Table 1 Structures of LPMOs

CAZy Family	Organism	Protein name	PDB code	ASU†	Crystallization and diffraction data: Protein conc. & buffer	Crystallization conditions	Space group	Resolution (Å)	Active site: Element (oxidation)‡	Residues	Specificity: Substrates	Site of attack	Comments	Reference
AA9	*Aspergillus fumigatus*	PMO-5 *Af*AA9_B Afum_AFUA_4G07850 Afu4g07850	5X6A	2	N/R	0.2M $MgCl_2$, 25% (w/v) PEG3350 0.1M BIS-TRIS pH 6.0	*P*1	1.70	-	His1 His86 Tyr175	N/D	N/D	Disordered active site His1. No active site metal	To be published
AA9	*Collariella virescens*	*Cv*AA9_A	5NLT	6	6.3 mg/ml 0.02M Na-acetate pH5.5	1.6 M $(NH_4)_2SO_4$ 0.1M NaCl 0.1 M HEPES pH 7.5	*P*1	1.95	Cu(I)	meHis1 His79 Tyr169	PASC Cellooligo-saccharides Xyloglucan Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate	Simmons et al. (2017)
AA9	*Heterobasidion irregulare*	*Hi*AA9_B *Hi*LPMO9B	5NNS	2	10 mg/ml 0.02 M HEPES pH 7.5 (0.15 M NaCl)	22%(w/v) Na-polyacrylic acid, 0.02 M $MgCl_2$ 0.1 M HEPES pH 7.5	*P*2_1	2.10	Cu	His1 His80 Tyr166	PASC	C1	The structure has been deposited in the Protein Data Bank, currently with the status HPUB (processing complete, entry on hold until publication)	Liu et al. (2018)(Liu et al. 2018)
AA9	*Lentinus similis*	*Ls*AA9_A	5ACF	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.6M NaCl 0.1M Citric acid pH4.0 (pH5.5)	*P*$4_1$32	1.80	Cu(II)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Cellotriose bound in the active site. Exogenous ligand (Cl^-) mimicking superoxide in the equatorial position	Frandsen *et al.*, (2016)
AA9	*Lentinus similis*	*Ls*AA9_A	5ACG	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.9M NaCl 0.1M Citric acid pH 4.0 (soaked in pH 5.5)	*P*$4_1$32	1.91	Cu(II)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate	Frandsen *et al.*, (2016)

											Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans			
AA9	*Lentinus similis*	*Ls*AA9_A	5ACH	1	8.5 mg/ml 0.02M Na-acetate pH5.5	3.0M NaCl 0.1M Citric acid pH 3.5 (soaked in pH 5.5)	$P4_132$	1.28	Cu(II)/Cu(I) 0.9	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate	Frandsen *et al.*, (2016)
AA9	*Lentinus similis*	*Ls*AA9_A	5ACI	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.6M NaCl 0.1M Citric acid pH 4.0 (soaked in pH 5.5)	$P4_132$	1.75	Cu(II)/Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Cellohexaose bound in the active site (pH 5.5).	Frandsen *et al.*, (2016)
AA9	*Lentinus similis*	*Ls*AA9_A	5ACJ	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.0M NaCl 0.1M Citric acid pH 3.5 (soaked in pH 5.5)	$P4_132$	1.70	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Cellotriose bound in the active site	Frandsen *et al.*, (2016)
AA9	*Lentinus similis*	*Ls*AA9_A	5N04	1	8.5 mg/ml 0.02M Na-acetate pH5.5	3.0M NaCl 0.1M Citric acid pH 3.5	$P4_132$	1.76	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Disordered active site His78, partially replaced by a chloride ion.	Frandsen *et al.*, (2017)

											Mixed-linkage (1;3,1;4)-β-D-glucans			
AA9	*Lentinus similis*	*Ls*AA9_A	5N05	1	8.5 mg/ml 0.02M Na-acetate pH5.5	3.4M NaCl 0.1M Citric acid pH 3.5	$P4_132$	1.58	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Cellohexaose bound in the active site.	Frandsen *et al.*, (2017)
AA9	*Lentinus similis*	*Ls*AA9_A	5NKW	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.3M NaCl 0.1M Citric acid pH 3.5 (soaked in pH 5.5)	$P4_132$	1.48	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Glucomannan oligosaccharide in the active site. Oligosaccharides modelled near Gln14	Simmons et al. (2017)
AA9	*Lentinus similis*	*Ls*AA9_A	5NLN	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.6M NaCl 0.1 M citric acid pH4.5 (soaked in pH5.5)	$P4_132$	1.90	Cu(II)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Xylopentaose oligosaccharide in the active site. The active site axial position is partially occupied by an exogenous ligand (Cl^-) mimicking an oxygen species.	Simmons et al. (2017)
AA9	*Lentinus similis*	*Ls*AA9_A	5NLO	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.6M NaCl 0.1 M citric acid pH4.5 (soaked in pH5.5)	$P4_132$	1.33	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Xylopentaose oligosaccharide modelled in the active site.	Simmons et al. (2017)

