



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2023 – 12:46 AM JST

PDB ID : 5YN3  
Title : Crystal structure of xylose isomerase from *Piromyces* sp. E2  
Authors : Son, H.-F.; Kim, K.-J.  
Deposited on : 2017-10-24  
Resolution : 2.70 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

<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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

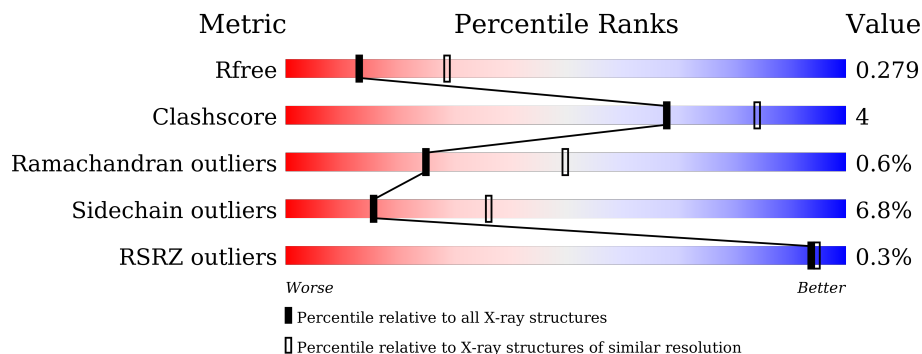
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	449	 84% 11% . .
1	B	449	 82% 13% . .
1	C	449	 83% 13% . .
1	D	449	 82% 14% . .

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14080 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
			Total	C	N	O	S			
1	A	435	3463	2198	581	665	19	0	0	0
1	B	435	3463	2198	581	665	19	0	0	0
1	C	435	3463	2198	581	665	19	0	0	0
1	D	435	3463	2198	581	665	19	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9P8C9
A	-10	ARG	-	expression tag	UNP Q9P8C9
A	-9	GLY	-	expression tag	UNP Q9P8C9
A	-8	SER	-	expression tag	UNP Q9P8C9
A	-7	HIS	-	expression tag	UNP Q9P8C9
A	-6	HIS	-	expression tag	UNP Q9P8C9
A	-5	HIS	-	expression tag	UNP Q9P8C9
A	-4	HIS	-	expression tag	UNP Q9P8C9
A	-3	HIS	-	expression tag	UNP Q9P8C9
A	-2	HIS	-	expression tag	UNP Q9P8C9
A	-1	GLY	-	expression tag	UNP Q9P8C9
A	0	SER	-	expression tag	UNP Q9P8C9
B	-11	MET	-	expression tag	UNP Q9P8C9
B	-10	ARG	-	expression tag	UNP Q9P8C9
B	-9	GLY	-	expression tag	UNP Q9P8C9
B	-8	SER	-	expression tag	UNP Q9P8C9
B	-7	HIS	-	expression tag	UNP Q9P8C9
B	-6	HIS	-	expression tag	UNP Q9P8C9
B	-5	HIS	-	expression tag	UNP Q9P8C9
B	-4	HIS	-	expression tag	UNP Q9P8C9
B	-3	HIS	-	expression tag	UNP Q9P8C9

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9P8C9
B	-1	GLY	-	expression tag	UNP Q9P8C9
B	0	SER	-	expression tag	UNP Q9P8C9
C	-11	MET	-	expression tag	UNP Q9P8C9
C	-10	ARG	-	expression tag	UNP Q9P8C9
C	-9	GLY	-	expression tag	UNP Q9P8C9
C	-8	SER	-	expression tag	UNP Q9P8C9
C	-7	HIS	-	expression tag	UNP Q9P8C9
C	-6	HIS	-	expression tag	UNP Q9P8C9
C	-5	HIS	-	expression tag	UNP Q9P8C9
C	-4	HIS	-	expression tag	UNP Q9P8C9
C	-3	HIS	-	expression tag	UNP Q9P8C9
C	-2	HIS	-	expression tag	UNP Q9P8C9
C	-1	GLY	-	expression tag	UNP Q9P8C9
C	0	SER	-	expression tag	UNP Q9P8C9
D	-11	MET	-	expression tag	UNP Q9P8C9
D	-10	ARG	-	expression tag	UNP Q9P8C9
D	-9	GLY	-	expression tag	UNP Q9P8C9
D	-8	SER	-	expression tag	UNP Q9P8C9
D	-7	HIS	-	expression tag	UNP Q9P8C9
D	-6	HIS	-	expression tag	UNP Q9P8C9
D	-5	HIS	-	expression tag	UNP Q9P8C9
D	-4	HIS	-	expression tag	UNP Q9P8C9
D	-3	HIS	-	expression tag	UNP Q9P8C9
D	-2	HIS	-	expression tag	UNP Q9P8C9
D	-1	GLY	-	expression tag	UNP Q9P8C9
D	0	SER	-	expression tag	UNP Q9P8C9

