



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:00 PM GMT

PDB ID : 1DLA  
Title : NOVEL NADPH-BINDING DOMAIN REVEALED BY THE CRYSTAL  
STRUCTURE OF ALDOSE REDUCTASE  
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Biellmann, J.-F.; Moras, D.  
Deposited on : 1993-02-08  
Resolution : 3.00 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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

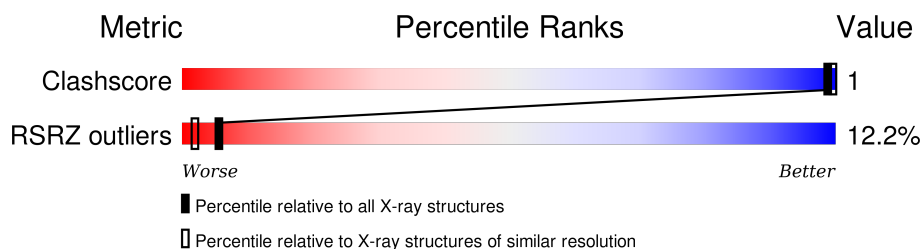
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	314	
1	B	314	
1	C	314	
1	D	314	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1242 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.

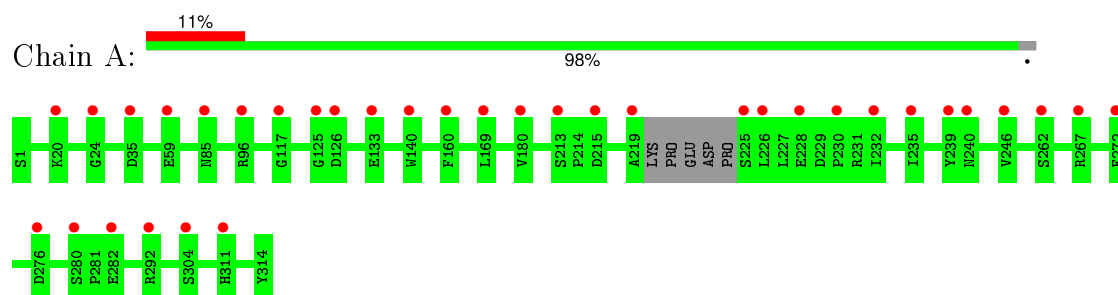
- Molecule 1 is a protein called ALDOSE REDUCTASE.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	309	Total	C	0	0	309
			309	309			
1	B	314	Total	C	0	0	314
			314	314			
1	C	311	Total	C	0	0	311
			311	311			
1	D	308	Total	C	0	0	308
			308	308			

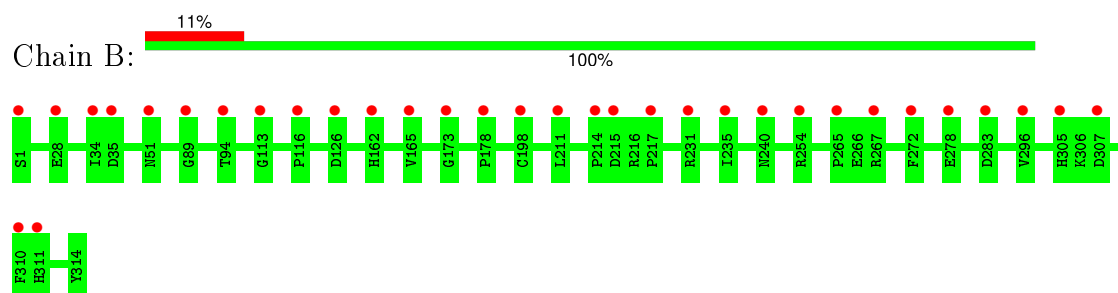
### 3 Residue-property plots [i](#)

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.

