



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 01:58 am BST

PDB ID : 3IWR
Title : Crystal structure of class I chitinase from *Oryza sativa* L. japonica
Authors : Kezuka, Y.; Watanabe, T.; Nonaka, T.
Deposited on : 2009-09-03
Resolution : 2.57 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 following versions of software and data (see [references ⓘ](#)) 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

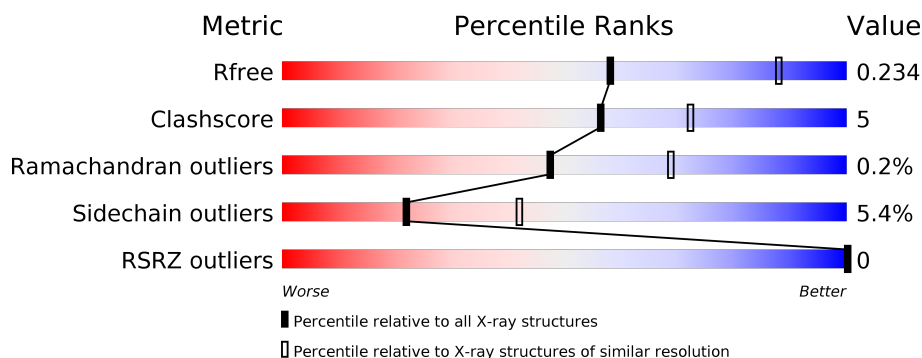
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 $\leq 5\%$. 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	309	<div> <div style="width: 68%; background-color: red;"></div> <div style="width: 9%; background-color: orange;"></div> <div style="width: 21%; background-color: grey;"></div> <div>68% 9% • 21%</div> </div>
1	B	309	<div> <div style="width: 73%; background-color: green;"></div> <div style="width: 5%; background-color: yellow;"></div> <div style="width: 20%; background-color: grey;"></div> <div>73% 5% • 20%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3925 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.

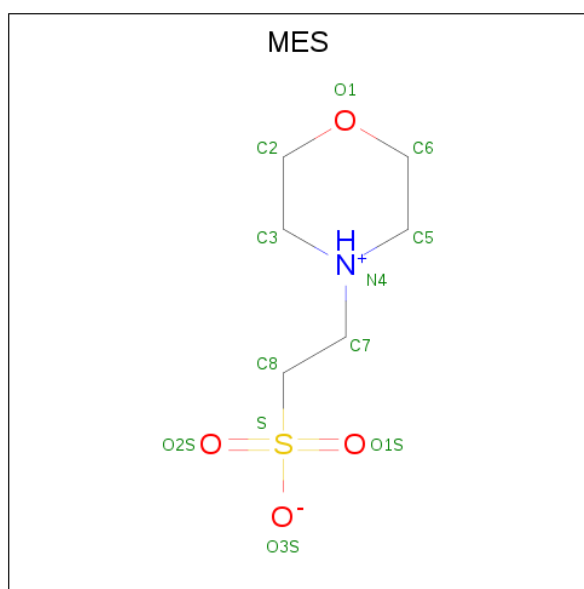
- Molecule 1 is a protein called Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	1	0
			1866	1182	332	344	8			
1	B	246	Total	C	N	O	S	0	4	0
			1898	1205	336	349	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	INITIATING METHIONINE	UNP Q7DNA1
B	32	MET	-	INITIATING METHIONINE	UNP Q7DNA1

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



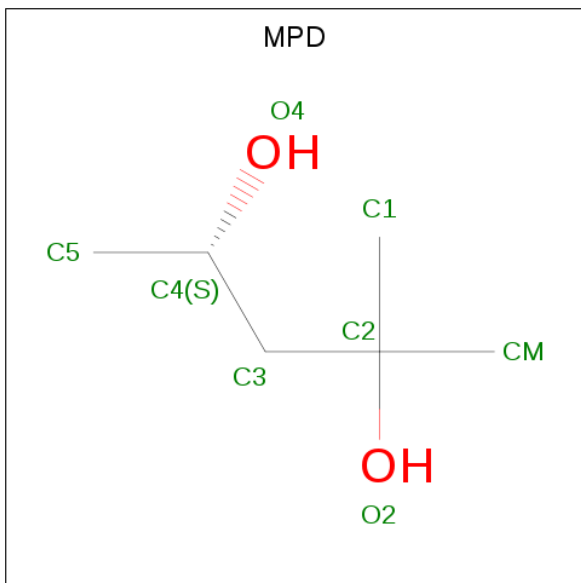
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	72	Total	O	0	0
			72	72		

- Molecule 1: Chitinase

	GLY	LEU	ALA	GLU	GLN	MET
L97						GLN
L101						CYS
M106						GLY
D107						ALA
R113						GLN
M136						GLY
T139						ALA
P140						ARG
H153						CYS
A193						LEU
R196						CYS
I204						SER
Q205						ARG
L206						TRP
S207						GLY
F208						TRP
A215						CYS
I219						THR
N226						SER
T235						ASP
K239						PHE
I259						CYS
A272						GLY
A275						GLY
N283						CYS
N301						SER
Y309						GLY
N320						CYS
Q326						GLY
R327						PRO
N330						THR
SER						PRO
GLY						THR
SER						PRO
SER						PRO
VAL						PRO
						SER
						D87
						V89
						T93

