



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:04 am GMT

PDB ID : 7ABP  
Title : SUGAR-BINDING AND CRYSTALLOGRAPHIC STUDIES OF AN ARABINOSE-BINDING PROTEIN MUTANT (MET108LEU) WHICH EXHIBITS ENHANCED AFFINITY AND ALTERED SPECIFICITY  
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Deposited on : 1991-04-25  
Resolution : 1.67 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

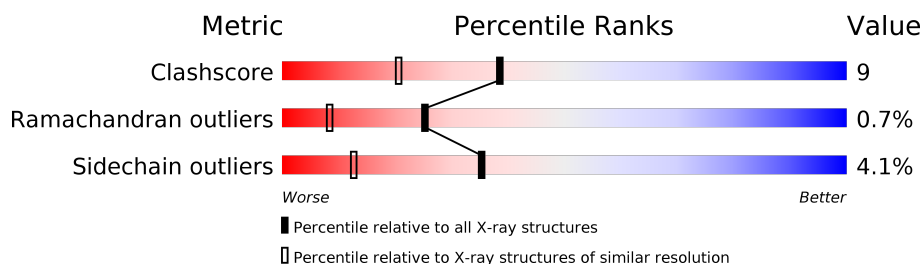
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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	112137	5803 (1.70-1.66)
Ramachandran outliers	110173	5704 (1.70-1.66)
Sidechain outliers	110143	5703 (1.70-1.66)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	 74% 22% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2531 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
1	A	305	Total	C	N	O	S	0	0	0
			2316	1474	389	443	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	LEU	MET	CONFLICT	UNP P02924

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			22	12	10		

- Molecule 3 is water.

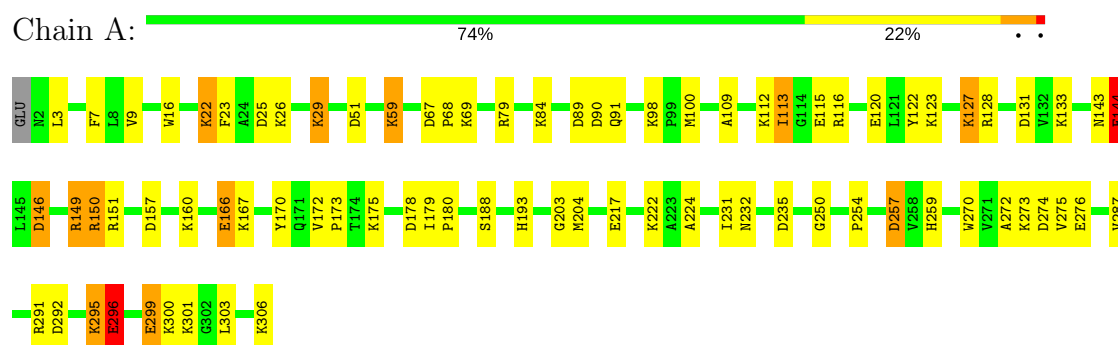
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	193	Total	O	0	0
			193	193		

### 3 Residue-property plots [i](#)

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

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 is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.75Å 71.83Å 78.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.67	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.67)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2531	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: FCA, FCB

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	1.26	5/2361 (0.2%)	1.93	65/3190 (2.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	GLY	N-CA	5.95	1.54	1.46
1	A	203	GLY	N-CA	5.91	1.54	1.46
1	A	9	VAL	C-O	5.56	1.33	1.23
1	A	120	GLU	CD-OE1	-5.17	1.20	1.25
1	A	188	SER	CB-OG	5.09	1.48	1.42

