



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 05:05 PM GMT

PDB ID : 4J18
Title : Crystal structure of H191L mutant of UDP-glucose pyrophosphorylase from Leishmania major
Authors : Fuehring, J.I.; Routier, F.H.; Lamerz, A.-C.; Baruch, P.; Gerardy-Schahn, R.; Fedorov, R.
Deposited on : 2013-02-01
Resolution : 2.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

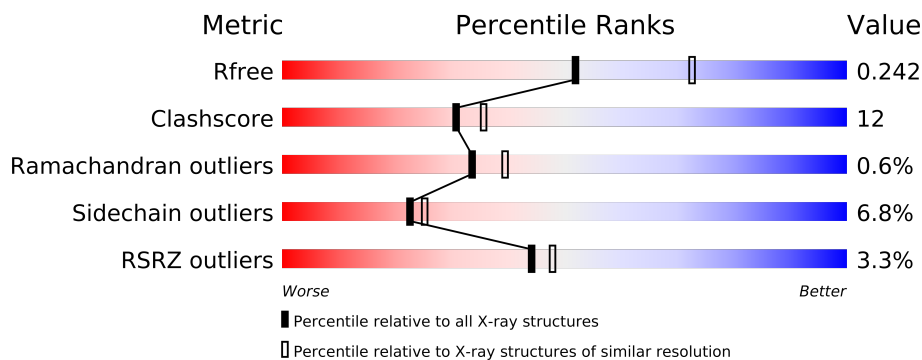
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	505	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4053 atoms, of which 0 are hydrogen and 0 are deuterium.

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-glucose pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	485	3744	2360	636	721	27	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	LEU	HIS	ENGINEERED MUTATION	UNP Q4QDU3
A	495	MET	-	EXPRESSION TAG	UNP Q4QDU3
A	496	ARG	-	EXPRESSION TAG	UNP Q4QDU3
A	497	PRO	-	EXPRESSION TAG	UNP Q4QDU3
A	498	LEU	-	EXPRESSION TAG	UNP Q4QDU3
A	499	GLU	-	EXPRESSION TAG	UNP Q4QDU3
A	500	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	501	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	502	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	503	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	504	HIS	-	EXPRESSION TAG	UNP Q4QDU3
A	505	HIS	-	EXPRESSION TAG	UNP Q4QDU3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	309	Total	O	0	0
			309	309		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	101.31Å 101.31Å 71.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.50 – 2.35 19.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.50-2.35) 99.4 (19.50-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.178 , 0.232 0.194 , 0.242	Depositor DCC
R_{free} test set	1511 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 28.9	EDS
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30206 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4053	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 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.47	1/3813 (0.0%)	0.89	13/5164 (0.3%)