											Mixed-linkage (1;3,1;4)-β-D-glucans			
AA9	*Lentinus similis*	*Ls*AA9_A	5NLP	1	19.2 mg/ml 0.02M Na-acetate pH5.5	4.1 M NaCl 0.1 M citric acid pH 4.0 (soaked pH 5.5)	$P4_132$	1.59	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Soaked with Xylotetraose Xylooligosaccharides modelled in the active site and near Gln14 and Tyr21	Simmons et al. (2017)
AA9	*Lentinus similis*	*Ls*AA9_A	5NLQ	1	19.2 mg/ml 0.02M Na-acetate pH5.5	4.4 M NaCl 0.1 M citric acid pH4.5 (soaked in pH 5.5)	$P4_132$	1.50	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Soaked with Xylotriose Xylooligosaccharides modelled in the active site and near Asp38 and the glycosylation (Asn33)	Simmons et al. (2017)
AA9	*Lentinus similis*	*Ls*AA9_A	5NLR	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.5 M NaCl 0.1 M citric acid, pH3.5	$P4_132$	2.00	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan Mixed-linkage (1;3,1;4)-β-D-glucans	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Soaked with 1,3:1,4-β-glucotetraose. Partially overlapping β(1,4)-gluco-oligosaccharides modelled in the active site	Simmons et al. (2017)
AA9	*Lentinus similis*	*Ls*AA9_A	5NLS	1	19.2 mg/ml 0.02M Na-acetate pH5.5	3.2 M NaCl 0.1 M citric acid, pH3.5 (soaked in pH 5.5)	$P4_132$	1.75	Cu(I)	meHis1 His78 Tyr164	PASC Cellooligo-saccharides Xyloglucan Xylan Xylooligo-saccharides Glucomannan	C4 (C1 products also detected from polysaccharides)	Preincubated with 1mM Cu(II)acetate Cellopentaose modelled in the active site	Simmons et al. (2017)

											Mixed-linkage (1;3,1;4)-β-D-glucans			
AA9	*Neurospora crassa*	*Nc*AA9_D *Nc*LPMO9D PMO-2 NCU01050 GH61-4	4EIR	2	- 0.15M NaCl 0.010 M Tris pH 8.5	PEG3350 (pH 6.7)	*$P2_1$*	1.10	Cu(II)/Cu(I)	meH1 His84 Tyr168	PASC	C4	Proposed O_2 molecule Near the active site axial position	Li *et al.*, (2012) Phillips *et al.*, (2011)
AA9	*Neurospora crassa*	*Nc*AA9_D *Nc*LPMO9D PMO-2 NCU01050 GH61-4	5TKF	4	12.6 mg/ml 0.02M Na-acetate pH 5.0	22 %(w/v) PEG3350 0.1 M HEPES pH 6.4	*P*1	2.10	Cu(I)	meH1 His84 Tyr168	PASC	C4	In chain B and D O_2 molecules are modelled near the active site interacting with His157 and Gln166	O'Dell, Swartz et al (2017)
AA9	*Neurospora crassa*	*Nc*AA9_D *Nc*LPMO9D PMO-2 NCU01050 GH61-4	5TKG	2	12.5 mg/ml 0.02M Na-acetate pH 5.0	25 %(w/v) PEG3350 0.1 M HEPES pH 6.0	*$P2_1$*	1.20	Cu(II)	meH1 His84 Tyr168	PASC	C4	Additinal details on crystallzation in O'Dell, Swartz et al (2017)	O'Dell, Agarwal (2017)
AA9	*Neurospora crassa*	*Nc*AA9_D *Nc*LPMO9D PMO-2 NCU01050 GH61-4	5TKH	2	N/R	25 %(w/v) PEG3350 0.1 M HEPES pH 6.0	*$P2_1$*	1.20	Cu(II)/Cu(I)	meH1 His84 Tyr168	PASC	C4	Proposed peroxide ion modelled in the active site equatorial position interacting with His157 and Gln166	O'Dell, Agarwal (2017)
AA9	*Neurospora crassa*	*Nc*AA9_D *Nc*LPMO9D PMO-2 NCU01050 GH61-4	5TKI (X-ray)	2	12.2 mg/ml 0.02M Na-acetate pH 5.0	25 %(w/v) PEG3350 0.09 M HEPES pH 6.0	*$P2_1$*	1.50	Cu(II)	meH1 His84 Tyr168	PASC	C4	Room temperature X-ray data collection Joint X-ray and neutron crystal structure Additinal crystallzation conditions in O'Dell, Swartz et al (2017)	O'Dell, Agarwal (2017)
AA9	*Neurospora crassa*	*Nc*AA9_D *Nc*LPMO9D PMO-2 NCU01050 GH61-4	5TKI (neutron)	2	12.2 mg/ml 0.02M Na-acetate pH 5.0	25 %(w/v) PEG3350 0.09 M HEPES pH 6.0	*$P2_1$*	2.12	Cu	meH1 His84 Tyr168	PASC	C4	Joint X-ray and neutron crystal structure Additinal crystallzation conditions in O'Dell, Swartz et al (2017)	O'Dell, Agarwal (2017)
AA9	*Neurospora crassa*	*Nc*AA9_F *Nc*LPMO9F PMO-03328 NCU03328 GH61-6	4QI8	2	-	0.2M NH_4NO_3 20%(w/v) PEG3350 pH 7.0	*$P2_12_12$*	1.10	Cu(II)	His1 His72 Tyr157	PASC	C1	Regiospecificity in Vu, Beeson, Phillips et al. (2014).	Tan *et al.*, (2015) Phillips *et al.*, (2011)
AA9	*Neurospora crassa*	*Nc*AA9_M *Nc*LPMO9M NcPMO-3 PMO-3	4EIS	2	10 mg/ml 0.010 M Tris pH 8.5	0.1M NaCl 0.010 M Tris pH 8.5	*$P2_1$*	1. 37	Cu(I)	MeHis1 His82 Tyr171	PASC	C1/C4	Proposed peroxide ion near active site. Tyr24 oxidation.	Li *et al.*,(2012), Phillips *et al.*, (2011)

