



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:45 PM UTC

PDB ID : 1OAD / pdb\_00001oad  
Title : Glucose isomerase from Streptomyces rubiginosus in P21212 crystal form  
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Deposited on : 2003-01-08  
Resolution : 1.50 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](mailto: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>.

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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

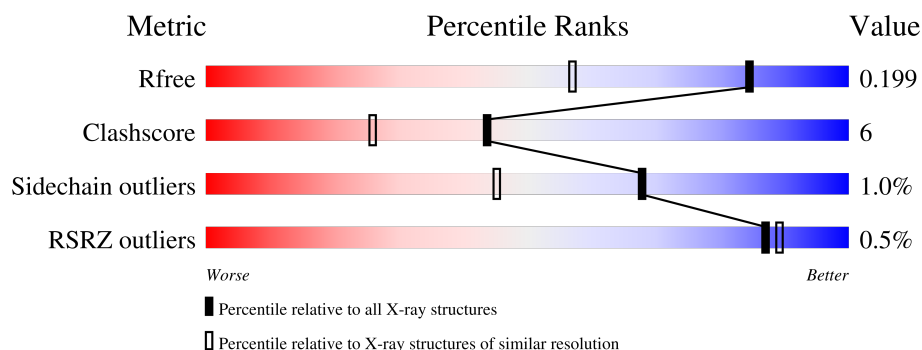
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>44%</div> <div>.</div> </div> </div>
1	B	388	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7120 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	5	0
			3060	1922	552	577	9			
1	B	386	Total	C	N	O	S	0	13	0
			3095	1941	560	585	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	GLN	conflict	UNP P24300
B	21	GLU	GLN	conflict	UNP P24300

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

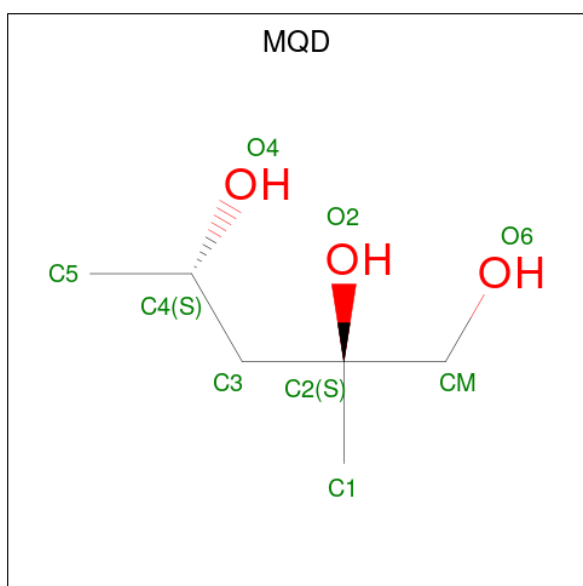
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is 2-METHYLPENTANE-1,2,4-TRIOL (CCD ID: MQD) (formula:  $C_6H_{14}O_3$ ).



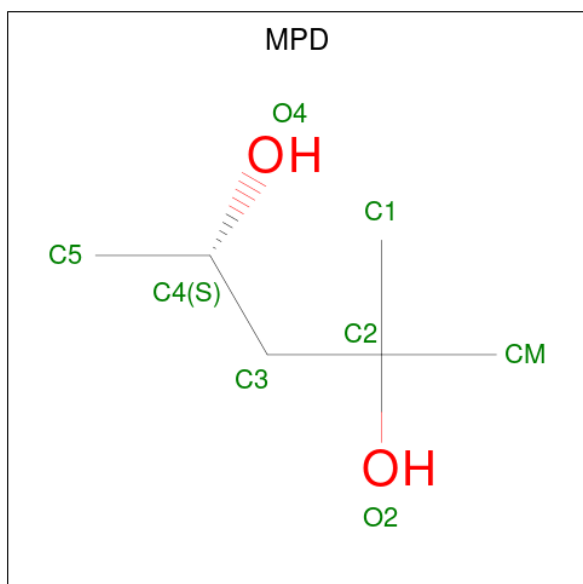
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	6	3		
5	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	8	4	1	3	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	8	6	2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	474	Total 474	O 474	1	0
8	B	437	Total 437	O 437	0	0



A344	D346	G346	L347	Q348	A349	L350	R354	S355	A356	V362	D363	A364	A365	R368	A371	R374	L375	D376	Q377	L378	D381	H382	R387	GLY
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.45Å 129.59Å 78.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 20.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-1.50) 97.9 (20.00-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.71 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.163 , 0.186 (Not available) , 0.199	Depositor DCC
$R_{free}$ test set	7880 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.7	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MQD, MN, TRS, MRD, MG, MPD

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	1.79	42/3158 (1.3%)	2.52	224/4270 (5.2%)
1	B	1.70	31/3231 (1.0%)	2.48	259/4368 (5.9%)
All	All	1.74	73/6389 (1.1%)	2.50	483/8638 (5.6%)

