

# Integrative Structure Validation Report

March 27, 2025 - 10:12 AM PDT

The following software was used in the production of this report:

*Integrative Modeling Validation* Version 2.0


*Python-IHM* Version 1.8

*MolProbity* Version 4.5.2

PDB ID	9A3U
PDB-Dev ID	PDBDEV_00000215
Structure Title	A representative atomistic model of the Populus Secondary Cell Wall
Structure Authors	Bharadwaj, V.S.; Bu, L.; Crowley, M.F.; Crowley, M.F.; Ciesielski, P.; Brooks, B.R.
Deposited on	2023-10-02

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at [helpdesk@pdb-ihm.org](mailto:helpdesk@pdb-ihm.org)

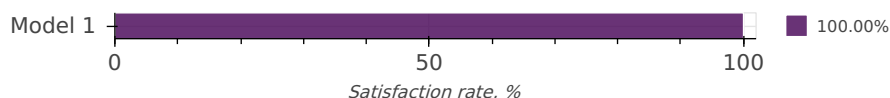
A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the  symbol.

List of references used to build this report is available [here](#).

## Overall quality

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

### Model Quality: Excluded Volume Analysis



## Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 2 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	Lignin	A [L10]	20	-	1-20	100.00 / 100.00	Atomic
				B [L21]					
				C [L32]					
				D [L43]					
				E [L54]					
				F [L65]					
				G [L76]					
				H [L87]					
				I [L98]					
				J [L109]					
				K [L11a]					
				L [L12b]					
				M [L13c]					
				N [L14d]					
				O [L15e]					
				P [L16f]					
				Q [L17g]					
				R [L18h]					
				S [L19i]					
				T [L20j]					
				U [L21k]					
				V [L22l]					
				W [L23m]					
				X [L24n]					
				Y [L25o]					
				Z [L26p]					
				AA [L27q]					
				AB [L53Q]					
				AC [L79k]					
				AD [L105K]					
				BA [L28r]					
				BB [L54R]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				BC [L80l]					
				BD [L106L]					
				CA [L29s]					
				CB [L55S]					
				CC [L81m]					
				CD [L107M]					
				DA [L30t]					
				DB [L56T]					
				DC [L82n]					
				DD [L108N]					
				EA [L31u]					
				EB [L57U]					
				EC [L83o]					
				ED [L109O]					
				FA [L32v]					
				FB [L58V]					
				FC [L84p]					
				FD [L110P]					
				GA [L33w]					
				GB [L590]					
				GC [L85q]					
				GD [L111Q]					
				HA [L34x]					
				HB [L60l]					
				HC [L86r]					
				HD [L112R]					
				IA [L35y]					
				IB [L612]					
				IC [L87s]					
				ID [L113S]					
				JA [L36z]					
				JB [L623]					
				JC [L88t]					
				JD [L114T]					
				KA [L37A]					
				KB [L634]					
				KC [L89u]					
				KD [L115U]					
				LA [L38B]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				LB [L645]					
				LC [L90v]					
				MA [L39C]					
				MB [L656]					
				MC [L91w]					
				NA [L40D]					
				NB [L667]					
				NC [L92x]					
				OA [L41E]					
				OB [L678]					
				OC [L93y]					
				PA [L42F]					
				PB [L689]					
				PC [L94z]					
				QA [L43G]					
				QB [L69a]					
				QC [L95A]					
				RA [L44H]					
				RB [L70b]					
				RC [L96B]					
				SA [L45I]					
				SB [L71c]					
				SC [L97C]					
				TA [L46J]					
				TB [L72d]					
				TC [L98D]					
				UA [L47K]					
				UB [L73e]					
				UC [L99E]					
				VA [L48L]					
				VB [L74f]					
				VC [L100F]					
				WA [L49M]					
				WB [L75g]					
				WC [L101G]					
				XA [L50N]					
				XB [L76h]					
				XC [L102H]					
				YA [L51O]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				YB [L77i]					
				YC [L103I]					
				ZA [L52P]					
