Integrative Structure Validation Report

July 22, 2024 - 05:27 PM PDT

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

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.

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

We welcome your comments at pdb-dev@mail.wwpdb.org

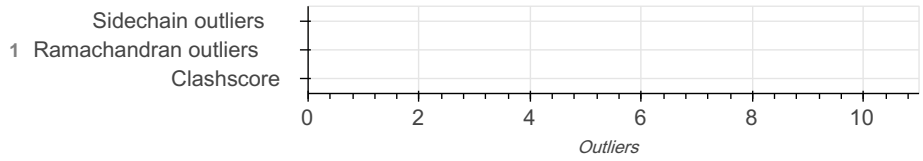
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the symbol.

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 assessment for SAS datasets and fit to model assessments for SAS 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: MolProbity Analysis



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 723 subunits in each model. A total of 2 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 723 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry.This model is titled None/8-cellulose fiber (each fiber containing 18 elementary chains) system with 70% cellulose-bound xylan (Model with the Best scores for agreement with ssNMR data).

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Lignin	A	L10	20
1	2	1	Lignin	B	L21	20
1	3	1	Lignin	C	L32	20
1	4	1	Lignin	D	L43	20
1	5	1	Lignin	E	L54	20
1	6	1	Lignin	F	L65	20
1	7	1	Lignin	G	L76	20
1	8	1	Lignin	H	L87	20
1	9	1	Lignin	I	L98	20
1	10	1	Lignin	J	L109	20
1	11	1	Lignin	K	L11a	20
1	12	1	Lignin	L	L12b	20
1	13	1	Lignin	M	L13c	20
1	14	1	Lignin	N	L14d	20
1	15	1	Lignin	O	L15e	20
1	16	1	Lignin	P	L16f	20
1	17	1	Lignin	Q	L17g	20
1	18	1	Lignin	R	L18h	20
1	19	1	Lignin	S	L19i	20
1	20	1	Lignin	T	L20j	20
1	21	1	Lignin	U	L21k	20

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	22	1	Lignin	V	L22l	20
1	23	1	Lignin	W	L23m	20
1	24	1	Lignin	X	L24n	20
1	25	1	Lignin	Y	L25o	20
1	26	1	Lignin	Z	L26p	20
1	27	1	Lignin	AA	L27q	20
1	28	1	Lignin	BA	L28r	20
1	29	1	Lignin	CA	L29s	20
1	30	1	Lignin	DA	L30t	20
1	31	1	Lignin	EA	L31u	20
1	32	1	Lignin	FA	L32v	20
1	33	1	Lignin	GA	L33w	20
1	34	1	Lignin	HA	L34x	20
1	35	1	Lignin	IA	L35y	20
1	36	1	Lignin	JA	L36z	20
1	37	1	Lignin	KA	L37A	20
1	38	1	Lignin	LA	L38B	20
1	39	1	Lignin	MA	L39C	20
1	40	1	Lignin	NA	L40D	20
1	41	1	Lignin	OA	L41E	20
1	42	1	Lignin	PA	L42F	20
1	43	1	Lignin	QA	L43G	20
1	44	1	Lignin	RA	L44H	20
1	45	1	Lignin	SA	L45I	20
1	46	1	Lignin	TA	L46J	20
1	47	1	Lignin	UA	L47K	20
1	48	1	Lignin	VA	L48L	20

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	49	1	Lignin	WA	L49M	20
1	50	1	Lignin	XA	L50N	20
1	51	1	Lignin	YA	L51O	20
1	52	1	Lignin	ZA	L52P	20
1	53	1	Lignin	AB	L53Q	20
1	54	1	Lignin	BB	L54R	20
1	55	1	Lignin	CB	L55S	20
1	56	1	Lignin	DB	L56T	20
1	57	1	Lignin	EB	L57U	20
1	58	1	Lignin	FB	L58V	20
1	59	1	Lignin	GB	L590	20
1	60	1	Lignin	HB	L601	20
1	61	1	Lignin	IB	L612	20
1	62	1	Lignin	JB	L623	20
1	63	1	Lignin	KB	L634	20
1	64	1	Lignin	LB	L645	20
1	65	1	Lignin	MB	L656	20
1	66	1	Lignin	NB	L667	20
1	67	1	Lignin	OB	L678	20
1	68	1	Lignin	PB	L689	20
1	69	1	Lignin	QB	L69a	20
1	70	1	Lignin	RB	L70b	20
1	71	1	Lignin	SB	L71c	20
1	72	1	Lignin	TB	L72d	20
1	73	1	Lignin	UB	L73e	20
1	74	1	Lignin	VB	L74f	20
1	75	1	Lignin	WB	L75g	20

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	76	1	Lignin	XB	L76h	20
1	77	1	Lignin	YB	L77i	20
1	78	1	Lignin	ZB	L78j	20
1	79	1	Lignin	AC	L79k	20
1	80	1	Lignin	BC	L80l	20
1	81	1	Lignin	CC	L81m	20
1	82	1	Lignin	DC	L82n	20
1	83	1	Lignin	EC	L83o	20
1	84	1	Lignin	FC	L84p	20
1	85	1	Lignin	GC	L85q	20
1	86	1	Lignin	HC	L86r	20
1	87	1	Lignin	IC	L87s	20
1	88	1	Lignin	JC	L88t	20
1	89	1	Lignin	KC	L89u	20
1	90	1	Lignin	LC	L90v	20
1	91	1	Lignin	MC	L91w	20
1	92	1	Lignin	NC	L92x	20
1	93	1	Lignin	OC	L93y	20
1	94	1	Lignin	PC	L94z	20
1	95	1	Lignin	QC	L95A	20
1	96	1	Lignin	RC	L96B	20
1	97	1	Lignin	SC	L97C	20
1	98	1	Lignin	TC	L98D	20
1	99	1	Lignin	UC	L99E	20
1	100	1	Lignin	VC	L100F	20
1	101	1	Lignin	WC	L101G	20
1	102	1	Lignin	XC	L102H	20

