Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2016 – 08:47 PM EST

PDB ID	:	5EQF
Title	:	Crystal strucutre of oxidized UDP-galactopyranose mutase from Corynebacterium diphtheriae with UDP bound in closed form
Authors	:	Wangkanont, K.; Kiessling, L.L.; Forest, K.T.
Deposited on	:	2015-11-12
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

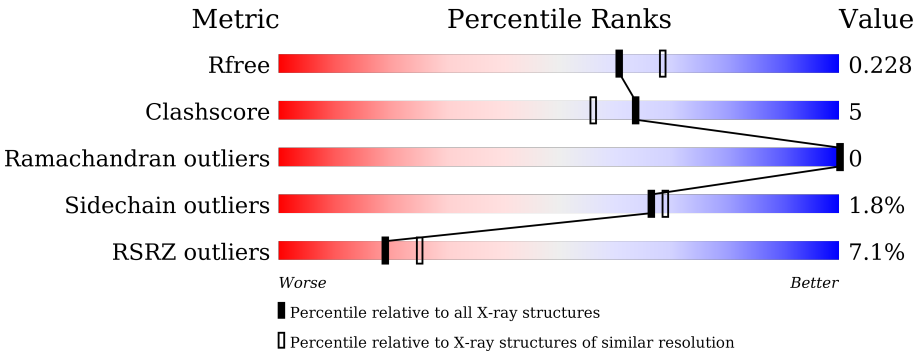
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

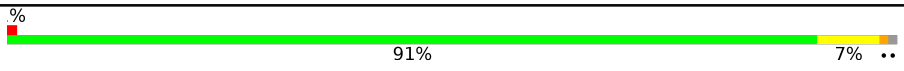
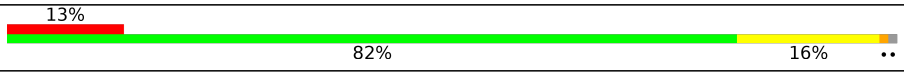
The reported resolution of this entry is 2.15 Å.

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	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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 <=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	390	
1	B	390	

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	SO4	A	406	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6758 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.

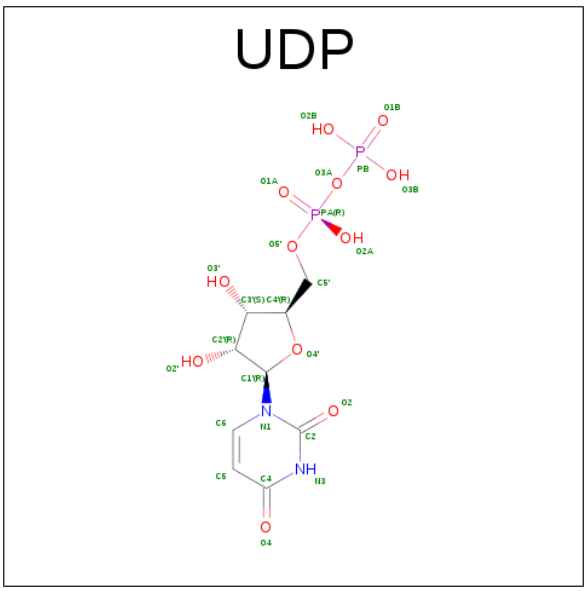
- Molecule 1 is a protein called UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	2	0
			3188	2026	544	609	9			
1	B	385	Total	C	N	O	S	0	0	0
			3156	2008	534	605	9			

There are 6 discrepancies between the modelled and reference sequences:

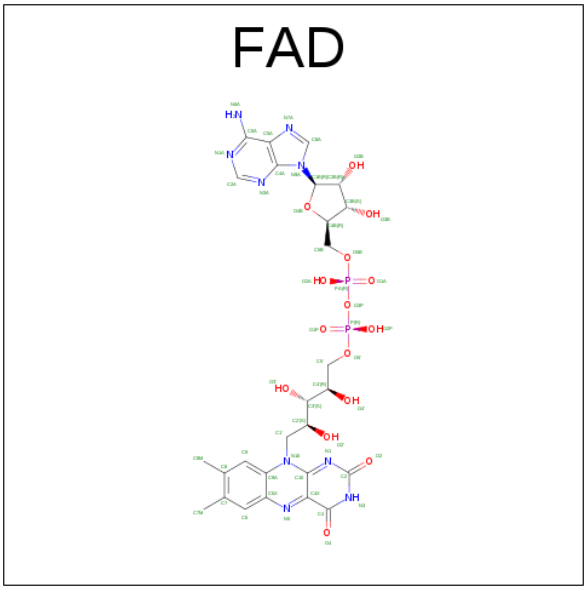
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q6NER4
A	-1	SER	-	expression tag	UNP Q6NER4
A	0	GLY	-	expression tag	UNP Q6NER4
B	-2	GLY	-	expression tag	UNP Q6NER4
B	-1	SER	-	expression tag	UNP Q6NER4
B	0	GLY	-	expression tag	UNP Q6NER4