		NCU07898 GH61-13												
AA9	*Neurospora crassa*	*Nc*AA9_C *Nc*LPMO9C NCU02916 PMO-02916 GH61-3	4D7U	2	1.4 mg/ml	0.2M NH_4-citrate 20%(w/v) PEG3350 pH 5.1	*P*2_1	1. 56	Cu(I)	His1 His83 Tyr166	PASC Cellooligo-saccharides Xyloglucan Glucomannan β-glucan	C4	-	Borisova *et al.*, (2015)
AA9	*Neurospora crassa*	*Nc*AA9_C *Nc*LPMO9C NCU02916 PMO-02916 GH61-3	4D7V	2	1.4 mg/ml	0.2M Zn(II)acetate 17.5% / 20.0 % (w/v)PEG3350 pH 8.0	*P*2_1	1.90	Zn(II)	His1 His83 Tyr166	PASC Cellooligo-saccharides Xyloglucan Glucomannan β-glucan	C4	-	Borisova *et al.*, (2015)
AA9	*Neurospora crassa*	*Nc*AA9_A *Nc*LPMO9A NCU02240 GH61-1	5FOH	1	-	0.2 M $LiSO_4$ 20%(w/v) PEG3350 pH 6.5	*P*$3_2$21	1. 60	Cu(I)	His1 His81 Tyr164	Avicel	N/D	Activity in Znameroski, E.A. *et al.* (2012)	To be published
AA9	*Phanerochaete chrysosporium*	*Pc*AA9_D PcLPMO9D PcGH61D GH61D	4B5Q	2	12 mg/ml 0.01M Na-acetate pH5.0	2.1M Malic Acid (racemic) pH 7.0	*C*2	1.75	Cu(I)	His1 His76 Tyr160	PASC Avicel	C1	-	Wu *et al.*,(2013)
AA9	*Thermoascus aurantiacus*	*Ta*AA9_A TaAA9A *Ta*GH61 *Ta*GH61A *Ta*LPMO9A	3ZUD	1	15 mg/ml 0.02M Na-acetate pH5.5	0.2M NaCl 0.1M HEPES pH7.5 25%(w/v) PEG3350	*P*2_1	1.25	Cu(II)/Cu(I) A 0.6 B 0.15	MeHis1 His86 Tyr175	PASC PCS	C1/C4	Crystal soaked in 10mM Cu(II)$(NO_3)_2$	Quinlan *et al.*, (2011)
AA9	*Thermoascus aurantiacus*	*Ta*AA9_A TaAA9A *Ta*GH61 *Ta*GH61A *Ta*LPMO9A	2YET	2	15 mg/ml 0.02M Na-acetate pH5.5	0.2M NaCl 0.1M HEPES pH8.0 25%(w/v) PEG3350	*P*2_1	1.50	Cu 0.2	MeHis1 His86 Tyr175	PASC PCS	C1/C4	-	Quinlan *et al.*, (2011)
	Thermothelomyces thermophila	*Mt*AA9_D *Mt*PMO3 MYCTH_92668	5UFV	6	20 mg/ml	18 %(w/v) PEG 6000 0.1 M Na-citrate pH 3.9	*P*2_1	2.45	Cu(I)	MeHis1 His75 Tyr169	PASC	C1	Reconstituted with excess $CuSO_4$ at pH 5.0 for 4 h	Span, Suess *et al.*, (2017)
AA9	*Thielavia terrestris*	*Tt*AA9_E *Tt*GH61E GH61E 131562	3EII	4	3.1 mg/ml (pH 7.6-5.0)	1.6M $MgSO_4$ 0.1 MES pH 6.5	*F*23	2.25	Zn(II)	His1 His68 Tyr153	PASC Avicel	C1	Crystal soaked in 1.8M $ZnSO_4$, Cacodylate pH 6.5 Regiospecificity inferred from Cannella et al. (2016).	Harris *et al.*, (2010)
AA9	*Thielavia terrestris*	*Tt*AA9_E *Tt*GH61E	3EJA	4	3.1 mg/ml (pH 7.6-5.0)	1.6M $MgSO_4$ 0.1 MES pH 6.5	*F*23	1.90	Mg^{2+}	His1 His68	PASC Avicel	C1	-	Harris *et al.*, (2010)

