



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:09 pm GMT

PDB ID : 1DLA  
Title : NOVEL NADPH-BINDING DOMAIN REVEALED BY THE CRYSTAL  
STRUCTURE OF ALDOSE REDUCTASE  
Authors : Rondeau, J.-M.; Tete-Favier, F.; Podjarny, A.; Reymann, J.-M.; Barth, P.;  
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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

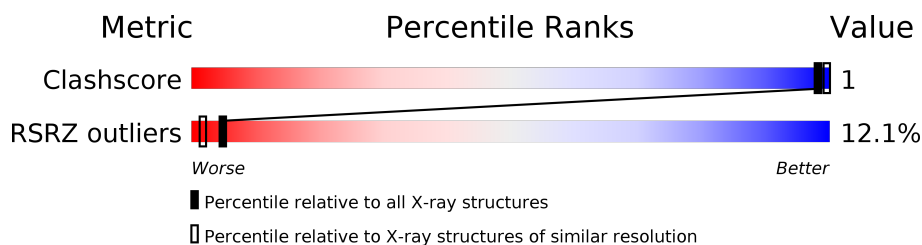
# 1 Overall quality at a glance

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	112137	2037 (3.00-3.00)
RSRZ outliers	101464	1716 (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.

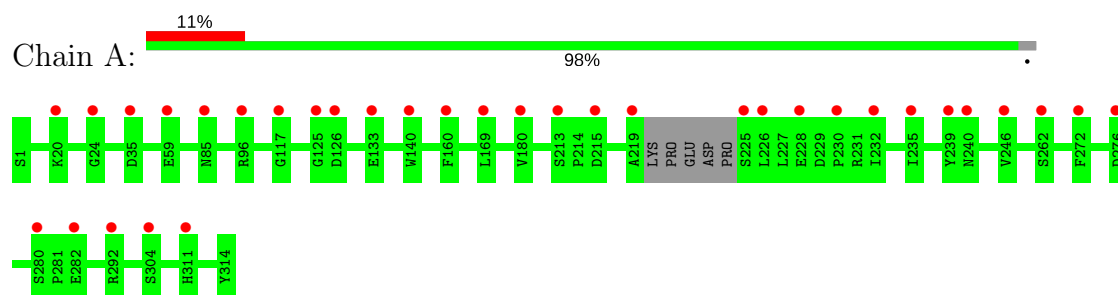
- Molecule 1 is a protein called ALDOSE REDUCTASE.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	309	Total 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

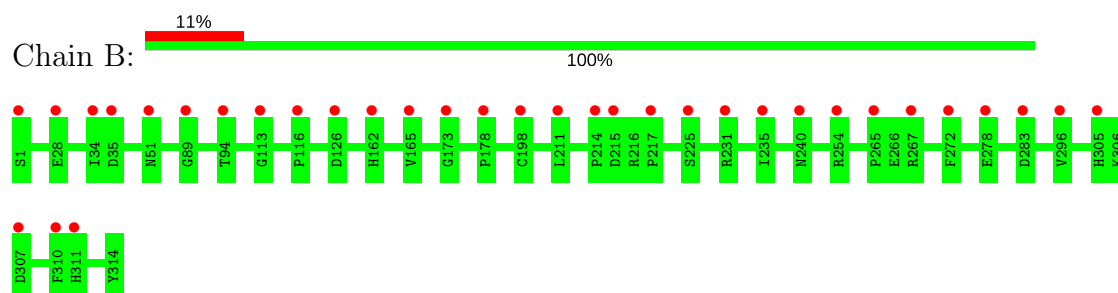
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

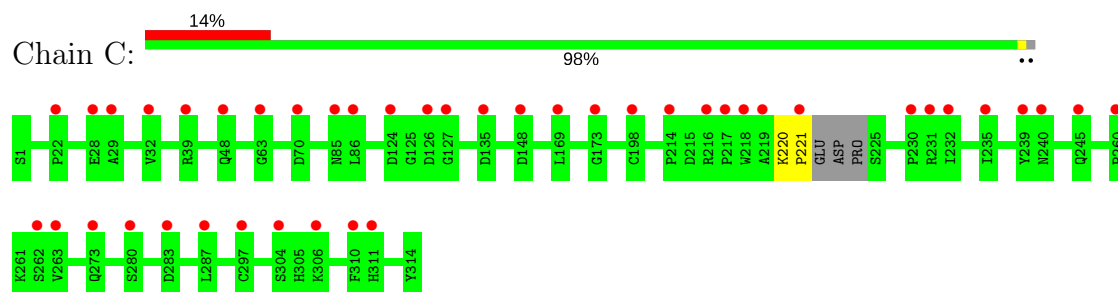
#### • Molecule 1: ALDOSE REDUCTASE



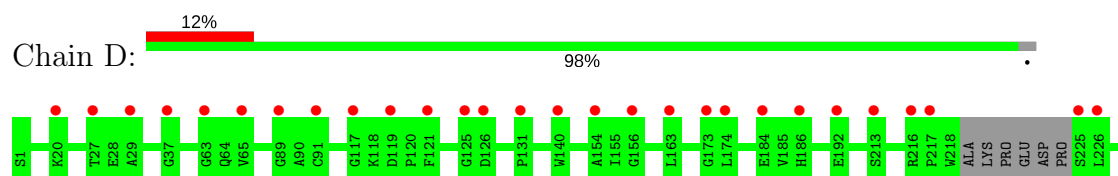
#### • Molecule 1: ALDOSE REDUCTASE

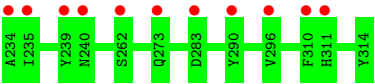


#### • Molecule 1: ALDOSE REDUCTASE



#### • 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) 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 3.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.219 , (Not available) (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	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> )	0.28 , 151.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.43	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, 0.333 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).