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



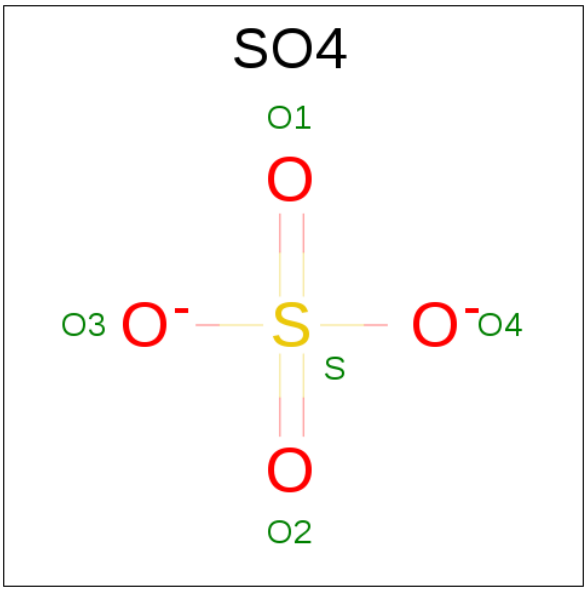
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

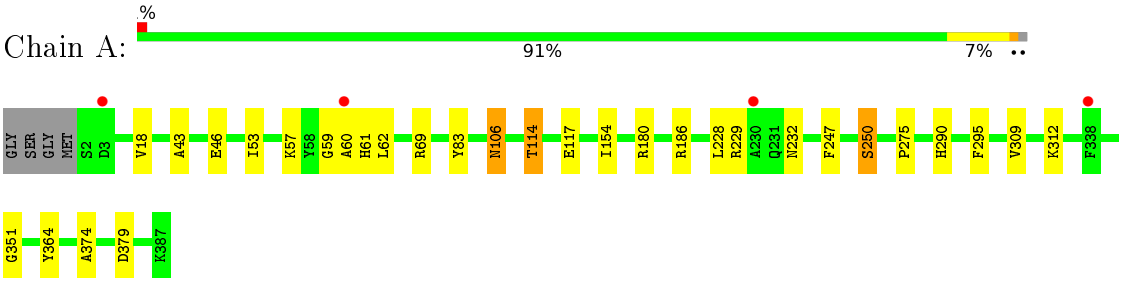
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	155	Total O 155 155	0	0
5	B	73	Total O 73 73	0	0

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.

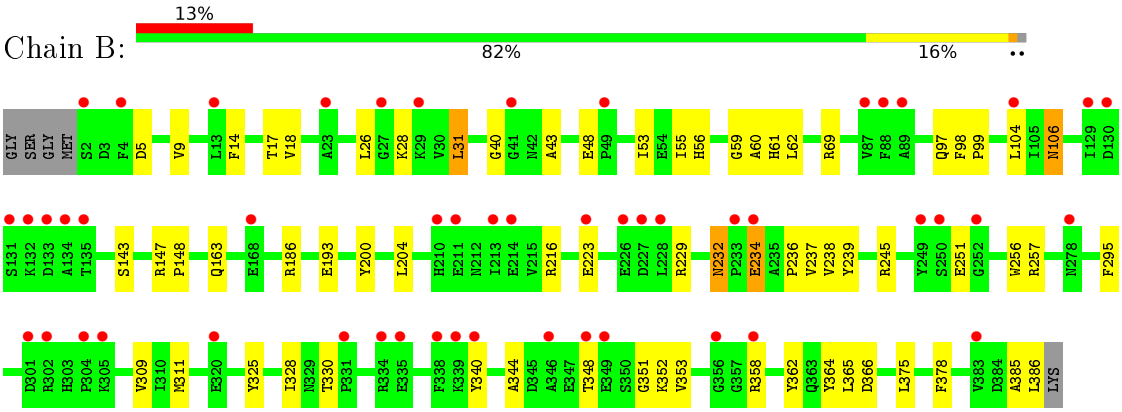
- Molecule 1: UDP-galactopyranose mutase