		GH61E 131562								Tyr153				
AA9	*Trichoderma reesei*	*Hj*AA9_B HjGH61B GH61B Cel61B EG7	2VTC	2	2.2 mg/ml 0.02M Na-phosphate pH 6.8	15-20%(w/v) PEG2000 0.1M TRIS pH8.4 0.010M $NiCl_2$	*P*65	1.60	Ni(II)	His1 His89 Tyr176	Cellulose	N/D	-	Karkehabadi *et al.*,(2008)
AA9	*Trichoderma reesei*	EGIV Egl4 EG4 LPMO4 *Hj*LPMO9A *Tr*AA9_A *Tr*Cel61A	5O2W	1	30 mg/ml 0.025 M Tris-HCl pH 7.5 0.025 M NaCl	1.6 M $(NH_4)_2SO_4$ 0.1 M citric acid pH 4.0	$P2_1$	1.78	Cu(I)	MeHis1 His86 Tyr174	PASC	C1/C4	Structure shows that a predicted linker is an integral part of the catalytic domain	Hansson, Karkehabadi et al (2017)
AA9	*Trichoderma reesei*	EGIV Egl4 EG4 LPMO4 *Hj*LPMO9A *Tr*AA9_A *Tr*Cel61A	5O2X	1	30 mg/ml 0.025 M Tris-HCl pH 7.5 0.025 M NaCl	1.6 M $(NH_4)_2SO_4$ 0.1 M citric acid pH 4.0	$P2_1$	0.95	Cu(II)	MeHis1 His86 Tyr174	PASC	C1/C4	Structure shows that a predicted linker is an integral part of the catalytic domain	Hansson, Karkehabadi et al (2017)
AA10	*Bacillus amylolique-faciens*	*Ba*AA10_A *Ba*CBM33 ChbB Rbam17540	2YOW	2	7.0 mg/ml 0.02 M Na-acetate pH5.0 0.25M NaCl	0.1M MMT pH 4.0, 25%(w/v) PEG1500	$P2_12_12$	1.80	-	His28 His125 Phe196	β-chitin	C1	C1 oxidation of β-chitin reported in Gregory et. al 2016	Hemsworth, Davies, *et al.*, (2013)
AA10	*Bacillus amylolique-faciens*	*Ba*AA10_A *Ba*CBM33 ChbB Rbam17540	2YOX	2	7.0 mg/ml 0.02 M Na-acetate pH5.0 0.25M NaCl	0.1M MMT pH 4.0, 25%(w/v) PEG1500	$P2_1$	1.90	Cu(I)	His28 His125 Phe196	β-chitin	C1	1mM $Cu(II)(NO_3)_2$ added to sample	Hemsworth, Davies, *et al.*, (2013)
AA10	*Bacillus amylolique-faciens*	*Ba*AA10_A *Ba*CBM33 ChbB Rbam17540	2YOY	2	7.0 mg/ml 0.02 M Na-acetate pH5.0 0.25M NaCl	0.1M MMT pH 4.0, 25%(w/v) PEG1500	$P2_12_12$	1.70	Cu(I)	His28 His125 Phe196	β-chitin	C1	-	Hemsworth, Davies, *et al.*, (2013)
AA10	*Bacillus amylolique-faciens*	*Ba*AA10_A *Ba*CBM33 ChbB Rbam17540	5IJU	2	4.7 mg/ml 0.02 M Na-acetate pH5.0 0.25M NaCl	20% (w/v) PEG6000 0.1M acetate pH5.0 0.2M $CaCl_2$ (+seed stock)	$P2_1$	1.70	Cu(II)	His28 His125 Phe196	β-chitin	C1	Microseeded using crystals grown in 0.1M MMT pH 4.0, 25%(w/v),PEG1500. $CuCl_2$ added in stoichiometric amounts C1 oxidation of β-chitin reported	Gregory *et al.* (2016).
AA10	*Bacillus amylolique-*	*Bl*LPMO10A *Bl*AA10_A	5LW4 (NMR)	1	0.8 mM BlLPMO10A	-	-	-	-	His1 His90	-	-	NMR structure 20 conformers No active site metal	To be published

