wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BL4
Title	:	LACTALDEHYDE:1,2-PROPANEDIOL OXIDOREDUCTASE OF ESCHERICHIA COLI
Authors	:	Montella, C.; Bellsolell, L.; Perez-Luque, R.; Badia, J.; Baldoma, L.; Coll, M.; Aguilar, J.
Deposited on	:	2005-03-01
Resolution	:	2.85 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 (i) symbol.

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

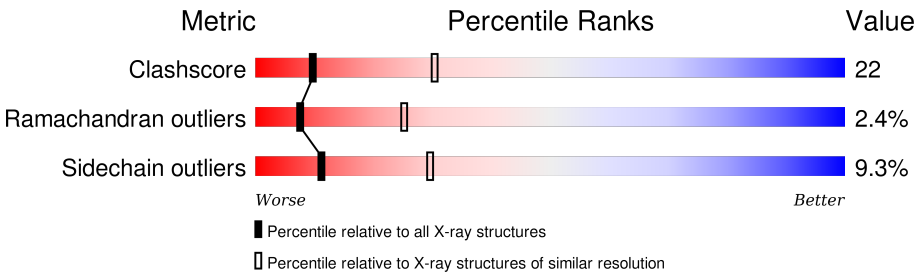
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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))
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	392	60% 32% 5% • •
1	B	392	57% 33% 7% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5828 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.

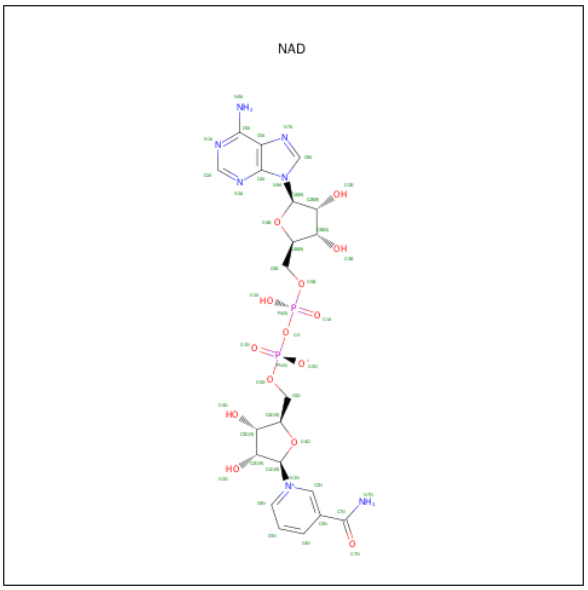
- Molecule 1 is a protein called LACTALDEHYDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	2845	1795	493	541	16	0	0	0
1	B	382	2845	1795	493	541	16	0	0	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	B	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	B	1	44	21	7	14	2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	20	20	20	0	0
			Total	O		
5	B	27	27	27	0	0

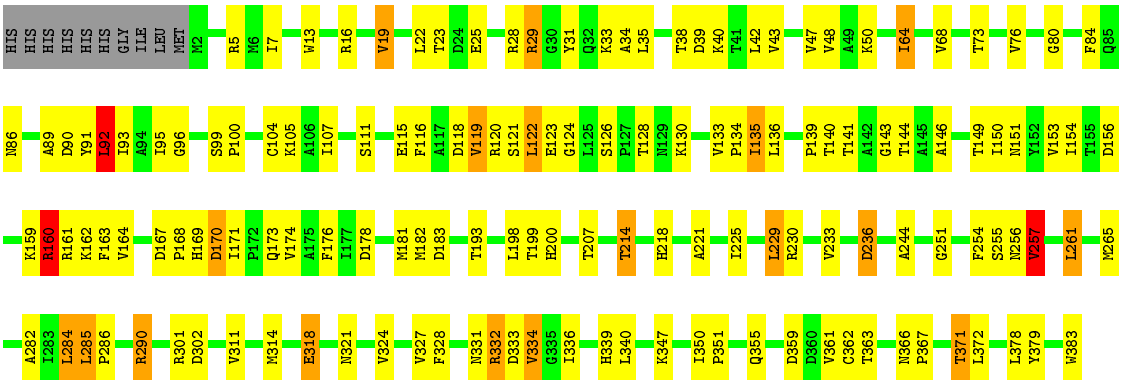
3 Residue-property plots (i)

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.

Note EDS was not executed.