				ZB [L78j]					
				ZC [L104J]					
		5	Xylan-m8	AE [X37f]	Non-polymeric	-	-	Not available / Not available	Atomic
				AF [X21F]					
				BE [X38g]					
				CE [X39h]					
				DE [X40i]					
				EE [X41j]					
				FE [X42k]					
				QF [X58V]					
				RF [X59W]					
				SF [X60X]					
				VE [X16A]					
				WE [X17B]					
				XE [X18C]					
				YE [X19D]					
				ZE [X20E]					
		6	Cellulose	AG [CEL17]	Non-polymeric	-	-	Not available / Not available	Atomic
				AH [CEL2x]					
				AI [CEL4n]					
				AJ [CEL5d]					
				AK [CEL73]					
				AL [CEL8t]					
				BG [CEL18]					
				BH [CEL2y]					
				BI [CEL4o]					
				BJ [CEL5e]					
				BK [CEL74]					
				BL [CEL8u]					
				CG [CEL19]					
				CH [CEL2z]					
				CI [CEL4p]					
				CJ [CEL5f]					
				CK [CEL75]					
				CL [CEL8v]					
				DG [CEL1a]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				DH [CEL30]					
				DI [CEL4q]					
				DJ [CEL5g]					
				DK [CEL76]					
				DL [CEL8w]					
				EG [CEL1b]					
				EH [CEL31]					
				EI [CEL4r]					
				EJ [CEL5h]					
				EK [CEL77]					
				EL [CEL8x]					
				FG [CEL1c]					
				FH [CEL32]					
				FI [CEL4s]					
				FJ [CEL6i]					
				FK [CEL78]					
				FL [CEL8y]					
				GG [CEL1d]					
				GH [CEL33]					
				GI [CEL4t]					
				GJ [CEL6j]					
				GK [CEL79]					
				GL [CEL8z]					
				HG [CEL1e]					
				HH [CEL34]					
				HI [CEL4u]					
				HJ [CEL6k]					
				HK [CEL7a]					
				IG [CEL1f]					
				IH [CEL35]					
				II [CEL4v]					
				IJ [CEL6l]					
				IK [CEL7b]					
				JG [CEL1g]					
				JH [CEL36]					
				JI [CEL4w]					
				JJ [CEL6m]					
				JK [CEL7c]					
				KG [CEL1h]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				KH [CEL37]					
				KI [CEL4x]					
				KJ [CEL6n]					
				KK [CEL7d]					
				LG [CEL2i]					
				LH [CEL38]					
				LI [CEL4y]					
				LJ [CEL6o]					
				LK [CEL7e]					
				MG [CEL2j]					
				MH [CEL39]					
				MI [CEL4z]					
				MJ [CEL6p]					
				MK [CEL7f]					
				NG [CEL2k]					
				NH [CEL3a]					
				NI [CEL50]					
				NJ [CEL6q]					
				NK [CEL7g]					
				OG [CEL2l]					
				OH [CEL3b]					
				OI [CEL51]					
				OJ [CEL6r]					
				OK [CEL7h]					
				PG [CEL2m]					
				PH [CEL3c]					
				PI [CEL52]					
				PJ [CEL6s]					
				PK [CEL8i]					
				QG [CEL2n]					
				QH [CEL3d]					
				QI [CEL53]					
				QJ [CEL6t]					
				QK [CEL8j]					
				RG [CEL2o]					
				RH [CEL3e]					
				RI [CEL54]					
				RJ [CEL6u]					
				RK [CEL8k]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				SG [CEL2p]					
				SH [CEL3f]					
				SI [CEL55]					
				SJ [CEL6v]					
				SK [CEL8l]					
				TF [CEL10]					
				TG [CEL2q]					
				TH [CEL3g]					
				TI [CEL56]					
				TJ [CEL6w]					
				TK [CEL8m]					
				UF [CEL11]					
				UG [CEL2r]					
				UH [CEL3h]					
				UI [CEL57]					
				UJ [CEL6x]					
				UK [CEL8n]					
				VF [CEL12]					
				VG [CEL2s]					
				VH [CEL4i]					
				VI [CEL58]					
				VJ [CEL6y]					
				VK [CEL8o]					
				WF [CEL13]					
				WG [CEL2t]					
				WH [CEL4j]					
				WI [CEL59]					
				WJ [CEL6z]					
				WK [CEL8p]					
				XF [CEL14]					
				XG [CEL2u]					
				XH [CEL4k]					
				XI [CEL5a]					
				XJ [CEL70]					
				XK [CEL8q]					
				YF [CEL15]					
				YG [CEL2v]					
				YH [CEL4l]					
				YI [CEL5b]					



ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				YJ [CEL71]					
				YK [CEL8r]					
				ZF [CEL16]					
				ZG [CEL2w]					
				ZH [CEL4m]					
				ZI [CEL5c]					
				ZJ [CEL72]					
				ZK [CEL8s]					
		7	SODIUM ION	AM [L13c]	Non-polymeric	-	-	Not available / Not available	Atomic
				AN [L24n]					
				AO [L30t]					
				AP [L40D]					
				AQ [L47K]					
				AR [L57U]					
				AS [L73e]					
				AT [L77i]					
				AU [L84p]					
				AV [L93y]					
				AW [L111Q]					
				BM [L13c]					
				BN [L25o]					
				BO [L31u]					
				BP [L40D]					
				BQ [L47K]					
				BR [L57U]					
				BS [L73e]					
				BT [L77i]					
				BU [L84p]					
				BV [L95A]					
				BW [L111Q]					
				CM [L14d]					
				CN [L25o]					
				CO [L33w]					
				CP [L40D]					
				CQ [L47K]					
				CR [L57U]					
				CS [L73e]					
				CT [L77i]					
				CU [L84p]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				CV [L95A]					
				CW [L111Q]					
				DM [L14d]					
				DN [L25o]					
				DO [L33w]					
				DP [L40D]					
				DQ [L48L]					
				DR [L57U]					
				DS [L73e]					
				DT [L77i]					
				DU [L84p]					
				DV [L95A]					
				DW [L111Q]					
				EM [L14d]					
				EN [L25o]					
				EO [L33w]					
				EP [L40D]					
				EQ [L49M]					
				ER [L57U]					
				ES [L73e]					
				ET [L77i]					
				EU [L84p]					
				EV [L95A]					
				EW [L111Q]					
				FM [L14d]					
				FN [L25o]					
				FO [L35y]					
				FP [L40D]					
				FQ [L49M]					
				FR [L57U]					
				FS [L73e]					
				FT [L77i]					
				FU [L84p]					
				FV [L96B]					
				FW [L111Q]					
				GM [L14d]					
				GN [L25o]					
				GO [L35y]					
				GP [L40D]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				GQ [L49M]					
				GR [L590]					
				GS [L73e]					
				GT [L77i]					
				GU [L84p]					
				GV [L96B]					
				GW [L111Q]					
				HL [L54]					
				HM [L15e]					
				HN [L25o]					
				HO [L35y]					
				HP [L40D]					
				HQ [L50N]					
				HR [L601]					
				HS [L73e]					
				HT [L77i]					
				HU [L84p]					
				HV [L96B]					
				HW [L111Q]					
				IL [L76]					
				IM [L16f]					
				IN [L25o]					
				IO [L35y]					
				IP [L40D]					
				IQ [L50N]					
				IR [L601]					
				IS [L73e]					
				IT [L77i]					
				IU [L84p]					
				IV [L96B]					
				IW [L111Q]					
				JL [L76]					
				JM [L16f]					
				JN [L25o]					
				JO [L36z]					
				JP [L40D]					
				JQ [L50N]					
				JR [L601]					
				JS [L73e]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				JT [L77i]					
				JU [L84p]					
				JV [L96B]					
				JW [L111Q]					
				KL [L76]					
				KM [L16f]					
				KN [L25o]					
				KO [L36z]					
				KP [L40D]					
				KQ [L50N]					
				KR [L601]					
				KS [L73e]					
				KT [L77i]					
				KU [L84p]					
				KV [L98D]					
				KW [L111Q]					
				LL [L76]					
				LM [L16f]					
				LN [L25o]					
				LO [L36z]					
				LP [L40D]					
				LQ [L52P]					
				LR [L601]					
				LS [L73e]					
				LT [L77i]					
				LU [L85q]					
				LV [L99E]					
				LW [L111Q]					
				ML [L76]					
				MM [L16f]					
				MN [L27q]					
				MO [L37A]					
				MP [L41E]					
				MQ [L55S]					
				MR [L612]					
				MS [L73e]					
				MT [L77i]					
				MU [L85q]					
