Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 01:50 pm GMT

PDB ID	:	2VDG
Title	:	Barley Aldose Reductase 1 complex with butanol
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Deposited on	:	2007-10-08
Resolution	:	1.92 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	1.13
EDS	:	NOT EXECUTED
buster-report	:	NOT EXECUTED
Percentile statistics	:	NOT EXECUTED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 Å.

There are no overall percentile quality scores available for this entry.

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	344	80% 10% 10%

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
4	1BO	A	1326	-	-	X	-

2 Entry composition (i)

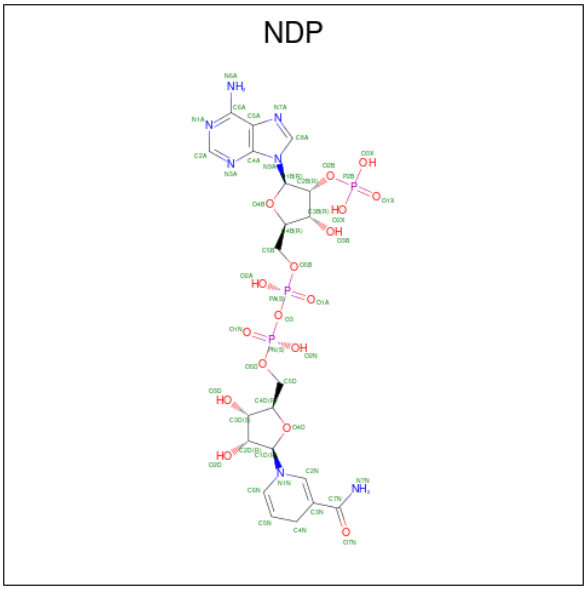
There are 5 unique types of molecules in this entry. The entry contains 2743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

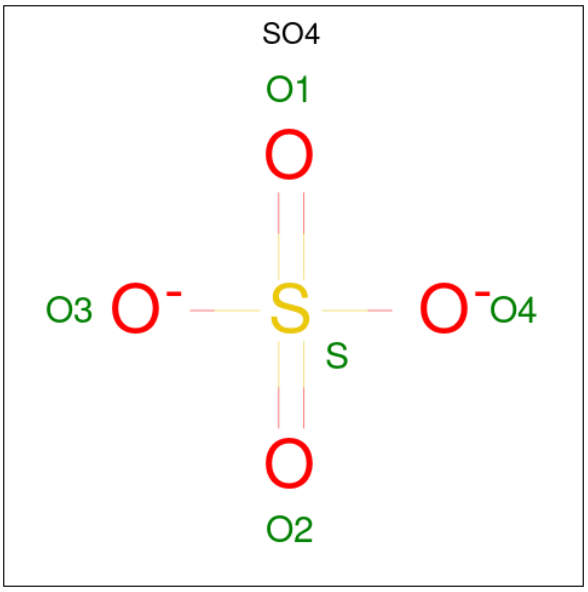
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2445	1550	431	452	12	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



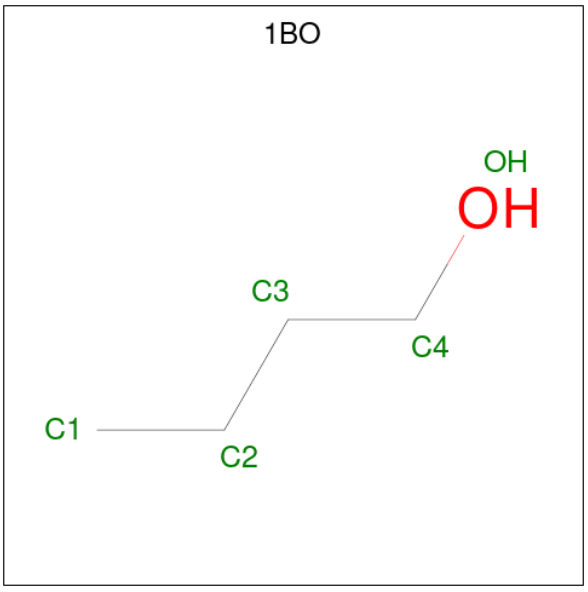
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is 1-BUTANOL (three-letter code: 1BO) (formula: $C_4H_{10}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	225	Total O 225 225	0	0

