



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:29 am GMT

PDB ID : 4B4H  
Title : Thermobifida fusca cellobiohydrolase Cel6B(E3) catalytic domain  
Authors : Sandgren, M.; Wu, M.; Stahlberg, J.; Karkehabadi, S.; Mitchinson, C.; Kelemen, B.R.; Larenas, E.A.; Hansson, H.  
Deposited on : 2012-07-30  
Resolution : 1.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

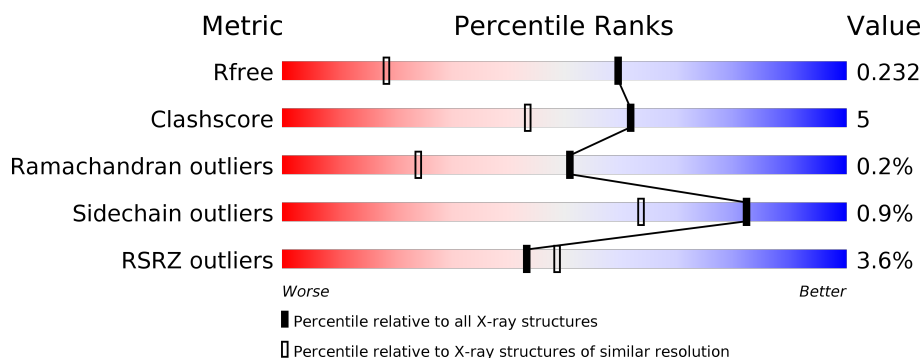
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	100719	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	420	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> </div>
1	B	420	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div></div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7239 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 BETA-1,4-EXOCELLULASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	9	0
			3215	2016	560	630	9			
1	B	413	Total	C	N	O	S	0	9	0
			3203	2006	555	633	9			

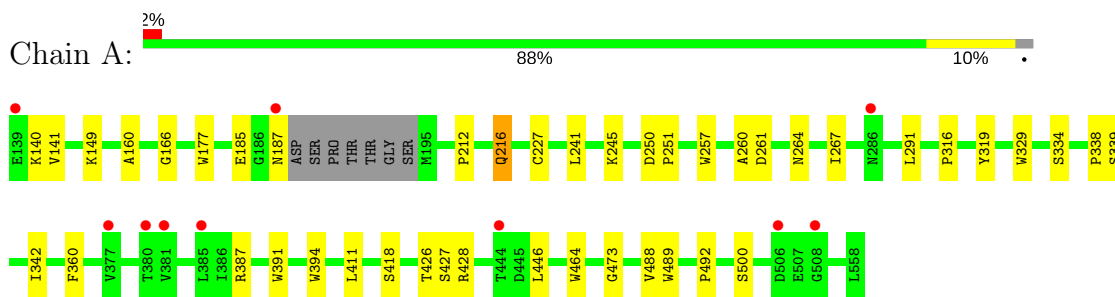
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	406	Total	O	0	0
			406	406		
2	B	415	Total	O	0	0
			415	415		

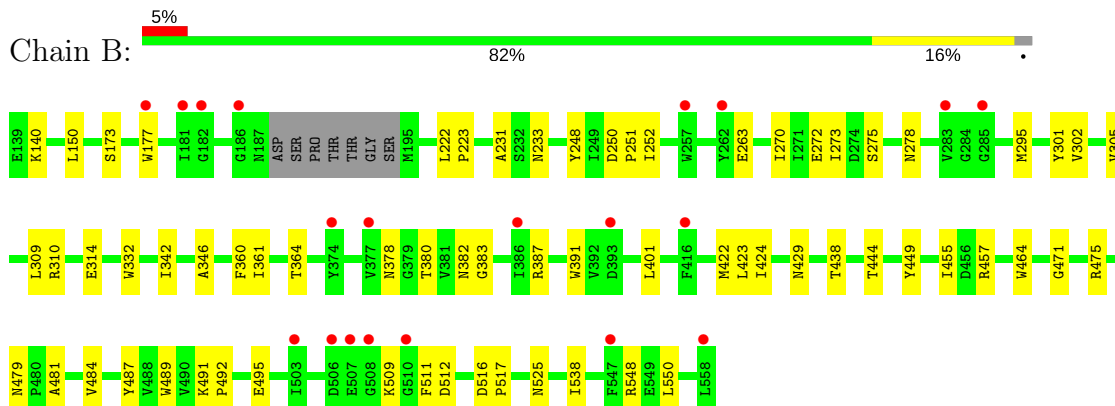
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: BETA-1,4-EXOCELLULASE