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	NE-CZ-NH1	17.11	128.85	120.30
1	A	291	ARG	NE-CZ-NH1	15.11	127.85	120.30
1	A	79	ARG	NE-CZ-NH1	14.16	127.38	120.30
1	A	149	ARG	NE-CZ-NH1	-13.62	113.49	120.30
1	A	235	ASP	CB-CG-OD1	10.40	127.66	118.30
1	A	170	TYR	CB-CG-CD2	-10.15	114.91	121.00
1	A	150	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	A	292	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	A	157	ASP	CB-CG-OD1	9.35	126.72	118.30
1	A	150	ARG	NE-CZ-NH1	-8.75	115.93	120.30
1	A	25	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	67	ASP	CB-CG-OD1	8.13	125.61	118.30
1	A	122	TYR	CB-CG-CD2	-8.02	116.19	121.00
1	A	296	GLU	CA-CB-CG	7.87	130.71	113.40
1	A	79	ARG	CA-CB-CG	7.50	129.90	113.40
1	A	51	ASP	CB-CG-OD1	7.34	124.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	GLU	N-CA-CB	7.34	123.81	110.60
1	A	89	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	151	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	116	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	170	TYR	CB-CG-CD1	6.74	125.04	121.00
1	A	115	GLU	OE1-CD-OE2	6.60	131.22	123.30
1	A	7	PHE	CB-CG-CD1	6.41	125.29	120.80
1	A	231	ILE	C-N-CA	6.37	137.62	121.70
1	A	144	GLU	CG-CD-OE1	6.19	130.68	118.30
1	A	79	ARG	CG-CD-NE	6.18	124.77	111.80
1	A	257	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	217	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	A	296	GLU	CB-CA-C	-5.97	98.46	110.40
1	A	22	LYS	CA-CB-CG	5.84	126.25	113.40
1	A	149	ARG	CD-NE-CZ	5.78	131.69	123.60
1	A	300	LYS	N-CA-CB	5.76	120.97	110.60
1	A	259	HIS	O-C-N	-5.73	113.46	123.20
1	A	29	LYS	N-CA-CB	5.64	120.75	110.60
1	A	23	PHE	CB-CG-CD1	-5.61	116.87	120.80
1	A	150	ARG	CD-NE-CZ	5.57	131.40	123.60
1	A	51	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	100	MET	CA-CB-CG	-5.56	103.85	113.30
1	A	203	GLY	N-CA-C	-5.55	99.23	113.10
1	A	303	LEU	C-N-CA	5.51	133.86	122.30
1	A	287	VAL	CA-CB-CG1	5.50	119.15	110.90
1	A	122	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	291	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	299	GLU	CG-CD-OE1	5.40	129.09	118.30
1	A	7	PHE	CB-CG-CD2	-5.38	117.03	120.80
1	A	69	LYS	O-C-N	-5.36	114.12	122.70
1	A	296	GLU	CG-CD-OE2	-5.36	107.59	118.30
1	A	151	ARG	CG-CD-NE	-5.27	100.73	111.80
1	A	90	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	23	PHE	CD1-CG-CD2	5.24	125.11	118.30
1	A	178	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	79	ARG	NH1-CZ-NH2	-5.23	113.64	119.40
1	A	274	ASP	N-CA-CB	5.21	119.98	110.60
1	A	157	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	113	ILE	CB-CG1-CD1	5.17	128.39	113.90
1	A	276	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	217	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	A	128	ARG	NE-CZ-NH1	-5.12	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	231	ILE	CA-C-N	5.09	128.39	117.20
1	A	16	TRP	O-C-N	-5.08	114.57	122.70
1	A	166	GLU	CG-CD-OE2	-5.08	108.14	118.30
1	A	292	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	193	HIS	CA-CB-CG	-5.03	105.06	113.60
1	A	299	GLU	CG-CD-OE2	-5.03	108.25	118.30

There are no chirality outliers.

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	2316	0	2326	40	0
2	A	22	0	11	0	0
3	A	193	0	0	5	0
All	All	2531	0	2337	40	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 9.

