



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 08:25 AM EDT

PDB ID : 2Z37
Title : Crystal structure of Brassica juncea chitinase catalytic module (Bjchi3)
Authors : Ubhayasekera, W.; Berglund, G.; Bergfors, T.; Mowbray, S.L.
Deposited on : unknown
Resolution : 1.53 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 : 4.02b-467
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

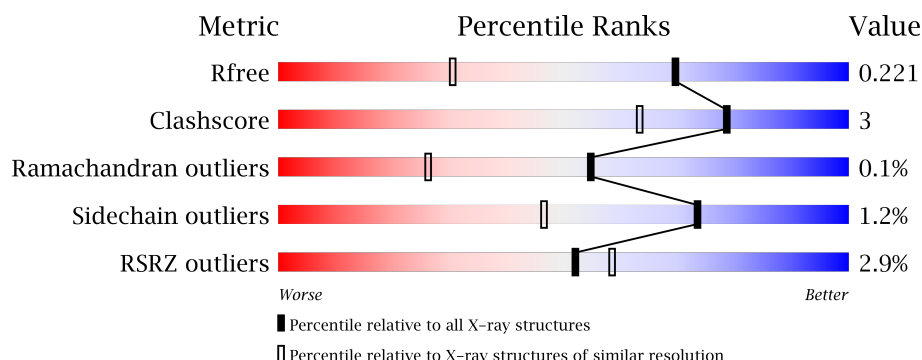
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	1773 (1.56-1.52)
Clashscore	112137	1845 (1.56-1.52)
Ramachandran outliers	110173	1810 (1.56-1.52)
Sidechain outliers	110143	1808 (1.56-1.52)
RSRZ outliers	101464	1774 (1.56-1.52)

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. 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	244	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
1	B	244	<div> <div>3%</div> <div>93%</div> <div>6%</div> </div>
1	C	244	<div> <div>3%</div> <div>95%</div> <div>• •</div> </div>
1	D	244	<div> <div>2%</div> <div>95%</div> <div>5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8402 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	6	0
			1930	1227	324	363	16			
1	B	244	Total	C	N	O	S	0	5	0
			1920	1221	320	362	17			
1	C	244	Total	C	N	O	S	0	2	0
			1909	1211	320	362	16			
1	D	244	Total	C	N	O	S	0	1	0
			1905	1208	320	361	16			

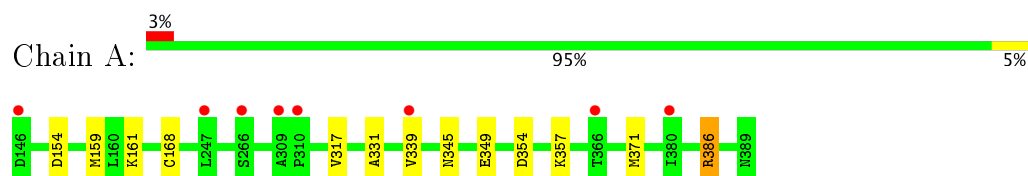
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	192	Total	O	0	0
			192	192		
2	B	184	Total	O	0	0
			184	184		
2	C	169	Total	O	0	0
			169	169		
2	D	193	Total	O	0	0
			193	193		

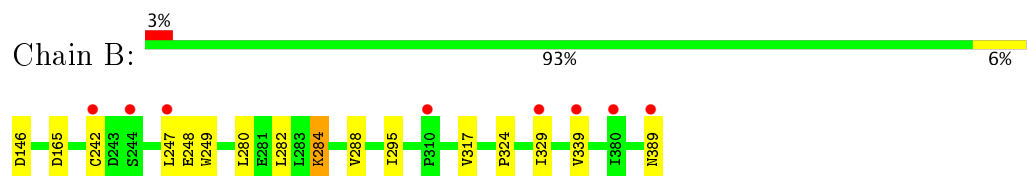
3 Residue-property plots [i](#)

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.

