



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:29 AM UTC

PDB ID : 1XIF / pdb_00001xif
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
Mogul	:	2022.3.0, CSD as543be (2022)
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

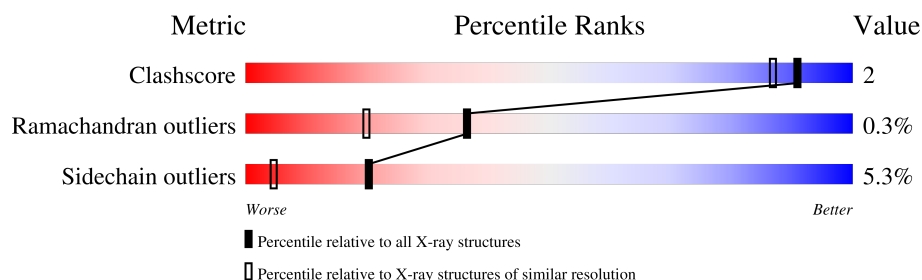
1 Overall quality at a glance

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3447 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.

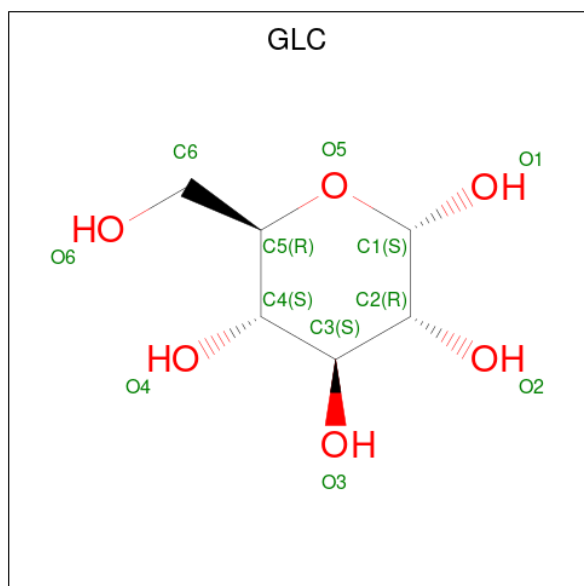
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3053	1917	550	577	9	0	2	0

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 alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	380	Total 380	O 380	0	0

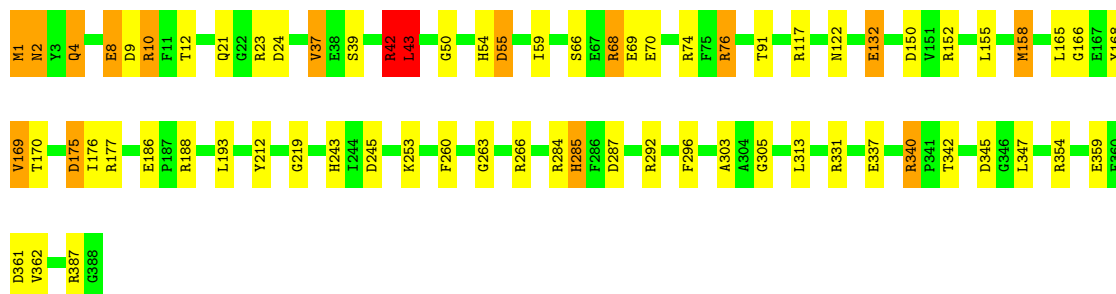
3 Residue-property plots

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: 



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	93.86Å 99.53Å 103.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.60)	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	3447	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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, GLC

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	1.04	3/3134 (0.1%)	1.76	68/4242 (1.6%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	LEU	C-O	7.21	1.27	1.23
1	A	37	VAL	N-CA	7.14	1.55	1.46
1	A	37	VAL	CA-CB	-5.41	1.47	1.54