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

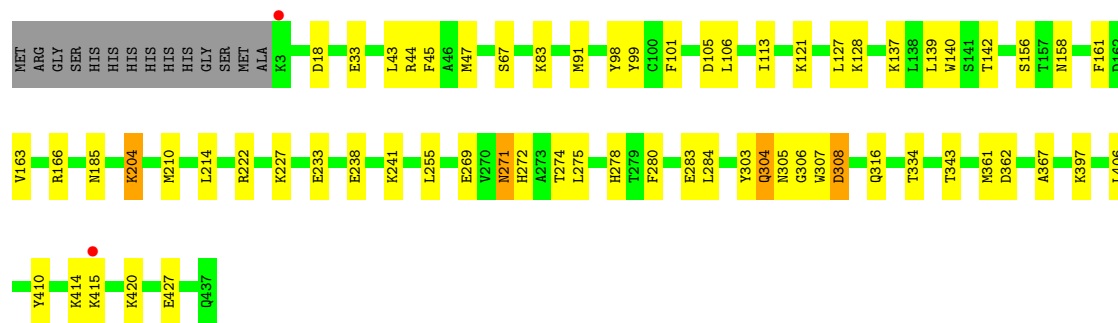
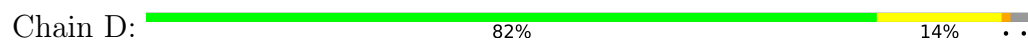


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			6	3 3		
3	A	1	Total	C O	0	0
			6	3 3		
3	B	1	Total	C O	0	0
			6	3 3		
3	C	1	Total	C O	0	0
			6	3 3		
3	D	1	Total	C O	0	0
			6	3 3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	42	Total	O	0	0
			42	42		
4	C	41	Total	O	0	0
			41	41		
4	D	54	Total	O	0	0
			54	54		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.47Å 126.42Å 171.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.38 – 2.70 37.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.4 (37.38-2.70) 91.5 (37.38-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.86 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.8.0218	Depositor
R, $R_{free}$	0.194 , 0.277 0.201 , 0.279	Depositor DCC
$R_{free}$ test set	2167 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1686e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 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: GOL, 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	0.53	0/3541	0.71	0/4768
1	B	0.54	0/3541	0.70	1/4768 (0.0%)
1	C	0.53	0/3541	0.71	0/4768
1	D	0.52	0/3541	0.72	0/4768
All	All	0.53	0/14164	0.71	1/19072 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	ARG	NE-CZ-NH1	5.02	122.81	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	3463	0	3346	29	0
1	B	3463	0	3346	32	0
1	C	3463	0	3346	24	0
1	D	3463	0	3346	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	12	0	15	3	0
3	B	6	0	7	3	0
3	C	6	0	7	1	0
3	D	6	0	7	2	0
4	A	53	0	0	1	0
4	B	42	0	0	0	0
4	C	41	0	0	0	0
4	D	54	0	0	0	0
All	All	14080	0	13420	104	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 4.