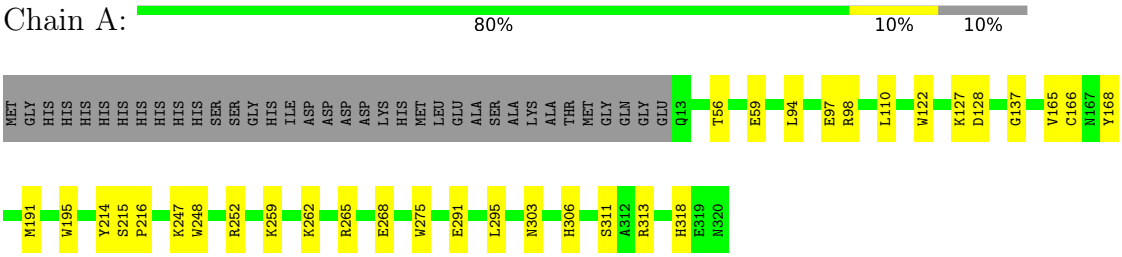
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: ALDOSE REDUCTASE

Chain A:



4 Data and refinement statistics (i)

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.07Å 61.24Å 87.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.20 – 1.92	Depositor
% Data completeness (in resolution range)	86.3 (16.20-1.92)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.214	Depositor
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.098	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2743	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1BO, NDP, SO4

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	0.75	2/2503 (0.1%)	0.76	0/3385

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	A	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	TYR	CD1-CE1	6.02	1.48	1.39
1	A	166	CYS	CB-SG	-5.51	1.72	1.81

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	211	ILE	CB

There are no planarity outliers.

5.2 Too-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 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	2445	0	2431	26	0
2	A	48	0	26	3	0
3	A	15	0	0	0	0
4	A	10	0	20	5	0
5	A	225	0	0	3	0
All	All	2743	0	2477	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.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASN:HD21	4:A:1326:1BO:H32	1.22	1.02
1:A:313:ARG:H	1:A:313:ARG:HD2	1.37	0.89
1:A:311:SER:HB2	1:A:313:ARG:HH11	1.57	0.68
1:A:97:GLU:H	1:A:97:GLU:CD	2.02	0.62
1:A:303:ASN:ND2	4:A:1326:1BO:H32	2.05	0.62
1:A:259:LYS:O	2:A:1321:NDP:H8A	2.01	0.60
1:A:306:HIS:CD2	4:A:1326:1BO:H31	2.36	0.60
1:A:262:LYS:HD3	5:A:2025:HOH:O	2.03	0.58
1:A:313:ARG:H	1:A:313:ARG:CD	2.14	0.56
1:A:127:LYS:HE3	1:A:137:GLY:O	2.05	0.56
1:A:318:HIS:HD2	5:A:2216:HOH:O	1.93	0.52
1:A:59:GLU:CG	4:A:1325:1BO:H12	2.42	0.49
1:A:306:HIS:HD2	4:A:1326:1BO:H31	1.78	0.47
1:A:248:TRP:CH2	1:A:252:ARG:HD2	2.50	0.47
1:A:94:LEU:HD11	1:A:122:TRP:O	2.14	0.47
1:A:311:SER:HB2	1:A:313:ARG:HD2	1.98	0.46
1:A:313:ARG:HG3	5:A:2213:HOH:O	2.16	0.45
1:A:191:MET:HA	1:A:195:TRP:O	2.17	0.45
1:A:165:VAL:HB	1:A:168:TYR:CD1	2.53	0.44
1:A:311:SER:HB2	1:A:313:ARG:CD	2.48	0.43
2:A:1321:NDP:H6N	2:A:1321:NDP:H3D	1.99	0.43
1:A:98:ARG:NH2	1:A:128:ASP:OD1	2.51	0.42
1:A:247:LYS:HE2	1:A:275:TRP:O	2.20	0.42
1:A:295:LEU:HD12	2:A:1321:NDP:H41N	2.02	0.41
1:A:56:THR:HG21	1:A:110:LEU:HD21	2.02	0.41
1:A:215:SER:N	1:A:216:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:HA	1:A:268:GLU:HB3	2.02	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	306/344 (89%)	299 (98%)	6 (2%)	1 (0%)	41 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLU

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)

Mogul was not executed - this section is therefore empty.

5.5 Carbohydrates (i)

Mogul was not executed - this section is therefore empty.

5.6 Ligand geometry (i)

Mogul was not executed - this section is therefore empty.

5.7 Other polymers (i)

Mogul was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.