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	103	1	Lignin	YC	L103I	20
1	104	1	Lignin	ZC	L104J	20
1	105	1	Lignin	AD	L105K	20
1	106	1	Lignin	BD	L106L	20
1	107	1	Lignin	CD	L107M	20
1	108	1	Lignin	DD	L108N	20
1	109	1	Lignin	ED	L109O	20
1	110	1	Lignin	FD	L110P	20
1	111	1	Lignin	GD	L111Q	20
1	112	1	Lignin	HD	L112R	20
1	113	1	Lignin	ID	L113S	20
1	114	1	Lignin	JD	L114T	20
1	115	1	Lignin	KD	L115U	20
1	116	2	Xylan-m2	LD	X220	45
1	117	2	Xylan-m2	MD	X231	45
1	118	2	Xylan-m2	ND	X242	45
1	119	2	Xylan-m2	OD	X253	45
1	120	2	Xylan-m2	PD	X264	45
1	121	2	Xylan-m2	GE	X1I	45
1	122	2	Xylan-m2	HE	X2m	45
1	123	2	Xylan-m2	IE	X3n	45
1	124	2	Xylan-m2	JE	X4o	45
1	125	2	Xylan-m2	KE	X5p	45
1	126	2	Xylan-m2	BF	X43G	45
1	127	2	Xylan-m2	CF	X44H	45
1	128	2	Xylan-m2	DF	X45I	45
1	129	2	Xylan-m2	EF	X46J	45

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	130	2	Xylan-m2	FF	X47K	45
1	131	3	Xylan-m4	QD	X275	45
1	132	3	Xylan-m4	RD	X286	45
1	133	3	Xylan-m4	SD	X297	45
1	134	3	Xylan-m4	TD	X308	45
1	135	3	Xylan-m4	UD	X319	45
1	136	3	Xylan-m4	LE	X6q	45
1	137	3	Xylan-m4	ME	X7r	45
1	138	3	Xylan-m4	NE	X8s	45
1	139	3	Xylan-m4	OE	X9t	45
1	140	3	Xylan-m4	PE	X10u	45
1	141	3	Xylan-m4	GF	X48L	45
1	142	3	Xylan-m4	HF	X49M	45
1	143	3	Xylan-m4	IF	X50N	45
1	144	3	Xylan-m4	JF	X51O	45
1	145	3	Xylan-m4	KF	X52P	45
1	146	4	Xylan-m6	VD	X32a	45
1	147	4	Xylan-m6	WD	X33b	45
1	148	4	Xylan-m6	XD	X34c	45
1	149	4	Xylan-m6	YD	X35d	45
1	150	4	Xylan-m6	ZD	X36e	45
1	151	4	Xylan-m6	QE	X11v	45
1	152	4	Xylan-m6	RE	X12w	45
1	153	4	Xylan-m6	SE	X13x	45
1	154	4	Xylan-m6	TE	X14y	45
1	155	4	Xylan-m6	UE	X15z	45
1	156	4	Xylan-m6	LF	X53Q	45

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	157	4	Xylan-m6	MF	X54R	45
1	158	4	Xylan-m6	NF	X55S	45
1	159	4	Xylan-m6	OF	X56T	45
1	160	4	Xylan-m6	PF	X57U	45
1	161	5	Xylan-m8	AE	X37f	45
1	162	5	Xylan-m8	BE	X38g	45
1	163	5	Xylan-m8	CE	X39h	45
1	164	5	Xylan-m8	DE	X40i	45
1	165	5	Xylan-m8	EE	X41j	45
1	166	5	Xylan-m8	FE	X42k	45
1	167	5	Xylan-m8	VE	X16A	45
1	168	5	Xylan-m8	WE	X17B	45
1	169	5	Xylan-m8	XE	X18C	45
1	170	5	Xylan-m8	YE	X19D	45
1	171	5	Xylan-m8	ZE	X20E	45
1	172	5	Xylan-m8	AF	X21F	45
1	173	5	Xylan-m8	QF	X58V	45
1	174	5	Xylan-m8	RF	X59W	45
1	175	5	Xylan-m8	SF	X60X	45
1	176	6	Cellulose	TF	CEL10	40
1	177	6	Cellulose	UF	CEL11	40
1	178	6	Cellulose	VF	CEL12	40
1	179	6	Cellulose	WF	CEL13	40
1	180	6	Cellulose	XF	CEL14	40
1	181	6	Cellulose	YF	CEL15	40
1	182	6	Cellulose	ZF	CEL16	40
1	183	6	Cellulose	AG	CEL17	40

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	184	6	Cellulose	BG	CEL18	40
1	185	6	Cellulose	CG	CEL19	40
1	186	6	Cellulose	DG	CEL1a	40
1	187	6	Cellulose	EG	CEL1b	40
1	188	6	Cellulose	FG	CEL1c	40
1	189	6	Cellulose	GG	CEL1d	40
1	190	6	Cellulose	HG	CEL1e	40
1	191	6	Cellulose	IG	CEL1f	40
1	192	6	Cellulose	JG	CEL1g	40
1	193	6	Cellulose	KG	CEL1h	40
1	194	6	Cellulose	LG	CEL2i	40
1	195	6	Cellulose	MG	CEL2j	40
1	196	6	Cellulose	NG	CEL2k	40
1	197	6	Cellulose	OG	CEL2l	40
1	198	6	Cellulose	PG	CEL2m	40
1	199	6	Cellulose	QG	CEL2n	40
1	200	6	Cellulose	RG	CEL2o	40
1	201	6	Cellulose	SG	CEL2p	40
1	202	6	Cellulose	TG	CEL2q	40
1	203	6	Cellulose	UG	CEL2r	40
1	204	6	Cellulose	VG	CEL2s	40
1	205	6	Cellulose	WG	CEL2t	40
1	206	6	Cellulose	XG	CEL2u	40
1	207	6	Cellulose	YG	CEL2v	40
1	208	6	Cellulose	ZG	CEL2w	40
1	209	6	Cellulose	AH	CEL2x	40
1	210	6	Cellulose	BH	CEL2y	40

