

Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 - 07:00 AM EDT

PDB ID	:	2IQD
Title	:	Crystal Structure of Aldose Reductase complexed with Lipoic Acid
Authors	:	Harrison, D.H.T.; Carlson, E.; Pape, E.; Brownlee, J.M.
Deposited on		
Resolution	:	2.00 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

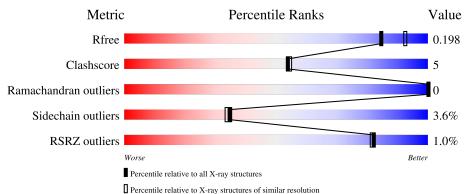
Xtriage (Phenix) EDS buster-report	: : :	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.35 1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019)
	: :	0

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	А	315	86%	12%	••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LPA	А	351	-	Х	-	-



2 Entry composition (i)

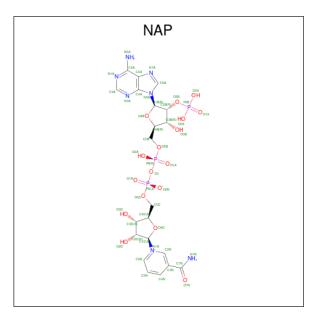
There are 4 unique types of molecules in this entry. The entry contains 2731 atoms, of which 0 are hydrogens and 0 are deuteriums.

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		At	oms			ZeroOcc	AltConf	Trace
1	А	315	Total 2517	C 1617	N 425	O 463	S 12	0	0	0

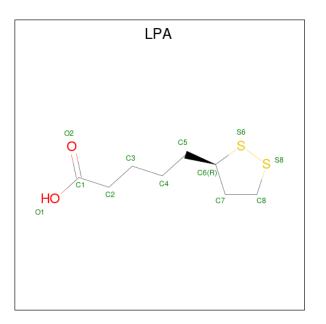
• Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
2	А	1	Total 48			0 17	Р 3	0	0

• Molecule 3 is LIPOIC ACID (three-letter code: LPA) (formula: $C_8H_{14}O_2S_2$).





N	Iol	Chain	Residues	Atoms			ZeroOcc	AltConf
	3	А	1	Total 8	C 6	O 2	0	0

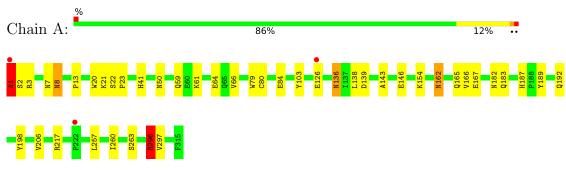
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	158	Total O 158 158	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	50.01Å 67.02Å 91.98Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 2.00	Depositor
Resolution (A)	19.95 - 2.00	EDS
% Data completeness	79.4 (20.00-2.00)	Depositor
(in resolution range)	80.1 (19.95 - 2.00)	EDS
R _{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$14.61 (at 2.01 \text{\AA})$	Xtriage
Refinement program	CNS, X-PLOR 3.851	Depositor
D D.	0.193 , 0.239	Depositor
R, R_{free}	0.166 , 0.198	DCC
R_{free} test set	824 reflections $(4.79%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	16.0	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 45.3	EDS
L-test for twinning ²	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2731	wwPDB-VP
Average B, all atoms $(Å^2)$	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.48% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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, LPA

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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.42	1/2579~(0.0%)	0.56	2/3502~(0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	1	ALA	N-CA	6.32	1.58	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	296	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	А	296	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1	ALA	Mainchain,Peptide
1	А	2	SER	Mainchain
1	А	296	ARG	Sidechain



