



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:12 PM GMT

PDB ID : 4ZGS  
Title : Identification of the pyruvate reductase of Chlamydomonas reinhardtii  
Authors : Burgess, S.J.; Hussein, T.; Yeoman, J.A.; Iamshanova, O.; Boehm, M.; Bundy, J.; Bialek, W.; Murray, J.W.; Nixon, P.J.  
Deposited on : 2015-04-23  
Resolution : 2.46 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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-20026982  
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-20026982

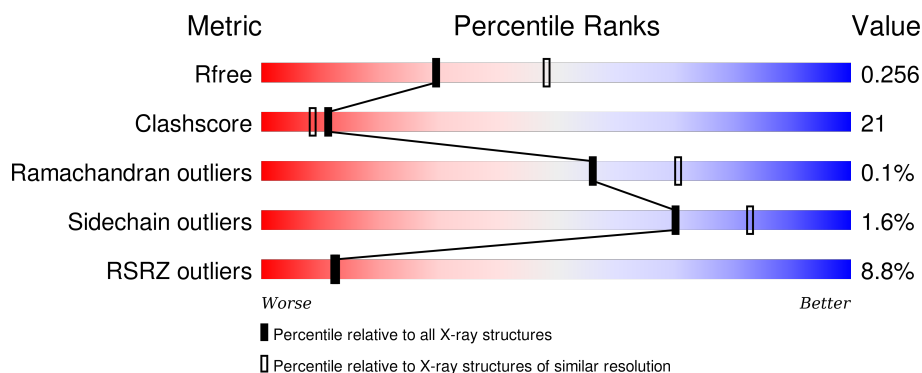
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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  $\geq 3$ , 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	386	<div> <div>13%</div> <div>59%</div> <div>30%</div> <div>10%</div> </div>
1	B	386	<div> <div>13%</div> <div>54%</div> <div>33%</div> <div>12%</div> </div>
1	C	386	<div> <div>12%</div> <div>55%</div> <div>33%</div> <div>11%</div> </div>
1	D	386	<div> <div>6%</div> <div>59%</div> <div>29%</div> <div>10%</div> </div>
1	E	386	<div> <div>7%</div> <div>59%</div> <div>28%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	386	
1	G	386	
1	H	386	

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	NAD	A	1000	-	-	-	X
2	NAD	B	1000	-	-	-	X
2	NAD	C	1000	-	-	-	X
2	NAD	D	1000	-	-	-	X
2	NAD	E	1000	-	-	-	X
2	NAD	F	1000	-	-	-	X
2	NAD	G	1000	-	-	-	X
2	NAD	H	1000	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21903 atoms, of which 208 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 Putative D-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2661	1695	459	492	15			
1	B	338	Total	C	N	O	S	0	0	0
			2599	1657	449	478	15			
1	C	342	Total	C	N	O	S	0	0	0
			2633	1677	454	487	15			
1	D	346	Total	C	N	O	S	0	0	0
			2664	1697	458	494	15			
1	E	344	Total	C	N	O	S	0	0	0
			2648	1687	456	490	15			
1	F	343	Total	C	N	O	S	0	0	0
			2640	1682	455	488	15			
1	G	343	Total	C	N	O	S	0	0	0
			2640	1682	455	488	15			
1	H	343	Total	C	N	O	S	0	0	0
			2640	1681	455	489	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B0LUZ5
A	379	LEU	-	expression tag	UNP B0LUZ5
A	380	GLU	-	expression tag	UNP B0LUZ5
A	381	HIS	-	expression tag	UNP B0LUZ5
A	382	HIS	-	expression tag	UNP B0LUZ5
A	383	HIS	-	expression tag	UNP B0LUZ5
A	384	HIS	-	expression tag	UNP B0LUZ5
A	385	HIS	-	expression tag	UNP B0LUZ5
A	386	HIS	-	expression tag	UNP B0LUZ5
B	1	MET	-	initiating methionine	UNP B0LUZ5
B	379	LEU	-	expression tag	UNP B0LUZ5
B	380	GLU	-	expression tag	UNP B0LUZ5
B	381	HIS	-	expression tag	UNP B0LUZ5