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	211	6	Cellulose	CH	CEL2z	40
1	212	6	Cellulose	DH	CEL30	40
1	213	6	Cellulose	EH	CEL31	40
1	214	6	Cellulose	FH	CEL32	40
1	215	6	Cellulose	GH	CEL33	40
1	216	6	Cellulose	HH	CEL34	40
1	217	6	Cellulose	IH	CEL35	40
1	218	6	Cellulose	JH	CEL36	40
1	219	6	Cellulose	KH	CEL37	40
1	220	6	Cellulose	LH	CEL38	40
1	221	6	Cellulose	MH	CEL39	40
1	222	6	Cellulose	NH	CEL3a	40
1	223	6	Cellulose	OH	CEL3b	40
1	224	6	Cellulose	PH	CEL3c	40
1	225	6	Cellulose	QH	CEL3d	40
1	226	6	Cellulose	RH	CEL3e	40
1	227	6	Cellulose	SH	CEL3f	40
1	228	6	Cellulose	TH	CEL3g	40
1	229	6	Cellulose	UH	CEL3h	40
1	230	6	Cellulose	VH	CEL4i	40
1	231	6	Cellulose	WH	CEL4j	40
1	232	6	Cellulose	XH	CEL4k	40
1	233	6	Cellulose	YH	CEL4l	40
1	234	6	Cellulose	ZH	CEL4m	40
1	235	6	Cellulose	AI	CEL4n	40
1	236	6	Cellulose	BI	CEL4o	40
1	237	6	Cellulose	CI	CEL4p	40

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	238	6	Cellulose	DI	CEL4q	40
1	239	6	Cellulose	EI	CEL4r	40
1	240	6	Cellulose	FI	CEL4s	40
1	241	6	Cellulose	GI	CEL4t	40
1	242	6	Cellulose	HI	CEL4u	40
1	243	6	Cellulose	II	CEL4v	40
1	244	6	Cellulose	JI	CEL4w	40
1	245	6	Cellulose	KI	CEL4x	40
1	246	6	Cellulose	LI	CEL4y	40
1	247	6	Cellulose	MI	CEL4z	40
1	248	6	Cellulose	NI	CEL50	40
1	249	6	Cellulose	OI	CEL51	40
1	250	6	Cellulose	PI	CEL52	40
1	251	6	Cellulose	QI	CEL53	40
1	252	6	Cellulose	RI	CEL54	40
1	253	6	Cellulose	SI	CEL55	40
1	254	6	Cellulose	TI	CEL56	40
1	255	6	Cellulose	UI	CEL57	40
1	256	6	Cellulose	VI	CEL58	40
1	257	6	Cellulose	WI	CEL59	40
1	258	6	Cellulose	XI	CEL5a	40
1	259	6	Cellulose	YI	CEL5b	40
1	260	6	Cellulose	ZI	CEL5c	40
1	261	6	Cellulose	AJ	CEL5d	40
1	262	6	Cellulose	BJ	CEL5e	40
1	263	6	Cellulose	CJ	CEL5f	40
1	264	6	Cellulose	DJ	CEL5g	40

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	265	6	Cellulose	EJ	CEL5h	40
1	266	6	Cellulose	FJ	CEL6i	40
1	267	6	Cellulose	GJ	CEL6j	40
1	268	6	Cellulose	HJ	CEL6k	40
1	269	6	Cellulose	IJ	CEL6l	40
1	270	6	Cellulose	JJ	CEL6m	40
1	271	6	Cellulose	KJ	CEL6n	40
1	272	6	Cellulose	LJ	CEL6o	40
1	273	6	Cellulose	MJ	CEL6p	40
1	274	6	Cellulose	NJ	CEL6q	40
1	275	6	Cellulose	OJ	CEL6r	40
1	276	6	Cellulose	PJ	CEL6s	40
1	277	6	Cellulose	QJ	CEL6t	40
1	278	6	Cellulose	RJ	CEL6u	40
1	279	6	Cellulose	SJ	CEL6v	40
1	280	6	Cellulose	TJ	CEL6w	40
1	281	6	Cellulose	UJ	CEL6x	40
1	282	6	Cellulose	VJ	CEL6y	40
1	283	6	Cellulose	WJ	CEL6z	40
1	284	6	Cellulose	XJ	CEL70	40
1	285	6	Cellulose	YJ	CEL71	40
1	286	6	Cellulose	ZJ	CEL72	40
1	287	6	Cellulose	AK	CEL73	40
1	288	6	Cellulose	BK	CEL74	40
1	289	6	Cellulose	CK	CEL75	40
1	290	6	Cellulose	DK	CEL76	40
1	291	6	Cellulose	EK	CEL77	40

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	292	6	Cellulose	FK	CEL78	40
1	293	6	Cellulose	GK	CEL79	40
1	294	6	Cellulose	HK	CEL7a	40
1	295	6	Cellulose	IK	CEL7b	40
1	296	6	Cellulose	JK	CEL7c	40
1	297	6	Cellulose	KK	CEL7d	40
1	298	6	Cellulose	LK	CEL7e	40
1	299	6	Cellulose	MK	CEL7f	40
1	300	6	Cellulose	NK	CEL7g	40
1	301	6	Cellulose	OK	CEL7h	40
1	302	6	Cellulose	PK	CEL8i	40
1	303	6	Cellulose	QK	CEL8j	40
1	304	6	Cellulose	RK	CEL8k	40
1	305	6	Cellulose	SK	CEL8l	40
1	306	6	Cellulose	TK	CEL8m	40
1	307	6	Cellulose	UK	CEL8n	40
1	308	6	Cellulose	VK	CEL8o	40
1	309	6	Cellulose	WK	CEL8p	40
1	310	6	Cellulose	XK	CEL8q	40
1	311	6	Cellulose	YK	CEL8r	40
1	312	6	Cellulose	ZK	CEL8s	40
1	313	6	Cellulose	AL	CEL8t	40
1	314	6	Cellulose	BL	CEL8u	40
1	315	6	Cellulose	CL	CEL8v	40
1	316	6	Cellulose	DL	CEL8w	40
1	317	6	Cellulose	EL	CEL8x	40
1	318	6	Cellulose	FL	CEL8y	40