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	А	2517	0	2533	27	0
2	А	48	0	25	3	0
3	А	8	0	8	0	0
4	А	158	0	0	1	0
All	All	2731	0	2566	27	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 5.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:217:ARG:HD3	1:A:297:VAL:HG13	1.76	0.66
1:A:162:ASN:C	1:A:162:ASN:HD22	2.00	0.65
1:A:8:ASN:HD22	1:A:8:ASN:H	1.50	0.59
1:A:20:TRP:O	1:A:21:LYS:HB2	2.06	0.55
1:A:103:TYR:CD2	1:A:154:LYS:HD3	2.42	0.54
1:A:187:HIS:HD2	1:A:189:TYR:H	1.57	0.51
1:A:136:ASN:HD22	1:A:138:LEU:H	1.59	0.51
1:A:206:VAL:HB	1:A:257:LEU:HD22	1.93	0.51
1:A:64:GLU:HB3	1:A:66:VAL:HG23	1.93	0.50
1:A:162:ASN:ND2	1:A:165:GLN:H	2.10	0.49
1:A:8:ASN:HD22	1:A:8:ASN:N	2.12	0.47
1:A:79:TRP:CG	1:A:80:CYS:N	2.83	0.47
1:A:59:GLN:HG2	4:A:599:HOH:O	2.17	0.45
1:A:162:ASN:O	1:A:166:VAL:HG23	2.17	0.44
1:A:183:GLN:NE2	2:A:316:NAP:H2N	2.33	0.44
1:A:260:ILE:O	1:A:260:ILE:HG13	2.18	0.44
1:A:183:GLN:NE2	2:A:316:NAP:H71N	2.16	0.43
1:A:167:GLU:HG2	1:A:198:TYR:OH	2.20	0.42
1:A:1:ALA:O	1:A:3:ARG:HG3	2.20	0.41
1:A:61:LYS:HA	1:A:61:LYS:HD2	1.77	0.41
1:A:13:PRO:HB2	1:A:41:HIS:HB2	2.03	0.41
1:A:21:LYS:HB2	1:A:21:LYS:NZ	2.37	0.40
1:A:22:SER:HA	1:A:23:PRO:HD3	1.91	0.40

Continued on next page...



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:136:ASN:HD22	1:A:138:LEU:N	2.19	0.40	
1:A:263:SER:HA	2:A:316:NAP:O1X	2.22	0.40	
1:A:136:ASN:ND2	1:A:139:ASP:H	2.19	0.40	
1:A:143:ALA:O	1:A:146:GLU:HG2	2.22	0.40	

Continued from previous page...

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	Analysed Favoured Allowed		Outliers		
1	А	313/315~(99%)	306 (98%)	7~(2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.

M	bl	Chain	Analysed	Analysed Rotameric		Percentiles	
1		А	280/280~(100%)	270~(96%)	10 (4%)	35 34	

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	7	ASN
1	А	8	ASN

Continued on next page...



Conti	Continuea from previous page								
Mol	l Chain Res		Type						
1	А	50	ASN						
1	А	84	GLU						
1	А	126	GLU						
1	А	136	ASN						
1	А	162	ASN						
1	А	182	ASN						
1	А	192	GLN						
1	А	296	ARG						

Continued from previous page...

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	8	ASN
1	А	50	ASN
1	А	136	ASN
1	А	160	ASN
1	А	162	ASN
1	А	182	ASN
1	А	183	GLN
1	А	187	HIS
1	А	200	GLN
1	А	283	GLN
1	A	312	HIS

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 monosaccharides 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	Mol Type Chain Beg		Link	Bo	ond leng	\mathbf{ths}	B	ond ang	les	
MOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAP	А	316	-	45,52,52	1.17	3 (6%)	56,80,80	1.40	6 (10%)
3	LPA	А	351	-	7,7,12	2.17	2 (28%)	7,7,14	1.39	1 (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	А	316	-	-	7/31/67/67	0/5/5/5
3	LPA	А	351	-	-	5/5/5/14	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	351	LPA	C2-C1	4.59	1.61	1.50
2	А	316	NAP	C2N-N1N	3.88	1.39	1.35
2	А	316	NAP	O4B-C1B	2.49	1.44	1.41
3	А	351	LPA	O1-C1	-2.47	1.22	1.30
2	А	316	NAP	C6N-N1N	2.22	1.40	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	316	NAP	N3A-C2A-N1A	-5.36	120.30	128.68
2	А	316	NAP	C2D-C3D-C4D	-3.41	96.02	102.64
2	А	316	NAP	C6N-N1N-C2N	-2.95	119.28	121.97
2	А	316	NAP	PN-O3-PA	2.25	140.54	132.83
2	А	316	NAP	O3X-P2B-O2X	2.24	116.21	107.64
2	А	316	NAP	C3N-C7N-N7N	-2.23	115.07	117.75
3	А	351	LPA	O2-C1-C2	-2.15	116.16	123.08