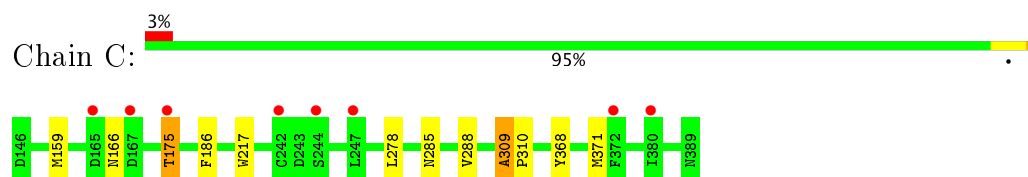
• Molecule 1: Chitinase



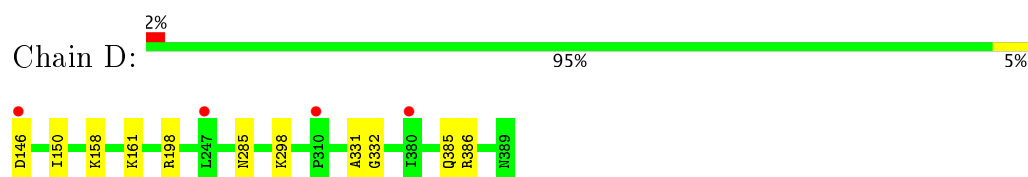
• Molecule 1: Chitinase



• Molecule 1: Chitinase



• Molecule 1: Chitinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.25Å 61.82Å 75.36Å 79.34° 89.52° 88.90°	Depositor
Resolution (Å)	42.23 – 1.53 42.23 – 1.53	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.23-1.53) 89.8 (42.23-1.53)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 1.53Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.222 0.185 , 0.221	Depositor DCC
R_{free} test set	7824 reflections (6.36%)	DCC
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8402	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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](#)

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	0.43	0/2007	0.55	0/2725
1	B	0.44	0/1994	0.54	0/2709
1	C	0.43	0/1974	0.55	0/2682
1	D	0.44	0/1967	0.57	0/2672
All	All	0.44	0/7942	0.55	0/10788

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 [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	1930	0	1819	21	0
1	B	1920	0	1801	7	0
1	C	1909	0	1781	14	0
1	D	1905	0	1774	7	0
2	A	192	0	0	7	0
2	B	184	0	0	2	0
2	C	169	0	0	1	0
2	D	193	0	0	1	0
All	All	8402	0	7175	49	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.

All (49) 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:159:MET:HG2	1:A:371:MET:HE1	1.28	1.13
1:C:159:MET:HG2	1:C:371:MET:HE1	1.22	1.11
1:C:159:MET:HG2	1:C:371:MET:CE	1.99	0.92
1:A:349:GLU:HG2	1:A:357:LYS:HE3	1.59	0.85
1:A:159:MET:HG2	1:A:371:MET:CE	2.07	0.84
1:A:154:ASP:OD1	2:A:581:HOH:O	1.96	0.83
1:A:159:MET:CG	1:A:371:MET:HE1	2.13	0.72
1:A:354:ASP:CG	1:A:357:LYS:HE2	2.09	0.72
1:A:168:CYS:O	2:A:494:HOH:O	2.07	0.72
1:D:158:LYS:O	1:D:161:LYS:HG2	1.90	0.72
1:C:309:ALA:CB	1:C:310:PRO:CD	2.69	0.70
1:B:146:ASP:N	2:B:551:HOH:O	2.25	0.70
1:B:317:VAL:HG11	1:B:339[B]:VAL:HG13	1.74	0.68
1:C:175[A]:THR:HG22	2:C:400:HOH:O	1.97	0.65
1:C:309:ALA:HB1	1:C:310:PRO:CD	2.27	0.64
1:A:354:ASP:CB	1:A:357:LYS:HE2	2.30	0.61
1:D:331:ALA:HB1	1:D:386:ARG:HB2	1.83	0.61
1:C:309:ALA:HB3	1:C:310:PRO:HD2	1.84	0.58
1:B:284:LYS:HD3	2:B:439:HOH:O	2.03	0.58
1:C:309:ALA:HB1	1:C:310:PRO:HD3	1.86	0.57
1:A:159:MET:CG	1:A:371:MET:CE	2.79	0.56
1:B:248:GLU:HG3	1:B:249:TRP:CE2	2.42	0.55
1:D:150:ILE:HD11	1:D:198:ARG:NH2	2.22	0.54
1:B:280:LEU:HD11	1:B:295:ILE:HD12	1.89	0.53
1:A:349:GLU:CG	1:A:357:LYS:HE3	2.33	0.53
1:C:309:ALA:CB	1:C:310:PRO:HD2	2.37	0.53
1:D:150:ILE:HD11	1:D:198:ARG:CZ	2.39	0.53
1:A:357:LYS:HD2	2:A:440:HOH:O	2.09	0.52
1:A:161:LYS:HE2	2:A:506:HOH:O	2.09	0.51
1:A:354:ASP:HB3	1:A:357:LYS:HE2	1.90	0.51
1:D:298:LYS:NZ	2:D:543:HOH:O	2.37	0.49
1:C:368:TYR:HA	1:C:371:MET:HE2	1.96	0.48
1:A:349:GLU:HG2	1:A:357:LYS:CE	2.38	0.47
1:D:150:ILE:HD12	1:D:150:ILE:N	2.30	0.47
1:A:345:ASN:ND2	2:A:439:HOH:O	2.48	0.46
1:A:154:ASP:CG	2:A:581:HOH:O	2.50	0.46
1:C:159:MET:CG	1:C:371:MET:CE	2.85	0.45
1:B:324:PRO:HB2	1:B:329[A]:ILE:HD11	1.99	0.45
1:C:186:PHE:HZ	1:C:278:LEU:HD21	1.81	0.45
1:B:282:LEU:HD23	1:B:288:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:420:HOH:O	1:C:217:TRP:HD1	2.00	0.44
1:A:354:ASP:OD2	1:A:357:LYS:CE	2.66	0.44
1:A:354:ASP:OD2	1:A:357:LYS:HE2	2.18	0.44
1:D:332:GLY:O	1:D:385:GLN:HG2	2.18	0.43
1:A:331:ALA:HB1	1:A:386:ARG:HB2	2.02	0.42
1:A:371:MET:HE2	1:A:371:MET:HB2	1.75	0.41
1:C:285:ASN:O	1:C:288:VAL:HG22	2.20	0.41
1:A:317:VAL:HG11	1:A:339[A]:VAL:CG1	2.51	0.40
1:C:371:MET:HE2	1:C:371:MET:HB2	1.94	0.40

