



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 08:09 AM BST

PDB ID : 1XIN
Title : PROTEIN ENGINEERING OF XYLOSE (GLUCOSE) ISOMERASE FROM ACTINOPLANES MISSOURIENSIS. 1. CRYSTALLOGRAPHY AND SITE-DIRECTED MUTAGENESIS OF METAL BINDING SITES
Authors : Janin, J.
Deposited on : 1992-04-06
Resolution : 2.40 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

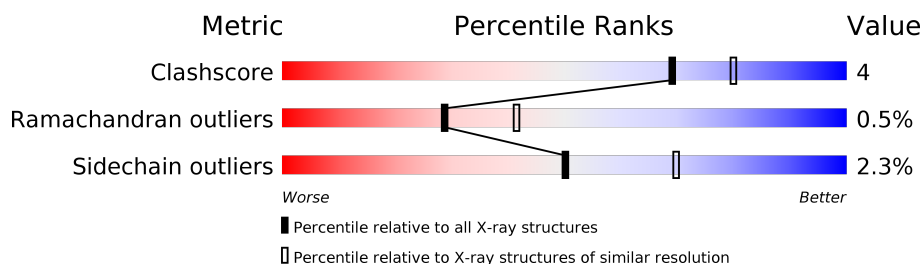
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 ≥ 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	393	
1	B	393	
1	C	393	
1	D	393	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13137 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.

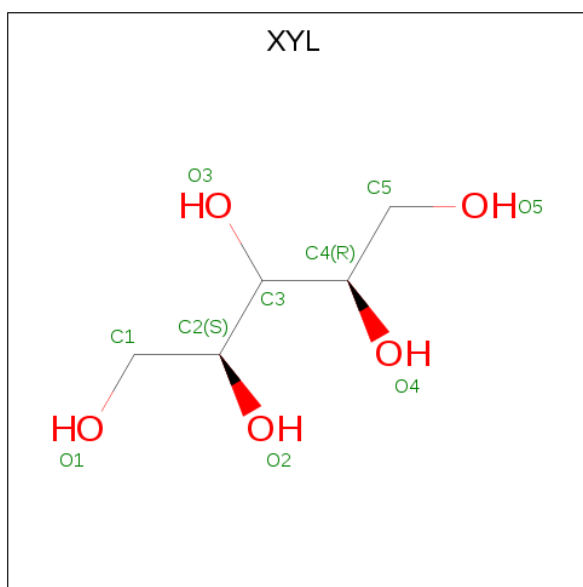
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	B	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	C	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	D	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	ASN	HIS	conflict	UNP P12851
B	220	ASN	HIS	conflict	UNP P12851
C	220	ASN	HIS	conflict	UNP P12851
D	220	ASN	HIS	conflict	UNP P12851

- Molecule 2 is Xylitol (three-letter code: XYL) (formula: C₅H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	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	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		

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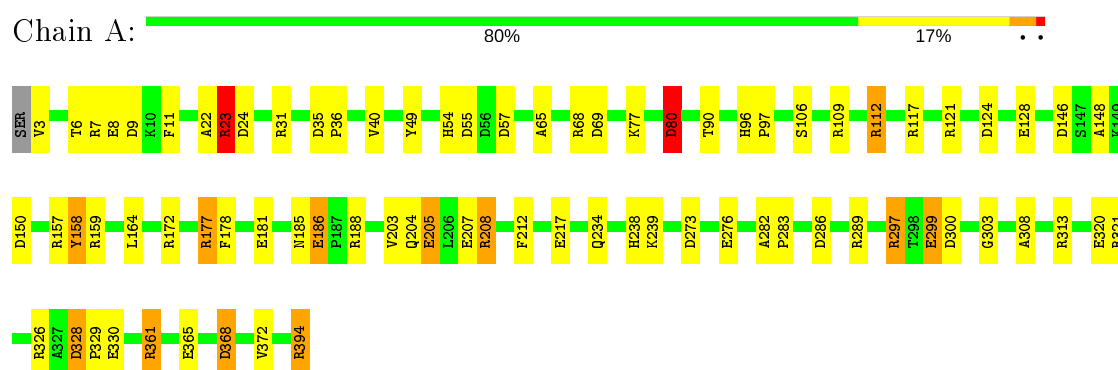
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	217	Total 217	O 217	0	0
4	C	232	Total 232	O 232	0	0
4	D	220	Total 220	O 220	0	0

3 Residue-property plots

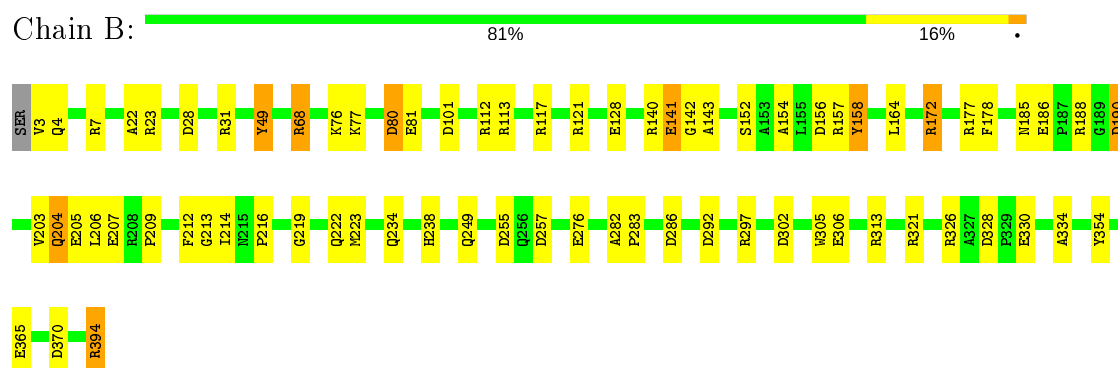
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