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	319	6	Cellulose	GL	CEL8z	40
1	320	7	SODIUM ION	HL	L54	Not available
1	321	7	SODIUM ION	IL	L76	Not available
1	322	7	SODIUM ION	JL	L76	Not available
1	323	7	SODIUM ION	KL	L76	Not available
1	324	7	SODIUM ION	LL	L76	Not available
1	325	7	SODIUM ION	ML	L76	Not available
1	326	7	SODIUM ION	NL	L76	Not available
1	327	7	SODIUM ION	OL	L76	Not available
1	328	7	SODIUM ION	PL	L76	Not available
1	329	7	SODIUM ION	QL	L87	Not available
1	330	7	SODIUM ION	RL	L87	Not available
1	331	7	SODIUM ION	SL	L87	Not available
1	332	7	SODIUM ION	TL	L87	Not available
1	333	7	SODIUM ION	UL	L87	Not available
1	334	7	SODIUM ION	VL	L98	Not available
1	335	7	SODIUM ION	WL	L98	Not available
1	336	7	SODIUM ION	XL	L98	Not available
1	337	7	SODIUM ION	YL	L12b	Not available
1	338	7	SODIUM ION	ZL	L12b	Not available
1	339	7	SODIUM ION	AM	L13c	Not available
1	340	7	SODIUM ION	BM	L13c	Not available
1	341	7	SODIUM ION	CM	L14d	Not available
1	342	7	SODIUM ION	DM	L14d	Not available
1	343	7	SODIUM ION	EM	L14d	Not available
1	344	7	SODIUM ION	FM	L14d	Not available
1	345	7	SODIUM ION	GM	L14d	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	346	7	SODIUM ION	HM	L15e	Not available
1	347	7	SODIUM ION	IM	L16f	Not available
1	348	7	SODIUM ION	JM	L16f	Not available
1	349	7	SODIUM ION	KM	L16f	Not available
1	350	7	SODIUM ION	LM	L16f	Not available
1	351	7	SODIUM ION	MM	L16f	Not available
1	352	7	SODIUM ION	NM	L16f	Not available
1	353	7	SODIUM ION	OM	L18h	Not available
1	354	7	SODIUM ION	PM	L18h	Not available
1	355	7	SODIUM ION	QM	L18h	Not available
1	356	7	SODIUM ION	RM	L18h	Not available
1	357	7	SODIUM ION	SM	L19i	Not available
1	358	7	SODIUM ION	TM	L21k	Not available
1	359	7	SODIUM ION	UM	L22l	Not available
1	360	7	SODIUM ION	VM	L23m	Not available
1	361	7	SODIUM ION	WM	L24n	Not available
1	362	7	SODIUM ION	XM	L24n	Not available
1	363	7	SODIUM ION	YM	L24n	Not available
1	364	7	SODIUM ION	ZM	L24n	Not available
1	365	7	SODIUM ION	AN	L24n	Not available
1	366	7	SODIUM ION	BN	L25o	Not available
1	367	7	SODIUM ION	CN	L25o	Not available
1	368	7	SODIUM ION	DN	L25o	Not available
1	369	7	SODIUM ION	EN	L25o	Not available
1	370	7	SODIUM ION	FN	L25o	Not available
1	371	7	SODIUM ION	GN	L25o	Not available
1	372	7	SODIUM ION	HN	L25o	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	373	7	SODIUM ION	IN	L25o	Not available
1	374	7	SODIUM ION	JN	L25o	Not available
1	375	7	SODIUM ION	KN	L25o	Not available
1	376	7	SODIUM ION	LN	L25o	Not available
1	377	7	SODIUM ION	MN	L27q	Not available
1	378	7	SODIUM ION	NN	L27q	Not available
1	379	7	SODIUM ION	ON	L27q	Not available
1	380	7	SODIUM ION	PN	L27q	Not available
1	381	7	SODIUM ION	QN	L27q	Not available
1	382	7	SODIUM ION	RN	L27q	Not available
1	383	7	SODIUM ION	SN	L27q	Not available
1	384	7	SODIUM ION	TN	L27q	Not available
1	385	7	SODIUM ION	UN	L28r	Not available
1	386	7	SODIUM ION	VN	L29s	Not available
1	387	7	SODIUM ION	WN	L29s	Not available
1	388	7	SODIUM ION	XN	L29s	Not available
1	389	7	SODIUM ION	YN	L29s	Not available
1	390	7	SODIUM ION	ZN	L30t	Not available
1	391	7	SODIUM ION	AO	L30t	Not available
1	392	7	SODIUM ION	BO	L31u	Not available
1	393	7	SODIUM ION	CO	L33w	Not available
1	394	7	SODIUM ION	DO	L33w	Not available
1	395	7	SODIUM ION	EO	L33w	Not available
1	396	7	SODIUM ION	FO	L35y	Not available
1	397	7	SODIUM ION	GO	L35y	Not available
1	398	7	SODIUM ION	HO	L35y	Not available
1	399	7	SODIUM ION	IO	L35y	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	400	7	SODIUM ION	JO	L36z	Not available
1	401	7	SODIUM ION	KO	L36z	Not available
1	402	7	SODIUM ION	LO	L36z	Not available
1	403	7	SODIUM ION	MO	L37A	Not available
1	404	7	SODIUM ION	NO	L37A	Not available
1	405	7	SODIUM ION	OO	L37A	Not available
1	406	7	SODIUM ION	PO	L37A	Not available
1	407	7	SODIUM ION	QO	L37A	Not available
1	408	7	SODIUM ION	RO	L37A	Not available
1	409	7	SODIUM ION	SO	L38B	Not available
1	410	7	SODIUM ION	TO	L38B	Not available
1	411	7	SODIUM ION	UO	L38B	Not available
1	412	7	SODIUM ION	VO	L38B	Not available
1	413	7	SODIUM ION	WO	L38B	Not available
1	414	7	SODIUM ION	XO	L38B	Not available
1	415	7	SODIUM ION	YO	L38B	Not available
1	416	7	SODIUM ION	ZO	L38B	Not available
1	417	7	SODIUM ION	AP	L40D	Not available
1	418	7	SODIUM ION	BP	L40D	Not available
1	419	7	SODIUM ION	CP	L40D	Not available
1	420	7	SODIUM ION	DP	L40D	Not available
1	421	7	SODIUM ION	EP	L40D	Not available
1	422	7	SODIUM ION	FP	L40D	Not available
1	423	7	SODIUM ION	GP	L40D	Not available
1	424	7	SODIUM ION	HP	L40D	Not available
1	425	7	SODIUM ION	IP	L40D	Not available
1	426	7	SODIUM ION	JP	L40D	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	427	7	SODIUM ION	KP	L40D	Not available
1	428	7	SODIUM ION	LP	L40D	Not available
1	429	7	SODIUM ION	MP	L41E	Not available
1	430	7	SODIUM ION	NP	L41E	Not available
1	431	7	SODIUM ION	OP	L42F	Not available
1	432	7	SODIUM ION	PP	L43G	Not available
1	433	7	SODIUM ION	QP	L45I	Not available
1	434	7	SODIUM ION	RP	L46J	Not available
1	435	7	SODIUM ION	SP	L46J	Not available
1	436	7	SODIUM ION	TP	L47K	Not available
1	437	7	SODIUM ION	UP	L47K	Not available
1	438	7	SODIUM ION	VP	L47K	Not available
1	439	7	SODIUM ION	WP	L47K	Not available
1	440	7	SODIUM ION	XP	L47K	Not available
1	441	7	SODIUM ION	YP	L47K	Not available
1	442	7	SODIUM ION	ZP	L47K	Not available
1	443	7	SODIUM ION	AQ	L47K	Not available
1	444	7	SODIUM ION	BQ	L47K	Not available
1	445	7	SODIUM ION	CQ	L47K	Not available
1	446	7	SODIUM ION	DQ	L48L	Not available
1	447	7	SODIUM ION	EQ	L49M	Not available
1	448	7	SODIUM ION	FQ	L49M	Not available
1	449	7	SODIUM ION	GQ	L49M	Not available
1	450	7	SODIUM ION	HQ	L50N	Not available
1	451	7	SODIUM ION	IQ	L50N	Not available
1	452	7	SODIUM ION	JQ	L50N	Not available
1	453	7	SODIUM ION	KQ	L50N	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	454	7	SODIUM ION	LQ	L52P	Not available
1	455	7	SODIUM ION	MQ	L55S	Not available
1	456	7	SODIUM ION	NQ	L55S	Not available
1	457	7	SODIUM ION	OQ	L55S	Not available
1	458	7	SODIUM ION	PQ	L55S	Not available
1	459	7	SODIUM ION	QQ	L55S	Not available
1	460	7	SODIUM ION	RQ	L55S	Not available
1	461	7	SODIUM ION	SQ	L55S	Not available
1	462	7	SODIUM ION	TQ	L55S	Not available
1	463	7	SODIUM ION	UQ	L55S	Not available
1	464	7	SODIUM ION	VQ	L56T	Not available
1	465	7	SODIUM ION	WQ	L56T	Not available
1	466	7	SODIUM ION	XQ	L56T	Not available
1	467	7	SODIUM ION	YQ	L57U	Not available
