



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:20 PM GMT

PDB ID : 1ABE
Title : NOVEL STEREOSPECIFICITY OF THE L-ARABINOSE-BINDING PROTEIN
Authors : Vyas, N.K.; Quijcho, F.A.
Deposited on : 1992-04-23
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

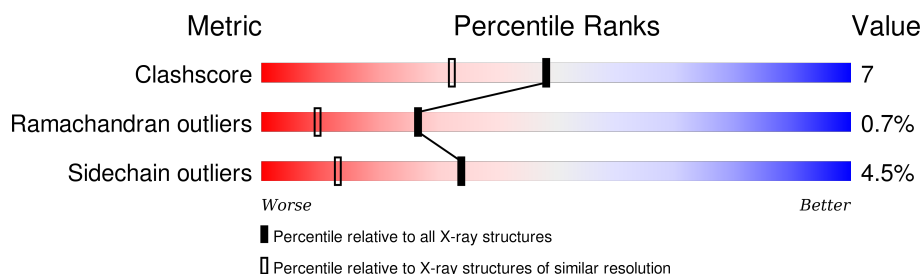
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	

2 Entry composition [i](#)

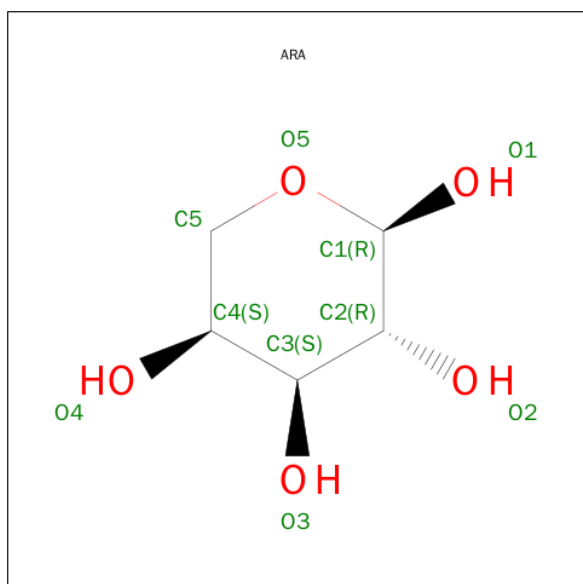
There are 4 unique types of molecules in this entry. The entry contains 2563 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ARABINOSE-BINDING PROTEIN.

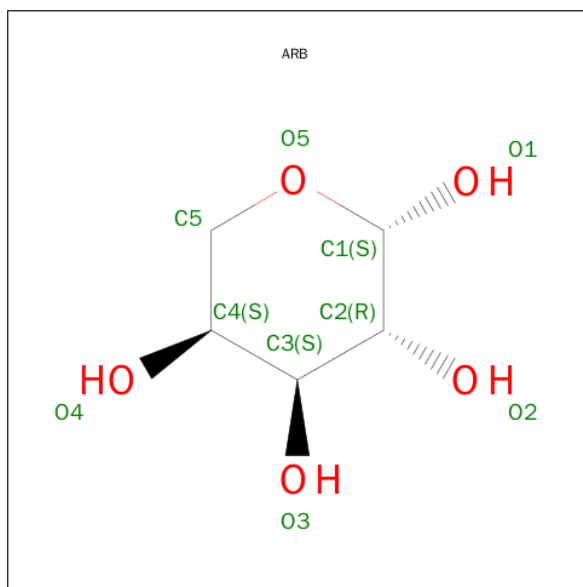
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2316	1473	389	443	11	0	0	0

- Molecule 2 is SUGAR (2-MER) (three-letter code: ARA) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	10	5	5	0	1

- Molecule 3 is water (three-letter code: ARB) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			10	5	5		

- Molecule 4 is water.

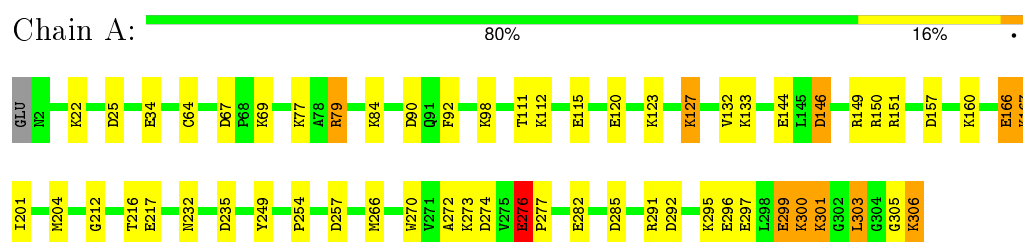
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		

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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

• Molecule 1: L-ARABINOSE-BINDING PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.46Å 71.82Å 77.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.137 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2563	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.99	2/2361 (0.1%)	1.79	45/3189 (1.4%)

