



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:00 PM GMT

PDB ID : 1DLA  
Title : NOVEL NADPH-BINDING DOMAIN REVEALED BY THE CRYSTAL  
STRUCTURE OF ALDOSE REDUCTASE  
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Deposited on : 1993-02-08  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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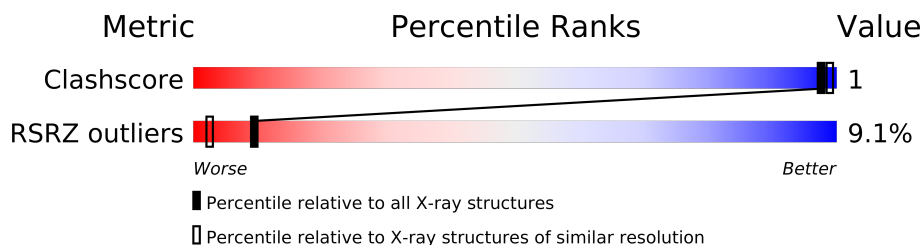
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance





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	79885	1594 (3.00-3.00)
RSRZ outliers	66119	1217 (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. 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	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 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.

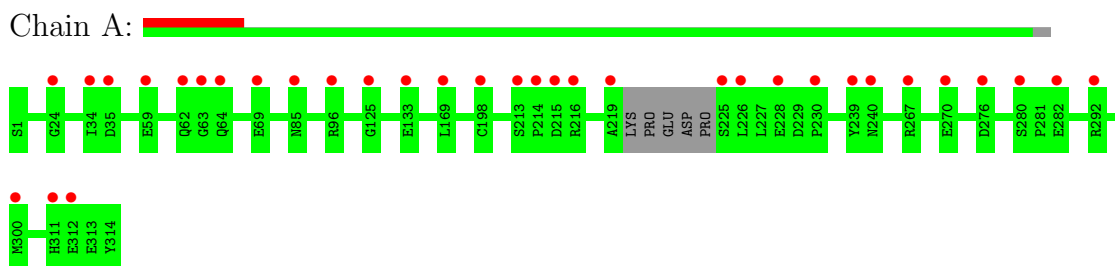
- Molecule 1 is a protein called ALDOSE REDUCTASE.

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

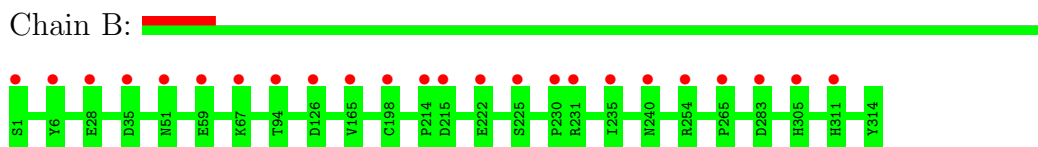
### 3 Residue-property plots

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.

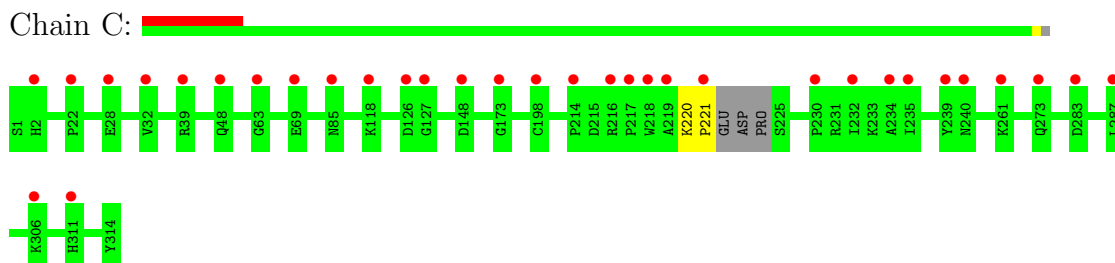
#### • Molecule 1: ALDOSE REDUCTASE



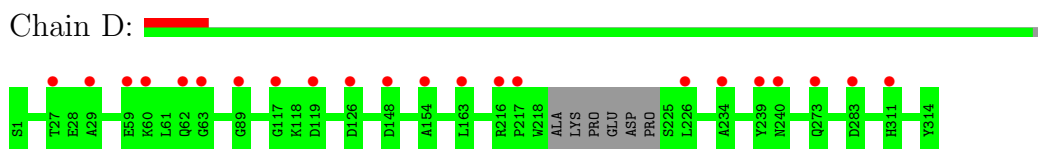
#### • Molecule 1: ALDOSE REDUCTASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	81.30Å 85.90Å 56.60Å 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) 95.2 (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 3.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.219 , (Not available) 0.476 , (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> )	0.14 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 27129 reflections	Xtriage
$F_o, F_c$ correlation	0.40	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.