1	468	7	SODIUM ION	ZQ	L57U	Not available
1	469	7	SODIUM ION	AR	L57U	Not available
1	470	7	SODIUM ION	BR	L57U	Not available
1	471	7	SODIUM ION	CR	L57U	Not available
1	472	7	SODIUM ION	DR	L57U	Not available
1	473	7	SODIUM ION	ER	L57U	Not available
1	474	7	SODIUM ION	FR	L57U	Not available
1	475	7	SODIUM ION	GR	L590	Not available
1	476	7	SODIUM ION	HR	L601	Not available
1	477	7	SODIUM ION	IR	L601	Not available
1	478	7	SODIUM ION	JR	L601	Not available
1	479	7	SODIUM ION	KR	L601	Not available
1	480	7	SODIUM ION	LR	L601	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	481	7	SODIUM ION	MR	L612	Not available
1	482	7	SODIUM ION	NR	L634	Not available
1	483	7	SODIUM ION	OR	L645	Not available
1	484	7	SODIUM ION	PR	L645	Not available
1	485	7	SODIUM ION	QR	L645	Not available
1	486	7	SODIUM ION	RR	L645	Not available
1	487	7	SODIUM ION	SR	L645	Not available
1	488	7	SODIUM ION	TR	L645	Not available
1	489	7	SODIUM ION	UR	L645	Not available
1	490	7	SODIUM ION	VR	L667	Not available
1	491	7	SODIUM ION	WR	L69a	Not available
1	492	7	SODIUM ION	XR	L69a	Not available
1	493	7	SODIUM ION	YR	L69a	Not available
1	494	7	SODIUM ION	ZR	L70b	Not available
1	495	7	SODIUM ION	AS	L73e	Not available
1	496	7	SODIUM ION	BS	L73e	Not available
1	497	7	SODIUM ION	CS	L73e	Not available
1	498	7	SODIUM ION	DS	L73e	Not available
1	499	7	SODIUM ION	ES	L73e	Not available
1	500	7	SODIUM ION	FS	L73e	Not available
1	501	7	SODIUM ION	GS	L73e	Not available
1	502	7	SODIUM ION	HS	L73e	Not available
1	503	7	SODIUM ION	IS	L73e	Not available
1	504	7	SODIUM ION	JS	L73e	Not available
1	505	7	SODIUM ION	KS	L73e	Not available
1	506	7	SODIUM ION	LS	L73e	Not available
1	507	7	SODIUM ION	MS	L73e	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	508	7	SODIUM ION	NS	L73e	Not available
1	509	7	SODIUM ION	OS	L73e	Not available
1	510	7	SODIUM ION	PS	L73e	Not available
1	511	7	SODIUM ION	QS	L73e	Not available
1	512	7	SODIUM ION	RS	L73e	Not available
1	513	7	SODIUM ION	SS	L73e	Not available
1	514	7	SODIUM ION	TS	L73e	Not available
1	515	7	SODIUM ION	US	L74f	Not available
1	516	7	SODIUM ION	VS	L76h	Not available
1	517	7	SODIUM ION	WS	L76h	Not available
1	518	7	SODIUM ION	XS	L76h	Not available
1	519	7	SODIUM ION	YS	L77i	Not available
1	520	7	SODIUM ION	ZS	L77i	Not available
1	521	7	SODIUM ION	AT	L77i	Not available
1	522	7	SODIUM ION	BT	L77i	Not available
1	523	7	SODIUM ION	CT	L77i	Not available
1	524	7	SODIUM ION	DT	L77i	Not available
1	525	7	SODIUM ION	ET	L77i	Not available
1	526	7	SODIUM ION	FT	L77i	Not available
1	527	7	SODIUM ION	GT	L77i	Not available
1	528	7	SODIUM ION	HT	L77i	Not available
1	529	7	SODIUM ION	IT	L77i	Not available
1	530	7	SODIUM ION	JT	L77i	Not available
1	531	7	SODIUM ION	KT	L77i	Not available
1	532	7	SODIUM ION	LT	L77i	Not available
1	533	7	SODIUM ION	MT	L77i	Not available
1	534	7	SODIUM ION	NT	L78j	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	535	7	SODIUM ION	OT	L79k	Not available
1	536	7	SODIUM ION	PT	L80l	Not available
1	537	7	SODIUM ION	QT	L80l	Not available
1	538	7	SODIUM ION	RT	L81m	Not available
1	539	7	SODIUM ION	ST	L82n	Not available
1	540	7	SODIUM ION	TT	L83o	Not available
1	541	7	SODIUM ION	UT	L84p	Not available
1	542	7	SODIUM ION	VT	L84p	Not available
1	543	7	SODIUM ION	WT	L84p	Not available
1	544	7	SODIUM ION	XT	L84p	Not available
1	545	7	SODIUM ION	YT	L84p	Not available
1	546	7	SODIUM ION	ZT	L84p	Not available
1	547	7	SODIUM ION	AU	L84p	Not available
1	548	7	SODIUM ION	BU	L84p	Not available
1	549	7	SODIUM ION	CU	L84p	Not available
1	550	7	SODIUM ION	DU	L84p	Not available
1	551	7	SODIUM ION	EU	L84p	Not available
1	552	7	SODIUM ION	FU	L84p	Not available
1	553	7	SODIUM ION	GU	L84p	Not available
1	554	7	SODIUM ION	HU	L84p	Not available
1	555	7	SODIUM ION	IU	L84p	Not available
1	556	7	SODIUM ION	JU	L84p	Not available
1	557	7	SODIUM ION	KU	L84p	Not available
1	558	7	SODIUM ION	LU	L85q	Not available
1	559	7	SODIUM ION	MU	L85q	Not available
1	560	7	SODIUM ION	NU	L86r	Not available
1	561	7	SODIUM ION	OU	L91w	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	562	7	SODIUM ION	PU	L91w	Not available
1	563	7	SODIUM ION	QU	L91w	Not available
1	564	7	SODIUM ION	RU	L91w	Not available
1	565	7	SODIUM ION	SU	L91w	Not available
1	566	7	SODIUM ION	TU	L92x	Not available
1	567	7	SODIUM ION	UU	L92x	Not available
1	568	7	SODIUM ION	VU	L92x	Not available
1	569	7	SODIUM ION	WU	L92x	Not available
1	570	7	SODIUM ION	XU	L92x	Not available
1	571	7	SODIUM ION	YU	L92x	Not available
1	572	7	SODIUM ION	ZU	L92x	Not available
1	573	7	SODIUM ION	AV	L93y	Not available
1	574	7	SODIUM ION	BV	L95A	Not available
1	575	7	SODIUM ION	CV	L95A	Not available
1	576	7	SODIUM ION	DV	L95A	Not available
1	577	7	SODIUM ION	EV	L95A	Not available
1	578	7	SODIUM ION	FV	L96B	Not available
1	579	7	SODIUM ION	GV	L96B	Not available
1	580	7	SODIUM ION	HV	L96B	Not available
1	581	7	SODIUM ION	IV	L96B	Not available
1	582	7	SODIUM ION	JV	L96B	Not available
1	583	7	SODIUM ION	KV	L98D	Not available
1	584	7	SODIUM ION	LV	L99E	Not available
1	585	7	SODIUM ION	MV	L99E	Not available
1	586	7	SODIUM ION	NV	L100F	Not available
1	587	7	SODIUM ION	OV	L100F	Not available
1	588	7	SODIUM ION	PV	L100F	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	589	7	SODIUM ION	QV	L100F	Not available
1	590	7	SODIUM ION	RV	L100F	Not available
1	591	7	SODIUM ION	SV	L100F	Not available
1	592	7	SODIUM ION	TV	L102H	Not available
1	593	7	SODIUM ION	UV	L104J	Not available
1	594	7	SODIUM ION	VV	L105K	Not available
1	595	7	SODIUM ION	WV	L105K	Not available
1	596	7	SODIUM ION	XV	L106L	Not available
1	597	7	SODIUM ION	YV	L107M	Not available
1	598	7	SODIUM ION	ZV	L111Q	Not available
1	599	7	SODIUM ION	AW	L111Q	Not available
1	600	7	SODIUM ION	BW	L111Q	Not available
1	601	7	SODIUM ION	CW	L111Q	Not available
1	602	7	SODIUM ION	DW	L111Q	Not available
1	603	7	SODIUM ION	EW	L111Q	Not available
1	604	7	SODIUM ION	FW	L111Q	Not available
1	605	7	SODIUM ION	GW	L111Q	Not available
1	606	7	SODIUM ION	HW	L111Q	Not available
1	607	7	SODIUM ION	IW	L111Q	Not available
1	608	7	SODIUM ION	JW	L111Q	Not available
1	609	7	SODIUM ION	KW	L111Q	Not available
1	610	7	SODIUM ION	LW	L111Q	Not available
1	611	7	SODIUM ION	MW	L111Q	Not available
1	612	7	SODIUM ION	NW	L111Q	Not available
1	613	7	SODIUM ION	OW	L111Q	Not available
1	614	7	SODIUM ION	PW	L111Q	Not available
1	615	7	SODIUM ION	QW	L111Q	Not available

