Full wwPDB X-ray Structure Validation Report (i)

Jun 29, 2016 – 02:27 PM EDT

PDB ID	:	4UUL
Title	:	Apo trichomonas vaginalis lactate dehydrogenase L91R
Authors	:	Steindel, P.A.; Chen, E.H.; L Theobald, D.
Deposited on	:	2014-07-29
Resolution	:	1.28 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:

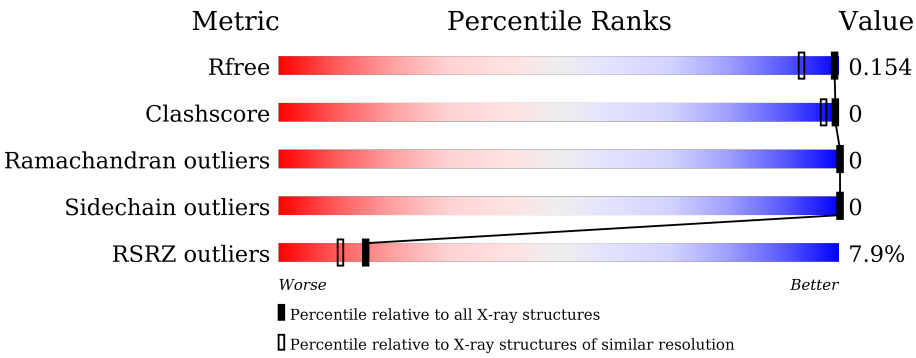
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 1.28 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	1194 (1.30-1.26)
Clashscore	102246	1271 (1.30-1.26)
Ramachandran outliers	100387	1217 (1.30-1.26)
Sidechain outliers	100360	1216 (1.30-1.26)
RSRZ outliers	91569	1194 (1.30-1.26)

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	341	10% 97%
1	B	341	5% 96%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11882 atoms, of which 5432 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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	334	5390	1742	2691	448	495	14	0	16	0
1	B	337	5487	1766	2741	461	505	14	0	18	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	LEU	-	EXPRESSION TAG	UNP O96445
A	335	GLU	-	EXPRESSION TAG	UNP O96445
A	336	HIS	-	EXPRESSION TAG	UNP O96445
A	337	HIS	-	EXPRESSION TAG	UNP O96445
A	338	HIS	-	EXPRESSION TAG	UNP O96445
A	339	HIS	-	EXPRESSION TAG	UNP O96445
A	340	HIS	-	EXPRESSION TAG	UNP O96445
A	341	HIS	-	EXPRESSION TAG	UNP O96445
A	91	ARG	LEU	ENGINEERED MUTATION	UNP O96445
B	334	LEU	-	EXPRESSION TAG	UNP O96445
B	335	GLU	-	EXPRESSION TAG	UNP O96445
B	336	HIS	-	EXPRESSION TAG	UNP O96445
B	337	HIS	-	EXPRESSION TAG	UNP O96445
B	338	HIS	-	EXPRESSION TAG	UNP O96445
B	339	HIS	-	EXPRESSION TAG	UNP O96445
B	340	HIS	-	EXPRESSION TAG	UNP O96445
B	341	HIS	-	EXPRESSION TAG	UNP O96445
B	91	ARG	LEU	ENGINEERED MUTATION	UNP O96445

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	498	498	498	0	0

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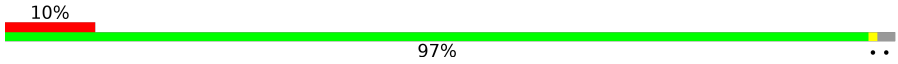
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	507	507	507	0	0

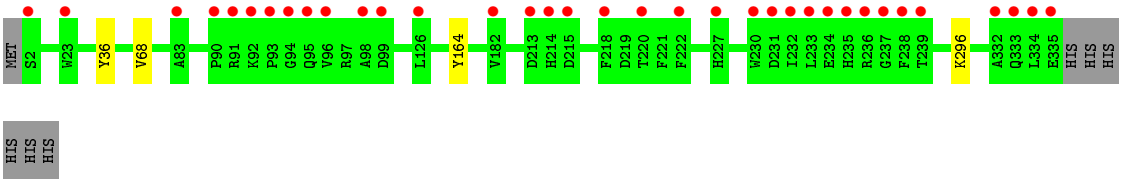
3 Residue-property plots (i)

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: L-LACTATE DEHYDROGENASE

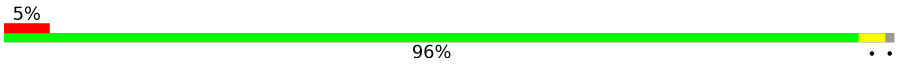
Chain A:

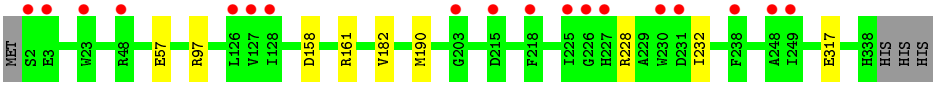




- Molecule 1: L-LACTATE DEHYDROGENASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.57Å 59.61Å 86.49Å 90.00° 116.18° 90.00°	Depositor
Resolution (Å)	30.71 – 1.28 30.71 – 1.28	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.71-1.28) 90.3 (30.71-1.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 1.28Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.129 , 0.154 0.128 , 0.154	Depositor DCC
R_{free} test set	8787 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	11882	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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 (i)

5.1 Standard geometry (i)

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	0.64	0/2809	0.71	0/3816
1	B	0.66	1/2855 (0.0%)	0.73	3/3876 (0.1%)
All	All	0.65	1/5664 (0.0%)	0.72	3/7692 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	GLU	CD-OE2	-6.15	1.18	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	97	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	161	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	158	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	2699	2691	2637	3	0
1	B	2746	2741	2690	3	0
2	A	498	0	0	1	0
2	B	507	0	0	0	0
All	All	6450	5432	5327	5	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 0.

All (5) 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:36:TYR:HE1	1:A:68[B]:VAL:HG23	1.68	0.57
1:A:296:LYS:HD3	2:A:2437:HOH:O	2.09	0.52
1:A:164[B]:TYR:CZ	1:B:57:GLU:HG2	2.48	0.48
1:B:228:ARG:O	1:B:232[A]:ILE:HG12	2.14	0.48
1:B:182:VAL:CG1	1:B:190[B]:MET:HE2	2.50	0.41

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	348/341 (102%)	341 (98%)	7 (2%)	0	100	100
1	B	353/341 (104%)	349 (99%)	4 (1%)	0	100	100
All	All	701/682 (103%)	690 (98%)	11 (2%)	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	294/287 (102%)	294 (100%)	0	100	100
1	B	301/287 (105%)	301 (100%)	0	100	100
All	All	595/574 (104%)	595 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

There are no ligands in this entry.

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, 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	334/341 (97%)	0.30	35 (10%)	8	6	12, 19, 45, 60	0
1	B	337/341 (98%)	0.10	18 (5%)	30	25	12, 19, 40, 55	0
All	All	671/682 (98%)	0.20	53 (7%)	15	11	12, 19, 43, 60	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230[A]	TRP	10.3
1	B	230	TRP	7.9
1	A	93	PRO	7.0
1	A	238	PHE	7.0
1	A	233	LEU	6.0
1	B	227	HIS	5.5
1	A	94	GLY	5.2
1	A	95	GLN	5.1
1	B	226	GLY	5.0
1	A	92	LYS	4.5
1	A	334	LEU	4.2
1	B	238	PHE	4.2
1	A	237	GLY	4.1
1	A	227	HIS	4.0
1	B	2	SER	4.0
1	A	96	VAL	3.9
1	A	91	ARG	3.6
1	A	235	HIS	3.5
1	A	231	ASP	3.5
1	B	249[A]	ILE	3.4
1	A	333	GLN	3.3
1	A	234	GLU	3.3
1	A	2	SER	3.1
1	A	239	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	215	ASP	3.0
1	A	232	ILE	2.9
1	A	98	ALA	2.9
1	B	23[A]	TRP	2.9
1	A	335	GLU	2.8
1	A	332	ALA	2.8
1	A	213	ASP	2.7
1	B	48	ARG	2.6
1	B	3	GLU	2.6
1	A	218	PHE	2.6
1	A	99	ASP	2.4
1	B	215	ASP	2.4
1	A	83	ALA	2.3
1	A	220	THR	2.3
1	A	214	HIS	2.3
1	B	218	PHE	2.3
1	B	126	LEU	2.3
1	B	127	VAL	2.3
1	A	236	ARG	2.2
1	A	23[A]	TRP	2.2
1	A	222	PHE	2.2
1	A	126	LEU	2.2
1	B	128	ILE	2.2
1	A	182[A]	VAL	2.2
1	B	231	ASP	2.2
1	A	90	PRO	2.2
1	B	203	GLY	2.1
1	B	225	ILE	2.1
1	B	248	ALA	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.