



wwPDB Geometry-Only Validation Summary Report ⓘ

May 23, 2024 – 09:35 AM EDT

PDB ID : 3CWH
Title : D-xylose Isomerase in complex with linear product, per-deuterated xylulose
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Deposited on : 2008-04-21
Resolution : 2.20 Å(reported)

This is a wwPDB Geometry-Only 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 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)
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) : 2.36.2

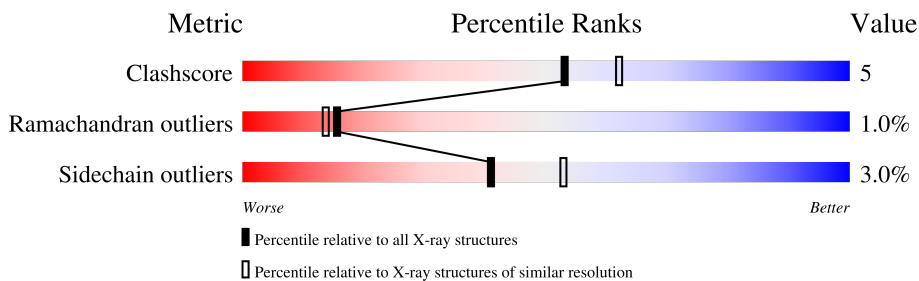
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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](#)

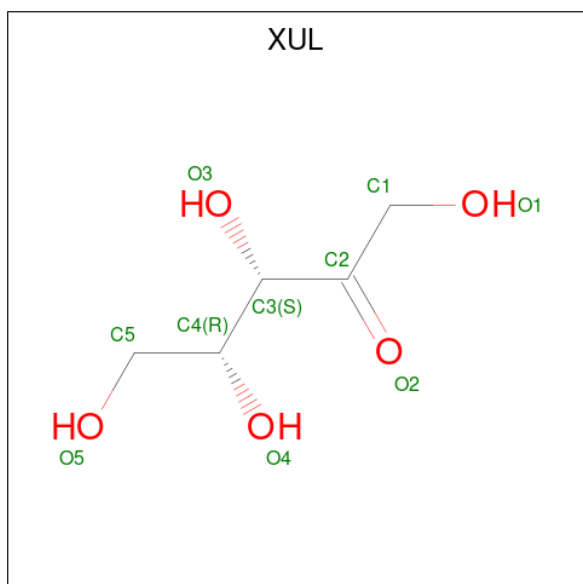
There are 5 unique types of molecules in this entry. The entry contains 6674 atoms, of which 2244 are hydrogens and 1144 are deuteriums.

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	D	H	N	O	S			
1	A	387	5970	1913	680	2244	550	575	8	67	0	0

- Molecule 2 is D-XYLULOSE (three-letter code: XUL) (formula: $C_5H_{10}O_5$).

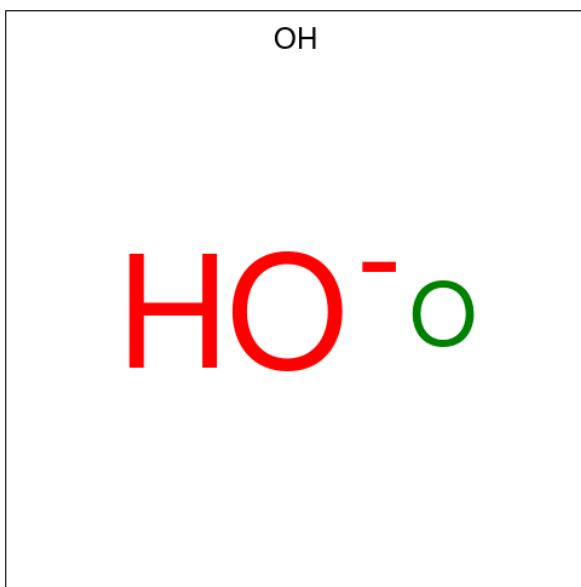


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	D	O		
2	A	1	19	5	9	5	0	0

- 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 HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	D	O	0	0
			2	1	1		

- Molecule 5 is water.


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	227	Total	D	O	0	0
			681	454	227		

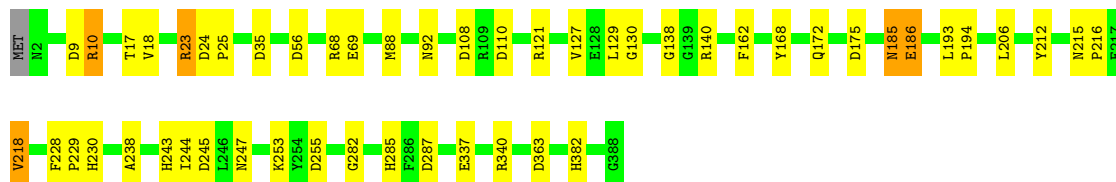
3 Residue-property plots [i](#)

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

Chain A:  87% 12% .



4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OH, XUL, DOD, MG

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	0.38	0/3118	0.60	3/4219 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	287	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	287	ASP	CB-CG-OD2	-5.16	113.66	118.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	3726	2244	2914	31	0
2	A	19	0	10	1	0
3	A	2	0	0	0	0
4	A	2	0	0	1	0
5	A	681	0	0	9	3
All	All	4430	2244	2924	32	3

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 5.

The worst 5 of 32 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:218:VAL:HB	1:A:247:ASN:OD1	1.81	0.76
1:A:68:ARG:NH2	5:A:1057:DOD:O	2.19	0.75
1:A:129:LEU:O	5:A:1153:DOD:O	2.09	0.70
1:A:121:ARG:NE	5:A:1111:DOD:O	2.34	0.60
1:A:215:ASN:OD1	1:A:243:HIS:ND1	2.40	0.55

All (3) 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)
5:A:1133:DOD:O	5:A:1155:DOD:D2[4_566]	1.55	0.65
5:A:1038:DOD:D1	5:A:1094:DOD:O[4_566]	1.57	0.63
5:A:1087:DOD:O	5:A:1198:DOD:D2[3_556]	1.59	0.61

4.3 Torsion angles [i](#)

4.3.1 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	385/388 (99%)	356 (92%)	25 (6%)	4 (1%)	15 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	VAL
1	A	186	GLU
1	A	253	LYS
1	A	282	GLY

4.3.2 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	303/304 (100%)	294 (97%)	9 (3%)	41 53

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
1	A	363	ASP
1	A	35	ASP
1	A	69	GLU
1	A	175	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	234	GLN
1	A	348	GLN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - 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	XUL	A	401	3	7,9,9	3.19	2 (28%)	5,11,11	1.50	1 (20%)

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	XUL	A	401	3	-	3/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	XUL	O2-C2	7.66	1.34	1.21
2	A	401	XUL	C1-C2	2.01	1.56	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	XUL	O4-C4-C5	-2.08	104.26	109.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	XUL	O2-C2-C3-O3
2	A	401	XUL	O4-C4-C5-O5
2	A	401	XUL	C3-C4-C5-O5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	XUL	1	0

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.