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wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Apr 26, 2022 – 10:11 am BST

PDB ID	:	7YWG
Title	:	Monocot chimeric jacalin JAC1 from Oryza sativa: lectin domain (crystal form 1)
Authors	:	Huwa, N.; Classen, T.; Weiergraeber, O.H.
Deposited on	:	2022-02-14
Resolution	:	1.10 Å(reported)

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

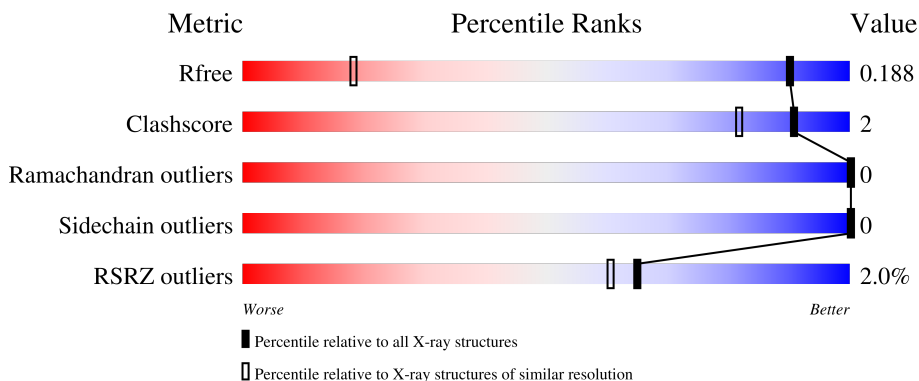|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

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 1.10 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	Percentile Ranks	Value
Rfree		0.188
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		2.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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 <=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	170	% 82% • 14%
1	B	170	2% 83% • 13%

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2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2870 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 Dirigent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	10	0
			1195	757	198	237	3			
1	B	148	Total	C	N	O	S	0	13	0
			1229	784	202	241	2			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	MET	-	initiating methionine	UNP Q306J3
A	138	GLY	-	expression tag	UNP Q306J3
A	139	SER	-	expression tag	UNP Q306J3
A	140	SER	-	expression tag	UNP Q306J3
A	141	HIS	-	expression tag	UNP Q306J3
A	142	HIS	-	expression tag	UNP Q306J3
A	143	HIS	-	expression tag	UNP Q306J3
A	144	HIS	-	expression tag	UNP Q306J3
A	145	HIS	-	expression tag	UNP Q306J3
A	146	HIS	-	expression tag	UNP Q306J3
A	147	SER	-	expression tag	UNP Q306J3
A	148	SER	-	expression tag	UNP Q306J3
A	149	GLY	-	expression tag	UNP Q306J3
A	150	LEU	-	expression tag	UNP Q306J3
A	151	VAL	-	expression tag	UNP Q306J3
A	152	PRO	-	expression tag	UNP Q306J3
A	153	ARG	-	expression tag	UNP Q306J3
A	154	GLY	-	expression tag	UNP Q306J3
A	155	SER	-	expression tag	UNP Q306J3
A	156	HIS	-	expression tag	UNP Q306J3
A	157	MET	-	expression tag	UNP Q306J3
A	158	LEU	-	expression tag	UNP Q306J3
A	159	GLU	-	expression tag	UNP Q306J3
B	137	MET	-	initiating methionine	UNP Q306J3
B	138	GLY	-	expression tag	UNP Q306J3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	139	SER	-	expression tag	UNP Q306J3
B	140	SER	-	expression tag	UNP Q306J3
B	141	HIS	-	expression tag	UNP Q306J3
B	142	HIS	-	expression tag	UNP Q306J3
B	143	HIS	-	expression tag	UNP Q306J3
B	144	HIS	-	expression tag	UNP Q306J3
B	145	HIS	-	expression tag	UNP Q306J3
B	146	HIS	-	expression tag	UNP Q306J3
B	147	SER	-	expression tag	UNP Q306J3
B	148	SER	-	expression tag	UNP Q306J3
B	149	GLY	-	expression tag	UNP Q306J3
B	150	LEU	-	expression tag	UNP Q306J3
B	151	VAL	-	expression tag	UNP Q306J3
B	152	PRO	-	expression tag	UNP Q306J3
B	153	ARG	-	expression tag	UNP Q306J3
B	154	GLY	-	expression tag	UNP Q306J3
B	155	SER	-	expression tag	UNP Q306J3
B	156	HIS	-	expression tag	UNP Q306J3
B	157	MET	-	expression tag	UNP Q306J3
B	158	LEU	-	expression tag	UNP Q306J3
B	159	GLU	-	expression tag	UNP Q306J3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
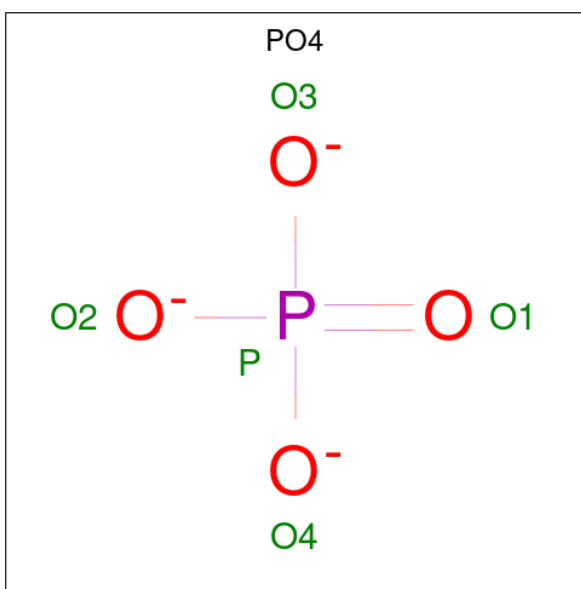
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 5	O 4	P 1	0	1

• Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	250	Total 257	O 257	0	7
3	B	182	Total 184	O 184	0	3

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: Dirigent protein

Chain A:

- Molecule 1: Dirigent protein

Chain B:
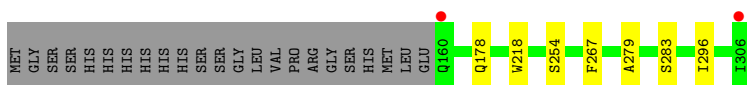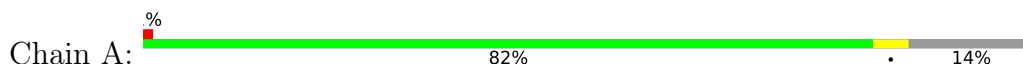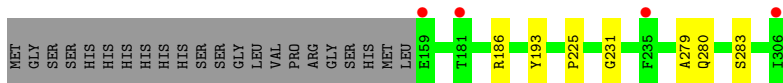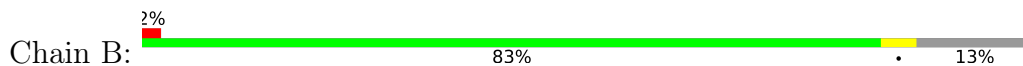
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	34.93Å 63.51Å 105.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.46 – 1.10 54.46 – 1.10	Depositor EDS
% Data completeness (in resolution range)	90.9 (54.46-1.10) 90.9 (54.46-1.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.155 , 0.188 0.155 , 0.188	Depositor DCC
R_{free} test set	4378 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	0.98	EDS
Total number of atoms	2870	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0214e-03.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.44	0/1230	0.69	0/1670
1	B	0.42	0/1266	0.67	0/1720
All	All	0.43	0/2496	0.68	0/3390

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 ⓘ

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	1195	0	1116	4	0
1	B	1229	0	1136	4	0
2	B	5	0	0	0	0
3	A	257	0	0	0	0
3	B	184	0	0	1	0
All	All	2870	0	2252	8	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.

The worst 5 of 8 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:280:GLN:NE2	3:B:503:HOH:O	2.32	0.63
1:A:218:TRP:O	1:A:296[B]:ILE:HD11	2.01	0.60
1:B:193:TYR:CZ	1:B:225:PRO:HB3	2.49	0.47
1:B:186:ARG:NH2	1:B:231:GLY:O	2.48	0.46
1:B:279:ALA:HB1	1:B:283[A]:SER:OG	2.19	0.42

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	156/170 (92%)	152 (97%)	4 (3%)	0	100	100
1	B	160/170 (94%)	155 (97%)	5 (3%)	0	100	100
All	All	316/340 (93%)	307 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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	131/142 (92%)	131 (100%)	0	100	100
1	B	131/142 (92%)	131 (100%)	0	100	100
All	All	262/284 (92%)	262 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 monosaccharides in this entry.

5.6   Ligand geometry   ⓘ

1 ligand is modelled in this entry.

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	$\#|Z| > 2$
2	PO4	B	401[A]	-	4,4,4	0.90	0	6,6,6	0.89	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data   ⓘ

6.1   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	147/170 (86%)	-0.36	2 (1%)	75	71	10, 15, 26, 41	0
1	B	148/170 (87%)	-0.22	4 (2%)	54	51	10, 16, 28, 45	0
All	All	295/340 (86%)	-0.29	6 (2%)	65	60	10, 16, 27, 45	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ILE	5.1
1	A	160	GLN	2.9
1	A	306	ILE	2.7
1	B	159	GLU	2.6
1	B	235	PHE	2.4

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

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

6.3   Carbohydrates   ⓘ

There are no monosaccharides in this entry.

6.4   Ligands   ⓘ

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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	B	401[A]	5/5	0.97	0.08	11,12,14,16	5

6.5   Other polymers ⓘ

There are no such residues in this entry.