



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:56 PM UTC

PDB ID : 1XIB / pdb_00001xib
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

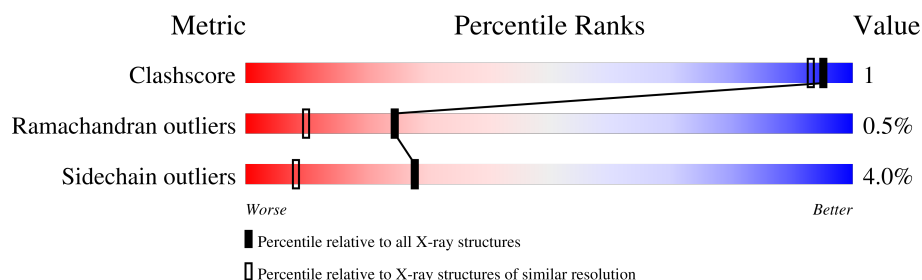
1 Overall quality at a glance

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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	

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 (CCD ID: 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		

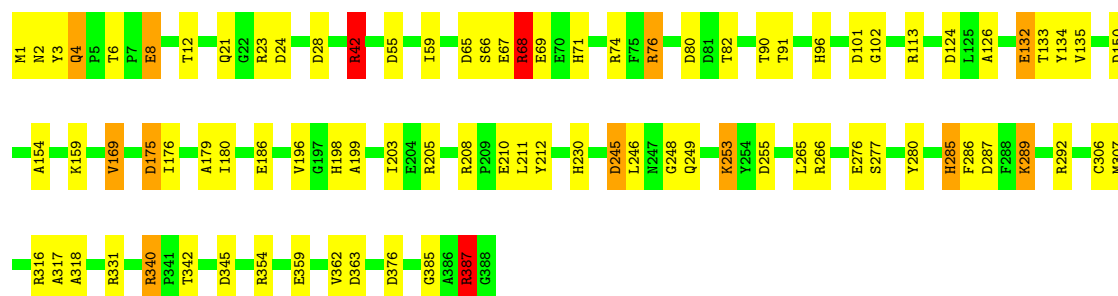
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: D-XYLOSE ISOMERASE

Chain A:  78% 19% ..



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, α , β , γ	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 ²)	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	1.74	26/3130 (0.8%)	2.17	92/4236 (2.2%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	GLY	N-CA	7.95	1.52	1.45
1	A	6	THR	CA-CB	6.68	1.62	1.54
1	A	82	THR	CA-CB	6.62	1.64	1.54
1	A	196	VAL	CA-CB	6.55	1.62	1.54
1	A	248	GLY	CA-C	6.17	1.57	1.52
1	A	134	TYR	N-CA	6.14	1.53	1.46
1	A	68	ARG	CD-NE	6.13	1.54	1.46
1	A	90	THR	N-CA	6.04	1.53	1.46
1	A	307	MET	N-CA	5.93	1.53	1.46
1	A	316	ARG	CD-NE	5.87	1.54	1.46
1	A	180	ILE	CA-CB	5.84	1.62	1.54
1	A	175	ASP	C-O	5.84	1.31	1.23
1	A	253[1]	LYS	C-O	5.79	1.29	1.24
1	A	253[2]	LYS	C-O	5.79	1.29	1.24
1	A	340	ARG	CZ-NH2	5.66	1.40	1.33
1	A	159	LYS	N-CA	5.60	1.53	1.46
1	A	292	ARG	CZ-NH1	5.52	1.40	1.32
1	A	340	ARG	CD-NE	-5.46	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	ALA	N-CA	5.34	1.52	1.46
1	A	317	ALA	N-CA	5.30	1.53	1.46
1	A	198	HIS	CE1-NE2	5.22	1.37	1.32
1	A	249	GLN	N-CA	5.20	1.52	1.46
1	A	80	ASP	N-CA	5.16	1.52	1.46
1	A	230	HIS	N-CA	5.10	1.52	1.46
1	A	246	LEU	N-CA	5.05	1.52	1.46
1	A	135	VAL	N-CA	5.03	1.51	1.46