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
2	А	316	NAP	C5D-O5D-PN-O1N
3	А	351	LPA	C2-C3-C4-C5
3	А	351	LPA	C1-C2-C3-C4
2	А	316	NAP	PA-O3-PN-O5D
2	А	316	NAP	C2B-O2B-P2B-O2X
2	А	316	NAP	C2B-O2B-P2B-O3X
2	А	316	NAP	C4D-C5D-O5D-PN
3	А	351	LPA	O1-C1-C2-C3
3	А	351	LPA	O2-C1-C2-C3
3	А	351	LPA	C3-C4-C5-C6
2	А	316	NAP	C5D-O5D-PN-O3
2	А	316	NAP	PA-O3-PN-O2N

All (12) torsion outliers are listed below:

There are no ring outliers.

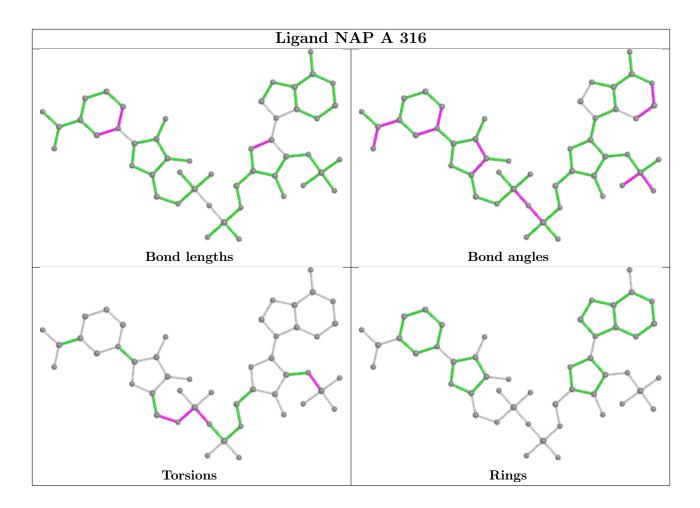
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	316	NAP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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^{th} 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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	315/315~(100%)	-0.55	3 (0%) 82	81	3,10,24,55	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1	ALA	8.1
1	А	222	PRO	2.7
1	А	126	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

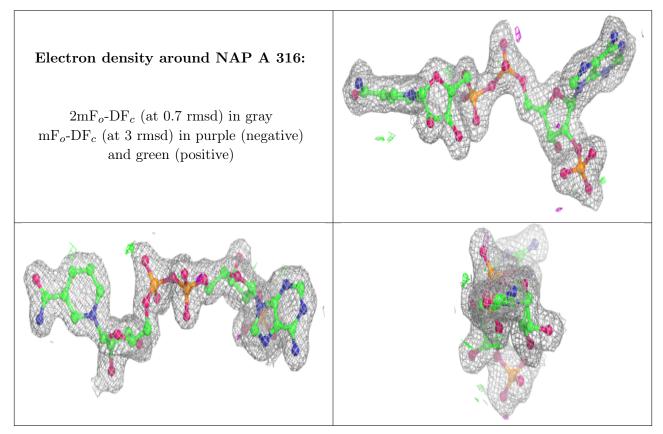
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	LPA	А	351	8/12	0.81	0.24	23,30,37,38	0
2	NAP	А	316	48/48	0.98	0.07	2,5,9,12	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

