



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:41 AM BST

PDB ID : 2XIS  
Title : A METAL-MEDIATED HYDRIDE SHIFT MECHANISM FOR XYLOSE ISOMERASE BASED ON THE 1.6 ANGSTROMS STREPTOMYCES RUBIGINOSUS STRUCTURES WITH XYLITOL AND D-XYLOSE  
Authors : Whitlow, M.; Howard, A.J.  
Deposited on : 1991-03-25  
Resolution : 1.71 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

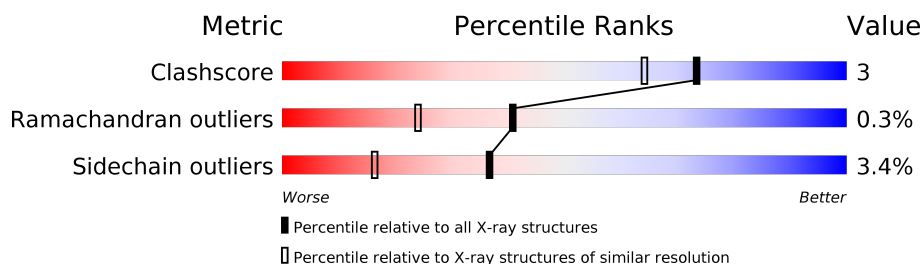
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 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	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)

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  $\geq 3$ , 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	387	

## 2 Entry composition [i](#)

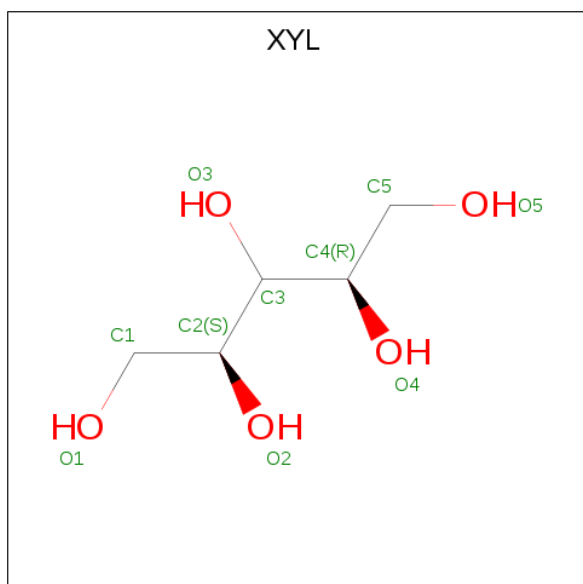
There are 4 unique types of molecules in this entry. The entry contains 3406 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	8	1
			3049	1910	560	571	8			

- Molecule 2 is Xylitol (three-letter code: XYL) (formula:  $C_5H_{12}O_5$ ).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

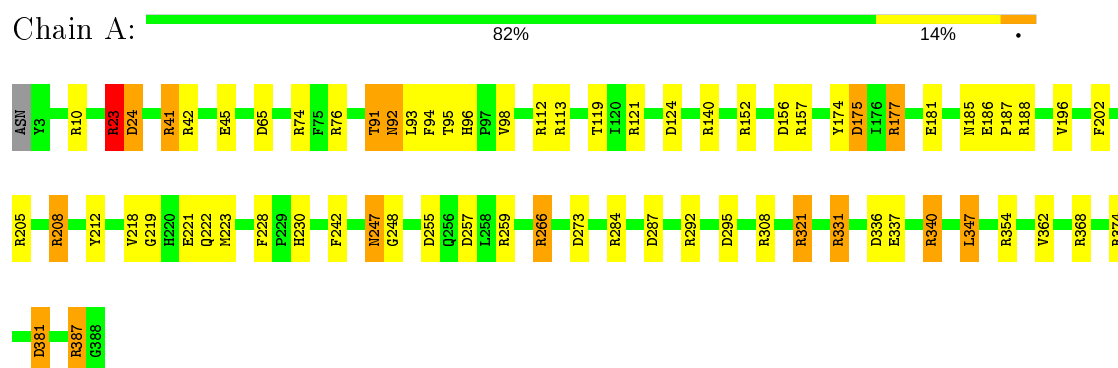
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	345	Total 345	O 345	0	0

### 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: 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, $\alpha$ , $\beta$ , $\gamma$	94.64Å 99.97Å 103.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.71	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.71)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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: MG, XYL

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	1.22	3/3171 (0.1%)	1.87	81/4290 (1.9%)

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	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	ARG	CZ-NH2	6.12	1.41	1.33
1	A	340	ARG	CD-NE	-5.82	1.36	1.46
1	A	222	GLN	C-O	5.61	1.34	1.23