				MV [L99E]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				MW [L111Q]					
				NL [L76]					
				NM [L16f]					
				NN [L27q]					
				NO [L37A]					
				NP [L41E]					
				NQ [L55S]					
				NR [L634]					
				NS [L73e]					
				NT [L78]					
				NU [L86r]					
				NV [L100F]					
				NW [L111Q]					
				OL [L76]					
				OM [L18h]					
				ON [L27q]					
				OO [L37A]					
				OP [L42F]					
				OQ [L55S]					
				OR [L645]					
				OS [L73e]					
				OT [L79k]					
				OU [L91w]					
				OV [L100F]					
				OW [L111Q]					
				PL [L76]					
				PM [L18h]					
				PN [L27q]					
				PO [L37A]					
				PP [L43G]					
				PQ [L55S]					
				PR [L645]					
				PS [L73e]					
				PT [L80I]					
				PU [L91w]					
				PV [L100F]					
				PW [L111Q]					
				QL [L87]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				QM [L18h]					
				QN [L27q]					
				QO [L37A]					
				QP [L45I]					
				QQ [L55S]					
				QR [L645]					
				QS [L73e]					
				QT [L80I]					
				QU [L91w]					
				QV [L100F]					
				QW [L111Q]					
				RL [L87]					
				RM [L18h]					
				RN [L27q]					
				RO [L37A]					
				RP [L46J]					
				RQ [L55S]					
				RR [L645]					
				RS [L73e]					
				RT [L81m]					
				RU [L91w]					
				RV [L100F]					
				RW [L111Q]					
				SL [L87]					
				SM [L19i]					
				SN [L27q]					
				SO [L38B]					
				SP [L46J]					
				SQ [L55S]					
				SR [L645]					
				SS [L73e]					
				ST [L82n]					
				SU [L91w]					
				SV [L100F]					
				SW [L111Q]					
				TL [L87]					
				TM [L21k]					
				TN [L27q]					
				TO [L38B]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				TP [L47K]					
				TQ [L55S]					
				TR [L645]					
				TS [L73e]					
				TT [L83o]					
				TU [L92x]					
				TV [L102H]					
				TW [L114T]					
				UL [L87]					
				UM [L22l]					
				UN [L28r]					
				UO [L38B]					
				UP [L47K]					
				UQ [L55S]					
				UR [L645]					
				US [L74f]					
				UT [L84p]					
				UU [L92x]					
				UV [L104J]					
				UW [L114T]					
				VL [L98]					
				VM [L23m]					
				VN [L29s]					
				VO [L38B]					
				VP [L47K]					
				VQ [L56T]					
				VR [L667]					
				VS [L76h]					
				VT [L84p]					
				VU [L92x]					
				VV [L105K]					
				WL [L98]					
				WM [L24n]					
				WN [L29s]					
				WO [L38B]					
				WP [L47K]					
				WQ [L56T]					
				WR [L69a]					
				WS [L76h]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				WT [L84p]					
				WU [L92x]					
				WV [L105K]					
				XL [L98]					
				XM [L24n]					
				XN [L29s]					
				XO [L38B]					
				XP [L47K]					
				XQ [L56T]					
				XR [L69a]					
				XS [L76h]					
				XT [L84p]					
				XU [L92x]					
				XV [L106L]					
				YL [L12b]					
				YM [L24n]					
				YN [L29s]					
				YO [L38B]					
				YP [L47K]					
				YQ [L57U]					
				YR [L69a]					
				YS [L77i]					
				YT [L84p]					
				YU [L92x]					
				YV [L107M]					
				ZL [L12b]					
				ZM [L24n]					
				ZN [L30t]					
				ZO [L38B]					
				ZP [L47K]					
				ZQ [L57U]					
				ZR [L70b]					
				ZS [L77i]					
				ZT [L84p]					
				ZU [L92x]					
				ZV [L111Q]					
		8	water	AX [L87]	Non-polymeric	-	-	Not available / Not available	Atomic
				AY [L37A]					
				AZ [L645]					



ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				BX [L98]					
				BY [L38B]					
				BZ [L656]					
				CX [L11a]					
				CY [L39C]					
				CZ [L667]					
				DX [L12b]					
				DY [L40D]					
				DZ [L69a]					
				EX [L13c]					
				EY [L41E]					
				EZ [L70b]					
				FX [L14d]					
				FY [L42F]					
				FZ [L71c]					
				GX [L15e]					
				GY [L43G]					
				GZ [L73e]					
				HX [L16f]					
				HY [L44H]					
				HZ [L74f]					
				IX [L17g]					
				IY [L45I]					
				IZ [L75g]					
				JX [L18h]					
				JY [L46J]					
				JZ [L76h]					
				KX [L19i]					
				KY [L47K]					
				KZ [L77i]					
				LX [L21k]					
				LY [L48L]					
				LZ [L78j]					
				MX [L22l]					
				MY [L49M]					
				MZ [L79k]					
				NX [L23m]					
				NY [L50N]					
				NZ [L80l]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				OX [L24n]					
				OY [L51O]					
				OZ [L81m]					
				PX [L25o]					
				PY [L52P]					
				PZ [L82n]					
				QX [L26p]					
				QY [L54R]					
				QZ [L83o]					
				RX [L27q]					
				RY [L55S]					
				RZ [L84p]					
				SX [L28r]					
				SY [L56T]					
				SZ [L85q]					
				TX [L29s]					
				TY [L57U]					
				TZ [L86r]					
				UX [L30t]					
				UY [L58V]					
				UZ [L87s]					
				VW [L10]					
				VX [L31u]					
				VY [L590]					
				VZ [L88t]					
				WW [L21]					
				WX [L33w]					
				WY [L601]					
				WZ [L89u]					
				XW [L43]					
				XX [L34x]					
				XY [L612]					
				XZ [L91w]					
				YW [L54]					
				YX [L35y]					
				YY [L623]					
				YZ [L92x]					
				ZW [L76]					
				ZX [L36z]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				ZY [L634]					
				ZZ [L93y]					
				AAA [L94z]					
				BAA [L95A]					
				CAA [L96B]					
				DAA [L97C]					
				EAA [L98D]					
				FAA [L99E]					
				GAA [L100F]					
				HAA [L101G]					
				IAA [L102H]					
				JAA [L103I]					
				KAA [L104J]					
				LAA [L105K]					
				MAA [L106L]					
				NAA [L107M]					
				OAA [L108N]					
				PAA [L109O]					
				QAA [L110P]					
				RAA [L111Q]					
				SAA [L112R]					
				TAA [L113S]					
				UAA [L114T]					
		2	Xylan-m2	BF [X43G]	Non-polymeric	-	-	Not available / Not available	Atomic
				CF [X44H]					
				DF [X45I]					
				EF [X46J]					
				FF [X47K]					
				GE [X1I]					
				HE [X2m]					
				IE [X3n]					
				JE [X4o]					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				KE [X5p]					
				LD [X220]					
				MD [X231]					
				ND [X242]					
				OD [X253]					
				PD [X264]					
		3	Xylan-m4	GF [X48L]	Non-polymeric	-	-	Not available / Not available	Atomic
				HF [X49M]					
				IF [X50N]					
				JF [X51O]					
				KF [X52P]					
				LE [X6q]					
				ME [X7r]					
				NE [X8s]					
				OE [X9t]					
				PE [X10u]					
				QD [X275]					
				RD [X286]					
				SD [X297]					
				TD [X308]					
				UD [X319]					
		4	Xylan-m6	LF [X53Q]	Non-polymeric	-	-	Not available / Not available	Atomic
				MF [X54R]					
				NF [X55S]					
				OF [X56T]					
				PF [X57U]					
				QE [X11v]					
				RE [X12w]					
				SE [X13x]					
				TE [X14y]					
				UE [X15z]					
				VD [X32a]					
				WD [X33b]					
				XD [X34c]					
				YD [X35d]					
				ZD [X36e]					