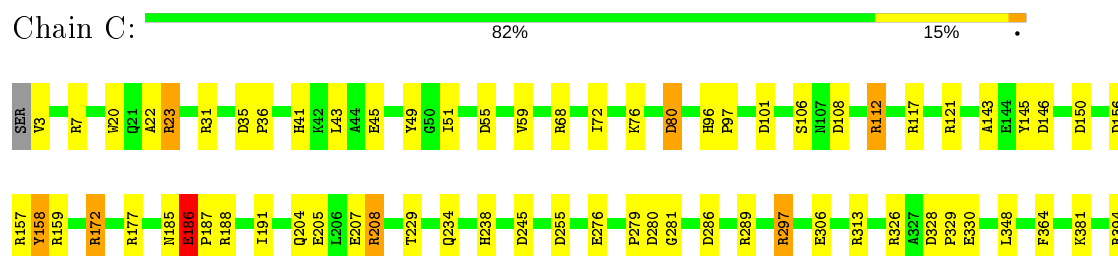
• Molecule 1: D-XYLOSE ISOMERASE



• Molecule 1: D-XYLOSE ISOMERASE



• Molecule 1: D-XYLOSE ISOMERASE



• Molecule 1: D-XYLOSE ISOMERASE

Chain D:

81%

16%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.45Å 143.45Å 231.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13137	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: MG, XYZ

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	0.83	0/3122	1.75	71/4229 (1.7%)
1	B	0.83	0/3122	1.77	56/4229 (1.3%)
1	C	0.83	1/3122 (0.0%)	1.69	55/4229 (1.3%)
1	D	0.84	0/3122	1.74	58/4229 (1.4%)
All	All	0.83	1/12488 (0.0%)	1.74	240/16916 (1.4%)

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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	GLU	CD-OE2	-5.38	1.19	1.25

The worst 5 of 240 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ARG	NE-CZ-NH1	20.25	130.42	120.30
1	B	172	ARG	NE-CZ-NH1	18.18	129.39	120.30
1	B	394	ARG	NE-CZ-NH2	-17.48	111.56	120.30
1	B	157	ARG	NE-CZ-NH1	15.69	128.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ARG	NE-CZ-NH2	-15.12	112.74	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	B	172	ARG	Sidechain
1	C	172	ARG	Sidechain
1	D	208	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	3051	0	2953	26	0
1	B	3051	0	2953	28	0
1	C	3051	0	2953	21	0
1	D	3051	0	2953	24	0
2	A	10	0	12	0	0
2	B	10	0	12	1	0
2	C	10	0	11	1	0
2	D	10	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	220	0	0	1	0
4	B	217	0	0	2	0
4	C	232	0	0	2	0
4	D	220	0	0	4	0
All	All	13137	0	11859	89	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 89 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:204:GLN:OE1	1:C:204:GLN:OE1	1.65	1.13
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.70	1.08
1:D:208:ARG:HH11	1:D:208:ARG:HG2	1.27	1.00
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.18	0.92
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.19	0.87

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	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	41	55
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	41	55
1	C	390/393 (99%)	374 (96%)	12 (3%)	4 (1%)	15	23
1	D	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	29	41
All	All	1560/1572 (99%)	1504 (96%)	48 (3%)	8 (0%)	29	41

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	279	PRO

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	306/310 (99%)	297 (97%)	9 (3%)	42	62
1	B	306/310 (99%)	301 (98%)	5 (2%)	62	79
1	C	306/310 (99%)	301 (98%)	5 (2%)	62	79
1	D	306/310 (99%)	297 (97%)	9 (3%)	42	62
All	All	1224/1240 (99%)	1196 (98%)	28 (2%)	50	70

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	185	ASN
1	C	49	TYR
1	D	208	ARG
1	B	394	ARG
1	C	3	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	238	HIS
1	C	41	HIS
1	C	238	HIS
1	B	204	GLN
1	C	222	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	C	397	3	9,9,9	0.55	0	11,11,11	1.70	2 (18%)
2	XYL	A	397	3	9,9,9	0.53	0	11,11,11	1.43	1 (9%)
2	XYL	D	397	3	9,9,9	0.55	0	11,11,11	1.76	3 (27%)
2	XYL	B	397	3	9,9,9	0.48	0	11,11,11	2.29	4 (36%)

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	C	397	3	-	0/12/12/12	-
2	XYL	A	397	3	-	1/12/12/12	-
2	XYL	D	397	3	-	2/12/12/12	-
2	XYL	B	397	3	-	2/12/12/12	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XYL	O4-C4-C3	4.81	120.80	109.10
2	B	397	XYL	C1-C2-C3	4.57	122.32	112.41
2	A	397	XYL	O4-C4-C3	3.77	118.25	109.10
2	D	397	XYL	C5-C4-C3	3.76	120.56	112.41
2	C	397	XYL	O4-C4-C3	3.69	118.07	109.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	397	XYL	O4-C4-C5-O5
2	D	397	XYL	C2-C3-C4-C5
2	A	397	XYL	O4-C4-C5-O5
2	B	397	XYL	O3-C3-C4-C5
2	D	397	XYL	O3-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	397	XYL	1	0
2	B	397	XYL	1	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 ⓘ

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.