



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 11:06 PM EDT

PDB ID : 1WS4
Title : Crystal structure of Jacalin- Me-alpha-Mannose complex: Promiscuity vs Specificity
Authors : Jeyaprakash, A.A.; Jayashree, G.; Mahanta, S.K.; Sekar, K.; Surolia, A.; Vijayan, M.
Deposited on : unknown
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/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 : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

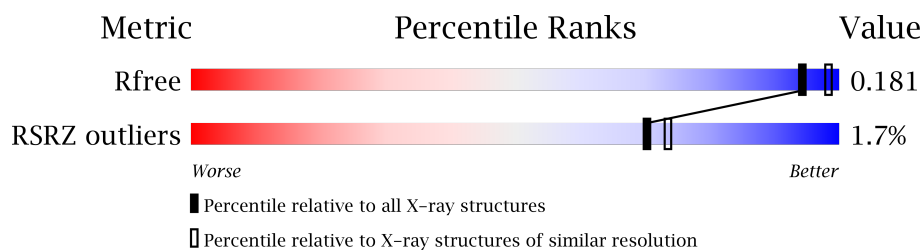
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4916 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 Agglutinin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1038	678	159	199	2			
1	G	133	Total	C	N	O	S	0	0	0
			1038	678	159	199	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	VAL	LYS	CONFLICT	UNP P18670
G	45	VAL	LYS	CONFLICT	UNP P18670

- Molecule 2 is a protein called Agglutinin beta-3 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O		0	0	0
			110	71	19	20				
2	D	16	Total	C	N	O		0	0	0
			110	71	19	20				
2	F	18	Total	C	N	O		0	0	0
			122	77	21	24				
2	H	16	Total	C	N	O		0	0	0
			110	71	19	20				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	SER	VAL	CONFLICT	UNP P18673
B	20	ALA	SER	CONFLICT	UNP P18673
D	19	SER	VAL	CONFLICT	UNP P18673
D	20	ALA	SER	CONFLICT	UNP P18673
F	19	SER	VAL	CONFLICT	UNP P18673
F	20	ALA	SER	CONFLICT	UNP P18673

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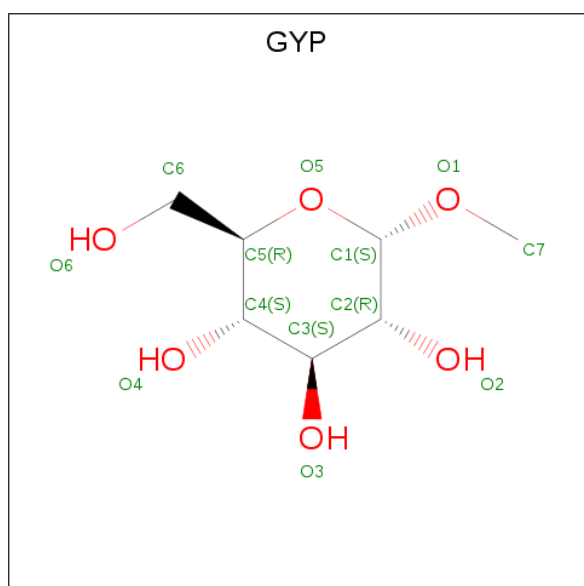
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Chain	Residue	Modelled	Actual	Comment	Reference
H	19	SER	VAL	CONFLICT	UNP P18673
H	20	ALA	SER	CONFLICT	UNP P18673

- Molecule 3 is a protein called Agglutinin alpha chain.

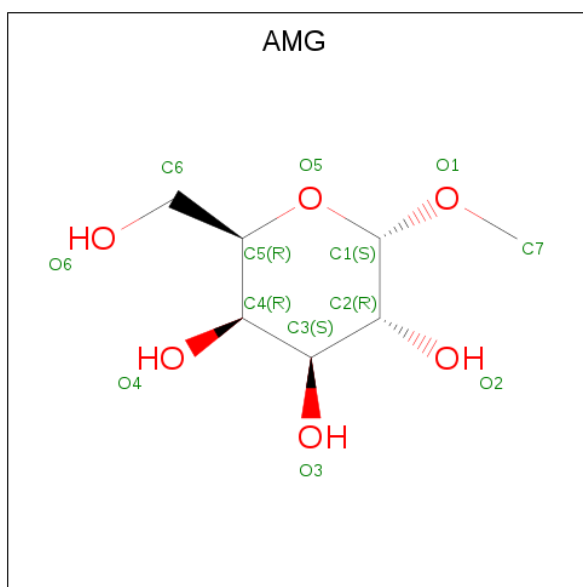
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			
3	E	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			

- Molecule 4 is METHYL-ALPHA-D-GLUCOPYRANOSIDE (three-letter code: GYP) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	7	6		
4	C	1	Total	C	O	0	0
			13	7	6		
4	G	1	Total	C	O	0	1
			14	7	7		

- Molecule 5 is ALPHA-METHYL-D-GALACTOSIDE (three-letter code: AMG) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	1
			14	7	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	B	5	Total	O	0	0
			5	5		
6	C	63	Total	O	0	0
			63	63		
6	D	6	Total	O	0	0
			6	6		
6	E	54	Total	O	0	0
			54	54		
6	F	5	Total	O	0	0
			5	5		
6	G	61	Total	O	0	0
			61	61		
6	H	6	Total	O	0	0
			6	6		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.29 Å 99.42 Å 105.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.06 – 1.90 28.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.06-1.90) 99.2 (28.06-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.91 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.184 , 0.205 0.185 , 0.181	Depositor DCC
R_{free} test set	3341 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4916	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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4.5 Carbohydrates [i](#)

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4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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	133/133 (100%)	-0.17	1 (0%) 86 87	19, 24, 33, 40	0
1	G	133/133 (100%)	-0.16	0 100 100	17, 24, 36, 45	0
2	B	16/20 (80%)	0.41	2 (12%) 4 5	18, 25, 48, 54	0
2	D	16/20 (80%)	0.30	2 (12%) 4 5	19, 26, 48, 53	0
2	F	18/20 (90%)	0.47	1 (5%) 25 28	19, 25, 49, 52	0
2	H	16/20 (80%)	0.28	2 (12%) 4 5	18, 24, 49, 53	0
3	C	133/133 (100%)	-0.21	0 100 100	17, 24, 34, 41	0
3	E	133/133 (100%)	0.01	2 (1%) 74 77	19, 26, 37, 43	0
All	All	598/612 (97%)	-0.08	10 (1%) 70 73	17, 25, 38, 54	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	18	LYS	3.8
2	F	3	GLN	3.6
2	B	18	LYS	3.5
2	B	3	GLN	3.2
3	E	122	TYR	3.0
2	D	18	LYS	3.0
2	D	3	GLN	3.0
2	H	3	GLN	2.9
3	E	21	LYS	2.5
1	A	98	VAL	2.4

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
4	GYP	G	504[A]	13/13	0.91	0.14	1.44	28,38,42,44	2
4	GYP	G	504[B]	13/13	0.91	0.14	1.44	28,38,42,44	2
4	GYP	C	502	13/13	0.95	0.10	0.53	26,31,36,36	0
5	AMG	E	503[A]	13/13	0.92	0.11	-0.05	26,36,39,42	2
5	AMG	E	503[B]	13/13	0.92	0.11	-0.05	26,36,39,41	2
4	GYP	A	501	13/13	0.96	0.09	-0.27	17,26,29,30	0

5.5 Other polymers [i](#)

There are no such residues in this entry.