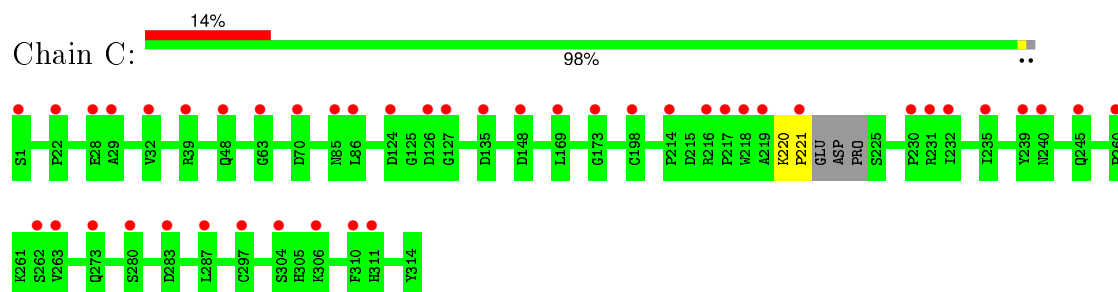
#### • Molecule 1: ALDOSE REDUCTASE



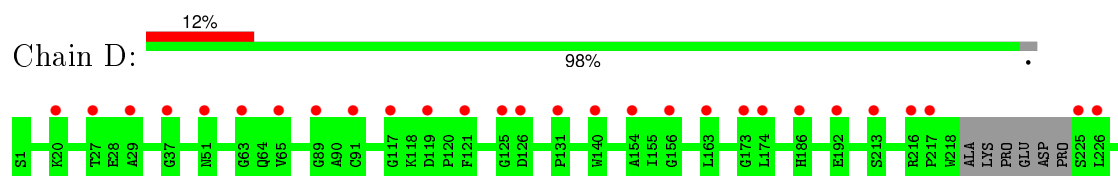
#### • Molecule 1: ALDOSE REDUCTASE

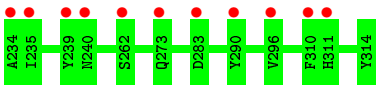


#### • Molecule 1: ALDOSE REDUCTASE



#### • Molecule 1: ALDOSE REDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.30 Å 85.90 Å 56.60 Å 102.30° 103.30° 79.00°	Depositor
Resolution (Å)	(Not available) – 3.00 30.45 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 89.9 (30.45-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.89 (at 3.00 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.219 , (Not available) 0.452 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 170.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 27129 reflections	Xtriage
$F_o, F_c$ correlation	0.42	EDS
Total number of atoms	1242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	309	0	0	0	0
1	B	314	0	0	0	0
1	C	311	0	0	1	0
1	D	308	0	0	0	0
All	All	1242	0	0	1	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 1.

All (1) 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:220:LYS:CA	1:C:221:PRO:CA	2.83	0.56

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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

