



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:20 pm BST

PDB ID : 2B42  
Title : Crystal structure of the Triticum xylanase inhibitor-I in complex with bacillus subtilis xylanase  
Authors : Sansen, S.; Dewilde, M.; De Ranter, C.J.; Gebruers, K.; Brijs, K.; Courtin, C.M.; Delcour, J.A.; Rabijns, A.  
Deposited on : 2005-09-22  
Resolution : 2.50 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](mailto: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  
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

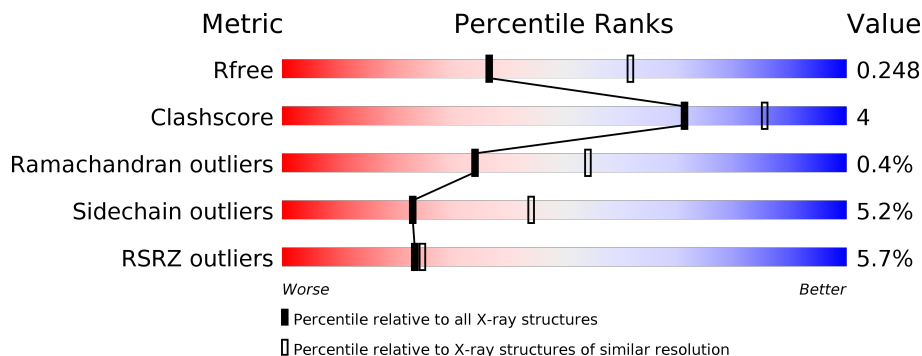
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	381	
2	B	185	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4112 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 xylanase inhibitor-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2604	1661	444	480	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	LYS	ASP	CONFLICT	GB 23954367
A	274	VAL	GLU	CONFLICT	GB 23954367

- Molecule 2 is a protein called Endo-1,4-beta-xylanase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	184	1443	909	248	284	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	THR	SER	CONFLICT	UNP P18429

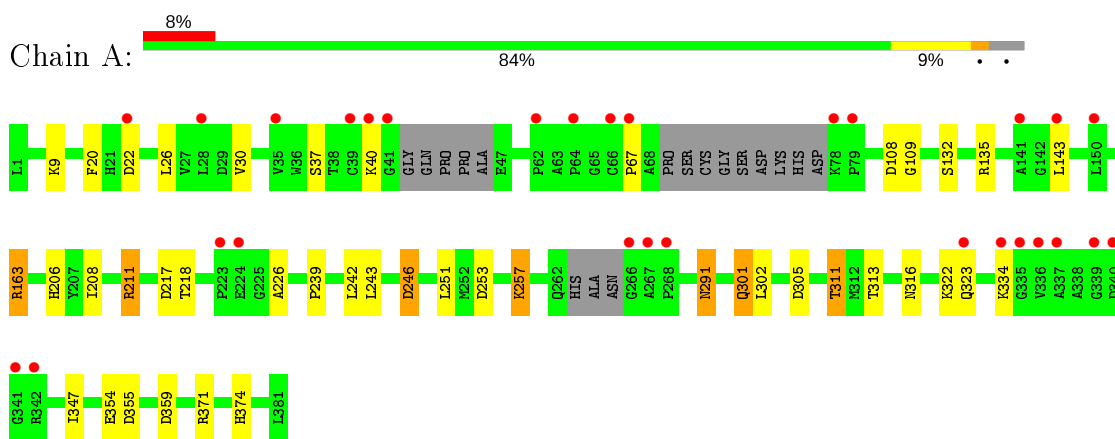
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	27	Total	O	0	0
			27	27		

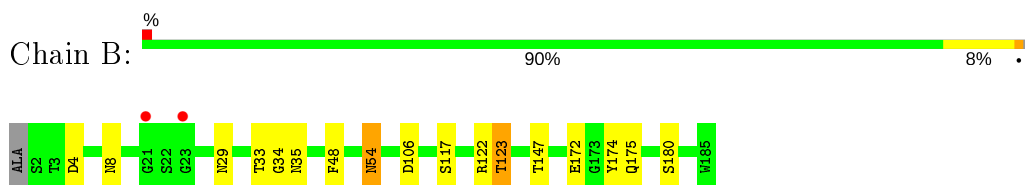
### 3 Residue-property plots [i](#)

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: xylanase inhibitor-I



- Molecule 2: Endo-1,4-beta-xylanase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.89Å 95.34Å 69.31Å 90.00° 122.24° 90.00°	Depositor
Resolution (Å)	29.36 – 2.50 29.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.36-2.50) 97.8 (29.31-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, $R_{free}$	0.183 , 0.240 0.192 , 0.248	Depositor DCC
$R_{free}$ test set	1968 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	0.58	0/2667	0.79	5/3644 (0.1%)
2	B	0.58	0/1491	0.82	2/2043 (0.1%)
All	All	0.58	0/4158	0.80	7/5687 (0.1%)

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
2	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	106	ASP	CB-CG-OD2	6.83	124.44	118.30
1	A	355	ASP	CB-CG-OD2	6.35	124.02	118.30
2	B	4	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	108	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	22	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	246	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	135	ARG	NE-CZ-NH1	5.41	123.00	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	33	THR	Peptide

## 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	2604	0	2628	21	0
2	B	1443	0	1314	11	0
3	A	38	0	0	1	0
3	B	27	0	0	1	0
All	All	4112	0	3942	28	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 4.