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	ARG	NE-CZ	9.42	1.43	1.33
1	A	201	ALA	C-O	7.65	1.33	1.24
1	A	14	GLY	C-O	7.34	1.31	1.23
1	A	307	MET	C-N	7.20	1.43	1.33
1	B	220	HIS	CE1-NE2	7.05	1.39	1.32

The worst 5 of 483 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	GLN	O-C-N	14.38	137.36	122.12
1	A	247	ASN	OD1-CG-ND2	13.01	135.61	122.60
1	B	306	CYS	O-C-N	12.88	135.34	122.07
1	B	157	ARG	NE-CZ-NH1	12.41	133.91	121.50
1	A	292	ARG	NE-CZ-NH1	-12.33	109.17	121.50

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 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	3060	0	2925	34	0
1	B	3095	0	2955	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	14	0	0
4	B	8	0	14	0	0
5	A	9	0	14	1	0
5	B	9	0	14	0	0
6	A	8	0	12	0	0
7	B	8	0	14	5	0
8	A	474	0	0	11	1
8	B	437	0	0	9	0
All	All	7120	0	5962	74	1

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 6.

The worst 5 of 74 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:B:132[B]:GLU:HG3	8:B:2187:HOH:O	1.28	1.26
1:A:10[B]:ARG:HH21	1:A:284:ARG:NH1	1.35	1.24
1:A:10[B]:ARG:NH2	1:A:284:ARG:NH1	1.86	1.23
1:A:10[B]:ARG:HH21	1:A:284:ARG:CZ	1.64	1.09
1:B:132[B]:GLU:OE2	8:B:2188:HOH:O	1.77	1.00

All (1) 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)
8:A:2136:HOH:O	8:A:2233:HOH:O[2_665]	2.08	0.12

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 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	307/304 (101%)	303 (99%)	4 (1%)	61	35
1	B	315/304 (104%)	311 (99%)	4 (1%)	61	35
All	All	622/608 (102%)	614 (99%)	8 (1%)	68	35

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	245	ASP
1	B	66	SER
1	B	42[A]	ARG
1	A	245	ASP
1	B	42[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	HIS
1	B	172	GLN

### 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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
4	MRD	A	394	-	7,7,7	0.66	0	9,10,10	0.98	0
5	MQD	B	395	3	7,8,8	0.96	1 (14%)	6,11,11	1.10	0
7	MPD	B	396	-	7,7,7	0.94	0	9,10,10	2.25	4 (44%)
6	TRS	A	396	-	7,7,7	0.99	0	9,9,9	1.61	2 (22%)
5	MQD	A	395	3	7,8,8	0.74	0	6,11,11	0.96	0
4	MRD	B	394	-	7,7,7	0.47	0	9,10,10	0.88	0

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
4	MRD	A	394	-	-	2/5/5/5	-
5	MQD	B	395	3	-	1/8/8/8	-
7	MPD	B	396	-	-	3/5/5/5	-
6	TRS	A	396	-	-	0/9/9/9	-
5	MQD	A	395	3	-	5/8/8/8	-
4	MRD	B	394	-	-	1/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	395	MQD	C1-C2	2.05	1.54	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	396	MPD	O2-C2-C1	4.08	120.72	107.99
6	A	396	TRS	C3-C-N	3.37	116.78	108.17
7	B	396	MPD	O2-C2-CM	3.22	118.03	107.99
6	A	396	TRS	C3-C-C1	-2.82	103.14	110.66
7	B	396	MPD	C1-C2-C3	-2.60	98.96	110.20

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	395	MQD	C1-C2-CM-O6
5	A	395	MQD	O2-C2-CM-O6
4	B	394	MRD	O2-C2-C3-C4
5	A	395	MQD	C3-C2-CM-O6
5	A	395	MQD	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	396	MPD	5	0
5	A	395	MQD	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	387/388 (99%)	-0.61	2 (0%) 87 89	8, 13, 24, 34	4 (1%)
1	B	386/388 (99%)	-0.55	2 (0%) 87 89	8, 14, 27, 44	12 (3%)
All	All	773/776 (99%)	-0.58	4 (0%) 87 89	8, 13, 26, 44	16 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	PRO	3.4
1	A	25	PRO	3.3
1	B	296	PHE	3.2
1	A	2	ASN	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MPD	B	396	8/8	0.80	0.27	5,20,28,33	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MRD	A	394	8/8	0.83	0.14	24,31,38,38	0
6	TRS	A	396	8/8	0.87	0.11	28,30,32,35	0
4	MRD	B	394	8/8	0.92	0.09	21,27,32,34	0
5	MQD	A	395	9/9	0.93	0.10	18,25,27,27	0
5	MQD	B	395	9/9	0.94	0.09	21,24,25,29	0
3	MG	A	392	1/1	0.99	0.03	11,11,11,11	0
3	MG	B	392	1/1	0.99	0.04	12,12,12,12	0
2	MN	A	390	1/1	1.00	0.01	14,14,14,14	0
2	MN	B	390	1/1	1.00	0.03	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.