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	616	7	SODIUM ION	RW	L111Q	Not available
1	617	7	SODIUM ION	SW	L111Q	Not available
1	618	7	SODIUM ION	TW	L114T	Not available
1	619	7	SODIUM ION	UW	L114T	Not available
1	620	8	water	VW	L10	2
1	621	8	water	WW	L21	4
1	622	8	water	XW	L43	2
1	623	8	water	YW	L54	2
1	624	8	water	ZW	L76	45
1	625	8	water	AX	L87	43
1	626	8	water	BX	L98	17
1	627	8	water	CX	L11a	8
1	628	8	water	DX	L12b	4
1	629	8	water	EX	L13c	11
1	630	8	water	FX	L14d	41
1	631	8	water	GX	L15e	10
1	632	8	water	HX	L16f	47
1	633	8	water	IX	L17g	5
1	634	8	water	JX	L18h	54
1	635	8	water	KX	L19i	1
1	636	8	water	LX	L21k	8
1	637	8	water	MX	L22l	3
1	638	8	water	NX	L23m	10
1	639	8	water	OX	L24n	69
1	640	8	water	PX	L25o	105
1	641	8	water	QX	L26p	4
1	642	8	water	RX	L27q	134

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	643	8	water	SX	L28r	16
1	644	8	water	TX	L29s	29
1	645	8	water	UX	L30t	21
1	646	8	water	VX	L31u	10
1	647	8	water	WX	L33w	25
1	648	8	water	XX	L34x	1
1	649	8	water	YX	L35y	61
1	650	8	water	ZX	L36z	22
1	651	8	water	AY	L37A	72
1	652	8	water	BY	L38B	97
1	653	8	water	CY	L39C	2
1	654	8	water	DY	L40D	241
1	655	8	water	EY	L41E	36
1	656	8	water	FY	L42F	19
1	657	8	water	GY	L43G	22
1	658	8	water	HY	L44H	2
1	659	8	water	IY	L45I	23
1	660	8	water	JY	L46J	11
1	661	8	water	KY	L47K	148
1	662	8	water	LY	L48L	6
1	663	8	water	MY	L49M	21
1	664	8	water	NY	L50N	20
1	665	8	water	OY	L51O	2
1	666	8	water	PY	L52P	7
1	667	8	water	QY	L54R	2
1	668	8	water	RY	L55S	110
1	669	8	water	SY	L56T	47