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	CD-NE-CZ	31.44	168.42	124.40
1	A	175	ASP	CA-CB-CG	-13.37	99.23	112.60
1	A	68	ARG	NE-CZ-NH2	12.01	130.00	119.20
1	A	340	ARG	NE-CZ-NH1	11.59	133.09	121.50
1	A	340	ARG	NE-CZ-NH2	-10.88	109.41	119.20
1	A	68	ARG	CA-CB-CG	10.47	135.05	114.10
1	A	68	ARG	NH1-CZ-NH2	-9.47	106.99	119.30
1	A	74	ARG	NE-CZ-NH2	-9.39	110.75	119.20
1	A	69	GLU	CB-CG-CD	9.09	128.05	112.60
1	A	68	ARG	CD-NE-CZ	-8.82	112.06	124.40
1	A	21	GLN	OE1-CD-NE2	8.34	130.94	122.60
1	A	28	ASP	CA-CB-CG	-8.21	104.39	112.60
1	A	24	ASP	CB-CA-C	7.82	125.57	110.17
1	A	362	VAL	O-C-N	7.70	129.76	121.83
1	A	132	GLU	N-CA-CB	-7.69	99.07	110.53
1	A	96	HIS	CA-CB-CG	-7.41	106.39	113.80
1	A	2	ASN	CB-CA-C	7.36	124.08	110.24
1	A	387	ARG	N-CA-C	7.33	126.41	110.80
1	A	362	VAL	CA-C-O	-7.33	113.08	120.85
1	A	253[1]	LYS	CA-C-O	-7.28	113.37	120.94
1	A	253[2]	LYS	CA-C-O	-7.28	113.37	120.94
1	A	342	THR	O-C-N	7.21	130.36	122.15
1	A	150	ASP	CA-CB-CG	-7.13	105.47	112.60
1	A	133	THR	CA-C-N	-7.10	112.99	123.00
1	A	133	THR	C-N-CA	-7.10	112.99	123.00
1	A	68	ARG	CB-CG-CD	6.99	127.36	111.30
1	A	76	ARG	NE-CZ-NH2	-6.93	112.96	119.20
1	A	287	ASP	CA-CB-CG	-6.92	105.68	112.60
1	A	316	ARG	CD-NE-CZ	-6.75	114.95	124.40
1	A	42	ARG	CD-NE-CZ	6.74	133.84	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	196	VAL	CA-CB-CG2	-6.61	99.16	110.40
1	A	266	ARG	NE-CZ-NH2	-6.61	113.25	119.20
1	A	306	CYS	O-C-N	6.48	128.83	122.09
1	A	277	SER	CB-CA-C	6.44	123.52	110.38
1	A	12	THR	O-C-N	6.29	131.33	123.15
1	A	169	VAL	CA-CB-CG1	6.29	121.08	110.40
1	A	133	THR	CA-CB-OG1	-6.28	100.17	109.60
1	A	76	ARG	CG-CD-NE	-6.28	98.19	112.00
1	A	203	ILE	O-C-N	6.24	127.93	121.87
1	A	286	PHE	CA-CB-CG	-6.19	107.61	113.80
1	A	199	ALA	CA-C-O	-6.17	113.88	120.42
1	A	265	LEU	CA-C-O	-6.00	114.06	120.42
1	A	385	GLY	N-CA-C	-5.95	104.60	114.48
1	A	210	GLU	CB-CG-CD	5.93	122.68	112.60
1	A	113	ARG	NE-CZ-NH2	-5.91	113.88	119.20
1	A	331	ARG	NE-CZ-NH2	-5.88	113.91	119.20
1	A	376	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	211	LEU	CA-C-N	-5.85	113.25	122.73
1	A	211	LEU	C-N-CA	-5.85	113.25	122.73
1	A	23	ARG	CD-NE-CZ	5.85	132.59	124.40
1	A	277	SER	CA-CB-OG	-5.84	99.42	111.10
1	A	292	ARG	CD-NE-CZ	5.78	132.49	124.40
1	A	71	HIS	CA-CB-CG	-5.73	108.07	113.80
1	A	132	GLU	CB-CA-C	-5.72	99.69	109.65
1	A	6	THR	O-C-N	5.71	126.17	121.32
1	A	76	ARG	NH1-CZ-NH2	5.66	126.65	119.30
1	A	4	GLN	CB-CG-CD	5.61	122.13	112.60
1	A	8	GLU	CA-CB-CG	5.59	125.28	114.10
1	A	3	TYR	N-CA-CB	-5.57	102.41	112.27
1	A	286	PHE	CA-C-N	-5.57	114.49	123.23
1	A	286	PHE	C-N-CA	-5.57	114.49	123.23
1	A	342	THR	CA-CB-OG1	-5.52	101.32	109.60
1	A	55	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	280	TYR	CA-C-N	-5.47	113.90	122.49
1	A	280	TYR	C-N-CA	-5.47	113.90	122.49
1	A	101	ASP	CA-C-N	-5.46	115.31	122.63
1	A	101	ASP	C-N-CA	-5.46	115.31	122.63
1	A	318	ALA	CA-C-O	-5.45	114.64	120.42
1	A	285	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	A	65	ASP	CB-CA-C	5.41	120.96	110.46
1	A	363	ASP	CA-CB-CG	-5.35	107.25	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	VAL	N-CA-CB	5.35	118.61	110.58
1	A	176	ILE	N-CA-C	-5.32	101.33	108.35
1	A	74	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	A	362	VAL	CA-CB-CG2	5.25	119.33	110.40
1	A	289	LYS	CA-C-N	-5.24	114.98	120.38
1	A	289	LYS	C-N-CA	-5.24	114.98	120.38
1	A	245	ASP	O-C-N	5.24	129.34	123.27
1	A	133	THR	O-C-N	5.23	129.65	123.27
1	A	255	ASP	N-CA-CB	-5.23	101.57	109.94
1	A	276	GLU	N-CA-C	-5.22	105.66	112.23
1	A	285	HIS	CA-C-O	-5.20	115.03	120.80
1	A	208	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	124	ASP	CA-C-O	-5.18	115.06	120.55
1	A	59	ILE	O-C-N	5.17	126.99	121.10
1	A	67	GLU	CG-CD-OE2	-5.12	106.62	118.40
1	A	126	ALA	O-C-N	5.12	127.34	122.07
1	A	387	ARG	CD-NE-CZ	5.12	131.56	124.40
1	A	2	ASN	N-CA-CB	5.11	118.71	111.05
1	A	154	ALA	CA-C-O	-5.08	115.03	120.42
1	A	203	ILE	CA-C-O	-5.06	115.68	120.95

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

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles [i](#)

5.2.1 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	387/388 (100%)	373 (96%)	12 (3%)	2 (0%)	24 10

All (2) Ramachandran outliers are listed below:

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

5.2.2 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	303/304 (100%)	291 (96%)	12 (4%)	28 8

All (12) 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	169	VAL
1	A	175	ASP
1	A	340	ARG

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

Mol	Chain	Res	Type
1	A	234	GLN
1	A	285	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	GLN

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.5 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.

5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 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.