#### • Molecule 1: BETA-1,4-EXOCELLULASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.75Å 93.35Å 96.59Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	39.09 – 1.50 38.87 – 1.50	Depositor EDS
% Data completeness (in resolution range)	89.3 (39.09-1.50) 89.3 (38.87-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.196 , 0.232 0.195 , 0.232	Depositor DCC
$R_{free}$ test set	5441 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.9	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 23.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.065 for -h,l,k 0.066 for -h,-l,-k 0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.515 for H, K, L 0.485 for H, -K, -L	Depositor
Outliers	0 of 108166 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7239	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.58	6/3324 (0.2%)	0.65	1/4532 (0.0%)
1	B	0.53	4/3312 (0.1%)	0.57	0/4517
All	All	0.56	10/6636 (0.2%)	0.61	1/9049 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLN	C-O	-6.55	1.10	1.23
1	A	177	TRP	CD2-CE2	5.29	1.47	1.41
1	A	464	TRP	CD2-CE2	5.28	1.47	1.41
1	B	489	TRP	CD2-CE2	5.24	1.47	1.41
1	A	391	TRP	CD2-CE2	5.22	1.47	1.41
1	A	257	TRP	CD2-CE2	5.16	1.47	1.41
1	B	332	TRP	CD2-CE2	5.05	1.47	1.41
1	B	391	TRP	CD2-CE2	5.03	1.47	1.41
1	A	329	TRP	CD2-CE2	5.00	1.47	1.41
1	B	177	TRP	CD2-CE2	5.00	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ARG	NE-CZ-NH1	5.29	122.94	120.30

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	3215	0	3048	23	0
1	B	3203	0	3025	42	0
2	A	406	0	0	5	0
2	B	415	0	0	9	0
All	All	7239	0	6073	64	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 (64) 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:B:429:ASN:OD1	2:B:2308:HOH:O	2.12	0.68
1:B:438:THR:HB	2:B:2316:HOH:O	1.93	0.67
1:A:160:ALA:O	1:A:166:GLY:HA3	1.97	0.64
1:B:495:GLU:O	2:B:2306:HOH:O	2.15	0.63
1:B:387:ARG:HD3	2:B:2273:HOH:O	1.99	0.63
1:A:140:LYS:HB3	1:A:319:TYR:CE2	2.34	0.62
1:B:509:LYS:HD2	1:B:538:ILE:CG2	2.33	0.58
1:A:216:GLN:HE22	1:A:488:VAL:HB	1.68	0.58
1:B:273:ILE:HG21	1:B:364:THR:HG21	1.88	0.54
1:B:471:GLY:HA2	1:B:550:LEU:HA	1.89	0.53
1:A:241:LEU:HG	1:A:245:LYS:HE3	1.90	0.53
1:B:424:ILE:HD12	1:B:487:TYR:CE1	2.44	0.52
1:B:360:PHE:O	1:B:422:MET:HA	2.10	0.52
1:A:140:LYS:HB3	1:A:319:TYR:CZ	2.46	0.51
1:A:426:THR:O	1:A:473:GLY:HA3	2.11	0.51
1:B:361:ILE:HB	1:B:423:LEU:HB2	1.91	0.51
1:B:305:VAL:HG12	1:B:309:LEU:HD11	1.93	0.50
1:A:212:PRO:HA	1:A:264:ASN:O	2.10	0.50
1:A:260:ALA:HB1	1:A:316:PRO:HG2	1.92	0.50
1:A:261:ASP:HB2	1:B:383:GLY:O	2.12	0.50
1:A:500:SER:O	2:A:2352:HOH:O	2.19	0.50
1:B:263:GLU:HG3	1:B:263:GLU:O	2.13	0.49
1:A:227:CYS:HA	1:A:291:LEU:HD23	1.94	0.49
1:B:424:ILE:HD12	1:B:487:TYR:HE1	1.78	0.48
1:B:525:ASN:HB3	2:B:2376:HOH:O	2.12	0.48
1:B:302:VAL:HG13	1:B:346:ALA:HA	1.96	0.47
1:B:305:VAL:O	1:B:309:LEU:HG	2.14	0.47
1:B:479:ASN:HA	1:B:484:VAL:O	2.16	0.46
1:B:273:ILE:CG2	1:B:364:THR:HG21	2.46	0.46
1:B:275:SER:O	1:B:278:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:C	1:A:187:ASN:H	2.20	0.45
1:B:250:ASP:HB2	1:B:251:PRO:HD3	1.99	0.45
1:B:449:TYR:C	1:B:449:TYR:CD1	2.90	0.45
1:B:511:PHE:CZ	1:B:516:ASP:HB2	2.52	0.45
1:B:231:ALA:HB3	1:B:512:ASP:HB2	1.99	0.45
1:B:233:ASN:OD1	1:B:509:LYS:HA	2.17	0.44
1:A:267:ILE:HD12	2:A:2133:HOH:O	2.17	0.44
1:A:387[B]:ARG:NH1	2:A:2257:HOH:O	2.31	0.44
1:B:270:ILE:HG23	1:B:361:ILE:HG21	1.98	0.44
1:B:517:PRO:HB3	2:B:2391:HOH:O	2.18	0.44
1:B:382:ASN:OD1	1:B:444:THR:HG22	2.18	0.44
1:B:491:LYS:HA	1:B:492:PRO:HD3	1.84	0.44
1:B:295:MET:HG3	1:B:301:TYR:CE1	2.53	0.43
1:B:401:LEU:HD11	1:B:481:ALA:CB	2.48	0.43
1:B:548:ARG:HG2	2:B:2033:HOH:O	2.18	0.43
1:B:509:LYS:HD2	1:B:538:ILE:HG21	1.98	0.43
1:A:446:LEU:HD23	2:A:2259:HOH:O	2.18	0.43
1:B:222:LEU:HD23	1:B:223:PRO:HD2	2.00	0.43
1:B:429:ASN:HB3	2:B:2251:HOH:O	2.18	0.43
1:A:334:SER:O	1:A:338:PRO:HG2	2.18	0.43
1:B:248:TYR:CE1	1:B:252:ILE:HD11	2.54	0.43
1:B:310:ARG:O	1:B:314:GLU:HG3	2.19	0.43
1:B:150:LEU:HB3	1:B:173:SER:CB	2.48	0.42
1:A:339:SER:O	1:A:342:ILE:HG22	2.20	0.42
1:A:387[A]:ARG:HD3	1:A:394:TRP:CZ3	2.54	0.42
1:B:464:TRP:HB3	2:B:2256:HOH:O	2.20	0.42
1:A:492:PRO:HD2	2:A:2346:HOH:O	2.19	0.42
1:B:516:ASP:C	1:B:516:ASP:OD1	2.57	0.42
1:A:360:PHE:CE1	1:A:411:LEU:HD13	2.55	0.42
1:A:141:VAL:HG22	1:A:319:TYR:OH	2.20	0.41
1:A:427:SER:HA	1:A:489:TRP:CD1	2.56	0.41
1:B:360:PHE:HB2	1:B:422:MET:CE	2.51	0.41
1:A:250:ASP:N	1:A:251:PRO:HD2	2.36	0.40
1:B:455:ILE:O	1:B:457:ARG:HG3	2.22	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	418/420 (100%)	406 (97%)	12 (3%)	0	100	100
1	B	418/420 (100%)	395 (94%)	21 (5%)	2 (0%)	32	10
All	All	836/840 (100%)	801 (96%)	33 (4%)	2 (0%)	51	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	LYS
1	B	272	GLU