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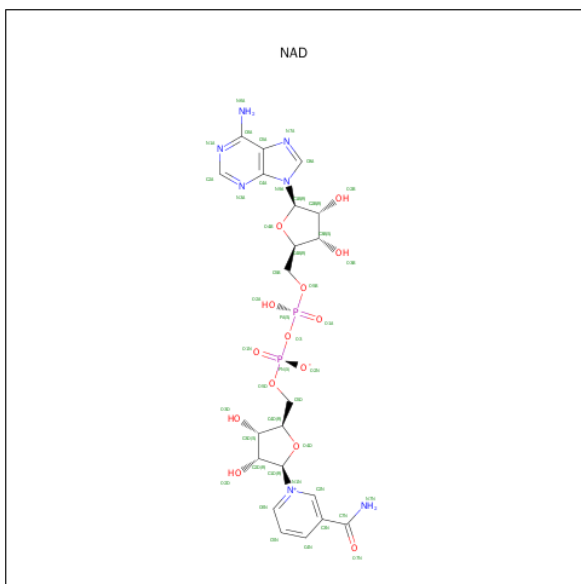
Chain	Residue	Modelled	Actual	Comment	Reference
B	382	HIS	-	expression tag	UNP B0LUZ5
B	383	HIS	-	expression tag	UNP B0LUZ5
B	384	HIS	-	expression tag	UNP B0LUZ5
B	385	HIS	-	expression tag	UNP B0LUZ5
B	386	HIS	-	expression tag	UNP B0LUZ5
C	1	MET	-	initiating methionine	UNP B0LUZ5
C	379	LEU	-	expression tag	UNP B0LUZ5
C	380	GLU	-	expression tag	UNP B0LUZ5
C	381	HIS	-	expression tag	UNP B0LUZ5
C	382	HIS	-	expression tag	UNP B0LUZ5
C	383	HIS	-	expression tag	UNP B0LUZ5
C	384	HIS	-	expression tag	UNP B0LUZ5
C	385	HIS	-	expression tag	UNP B0LUZ5
C	386	HIS	-	expression tag	UNP B0LUZ5
D	1	MET	-	initiating methionine	UNP B0LUZ5
D	379	LEU	-	expression tag	UNP B0LUZ5
D	380	GLU	-	expression tag	UNP B0LUZ5
D	381	HIS	-	expression tag	UNP B0LUZ5
D	382	HIS	-	expression tag	UNP B0LUZ5
D	383	HIS	-	expression tag	UNP B0LUZ5
D	384	HIS	-	expression tag	UNP B0LUZ5
D	385	HIS	-	expression tag	UNP B0LUZ5
D	386	HIS	-	expression tag	UNP B0LUZ5
E	1	MET	-	initiating methionine	UNP B0LUZ5
E	379	LEU	-	expression tag	UNP B0LUZ5
E	380	GLU	-	expression tag	UNP B0LUZ5
E	381	HIS	-	expression tag	UNP B0LUZ5
E	382	HIS	-	expression tag	UNP B0LUZ5
E	383	HIS	-	expression tag	UNP B0LUZ5
E	384	HIS	-	expression tag	UNP B0LUZ5
E	385	HIS	-	expression tag	UNP B0LUZ5
E	386	HIS	-	expression tag	UNP B0LUZ5
F	1	MET	-	initiating methionine	UNP B0LUZ5
F	379	LEU	-	expression tag	UNP B0LUZ5
F	380	GLU	-	expression tag	UNP B0LUZ5
F	381	HIS	-	expression tag	UNP B0LUZ5
F	382	HIS	-	expression tag	UNP B0LUZ5
F	383	HIS	-	expression tag	UNP B0LUZ5
F	384	HIS	-	expression tag	UNP B0LUZ5
F	385	HIS	-	expression tag	UNP B0LUZ5
F	386	HIS	-	expression tag	UNP B0LUZ5
G	1	MET	-	initiating methionine	UNP B0LUZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	379	LEU	-	expression tag	UNP B0LUZ5
G	380	GLU	-	expression tag	UNP B0LUZ5
G	381	HIS	-	expression tag	UNP B0LUZ5
G	382	HIS	-	expression tag	UNP B0LUZ5
G	383	HIS	-	expression tag	UNP B0LUZ5
G	384	HIS	-	expression tag	UNP B0LUZ5
G	385	HIS	-	expression tag	UNP B0LUZ5
G	386	HIS	-	expression tag	UNP B0LUZ5
H	1	MET	-	initiating methionine	UNP B0LUZ5
H	379	LEU	-	expression tag	UNP B0LUZ5
H	380	GLU	-	expression tag	UNP B0LUZ5
H	381	HIS	-	expression tag	UNP B0LUZ5
H	382	HIS	-	expression tag	UNP B0LUZ5
H	383	HIS	-	expression tag	UNP B0LUZ5
H	384	HIS	-	expression tag	UNP B0LUZ5
H	385	HIS	-	expression tag	UNP B0LUZ5
H	386	HIS	-	expression tag	UNP B0LUZ5

