



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 02:28 pm GMT

PDB ID : 4B4F
Title : Thermobifida fusca Cel6B(E3) co-crystallized with cellobiose
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 : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

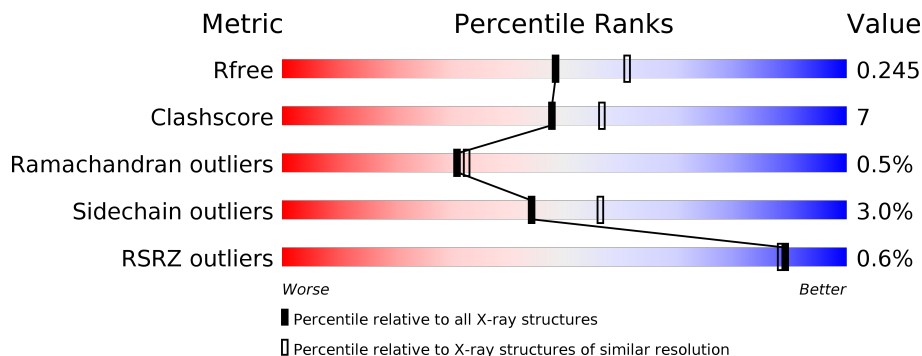
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	A	420	<div> <div></div> <div>87%</div> <div>11%</div> <div>•</div> </div>
1	B	420	<div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div>

2 Entry composition [i](#)

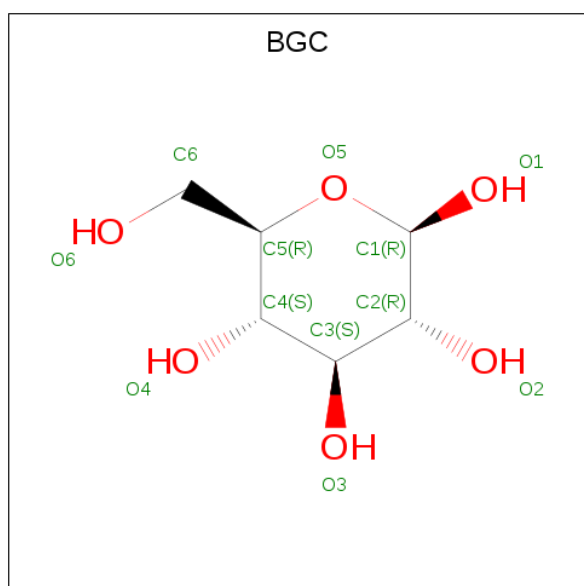
There are 4 unique types of molecules in this entry. The entry contains 7226 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	420	Total	C	N	O	S	0	4	0
			3234	2022	562	641	9			
1	B	420	Total	C	N	O	S	0	2	0
			3222	2016	558	639	9			

- Molecule 2 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	341	Total	O	0	0
			341	341		
4	B	314	Total	O	0	0
			314	314		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.95Å 106.70Å 92.47Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	19.92 – 2.20 19.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.92-2.20) 98.0 (19.92-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.244 0.186 , 0.245	Depositor DCC
R_{free} test set	2076 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7226	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BGC

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	0.54	6/3330 (0.2%)	0.56	0/4545
1	B	0.54	4/3312 (0.1%)	0.56	0/4522
All	All	0.54	10/6642 (0.2%)	0.56	0/9067

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	TRP	CD2-CE2	5.31	1.47	1.41
1	A	464	TRP	CD2-CE2	5.26	1.47	1.41
1	A	177	TRP	CD2-CE2	5.12	1.47	1.41
1	A	332	TRP	CD2-CE2	5.12	1.47	1.41
1	B	257	TRP	CD2-CE2	5.10	1.47	1.41

There are no bond angle outliers.

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	3234	0	3041	33	0
1	B	3222	0	3026	51	0
2	A	67	0	57	3	0
2	B	45	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	341	0	0	0	0
4	B	314	0	0	0	0
All	All	7226	0	6163	84	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 7.

