



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:05 AM GMT

PDB ID : 2PDY  
Title : Human aldose reductase double mutant S302R-C303D complexed with fidarestat.  
Authors : Steuber, H.; Heine, A.; Klebe, G.  
Deposited on : 2007-04-01  
Resolution : 1.65 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

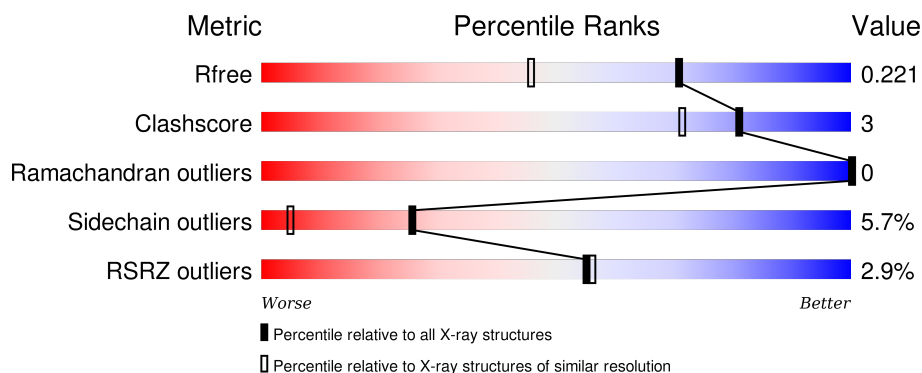
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	316	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2919 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.

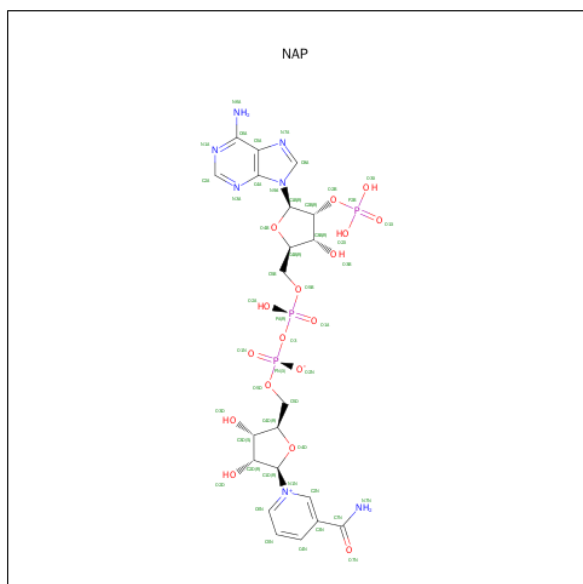
- Molecule 1 is a protein called Aldose reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2536	1628	429	468	11	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

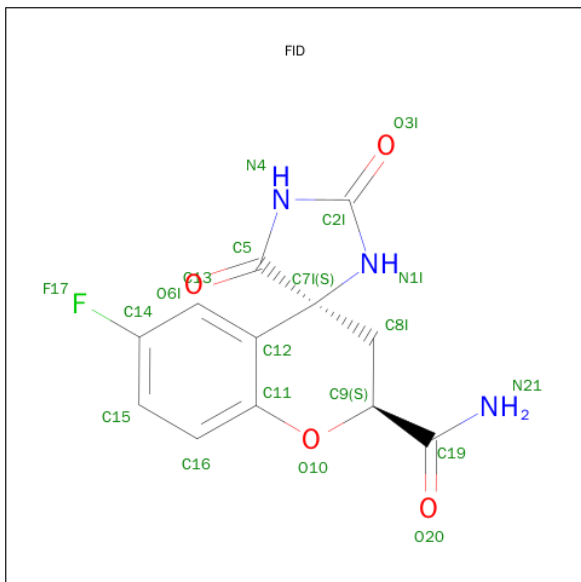
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ILE	LEU	CONFLICT	UNP P15121
A	302	ARG	SER	ENGINEERED	UNP P15121
A	303	ASP	CYS	ENGINEERED	UNP P15121

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is (2S,4S)-2-AMINOFORMYL-6-FLUORO-SPIRO[CHROMAN-4,4'-IMIDAZOLIDINE]-2',5'-DIONE (three-letter code: FID) (formula: C<sub>12</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			20	12	1	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	315	Total	O	0	0
			315	315		



- Molecule 1: Aldose reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.41Å 66.71Å 47.51Å 90.00° 91.56° 90.00°	Depositor
Resolution (Å)	30.00 – 1.65 20.18 – 1.65	Depositor EDS
% Data completeness (in resolution range)	89.2 (30.00-1.65) 89.3 (20.18-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 1.65Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.160 , 0.224 0.165 , 0.221	Depositor DCC
$R_{free}$ test set	1645 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.9	EDS
Estimated twinning fraction	0.002 for -l,k,h 0.035 for -h,-k,l 0.025 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33366 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, FID

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	0.44	0/2610	1.18	14/3544 (0.4%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	TYR	CA-CB-CG	9.20	130.88	113.40
1	A	69	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	307	LYS	C-N-CA	7.96	141.59	121.70
1	A	302	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	209	TYR	CB-CG-CD1	6.98	125.19	121.00
1	A	309	TYR	CB-CG-CD1	6.87	125.12	121.00
1	A	283	GLN	CG-CD-OE1	6.41	134.43	121.60
1	A	209	TYR	CG-CD1-CE1	6.37	126.40	121.30
1	A	40	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	288	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	268	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	126	GLU	CA-CB-CG	5.77	126.09	113.40
1	A	232	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	39	TYR	CA-CB-CG	5.54	123.92	113.40

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	2536	0	2546	17	0
2	A	48	0	25	2	0
3	A	20	0	10	0	0
4	A	315	0	0	7	0
All	All	2919	0	2581	17	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 3.