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ARG	CD-NE-CZ	12.60	142.04	124.40
1	A	2	ASN	CA-CB-CG	-9.25	103.35	112.60
1	A	76	ARG	NE-CZ-NH2	-8.95	111.14	119.20
1	A	158	MET	CA-CB-CG	-8.53	97.04	114.10
1	A	175	ASP	CA-CB-CG	-8.50	104.10	112.60
1	A	68	ARG	NE-CZ-NH2	8.12	126.51	119.20
1	A	23	ARG	CD-NE-CZ	8.10	135.73	124.40
1	A	169	VAL	N-CA-CB	-7.89	99.81	110.54
1	A	55	ASP	CA-CB-CG	7.55	120.15	112.60
1	A	387	ARG	CD-NE-CZ	7.43	134.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ARG	NH1-CZ-NH2	7.39	128.91	119.30
1	A	266	ARG	CD-NE-CZ	7.25	134.54	124.40
1	A	150	ASP	CA-C-O	-7.17	112.50	120.60
1	A	362	VAL	CA-C-O	-7.01	112.90	120.47
1	A	387	ARG	NE-CZ-NH2	-6.93	112.96	119.20
1	A	4	GLN	CB-CG-CD	6.86	124.26	112.60
1	A	24	ASP	CB-CA-C	6.57	123.11	110.17
1	A	345	ASP	CA-CB-CG	6.53	119.12	112.60
1	A	253[1]	LYS	CA-C-O	-6.51	114.17	120.94
1	A	253[2]	LYS	CA-C-O	-6.51	114.17	120.94
1	A	342	THR	O-C-N	6.44	129.49	122.15
1	A	74	ARG	CD-NE-CZ	6.36	133.30	124.40
1	A	132	GLU	N-CA-CB	-6.19	101.43	110.53
1	A	10	ARG	CD-NE-CZ	6.17	133.03	124.40
1	A	37	VAL	CA-CB-CG2	6.16	120.87	110.40
1	A	287	ASP	CA-CB-CG	-6.09	106.50	112.60
1	A	69	GLU	CA-C-N	6.06	128.31	120.44
1	A	69	GLU	C-N-CA	6.06	128.31	120.44
1	A	4	GLN	CG-CD-NE2	5.98	125.37	116.40
1	A	12	THR	O-C-N	5.98	130.93	123.15
1	A	117	ARG	NE-CZ-NH1	5.94	127.44	121.50
1	A	340	ARG	CA-C-O	-5.85	115.33	120.60
1	A	132	GLU	CB-CG-CD	5.81	122.47	112.60
1	A	219	GLY	CA-C-O	-5.75	113.97	120.30
1	A	331	ARG	CG-CD-NE	-5.67	99.53	112.00
1	A	155	LEU	O-C-N	5.66	128.12	122.12
1	A	158	MET	CG-SD-CE	5.62	113.26	100.90
1	A	76	ARG	CG-CD-NE	-5.59	99.69	112.00
1	A	4	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	A	284	ARG	NE-CZ-NH2	-5.54	114.22	119.20
1	A	340	ARG	CG-CD-NE	-5.49	99.92	112.00
1	A	168	TYR	CA-C-O	5.49	126.58	120.82
1	A	331	ARG	NH1-CZ-NH2	5.46	126.40	119.30
1	A	176	ILE	N-CA-C	-5.44	101.17	108.35
1	A	1	MET	O-C-N	5.42	131.68	123.00
1	A	331	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	A	305	GLY	CA-C-O	-5.34	114.43	120.30
1	A	292	ARG	CD-NE-CZ	5.32	131.85	124.40
1	A	122	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	74	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	188	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	303	ALA	O-C-N	-5.22	116.59	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	LEU	CA-C-O	-5.20	115.04	120.55
1	A	21	GLN	OE1-CD-NE2	5.17	127.78	122.60
1	A	361	ASP	CA-C-O	-5.17	115.54	120.92
1	A	177	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	243	HIS	CA-CB-CG	5.16	118.96	113.80
1	A	8	GLU	CA-CB-CG	5.15	124.39	114.10
1	A	43	LEU	N-CA-CB	-5.11	102.60	110.16
1	A	165	LEU	CA-C-N	5.09	125.60	120.00
1	A	165	LEU	C-N-CA	5.09	125.60	120.00
1	A	285	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	296	PHE	CA-C-O	-5.08	114.36	120.10
1	A	50	GLY	CA-C-O	-5.07	116.81	121.63
1	A	243	HIS	CA-C-O	-5.06	116.02	121.38
1	A	263	GLY	CA-C-O	5.05	127.00	120.89
1	A	152	ARG	CA-C-O	-5.04	115.53	120.82
1	A	260	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ASN	Peptide

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	3053	0	2919	10	0
2	A	12	0	11	0	0
3	A	2	0	0	0	0
4	A	380	0	0	1	1
All	All	3447	0	2930	10	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 2.

All (10) 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:59:ILE:HG21	1:A:68:ARG:HG3	1.80	0.63
1:A:354:ARG:HB3	1:A:359:GLU:HG3	1.88	0.56
1:A:212:TYR:HB3	4:A:739:HOH:O	2.11	0.49
1:A:337:GLU:HG2	1:A:340:ARG:NH1	2.30	0.45
1:A:245:ASP:OD1	1:A:285:HIS:HD2	2.02	0.43
1:A:166:GLY:O	1:A:170:THR:HG23	2.19	0.42
1:A:9:ASP:O	1:A:10:ARG:HB2	2.18	0.42
1:A:54:HIS:O	1:A:55:ASP:C	2.63	0.41
1:A:39:SER:O	1:A:43:LEU:HB2	2.20	0.41
1:A:42:ARG:HE	1:A:42:ARG:HA	1.86	0.40

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)
4:A:629:HOH:O	4:A:715:HOH:O[3_656]	2.17	0.03

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	388/388 (100%)	373 (96%)	14 (4%)	1 (0%)	36 20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	302/304 (99%)	286 (95%)	16 (5%)	20 4

All (16) 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	37	VAL
1	A	42	ARG
1	A	43	LEU
1	A	66	SER
1	A	70	GLU
1	A	76	ARG
1	A	91	THR
1	A	132	GLU
1	A	158	MET
1	A	169	VAL
1	A	175	ASP
1	A	313	LEU
1	A	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	GLN
1	A	234	GLN
1	A	285	HIS
1	A	348	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	GLC	A	389	3	12,12,12	1.05	0	17,17,17	1.98	5 (29%)

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	GLC	A	389	3	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	GLC	O5-C5-C6	-4.92	94.25	106.44
2	A	389	GLC	O3-C3-C4	-3.08	103.12	110.38
2	A	389	GLC	C6-C5-C4	2.65	119.53	113.02
2	A	389	GLC	O2-C2-C1	2.53	115.08	109.25
2	A	389	GLC	C4-C3-C2	-2.25	106.88	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	GLC	C4-C5-C6-O6
2	A	389	GLC	O5-C5-C6-O6

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.