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	670	8	water	TY	L57U	31
1	671	8	water	UY	L58V	5
1	672	8	water	VY	L590	5
1	673	8	water	WY	L601	41
1	674	8	water	XY	L612	10
1	675	8	water	YY	L623	1
1	676	8	water	ZY	L634	10
1	677	8	water	AZ	L645	29
1	678	8	water	BZ	L656	1
1	679	8	water	CZ	L667	10
1	680	8	water	DZ	L69a	9
1	681	8	water	EZ	L70b	20
1	682	8	water	FZ	L71c	1
1	683	8	water	GZ	L73e	251
1	684	8	water	HZ	L74f	4
1	685	8	water	IZ	L75g	1
1	686	8	water	JZ	L76h	29
1	687	8	water	KZ	L77i	147
1	688	8	water	LZ	L78j	3
1	689	8	water	MZ	L79k	3
1	690	8	water	NZ	L80l	13
1	691	8	water	OZ	L81m	13
1	692	8	water	PZ	L82n	3
1	693	8	water	QZ	L83o	12
1	694	8	water	RZ	L84p	234
1	695	8	water	SZ	L85q	13
1	696	8	water	TZ	L86r	7

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	697	8	water	UZ	L87s	1
1	698	8	water	VZ	L88t	1
1	699	8	water	WZ	L89u	5
1	700	8	water	XZ	L91w	55
1	701	8	water	YZ	L92x	79
1	702	8	water	ZZ	L93y	8
1	703	8	water	AAA	L94z	2
1	704	8	water	BAA	L95A	40
1	705	8	water	CAA	L96B	68
1	706	8	water	DAA	L97C	2
1	707	8	water	EAA	L98D	13
1	708	8	water	FAA	L99E	9
1	709	8	water	GAA	L100F	100
1	710	8	water	HAA	L101G	6
1	711	8	water	IAA	L102H	9
1	712	8	water	JAA	L103I	2
1	713	8	water	KAA	L104J	15
1	714	8	water	LAA	L105K	50
1	715	8	water	MAA	L106L	5
1	716	8	water	NAA	L107M	1
1	717	8	water	OAA	L108N	6
1	718	8	water	PAA	L109O	14
1	719	8	water	QAA	L110P	5
1	720	8	water	RAA	L111Q	263
1	721	8	water	SAA	L112R	2
1	722	8	water	TAA	L113S	2
1	723	8	water	UAA	L114T	15

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	BMRB	big94
1	De Novo model	File	10.5281/zenodo.10179190

Representation

This entry has only one representation and includes 0 rigid bodies and 723 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-20
B	-	1-20
C	-	1-20
D	-	1-20
E	-	1-20
F	-	1-20
G	-	1-20
H	-	1-20
I	-	1-20
J	-	1-20
K	-	1-20
L	-	1-20
M	-	1-20
N	-	1-20
O	-	1-20
P	-	1-20
Q	-	1-20
R	-	1-20

Chain ID	Rigid bodies	Non-rigid segments
S	-	1-20
T	-	1-20
U	-	1-20
V	-	1-20
W	-	1-20
X	-	1-20
Y	-	1-20
Z	-	1-20
AA	-	1-20
BA	-	1-20
CA	-	1-20
DA	-	1-20
EA	-	1-20
FA	-	1-20
GA	-	1-20
HA	-	1-20
IA	-	1-20
JA	-	1-20
KA	-	1-20
LA	-	1-20
MA	-	1-20
NA	-	1-20
OA	-	1-20
PA	-	1-20
QA	-	1-20
RA	-	1-20
SA	-	1-20

Chain ID	Rigid bodies	Non-rigid segments
TA	-	1-20
UA	-	1-20
VA	-	1-20
WA	-	1-20
XA	-	1-20
YA	-	1-20
ZA	-	1-20
AB	-	1-20
BB	-	1-20
CB	-	1-20
DB	-	1-20
EB	-	1-20
FB	-	1-20
GB	-	1-20
HB	-	1-20
IB	-	1-20
JB	-	1-20
KB	-	1-20
LB	-	1-20
MB	-	1-20
NB	-	1-20
OB	-	1-20
PB	-	1-20
QB	-	1-20
RB	-	1-20
SB	-	1-20
TB	-	1-20

Chain ID	Rigid bodies	Non-rigid segments
UB	-	1-20
VB	-	1-20
WB	-	1-20
XB	-	1-20
YB	-	1-20
ZB	-	1-20
AC	-	1-20
BC	-	1-20
CC	-	1-20
DC	-	1-20
EC	-	1-20
FC	-	1-20
GC	-	1-20
HC	-	1-20
IC	-	1-20
JC	-	1-20
KC	-	1-20
LC	-	1-20
MC	-	1-20
NC	-	1-20
OC	-	1-20
PC	-	1-20
QC	-	1-20
RC	-	1-20
SC	-	1-20
TC	-	1-20
UC	-	1-20

