



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 09:26 PM GMT

PDB ID : 2IKI  
Title : Human aldose reductase complexed with halogenated IDD-type inhibitor  
Authors : Steuber, H.; Koch, C.; Heine, A.; Klebe, G.  
Deposited on : 2006-10-02  
Resolution : 1.47 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>

---

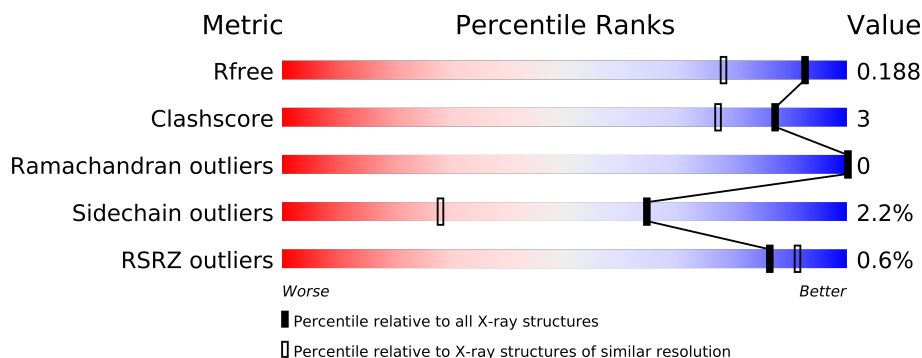
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.47 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))
$R_{free}$	66092	2222 (1.50-1.46)
Clashscore	79885	2555 (1.50-1.46)
Ramachandran outliers	78287	2496 (1.50-1.46)
Sidechain outliers	78261	2494 (1.50-1.46)
RSRZ outliers	66119	2223 (1.50-1.46)

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	316	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2975 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.

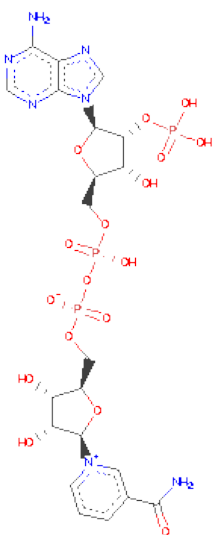
- Molecule 1 is a protein called Aldose reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	2497	1603	420	461	13	0	6	0

There is a discrepancy between the modelled and reference sequences:

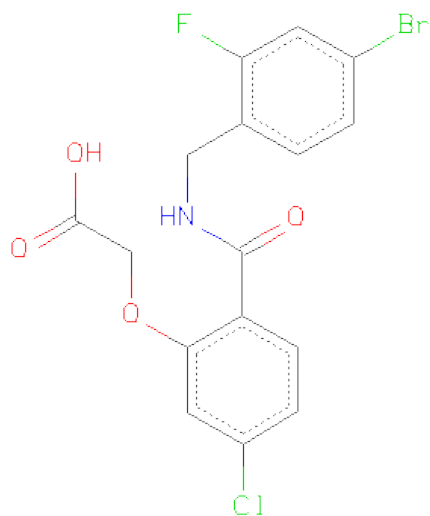
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ILE	LEU	SEE REMARK 999	UNP P15121

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

- Molecule 3 is (2-([(4-BROMO-2-FLUOROBENZYL)AMINO]CARBONYL}-5-CHLOROPHENOXY)ACETICACID (three-letter code: 388) (formula:  $C_{16}H_{12}BrClFNO_4$ ).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	F	N	O	0	0
			24	1	16	1	1	1	4		

- Molecule 4 is water.

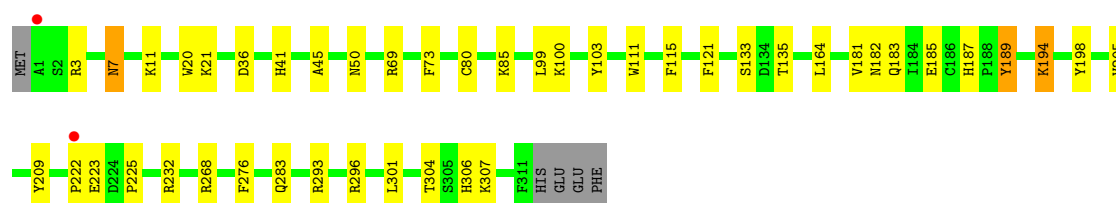
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	406	Total	O	0	0
			406	406		

### 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

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.36Å 66.80Å 47.32Å 90.00° 92.37° 90.00°	Depositor
Resolution (Å)	25.00 – 1.47 24.12 – 1.47	Depositor EDS
% Data completeness (in resolution range)	89.8 (25.00-1.47) 89.3 (24.12-1.47)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.31 (at 1.47Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.148 , 0.183 0.157 , 0.188	Depositor DCC
$R_{free}$ test set	2324 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.5	EDS
Estimated twinning fraction	0.004 for -l,k,h 0.028 for -h,-k,l 0.022 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46658 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 388, NAP