All (17) 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:A:274:LYS:HE3	4:A:679:HOH:O	1.85	0.77
1:A:85:LYS:HE3	4:A:655:HOH:O	1.95	0.67
1:A:244[B]:THR:HG22	4:A:648:HOH:O	2.00	0.61
1:A:189:TYR:CE2	1:A:225:PRO:HB2	2.39	0.58
1:A:185:GLU:OE2	1:A:187:HIS:HE1	1.86	0.58
1:A:302:ARG:HD2	4:A:795:HOH:O	2.04	0.57
1:A:181:VAL:HA	1:A:205:VAL:O	2.09	0.53
1:A:20:TRP:CE3	1:A:21:LYS:HE3	2.45	0.51
1:A:215:PRO:HD2	2:A:500:NAP:H4B	1.92	0.51
1:A:262:LYS:O	2:A:500:NAP:H8A	2.14	0.48
1:A:7:ASN:ND2	4:A:689:HOH:O	2.49	0.45
1:A:85:LYS:HG3	4:A:655:HOH:O	2.16	0.45
1:A:242:LYS:HE3	1:A:246:GLN:OE1	2.19	0.43
1:A:41:HIS:HA	1:A:73:PHE:O	2.21	0.41
1:A:194:LYS:NZ	4:A:705:HOH:O	2.54	0.40
1:A:217:ARG:CD	1:A:297:VAL:HG13	2.51	0.40
1:A:96:LEU:HD23	1:A:104:LEU:HD13	2.04	0.40

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	316/316 (100%)	314 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	283/281 (101%)	267 (94%)	16 (6%)	25	5

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	LEU
1	A	7	ASN
1	A	50	ASN
1	A	60	GLU
1	A	85	LYS
1	A	104	LEU
1	A	119	LYS
1	A	126	GLU
1	A	136	ASN
1	A	168	MET
1	A	170	LEU
1	A	194	LYS
1	A	209	TYR
1	A	288	LEU
1	A	293	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	50	ASN
1	A	136	ASN
1	A	182	ASN
1	A	187	HIS
1	A	283	GLN

### 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](#)

2 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	NAP	A	500	-	42,52,52	1.48	6 (14%)	54,80,80	2.02	16 (29%)
3	FID	A	600	-	20,22,22	0.70	0	23,34,34	2.00	8 (34%)

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	NAP	A	500	-	-	0/27/67/67	0/5/5/5
3	FID	A	600	-	-	0/4/34/34	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAP	C5B-C4B	2.38	1.59	1.51
2	A	500	NAP	C6N-N1N	2.48	1.42	1.35
2	A	500	NAP	C2A-N1A	2.69	1.39	1.33
2	A	500	NAP	C4A-N3A	2.79	1.39	1.35
2	A	500	NAP	O4D-C1D	3.07	1.45	1.41
2	A	500	NAP	C2A-N3A	3.17	1.37	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	NAP	N3A-C2A-N1A	-8.16	122.65	128.89
2	A	500	NAP	C3N-C7N-N7N	-3.66	113.81	117.82
3	A	600	FID	C5-N4-C2I	-3.57	108.25	111.60
3	A	600	FID	C16-C11-C12	-3.47	116.24	121.37
2	A	500	NAP	O7N-C7N-C3N	-3.30	115.99	119.59
2	A	500	NAP	O4D-C1D-N1N	-3.03	104.80	108.13
3	A	600	FID	O3I-C2I-N4	-2.80	120.39	125.44
2	A	500	NAP	C3N-C2N-N1N	-2.69	117.26	120.36
2	A	500	NAP	O3-PA-O5B	-2.69	95.80	102.94
2	A	500	NAP	O4D-C4D-C3D	-2.06	101.00	105.15
2	A	500	NAP	O3D-C3D-C2D	2.12	118.73	111.83
2	A	500	NAP	P2B-O2B-C2B	2.16	126.73	121.56
3	A	600	FID	C8I-C7I-C5	2.17	114.20	109.65
2	A	500	NAP	O2A-PA-O1A	2.31	125.03	112.53
3	A	600	FID	C8I-C7I-N1I	2.49	116.51	112.09
2	A	500	NAP	C2N-C3N-C4N	2.91	121.53	118.29
2	A	500	NAP	PN-O3-PA	2.94	140.98	132.73
2	A	500	NAP	O3X-P2B-O2X	2.95	118.62	107.38
3	A	600	FID	C11-O10-C9	2.96	122.49	115.51
2	A	500	NAP	C2A-N1A-C6A	2.99	124.11	118.77
2	A	500	NAP	O7N-C7N-N7N	3.07	126.91	122.59
2	A	500	NAP	C4B-O4B-C1B	3.83	113.92	109.72
3	A	600	FID	C13-C12-C11	3.84	122.52	116.67
3	A	600	FID	N4-C2I-N1I	4.01	112.22	107.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAP	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](#)

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	315/316 (99%)	0.46	9 (2%) 55 56	11, 17, 33, 59	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	PRO	5.2
1	A	126	GLU	4.0
1	A	315	PHE	3.5
1	A	314	GLU	3.4
1	A	1	ALA	2.6
1	A	276	PHE	2.3
1	A	313	GLU	2.3
1	A	135	THR	2.2
1	A	134[A]	ASP	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](#)

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( $\text{\AA}^2$ )	Q<0.9
3	FID	A	600	20/20	0.93	0.09	-0.36	11,14,17,19	0
2	NAP	A	500	48/48	0.97	0.08	-1.23	9,13,17,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.