	faciens				0.025 M Na-phosphate pH 5.0 0.01 M NaCl (90%/10% H2O/D2O)					Phe161			Active site disorder reminiscent of *Ao*AA13 (PDB 5T7K)	
	Bacillus thuringiensis serovar	*Bt*AA10_A LPMO10A *Bt*LPMO10A	5WSZ	4	-	0.2M Mg-acetate 0.1M Na-cacodylate pH 6.5, 20% (w/v) PEG8000	$P2_12_12$	2.57	Cu(I)	His1 His85 Phe158	-	-	-	To be published
AA10	*Burkholderia pseudomallei*	*Bp*AA10_A	3UAM	6	21 mg/ml	0.1M Bis-Tris-propane pH 6.77 0.2M $NaNO_3$ 20.54%(w/v) PEG3500	$P1$	2.00	-	His19 His122 Phe205	N/D	N/D	Mentioned in (Book *et al.*, 2014)	To be published
AA10	*Cellvibrio japonicus*	*Cf*AA10_A *Cj*LPMO10A CJA_2191 Cbp33A Lpmo10A	5FJQ	3	9 mg/ml 0.02 M TRIS pH8.0	0.1 M Na-acetate pH 5.2 22%(w/v) PEG4000	$C2$	1.85	Cu(I) (Chain B Cu(II))	His37 His136 Phe205	α-chitin β-chitin	C1	Cu(II)-saturated sample	Forsberg *et al.*, (2016)
AA10	*Enterococcus faecalis*	*Ef*AA10_A EfCBM33A EfaCBM33 EF0362	4A02	1	25 mg/ml 0.02 M TRIS pH8.0	1.0M K/Na-tartrate 0.1M imidazole pH 8.0 0.2M NaCl	$P3_2$	0.95	-	His29 His114 Phe185	α-chitin β-chitin	C1	-	Vaaje-Kolstad *et al.*, (2012)
AA10	*Enterococcus faecalis*	*Ef*AA10_A EfCBM33A EfaCBM33 EF0362	4ALC	1	25 mg/ml 0.02 M TRIS pH8.0	0.1 M HEPES pH 7.5 20%(w/v) PEG8000	$P2_12_12$	1.49	Cu(II)	His29 His114 Phe185	α-chitin β-chitin	C1	Preincubated with 1mM $CuSO_4$	Gudmundsson *et al.*, (2014)
AA10	*Enterococcus faecalis*	*Ef*AA10_A EfCBM33A EfaCBM33 EF0362	4ALE	1	25 mg/ml 0.02 M TRIS pH8.0	0.1 M HEPES pH 7.5 20%(w/v) PEG8000	$P2_12_12$	1.48	Cu(II)/(I)	His29 His114 Phe185	α-chitin β-chitin	C1	Preincubated with 1mM $CuSO_4$	Gudmundsson *et al.*, (2014)
AA10	*Enterococcus faecalis*	*Ef*AA10_A EfCBM33A EfaCBM33 EF0362	4ALQ	1	25 mg/ml 0.02 M TRIS pH8.0	0.1 M HEPES pH 7.5 20%(w/v) PEG8000	$P2_12_12$	1.48	Cu(II)/(I)	His29 His114 Phe185	α-chitin β-chitin	C1	Preincubated with 1mM $CuSO_4$	Gudmundsson *et al.*, (2014)
AA10	*Enterococcus faecalis*	*Ef*AA10_A EfCBM33A EfaCBM33 EF0362	4ALR	1	25 mg/ml 0.02 M TRIS pH8.0	0.1 M HEPES pH 7.5 20%(w/v) PEG8000	$P2_12_12$	1.49	Cu(II)/(I)	His29 His114 Phe185	α-chitin β-chitin	C1	Preincubated with 1mM $CuSO_4$	Gudmundsson *et al.*, (2014)
AA10	*Enterococcus faecalis*	*Ef*AA10_A EfCBM33A EfaCBM33 EF0362	4ALS	1	25 mg/ml 0.02 M TRIS pH8.0	0.1 M HEPES pH 7.5 20%(w/v) PEG8000	$P2_12_12$	1.47	Cu(II)/(I)	His29 His114 Phe185	α-chitin β-chitin	C1	Preincubated with 1mM $CuSO_4$	Gudmundsson *et al.*, (2014)
AA10	*Enterococcus faecalis*	*Ef*AA10_A EfCBM33A EfaCBM33 EF0362	4ALT	1	25 mg/ml 0.02 M TRIS pH8.0	0.1 M HEPES pH 7.5 20%(w/v) PEG8000	$P2_12_12$	1.49	Cu(I)	His29 His114 Phe185	α-chitin β-chitin	C1	Preincubated with 1mM $CuSO_4$	Gudmundsson *et al.*, (2014)

