



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:25 PM UTC

PDB ID : 1XND / pdb_00001xnd
Title : HIGH-RESOLUTION STRUCTURES OF XYLANASES FROM B. CIRCULANS AND T. HARZIANUM IDENTIFY A NEW FOLDING PATTERN AND IMPLICATIONS FOR THE ATOMIC BASIS OF THE CATALYSIS
Authors : Campbell, R.L.; Rose, D.R.
Deposited on : 1994-06-01
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

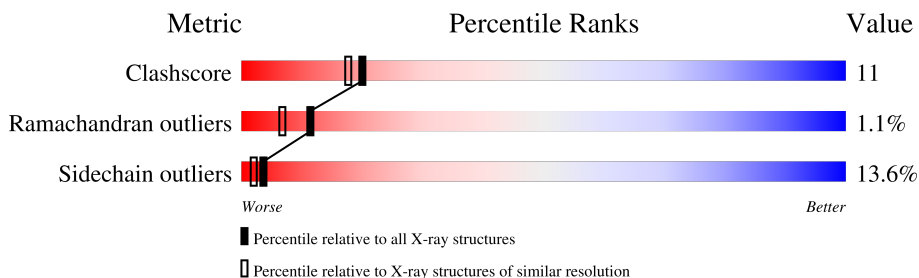
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	190	 62% 23% 9% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1530 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1471	928	251	291	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total	O	0	0
			59	59		

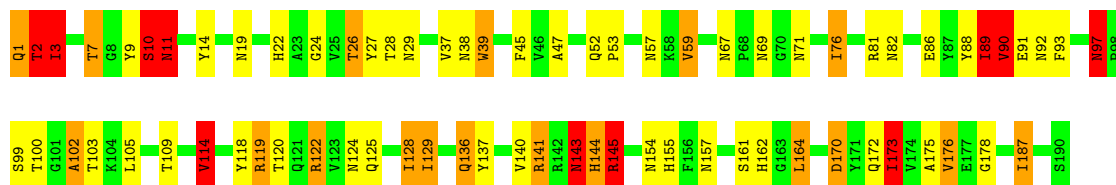
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: XYLANASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.67Å 94.65Å 51.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1530	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

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	1.32	15/1517 (1.0%)	2.31	71/2069 (3.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	ASP	CA-CB	-15.43	1.27	1.53
1	A	89	ILE	CA-CB	10.20	1.66	1.53
1	A	22	HIS	CD2-NE2	-7.49	1.29	1.37
1	A	90	VAL	CA-CB	7.33	1.62	1.54
1	A	155	HIS	CG-ND1	-6.30	1.31	1.38
1	A	155	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	59	VAL	CA-CB	5.84	1.61	1.54
1	A	144	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	129	ILE	CA-CB	5.61	1.60	1.54
1	A	176	VAL	CA-CB	5.54	1.60	1.54
1	A	22	HIS	CG-ND1	-5.46	1.32	1.38
1	A	187	ILE	CA-CB	5.33	1.64	1.55
1	A	119	ARG	NE-CZ	5.29	1.38	1.33
1	A	26	THR	CA-CB	5.06	1.61	1.53
1	A	114	VAL	CA-CB	5.02	1.62	1.54

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ASP	CA-CB-CG	30.30	142.91	112.60
1	A	170	ASP	N-CA-CB	24.51	151.91	110.49
1	A	170	ASP	CB-CA-C	-12.34	85.86	110.42
1	A	10	SER	N-CA-C	11.95	124.51	110.41
1	A	129	ILE	N-CA-CB	-10.41	98.83	112.26
1	A	141	ARG	NE-CZ-NH2	-10.23	109.99	119.20
1	A	100	THR	O-C-N	-10.13	110.38	122.95
1	A	11	ASN	CA-CB-CG	-9.30	103.30	112.60
1	A	2	THR	N-CA-C	-8.29	93.14	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	NE-CZ-NH1	8.21	129.71	121.50
1	A	76	ILE	N-CA-C	-8.04	97.00	108.58
1	A	92	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	A	10	SER	CA-C-O	7.96	128.19	121.02
1	A	22	HIS	CB-CG-CD2	-7.88	120.96	131.20
1	A	141	ARG	NE-CZ-NH1	7.86	129.36	121.50
1	A	141	ARG	CD-NE-CZ	7.85	135.40	124.40
1	A	102	ALA	N-CA-C	7.68	120.92	110.55
1	A	19	ASN	CA-CB-CG	7.66	120.25	112.60
1	A	69	ASN	OD1-CG-ND2	-7.61	115.00	122.60
1	A	100	THR	CA-C-N	-7.50	111.53	123.31
1	A	100	THR	C-N-CA	-7.50	111.53	123.31
1	A	69	ASN	CB-CG-ND2	7.44	127.56	116.40
1	A	92	ASN	CB-CG-ND2	7.39	127.49	116.40
1	A	11	ASN	O-C-N	7.13	132.07	122.59
1	A	145	ARG	CB-CG-CD	6.99	127.37	111.30
1	A	128	ILE	N-CA-CB	-6.88	99.88	111.23
1	A	1	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	A	124	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	173	ILE	N-CA-CB	-6.57	99.77	111.93
1	A	162	HIS	CB-CG-CD2	-6.50	122.76	131.20
1	A	129	ILE	CB-CA-C	6.48	119.24	111.20
1	A	162	HIS	N-CA-C	-6.45	105.04	113.17
1	A	37	VAL	N-CA-C	-6.43	98.78	108.17
1	A	89	ILE	CB-CG1-CD1	-6.42	100.33	113.80
1	A	97	ASN	CA-C-N	6.31	126.22	119.28
1	A	97	ASN	C-N-CA	6.31	126.22	119.28
1	A	3	ILE	CA-CB-CG2	6.25	121.13	110.50
1	A	144	HIS	CB-CG-CD2	-6.24	123.08	131.20
1	A	143	ASN	CA-CB-CG	-6.20	106.40	112.60
1	A	82	ASN	OD1-CG-ND2	-6.14	116.45	122.60
1	A	124	ASN	CB-CG-ND2	6.11	125.56	116.40
1	A	71	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	136	GLN	OE1-CD-NE2	-6.00	116.59	122.60
1	A	144	HIS	CB-CG-ND1	5.92	131.58	122.70
1	A	67	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	1	GLN	N-CA-C	-5.90	94.48	111.00
1	A	136	GLN	N-CA-CB	-5.88	101.48	110.65
1	A	9	TYR	CA-C-O	-5.80	114.56	121.11
1	A	57	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	A	2	THR	CA-CB-OG1	-5.78	100.93	109.60
1	A	173	ILE	CA-CB-CG2	5.73	120.25	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	175	ALA	N-CA-C	5.65	118.67	109.24
1	A	93	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	125	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	A	173	ILE	CA-CB-CG1	-5.62	100.85	110.40
1	A	154	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	39	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	A	89	ILE	CB-CA-C	5.37	117.82	111.32
1	A	39	TRP	CE2-CD2-CG	-5.32	100.81	107.20
1	A	89	ILE	N-CA-C	-5.32	98.26	106.72
1	A	157	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	143	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	A	88	TYR	CA-C-N	-5.25	115.96	123.10
1	A	88	TYR	C-N-CA	-5.25	115.96	123.10
1	A	3	ILE	CA-CB-CG1	-5.19	101.58	110.40
1	A	3	ILE	CB-CA-C	5.18	118.80	110.82
1	A	82	ASN	CB-CG-ND2	5.18	124.17	116.40
1	A	175	ALA	CA-C-N	-5.14	116.45	122.93
1	A	175	ALA	C-N-CA	-5.14	116.45	122.93
1	A	7	THR	N-CA-CB	-5.05	102.18	111.37