The worst 5 of 84 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:464:TRP:HE1	1:B:524[B]:ARG:NH2	1.55	1.05
1:A:366:ASN:HD22	1:A:367:TYR:H	1.04	0.98
1:B:366:ASN:HD22	1:B:367:TYR:H	1.13	0.94
1:B:152:VAL:H	1:B:207:GLN:HE22	1.26	0.83
1:A:366:ASN:ND2	1:A:367:TYR:H	1.78	0.80

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	422/420 (100%)	405 (96%)	15 (4%)	2 (0%)	31	33
1	B	420/420 (100%)	409 (97%)	9 (2%)	2 (0%)	31	33
All	All	842/840 (100%)	814 (97%)	24 (3%)	4 (0%)	31	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	GLU
1	A	272	GLU
1	B	381	VAL
1	A	381	VAL

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	339/335 (101%)	331 (98%)	8 (2%)	52	65
1	B	337/335 (101%)	324 (96%)	13 (4%)	35	44
All	All	676/670 (101%)	655 (97%)	21 (3%)	44	55

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	171	ASN
1	B	241	LEU
1	B	395	ASN
1	B	143	ASN
1	B	477	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	ASN
1	B	278	ASN
1	B	467	GLN
1	B	207	GLN
1	A	363	ASN

5.3.3 RNA ⓘ

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](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	A	601	2	11,11,12	0.56	0	15,15,17	1.03	1 (6%)
2	BGC	A	602	2	11,11,12	0.63	0	15,15,17	2.31	4 (26%)
2	BGC	A	603	2	11,11,12	0.66	0	15,15,17	1.50	3 (20%)
2	BGC	A	604	2	11,11,12	0.57	0	15,15,17	1.34	1 (6%)
2	BGC	A	605	2	11,11,12	0.59	0	15,15,17	0.97	1 (6%)
2	BGC	A	606	2	12,12,12	0.53	0	17,17,17	0.72	0
2	BGC	B	601	2	11,11,12	0.54	0	15,15,17	0.93	1 (6%)
2	BGC	B	602	2	11,11,12	0.64	0	15,15,17	2.64	4 (26%)
2	BGC	B	603	2	11,11,12	0.68	0	15,15,17	1.36	2 (13%)
2	BGC	B	604	2	12,12,12	0.58	0	17,17,17	0.86	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	601	2	-	0/2/19/22	0/1/1/1
2	BGC	A	602	2	-	0/2/19/22	0/1/1/1
2	BGC	A	603	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	604	2	-	0/2/19/22	0/1/1/1
2	BGC	A	605	2	-	0/2/19/22	0/1/1/1
2	BGC	A	606	2	-	0/2/22/22	0/1/1/1
2	BGC	B	601	2	-	0/2/19/22	0/1/1/1
2	BGC	B	602	2	-	0/2/19/22	0/1/1/1
2	BGC	B	603	2	-	0/2/19/22	0/1/1/1
2	BGC	B	604	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	BGC	C3-C4-C5	-2.11	106.46	110.24
2	B	602	BGC	C2-C3-C4	2.08	114.48	110.87
2	B	601	BGC	C1-O5-C5	2.15	115.14	112.19
2	B	604	BGC	C4-C3-C2	2.15	114.60	110.83
2	A	603	BGC	C1-C2-C3	2.20	112.44	109.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	BGC	1	0
2	A	602	BGC	1	0
2	A	603	BGC	1	0
2	B	601	BGC	1	0
2	B	602	BGC	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	420/420 (100%)	-0.57	3 (0%) 87 86	11, 16, 28, 52	0
1	B	420/420 (100%)	-0.51	2 (0%) 90 90	12, 17, 28, 55	0
All	All	840/840 (100%)	-0.54	5 (0%) 89 88	11, 17, 28, 55	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	ASN	4.0
1	A	285	GLY	3.8
1	A	286	ASN	2.2
1	A	284	GLY	2.1
1	B	284	GLY	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	A	603	11/12	0.81	0.16	28,30,31,31	0
2	BGC	A	604	11/12	0.82	0.19	32,33,34,34	0
2	BGC	A	606	12/12	0.84	0.16	42,44,45,46	0
2	BGC	B	604	12/12	0.85	0.17	32,33,34,35	0
2	BGC	B	603	11/12	0.86	0.17	27,28,30,30	0
2	BGC	A	605	11/12	0.87	0.14	35,40,41,42	0
2	BGC	B	601	11/12	0.91	0.12	16,18,19,19	0
2	BGC	A	602	11/12	0.91	0.13	21,24,26,26	0
2	BGC	A	601	11/12	0.93	0.13	18,19,20,20	0
3	CA	A	608	1/1	0.94	0.05	48,48,48,48	0
2	BGC	B	602	11/12	0.95	0.10	20,22,23,24	0
3	CA	B	607	1/1	0.99	0.06	20,20,20,20	0
3	CA	A	607	1/1	0.99	0.04	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.