All (40) 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:127:LYS:NZ	1:A:127:LYS:HB2	1.22	1.16
1:A:127:LYS:NZ	1:A:127:LYS:CB	2.07	1.12
1:A:127:LYS:HZ3	1:A:127:LYS:CB	1.64	1.04
1:A:127:LYS:HZ2	1:A:127:LYS:HB2	1.30	0.96
1:A:160:LYS:HD3	1:A:166:GLU:HG2	1.48	0.95
1:A:127:LYS:HZ3	1:A:127:LYS:HB2	0.72	0.71
1:A:131:ASP:OD2	1:A:133:LYS:HG3	1.91	0.70
1:A:127:LYS:HZ2	1:A:127:LYS:CB	1.90	0.68
1:A:295:LYS:NZ	1:A:306:LYS:O	2.27	0.67
1:A:127:LYS:HE2	3:A:359:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD12	1:A:59:LYS:HG2	1.81	0.62
1:A:146:ASP:O	1:A:150:ARG:HG3	2.01	0.60
1:A:167:LYS:HG2	3:A:426:HOH:O	2.02	0.59
1:A:160:LYS:CD	1:A:166:GLU:HG2	2.27	0.59
1:A:273:LYS:HB2	1:A:275:VAL:HG23	1.87	0.57
1:A:3:LEU:CD1	1:A:59:LYS:CG	2.83	0.56
1:A:3:LEU:CD1	1:A:59:LYS:HG2	2.38	0.53
1:A:109:ALA:O	1:A:113:ILE:HD12	2.09	0.52
1:A:3:LEU:CD1	1:A:59:LYS:HG3	2.40	0.51
1:A:68:PRO:HB3	1:A:91:GLN:O	2.11	0.51
1:A:144:GLU:CD	1:A:144:GLU:H	2.15	0.50
1:A:84:LYS:HE2	3:A:479:HOH:O	2.12	0.49
1:A:257:ASP:OD2	1:A:301:LYS:NZ	2.46	0.47
1:A:3:LEU:HD11	1:A:59:LYS:CG	2.45	0.47
1:A:222:LYS:HE2	1:A:224:ALA:HB3	1.95	0.46
1:A:272:ALA:C	1:A:273:LYS:HG3	2.36	0.45
1:A:84:LYS:HD2	1:A:270:TRP:CZ2	2.53	0.43
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.98	0.43
1:A:22:LYS:HB2	1:A:22:LYS:HE2	1.13	0.42
1:A:295:LYS:CE	1:A:306:LYS:O	2.67	0.42
1:A:296:GLU:CD	3:A:402:HOH:O	2.58	0.42
1:A:3:LEU:HD12	1:A:59:LYS:CG	2.44	0.42
1:A:172:VAL:HA	1:A:173:PRO:HD3	1.91	0.42
1:A:143:ASN:OD1	1:A:149:ARG:HG3	2.20	0.42
1:A:3:LEU:HD11	1:A:59:LYS:HG3	2.01	0.42
1:A:295:LYS:CD	3:A:450:HOH:O	2.68	0.41
1:A:84:LYS:HD2	1:A:270:TRP:CE2	2.55	0.41
1:A:112:LYS:HA	1:A:112:LYS:HD3	1.59	0.41
1:A:26:LYS:HA	1:A:29:LYS:HD2	2.03	0.40
1:A:59:LYS:HA	1:A:59:LYS:HZ3	1.86	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	303/306 (99%)	296 (98%)	5 (2%)	2 (1%)	25 8

All (2) Ramachandran outliers are listed below:

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

### 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	243/246 (99%)	233 (96%)	10 (4%)	35 13

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

Mol	Chain	Res	Type
1	A	59	LYS
1	A	98	LYS
1	A	123	LYS
1	A	127	LYS
1	A	144	GLU
1	A	175	LYS
1	A	204	MET
1	A	295	LYS
1	A	296	GLU
1	A	299	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN

### 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 ⓘ

2 carbohydrates 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	FCA	A	307	2	11,11,11	1.09	1 (9%)	15,16,16	1.19	1 (6%)
2	FCB	A	308	2	11,11,11	2.47	3 (27%)	15,16,16	1.75	4 (26%)

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	FCA	A	307	2	-	0/0/20/20	0/1/1/1
2	FCB	A	308	2	-	0/0/20/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	308	FCB	C3-C2	-6.36	1.36	1.52
2	A	307	FCA	O2-C2	2.01	1.47	1.43
2	A	308	FCB	C4-C3	3.23	1.60	1.52
2	A	308	FCB	O3-C3	3.57	1.51	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	308	FCB	O3-C3-C4	-3.74	102.22	110.36
2	A	308	FCB	O5-C5-C6	-2.03	102.40	106.69
2	A	307	FCA	C1-C2-C3	2.23	114.68	110.65
2	A	308	FCB	C4-C3-C2	2.57	115.37	110.84
2	A	308	FCB	O3-C3-C2	3.10	117.11	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

### 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.