



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:37 am GMT

PDB ID : 1XIB  
Title : MODES OF BINDING SUBSTRATES AND THEIR ANALOGUES TO THE  
ENZYME D-XYLOSE ISOMERASE  
Authors : Carrell, H.L.; Glusker, J.P.  
Deposited on : 1994-03-07  
Resolution : 1.60 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  
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

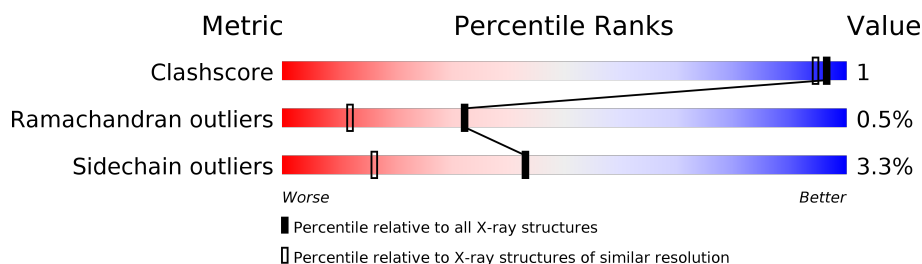
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)

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	388	 80% <span style="float: right;">17% ..</span>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3432 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 D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	1	0
			3052	1917	550	576	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLN	ARG	CONFLICT	UNP P24300

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

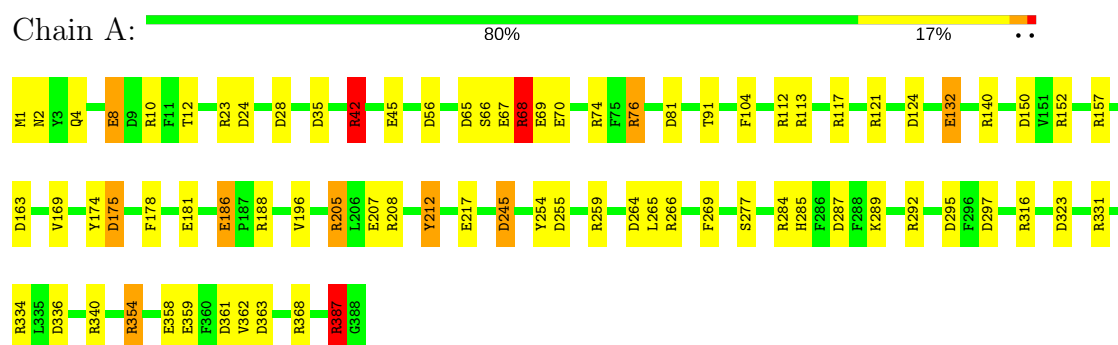
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	378	Total	O	0	0
			378	378		

### 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: D-XYLOSE ISOMERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.88Å 99.68Å 102.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-1.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3432	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: MN

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	1.36	6/3130 (0.2%)	2.14	116/4236 (2.7%)