The worst 5 of 104 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:C:102:HIS:NE2	3:C:503:GOL:O2	2.16	0.77
1:A:102:HIS:NE2	3:A:503:GOL:H31	2.00	0.76
1:D:233:GLU:OE1	3:D:503:GOL:H32	1.95	0.67
1:D:280:PHE:CE2	1:D:284:LEU:HD11	2.33	0.64
1:B:233:GLU:OE1	3:B:503:GOL:C1	2.46	0.62

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	433/449 (96%)	411 (95%)	19 (4%)	3 (1%)	22 46
1	B	433/449 (96%)	410 (95%)	20 (5%)	3 (1%)	22 46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	433/449 (96%)	415 (96%)	16 (4%)	2 (0%)	29	54
1	D	433/449 (96%)	411 (95%)	20 (5%)	2 (0%)	29	54
All	All	1732/1796 (96%)	1647 (95%)	75 (4%)	10 (1%)	25	50

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	GLY
1	B	306	GLY
1	D	306	GLY
1	A	238	GLU
1	B	314	ILE

### 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	357/368 (97%)	330 (92%)	27 (8%)	13	30
1	B	357/368 (97%)	336 (94%)	21 (6%)	19	43
1	C	357/368 (97%)	333 (93%)	24 (7%)	16	37
1	D	357/368 (97%)	332 (93%)	25 (7%)	15	35
All	All	1428/1472 (97%)	1331 (93%)	97 (7%)	16	36

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	222	ARG
1	C	422	THR
1	C	227	LYS
1	C	279	THR
1	D	67	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	408	GLN
1	C	185	ASN
1	D	305	ASN
1	C	119	ASN
1	C	242	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z  > 2$
3	GOL	C	503	2	5,5,5	0.45	0	5,5,5	0.63	0
3	GOL	B	503	2	5,5,5	0.21	0	5,5,5	0.34	0
3	GOL	D	503	2	5,5,5	0.31	0	5,5,5	0.88	0
3	GOL	A	504	-	5,5,5	0.47	0	5,5,5	0.46	0
3	GOL	A	503	2	5,5,5	0.36	0	5,5,5	0.67	0

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
3	GOL	C	503	2	-	2/4/4/4	-
3	GOL	B	503	2	-	4/4/4/4	-
3	GOL	D	503	2	-	2/4/4/4	-
3	GOL	A	504	-	-	0/4/4/4	-
3	GOL	A	503	2	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
3	B	503	GOL	O2-C2-C3-O3
3	C	503	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	GOL	1	0
3	B	503	GOL	3	0
3	D	503	GOL	2	0
3	A	504	GOL	1	0
3	A	503	GOL	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	435/449 (96%)	-0.44	1 (0%) 95 96	10, 16, 26, 54	0
1	B	435/449 (96%)	-0.36	1 (0%) 95 96	11, 18, 29, 60	0
1	C	435/449 (96%)	-0.34	2 (0%) 91 92	9, 18, 29, 65	0
1	D	435/449 (96%)	-0.36	2 (0%) 91 92	9, 16, 28, 52	0
All	All	1740/1796 (96%)	-0.38	6 (0%) 94 95	9, 17, 28, 65	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	114	GLU	2.8
1	B	8	GLN	2.6
1	A	3	LYS	2.3
1	D	415	LYS	2.3
1	C	8	GLN	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	504	6/6	0.83	0.19	44,46,47,48	0
3	GOL	C	503	6/6	0.90	0.23	32,33,35,38	0
2	MN	B	502	1/1	0.93	0.10	53,53,53,53	0
3	GOL	A	503	6/6	0.93	0.19	30,30,30,31	0
3	GOL	B	503	6/6	0.94	0.26	35,37,37,41	0
3	GOL	D	503	6/6	0.94	0.20	38,39,39,42	0
2	MN	A	502	1/1	0.96	0.08	36,36,36,36	0
2	MN	D	502	1/1	0.97	0.10	37,37,37,37	0
2	MN	B	501	1/1	0.97	0.06	34,34,34,34	0
2	MN	A	501	1/1	0.97	0.08	47,47,47,47	0
2	MN	C	501	1/1	0.98	0.07	27,27,27,27	0
2	MN	C	502	1/1	0.98	0.06	41,41,41,41	0
2	MN	D	501	1/1	0.99	0.04	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.