



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:09 AM UTC

PDB ID : 3KCL / pdb_00003kcl
Title : Room temperature neutron structure of D-Xylose Isomerase in complex with two Cd²⁺ cations and d12-D-alpha-glucose in the ring form (refined jointly with X-ray structure 3KBM)
Authors : Kovalevsky, A.Y.; Langan, P.
Deposited on : 2009-10-21
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

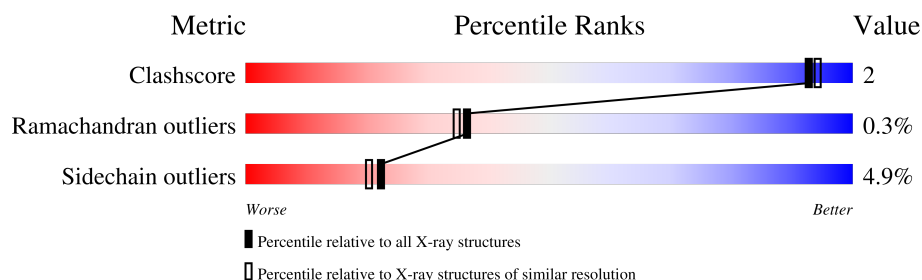
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION, X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	388	 93% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6606 atoms, of which 2252 are hydrogens and 1087 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.

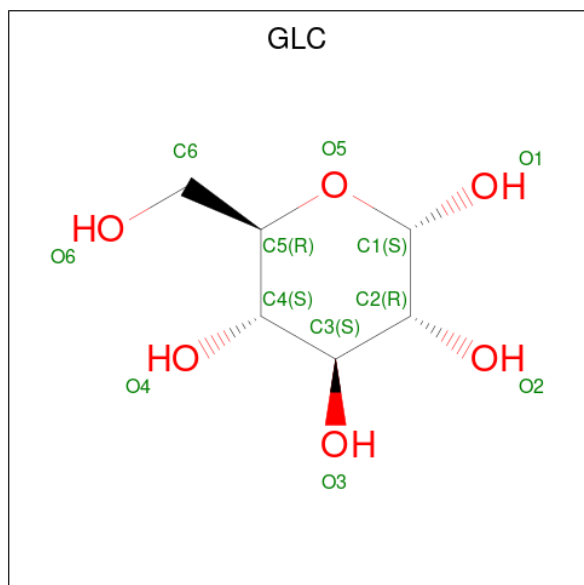
- Molecule 1 is a protein called Xylose isomerase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	388	5983	1918	677	2252	551	576	9	174	0	0

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cd	0	0
			2	2		

- Molecule 3 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	D	O	0	0
			24	6	12	6		

- Molecule 4 is water.

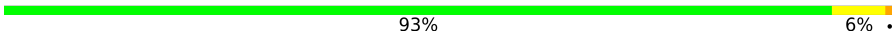
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	199	Total 597	D 398	O 199	0	0

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 failed to run properly.

- Molecule 1: Xylose isomerase

Chain A:  93% 6% •



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.20Å 99.43Å 102.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.01Å)	Xtriage
Refinement program	nCNS	Depositor
R, R_{free}	0.188 , 0.211	Depositor
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.301	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,-l,-k	Xtriage
Total number of atoms	6606	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOD, CD, GLC

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	0.61	2/3126 (0.1%)	0.97	9/4229 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	ARG	CZ-NH1	-5.31	1.25	1.32
1	A	387	ARG	CD-NE	-5.04	1.39	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	VAL	CB-CA-C	-11.76	93.94	112.16
1	A	387	ARG	NE-CZ-NH2	-7.99	112.01	119.20
1	A	24	ASP	CA-C-N	-7.11	112.48	119.87
1	A	24	ASP	C-N-CA	-7.11	112.48	119.87
1	A	146	GLY	N-CA-C	6.97	122.37	113.24
1	A	54	HIS	N-CA-C	-6.93	99.02	110.17
1	A	98	VAL	N-CA-CB	6.54	121.83	110.65
1	A	111	VAL	N-CA-CB	5.84	121.34	110.77
1	A	194	PRO	N-CA-C	5.72	121.02	113.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	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	3731	2252	2926	8	0
2	A	2	0	0	0	0
3	A	24	0	10	1	0
4	A	597	0	0	3	0
All	All	4354	2252	2936	9	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 2.

All (9) 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)
3:A:401:GLC:H62	4:A:1106:DOD:O	1.87	0.69
1:A:42:ARG:HE	1:A:42:ARG:HA	1.71	0.46
1:A:37:VAL:O	1:A:41:ARG:HG3	2.10	0.46
1:A:76:ARG:HD2	4:A:1181:DOD:O	2.10	0.45
1:A:387:ARG:O	1:A:388:GLY:OXT	2.35	0.45
1:A:42:ARG:HA	1:A:42:ARG:NE	2.26	0.44
1:A:251:GLY:HA3	4:A:1167:DOD:O	2.11	0.44
1:A:24:ASP:HB2	1:A:25:PRO:CD	2.46	0.41
1:A:354:ARG:HA	1:A:358:GLU:OE1	2.16	0.40

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	386/388 (100%)	374 (97%)	11 (3%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	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	304/304 (100%)	289 (95%)	15 (5%)	22	20

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLN
1	A	8	GLU
1	A	10	ARG
1	A	42	ARG
1	A	65	ASP
1	A	66	SER
1	A	67	GLU
1	A	69	GLU
1	A	91	THR

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Mol	Chain	Res	Type
1	A	98	VAL
1	A	111	VAL
1	A	169	VAL
1	A	253	LYS
1	A	328	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - 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
3	GLC	A	401	2	12,12,12	1.56	2 (16%)	17,17,17	1.20	2 (11%)

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	GLC	A	401	2	-	2/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GLC	C4-C5	3.43	1.60	1.53
3	A	401	GLC	C4-C3	3.00	1.60	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	GLC	O4-C4-C3	-2.71	103.98	110.38
3	A	401	GLC	C4-C3-C2	-2.01	107.30	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GLC	C4-C5-C6-O6
3	A	401	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GLC	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 [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.