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	0.57	0/2581	1.37	24/3506 (0.7%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	THR	C-N-CA	10.92	148.99	121.70
1	A	268	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	A	189	TYR	CB-CG-CD1	10.03	127.02	121.00
1	A	121	PHE	CB-CG-CD2	9.40	127.38	120.80
1	A	283	GLN	CG-CD-OE1	8.68	138.96	121.60
1	A	209	TYR	CA-CB-CG	8.36	129.28	113.40
1	A	69	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	306	HIS	CG-ND1-CE1	7.67	118.94	108.20
1	A	276	PHE	CB-CG-CD1	6.83	125.58	120.80
1	A	307	LYS	C-N-CA	6.68	138.41	121.70
1	A	296	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	A	121	PHE	CD1-CG-CD2	-6.28	110.14	118.30
1	A	115	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	A	232	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	36	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	198	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	A	194	LYS	CA-CB-CG	5.84	126.24	113.40
1	A	301	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	268	ARG	NH1-CZ-NH2	5.66	125.63	119.40
1	A	103	TYR	CB-CG-CD1	5.64	124.38	121.00
1	A	209	TYR	CG-CD1-CE1	5.52	125.71	121.30
1	A	293	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	45	ALA	N-CA-CB	5.39	117.65	110.10
1	A	189	TYR	CB-CG-CD2	-5.22	117.87	121.00

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	2497	0	2513	13	0
2	A	48	0	25	1	0
3	A	24	0	11	0	0
4	A	406	0	0	1	0
All	All	2975	0	2549	13	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 3.

All (13) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:PRO:HG2	1:A:223:GLU:OE1	1.94	0.68
1:A:185:GLU:OE2	1:A:187:HIS:HE1	1.89	0.56
1:A:20:TRP:CE3	1:A:21:LYS:HE3	2.43	0.53
1:A:3:ARG:NH2	1:A:11:LYS:HD2	2.24	0.52
1:A:189:TYR:CE2	1:A:225:PRO:HB2	2.45	0.51
1:A:20:TRP:CD2	1:A:21:LYS:HE3	2.49	0.47
1:A:133[A]:SER:OG	1:A:135:THR:HG23	2.15	0.47
1:A:181:VAL:HA	1:A:205:VAL:O	2.18	0.44
1:A:41:HIS:HA	1:A:73:PHE:O	2.19	0.43
1:A:7:ASN:ND2	4:A:1059:HOH:O	2.53	0.42
1:A:183:GLN:OE1	2:A:500:NAP:H2N	2.20	0.41
1:A:80:CYS:SG	1:A:111:TRP:HB2	2.61	0.40
1:A:99:LEU:O	1:A:100:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	315/316 (100%)	311 (99%)	4 (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	282/281 (100%)	276 (98%)	6 (2%)	66	30

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	50	ASN
1	A	85	LYS
1	A	164	LEU
1	A	182	ASN
1	A	194	LYS

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	182	ASN
1	A	187	HIS
1	A	200	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	283	GLN

### 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 ⓘ

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	-	52,52,52	1.30	7 (13%)	80,80,80	1.53	11 (13%)
3	388	A	600	-	25,25,25	1.25	3 (12%)	34,34,34	1.33	5 (14%)

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	-	-	0/35/67/67	0/3/5/5
3	388	A	600	-	-	0/14/14/14	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	388	O24-C22	3.14	1.33	1.22
2	A	500	NAP	C2A-N1A	2.70	1.39	1.33
3	A	600	388	C6-C7	2.49	1.42	1.37
2	A	500	NAP	C2N-N1N	2.49	1.38	1.35
2	A	500	NAP	O4D-C1D	2.49	1.45	1.41
2	A	500	NAP	P2B-O1X	2.27	1.58	1.51
3	A	600	388	O23-C22	-2.26	1.22	1.30
2	A	500	NAP	C2A-N3A	2.15	1.36	1.32
2	A	500	NAP	C4N-C3N	2.15	1.43	1.39
2	A	500	NAP	C6N-N1N	2.14	1.41	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	NAP	N3A-C2A-N1A	-4.90	124.61	128.71
2	A	500	NAP	C8A-N9A-C4A	-4.31	103.61	106.90
2	A	500	NAP	O4D-C1D-N1N	-4.18	103.67	107.95
2	A	500	NAP	C6A-C5A-C4A	3.06	122.87	117.25
3	A	600	388	C1-C2-C7	-2.82	116.05	121.20
2	A	500	NAP	O3X-P2B-O2B	-2.68	99.37	107.09
2	A	500	NAP	O4B-C1B-C2B	-2.61	104.51	106.95
3	A	600	388	C6-C7-C2	-2.60	120.46	124.16
3	A	600	388	O23-C22-C21	2.60	125.74	113.24
2	A	500	NAP	O3X-P2B-O2X	2.54	117.49	107.61
2	A	500	NAP	N3A-C4A-N9A	2.30	129.59	125.43
2	A	500	NAP	C5A-C6A-N6A	2.23	125.76	120.72
2	A	500	NAP	C8A-N9A-C1B	2.20	130.72	126.38
3	A	600	388	C1-C2-C3	2.13	125.69	121.02
3	A	600	388	C15-C8-C11	-2.12	122.85	126.17
2	A	500	NAP	O4D-C4D-C3D	-2.03	101.05	105.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	311/316 (98%)	-0.19	2 (0%) 86 91	7, 11, 24, 53	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	PRO	3.2
1	A	1	ALA	3.0

### 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAP	A	500	48/48	0.06	-1.26	5,9,11,14	0
3	388	A	600	24/24	0.05	-2.05	7,9,11,11	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.