Datasets used for modeling 

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
2	NMR data	Zenodo	<a href="https://zenodo.org/record/105281/files/8377844">10.5281/zenodo.8377844</a>
1	De Novo model	Zenodo	<a href="https://zenodo.org/record/105281/files/10179190">10.5281/zenodo.10179190</a>

## Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Initial Polymer Placement	Molecular Placement of Cellulose, Xylan and Lignin	None	None	False	False
2	1	Equilibration with Molecular Dynamics	A series of compression simulations to assemble the matrix polymers (xylan and lignin) onto the xylan coated cellulose microfibril. This is followed by the placement of water molecules and ions for charge neutrality. Experimentally observed density values are used as a validation metric at this stage. For further details see cited manuscript DOI:10.1126/sciadv.adi7965	None	None	False	False
3	1	Production Simulations in the NVT ensemble	This step involves running molecular dynamics for 100ns (50,000,000 steps with a 2fs timestep) to explore the dynamics of biopolymeric components. Periodic boundary conditions are considered for the simulations. For further details see cited manuscript DOI:10.1126/sciadv.adi7965 . CHARMM compatible files for this system are available for download, visualization and analysis at <a href="https://doi.org/10.5281/zenodo.10179190">https://doi.org/10.5281/zenodo.10179190</a>	None	None	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
4	1	Proximity Calculations for Reproduction of ssNMR Observables	This step involves calculating the fraction of 'sink' atom type within 1nm of a 'source' atom type. The source and sink atoms are chosen based on ssNMR experiments. There are two types of sources Xylan-sourced (methyl carbon on the acetate group attached to xylose) or Lignin-Sourced (Ring atoms C3 and C5 on the Syringyl residues and atoms C4 and C3 on the Guaicol residues of lignin). The sink atoms for Xylan-sources include Cellulose atoms (C4 atom on Glucose) and Lignin atoms (Ring atoms C3 and C5 on the Syringyl residues and atoms C4 and C3 on the Guaicol residues). The sink atoms for Lignin-sources include Cellulose atoms (C4 atom on Glucose) and Xylan atoms (methyl carbon (CA2) on the acetate group attached to xylose). For a chosen source atom in the system, a count of sink atoms within 1nm of that source atom is calculated. This is repeated for each and every source atom and the total count is used to calculate the fraction of sink atoms within 1nm of the source atom. This metric also measured by ssNMR, is used to validate the spatial arrangement of polymers in the atomistic model. For further details see cited manuscript DOI:10.1126/sciadv.adi7965	None	None	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	CHARMM	C44a	model building	<a href="https://www.charmm.org/">https://www.charmm.org/</a>

## Data quality ?

### NMR

Validation for this section is under development.

## Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

### Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	32017024725	1219509	100.00

### Fit of model to data used for modeling ?

#### NMR

Validation for this section is under development.

### Fit of model to data used for validation ?

Validation for this section is under development.

#### *Acknowledgments*

*The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.*

*Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.*

*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*