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 [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	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%)	0.58	34 (11%) 6 2	2, 6, 20, 32	0
1	B	314/314 (100%)	0.54	34 (10%) 6 2	2, 5, 18, 23	0
1	C	311/314 (99%)	0.68	43 (13%) 3 1	2, 6, 19, 35	0
1	D	308/314 (98%)	0.53	39 (12%) 4 2	2, 6, 19, 28	0
All	All	1242/1256 (98%)	0.58	150 (12%) 5 2	2, 6, 19, 35	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	240	ASN	12.7
1	B	126	ASP	12.0
1	A	219	ALA	11.1
1	C	85	ASN	10.2
1	B	240	ASN	9.7
1	C	28	GLU	9.7
1	B	311	HIS	8.8
1	D	186	HIS	8.5
1	A	311	HIS	8.2
1	A	169	LEU	8.0
1	D	273	GLN	7.8
1	A	240	ASN	7.7
1	C	126	ASP	7.7
1	C	287	LEU	7.5
1	C	173	GLY	7.5
1	A	35	ASP	7.3
1	D	310	PHE	6.9
1	C	148	ASP	6.8
1	D	217	PRO	6.8
1	A	85	ASN	6.8
1	C	221	PRO	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	240	ASN	6.6
1	B	35	ASP	6.2
1	B	235	ILE	6.2
1	D	126	ASP	6.1
1	A	215	ASP	6.0
1	C	217	PRO	5.9
1	C	63	GLY	5.9
1	D	89	GLY	5.9
1	D	63	GLY	5.8
1	A	239	TYR	5.8
1	A	133	GLU	5.7
1	C	310	PHE	5.6
1	C	216	ARG	5.6
1	A	125	GLY	5.3
1	C	48	GLN	5.2
1	B	307	ASP	5.1
1	A	276	ASP	5.1
1	C	32	VAL	5.1
1	C	127	GLY	5.0
1	B	34	ILE	4.7
1	D	216	ARG	4.6
1	C	218	TRP	4.5
1	B	265	PRO	4.5
1	B	51	ASN	4.4
1	D	226	LEU	4.4
1	D	239	TYR	4.3
1	B	1	SER	4.3
1	C	311	HIS	4.3
1	A	126	ASP	4.2
1	C	235	ILE	4.2
1	C	232	ILE	4.1
1	D	156	GLY	4.1
1	C	283	ASP	4.0
1	B	94	THR	4.0
1	B	113	GLY	4.0
1	D	27	THR	4.0
1	D	154	ALA	4.0
1	A	230	PRO	4.0
1	B	231	ARG	4.0
1	A	59	GLU	4.0
1	D	131	PRO	4.0
1	D	65	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	198	CYS	3.8
1	A	280	SER	3.8
1	C	239	TYR	3.8
1	C	214	PRO	3.8
1	C	219	ALA	3.8
1	B	28	GLU	3.7
1	D	121	PHE	3.7
1	A	180	VAL	3.6
1	A	228	GLU	3.6
1	B	305	HIS	3.6
1	D	29	ALA	3.6
1	B	214	PRO	3.5
1	C	306	LYS	3.5
1	C	262	SER	3.5
1	C	22	PRO	3.4
1	B	89	GLY	3.4
1	A	96	ARG	3.4
1	B	215	ASP	3.4
1	A	226	LEU	3.4
1	D	311	HIS	3.3
1	C	297	CYS	3.3
1	D	234	ALA	3.3
1	A	272	PHE	3.3
1	C	39	ARG	3.3
1	D	213	SER	3.2
1	D	91	CYS	3.2
1	C	124	ASP	3.1
1	A	225	SER	3.1
1	D	296	VAL	3.1
1	D	163	LEU	3.1
1	C	280	SER	3.0
1	C	198	CYS	3.0
1	D	225	SER	3.0
1	B	267	ARG	2.9
1	C	86	LEU	2.9
1	B	211	LEU	2.9
1	B	278	GLU	2.9
1	A	235	ILE	2.8
1	A	246	VAL	2.8
1	C	263	VAL	2.8
1	C	231	ARG	2.8
1	C	304	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	24	GLY	2.8
1	D	173	GLY	2.8
1	A	304	SER	2.8
1	C	230	PRO	2.8
1	C	260	PRO	2.7
1	D	235	ILE	2.7
1	D	117	GLY	2.7
1	C	169	LEU	2.6
1	B	217	PRO	2.6
1	B	162	HIS	2.6
1	D	174	LEU	2.5
1	C	273	GLN	2.5
1	B	310	PHE	2.5
1	A	262	SER	2.5
1	D	262	SER	2.5
1	D	140	TRP	2.5
1	C	29	ALA	2.5
1	B	296	VAL	2.5
1	D	37	GLY	2.4
1	D	125	GLY	2.4
1	B	254	ARG	2.4
1	B	165	VAL	2.4
1	D	192	GLU	2.4
1	D	119	ASP	2.3
1	C	70	ASP	2.3
1	B	116	PRO	2.3
1	B	178	PRO	2.3
1	A	117	GLY	2.3
1	B	283	ASP	2.3
1	C	245	GLN	2.2
1	A	232	ILE	2.2
1	C	135	ASP	2.2
1	A	20	LYS	2.2
1	B	173	GLY	2.2
1	D	20	LYS	2.2
1	A	160	PHE	2.2
1	B	272	PHE	2.2
1	A	282	GLU	2.1
1	A	213	SER	2.1
1	A	292	ARG	2.1
1	D	184	GLU	2.1
1	A	140	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	283	ASP	2.1
1	D	290	TYR	2.0
1	B	225	SER	2.0

## 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.