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

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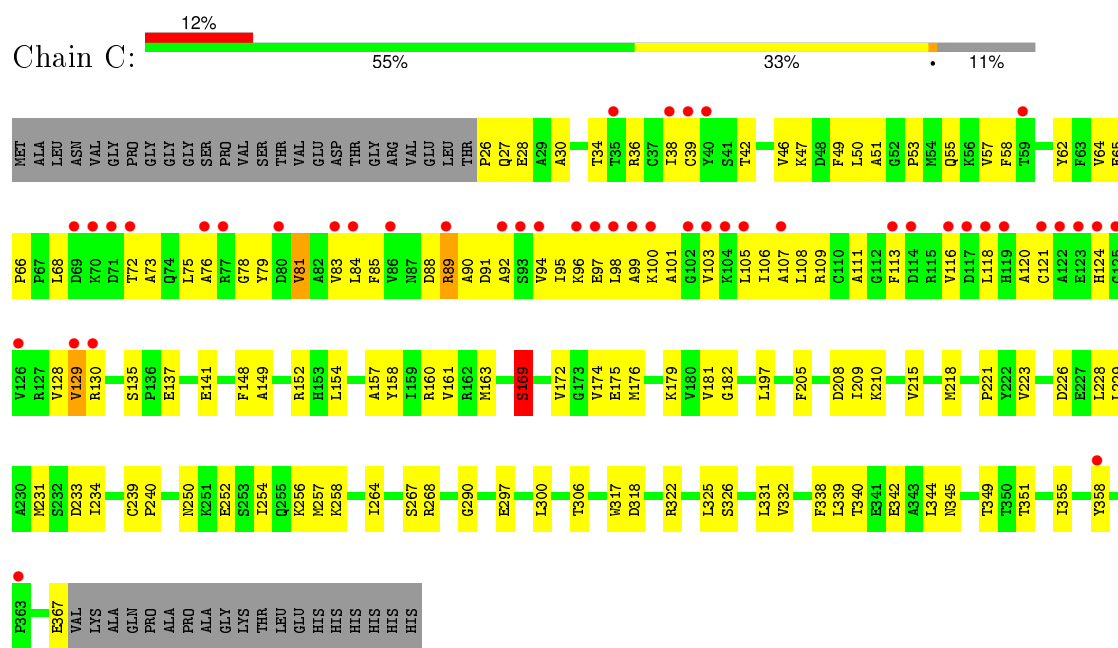
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total 70	C 21	H 26	N 7	O 14	P 2	0	0
2	D	1	Total 70	C 21	H 26	N 7	O 14	P 2	0	0
2	E	1	Total 70	C 21	H 26	N 7	O 14	P 2	0	0
2	F	1	Total 70	C 21	H 26	N 7	O 14	P 2	0	0
2	G	1	Total 70	C 21	H 26	N 7	O 14	P 2	0	0
2	H	1	Total 70	C 21	H 26	N 7	O 14	P 2	0	0

- Molecule 3 is water.