AA10	*Jonesia denitrificans*	*Jd*AA10_A *Jd*LPMO10A Jden_1381	5AA7	2	20 mg/ml 0.02 M TRIS pH8.0	1.9 M DL-malic acid pH 7	$P2_12_12_1$	1.55	Cu(I)	His32 His109 Phe164	α-chitin β-chitin	C1	-	Mekasha *et al.*, (2016)
AA10	*Jonesia denitrificans*	*Jd*AA10_A *Jd*LPMO10A Jden_1381	5VG0 (X-ray)	2	48 mg/ml 20 mM Tris-HCl pH 8.0	1.9 M DL-malic acid pH 7.0	$P2_12_12_1$	1.10	Cu(II)	His32 His109 Phe164	α-chitin β-chitin	C1	Incubated with a threefold molar excess of $CuSO_4$ for 30 min at room temperature Proposed peroxide ion in equatorial position	Bacik et al (2017)
AA10	*Jonesia denitrificans*	*Jd*AA10_A *Jd*LPMO10A Jden_1381	5VG1 (neutron)	2	48 mg/ml 20 mM Tris-HCl pH 8.0	1.9 M DL-malic acid pH 7.0	$P2_12_12_1$	2.10	Cu(II)	His32 His109 Phe164	α-chitin β-chitin	C1	Incubated with a threefold molar excess of $CuSO_4$ for 30 min at room temperature	Bacik et al (2017)
AA10	*Micromonospora aurantiaca*	*Ma*AA10_B *Ma*LPMO10B	5OPF	1	21.9 mg/ml, 0.02 M Bis-Tris pH 6.0	0.04 M potassium phosphate 16 %(w/v) PEG8000 20% (v/v) glycerol	$P2_12_12_1$	1.08	Cu(II)	His37 His144 Phe221	PASC β-chitin	C1/C4	The C-terminal G230 from a symmetry related molecule occupy the ligand position on the active site Cu, albeit with distorted geometry. Authors claim Cu(I)	Forsberg et al (2018)
AA10	*Serratia marcescens*	*Sm*AA10_A SmLPMO10A CBP21 Cbp21 Cbp	2BEM	3	20 mg/ml 0.05 M TRIS pH8.0	1.26 $(NH_4)_2SO_4$ 0.1M HEPES pH 7.5	$P2_12_12$	1.55	Na^{2+}	His28 His114 Phe187	α-chitin β-chitin	C1	Chain A and B have no active site metal	Vaaje-Kolstad, Houston, *et al.*, (2005)
AA10	*Serratia marcescens*	*Sm*AA10_A SmLPMO10A CBP21 Cbp21 Cbp	2BEN	2	17.5 mg/ml 0.05 M TRIS pH8.0	20%(w/v) PEG8000 0.1M CHAPS 0.2M NaCl	$P3_221$	1.80	-	His28 His114 Phe187	α-chitin β-chitin	C1	Y54A mutant	Vaaje-Kolstad, Houston, *et al.*, (2005)
AA10	*Serratia marcescens*	*Sm*AA10_A SmLPMO10A CBP21 Cbp21 Cbp	2LHS (NMR)	-	0.8-1.2mM 0.02M K_2PO_4 0.01M NaCl	pH 5.5	-	-	-	His28 His114 Phe187	α-chitin β-chitin	C1	NMR structure	Aachmann *et al.*, (2012)
AA10	*Streptomyces coelicolor*	*Sc*AA10_B *Sc*LPMO10B SCO0643 SCF91.03c	4OY6	1	10.3 mg/ml 0.02 M TRIS pH8.0	0.2 M Zn-acetate 0.1 M Na-cacodylate pH 6.5 9%(v/v) 2-propanol	$P3_121$	1.29	Cu(II)/Cu(I) 0.95	His43 His150 Tyr219	PASC Avicel β-chitin	C1/C4 (C1 on chitin)	Soaked in 1mM–20mM Cu(II)Cl_2 (Zn(II)-acetate reduced to 0.1M)	Forsberg, Mackenzie, *et al.*, (2014)

