



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6QRV / pdb_00006qrv
Title : X-ray radiation dose series on xylose isomerase - 2.63 MGy
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Deposited on : 2019-02-19
Resolution : 1.17 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 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	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

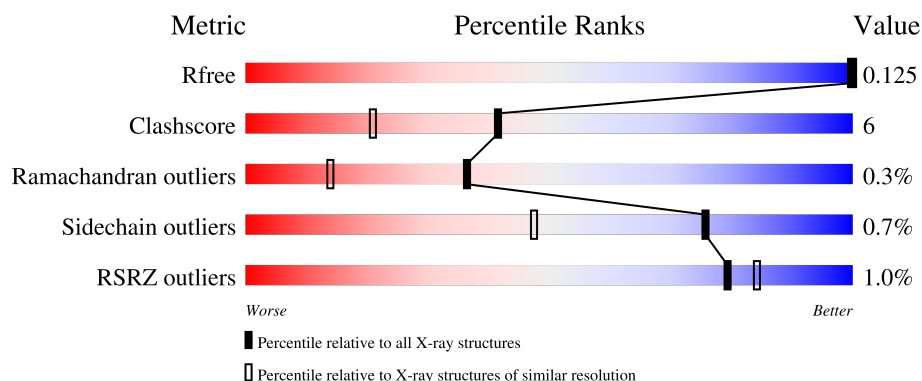
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.17 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}	1800	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7743 atoms, of which 3575 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	H	N	O	S			
1	A	387	7055	2254	3483	636	671	11	0	94	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	GLN	conflict	UNP P24300
A	8	VAL	GLU		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	1
			20	4	12	4		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 4	Mn 4	0	2

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Mg 2	0	1

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Na 2	0	0

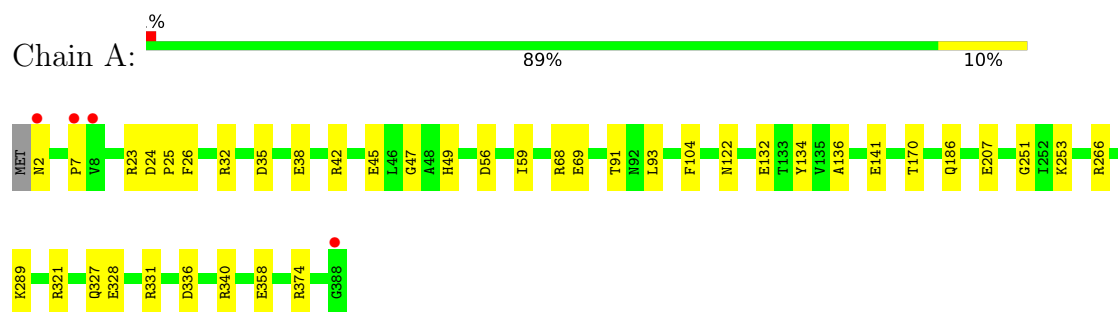
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	526	Total 528	O 528	0	2

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Xylose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.57Å 97.58Å 102.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.72 – 1.17 38.72 – 1.17	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.72-1.17) 99.3 (38.72-1.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.17Å)	Xtriage
Refinement program	PHENIX (1.14_3247: ???)	Depositor
R, R_{free}	0.104 , 0.124 0.105 , 0.125	Depositor DCC
R_{free} test set	7724 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtri

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: MG, EDO, NA, MN, IPA

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	0.39	0/3905	0.61	0/5278

There are no bond length outliers.

There are no bond angle outliers.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:412[A]:EDO:O1	7:A:501:HOH:O	1.67	1.11
1:A:289[B]:LYS:NZ	7:A:514:HOH:O	2.07	0.85
1:A:328[A]:GLU:OE2	7:A:505:HOH:O	1.95	0.84
1:A:47:GLY:O	7:A:506:HOH:O	1.98	0.82
1:A:56[B]:ASP:OD2	7:A:508:HOH:O	2.00	0.78

All (4) 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)
7:A:932:HOH:O	7:A:953:HOH:O[7_545]	1.98	0.22
1:A:23[A]:ARG:HH12	7:A:615:HOH:O[3_556]	1.54	0.06
7:A:534:HOH:O	7:A:936:HOH:O[3_556]	2.15	0.05
7:A:962:HOH:O	7:A:996:HOH:O[4_566]	2.18	0.02

5.3 Torsion angles ⓘ

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	384/303 (127%)	381 (99%)	3 (1%)	73 43

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69[A]	GLU
1	A	69[B]	GLU
1	A	91	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	411[B]	-	3,3,3	0.41	0	2,2,2	0.38	0
2	EDO	A	410	-	3,3,3	0.36	0	2,2,2	0.52	0
2	EDO	A	407[A]	-	3,3,3	0.34	0	2,2,2	0.12	0
2	EDO	A	401	4,5	3,3,3	0.45	0	2,2,2	0.45	0
2	EDO	A	403	-	3,3,3	0.30	0	2,2,2	0.67	0
3	IPA	A	413	-	3,3,3	0.50	0	3,3,3	0.32	0
2	EDO	A	402	-	3,3,3	0.22	0	2,2,2	0.86	0
2	EDO									

Mol	Chain	Res	Type	Atoms
2	A	409	EDO	O1-C1-C2-O2
2	A	411[B]	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	406	EDO	1	0
2	A	410	EDO	1	0
3	A	413	IPA	1	0
2	A	407[B]	EDO	1	0
2	A	412[A]	EDO	4	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, 95th 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 ²)	Q<0.9
1	A	387/388 (99%)	-0.56	4 (1%) 79 84	5, 13, 24, 62	69 (17%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	GLY	5.7
1	A	8[A]	VAL	5.6
1	A	7[A]	PRO	2.4
1	A	2	ASN	2.2

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IPA	A	413	4/4	0.84	0.14	39,47,48,48	12
2	EDO	A	412[A]	4/4	0.91	0.16	14,19,22,22	10
2	EDO	A	405	4/4	0.92	0.10	20,24,27,29	10
2	EDO	A	410	4/4	0.92	0.12	37,45,49,50	10
2	EDO	A	404	4/4	0.93	0.12	16,19,23,23	10
2	EDO	A	403	4/4	0.93	0.08	22,26,31,31	10
2	EDO	A	411[A]	4/4	0.96	0.08	17,21,25,25	10
2	EDO	A	411[B]	4/4	0.96	0.08	30,36,36,36	10
2	EDO	A	407[B]	4/4	0.96	0.08	23,28,28,30	10
2								