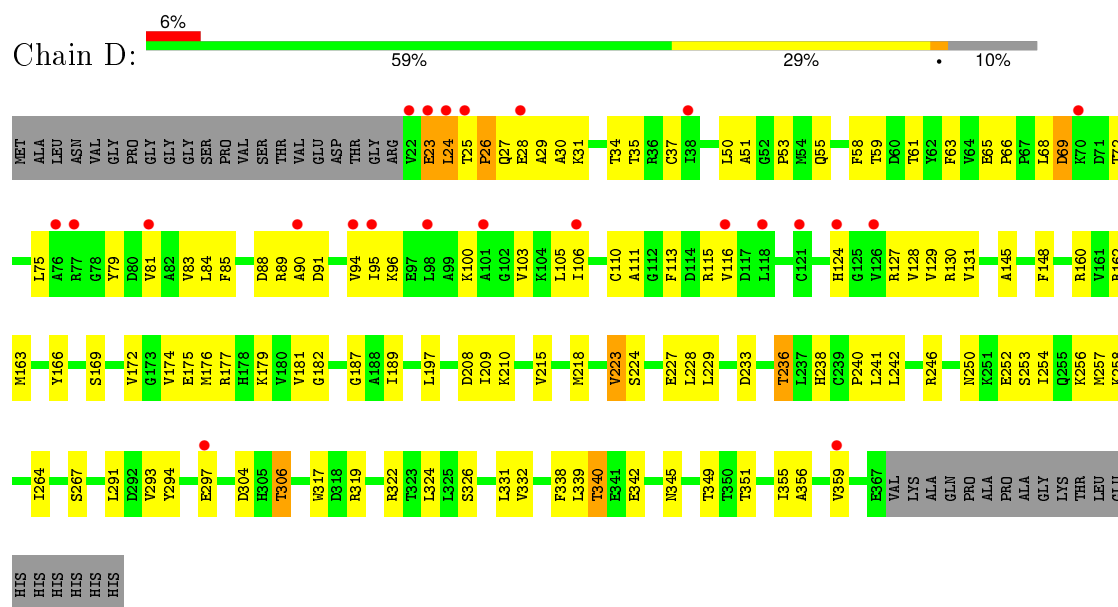
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	33	Total 33	O 33	0	0
3	C	25	Total 25	O 25	0	0
3	D	27	Total 27	O 27	0	0
3	E	33	Total 33	O 33	0	0
3	F	21	Total 21	O 21	0	0
3	G	20	Total 20	O 20	0	0
3	H	29	Total 29	O 29	0	0