AA10	*Streptomyces coelicolor*	*Sc*AA10_B *Sc*LPMO10B SCO0643 SCF91.03c	4OY8	1	10.3 mg/ml 0.02 M TRIS pH8.0	0.2 M Zn-acetate 0.1 M Na-cacodylate pH 6.5 9%(v/v) 2-propanol	$P3_121$	1.40	Zn(II) 0.8	His43 His150 Tyr219	PASC Avicel β-chitin	C1/C4 (C1 on chitin)	-	Forsberg, Mackenzie, *et al.*, (2014)
AA10	*Streptomyces coelicolor*	*Sc*AA10_C *Sc*LPMO10C LPMO10C CelS2 SCO1188 SCG11A.19	4OY7	8	9.2 mg/ml 0.02 M TRIS pH8.0	9%(w/v) PEG10.000 0.1M Na-citrate 0.1M Ca-acetate 5%(v/v)glycerol	$P2_12_12_1$	1.50	Cu(II)/Cu(I) 0.5	His35 His144 Phe219	PASC Avicel	C1	-	Forsberg, Mackenzie, *et al.*, (2014)
AA10	*Streptomyces lividans*	*Sl*AA10_E *Sli*LPMO10E SLI_3182	5FTZ	1	15 mg/ml 0.01M Na-acetate pH5.0 0.15M NaCl	0.1M Na-acetate pH 4.6 25%(w/v) PEG4000	*C*2	1.38	Cu(I) 0.8	His30 His120 Phe193	β-chitin	C1/(C4)	Definite C1 oxidation Indications of C4 ox.	Chaplin *et al.*, (2016)
AA10	*Thermobifida fusca*	*Tf*AA10_A *Tf*LPMO10A E7 Tfu_1268	4GBO	2	-	0.1M HEPES pH 7.5 4.3M NaCl	$P3_221$	2.00	Cu(I) 0.5	His37 His144 Tyr213	PASC Avicel β-chitin	C1/C4 (C1 on chitin)	Regiospecificity in (Forsberg, Mackenzie, *et al.*, 2014)	To be published
AA10	*Thermobifida fusca*	*Tf*AA10_A *Tf*LPMO10A E7 Tfu_1268	5UIZ	2	8.5 mg/ml 0.1M HEPES pH 7.5 0.1M NaCl 5% Glycerol 5% Ethylene-glycol	0.1M HEPES pH 7.5 4.3M NaCl - or - 0.1 M Na-acetate pH 4.6 20% (v/v) 2-propanol 0.2 M CaCl	$P3_221$	2.00	Cu(I) A 0.5 B 0.31	His37 His144 Tyr213	PASC Avicel β-chitin	C1/C4 (C1 on chitin)	Regiospecificity in (Forsberg, Mackenzie, *et al.*, 2014) Conflicting information on crystallizartion in publication and PDB deposition entry	Kruer-Zerhusen et al. (2017)
AA10	*Vibrio cholerae*	*Vc*AA10_B VCA0811 VcGbpA GbpA	2XWX	2	25 mg/ml 0.02M TRIS pH7.5	0.2M $Mg(HCO_3)_2$ 50%(w/v) PEG3350 3.33% (w/v) D-sorbitol pH 7.5	$P2_1$	1.80	-	His24 His121 Fis193	N/D	N/D	-	Wong *et al.*, (2012)
AA10	*Anomala cuprea* entomopox-virus	Fusolin (ACV034)	4YN1	1	-	In Vivo Crystallization (pH 7.0)	$P4_12_12$	1.90	-	His1 His142 Phe225	N/D	N/D	Intracellular Fusolin micro-crystals from EPV-infected larvae of *Anomala cuprea* moths	Chiu *et al.*, (2015)
AA10	Unidentified entomopox-virus	Fusolin (partial)	4YN2	1	-	In Vivo Crystallization (pH 7.0)	$P4_12_12$	2.02	Zn(II)	His1 His142 Phe222	N/D	N/D	Intracellular Fusolin micro-crystals from EPV-infected larvae of *Wiseana spp.* moths.	Chiu *et al.*, (2015)
AA10	Unidentified entomopox-virus *(Melolontha melolontha*	Fusolin	4OW5	1	-	In Vivo Crystallization	$P4_12_12$	1.90	(H_2O)	His1 His142 Phe225	N/D	N/D	Active site water molecule may be a low occupied metal ion. Chitin-binding domain <u>Mutations:</u>	Chiu *et al.*, (2015)

	entomopox-virus (MMEV))												G25D H192N, I351N, I352H, Q353T, D354G	
AA10	Unidentified entomopox-virus *(Melolontha melolontha* entomopox-virus (MMEV))	Fusolin	4X27	1	-	In Vivo Crystallization	$P4_12_12$	2.40	Cu(II) 0.79	His1 His142 Phe225	N/D	N/D	Soaked with $CuSO_4$ Cu(II))	Chiu *et al.*, (2015)
AA10	Unidentified entomopox-virus *(Melolontha melolontha* entomopox-virus (MMEV))	Fusolin	4X29	1	-	In Vivo Crystallization	$P4_12_12$	2.41	Zn(II)	His1 His142 Phe225	N/D	N/D	Soaked with $ZnSO_4$	Chiu *et al.*, (2015)
AA11	*Aspergillus oryzae*	*Ao*AA11 *Ao*(LPMO11) AO090102000501	4MAH	1	25 mg/ml 0.02M Na-acetate pH5.0	0.01M $ZnCl_2$ 0.1M MES pH 6.0 20%(w/v) PEG6000	$P2_12_12_1$	1.55	Zn(II)	His1 His60 Tyr140	β-chitin	C1	-	Hemsworth *et al.*, (2014)
AA11	*Aspergillus oryzae*	*Ao*AA11 *Ao*(LPMO11) AO090102000501	4MAI	1	25 mg/ml 0.02M Na-acetate pH5.0	0.01M $ZnCl_2$ 0.1M MES pH 6.0 20%(w/v) PEG6000	$P2_12_12_1$	1.40	Cu(I)	His1 His60 Tyr140	β-chitin	C1	Soaked in 2mM $Cu(II)Cl_2$	Hemsworth *et al.*, (2014)
AA13	*Aspergillus oryzae*	*Ao*AA13 AO090701000246 AOR_1_454114	4OPB	1	3 mg/ml 0.02M MES pH6.0 0.125M NaCl	0.14M $CaCl_2$ 0.07M Na-acetate pH 4.6 14%(v/v) 2-propanol 30%(v/v) Glycerol (+seed stock)	$P2_12_12_1$	1.55	Cu(I)	MeHis1 His91 Tyr224	N/D (starch)	N/D (C1)	Enzymes with 70-72% sequence identity [*An*AA13 in (Lo Leggio *et al.*, 2015) and *Nc*AA13 in (Vu *et al.*, 2014)] release C1-oxidized products from starch-related substrates	Lo Leggio *et al.*, (2015)
AA13	*Aspergillus oryzae*	*Ao*AA13 AO090701000246 AOR_1_454114	5T7J	1	3 mg/ml 0.02M MES pH6.0 0.125M NaCl	0.02M Zn-acetate 0.1M Malate/ MES/Tris pH 5.0 20%(w/v) PEG3000	$P2_12_12_1$	1.65	Zn(II)	MeHis1 His91 Tyr224	N/D (starch)	N/D (C1)	Activity inferred from Lo Leggio *et al.*, (2015) and Vu *et al.*, (2014)	Frandsen *et al.*, (2017)
AA13	*Aspergillus oryzae*	*Ao*AA13 AO090701000246 AOR_1_454114	5T7N	1	3 mg/ml 0.02M MES pH6.0	0.02M Zn-acetate 0.1M Malate/ MES/Tris pH 5.0	$P2_12_12_1$	1.60	Zn(II) 0.7	MeHis1 His91 Tyr224	N/D (starch)	N/D (C1)	Glucosyl-maltotriose bound outside the active site.	Frandsen *et al.*, (2017)

