



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:31 PM GMT

PDB ID : 1XND
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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

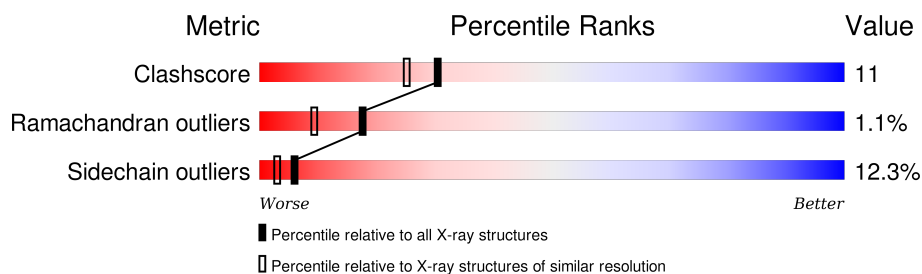
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	190	

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.

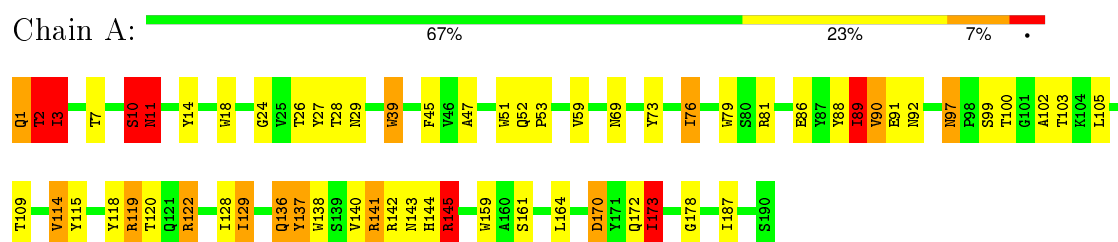
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total	O	0	0
			59	59		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

• Molecule 1: XYLANASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 ⓘ

5.1 Standard geometry ⓘ

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	1.06	2/1517 (0.1%)	2.02	50/2069 (2.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	ASP	CA-CB	-12.07	1.27	1.53
1	A	89	ILE	CA-CB	5.11	1.66	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ASP	N-CA-CB	22.95	151.91	110.60
1	A	141	ARG	NE-CZ-NH2	-20.61	109.99	120.30
1	A	145	ARG	NE-CZ-NH1	18.82	129.71	120.30
1	A	141	ARG	NE-CZ-NH1	18.11	129.36	120.30
1	A	170	ASP	CA-CB-CG	13.41	142.91	113.40
1	A	170	ASP	CB-CA-C	-12.27	85.86	110.40
1	A	145	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	39	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	A	141	ARG	CD-NE-CZ	8.43	135.40	123.60
1	A	142	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	79	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	A	39	TRP	CE2-CD2-CG	-8.11	100.81	107.30
1	A	51	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	A	100	THR	O-C-N	-7.54	110.38	123.20
1	A	11	ASN	CA-C-N	-7.51	101.19	116.20
1	A	138	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	79	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	A	122	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	18	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	A	73	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	A	2	THR	N-CA-C	-6.62	93.14	111.00
1	A	51	TRP	CE2-CD2-CG	-6.42	102.17	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	A	1	GLN	N-CA-C	-6.12	94.48	111.00
1	A	138	TRP	CD1-CG-CD2	6.08	111.17	106.30
1	A	145	ARG	CB-CG-CD	6.07	127.37	111.60
1	A	159	TRP	CE2-CD2-CG	-6.03	102.48	107.30
1	A	39	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	A	18	TRP	CD1-CG-CD2	6.00	111.10	106.30
1	A	88	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	A	39	TRP	CB-CG-CD1	-5.82	119.44	127.00
1	A	39	TRP	CG-CD1-NE1	-5.53	104.57	110.10
1	A	122	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	119	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	79	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	A	51	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	A	173	ILE	CA-CB-CG1	-5.34	100.85	111.00
1	A	18	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	A	159	TRP	CD1-CG-CD2	5.29	110.53	106.30
1	A	138	TRP	CG-CD2-CE3	5.26	138.63	133.90
1	A	11	ASN	O-C-N	5.22	132.07	123.20
1	A	129	ILE	N-CA-CB	-5.21	98.83	110.80
1	A	137	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	76	ILE	N-CA-C	-5.19	97.00	111.00
1	A	100	THR	C-N-CA	-5.13	111.53	122.30
1	A	3	ILE	CA-CB-CG2	5.11	121.13	110.90
1	A	115	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	136	GLN	N-CA-CB	-5.07	101.48	110.60
1	A	18	TRP	CG-CD2-CE3	5.03	138.42	133.90
1	A	10	SER	N-CA-C	5.00	124.51	111.00

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	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	59	0	0	1	0
All	All	1530	0	1345	31	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 (31) 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:HH11	1:A:122:ARG:HG3	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:HG13	1:A:89:ILE:O	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: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 [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	188/190 (99%)	178 (95%)	8 (4%)	2 (1%)	17 9

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%)	135 (88%)	19 (12%)	6 3

All (19) 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

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Mol	Chain	Res	Type
1	A	59	VAL
1	A	69	ASN
1	A	89	ILE
1	A	90	VAL
1	A	92	ASN
1	A	97	ASN
1	A	114	VAL
1	A	128	ILE
1	A	129	ILE
1	A	145	ARG
1	A	161	SER
1	A	173	ILE
1	A	187	ILE

Some 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 ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.