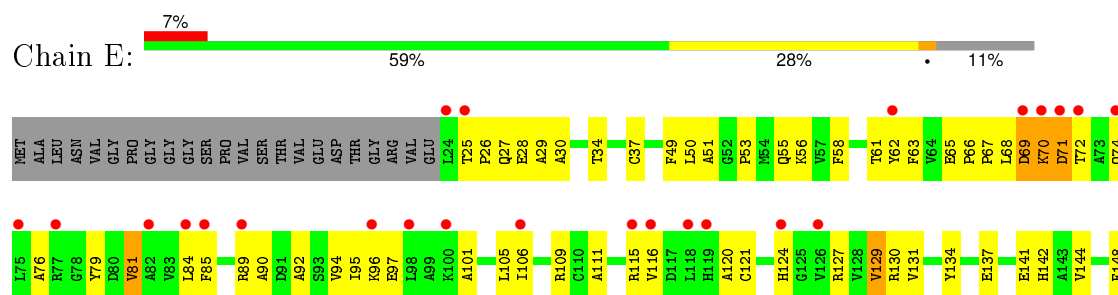


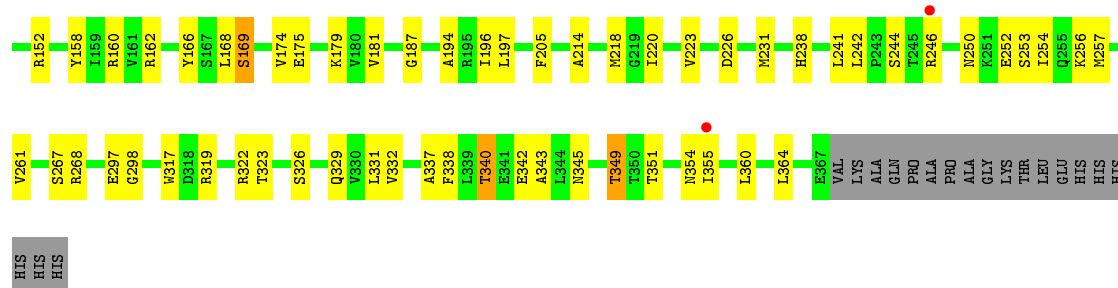


- Molecule 1: Putative D-lactate dehydrogenase

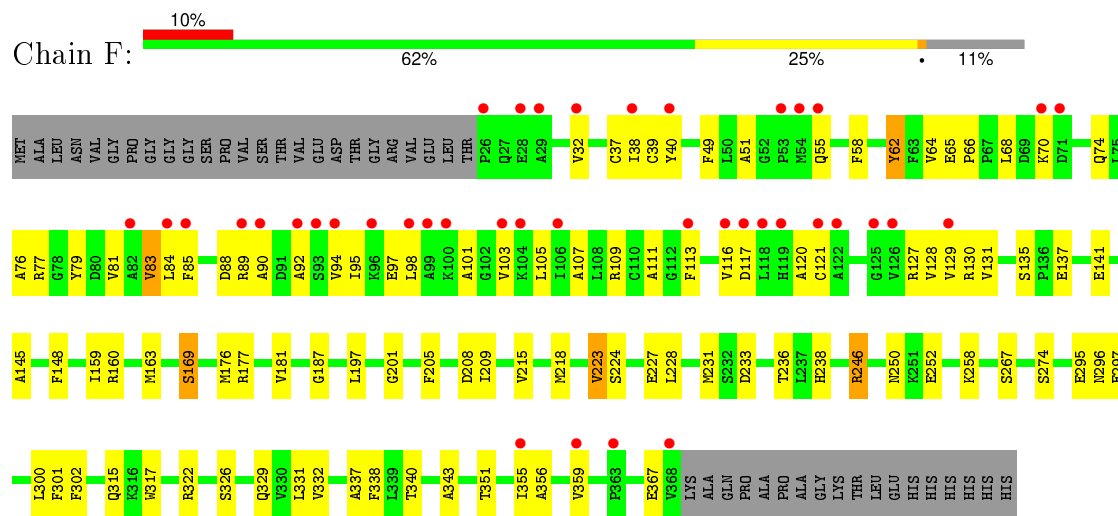


- Molecule 1: Putative D-lactate dehydrogenase

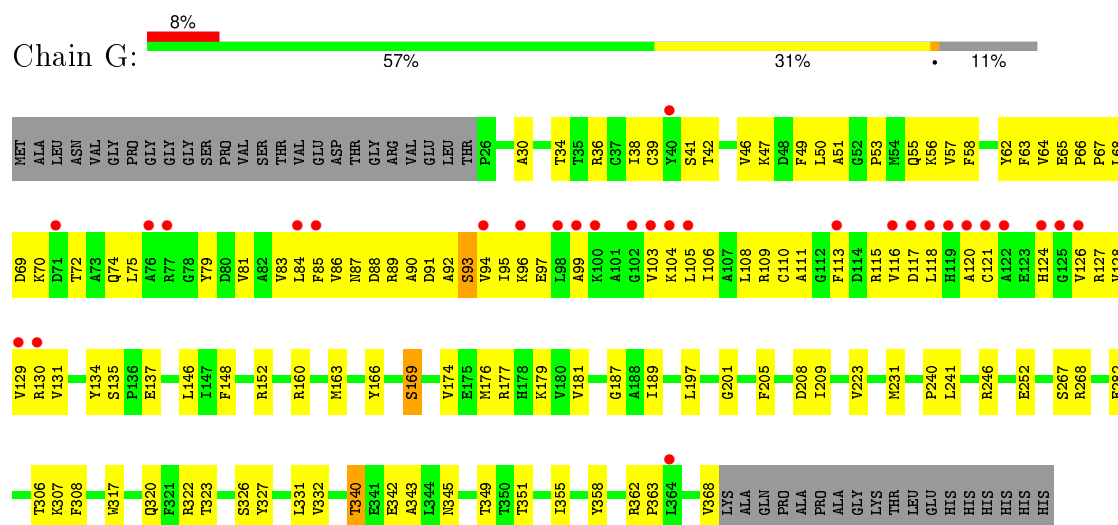




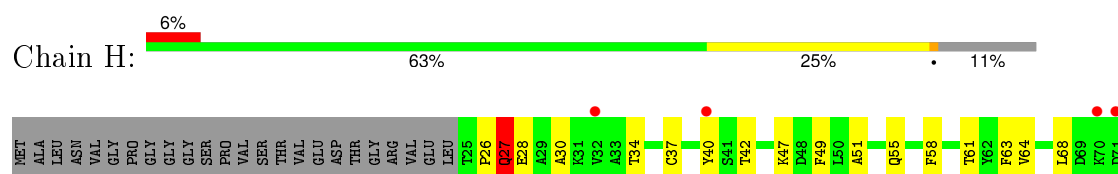
• Molecule 1: Putative D-lactate dehydrogenase

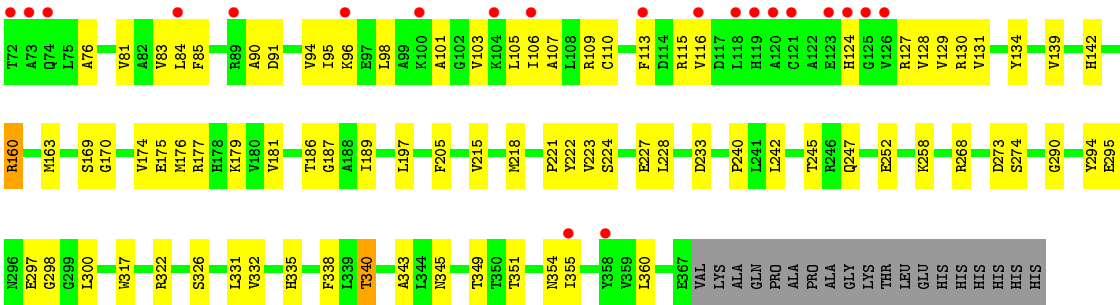


• Molecule 1: Putative D-lactate dehydrogenase



• Molecule 1: Putative D-lactate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.76Å 110.92Å 193.16Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	66.84 – 2.46 66.84 – 2.46	Depositor EDS
% Data completeness (in resolution range)	98.5 (66.84-2.46) 89.9 (66.84-2.46)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.202 , 0.254 0.210 , 0.256	Depositor DCC
$R_{free}$ test set	6341 reflections (5.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.878	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.8	EDS
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	9 of 126445 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	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 36.33 % 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 5.0847e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: NAD