All (28) 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)
2:B:29:ASN:HB3	3:B:195:HOH:O	1.74	0.88
3:A:382:HOH:O	2:B:175:GLN:HG3	1.74	0.84
1:A:374:HIS:H	2:B:35:ASN:HD21	1.27	0.81
1:A:313:THR:H	1:A:316:ASN:HD22	1.26	0.80
1:A:316:ASN:HD21	1:A:371:ARG:HH12	1.31	0.79
1:A:253:ASP:O	1:A:257:LYS:HG2	1.85	0.77
1:A:374:HIS:H	2:B:35:ASN:ND2	1.86	0.73
2:B:117:SER:OG	2:B:123:THR:HG21	1.90	0.71
1:A:316:ASN:ND2	1:A:371:ARG:HH12	1.91	0.69
1:A:301:GLN:OE1	1:A:311:THR:HB	2.00	0.61
2:B:34:GLY:O	2:B:174:TYR:HA	2.03	0.57
1:A:9:LYS:HE2	1:A:354:GLU:OE2	2.04	0.56
1:A:291:ASN:HD22	1:A:291:ASN:C	2.11	0.53
2:B:54:ASN:C	2:B:54:ASN:HD22	2.11	0.53
1:A:374:HIS:CD2	2:B:172:GLU:OE2	2.64	0.51
1:A:143:LEU:O	1:A:206:HIS:HE1	1.94	0.51
1:A:313:THR:H	1:A:316:ASN:ND2	2.02	0.49
1:A:211:ARG:HD3	1:A:305:ASP:OD1	2.13	0.49
1:A:20:PHE:HB2	1:A:26:LEU:HG	1.95	0.49
2:B:117:SER:CB	2:B:123:THR:HG21	2.43	0.48
1:A:163:ARG:HD2	1:A:359:ASP:OD1	2.14	0.47
1:A:243:LEU:HD11	1:A:251:LEU:HD23	1.96	0.46
1:A:226:ALA:HB1	1:A:246:ASP:OD2	2.15	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:THR:N	1:A:316:ASN:HD22	2.04	0.46
1:A:30:VAL:HA	1:A:143:LEU:HB2	1.97	0.46
2:B:48:PHE:HA	2:B:147:THR:HG23	2.01	0.43
1:A:242:LEU:HB2	1:A:347:ILE:HB	2.00	0.43
1:A:374:HIS:N	2:B:35:ASN:ND2	2.61	0.42

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	356/381 (93%)	342 (96%)	12 (3%)	2 (1%)	25	43
2	B	182/185 (98%)	177 (97%)	5 (3%)	0	100	100
All	All	538/566 (95%)	519 (96%)	17 (3%)	2 (0%)	34	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	PRO
1	A	109	GLY

### 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	275/288 (96%)	258 (94%)	17 (6%)	18	35
2	B	151/151 (100%)	146 (97%)	5 (3%)	38	64
All	All	426/439 (97%)	404 (95%)	22 (5%)	23	44

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	40	LYS
1	A	132	SER
1	A	163	ARG
1	A	208	ILE
1	A	211	ARG
1	A	217	ASP
1	A	218	THR
1	A	239	PRO
1	A	257	LYS
1	A	291	ASN
1	A	301	GLN
1	A	302	LEU
1	A	311	THR
1	A	322	LYS
1	A	323	GLN
1	A	334	LYS
2	B	8	ASN
2	B	54	ASN
2	B	122	ARG
2	B	123	THR
2	B	180	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	190	GLN
1	A	206	HIS
1	A	291	ASN
1	A	316	ASN
2	B	8	ASN
2	B	35	ASN
2	B	54	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	133	GLN
2	B	148	ASN
2	B	163	ASN

### 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	364/381 (95%)	0.27	29 (7%) <span style="border: 1px solid red; padding: 2px;">12</span> <span style="border: 1px solid red; padding: 2px;">12</span>	24, 40, 66, 82	0
2	B	184/185 (99%)	-0.13	2 (1%) <span style="border: 1px solid blue; padding: 2px;">80</span> <span style="border: 1px solid blue; padding: 2px;">82</span>	28, 35, 44, 54	0
All	All	548/566 (96%)	0.13	31 (5%) <span style="border: 1px solid red; padding: 2px;">23</span> <span style="border: 1px solid red; padding: 2px;">25</span>	24, 37, 64, 82	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	GLY	9.2
1	A	41	GLY	7.6
1	A	267	ALA	7.0
1	A	336	VAL	5.5
1	A	335	GLY	5.4
1	A	224	GLU	3.9
1	A	40	LYS	3.7
2	B	23	GLY	3.5
1	A	79	PRO	3.4
1	A	64	PRO	3.3
1	A	342	ARG	3.1
1	A	337	ALA	3.1
1	A	67	PRO	3.0
1	A	334	LYS	2.9
1	A	78	LYS	2.9
1	A	268	PRO	2.8
1	A	339	GLY	2.8
1	A	141	ALA	2.7
1	A	323	GLN	2.7
1	A	22	ASP	2.7
1	A	150	LEU	2.5
1	A	341	GLY	2.5
1	A	340	ASP	2.4
1	A	39	CYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	28	LEU	2.4
1	A	223	PRO	2.3
1	A	143	LEU	2.3
2	B	21	GLY	2.1
1	A	62	PRO	2.1
1	A	35	VAL	2.1
1	A	66	CYS	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.