### 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	338/335 (101%)	336 (99%)	2 (1%)	89	76
1	B	338/335 (101%)	334 (99%)	4 (1%)	75	52
All	All	676/670 (101%)	670 (99%)	6 (1%)	82	63

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	418	SER
1	B	342	ILE
1	B	378	ASN

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Mol	Chain	Res	Type
1	B	380	THR
1	B	475	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	A	435	ASN
1	A	520	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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	413/420 (98%)	0.28	10 (2%) 59 65	5, 11, 21, 31	0
1	B	413/420 (98%)	0.75	20 (4%) 31 35	14, 20, 26, 33	0
All	All	826/840 (98%)	0.51	30 (3%) 43 49	5, 17, 24, 33	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	VAL	5.9
1	B	506	ASP	4.1
1	A	381	VAL	4.0
1	B	508	GLY	3.8
1	B	558	LEU	3.8
1	B	510	GLY	3.5
1	A	187	ASN	3.3
1	B	283	VAL	3.0
1	B	182	GLY	2.9
1	B	547	PHE	2.9
1	A	139	GLU	2.9
1	B	416	PHE	2.8
1	A	385	LEU	2.7
1	A	508	GLY	2.7
1	B	285	GLY	2.7
1	B	262	TYR	2.5
1	A	444	THR	2.5
1	B	507	GLU	2.4
1	A	506	ASP	2.4
1	B	257	TRP	2.4
1	A	286	ASN	2.3
1	B	386	ILE	2.2
1	A	377	VAL	2.2
1	B	177	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	186	GLY	2.1
1	B	374	TYR	2.1
1	B	393	ASP	2.1
1	B	503	ILE	2.0
1	B	181	ILE	2.0
1	A	380	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.