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	0.55	0/2710	0.75	1/3679 (0.0%)
1	B	0.52	0/2647	0.73	2/3593 (0.1%)
1	C	0.51	0/2682	0.73	2/3640 (0.1%)
1	D	0.51	0/2713	0.71	1/3684 (0.0%)
1	E	0.51	0/2697	0.72	2/3662 (0.1%)
1	F	0.53	0/2689	0.73	1/3650 (0.0%)
1	G	0.56	0/2689	0.76	1/3650 (0.0%)
1	H	0.51	0/2689	0.71	2/3651 (0.1%)
All	All	0.52	0/21516	0.73	12/29209 (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	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	SER	C-N-CA	7.24	137.50	122.30
1	F	169	SER	C-N-CA	7.08	137.16	122.30
1	G	169	SER	C-N-CA	6.87	136.72	122.30
1	B	169	SER	C-N-CA	6.84	136.66	122.30
1	H	169	SER	C-N-CA	6.18	135.27	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ARG	Peptide
1	C	89	ARG	Peptide
1	E	71	ASP	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	2661	0	2707	107	0
1	B	2599	0	2646	137	0
1	C	2633	0	2674	134	0
1	D	2664	0	2706	109	0
1	E	2648	0	2691	112	0
1	F	2640	0	2683	106	0
1	G	2640	0	2683	142	0
1	H	2640	0	2680	89	0
2	A	44	26	26	6	0
2	B	44	26	26	8	0
2	C	44	26	26	6	0
2	D	44	26	26	5	0
2	E	44	26	26	3	0
2	F	44	26	26	4	0
2	G	44	26	26	9	0
2	H	44	26	26	5	0
3	A	30	0	0	3	0
3	B	33	0	0	6	0
3	C	25	0	0	1	0
3	D	27	0	0	3	0
3	E	33	0	0	3	0
3	F	21	0	0	2	0
3	G	20	0	0	1	0
3	H	29	0	0	2	0
All	All	21695	208	21678	889	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 21.

The worst 5 of 889 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:C:89:ARG:HB3	1:C:90:ALA:HA	1.21	1.16
1:F:38:ILE:HG22	1:F:62:TYR:HB3	1.18	1.15
1:E:70:LYS:HB3	1:E:71:ASP:HB2	1.31	1.12
1:C:106:ILE:HD11	1:C:128:VAL:HG13	1.31	1.09
1:G:89:ARG:HG3	1:G:115:ARG:HE	1.17	1.04

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	344/386 (89%)	336 (98%)	8 (2%)	0	100	100
1	B	336/386 (87%)	329 (98%)	7 (2%)	0	100	100
1	C	340/386 (88%)	331 (97%)	9 (3%)	0	100	100
1	D	344/386 (89%)	335 (97%)	7 (2%)	2 (1%)	30	35
1	E	342/386 (89%)	333 (97%)	9 (3%)	0	100	100
1	F	341/386 (88%)	335 (98%)	6 (2%)	0	100	100
1	G	341/386 (88%)	331 (97%)	10 (3%)	0	100	100
1	H	341/386 (88%)	334 (98%)	5 (2%)	2 (1%)	30	35
All	All	2729/3088 (88%)	2664 (98%)	61 (2%)	4 (0%)	56	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	24	LEU
1	H	27	GLN
1	H	26	PRO

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Mol	Chain	Res	Type
1	D	26	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	287/318 (90%)	285 (99%)	2 (1%)	88	93
1	B	280/318 (88%)	275 (98%)	5 (2%)	66	81
1	C	284/318 (89%)	281 (99%)	3 (1%)	80	88
1	D	288/318 (91%)	281 (98%)	7 (2%)	57	73
1	E	286/318 (90%)	279 (98%)	7 (2%)	57	73
1	F	285/318 (90%)	279 (98%)	6 (2%)	61	77
1	G	285/318 (90%)	281 (99%)	4 (1%)	74	85
1	H	285/318 (90%)	282 (99%)	3 (1%)	80	88
All	All	2280/2544 (90%)	2243 (98%)	37 (2%)	70	83

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	340	THR
1	E	129	VAL
1	H	27	GLN
1	E	49	PHE
1	E	69	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	366	ASN
1	H	247	GLN
1	F	151	ASN
1	B	151	ASN

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Mol	Chain	Res	Type
1	G	151	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 ⓘ

