



Full wwPDB Geometry-Only Validation Report ⓘ

May 29, 2020 – 06:23 pm BST

PDB ID : 3CWH
Title : D-xylose Isomerase in complex with linear product, per-deuterated xylulose
Authors : Kovalevsky, A.Y.; Langan, P.; Glusker, J.P.
Deposited on : 2008-04-21
Resolution : 2.20 Å(reported)

This is a Full wwPDB Geometry-Only Validation 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)
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) : 2.11

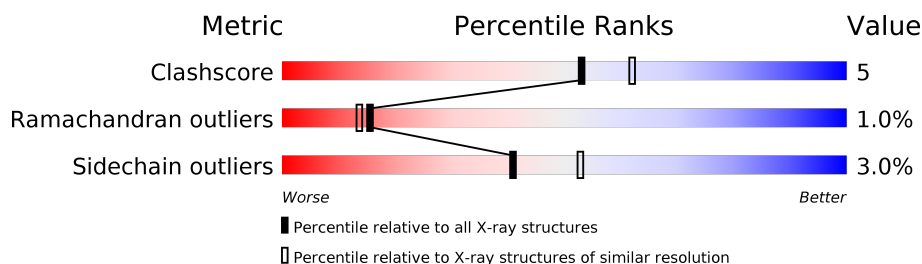
1 Overall quality at a glance

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 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	388	 87% 12%

2 Entry composition

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

- Molecule 2 is a ligand with the chemical component id XUL but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for XUL. ERROR THIS SHOULD NOT HAPPEN FOLLOWING ANNOTATION.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	D	O	0	0
			19	5	9	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 a ligand with the chemical component id OH but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for OH. ERROR THIS SHOULD NOT HAPPEN FOLLOWING ANNOTATION.

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

- Molecule 5 is water.

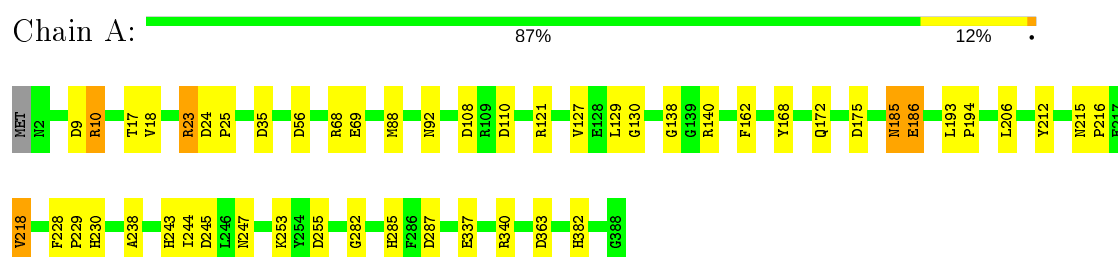
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	227	Total	D	O	0	0
			681	454	227		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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. 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 Model quality [i](#)

4.1 Standard geometry [i](#)

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

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($^{\circ}$)	Ideal($^{\circ}$)
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.

All (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
1:A:186:GLU:OE1	1:A:255:ASP:HB3	2.02	0.55
1:A:140:ARG:NH1	5:A:1006:DOD:O	2.41	0.53
2:A:401:XUL:C1	4:A:501:OH:O	2.59	0.50
1:A:162:PHE:O	1:A:212:TYR:OH	2.30	0.49
1:A:215:ASN:N	1:A:216:PRO:HD3	2.23	0.48
1:A:215:ASN:OD1	1:A:243:HIS:HB3	2.08	0.48
1:A:228:PHE:HB3	1:A:229:PRO:HD3	1.85	0.47
1:A:108:ASP:HB3	1:A:110:ASP:OD1	2.09	0.47
1:A:382:HIS:CE1	5:A:1049:DOD:O	2.69	0.46
1:A:244:ILE:O	1:A:285:HIS:HB3	2.11	0.45
1:A:17:THR:OG1	1:A:18:VAL:N	2.51	0.44
1:A:23:ARG:C	1:A:23:ARG:CD	2.86	0.44
1:A:337:GLU:HG2	1:A:340:ARG:NH2	2.28	0.43
1:A:88:MET:HE2	5:A:1119:DOD:O	2.12	0.43
1:A:9:ASP:O	1:A:10:ARG:HB2	2.12	0.43
1:A:206:LEU:HB3	5:A:1159:DOD:O	2.14	0.42
1:A:56:ASP:OD2	1:A:92:ASN:HB3	2.14	0.42
1:A:138:GLY:O	5:A:1002:DOD:O	2.25	0.41
1:A:127:VAL:O	1:A:130:GLY:N	2.53	0.41
1:A:215:ASN:N	1:A:216:PRO:CD	2.83	0.41
1:A:23:ARG:HD3	1:A:24:ASP:N	2.31	0.41
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.76	0.40
1:A:88:MET:C	1:A:88:MET:SD	3.00	0.40
1:A:193:LEU:N	1:A:194:PRO:CD	2.84	0.40
1:A:238:ALA:HB2	5:A:1133:DOD:O	2.15	0.40
1:A:168:TYR:O	1:A:172:GLN:HG2	2.16	0.40
1:A:185:ASN:O	1:A:186:GLU:HB3	2.17	0.40

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

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	23	ARG
1	A	25	PRO
1	A	35	ASP
1	A	69	GLU
1	A	175	ASP
1	A	185	ASN
1	A	230	HIS
1	A	363	ASP

Some 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 carbohydrates in this entry.

4.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.