	1.41
3	C	450	FAD	C6-C5X	-3.77	1.36	1.41

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	450	FAD	N3A-C2A-N1A	-12.85	119.06	128.89
3	D	450	FAD	N3A-C2A-N1A	-12.35	119.44	128.89
3	C	450	FAD	N3A-C2A-N1A	-12.32	119.46	128.89
3	J	450	FAD	N3A-C2A-N1A	-12.28	119.49	128.89
3	A	450	FAD	N3A-C2A-N1A	-12.12	119.61	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	FAD	1	0
3	B	450	FAD	2	0
2	B	500	GDU	3	0
3	C	450	FAD	1	0
2	C	500	GDU	1	0
2	D	500	GDU	3	0
2	E	500	GDU	1	0
3	F	450	FAD	1	0
2	F	500	GDU	2	0
3	G	450	FAD	3	0
2	G	500	GDU	3	0
2	H	500	GDU	1	0
3	I	450	FAD	1	0
2	I	500	GDU	4	0
3	J	450	FAD	1	0
2	J	500	GDU	2	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 [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, 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	365/397 (91%)	-0.39	6 (1%) 74 84	20, 30, 46, 75	0
1	B	364/397 (91%)	-0.27	11 (3%) 54 66	23, 34, 54, 80	1 (0%)
1	C	361/397 (90%)	0.00	13 (3%) 46 60	25, 39, 64, 82	6 (1%)
1	D	360/397 (90%)	-0.10	13 (3%) 46 60	20, 41, 65, 81	0
1	E	364/397 (91%)	-0.26	11 (3%) 54 66	24, 37, 57, 98	2 (0%)
1	F	363/397 (91%)	-0.33	9 (2%) 61 73	20, 32, 51, 75	1 (0%)
1	G	363/397 (91%)	-0.25	11 (3%) 54 66	20, 35, 55, 78	1 (0%)
1	H	364/397 (91%)	-0.30	8 (2%) 65 77	20, 32, 52, 76	0
1	I	363/397 (91%)	-0.35	6 (1%) 73 83	20, 32, 47, 70	1 (0%)
1	J	361/397 (90%)	-0.19	12 (3%) 50 63	20, 35, 59, 81	1 (0%)
All	All	3628/3970 (91%)	-0.24	100 (2%) 56 69	20, 34, 58, 98	13 (0%)

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	26	GLU	7.9
1	D	357	GLN	5.7
1	D	153	VAL	5.5
1	G	27	SER	5.5
1	F	153	VAL	5.4

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 [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	GDU	I	500	36/36	0.94	0.16	1.49	29,34,54,58	0
2	GDU	B	500	36/36	0.93	0.16	1.35	31,39,57,61	0
2	GDU	D	500	36/36	0.93	0.16	1.19	35,44,65,69	0
2	GDU	H	500	36/36	0.95	0.14	1.11	25,31,48,52	0
2	GDU	E	500	36/36	0.95	0.14	1.02	28,36,55,58	0
2	GDU	J	500	36/36	0.95	0.15	0.91	25,32,54,57	0
2	GDU	F	500	36/36	0.96	0.14	0.70	26,35,50,53	0
2	GDU	G	500	36/36	0.98	0.13	0.66	31,36,40,43	11
2	GDU	A	500	36/36	0.98	0.12	0.52	25,29,32,34	12
2	GDU	C	500	36/36	0.94	0.14	0.41	29,39,63,64	0
3	FAD	C	450	53/53	0.95	0.14	-0.08	23,29,36,51	0
3	FAD	E	450	53/53	0.97	0.10	-0.47	23,29,36,51	0
3	FAD	J	450	53/53	0.96	0.11	-0.51	23,29,36,51	0
3	FAD	G	450	53/53	0.96	0.11	-0.56	23,29,36,51	0
3	FAD	D	450	53/53	0.97	0.11	-0.56	23,29,36,51	0
3	FAD	B	450	53/53	0.96	0.09	-0.75	23,29,36,51	0
3	FAD	H	450	53/53	0.96	0.09	-0.90	23,29,36,51	0
3	FAD	F	450	53/53	0.96	0.09	-0.91	23,29,36,51	0
3	FAD	A	450	53/53	0.97	0.09	-1.11	23,29,36,51	0
3	FAD	I	450	53/53	0.97	0.08	-1.11	23,29,36,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.