- Molecule 1: Chitinase

L97	L101	E138	Q150	E176	S181	P186	G200	Q205	R217	L224	D228	N251	N286	R302	N330	GLY	GLY	VAL	GLN	ALA	GLU																														
Met	GLU	GLN	CYS	GLY	ALA	GLN	ALA	GLY	GLY	ALA	ARG	CYS	CYS	PRO	ASN	CYS	LEU	CYS	CYS	SER	THR	TRP	GLY	GLY	ASP	PHE	CYS	GLY	ASP	CYS	GLN	GLN	GLN	CYS	GLY	CYS	PRO	THR	PRO	THR	PRO	PRO	THR	PRO	PRO	SER	P85	S86	V89	I92	T93

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	117.08 Å 117.08 Å 77.97 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	101.53 – 2.57 101.40 – 2.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (101.53-2.57) 97.0 (101.40-2.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.14 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.236 0.181 , 0.234	Depositor DCC
R_{free} test set	967 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3925	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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.

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: MPD, MES

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	0.67	0/1932	0.67	0/2636
1	B	0.74	1/1975 (0.1%)	0.73	0/2695
All	All	0.71	1/3907 (0.0%)	0.70	0/5331

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	GLU	CG-CD	5.31	1.59	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	85	PRO	Peptide

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	1866	0	1738	24	0
1	B	1898	0	1774	12	0
2	A	12	0	13	1	0
2	B	12	0	13	0	0
3	A	8	0	14	0	0
3	B	8	0	14	1	0
4	A	49	0	0	1	0
4	B	72	0	0	1	0
All	All	3925	0	3566	37	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 5.

The worst 5 of 37 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:A:330:ASN:C	1:A:330:ASN:HD22	1.65	0.99
1:A:283:ASN:HD22	1:A:326:GLN:HE21	1.34	0.74
3:B:341:MPD:HM3	4:B:9:HOH:O	1.90	0.70
1:B:200:GLY:HA3	1:B:205[B]:GLN:NE2	2.07	0.68
1:A:330:ASN:ND2	1:A:330:ASN:C	2.38	0.68

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	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/309 (79%)	234 (96%)	8 (3%)	1 (0%)	34	55
1	B	248/309 (80%)	241 (97%)	7 (3%)	0	100	100
All	All	491/618 (79%)	475 (97%)	15 (3%)	1 (0%)	47	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PHE

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	186/235 (79%)	178 (96%)	8 (4%)	29	52
1	B	191/235 (81%)	179 (94%)	12 (6%)	18	35
All	All	377/470 (80%)	357 (95%)	20 (5%)	22	43

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	ILE
1	B	93	VAL
1	B	224	LEU
1	A	330	ASN
1	B	86	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	B	286	ASN
1	B	150	GLN
1	A	249	GLN
1	A	330	ASN

5.3.3 RNA ⓘ

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](#)

4 ligands are 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$
3	MPD	B	341	-	7,7,7	0.37	0	9,10,10	0.58	0
2	MES	B	2	-	12,12,12	2.05	1 (8%)	14,16,16	0.73	0
3	MPD	A	341	-	7,7,7	0.35	0	9,10,10	0.59	0
2	MES	A	1	-	12,12,12	1.99	1 (8%)	14,16,16	0.70	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
3	MPD	B	341	-	-	1/5/5/5	-
2	MES	B	2	-	-	1/6/14/14	0/1/1/1
3	MPD	A	341	-	-	0/5/5/5	-
2	MES	A	1	-	-	4/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	MES	C8-S	-6.62	1.68	1.77
2	A	1	MES	C8-S	-6.43	1.68	1.77

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	MES	N4-C7-C8-S
2	A	1	MES	N4-C7-C8-S
2	A	1	MES	C7-C8-S-O1S
2	A	1	MES	C7-C8-S-O3S
2	A	1	MES	C7-C8-S-O2S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	341	MPD	1	0
2	A	1	MES	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, 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	244/309 (78%)	-0.11	0 100 100	13, 24, 40, 47	0
1	B	246/309 (79%)	-0.15	0 100 100	9, 18, 35, 43	0
All	All	490/618 (79%)	-0.13	0 100 100	9, 22, 38, 47	0

There are no RSRZ outliers to report.

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, 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	B-factors(Å ²)	Q<0.9
3	MPD	B	341	8/8	0.89	0.21	38,41,42,42	0
2	MES	A	1	12/12	0.89	0.22	60,61,64,65	0
2	MES	B	2	12/12	0.95	0.20	53,53,54,55	0
3	MPD	A	341	8/8	0.96	0.14	33,35,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.