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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	PRO	N-CD	5.05	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	487	SER	C-N-CD	6.54	142.13	128.40
1	A	272	GLN	C-N-CD	6.46	141.96	128.40
1	A	284	GLU	CB-CA-C	-6.03	98.35	110.40
1	A	269	LYS	CB-CA-C	-5.88	98.64	110.40
1	A	346	SER	C-N-CD	5.59	140.15	128.40
1	A	189	PRO	CA-C-N	5.59	127.37	116.20
1	A	7	SER	CB-CA-C	-5.46	99.72	110.10
1	A	273	PRO	CA-N-CD	-5.44	103.88	111.50
1	A	249	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	7	SER	N-CA-C	5.06	124.66	111.00
1	A	423	MET	CA-CB-CG	-5.05	104.71	113.30
1	A	189	PRO	N-CA-C	5.04	125.20	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	PRO	Peptide
1	A	22	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3744	0	3737	88	0
2	A	309	0	0	21	0
All	All	4053	0	3737	88	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (88) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:268:GLY:HA2	1:A:269:LYS:CB	1.53	1.35
1:A:268:GLY:CA	1:A:269:LYS:HB2	1.62	1.30
1:A:249:ARG:HG2	1:A:305:PHE:HB2	1.33	1.03
1:A:351:GLN:HB3	2:A:1279:HOH:O	1.59	1.00
1:A:339:VAL:HG12	1:A:346:SER:HB2	1.59	0.84
1:A:268:GLY:HA2	1:A:269:LYS:HB2	0.83	0.83
1:A:271:GLY:C	1:A:273:PRO:HD3	2.00	0.82
1:A:5:MET:O	1:A:7:SER:HB3	1.80	0.80
1:A:268:GLY:CA	1:A:269:LYS:CB	2.40	0.78
1:A:152:GLN:HG2	2:A:1266:HOH:O	1.84	0.77
1:A:284:GLU:H	1:A:287:GLN:HE21	1.32	0.77
1:A:267:LYS:O	1:A:269:LYS:HB2	1.85	0.76
1:A:167:LYS:HE3	1:A:184:TYR:O	1.86	0.76
1:A:133:PHE:CE2	2:A:1092:HOH:O	2.41	0.73
1:A:267:LYS:O	1:A:269:LYS:HG3	1.88	0.73
1:A:249:ARG:CG	1:A:305:PHE:HB2	2.15	0.73
1:A:149:TRP:HB2	2:A:1108:HOH:O	1.91	0.70
1:A:6:LYS:HA	1:A:8:LEU:N	2.09	0.67
1:A:144:LYS:HB2	1:A:151:TYR:CD1	2.29	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:475:ILE:HG23	1:A:476:PRO:HD2	1.75	0.67
1:A:305:PHE:CD1	2:A:1240:HOH:O	2.46	0.67
1:A:74:GLN:OE1	1:A:122:SER:HB2	1.95	0.67
1:A:213:ARG:NH2	1:A:236:GLU:OE1	2.25	0.66
1:A:351:GLN:CG	2:A:1279:HOH:O	2.43	0.66
1:A:459:THR:HB	1:A:482:ASN:HD22	1.61	0.65
1:A:167:LYS:HD3	1:A:351:GLN:NE2	2.12	0.65
1:A:268:GLY:HA2	1:A:269:LYS:HB3	1.69	0.65
1:A:334:ARG:NH1	2:A:1009:HOH:O	2.28	0.64
1:A:169:LEU:HD12	1:A:174:GLU:HG2	1.79	0.63
1:A:7:SER:OG	1:A:7:SER:O	2.14	0.63
1:A:149:TRP:HE3	2:A:1108:HOH:O	1.82	0.62
1:A:351:GLN:HG2	2:A:1279:HOH:O	1.99	0.62
1:A:475:ILE:CG2	1:A:476:PRO:HD2	2.29	0.62
1:A:249:ARG:HG2	1:A:305:PHE:CB	2.21	0.61
1:A:395:VAL:HG22	1:A:401:LEU:CD2	2.32	0.60
1:A:284:GLU:H	1:A:287:GLN:NE2	1.99	0.59
1:A:98:LEU:HD23	1:A:106:PHE:HE1	1.68	0.59
1:A:290:LYS:HD2	2:A:1184:HOH:O	2.01	0.59
1:A:267:LYS:O	1:A:269:LYS:CG	2.51	0.58
1:A:144:LYS:HB2	1:A:151:TYR:CE1	2.39	0.58
1:A:180:GLU:HB2	2:A:1278:HOH:O	2.02	0.57
1:A:100:VAL:O	1:A:389:ARG:HG2	2.05	0.57
1:A:267:LYS:O	1:A:269:LYS:CB	2.53	0.56
1:A:351:GLN:CB	2:A:1279:HOH:O	2.31	0.55
1:A:415:ASP:HB3	1:A:445:THR:HG23	1.88	0.55
1:A:270:ASP:CG	1:A:270:ASP:O	2.45	0.55
1:A:98:LEU:HD23	1:A:106:PHE:CE1	2.42	0.54
1:A:6:LYS:HA	1:A:7:SER:C	2.28	0.54
1:A:459:THR:HB	1:A:482:ASN:ND2	2.24	0.52
1:A:74:GLN:HG2	2:A:1225:HOH:O	2.08	0.52
1:A:467:THR:HG22	2:A:1236:HOH:O	2.10	0.52
1:A:79:LEU:HD12	1:A:80:LYS:N	2.25	0.51
1:A:271:GLY:CA	1:A:273:PRO:HD3	2.40	0.51
1:A:461:THR:O	1:A:483:ASP:HA	2.10	0.51
1:A:191:LEU:HB2	2:A:1182:HOH:O	2.12	0.50
1:A:153:VAL:HB	1:A:157:GLU:HB2	1.92	0.49
1:A:74:GLN:CG	2:A:1225:HOH:O	2.61	0.48
1:A:178:TRP:HZ3	1:A:347:PRO:HD3	1.79	0.48
1:A:74:GLN:OE1	1:A:122:SER:CB	2.62	0.47
1:A:33:ILE:O	1:A:37:VAL:HG23	2.15	0.47
1:A:81:LEU:HD11	1:A:356:MET:SD	2.55	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:270:ASP:O	1:A:270:ASP:OD2	2.34	0.46
1:A:133:PHE:CD2	2:A:1092:HOH:O	2.64	0.46
1:A:235:MET:HG2	1:A:240:ILE:HB	1.97	0.46
1:A:395:VAL:HG22	1:A:401:LEU:HD21	1.96	0.45
1:A:267:LYS:C	1:A:269:LYS:HB2	2.37	0.45
1:A:482:ASN:OD1	1:A:483:ASP:HB2	2.17	0.45
1:A:25:ASN:ND2	1:A:27:ALA:H	2.15	0.44
1:A:6:LYS:HA	1:A:8:LEU:H	1.81	0.44
1:A:65:THR:HG23	2:A:1111:HOH:O	2.17	0.44
1:A:267:LYS:HG2	1:A:268:GLY:N	2.32	0.44
1:A:271:GLY:HA3	1:A:273:PRO:HD3	1.99	0.43
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.76	0.43
1:A:116:TYR:HA	2:A:1063:HOH:O	2.18	0.43
1:A:170:GLN:HG2	1:A:350:TYR:CZ	2.54	0.42
1:A:415:ASP:HB3	1:A:445:THR:HA	2.00	0.42
1:A:251:GLU:HB3	2:A:1306:HOH:O	2.19	0.42
1:A:343:ASN:O	1:A:346:SER:OG	2.34	0.42
1:A:176:ALA:O	1:A:185:GLU:HG2	2.21	0.41
1:A:404:ASP:OD1	1:A:405:ASP:N	2.53	0.41
1:A:182:PRO:O	1:A:185:GLU:HB2	2.21	0.41
1:A:287:GLN:NE2	2:A:1101:HOH:O	2.51	0.41
1:A:271:GLY:C	1:A:273:PRO:CD	2.82	0.41
1:A:167:LYS:HD3	1:A:351:GLN:HE21	1.85	0.40
1:A:457:VAL:C	1:A:458:LEU:HD12	2.42	0.40
1:A:458:LEU:N	1:A:458:LEU:CD1	2.84	0.40
1:A:453:GLY:H	1:A:456:ASN:ND2	2.19	0.40
1:A:482:ASN:O	1:A:484:THR:HG22	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	483/505 (96%)	473 (98%)	7 (1%)	3 (1%)	33	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	273	PRO
1	A	189	PRO