## 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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	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

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 1.

All (1) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

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

### 5.3.2 Protein sidechains ⓘ

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

### 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, 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%)	0.71	34 (11%) <b>6</b> <b>2</b>	2, 6, 20, 32	0
1	B	314/314 (100%)	0.54	24 (7%) <b>14</b> <b>3</b>	2, 5, 18, 23	0
1	C	311/314 (99%)	0.63	33 (10%) <b>7</b> <b>2</b>	2, 6, 19, 35	0
1	D	308/314 (98%)	0.51	22 (7%) <b>16</b> <b>4</b>	2, 6, 19, 28	0
All	All	1242/1256 (98%)	0.60	113 (9%) <b>9</b> <b>2</b>	2, 6, 19, 35	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	GLU	11.8
1	A	219	ALA	11.7
1	C	28	GLU	9.7
1	A	311	HIS	9.5
1	D	89	GLY	9.1
1	C	240	ASN	9.0
1	B	126	ASP	7.9
1	B	35	ASP	7.5
1	B	240	ASN	7.2
1	B	311	HIS	6.3
1	D	240	ASN	5.9
1	A	292	ARG	5.8
1	A	169	LEU	5.7
1	A	282	GLU	5.5
1	C	287	LEU	5.3
1	C	85	ASN	5.2
1	A	59	GLU	5.2
1	A	35	ASP	5.1
1	C	216	ARG	4.9
1	D	273	GLN	4.8
1	A	215	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	235	ILE	4.6
1	C	221	PRO	4.6
1	C	32	VAL	4.6
1	B	265	PRO	4.5
1	C	217	PRO	4.4
1	D	239	TYR	4.4
1	D	216	ARG	4.4
1	A	96	ARG	4.4
1	C	173	GLY	4.3
1	A	239	TYR	4.2
1	D	27	THR	4.2
1	C	311	HIS	4.2
1	C	39	ARG	4.2
1	B	94	THR	4.1
1	A	64	GLN	4.1
1	A	133	GLU	4.0
1	C	126	ASP	4.0
1	D	226	LEU	3.9
1	C	230	PRO	3.8
1	D	217	PRO	3.8
1	B	283	ASP	3.6
1	A	226	LEU	3.6
1	B	230	PRO	3.6
1	B	214	PRO	3.5
1	D	311	HIS	3.5
1	A	214	PRO	3.5
1	A	230	PRO	3.4
1	B	231	ARG	3.4
1	C	239	TYR	3.4
1	C	232	ILE	3.4
1	A	276	ASP	3.4
1	D	234	ALA	3.3
1	B	59	GLU	3.3
1	B	215	ASP	3.3
1	B	305	HIS	3.2
1	A	85	ASN	3.1
1	A	24	GLY	3.1
1	C	261	LYS	3.1
1	C	218	TRP	3.1
1	C	235	ILE	3.0
1	A	280	SER	3.0
1	D	154	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	125	GLY	3.0
1	A	213	SER	2.9
1	D	126	ASP	2.9
1	C	118	LYS	2.9
1	C	198	CYS	2.8
1	A	300	MET	2.8
1	C	48	GLN	2.8
1	A	62	GLN	2.8
1	D	163	LEU	2.8
1	A	240	ASN	2.7
1	D	59	GLU	2.7
1	C	69	GLU	2.6
1	B	51	ASN	2.6
1	A	267	ARG	2.6
1	A	270	GLU	2.6
1	B	225	SER	2.6
1	B	28	GLU	2.6
1	C	273	GLN	2.6
1	C	2	HIS	2.5
1	A	63	GLY	2.5
1	C	219	ALA	2.4
1	B	254	ARG	2.4
1	C	22	PRO	2.4
1	D	62	GLN	2.4
1	D	63	GLY	2.4
1	C	283	ASP	2.4
1	C	148	ASP	2.4
1	A	312	GLU	2.4
1	D	60	LYS	2.4
1	B	222	GLU	2.4
1	B	67	LYS	2.3
1	B	198	CYS	2.3
1	A	225	SER	2.3
1	A	198	CYS	2.3
1	A	216	ARG	2.3
1	C	214	PRO	2.2
1	C	306	LYS	2.2
1	C	63	GLY	2.2
1	B	165	VAL	2.2
1	A	69	GLU	2.2
1	D	119	ASP	2.2
1	D	148	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	283	ASP	2.2
1	C	234	ALA	2.1
1	D	117	GLY	2.1
1	C	127	GLY	2.1
1	D	29	ALA	2.1
1	B	1	SER	2.1
1	B	6	TYR	2.1
1	A	34	ILE	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.