Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:32 AM GMT

PDB ID	:	3B7M
Title	:	Crystal structure of a meso-active thermo-stable cellulase (MT Cel12A) derived by making non-contiguous mutations in the active surface of the Cel12A cellulase of Rhodothermus marinus
Authors	:	Karthikeyan, S.; Guptasarma, P.
Deposited on	:	2007-10-31
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

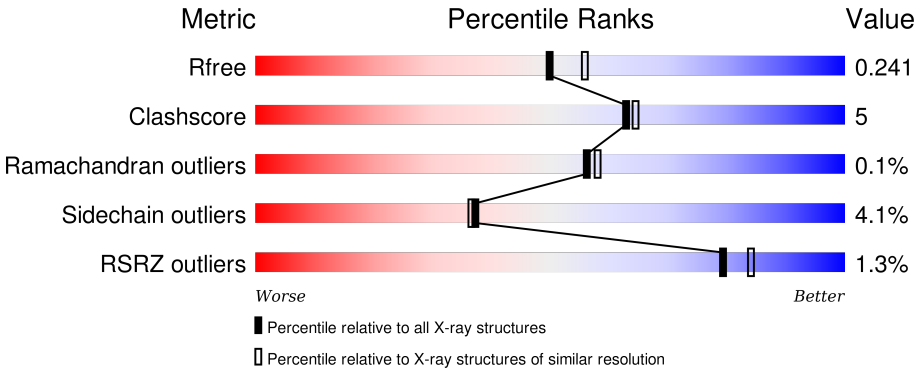
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	216	89% 10%
1	B	216	% 87% 12%
1	C	216	% 90% 9%
1	D	216	2% 88% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7062 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 CELLULASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	6	0
			1701	1077	287	332	5			
1	B	216	Total	C	N	O	S	0	2	0
			1688	1066	287	330	5			
1	C	216	Total	C	N	O	S	0	2	0
			1687	1066	287	328	6			
1	D	216	Total	C	N	O	S	0	3	0
			1693	1073	287	328	5			

- Molecule 2 is water.

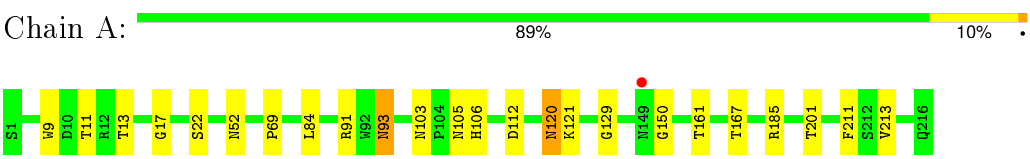
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	93	Total	O	0	0
			93	93		
2	B	73	Total	O	0	0
			73	73		
2	C	68	Total	O	0	0
			68	68		
2	D	59	Total	O	0	0
			59	59		

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 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 (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.

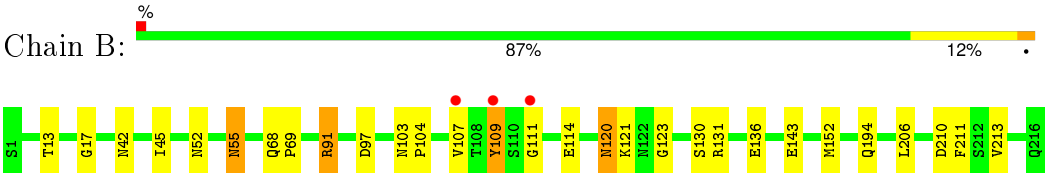
- Molecule 1: CELLULASE

Chain A:



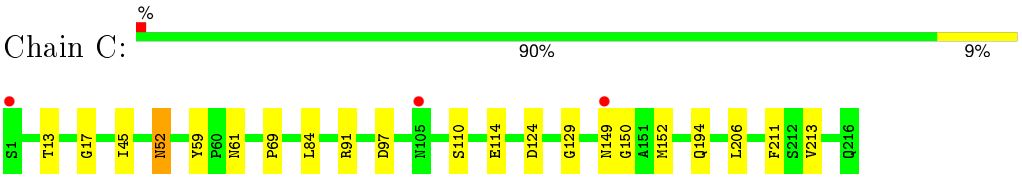
- Molecule 1: CELLULASE

Chain B:



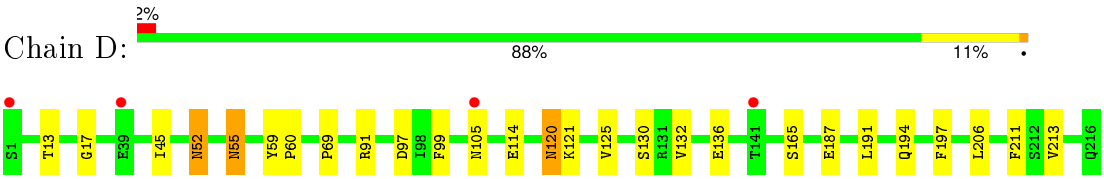
- Molecule 1: CELLULASE

Chain C:



- Molecule 1: CELLULASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.40Å 111.87Å 133.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.42 – 2.10 41.40 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.42-2.10) 97.5 (41.40-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.238 0.189 , 0.241	Depositor DCC
R_{free} test set	2666 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 52277 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7062	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0/1760	0.60	2/2412 (0.1%)
1	B	0.48	0/1735	0.61	1/2376 (0.0%)
1	C	0.47	0/1734	0.58	0/2374
1	D	0.43	0/1745	0.57	0/2390
All	All	0.47	0/6974	0.59	3/9552 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	91	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	91	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	1701	0	1642	23	0
1	B	1688	0	1613	30	0
1	C	1687	0	1616	13	0
1	D	1693	0	1621	18	0
2	A	93	0	0	2	0
2	B	73	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	68	0	0	1	0
2	D	59	0	0	1	0
All	All	7062	0	6492	70	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 5.

All (70) 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:13[B]:THR:HG21	1:B:68:GLN:HG2	1.51	0.93
1:A:11[B]:THR:HG21	1:B:104:PRO:HG2	1.62	0.82
1:A:120:ASN:HD22	1:A:121:LYS:H	1.25	0.81
1:D:55:ASN:H	1:D:55:ASN:HD22	1.29	0.81
1:B:120:ASN:HD22	1:B:121:LYS:H	1.29	0.80
1:D:120:ASN:HD22	1:D:121:LYS:H	1.32	0.77
1:A:93:ASN:HD22	1:A:93:ASN:C	1.88	0.76
1:A:112:ASP:HB2	2:A:300:HOH:O	1.87	0.74
1:B:55:ASN:HD22	1:B:55:ASN:H	1.41	0.69
1:A:11[B]:THR:HG21	1:B:104:PRO:CG	2.24	0.67
1:D:99[B]:PHE:HD1	1:D:191:LEU:HD12	1.59	0.67
1:A:11[B]:THR:CG2	1:B:104:PRO:HG2	2.26	0.65
1:A:120:ASN:HD22	1:A:121:LYS:N	1.96	0.64
1:B:13:THR:HG23	1:B:17:GLY:HA2	1.81	0.63
1:A:129:GLY:H	1:D:55:ASN:ND2	1.96	0.63
1:A:11[B]:THR:CG2	1:B:104:PRO:CG	2.77	0.63
1:A:129:GLY:H	1:D:55:ASN:HD21	1.45	0.62
1:B:55:ASN:HD21	1:C:129:GLY:H	1.47	0.62
1:C:110:SER:HB2	1:C:152[A]:MET:HE1	1.80	0.61
1:B:120:ASN:HD22	1:B:121:LYS:N	1.98	0.58
1:D:99[B]:PHE:CD1	1:D:191:LEU:HD12	2.39	0.57
1:B:69:PRO:HA	2:B:254:HOH:O	2.05	0.57
1:D:120:ASN:HD22	1:D:121:LYS:N	1.98	0.57
1:C:211:PHE:CZ	1:C:213:VAL:HG23	2.40	0.56
1:D:69:PRO:HA	2:D:260:HOH:O	2.07	0.55
1:B:42:ASN:HD21	1:B:210:ASP:H	1.55	0.54
1:B:211:PHE:CZ	1:B:213:VAL:HG23	2.43	0.54
1:C:61:ASN:ND2	1:D:105:ASN:OD1	2.40	0.53
1:A:11[B]:THR:HG23	1:B:104:PRO:HG3	1.91	0.52
1:C:13:THR:CG2	1:C:17:GLY:HA2	2.41	0.51
1:D:97:ASP:OD1	1:D:114:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:VAL:HG21	1:B:109:TYR:CE2	2.46	0.50
1:A:13[A]:THR:CG2	1:A:17:GLY:HA2	2.41	0.50
1:A:11[B]:THR:CG2	1:B:104:PRO:HG3	2.41	0.50
1:D:13:THR:CG2	1:D:17:GLY:HA2	2.41	0.50
1:B:55:ASN:ND2	1:C:129:GLY:H	2.09	0.49
1:C:149:ASN:OD1	1:C:150:GLY:N	2.45	0.49
1:A:13[A]:THR:HG22	1:A:17:GLY:HA2	1.94	0.49
1:D:121:LYS:HD2	1:D:125[A]:VAL:HG13	1.95	0.49
1:B:55:ASN:HD22	1:B:55:ASN:N	2.09	0.49
1:A:69:PRO:HA	2:A:289:HOH:O	2.11	0.48
1:C:97:ASP:OD1	1:C:114:GLU:HG3	2.14	0.48
1:C:211:PHE:CZ	1:C:213:VAL:CG2	2.97	0.48
1:B:107:VAL:HG21	1:B:109:TYR:CZ	2.49	0.47
1:D:45:ILE:HD12	1:D:206:LEU:HB2	1.96	0.47
1:B:91:ARG:HG2	1:B:123:GLY:HA3	1.95	0.47
1:D:59:TYR:HE2	1:D:194:GLN:HE21	1.62	0.47
1:D:55:ASN:ND2	1:D:55:ASN:H	2.05	0.47
1:C:45:ILE:HD12	1:C:206:LEU:HB2	1.97	0.47
1:B:55:ASN:H	1:B:55:ASN:ND2	2.11	0.46
1:C:59:TYR:HE2	1:C:194:GLN:HE21	1.62	0.46
1:B:211:PHE:CZ	1:B:213:VAL:CG2	2.99	0.46
1:C:52:ASN:O	1:C:91:ARG:NH2	2.49	0.46
1:A:211:PHE:CZ	1:A:213:VAL:HG23	2.52	0.45
1:A:211:PHE:CZ	1:A:213:VAL:CG2	3.00	0.45
1:B:45:ILE:HD12	1:B:206:LEU:HB2	1.98	0.45
1:A:93:ASN:ND2	1:A:93:ASN:C	2.62	0.45
1:B:107:VAL:HG11	1:B:109:TYR:CE1	2.53	0.43
1:B:111:GLY:O	1:B:152:MET:HG3	2.19	0.42
1:D:211:PHE:CZ	1:D:213:VAL:HG23	2.54	0.42
1:B:68:GLN:HA	1:B:69:PRO:HD2	1.80	0.42
1:D:52:ASN:O	1:D:91:ARG:NH2	2.53	0.42
1:A:103:ASN:HB3	1:A:106:HIS:O	2.20	0.42
1:A:9:TRP:CD1	1:B:103:ASN:ND2	2.88	0.42
1:A:11[B]:THR:HG23	1:B:104:PRO:CG	2.46	0.41
1:B:13:THR:CG2	1:B:17:GLY:HA2	2.48	0.41
1:B:97:ASP:OD1	1:B:114:GLU:HG3	2.20	0.41
1:C:69:PRO:HA	2:C:280:HOH:O	2.19	0.41
1:A:11[B]:THR:HG22	1:A:22:SER:OG	2.20	0.41
1:D:60:PRO:HD2	1:D:197:PHE:O	2.20	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	220/216 (102%)	214 (97%)	5 (2%)	1 (0%)	34 30
1	B	216/216 (100%)	208 (96%)	8 (4%)	0	100 100
1	C	216/216 (100%)	210 (97%)	6 (3%)	0	100 100
1	D	217/216 (100%)	210 (97%)	7 (3%)	0	100 100
All	All	869/864 (101%)	842 (97%)	26 (3%)	1 (0%)	56 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	GLY