Chain A:



- Molecule 1: UDP-galactopyranose mutase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.56Å 82.69Å 108.57Å 90.00° 112.64° 90.00°	Depositor
Resolution (Å)	28.25 – 2.15 29.11 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.1 (28.25-2.15) 92.1 (29.11-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.43 (at 2.14Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.176 , 0.228 0.174 , 0.228	Depositor DCC
R_{free} test set	2381 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6758	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, SO4, 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	0.46	0/3276	0.61	0/4437
1	B	0.40	0/3244	0.57	0/4398
All	All	0.43	0/6520	0.59	0/8835

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	3188	0	3001	22	0
1	B	3156	0	2964	43	1
2	A	25	0	11	0	0
2	B	25	0	11	0	0
3	A	53	0	30	2	0
3	B	53	0	31	4	0
4	A	20	0	0	1	0
4	B	10	0	0	0	0
5	A	155	0	0	3	0
5	B	73	0	0	3	0
All	All	6758	0	6048	65	1

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 5.

All (65) 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:B:14:PHE:O	5:B:501:HOH:O	1.88	0.91
1:A:114:THR:HG22	1:A:117:GLU:H	1.33	0.90
1:B:18:VAL:N	5:B:501:HOH:O	2.07	0.76
1:A:228:LEU:O	5:A:501:HOH:O	2.06	0.73
1:A:46:GLU:HG2	1:A:57:LYS:HD2	1.76	0.67
1:A:62:LEU:HD11	1:A:295:PHE:CE1	2.30	0.67
1:B:17:THR:N	5:B:501:HOH:O	2.28	0.66
1:A:59:GLY:HA3	3:A:402:FAD:HM72	1.76	0.66
1:B:229:ARG:HH22	1:B:352:LYS:HB2	1.61	0.66
1:B:69:ARG:HH12	1:B:375:LEU:HB3	1.60	0.65
1:B:59:GLY:O	1:B:61:HIS:ND1	2.28	0.65
1:B:62:LEU:O	3:B:402:FAD:N3	2.30	0.64
1:B:40:GLY:HA3	1:B:204:LEU:HD13	1.80	0.62
1:B:325:TYR:O	1:B:358:ARG:NH1	2.35	0.59
1:A:59:GLY:O	1:A:61:HIS:ND1	2.29	0.57
1:B:147:ARG:HB3	1:B:148:PRO:HD3	1.87	0.57
1:B:237:VAL:HB	1:B:353:VAL:HG22	1.86	0.56
1:B:5:ASP:O	1:B:236:PRO:HD2	2.08	0.54
1:B:186:ARG:NH2	1:B:193:GLU:OE2	2.42	0.54
1:A:61:HIS:O	1:A:62:LEU:HD13	2.08	0.53
1:B:28:LYS:HG3	1:B:386:LEU:HD22	1.91	0.51