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	248/244 (102%)	241 (97%)	7 (3%)	0	100	100
1	B	247/244 (101%)	239 (97%)	8 (3%)	0	100	100
1	C	244/244 (100%)	237 (97%)	6 (2%)	1 (0%)	38	14
1	D	243/244 (100%)	237 (98%)	6 (2%)	0	100	100
All	All	982/976 (101%)	954 (97%)	27 (3%)	1 (0%)	55	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	309	ALA

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	206/200 (103%)	205 (100%)	1 (0%)	91	79
1	B	205/200 (102%)	199 (97%)	6 (3%)	48	15
1	C	202/200 (101%)	199 (98%)	3 (2%)	70	40
1	D	201/200 (100%)	199 (99%)	2 (1%)	80	59
All	All	814/800 (102%)	802 (98%)	12 (2%)	73	40

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	386	ARG
1	B	165	ASP
1	B	242[A]	CYS
1	B	242[B]	CYS
1	B	247	LEU
1	B	284	LYS
1	B	389	ASN
1	C	166	ASN
1	C	175[A]	THR
1	C	175[B]	THR
1	D	146	ASP
1	D	285	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	GLN
1	C	270	ASN
1	D	245	ASN
1	D	285	ASN
1	D	321	GLN

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](#)

There are no ligands in this entry.

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 ⓘ

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	244/244 (100%)	0.09	8 (3%)	47	53	10, 19, 28, 37	6 (2%)
1	B	244/244 (100%)	0.14	8 (3%)	47	53	11, 19, 30, 36	5 (2%)
1	C	244/244 (100%)	0.16	8 (3%)	47	53	11, 20, 29, 35	2 (0%)
1	D	244/244 (100%)	0.09	4 (1%)	72	77	10, 18, 29, 36	1 (0%)
All	All	976/976 (100%)	0.12	28 (2%)	52	58	10, 19, 30, 37	14 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380[A]	ILE	3.8
1	A	309	ALA	3.5
1	B	339[A]	VAL	3.5
1	B	310	PRO	3.4
1	B	242[A]	CYS	3.3
1	A	339[A]	VAL	3.2
1	D	380[A]	ILE	3.2
1	D	146	ASP	3.0
1	A	310	PRO	2.9
1	C	242	CYS	2.9
1	B	247	LEU	2.7
1	C	380[A]	ILE	2.6
1	A	146	ASP	2.6
1	C	175[A]	THR	2.6
1	D	247	LEU	2.5
1	A	366[A]	THR	2.5
1	A	380[A]	ILE	2.4
1	B	329[A]	ILE	2.3
1	C	244	SER	2.3
1	A	266[A]	SER	2.2
1	B	389	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	310	PRO	2.2
1	C	247	LEU	2.2
1	B	244	SER	2.1
1	C	372	PHE	2.1
1	C	165	ASP	2.1
1	A	247	LEU	2.0
1	C	167	ASP	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.