Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:26 PM UTC

PDB ID	:	1HIX / pdb_00001hix
Title	:	CRYSTALLOGRAPHIC ANALYSES OF FAMILY 11 ENDO-BETA-1,4-XYLANASE XYL1 FROM STREPTOMYCES SP. S38
Authors	:	Wouters, J.; Georis, J.; Dusart, J.; Frere, J.M.; Depiereux, E.; Charlier, P.
Deposited on	:	2001-01-05
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:

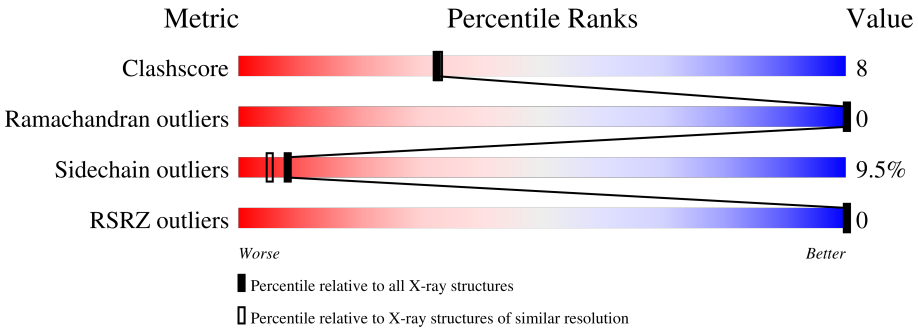
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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)
RSRZ outliers	180081	10067 (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 <=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	190	71% 22%
1	B	190	73% 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3077 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 ENDO-1,4-BETA-XYLANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	7	0	0
			1420	891	240	284	5			
1	B	187	Total	C	N	O	S	7	3	0
			1438	902	242	289	5			

- Molecule 2 is water.

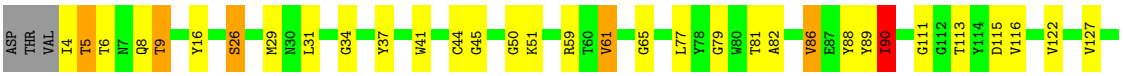
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total	O	0	0
			97	97		
2	B	122	Total	O	0	0
			122	122		

3 Residue-property plots (i)

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 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.

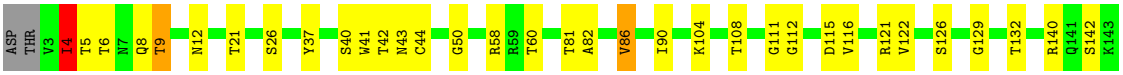
- Molecule 1: ENDO-1,4-BETA-XYLANASE

Chain A:



- Molecule 1: ENDO-1,4-BETA-XYLANASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.49Å 71.49Å 130.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.00 7.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	82.5 (7.00-2.00) 82.5 (7.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.204 , 0.309 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.66 , 110.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3077	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0550e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.51	1/1463 (0.1%)	1.39	19/1994 (1.0%)
1	B	0.44	0/1496	1.55	26/2040 (1.3%)
All	All	0.48	1/2959 (0.0%)	1.47	45/4034 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ARG	CB-CG	8.21	1.77	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	144	ARG	CD-NE-CZ	32.88	170.43	124.40
1	A	115	ASP	CA-C-N	-8.36	112.32	123.10
1	A	115	ASP	C-N-CA	-8.36	112.32	123.10
1	A	89	TYR	CA-C-N	-7.77	112.39	123.11
1	A	89	TYR	C-N-CA	-7.77	112.39	123.11
1	A	111	GLY	CA-C-N	-7.45	115.56	121.82
1	A	111	GLY	C-N-CA	-7.45	115.56	121.82
1	A	90	ILE	N-CA-CB	7.30	121.45	112.10
1	A	171	TYR	CA-C-N	7.07	132.43	121.76
1	A	171	TYR	C-N-CA	7.07	132.43	121.76
1	B	166	GLY	CA-C-N	6.94	130.73	120.87
1	B	166	GLY	C-N-CA	6.94	130.73	120.87
1	A	5	THR	CA-C-O	6.82	126.11	119.08
1	B	115	ASP	CA-C-N	-6.46	114.77	123.10
1	B	115	ASP	C-N-CA	-6.46	114.77	123.10
1	B	144	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	B	111	GLY	CA-C-N	-6.33	116.50	121.82
1	B	111	GLY	C-N-CA	-6.33	116.50	121.82
1	B	144	ARG	CA-CB-CG	6.15	126.41	114.10
1	B	171	TYR	CA-C-N	6.02	131.17	122.44
1	B	171	TYR	C-N-CA	6.02	131.17	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	144	ARG	CD-NE-CZ	5.90	132.66	124.40
1	B	90	ILE	CA-C-N	5.75	130.26	122.90
1	B	90	ILE	C-N-CA	5.75	130.26	122.90
1	A	90	ILE	CA-CB-CG1	5.75	120.17	110.40
1	B	144	ARG	CG-CD-NE	5.57	124.25	112.00
1	B	144	ARG	NH1-CZ-NH2	-5.33	112.37	119.30
1	A	186	SER	CA-C-N	-5.23	115.18	122.71
1	A	186	SER	C-N-CA	-5.23	115.18	122.71
1	A	90	ILE	CA-C-N	5.21	128.88	122.37
1	A	90	ILE	C-N-CA	5.21	128.88	122.37
1	A	166	GLY	CA-C-N	5.20	128.25	120.87
1	A	166	GLY	C-N-CA	5.20	128.25	120.87
1	B	151	ALA	CA-C-N	5.18	126.66	120.13
1	B	151	ALA	C-N-CA	5.18	126.66	120.13
1	B	4	ILE	CA-C-N	5.18	130.07	121.99
1	B	4	ILE	C-N-CA	5.18	130.07	121.99
1	B	153	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	40[A]	SER	CA-C-N	-5.10	112.83	121.85
1	B	40[A]	SER	C-N-CA	-5.10	112.83	121.85
1	B	40[B]	SER	CA-C-N	-5.10	112.83	121.85
1	B	40[B]	SER	C-N-CA	-5.10	112.83	121.85
1	B	60	THR	CA-C-N	5.07	128.71	122.37
1	B	60	THR	C-N-CA	5.07	128.71	122.37

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	1420	0	1290	24	0
1	B	1438	0	1313	19	0
2	A	97	0	0	3	0
2	B	122	0	0	6	0
All	All	3077	0	2603	43	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 8.