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	182/176 (103%)	172 (94%)	10 (6%)	27 23
1	B	178/176 (101%)	169 (95%)	9 (5%)	29 26
1	C	178/176 (101%)	175 (98%)	3 (2%)	68 74
1	D	179/176 (102%)	171 (96%)	8 (4%)	34 32
All	All	717/704 (102%)	687 (96%)	30 (4%)	37 35

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	84	LEU
1	A	93	ASN
1	A	105	ASN
1	A	120	ASN
1	A	161	THR
1	A	167[A]	THR
1	A	167[B]	THR
1	A	185	ARG
1	A	201	THR
1	B	52	ASN
1	B	55	ASN
1	B	109	TYR
1	B	120	ASN
1	B	130	SER
1	B	131	ARG
1	B	136	GLU
1	B	143	GLU
1	B	194	GLN
1	C	52	ASN
1	C	84	LEU
1	C	124	ASP
1	D	52	ASN
1	D	55	ASN
1	D	120	ASN
1	D	130	SER
1	D	132	VAL
1	D	136	GLU
1	D	165	SER
1	D	187	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	52	ASN
1	A	73	GLN
1	A	93	ASN
1	A	106	HIS
1	A	120	ASN
1	B	42	ASN
1	B	52	ASN
1	B	55	ASN

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Mol	Chain	Res	Type
1	B	61	ASN
1	B	120	ASN
1	C	52	ASN
1	C	63	GLN
1	C	153	ASN
1	D	52	ASN
1	D	55	ASN
1	D	63	GLN
1	D	120	ASN
1	D	153	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

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	216/216 (100%)	-0.22	1 (0%)	91	93	13, 21, 38, 44	0
1	B	216/216 (100%)	-0.10	3 (1%)	78	82	16, 26, 42, 48	0
1	C	216/216 (100%)	-0.15	3 (1%)	78	82	16, 26, 40, 44	0
1	D	216/216 (100%)	-0.00	4 (1%)	70	75	19, 32, 45, 50	0
All	All	864/864 (100%)	-0.12	11 (1%)	79	84	13, 26, 42, 50	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	ASN	5.5
1	A	149	ASN	4.1
1	D	1	SER	3.9
1	B	107	VAL	3.3
1	D	141	THR	3.0
1	B	109	TYR	2.7
1	D	105	ASN	2.6
1	C	105	ASN	2.6
1	C	1	SER	2.3
1	B	111	GLY	2.1
1	D	39	GLU	2.0

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.