

wwPDB X-ray Structure Validation Summary Report (i)

May 24, 2020 – 01:46 am BST

PDB ID : 3D51

Title : GOLGI MANNOSIDASE II complex with gluco-hydroxyiminolactam

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Deposited on : 2008-05-15

Resolution : 1.43 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

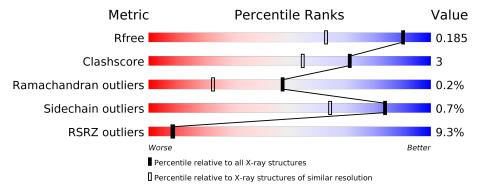
Ideal geometry (DNA, RNA) : Parkinson et al. (1996) Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.43 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	$egin{aligned} ext{Whole archive} \ (\# ext{Entries}) \end{aligned}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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 <=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		
			9%		
1	A	1045	91%	6%	- ∣



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9408 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 Alpha-mannosidase 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	1016	Total 8259	C 5257	N 1443	O 1517	S 42	6	12	0

There are 13 discrepancies between the modelled and reference sequences:

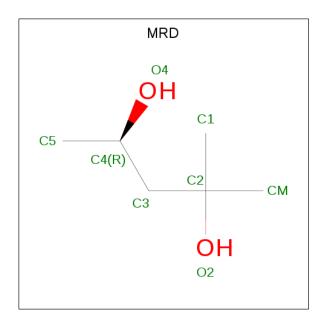
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	=	EXPRESSION TAG	UNP Q24451
A	2	SER	-	EXPRESSION TAG	UNP Q24451
A	3	SER	_	EXPRESSION TAG	UNP Q24451
A	4	HIS	_	EXPRESSION TAG	UNP Q24451
A	5	HIS	_	EXPRESSION TAG	UNP Q24451
A	6	HIS	_	EXPRESSION TAG	UNP Q24451
A	7	HIS	_	EXPRESSION TAG	UNP Q24451
A	8	HIS	_	EXPRESSION TAG	UNP Q24451
A	9	HIS	_	EXPRESSION TAG	UNP Q24451
A	10	GLY	_	EXPRESSION TAG	UNP Q24451
A	11	GLU	-	EXPRESSION TAG	UNP Q24451
A	12	PHE	-	EXPRESSION TAG	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

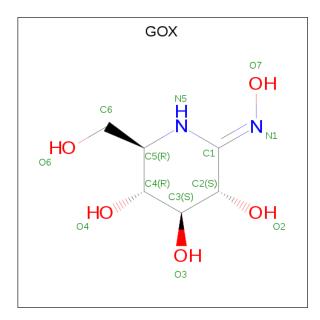
• Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).





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

• Molecule 4 is (2S,3S,4R,5R)-6-(HYDROXYAMINO)-2-(HYDROXYMETHYL)-2,3,4,5-TE TRAHYDROPYRIDINE-3,4,5-TRIOL (three-letter code: GOX) (formula: $C_6H_{12}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 13	C 6	N 2	O 5	0	0

• Molecule 5 is water.



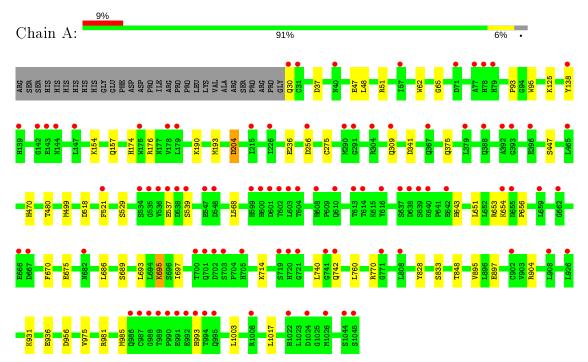
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1124	Total O 1127 1127	0	3



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 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: Alpha-mannosidase 2





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	68.74Å 109.12Å 137.69Å	Danagitan	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	40.00 - 1.43	Depositor	
resolution (A)	38.17 - 1.43	Depositor Depositor	
% Data completeness	96.4 (40.00-1.43)	Depositor	
(in resolution range)	96.4 (38.17-1.43)	EDS	
R_{merge}	0.08	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.82 (at 1.43Å)	Xtriage	
Refinement program	REFMAC, CNS	Depositor	
P. P.	0.187 , 0.201	Depositor	
R, R_{free}	0.181 , 0.185	DCC	
R_{free} test set	2773 reflections $(1.51%)$	wwPDB-VP	
Wilson B-factor (Å ²)	14.3	Xtriage	
Anisotropy	0.060	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40 , 54.2	EDS	
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	9408	wwPDB-VP	
Average B, all atoms (Å ²)	16.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: MRD, ZN, GOX

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).

Mal	Chain	Bond	lengths	Во	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.64	0/8518	0.77	1/11563~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	956	ASP	CB-CG-OD1	5.02	122.81	118.30

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	8259	0	8084	54	0
2	A	1	0	0	0	0
3	A	8	0	14	3	0
4	A	13	0	11	2	0
5	A	1127	0	0	17	0
All	All	9408	0	8109	57	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 3.



The worst 5 of 57 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:695[B]:LYS:HB3	1:A:695[B]:LYS:HZ3	1.15	1.05
1:A:695[B]:LYS:HB3	1:A:695[B]:LYS:NZ	1.69	1.01
1:A:47:GLU:OE2	1:A:51:ARG:HD3	1.63	0.95
1:A:309:GLN:HG3	5:A:1526:HOH:O	1.65	0.95
1:A:695[B]:LYS:CB	1:A:695[B]:LYS:NZ	2.38	0.87

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	${f Analysed}$	Favoured	Allowed	Outliers	Percenti	les
1	A	1026/1045 (98%)	1005 (98%)	19 (2%)	2 (0%)	47 23	3

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	204	ASP

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	915/929 (98%)	908 (99%)	7 (1%)	81 61	

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	SER
1	A	828	TYR
1	A	695[A]	LYS
1	A	275	CYS
1	A	695[B]	LYS

Some 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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		Dog	Link	Bond lengths			Bond angles		
MIOI	туре	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MRD	A	1047	-	7,7,7	0.37	0	9,10,10	0.54	0
4	GOX	A	1048	2	11,13,13	0.71	0	14,18,18	2.16	2 (14%)

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	MRD	A	1047	-	-	1/5/5/5	-
4	GOX	A	1048	2	_	0/3/24/24	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
4	A	1048	GOX	O7-N1-C1	6.60	116.38	110.18
4	A	1048	GOX	O3-C3-C2	-2.10	105.68	109.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms
3	A	1047	MRD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1047	MRD	3	0
4	A	1048	GOX	2	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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q<0.9
1	A	1016/1045 (97%)	0.68	94 (9%) 8 9	7, 14, 27, 46	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	603	LEU	9.0
1	A	534	SER	8.6
1	A	993	HIS	8.0
1	A	702	ASP	7.7
1	A	720	HIS	7.1

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 carbohydrates 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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	MRD	A	1047	8/8	0.86	0.12	14,20,24,25	0
4	GOX	A	1048	13/13	0.94	0.11	9,12,16,22	0
2	ZN	A	1046	1/1	1.00	0.07	9,9,9,9	0



6.5 Other polymers (i)

There are no such residues in this entry.

