



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:57 PM GMT

PDB ID : 1HIX
Title : CRYSTALLOGRAPHIC ANALYSES OF FAMILY 11 ENDO-BETA-1,4-XYLANASEXYL1 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 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/ValidationPDFNotes.html>

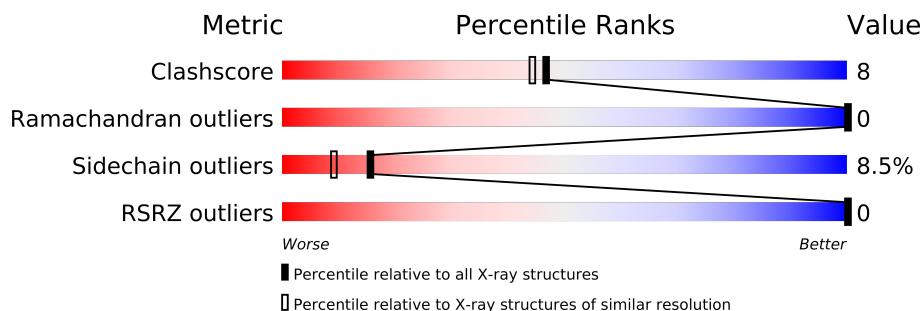
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	190	
1	B	190	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3077 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

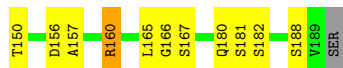
- Molecule 2 is water.

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

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

Age Group	Percentage
18-24	45%
25-34	35%
35-44	15%
45-54	5%
55-64	2%
65-74	1%
75-84	1%
85+	1%



4 Data and refinement statistics

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 6.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	82.5 (7.00-2.00) 84.8 (6.99-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.204 , 0.309 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.70 , 103.8	EDS
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 22088 reflections	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 58.23 % 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 2.1067e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.47	2/1463 (0.1%)	1.08	5/1994 (0.3%)
1	B	0.38	0/1496	1.29	8/2040 (0.4%)
All	All	0.43	2/2959 (0.1%)	1.19	13/4034 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ARG	CB-CG	9.09	1.77	1.52
1	A	144	ARG	CG-CD	5.53	1.65	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ARG	CD-NE-CZ	33.45	170.43	123.60
1	A	144	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	B	144	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	B	160	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	144	ARG	CD-NE-CZ	6.47	132.66	123.60
1	B	144	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
1	A	58	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	144	ARG	CG-CD-NE	5.93	124.25	111.80
1	B	144	ARG	CA-CB-CG	5.91	126.41	113.40
1	B	58	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	168	PHE	CB-CG-CD1	5.19	124.43	120.80
1	B	58	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	160	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1420	0	1290	23	0
1	B	1438	0	1313	21	0
2	A	97	0	0	3	0
2	B	122	0	0	6	0
All	All	3077	0	2603	44	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:144:ARG:CB	1:A:144:ARG:CG	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:CA	1:A:144:ARG:CG	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:HG13	1:A:90:ILE:O	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:B:58:ARG:NH2	1:B:156:ASP:OD1	2.50	0.44
1:A:82:ALA:HB3	1:A:169:ASN:ND2	2.33	0.44
1:A:79:GLY:HA3	1:A:88:TYR:CZ	2.52	0.44
1:B:126:SER:OG	1:B:129:GLY:O	2.29	0.42
1:B:110:ASP:OD1	1:B:150:THR:OG1	2.37	0.42
1:B:58:ARG:HH22	1:B:156:ASP:CG	2.23	0.42
1:B:140:ARG:HG2	1:B:142:SER:O	2.20	0.42
1:B:104:LYS:HE2	2:B:2074:HOH:O	2.20	0.42
1:A:122:VAL:HG23	1:A:122:VAL:O	2.20	0.42
1:B:6:THR:O	1:B:8:GLN:OE1	2.38	0.41
1:B:16:TYR:HH	1:B:18[B]:SER:HG	1.64	0.41
1:B:157:ALA:HA	1:B:160:ARG:NH1	2.35	0.41
1:A:39:THR:HG1	1:A:41:TRP:HZ3	1.69	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

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	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 ⓘ

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%)	12 6
1	B	151/151 (100%)	139 (92%)	12 (8%)	18 11
All	All	297/302 (98%)	271 (91%)	26 (9%)	15 8

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	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	142	SER
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	86	VAL
1	B	116	VAL
1	B	144	ARG
1	B	165	LEU
1	B	167	SER
1	B	188	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	8	GLN
1	A	118	GLN
1	A	134	ASN
1	A	141	GLN
1	A	153	ASN
1	B	7	ASN
1	B	8	GLN
1	B	13	ASN
1	B	55	ASN
1	B	118	GLN
1	B	153	ASN
1	B	180	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	185/190 (97%)	-0.29	0 100 100	12, 23, 34, 50	1 (0%)
1	B	187/190 (98%)	-0.33	0 100 100	12, 22, 34, 42	1 (0%)
All	All	372/380 (97%)	-0.31	0 100 100	12, 23, 34, 50	2 (0%)

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 carbohydrates 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.