All (43) 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:144:ARG:CG	1:A:144:ARG:CB	1.77	1.55
1:A:127:VAL:HG12	2:A:2018:HOH:O	1.88	0.72
1:A:113:THR:O	1:A:141:GLN:HG3	1.92	0.68
1:B:9[A]:THR:HG21	2:B:2014:HOH:O	1.98	0.63
1:A:81:THR:OG1	1:A:86:VAL:HG13	2.01	0.60
1:A:179:TYR:HB2	2:A:2093:HOH:O	2.00	0.60
1:B:81:THR:OG1	1:B:86:VAL:HG13	2.02	0.60
1:A:90:ILE:HD13	1:A:154:HIS:CE1	2.38	0.59
1:A:6:THR:O	1:A:8:GLN:HG2	2.04	0.57
1:B:42:THR:HG22	2:B:2034:HOH:O	2.06	0.55
1:B:4:ILE:HD11	2:B:2005:HOH:O	2.07	0.55
1:B:82:ALA:O	1:B:166:GLY:HA3	2.08	0.54
1:A:144:ARG:CG	1:A:144:ARG:CA	2.78	0.53
1:A:156:ASP:OD2	2:A:2083:HOH:O	2.18	0.53
1:B:108:THR:HG23	1:B:112:GLY:O	2.09	0.53
1:A:90:ILE:O	1:A:90:ILE:HG13	2.09	0.51
1:A:45:GLY:O	1:A:179:TYR:HA	2.10	0.51
1:A:37:TYR:CZ	1:A:50:GLY:HA2	2.46	0.49
1:A:61:VAL:HG21	1:A:77:LEU:HD22	1.93	0.49
1:A:65:GLY:HA3	1:A:186:SER:O	2.11	0.49
1:A:162:GLY:O	1:A:164:PRO:HD3	2.14	0.48
1:B:44:CYS:O	1:B:180:GLN:HA	2.13	0.47
1:B:12:ASN:HA	2:B:2011:HOH:O	2.13	0.47
1:B:41:TRP:CD1	1:B:182:SER:HA	2.49	0.47
1:A:44:CYS:O	1:A:180:GLN:HA	2.14	0.47
1:A:9:THR:HG23	1:A:16:TYR:CE1	2.50	0.47
1:B:58:ARG:HH22	1:B:156:ASP:CG	2.23	0.47
1:A:26:SER:O	1:A:41:TRP:HA	2.15	0.46
1:B:181:SER:HB3	2:B:2122:HOH:O	2.16	0.46
1:A:61:VAL:HG23	1:A:149:ILE:O	2.16	0.46
1:A:34:GLY:O	1:A:51:LYS:NZ	2.50	0.45
1:A:79:GLY:HA3	1:A:88:TYR:CZ	2.52	0.44
1:A:82:ALA:HB3	1:A:169:ASN:ND2	2.33	0.44
1:B:58:ARG:NH2	1:B:156:ASP:OD1	2.50	0.44
1:A:29:MET:HE2	1:A:31:LEU:CD2	2.48	0.43
1:B:126:SER:OG	1:B:129:GLY:O	2.29	0.42
1:B:140:ARG:HG2	1:B:142:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:O	1:A:122:VAL:HG23	2.20	0.42
1:B:104:LYS:HE2	2:B:2074:HOH:O	2.20	0.42
1:B:6:THR:O	1:B:8:GLN:OE1	2.38	0.41
1:B:157:ALA:HA	1:B:160:ARG:NH1	2.35	0.41
1:B:121:ARG:O	1:B:132:THR:HA	2.21	0.41
1:B:37:TYR:CZ	1:B:50:GLY:HA2	2.56	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	183/190 (96%)	175 (96%)	8 (4%)	0	100	100
1	B	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
All	All	371/380 (98%)	356 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	146/151 (97%)	132 (90%)	14 (10%)	8	5
1	B	151/151 (100%)	136 (90%)	15 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	297/302 (98%)	268 (90%)	29 (10%)	8 5

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	THR
1	A	9	THR
1	A	26	SER
1	A	59	ARG
1	A	61	VAL
1	A	86	VAL
1	A	90	ILE
1	A	116	VAL
1	A	165	LEU
1	A	167	SER
1	A	180	GLN
1	A	187	ILE
1	A	188	SER
1	B	4	ILE
1	B	5	THR
1	B	9[A]	THR
1	B	9[B]	THR
1	B	21	THR
1	B	26	SER
1	B	43	ASN
1	B	86	VAL
1	B	116	VAL
1	B	122	VAL
1	B	144	ARG
1	B	165	LEU
1	B	167	SER
1	B	188	SER
1	B	189	VAL

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

Mol	Chain	Res	Type
1	A	7	ASN
1	A	8	GLN
1	A	134	ASN

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Mol	Chain	Res	Type
1	A	135	GLN
1	A	153	ASN
1	B	8	GLN
1	B	13	ASN
1	B	123	ASN
1	B	134	ASN
1	B	135	GLN
1	B	141	GLN

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 (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^{th} 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	185/190 (97%)	-0.22	0	100	100	9, 23, 34, 50	1 (0%)
1	B	187/190 (98%)	-0.24	0	100	100	9, 22, 34, 42	4 (2%)
All	All	372/380 (97%)	-0.23	0	100	100	9, 23, 34, 50	5 (1%)

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.