### 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

### 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	309/314 (98%)	0.56	35 (11%) <b>7</b> <b>2</b>	2, 6, 20, 32	0
1	B	314/314 (100%)	0.52	33 (10%) <b>8</b> <b>3</b>	2, 5, 18, 23	0
1	C	311/314 (99%)	0.68	44 (14%) <b>4</b> <b>1</b>	2, 6, 19, 35	0
1	D	308/314 (98%)	0.51	39 (12%) <b>5</b> <b>2</b>	2, 6, 19, 28	0
All	All	1242/1256 (98%)	0.57	151 (12%) <b>5</b> <b>2</b>	2, 6, 19, 35	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	240	ASN	12.8
1	A	219	ALA	11.5
1	B	126	ASP	10.9
1	B	240	ASN	10.7
1	C	28	GLU	9.5
1	C	85	ASN	9.1
1	B	311	HIS	8.7
1	A	311	HIS	8.4
1	A	169	LEU	8.3
1	D	273	GLN	8.1
1	C	173	GLY	7.8
1	A	240	ASN	7.7
1	C	287	LEU	7.5
1	C	221	PRO	7.3
1	D	186	HIS	7.3
1	C	126	ASP	7.1
1	D	217	PRO	6.8
1	C	148	ASP	6.7
1	D	310	PHE	6.6
1	A	85	ASN	6.5
1	B	35	ASP	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	35	ASP	6.3
1	C	63	GLY	6.2
1	C	217	PRO	6.1
1	D	89	GLY	6.1
1	D	240	ASN	6.1
1	B	235	ILE	6.1
1	A	133	GLU	5.9
1	A	215	ASP	5.8
1	B	307	ASP	5.5
1	D	63	GLY	5.4
1	C	310	PHE	5.4
1	D	126	ASP	5.3
1	C	32	VAL	5.2
1	A	239	TYR	5.2
1	C	216	ARG	5.1
1	A	276	ASP	5.0
1	C	127	GLY	5.0
1	C	48	GLN	4.9
1	D	216	ARG	4.8
1	A	125	GLY	4.8
1	B	34	ILE	4.7
1	D	226	LEU	4.4
1	C	232	ILE	4.4
1	A	126	ASP	4.3
1	B	51	ASN	4.3
1	C	311	HIS	4.3
1	D	65	VAL	4.2
1	C	218	TRP	4.2
1	A	59	GLU	4.1
1	B	1	SER	4.1
1	B	265	PRO	4.0
1	B	94	THR	4.0
1	C	235	ILE	4.0
1	D	156	GLY	4.0
1	B	198	CYS	4.0
1	B	28	GLU	4.0
1	B	231	ARG	3.9
1	D	239	TYR	3.9
1	C	283	ASP	3.9
1	D	27	THR	3.9
1	B	113	GLY	3.9
1	A	280	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	131	PRO	3.8
1	D	234	ALA	3.7
1	D	311	HIS	3.7
1	A	180	VAL	3.7
1	C	214	PRO	3.7
1	A	230	PRO	3.7
1	B	305	HIS	3.7
1	D	154	ALA	3.6
1	C	239	TYR	3.6
1	C	22	PRO	3.6
1	C	219	ALA	3.6
1	A	96	ARG	3.6
1	D	121	PHE	3.6
1	D	29	ALA	3.5
1	C	306	LYS	3.5
1	C	297	CYS	3.5
1	B	89	GLY	3.5
1	C	39	ARG	3.5
1	B	214	PRO	3.4
1	B	215	ASP	3.4
1	C	198	CYS	3.4
1	B	267	ARG	3.3
1	A	228	GLU	3.2
1	C	262	SER	3.2
1	A	226	LEU	3.2
1	C	124	ASP	3.1
1	A	272	PHE	3.1
1	A	24	GLY	3.1
1	C	280	SER	3.0
1	D	91	CYS	3.0
1	A	235	ILE	3.0
1	D	296	VAL	3.0
1	D	173	GLY	3.0
1	C	86	LEU	3.0
1	A	225	SER	2.9
1	C	304	SER	2.9
1	D	213	SER	2.9
1	D	163	LEU	2.9
1	C	231	ARG	2.8
1	D	117	GLY	2.8
1	A	304	SER	2.8
1	D	225	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	246	VAL	2.7
1	B	162	HIS	2.7
1	C	263	VAL	2.7
1	C	169	LEU	2.6
1	D	119	ASP	2.6
1	C	29	ALA	2.6
1	B	254	ARG	2.6
1	B	278	GLU	2.6
1	D	192	GLU	2.6
1	C	230	PRO	2.5
1	D	235	ILE	2.5
1	B	217	PRO	2.5
1	C	260	PRO	2.5
1	C	273	GLN	2.5
1	A	232	ILE	2.5
1	D	20	LYS	2.5
1	A	117	GLY	2.4
1	D	125	GLY	2.4
1	A	20	LYS	2.4
1	D	140	TRP	2.4
1	B	165	VAL	2.4
1	C	1	SER	2.3
1	D	51	ASN	2.3
1	B	173	GLY	2.3
1	A	262	SER	2.3
1	B	283	ASP	2.3
1	A	140	TRP	2.3
1	B	211	LEU	2.3
1	C	70	ASP	2.3
1	B	178	PRO	2.3
1	D	37	GLY	2.2
1	C	245	GLN	2.2
1	B	296	VAL	2.2
1	A	160	PHE	2.2
1	D	262	SER	2.2
1	D	283	ASP	2.2
1	C	135	ASP	2.2
1	A	213	SER	2.2
1	D	174	LEU	2.2
1	B	272	PHE	2.2
1	B	310	PHE	2.2
1	A	292	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	267	ARG	2.1
1	B	116	PRO	2.1
1	A	282	GLU	2.1
1	D	290	TYR	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.