



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2017 – 02:24 AM EST

PDB ID : 1XLI  
Title : MECHANISM FOR ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE INVOLVING RING OPENING FOLLOWED BY A 1,2-HYDRIDE SHIFT  
Authors : Collyer, C.A.; Henrick, K.; Blow, D.M.  
Deposited on : unknown  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)  
Xtrriage (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) : rb-20030345

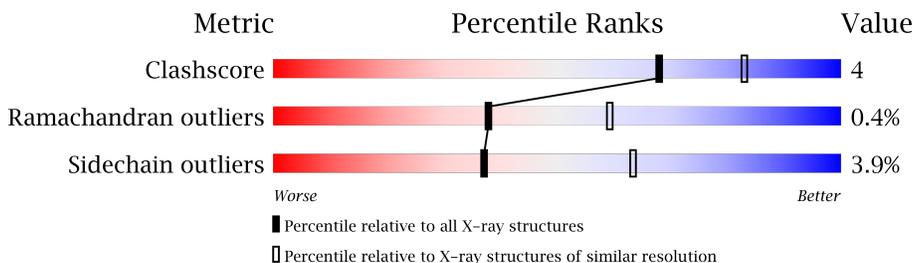
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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	394	
1	B	394	

## 2 Entry composition [i](#)

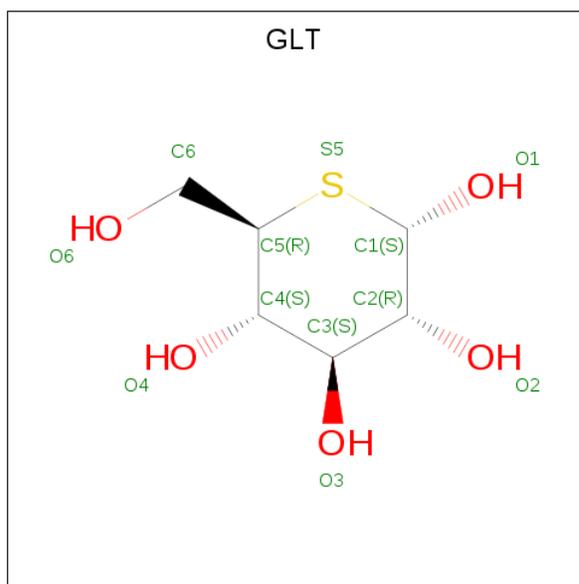
There are 4 unique types of molecules in this entry. The entry contains 6601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	393	Total 3027	C 1919	N 520	O 579	S 9	0	0	0
1	B	393	Total 3027	C 1919	N 520	O 579	S 9	0	0	0

- Molecule 2 is 5-DEOXY-5-THIO-ALPHA-D-GLUCOSE (three-letter code: GLT) (formula:  $C_6H_{12}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	Total 12	C 6	O 5	S 1	0	0
2	B	1	Total 12	C 6	O 5	S 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is water.

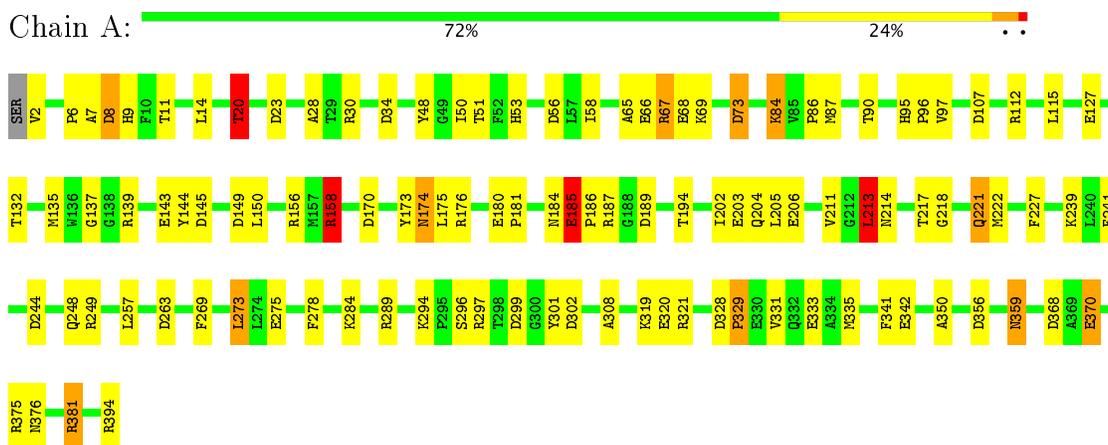
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	255	Total 255	O 255	0	0
4	B	264	Total 264	O 264	0	0