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	412/432 (95%)	384 (93%)	28 (7%)	22	25

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	6	LYS
1	A	17	LYS
1	A	23	LYS
1	A	49	ASP
1	A	73	LEU
1	A	74	GLN
1	A	79	LEU
1	A	118	ARG
1	A	130	MET
1	A	138	SER
1	A	141	SER
1	A	194	ILE
1	A	251	GLU
1	A	269	LYS
1	A	272	GLN
1	A	281	LEU
1	A	284	GLU
1	A	290	LYS
1	A	301	LYS
1	A	337	LYS
1	A	341	SER
1	A	346	SER
1	A	351	GLN

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Mol	Chain	Res	Type
1	A	403	LEU
1	A	440	GLU
1	A	442	LYS
1	A	484	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	113	GLN
1	A	170	GLN
1	A	219	ASN
1	A	287	GLN
1	A	309	ASN
1	A	322	GLN
1	A	351	GLN
1	A	456	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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, 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	485/505 (96%)	-0.06	16 (3%)	44 48	16, 33, 62, 120	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ASP	11.6
1	A	271	GLY	8.0
1	A	269	LYS	7.1
1	A	272	GLN	5.8
1	A	273	PRO	5.2
1	A	4	ASP	5.2
1	A	5	MET	5.1
1	A	342	SER	3.8
1	A	179	ALA	3.3
1	A	274	ASP	3.1
1	A	343	ASN	2.8
1	A	133	PHE	2.6
1	A	341	SER	2.4
1	A	482	ASN	2.1
1	A	464	ILE	2.1
1	A	344	SER	2.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.