8 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	NAD	A	1000	-	42,48,48	2.50	16 (38%)	46,73,73	2.13	9 (19%)
2	NAD	B	1000	-	42,48,48	2.46	16 (38%)	46,73,73	2.26	10 (21%)
2	NAD	C	1000	-	42,48,48	2.48	16 (38%)	46,73,73	2.23	10 (21%)
2	NAD	D	1000	-	42,48,48	2.47	16 (38%)	46,73,73	2.32	9 (19%)
2	NAD	E	1000	-	42,48,48	2.51	16 (38%)	46,73,73	2.29	12 (26%)
2	NAD	F	1000	-	42,48,48	2.47	16 (38%)	46,73,73	2.37	9 (19%)
2	NAD	G	1000	-	42,48,48	2.45	15 (35%)	46,73,73	2.41	12 (26%)
2	NAD	H	1000	-	42,48,48	2.49	16 (38%)	46,73,73	2.20	10 (21%)

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	NAD	A	1000	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1000	-	-	0/22/62/62	0/5/5/5
2	NAD	C	1000	-	-	0/22/62/62	0/5/5/5
2	NAD	D	1000	-	-	0/22/62/62	0/5/5/5
2	NAD	E	1000	-	-	0/22/62/62	0/5/5/5
2	NAD	F	1000	-	-	0/22/62/62	0/5/5/5
2	NAD	G	1000	-	-	0/22/62/62	0/5/5/5
2	NAD	H	1000	-	-	0/22/62/62	0/5/5/5

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1000	NAD	C2A-N1A	-5.99	1.22	1.33
2	C	1000	NAD	C2A-N1A	-5.93	1.22	1.33
2	E	1000	NAD	C2A-N1A	-5.91	1.22	1.33
2	B	1000	NAD	C2A-N1A	-5.91	1.22	1.33
2	A	1000	NAD	C2A-N1A	-5.87	1.22	1.33

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	NAD	N3A-C2A-N1A	-8.88	121.89	128.87
2	F	1000	NAD	N3A-C2A-N1A	-8.86	121.91	128.87
2	C	1000	NAD	N3A-C2A-N1A	-8.66	122.07	128.87
2	E	1000	NAD	N3A-C2A-N1A	-8.45	122.23	128.87
2	G	1000	NAD	N3A-C2A-N1A	-8.40	122.27	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	NAD	6	0
2	B	1000	NAD	8	0
2	C	1000	NAD	6	0
2	D	1000	NAD	5	0
2	E	1000	NAD	3	0
2	F	1000	NAD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1000	NAD	9	0
2	H	1000	NAD	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	346/386 (89%)	0.00	4 (1%) 81 83	30, 57, 95, 134	0
1	B	338/386 (87%)	0.58	50 (14%) 3 3	27, 61, 146, 199	0
1	C	342/386 (88%)	0.53	45 (13%) 4 4	32, 61, 160, 208	0
1	D	346/386 (89%)	0.21	23 (6%) 22 23	31, 58, 120, 175	0
1	E	344/386 (89%)	0.22	26 (7%) 17 17	30, 63, 133, 165	0
1	F	343/386 (88%)	0.43	40 (11%) 6 6	30, 58, 128, 170	0
1	G	343/386 (88%)	0.48	29 (8%) 13 13	29, 58, 163, 203	0
1	H	343/386 (88%)	0.36	25 (7%) 18 19	28, 59, 124, 173	0
All	All	2745/3088 (88%)	0.35	242 (8%) 12 13	27, 59, 138, 208	0

The worst 5 of 242 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	121	CYS	12.2
1	C	98	LEU	10.4
1	G	98	LEU	9.1
1	G	94	VAL	8.0
1	B	93	SER	7.9

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAD	C	1000	44/44	0.76	0.52	12.18	205,211,254,256	0
2	NAD	F	1000	44/44	0.73	0.43	9.21	172,177,213,216	0
2	NAD	H	1000	44/44	0.63	0.42	8.53	161,163,197,199	0
2	NAD	D	1000	44/44	0.74	0.38	8.00	156,163,195,204	0
2	NAD	A	1000	44/44	0.77	0.36	7.69	157,163,196,197	0
2	NAD	B	1000	44/44	0.70	0.41	7.37	169,174,209,214	0
2	NAD	E	1000	44/44	0.75	0.35	5.93	153,176,211,218	0
2	NAD	G	1000	44/44	0.86	0.28	2.92	112,128,155,161	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.