1:A:69:ARG:NH2	1:A:379:ASP:OD2	2.43	0.51
1:B:59:GLY:HA3	3:B:402:FAD:HM72	1.93	0.50
1:A:53:ILE:HD12	1:A:309:VAL:HG12	1.94	0.49
1:B:251:GLU:HB2	1:B:340:TYR:CZ	2.47	0.49
1:A:247:PHE:O	1:A:250:SER:OG	2.31	0.49
1:A:180:ARG:NE	4:A:405:SO4:O3	2.45	0.49
1:B:106:ASN:C	1:B:106:ASN:HD22	2.16	0.48
1:B:53:ILE:HD12	1:B:309:VAL:HG12	1.95	0.48
1:B:43:ALA:HA	1:B:61:HIS:CD2	2.48	0.48
1:B:26:LEU:HD13	1:B:378:PHE:HZ	1.78	0.48
1:A:186:ARG:NH1	5:A:513:HOH:O	2.46	0.48
1:B:344:ALA:O	1:B:348:THR:HG23	2.13	0.48
1:A:106:ASN:C	1:A:106:ASN:HD22	2.18	0.47
1:B:48:GLU:HB2	1:B:55:ILE:HD11	1.97	0.47
1:A:61:HIS:C	1:A:62:LEU:HD13	2.36	0.47
1:B:62:LEU:HD11	1:B:295:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:HB	1:B:239:TYR:HA	1.96	0.46
1:A:229:ARG:NH2	1:A:351:GLY:O	2.41	0.46
1:B:18:VAL:HG11	1:B:238:VAL:HG21	1.98	0.46
1:B:328:ILE:HG22	1:B:330:THR:HG23	1.98	0.46
1:A:83:TYR:OH	1:A:275:PRO:HG2	2.16	0.46
1:B:232:ASN:HA	1:B:232:ASN:HD22	1.62	0.45
1:B:61:HIS:O	1:B:200:TYR:OH	2.20	0.45
1:B:385:ALA:O	1:B:386:LEU:HG	2.17	0.45
1:B:232:ASN:C	1:B:234:GLU:H	2.19	0.45
1:A:60:ALA:HB2	1:A:290:HIS:ND1	2.31	0.45
1:A:46:GLU:CG	1:A:57:LYS:HD2	2.46	0.44
1:A:62:LEU:O	3:A:402:FAD:N3	2.43	0.44
1:B:229:ARG:NH2	1:B:352:LYS:HB2	2.31	0.44
1:B:56:HIS:ND1	1:B:60:ALA:HA	2.33	0.44
1:B:365:LEU:O	3:B:402:FAD:O3'	2.34	0.43
1:A:312:LYS:NZ	5:A:506:HOH:O	2.37	0.43
1:B:69:ARG:NH1	1:B:375:LEU:HB3	2.30	0.43
1:B:311:MET:HB2	1:B:311:MET:HE2	1.84	0.43
1:B:256:TRP:CZ2	1:B:362:TYR:HD1	2.37	0.42
1:B:366:ASP:HA	3:B:402:FAD:H1'2	2.00	0.42
1:B:97:GLN:O	1:B:104:LEU:HB2	2.20	0.42
1:B:98:PHE:CG	1:B:99:PRO:HA	2.55	0.41
1:B:31:LEU:HD11	1:B:216:ARG:HG3	2.03	0.41
1:A:18:VAL:HG13	1:A:374:ALA:HB1	2.03	0.41
1:B:251:GLU:HB2	1:B:340:TYR:CE2	2.55	0.41
1:A:43:ALA:HA	1:A:61:HIS:CD2	2.56	0.41
1:B:229:ARG:NH1	1:B:351:GLY:O	2.50	0.40
1:B:163:GLN:HB2	1:B:257:ARG:NH1	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLU:OE2	1:B:245:ARG:NH2[2_655]	2.04	0.16