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

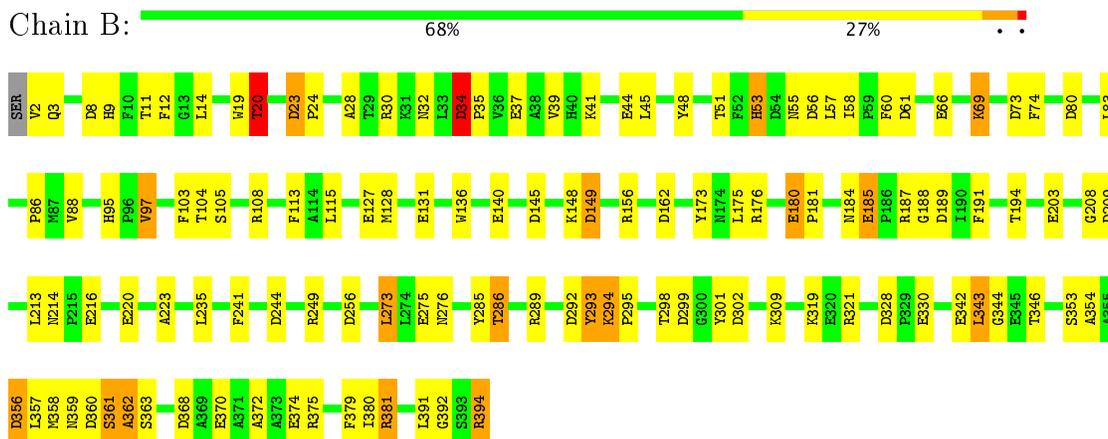
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



- Molecule 1: D-XYLOSE ISOMERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.80Å 105.80Å 153.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.150 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GLT

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	1.09	1/3101 (0.0%)	2.15	108/4204 (2.6%)
1	B	1.15	3/3101 (0.1%)	2.06	113/4204 (2.7%)
All	All	1.12	4/6202 (0.1%)	2.11	221/8408 (2.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	SER	C-N	17.91	1.75	1.34
1	B	374	GLU	CD-OE1	-5.12	1.20	1.25
1	B	344	GLY	N-CA	-5.04	1.38	1.46
1	A	187	ARG	NE-CZ	5.03	1.39	1.33

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	25.75	159.66	123.60
1	B	187	ARG	NE-CZ-NH2	-19.49	110.55	120.30
1	A	187	ARG	NE-CZ-NH2	-19.38	110.61	120.30
1	B	361	SER	C-N-CA	18.01	166.74	121.70
1	A	394	ARG	NE-CZ-NH1	16.01	128.31	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3027	0	2881	26	1
1	B	3027	0	2879	27	7
2	A	12	0	10	0	0
2	B	12	0	11	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	255	0	0	3	2
4	B	264	0	0	2	7
All	All	6601	0	5781	52	9

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 4.

The worst 5 of 52 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:B:361:SER:C	1:B:362:ALA:N	1.75	1.38
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.58	0.82
1:A:58:ILE:HD13	1:A:67:ARG:HD2	1.73	0.71
1:A:95:HIS:HD2	1:A:97:VAL:H	1.41	0.67
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.76	0.67

The worst 5 of 9 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)
1:B:105:SER:CA	4:B:846(B):HOH:O[4_555]	1.16	1.04
1:B:105:SER:N	4:B:846(B):HOH:O[4_555]	1.32	0.88
4:A:564(A):HOH:O	4:B:668(B):HOH:O[4_555]	1.81	0.39
4:B:761(B):HOH:O	4:B:829(B):HOH:O[4_555]	1.90	0.30
1:B:104:THR:C	4:B:846(B):HOH:O[4_555]	1.92	0.28

## 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	391/394 (99%)	371 (95%)	19 (5%)	1 (0%)	44	66
1	B	391/394 (99%)	376 (96%)	13 (3%)	2 (0%)	32	53
All	All	782/788 (99%)	747 (96%)	32 (4%)	3 (0%)	38	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	3	GLN
1	B	185	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	305/310 (98%)	293 (96%)	12 (4%)	37	63
1	B	305/310 (98%)	293 (96%)	12 (4%)	37	63
All	All	610/620 (98%)	586 (96%)	24 (4%)	37	63

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	B	34	ASP
1	B	293	TYR
1	A	370	GLU
1	B	20	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	GLN
1	B	40	HIS
1	B	184	ASN
1	A	221	GLN
1	B	95	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	GLT	A	400	3	11,12,12	1.79	4 (36%)	11,17,17	3.14	5 (45%)
2	GLT	B	400	3	11,12,12	1.02	0	11,17,17	2.85	6 (54%)

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	GLT	A	400	3	-	0/2/22/22	0/1/1/1
2	GLT	B	400	3	-	0/2/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	GLT	C4-C5	-3.53	1.50	1.53
2	A	400	GLT	C6-C5	-2.14	1.50	1.52
2	A	400	GLT	O3-C3	2.02	1.47	1.43
2	A	400	GLT	C5-S5	2.75	1.86	1.82

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	GLT	O4-C4-C5	-3.41	101.04	108.83
2	A	400	GLT	O1-C1-C2	2.11	114.78	110.08
2	B	400	GLT	O2-C2-C1	2.37	114.99	110.27
2	A	400	GLT	O2-C2-C1	2.63	115.51	110.27
2	B	400	GLT	O1-C1-C2	2.96	116.67	110.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	GLT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	361:SER	C	362:ALA	N	1.75

## 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.