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	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	GLU	CD-OE1	-6.40	1.18	1.25
1	A	186	GLU	CD-OE2	-6.38	1.18	1.25
1	A	217	GLU	CD-OE2	-5.98	1.19	1.25
1	A	340	ARG	CZ-NH2	5.97	1.40	1.33
1	A	292	ARG	CZ-NH1	5.71	1.40	1.33
1	A	112	ARG	CZ-NH2	5.03	1.39	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	CD-NE-CZ	32.02	168.42	123.60
1	A	340	ARG	NE-CZ-NH1	25.57	133.09	120.30
1	A	340	ARG	NE-CZ-NH2	-21.78	109.41	120.30
1	A	68	ARG	NE-CZ-NH2	19.41	130.00	120.30
1	A	74	ARG	NE-CZ-NH2	-19.11	110.75	120.30
1	A	76	ARG	NE-CZ-NH2	-14.68	112.96	120.30
1	A	266	ARG	NE-CZ-NH2	-14.09	113.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	A	113	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	A	331	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	A	212	TYR	CB-CG-CD1	-11.92	113.85	121.00
1	A	363	ASP	CB-CG-OD2	-11.85	107.64	118.30
1	A	316	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	A	208	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	A	68	ARG	NH1-CZ-NH2	-11.28	106.99	119.40
1	A	368	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	368	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	A	28	ASP	CB-CG-OD1	11.00	128.20	118.30
1	A	124	ASP	CB-CG-OD1	10.63	127.87	118.30
1	A	23	ARG	NE-CZ-NH1	10.57	125.58	120.30
1	A	113	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	A	121	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	A	117	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	68	ARG	CA-CB-CG	9.84	135.05	113.40
1	A	287	ASP	CB-CG-OD1	9.45	126.80	118.30
1	A	316	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	A	284	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	A	104	PHE	CB-CG-CD2	-8.94	114.54	120.80
1	A	354	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	A	266	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	259	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	68	ARG	CD-NE-CZ	-8.24	112.06	123.60
1	A	284	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	361	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	A	196	VAL	CA-CB-CG2	-7.83	99.16	110.90
1	A	152	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	363	ASP	CB-CG-OD1	7.78	125.30	118.30
1	A	28	ASP	CB-CG-OD2	-7.74	111.33	118.30
1	A	152	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	24	ASP	CB-CA-C	7.58	125.57	110.40
1	A	245	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	124	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	A	157	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	188	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	42	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	35	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	42	ARG	CD-NE-CZ	7.31	133.84	123.60
1	A	56	ASP	CB-CG-OD1	7.18	124.77	118.30
1	A	175	ASP	CB-CG-OD1	-7.17	111.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	277	SER	CB-CA-C	7.06	123.52	110.10
1	A	212	TYR	CB-CG-CD2	7.02	125.21	121.00
1	A	121	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	174	TYR	CB-CG-CD1	6.90	125.14	121.00
1	A	2	ASN	CB-CA-C	6.84	124.08	110.40
1	A	297	ASP	CB-CG-OD1	6.79	124.42	118.30
1	A	188	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	169	VAL	CA-CB-CG1	6.79	121.08	110.90
1	A	254	TYR	CB-CG-CD2	-6.66	117.00	121.00
1	A	169	VAL	CG1-CB-CG2	6.62	121.49	110.90
1	A	76	ARG	NH1-CZ-NH2	6.59	126.65	119.40
1	A	76	ARG	CG-CD-NE	-6.48	98.19	111.80
1	A	264	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	175	ASP	CA-CB-CG	-6.44	99.23	113.40
1	A	23	ARG	CD-NE-CZ	6.42	132.59	123.60
1	A	208	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	334	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	132	GLU	N-CA-CB	-6.41	99.07	110.60
1	A	295	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	292	ARG	CD-NE-CZ	6.35	132.49	123.60
1	A	181	GLU	OE1-CD-OE2	6.34	130.91	123.30
1	A	205	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	323	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	292	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	316	ARG	CD-NE-CZ	-6.18	114.95	123.60
1	A	354	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	68	ARG	CB-CG-CD	6.06	127.36	111.60
1	A	10	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	336	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	23	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	358	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	A	175	ASP	OD1-CG-OD2	5.88	134.47	123.30
1	A	387	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	67	GLU	CG-CD-OE2	-5.84	106.62	118.30
1	A	269	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	A	140	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	387	ARG	N-CA-C	5.71	126.41	111.00
1	A	387	ARG	CD-NE-CZ	5.69	131.56	123.60
1	A	70	GLU	CG-CD-OE2	-5.68	106.94	118.30
1	A	255	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	362	VAL	CA-CB-CG2	5.62	119.33	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	205	ARG	CD-NE-CZ	5.54	131.36	123.60
1	A	45	GLU	CG-CD-OE2	-5.50	107.30	118.30
1	A	65	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	266	ARG	CD-NE-CZ	5.47	131.26	123.60
1	A	35	ASP	N-CA-CB	-5.44	100.81	110.60
1	A	331	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	A	8	GLU	CA-CB-CG	5.40	125.28	113.40
1	A	12	THR	O-C-N	5.39	131.33	122.70
1	A	132	GLU	CB-CA-C	-5.35	99.69	110.40
1	A	265	LEU	CB-CG-CD2	-5.34	101.93	111.00
1	A	207	GLU	CG-CD-OE1	-5.32	107.67	118.30
1	A	68	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	163	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	175	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	207	GLU	CG-CD-OE2	5.29	128.88	118.30
1	A	178	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	A	65	ASP	CB-CA-C	5.28	120.96	110.40
1	A	259	ARG	NH1-CZ-NH2	-5.22	113.65	119.40
1	A	117	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	150	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	69	GLU	CB-CG-CD	5.13	128.05	114.20
1	A	196	VAL	CG1-CB-CG2	-5.04	102.83	110.90
1	A	264	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	255	ASP	N-CA-CB	-5.02	101.57	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	ARG	Sidechain
1	A	42	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	3052	0	2918	7	0
2	A	2	0	0	0	0
3	A	378	0	0	3	1
All	All	3432	0	2918	7	1

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 1.

All (7) 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:289:LYS:HE2	3:A:727:HOH:O	1.92	0.69
1:A:354:ARG:HB3	1:A:359:GLU:HG3	1.83	0.59
1:A:245:ASP:OD1	1:A:285:HIS:HD2	1.99	0.45
1:A:205:ARG:HD2	3:A:772:HOH:O	2.16	0.44
1:A:212:TYR:HB3	3:A:739:HOH:O	2.17	0.44
1:A:387:ARG:HA	1:A:387:ARG:HD2	1.79	0.43
1:A:68:ARG:HH11	1:A:68:ARG:HD3	1.57	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:629:HOH:O	3:A:715:HOH:O[3_656]	1.98	0.22

## 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	387/388 (100%)	373 (96%)	12 (3%)	2 (0%)	32 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	ARG
1	A	186	GLU

### 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	303/304 (100%)	293 (97%)	10 (3%)	43	16

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLN
1	A	8	GLU
1	A	42	ARG
1	A	66	SER
1	A	68	ARG
1	A	76	ARG
1	A	91	THR
1	A	132	GLU
1	A	175	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	234	GLN
1	A	285	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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.