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	386/390 (99%)	381 (99%)	5 (1%)	0	100	100
1	B	383/390 (98%)	377 (98%)	6 (2%)	0	100	100
All	All	769/780 (99%)	758 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	333/333 (100%)	327 (98%)	6 (2%)	66	69
1	B	330/333 (99%)	324 (98%)	6 (2%)	66	69
All	All	663/666 (100%)	651 (98%)	12 (2%)	66	69

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	114	THR
1	A	154	ILE
1	A	232	ASN
1	A	250	SER
1	A	364	TYR
1	B	31	LEU
1	B	106	ASN

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Mol	Chain	Res	Type
1	B	143	SER
1	B	232	ASN
1	B	234	GLU
1	B	364	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	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

10 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	UDP	A	401	-	20,26,26	2.02	4 (20%)	24,40,40	2.54	7 (29%)
3	FAD	A	402	-	52,58,58	2.24	17 (32%)	52,89,89	2.37	8 (15%)
4	SO4	A	403	-	4,4,4	0.27	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	404	-	4,4,4	0.24	0	6,6,6	0.18	0
4	SO4	A	405	-	4,4,4	0.18	0	6,6,6	0.32	0
4	SO4	A	406	-	4,4,4	0.19	0	6,6,6	0.11	0
2	UDP	B	401	-	20,26,26	2.16	6 (30%)	24,40,40	2.53	6 (25%)
3	FAD	B	402	-	52,58,58	2.27	16 (30%)	52,89,89	2.24	8 (15%)
4	SO4	B	403	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	B	404	-	4,4,4	0.19	0	6,6,6	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	A	401	-	-	0/12/32/32	0/2/2/2
3	FAD	A	402	-	-	0/30/50/50	0/6/6/6
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
4	SO4	A	404	-	-	0/0/0/0	0/0/0/0
4	SO4	A	405	-	-	0/0/0/0	0/0/0/0
4	SO4	A	406	-	-	0/0/0/0	0/0/0/0
2	UDP	B	401	-	-	0/12/32/32	0/2/2/2
3	FAD	B	402	-	-	0/30/50/50	0/6/6/6
4	SO4	B	403	-	-	0/0/0/0	0/0/0/0
4	SO4	B	404	-	-	0/0/0/0	0/0/0/0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	FAD	C2B-C1B	-4.73	1.46	1.53
3	A	402	FAD	C2B-C1B	-4.70	1.46	1.53
3	B	402	FAD	C2B-C3B	-3.67	1.43	1.53
3	A	402	FAD	C2B-C3B	-3.49	1.44	1.53
3	A	402	FAD	O3'-C3'	-3.01	1.35	1.43
2	A	401	UDP	O5'-C5'	-2.85	1.33	1.44
3	B	402	FAD	O2'-C2'	-2.83	1.37	1.43
2	B	401	UDP	O5'-C5'	-2.82	1.33	1.44
3	A	402	FAD	C3B-C4B	-2.80	1.45	1.53
3	B	402	FAD	C3B-C4B	-2.57	1.46	1.53
3	B	402	FAD	O3'-C3'	-2.52	1.37	1.43
3	A	402	FAD	O2'-C2'	-2.49	1.37	1.43
3	A	402	FAD	O4'-C4'	-2.15	1.38	1.43
3	A	402	FAD	C4A-N3A	-2.07	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	FAD	C5'-C4'	-2.05	1.48	1.51
3	B	402	FAD	O4'-C4'	-2.03	1.38	1.43
2	A	401	UDP	C6-N1	2.06	1.38	1.35
2	B	401	UDP	C5'-C4'	2.11	1.58	1.51
2	B	401	UDP	C2'-C1'	2.11	1.57	1.53
3	B	402	FAD	C4-C4X	2.13	1.45	1.41
3	A	402	FAD	C6A-N6A	2.45	1.44	1.34
3	B	402	FAD	C6A-N6A	2.48	1.44	1.34
2	B	401	UDP	C6-N1	2.73	1.39	1.35
3	A	402	FAD	C2-N3	2.92	1.44	1.38
3	A	402	FAD	C2A-N3A	2.94	1.37	1.32
3	A	402	FAD	C4-N3	3.16	1.38	1.33
3	B	402	FAD	C4-N3	3.18	1.38	1.33
3	B	402	FAD	C9A-N10	3.19	1.43	1.38
3	A	402	FAD	O4B-C1B	3.20	1.45	1.41
3	B	402	FAD	C2-N3	3.27	1.45	1.38
3	B	402	FAD	C2A-N3A	3.38	1.38	1.32
3	B	402	FAD	O4B-C1B	3.96	1.46	1.41
3	A	402	FAD	C9A-N10	4.13	1.44	1.38
2	A	401	UDP	C4-N3	4.66	1.41	1.33
2	B	401	UDP	C4-N3	4.92	1.41	1.33
3	B	402	FAD	C2-N1	5.40	1.49	1.38
2	A	401	UDP	PA-O5'	5.47	1.82	1.59
3	A	402	FAD	C4X-C10	5.64	1.51	1.40
3	B	402	FAD	C4X-C10	5.72	1.51	1.40
3	A	402	FAD	C2-N1	5.83	1.50	1.38
2	B	401	UDP	PA-O5'	5.87	1.84	1.59
3	A	402	FAD	C5X-N5	6.39	1.45	1.35