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	1471	0	1345	32	0
2	A	59	0	0	1	0
All	All	1530	0	1345	32	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 11.

All (32) 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:137:TYR:CE1	1:A:164:LEU:HG	2.23	0.73
1:A:141:ARG:HD3	1:A:143:ASN:O	1.91	0.71
1:A:102:ALA:HB1	1:A:118:TYR:HB3	1.82	0.61
1:A:10:SER:O	1:A:11:ASN:HB2	2.01	0.61
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.64	0.60
1:A:27:TYR:CD2	1:A:47:ALA:HB1	2.37	0.59
1:A:144:HIS:HD2	2:A:219:HOH:O	1.85	0.58
1:A:90:VAL:HG13	1:A:140:VAL:HA	1.86	0.58
1:A:1:GLN:N	1:A:3:ILE:HD13	2.23	0.53
1:A:97:ASN:HD22	1:A:99:SER:H	1.56	0.52
1:A:52:GLN:HE22	1:A:170:ASP:HB3	1.76	0.49
1:A:89:ILE:O	1:A:89:ILE:HG13	2.12	0.49
1:A:137:TYR:CE2	1:A:164:LEU:HB3	2.49	0.48
1:A:105:LEU:HD11	1:A:119:ARG:HB3	1.96	0.47
1:A:1:GLN:H3	1:A:3:ILE:HD13	1.80	0.47
1:A:120:THR:OG1	1:A:136:GLN:HB3	2.15	0.46
1:A:24:GLY:O	1:A:39:TRP:HA	2.15	0.46
1:A:103:THR:O	1:A:105:LEU:HD12	2.16	0.46
1:A:2:THR:H	1:A:28:THR:HA	1.83	0.44
1:A:109:THR:HA	1:A:114:VAL:HA	2.00	0.44
1:A:2:THR:O	1:A:3:ILE:HD12	2.18	0.43
1:A:97:ASN:ND2	1:A:99:SER:H	2.16	0.43
1:A:45:PHE:CE1	1:A:178:GLY:HA3	2.52	0.43
1:A:97:ASN:ND2	1:A:99:SER:OG	2.52	0.42
1:A:14:TYR:HD2	1:A:173:ILE:HD11	1.84	0.42
1:A:86:GLU:O	1:A:136:GLN:HA	2.20	0.42
1:A:27:TYR:CE2	1:A:47:ALA:HB1	2.55	0.41
1:A:27:TYR:HD2	1:A:47:ALA:HB1	1.83	0.41
1:A:76:ILE:HB	1:A:89:ILE:HG13	2.03	0.41
1:A:91:GLU:OE1	1:A:145:ARG:HD2	2.20	0.41
1:A:81:ARG:CZ	1:A:170:ASP:OD1	2.69	0.40
1:A:172:GLN:O	1:A:173:ILE:HD12	2.21	0.40

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	188/190 (99%)	178 (95%)	8 (4%)	2 (1%)	11 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	2	THR

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	154/154 (100%)	133 (86%)	21 (14%)	3 2

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	7	THR
1	A	10	SER
1	A	26	THR
1	A	29	ASN
1	A	53	PRO
1	A	59	VAL
1	A	89	ILE
1	A	90	VAL
1	A	97	ASN
1	A	114	VAL
1	A	122	ARG
1	A	128	ILE
1	A	129	ILE
1	A	143	ASN
1	A	145	ARG
1	A	161	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	LEU
1	A	173	ILE
1	A	176	VAL
1	A	187	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	92	ASN
1	A	97	ASN
1	A	124	ASN
1	A	144	HIS
1	A	154	ASN
1	A	157	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.