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ARG	NE-CZ-NH1	19.93	130.27	120.30
1	A	354[A]	ARG	CD-NE-CZ	19.69	151.16	123.60
1	A	354[B]	ARG	CD-NE-CZ	19.69	151.16	123.60
1	A	331	ARG	NE-CZ-NH1	17.46	129.03	120.30
1	A	266	ARG	NE-CZ-NH1	15.86	128.23	120.30
1	A	340	ARG	CD-NE-CZ	15.13	144.78	123.60
1	A	354[A]	ARG	NE-CZ-NH2	14.11	127.35	120.30
1	A	354[B]	ARG	NE-CZ-NH2	14.11	127.35	120.30
1	A	266	ARG	CD-NE-CZ	13.35	142.29	123.60
1	A	266	ARG	NE-CZ-NH2	-13.16	113.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	NE-CZ-NH2	-13.09	113.76	120.30
1	A	340	ARG	NE-CZ-NH1	12.92	126.76	120.30
1	A	113	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	A	295	ASP	CB-CG-OD1	11.41	128.57	118.30
1	A	331	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	A	152	ARG	CD-NE-CZ	10.30	138.03	123.60
1	A	124	ASP	CB-CG-OD1	9.78	127.10	118.30
1	A	259	ARG	NE-CZ-NH2	9.45	125.02	120.30
1	A	23	ARG	CD-NE-CZ	9.32	136.65	123.60
1	A	152	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	A	177	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	208	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	23	ARG	CG-CD-NE	8.43	129.50	111.80
1	A	74	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	A	284	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	284	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	177	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	76[A]	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	76[B]	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	387[A]	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	387[B]	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	121	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	212	TYR	CB-CG-CD1	-7.49	116.51	121.00
1	A	112	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	A	10	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	242	PHE	CB-CG-CD2	-7.07	115.85	120.80
1	A	76[A]	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	76[B]	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	212	TYR	CB-CG-CD2	6.98	125.19	121.00
1	A	205[A]	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	205[B]	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	74	ARG	CD-NE-CZ	6.67	132.94	123.60
1	A	340	ARG	CG-CD-NE	6.48	125.40	111.80
1	A	188	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	121	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	41	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	228	PHE	CB-CG-CD1	-6.24	116.44	120.80
1	A	368	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	181	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	A	42	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	74	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	221	GLU	CG-CD-OE1	5.98	130.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	VAL	CG1-CB-CG2	-5.95	101.37	110.90
1	A	205[A]	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	205[B]	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	202	PHE	CB-CG-CD1	-5.88	116.69	120.80
1	A	10	ARG	CA-CB-CG	5.87	126.31	113.40
1	A	24	ASP	CB-CA-C	5.77	121.94	110.40
1	A	336	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	257	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	374	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	65	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	10	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	381	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	331	ARG	CD-NE-CZ	5.48	131.28	123.60
1	A	45	GLU	CA-CB-CG	5.36	125.19	113.40
1	A	157	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	273	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	A	188	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	A	177	ARG	CD-NE-CZ	5.27	130.98	123.60
1	A	76[A]	ARG	CA-CB-CG	5.22	124.89	113.40
1	A	76[B]	ARG	CA-CB-CG	5.22	124.89	113.40
1	A	308	ARG	CD-NE-CZ	5.19	130.87	123.60
1	A	156	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	174	TYR	CB-CG-CD1	5.13	124.08	121.00
1	A	292	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	347	LEU	CB-CG-CD2	5.06	119.61	111.00
1	A	175	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	287	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	A	140	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	321	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	331	ARG	Sidechain
1	A	41	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	3049	0	2895	20	0
2	A	10	0	10	0	0
3	A	2	0	0	0	0
4	A	345	0	0	6	0
All	All	3406	0	2905	20	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 3.

All (20) 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:92:ASN:HD21	1:A:95:THR:H	1.24	0.86
1:A:96:HIS:HD2	1:A:98:VAL:H	1.30	0.80
1:A:93:LEU:HD21	4:A:618:HOH:O	1.96	0.65
1:A:219:GLY:H	1:A:247:ASN:HD21	1.43	0.64
1:A:248:GLY:HA2	4:A:608:HOH:O	2.01	0.60
1:A:92:ASN:ND2	1:A:94:PHE:H	2.00	0.59
1:A:218:VAL:HG11	4:A:608:HOH:O	2.03	0.58
1:A:92:ASN:ND2	1:A:95:THR:H	1.98	0.57
1:A:92:ASN:HD22	1:A:94:PHE:H	1.52	0.55
1:A:96:HIS:CD2	1:A:98:VAL:H	2.18	0.53
1:A:266:ARG:HG3	4:A:454:HOH:O	2.14	0.47
1:A:223:MET:SD	1:A:255[B]:ASP:HB2	2.56	0.46
1:A:91:THR:HG21	4:A:618:HOH:O	2.15	0.46
1:A:92:ASN:C	1:A:92:ASN:HD22	2.19	0.45
1:A:223:MET:SD	1:A:255[A]:ASP:HB3	2.57	0.44
1:A:337:GLU:HG2	1:A:340:ARG:NH2	2.32	0.44
1:A:23:ARG:HD3	1:A:24:ASP:N	2.33	0.44
1:A:119:THR:N	4:A:618:HOH:O	2.49	0.43
1:A:92:ASN:HD21	1:A:95:THR:N	2.05	0.41
1:A:381:ASP:HB3	1:A:387[B]:ARG:HD2	2.03	0.41

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	392/387 (101%)	377 (96%)	13 (3%)	2 (0%)	29 13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186[A]	GLU
1	A	186[B]	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	306/303 (101%)	296 (97%)	10 (3%)	38 17

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

Mol	Chain	Res	Type
1	A	23	ARG
1	A	91	THR
1	A	92	ASN
1	A	175	ASP
1	A	185	ASN
1	A	187	PRO
1	A	230	HIS
1	A	247	ASN
1	A	347	LEU

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Mol	Chain	Res	Type
1	A	362	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	96	HIS
1	A	185	ASN
1	A	215	ASN
1	A	230	HIS
1	A	247	ASN

### 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 monosaccharides 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	XYL	A	390	3	9,9,9	1.14	1 (11%)	11,11,11	1.32	1 (9%)

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	XYL	A	390	3	-	1/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	390	XYL	C1-C2	2.27	1.58	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	390	XYL	C1-C2-C3	-2.90	106.13	112.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	390	XYL	O4-C4-C5-O5

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.