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	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	LYS	C-O	9.86	1.42	1.23
1	A	306	LYS	CA-C	7.82	1.73	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	CD-NE-CZ	14.73	144.23	123.60
1	A	149	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	A	67	ASP	CB-CG-OD1	10.00	127.30	118.30
1	A	306	LYS	CA-C-O	-9.73	99.66	120.10
1	A	257	ASP	CB-CG-OD2	9.44	126.79	118.30
1	A	150	ARG	NE-CZ-NH1	-9.40	115.60	120.30
1	A	235	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	A	79	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	A	235	ASP	CB-CG-OD1	8.98	126.39	118.30
1	A	79	ARG	CA-CB-CG	8.84	132.86	113.40
1	A	292	ASP	CB-CG-OD2	-7.52	111.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	LYS	CA-CB-CG	7.41	129.71	113.40
1	A	285	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	67	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	285	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	291	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	276	GLU	OE1-CD-OE2	6.85	131.52	123.30
1	A	249	TYR	CG-CD1-CE1	-6.71	115.93	121.30
1	A	25	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	157	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	144	GLU	CG-CD-OE1	6.38	131.06	118.30
1	A	299	GLU	CG-CD-OE1	6.34	130.99	118.30
1	A	120	GLU	OE1-CD-OE2	6.23	130.78	123.30
1	A	276	GLU	CA-CB-CG	6.11	126.85	113.40
1	A	64	CYS	N-CA-CB	6.01	121.42	110.60
1	A	157	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	166	GLU	CG-CD-OE1	-5.96	106.39	118.30
1	A	90	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	299	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	A	34	GLU	OE1-CD-OE2	5.68	130.12	123.30
1	A	299	GLU	CB-CG-CD	5.66	129.48	114.20
1	A	34	GLU	CG-CD-OE2	-5.62	107.05	118.30
1	A	249	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	A	282	GLU	CG-CD-OE2	5.52	129.34	118.30
1	A	257	ASP	OD1-CG-OD2	-5.49	112.88	123.30
1	A	249	TYR	CD1-CG-CD2	5.46	123.90	117.90
1	A	149	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	274	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	120	GLU	CG-CD-OE2	-5.25	107.80	118.30
1	A	92	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	A	249	TYR	CZ-CE2-CD2	-5.19	115.13	119.80
1	A	217	GLU	CG-CD-OE2	-5.18	107.94	118.30
1	A	291	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	146	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	199	TRP	CB-CA-C	-5.03	100.35	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain

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	2316	0	2326	34	0
2	A	10	0	10	0	0
3	A	10	0	10	0	0
4	A	227	0	0	11	0
All	All	2563	0	2346	34	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 7.

All (34) 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:146:ASP:HB2	4:A:497:HOH:O	1.54	1.07
1:A:160:LYS:HD3	1:A:166:GLU:HG2	1.56	0.86
1:A:115:GLU:OE1	4:A:487:HOH:O	1.99	0.81
1:A:22:LYS:HE3	4:A:479:HOH:O	1.80	0.80
1:A:167:LYS:HG3	4:A:506:HOH:O	1.86	0.74
1:A:295:LYS:HE3	1:A:306:LYS:CA	2.21	0.71
1:A:69:LYS:NZ	4:A:484:HOH:O	2.24	0.70
1:A:305:GLY:O	1:A:306:LYS:C	2.31	0.69
1:A:22:LYS:HB2	1:A:22:LYS:HZ3	1.59	0.68
1:A:22:LYS:HB2	1:A:22:LYS:NZ	1.94	0.68
1:A:297:GLU:OE1	4:A:420:HOH:O	2.11	0.67
1:A:22:LYS:CB	1:A:22:LYS:NZ	2.55	0.65
1:A:295:LYS:CE	1:A:306:LYS:CA	2.76	0.64
1:A:296:GLU:CD	4:A:417:HOH:O	2.37	0.63
1:A:84:LYS:HD2	1:A:270:TRP:CE2	2.37	0.59
1:A:123:LYS:NZ	4:A:486:HOH:O	2.36	0.57
1:A:132:VAL:HG13	1:A:133:LYS:N	2.22	0.53
1:A:112:LYS:HE2	1:A:115:GLU:OE1	2.09	0.53
1:A:201:ILE:HD11	1:A:216:THR:HG21	1.90	0.52
1:A:22:LYS:CE	4:A:479:HOH:O	2.50	0.50
1:A:160:LYS:CD	1:A:166:GLU:HG2	2.36	0.50
1:A:266:MET:HE3	1:A:277:PRO:HB3	1.95	0.49
1:A:132:VAL:CG1	1:A:133:LYS:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:CB	1:A:22:LYS:HZ3	2.21	0.47
1:A:272:ALA:C	1:A:273:LYS:HG3	2.31	0.47
1:A:301:LYS:HD3	1:A:303:LEU:HD11	1.97	0.46
1:A:127:LYS:HB2	1:A:127:LYS:NZ	2.19	0.45
1:A:212:GLY:O	1:A:216:THR:HG23	2.17	0.44
1:A:296:GLU:HG3	4:A:342:HOH:O	2.17	0.44
1:A:167:LYS:HD2	4:A:506:HOH:O	2.17	0.43
1:A:296:GLU:O	1:A:300:LYS:HB2	2.19	0.43
1:A:276:GLU:OE1	1:A:276:GLU:HA	2.19	0.41
1:A:111:THR:O	1:A:115:GLU:HG3	2.21	0.41
1:A:22:LYS:HB2	1:A:22:LYS:HE2	1.35	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	303/306 (99%)	295 (97%)	6 (2%)	2 (1%)	26 9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	254	PRO

5.3.2 Protein sidechains [i](#)

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	243/246 (99%)	232 (96%)	11 (4%)	34 13

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	98	LYS
1	A	127	LYS
1	A	167	LYS
1	A	175	LYS
1	A	204	MET
1	A	276	GLU
1	A	299	GLU
1	A	300	LYS
1	A	301	LYS
1	A	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	ARA	A	307[A]	-	10,10,10	0.93	1 (10%)	12,14,14	1.05	1 (8%)
3	ARB	A	308[B]	-	10,10,10	1.20	2 (20%)	12,14,14	0.86	0

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	ARA	A	307[A]	-	-	0/0/17/17	0/1/1/1
3	ARB	A	308[B]	-	-	0/0/17/17	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	308[B]	ARB	O5-C5	2.07	1.47	1.43
2	A	307[A]	ARA	O5-C5	2.46	1.47	1.43
3	A	308[B]	ARB	O5-C1	2.65	1.46	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	307[A]	ARA	O5-C5-C4	-2.38	107.00	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.