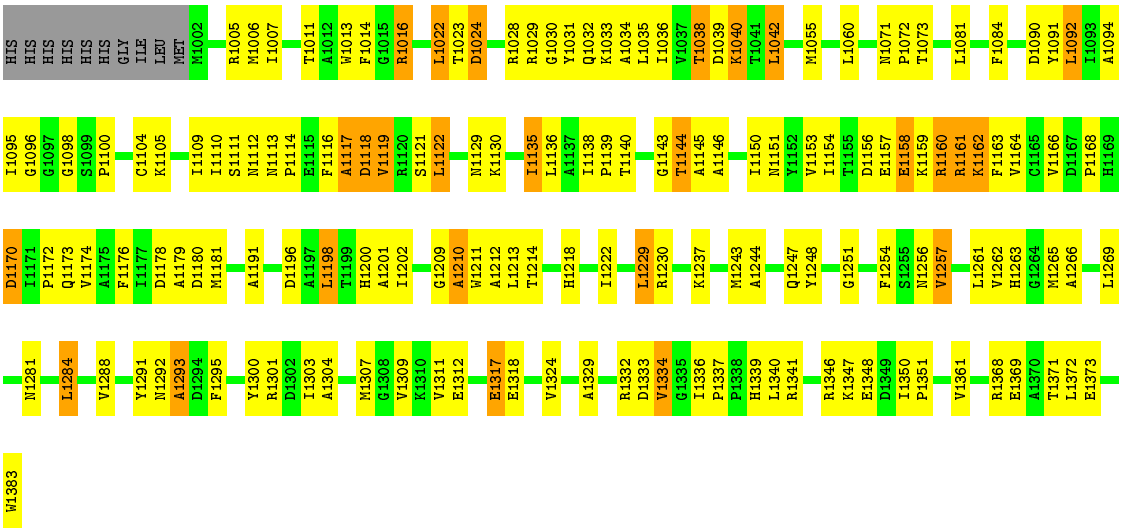
- Molecule 1: LACTALDEHYDE REDUCTASE

Chain A: 60% 32% 5%



- Molecule 1: LACTALDEHYDE REDUCTASE

Chain B: 57% 33% 7%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.42Å 109.42Å 182.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.00 – 2.85	Depositor
% Data completeness (in resolution range)	88.3 (28.00-2.85)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.251 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5828	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

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: FE2, NAD, CL

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	0.75	1/2899 (0.0%)	0.85	3/3944 (0.1%)
1	B	0.80	2/2899 (0.1%)	0.84	2/3944 (0.1%)
All	All	0.77	3/5798 (0.1%)	0.85	5/7888 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1040	LYS	CE-NZ	16.05	1.89	1.49
1	B	1040	LYS	CD-CE	8.43	1.72	1.51
1	A	362	CYS	CB-SG	-5.26	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1040	LYS	CD-CE-NZ	-6.48	96.79	111.70
1	A	170	ASP	CB-CA-C	-6.15	98.11	110.40
1	A	236	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	1092	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	92	LEU	CA-CB-CG	5.48	127.90	115.30

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	2845	0	2840	126	0
1	B	2845	0	2840	135	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	26	4	0
3	B	44	0	26	2	0
4	A	1	0	0	1	0
5	A	20	0	0	0	0
5	B	27	0	0	1	0
All	All	5828	0	5732	257	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 22.

The worst 5 of 257 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:1040:LYS:NZ	1:B:1040:LYS:CE	1.89	1.34
1:A:290:ARG:HH11	1:A:290:ARG:HG3	1.09	1.09
1:B:1104:CYS:SG	1:B:1135:ILE:HD12	2.14	0.88
1:A:38:THR:HG22	1:A:39:ASP:H	1.40	0.87
1:B:1024:ASP:HB3	1:B:1028:ARG:HH12	1.41	0.86

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	380/392 (97%)	344 (90%)	30 (8%)	6 (2%)	12 36
1	B	380/392 (97%)	342 (90%)	26 (7%)	12 (3%)	5 18
All	All	760/784 (97%)	686 (90%)	56 (7%)	18 (2%)	7 25

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	160	ARG
1	B	1119	VAL
1	B	1122	LEU
1	B	1144	THR

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	291/300 (97%)	262 (90%)	29 (10%)	9 26
1	B	291/300 (97%)	266 (91%)	25 (9%)	13 34
All	All	582/600 (97%)	528 (91%)	54 (9%)	11 29

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	ASP
1	B	1024	ASP
1	B	1317	GLU
1	A	318	GLU
1	A	334	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1071	ASN
1	B	1086	ASN
1	B	1151	ASN
1	B	1044	GLN
1	B	1112	ASN

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)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	NAD	A	1385	-	38,48,48	1.88	6 (15%)	47,73,73	2.65	10 (21%)
3	NAD	B	2385	-	38,48,48	1.91	5 (13%)	47,73,73	2.55	14 (29%)

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	NAD	A	1385	-	-	0/22/62/62	0/5/5/5
3	NAD	B	2385	-	-	0/22/62/62	0/5/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1385	NAD	PN-O2N	-2.03	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1385	NAD	C3N-C7N	2.54	1.54	1.50
3	B	2385	NAD	C3N-C7N	2.80	1.54	1.50
3	A	1385	NAD	C2A-N1A	2.81	1.39	1.33
3	B	2385	NAD	C2A-N1A	3.05	1.39	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2385	NAD	N3A-C2A-N1A	-11.36	120.20	128.89
3	A	1385	NAD	N3A-C2A-N1A	-11.09	120.41	128.89
3	B	2385	NAD	O7N-C7N-N7N	-6.30	113.72	122.59
3	A	1385	NAD	O7N-C7N-N7N	-5.60	114.71	122.59
3	A	1385	NAD	C4A-C5A-N7A	-3.03	106.69	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1385	NAD	4	0
3	B	2385	NAD	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.