					0.125M NaCl	20%(w/v) PEG3000							Activity inferred from Lo Leggio *et al.*, (2015) and Vu *et al.*, (2014)	
AA13	*Aspergillus oryzae*	*Ao*AA13 AO090701000246 AOR_1_454114	5T7K	1	3 mg/ml 0.02M MES pH6.0 0.125M NaCl	0.02M Zn-acetate 0.1M Malate/ MES/Tris pH 5.0 20%(w/v) PEG3000	$P2_12_12_1$	1.30	Zn(II) 0.2	MeHis1 His91 Tyr224	N/D (starch)	N/D (C1)	His91 flipped out of active site. Stacking with Phe166. Activity inferred from Lo Leggio *et al.*, (2015) and Vu *et al.*, (2014)	Frandsen *et al.*, (2017)
AA13	*Aspergillus oryzae*	*Ao*AA13 AO090701000246 AOR_1_454114	5LSV	1	3 mg/ml 0.02M MES pH6.0 0.125M NaCl	0.02M Zn-acetate 0.1M Malate/ MES/Tris pH 5.0 20%(w/v) PEG3000	$P2_12_12_1$	1.10	Zn(II) A 0.8 B 0.2	MeHis1 His91 Tyr224	N/D (starch)	N/D (C1)	Maltose bound outside the active site. Activity inferred from Lo Leggio *et al.*, (2015) and Vu *et al.*, (2014)	Frandsen *et al.*, (2017)
AA14	*Pycnoporus coccineus*	*Pc*AA14B *Pc*AA14_B	5NO7	2	28 mg/ml 0.05M Na-acetate pH 5.2	2.4 M $(NH_4)_2SO_4$ 0.1 M citric acid pH 4.4	$P4_22_12_1$	3.01	-	His1 His99 Tyr176	Xylan (cellulose-associated)	C1	C1-oxidized xylo-oligosaccharides released after synergistic action with GH11 xylanases	Couturier et al (2018)
AA15	*Thermobia domestica*	*Td*AA15A *Td*AA15_A	5MSZ	1	28 mg/ml 0.05M Na-acetate pH 5.2	0.1 M Na-citrate pH 5.5 0.1 M LiCl, 10-25% (w/v) PEG6000	$P22_12_1$	1.10	Cu(I)	His1 His91 Tyr184	Avicel β-chitin	C1	First structure of an LPMO belonging to the phylum of Arthropoda	Sabbadin et al (2018)

† Number of molecules in the asymmetric unit. ‡ The criteria for assigning a Cu(II) or Cu(I) state were informed by structures where both states have been characterized (Gudmundsson *et al.*, 2014). The electron density of the equatorial exogenous ligand to the Cu (from weighed 2Fobs-Fcalc) should be more than 2 σ with more than 0.5 occupancy and distance to the copper less than 2.4 Å with similar criteria applying to the exogenous axial ligand, although with a distance of 2.8 Å. In structures where a distorted geometry is observed because of significant steric effects (most AA10), structures with a single exogenous ligand within 2.5 Å distance are taken as Cu(II). The occupancy of the metal is 1.00 if nothing else is indicated. If there is significant metal-site disorder with characteristics that could fit both states, the site is described as Cu(II)/Cu(I). When the copper occupancy was lower than 0.5, no oxidation state was assigned.

N/R: non reported; N/D: non determined

Additional references for the updated table not present in the review (Frandsen, K. E. H. & Lo Leggio, L. (2016). *IUCrJ* **3**, 448-467):

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