3	B	402	FAD	C5X-N5	7.05	1.46	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	FAD	N3A-C2A-N1A	-11.11	120.14	128.87
3	B	402	FAD	N3A-C2A-N1A	-10.90	120.31	128.87
3	A	402	FAD	C4X-C10-N10	-6.46	115.82	120.52
3	A	402	FAD	C4B-O4B-C1B	-5.36	103.96	109.64
3	B	402	FAD	C4X-C10-N10	-4.77	117.05	120.52
3	B	402	FAD	N3-C2-N1	-4.74	119.70	127.69
3	A	402	FAD	N3-C2-N1	-4.04	120.89	127.69
2	B	401	UDP	C5-C4-N3	-3.46	114.78	123.28
2	A	401	UDP	C5-C4-N3	-3.43	114.87	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	FAD	C4B-O4B-C1B	-3.39	106.05	109.64
2	B	401	UDP	O5'-PA-O1A	-3.02	96.83	109.21
2	A	401	UDP	O5'-PA-O1A	-2.67	98.27	109.21
3	A	402	FAD	C4X-C4-N3	-2.64	120.07	123.52
3	B	402	FAD	C4X-C4-N3	-2.61	120.11	123.52
2	B	401	UDP	O2A-PA-O5'	-2.37	96.93	108.24
2	A	401	UDP	O2A-PA-O5'	-2.36	96.98	108.24
3	B	402	FAD	C2B-C3B-C4B	2.08	106.89	102.64
2	A	401	UDP	O2A-PA-O3A	2.27	115.01	105.27
2	A	401	UDP	C6-C5-C4	2.36	121.67	117.30
2	B	401	UDP	O2A-PA-O3A	2.41	115.61	105.27
3	B	402	FAD	C4X-N5-C5X	2.44	119.59	116.72
3	A	402	FAD	C4X-N5-C5X	2.44	119.59	116.72
2	B	401	UDP	C6-C5-C4	2.45	121.84	117.30
2	A	401	UDP	O3B-PB-O2B	2.50	116.62	107.44
3	A	402	FAD	C6-C5X-C9A	2.80	122.19	119.11
3	A	402	FAD	C4-N3-C2	6.02	120.18	115.16
3	B	402	FAD	C4-N3-C2	6.60	120.66	115.16
2	B	401	UDP	C4-N3-C2	10.02	124.76	114.21
2	A	401	UDP	C4-N3-C2	10.05	124.80	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	FAD	2	0
4	A	405	SO4	1	0
3	B	402	FAD	4	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^{th} 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	386/390 (98%)	-0.12	4 (1%) 84 88	30, 45, 68, 113	0
1	B	385/390 (98%)	0.66	51 (13%) 4 7	36, 66, 111, 137	0
All	All	771/780 (98%)	0.27	55 (7%) 19 25	30, 52, 99, 137	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	ALA	6.0
1	B	338	PHE	5.7
1	B	129	ILE	4.6
1	B	130	ASP	4.4
1	B	234	GLU	4.0
1	B	331	PRO	4.0
1	B	133	ASP	3.7
1	B	131	SER	3.6
1	B	304	PRO	3.6
1	B	211	GLU	3.5
1	B	383	VAL	3.5
1	B	228	LEU	3.4
1	B	4	PHE	3.4
1	B	27	GLY	3.3
1	B	89	ALA	3.2
1	B	223	GLU	3.2
1	B	349	GLU	3.2
1	B	210	HIS	3.1
1	A	3	ASP	3.1
1	B	227	ASP	3.1
1	A	60	ALA	2.9
1	B	29	LYS	2.9
1	A	338	PHE	2.9
1	B	346	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	132	LYS	2.9
1	B	335	GLU	2.7
1	B	135	THR	2.7
1	B	358	ARG	2.7
1	B	213	ILE	2.7
1	B	356	GLY	2.6
1	B	226	GLU	2.6
1	B	168	GLU	2.6
1	B	340	TYR	2.6
1	B	214	GLU	2.4
1	B	249	TYR	2.4
1	B	88	PHE	2.4
1	B	339	LYS	2.4
1	B	13	LEU	2.3
1	B	233	PRO	2.3
1	B	252	GLY	2.3
1	B	2	SER	2.3
1	B	41	GLY	2.3
1	A	230	ALA	2.3
1	B	320	GLU	2.2
1	B	23	ALA	2.2
1	B	302	ARG	2.2
1	B	305	LYS	2.2
1	B	87	VAL	2.1
1	B	301	ASP	2.1
1	B	334	ARG	2.1
1	B	104	LEU	2.1
1	B	278	ASN	2.1
1	B	250	SER	2.0
1	B	49	PRO	2.0
1	B	348	THR	2.0

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^{th} 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
4	SO4	A	406	5/5	0.77	0.28	11.88	94,99,102,103	5
4	SO4	A	403	5/5	0.98	0.12	0.43	45,50,54,62	5
3	FAD	B	402	53/53	0.92	0.17	0.11	54,87,97,126	0
4	SO4	B	404	5/5	0.92	0.13	0.01	90,92,94,94	5
3	FAD	A	402	53/53	0.95	0.14	-0.04	37,49,69,77	0
2	UDP	A	401	25/25	0.98	0.12	-0.26	31,37,41,47	0
2	UDP	B	401	25/25	0.98	0.10	-1.23	44,54,64,66	0
4	SO4	A	405	5/5	0.89	0.18	-	61,63,67,77	5
4	SO4	B	403	5/5	0.86	0.15	-	68,68,72,72	5
4	SO4	A	404	5/5	0.96	0.10	-	89,93,95,98	0

6.5 Other polymers

There are no such residues in this entry.