Chain ID	Rigid bodies	Non-rigid segments
VC	-	1-20
WC	-	1-20
XC	-	1-20
YC	-	1-20
ZC	-	1-20
AD	-	1-20
BD	-	1-20
CD	-	1-20
DD	-	1-20
ED	-	1-20
FD	-	1-20
GD	-	1-20
HD	-	1-20
ID	-	1-20
JD	-	1-20
KD	-	1-20
LD	-	1-45
MD	-	1-45
ND	-	1-45
OD	-	1-45
PD	-	1-45
GE	-	1-45
HE	-	1-45
IE	-	1-45
JE	-	1-45
KE	-	1-45
BF	-	1-45

Chain ID	Rigid bodies	Non-rigid segments
CF	-	1-45
DF	-	1-45
EF	-	1-45
FF	-	1-45
QD	-	1-45
RD	-	1-45
SD	-	1-45
TD	-	1-45
UD	-	1-45
LE	-	1-45
ME	-	1-45
NE	-	1-45
OE	-	1-45
PE	-	1-45
GF	-	1-45
HF	-	1-45
IF	-	1-45
JF	-	1-45
KF	-	1-45
VD	-	1-45
WD	-	1-45
XD	-	1-45
YD	-	1-45
ZD	-	1-45
QE	-	1-45
RE	-	1-45
SE	-	1-45

Chain ID	Rigid bodies	Non-rigid segments
TE	-	1-45
UE	-	1-45
LF	-	1-45
MF	-	1-45
NF	-	1-45
OF	-	1-45
PF	-	1-45
AE	-	1-45
BE	-	1-45
CE	-	1-45
DE	-	1-45
EE	-	1-45
FE	-	1-45
VE	-	1-45
WE	-	1-45
XE	-	1-45
YE	-	1-45
ZE	-	1-45
AF	-	1-45
QF	-	1-45
RF	-	1-45
SF	-	1-45
TF	-	1-40
UF	-	1-40
VF	-	1-40
WF	-	1-40
XF	-	1-40

Chain ID	Rigid bodies	Non-rigid segments
YF	-	1-40
ZF	-	1-40
AG	-	1-40
BG	-	1-40
CG	-	1-40
DG	-	1-40
EG	-	1-40
FG	-	1-40
GG	-	1-40
HG	-	1-40
IG	-	1-40
JG	-	1-40
KG	-	1-40
LG	-	1-40
MG	-	1-40
NG	-	1-40
OG	-	1-40
PG	-	1-40
QG	-	1-40
RG	-	1-40
SG	-	1-40
TG	-	1-40
UG	-	1-40
VG	-	1-40
WG	-	1-40
XG	-	1-40
YG	-	1-40

Chain ID	Rigid bodies	Non-rigid segments
ZG	-	1-40
AH	-	1-40
BH	-	1-40
CH	-	1-40
DH	-	1-40
EH	-	1-40
FH	-	1-40
GH	-	1-40
HH	-	1-40
IH	-	1-40
JH	-	1-40
KH	-	1-40
LH	-	1-40
MH	-	1-40
NH	-	1-40
OH	-	1-40
PH	-	1-40
QH	-	1-40
RH	-	1-40
SH	-	1-40
TH	-	1-40
UH	-	1-40
VH	-	1-40
WH	-	1-40
XH	-	1-40
YH	-	1-40
ZH	-	1-40

Chain ID	Rigid bodies	Non-rigid segments
AI	-	1-40
BI	-	1-40
CI	-	1-40
DI	-	1-40
EI	-	1-40
FI	-	1-40
GI	-	1-40
HI	-	1-40
II	-	1-40
JI	-	1-40
KI	-	1-40
LI	-	1-40
MI	-	1-40
NI	-	1-40
OI	-	1-40
PI	-	1-40
QI	-	1-40
RI	-	1-40
SI	-	1-40
TI	-	1-40
UI	-	1-40
VI	-	1-40
WI	-	1-40
XI	-	1-40
YI	-	1-40
ZI	-	1-40
AJ	-	1-40

Chain ID	Rigid bodies	Non-rigid segments
BJ	-	1-40
CJ	-	1-40
DJ	-	1-40
EJ	-	1-40
FJ	-	1-40
GJ	-	1-40
HJ	-	1-40
IJ	-	1-40
JJ	-	1-40
KJ	-	1-40
LJ	-	1-40
MJ	-	1-40
NJ	-	1-40
OJ	-	1-40
PJ	-	1-40
QJ	-	1-40
RJ	-	1-40
SJ	-	1-40
TJ	-	1-40
UJ	-	1-40
VJ	-	1-40
WJ	-	1-40
XJ	-	1-40
YJ	-	1-40
ZJ	-	1-40
AK	-	1-40
BK	-	1-40

Chain ID	Rigid bodies	Non-rigid segments
CK	-	1-40
DK	-	1-40
EK	-	1-40
FK	-	1-40
GK	-	1-40
HK	-	1-40
IK	-	1-40
JK	-	1-40
KK	-	1-40
LK	-	1-40
MK	-	1-40
NK	-	1-40
OK	-	1-40
PK	-	1-40
QK	-	1-40
RK	-	1-40
SK	-	1-40
TK	-	1-40
UK	-	1-40
VK	-	1-40
WK	-	1-40
XK	-	1-40
YK	-	1-40
ZK	-	1-40
AL	-	1-40
BL	-	1-40
CL	-	1-40

Chain ID	Rigid bodies	Non-rigid segments
DL	-	1-40
EL	-	1-40
FL	-	1-40
GL	-	1-40
HL	-	None-None
IL	-	None-None
JL	-	None-None
KL	-	None-None
LL	-	None-None
ML	-	None-None
NL	-	None-None
OL	-	None-None
PL	-	None-None
QL	-	None-None
RL	-	None-None
SL	-	None-None
TL	-	None-None
UL	-	None-None
VL	-	None-None
WL	-	None-None
XL	-	None-None
YL	-	None-None
ZL	-	None-None
AM	-	None-None
BM	-	None-None
CM	-	None-None
DM	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
EM	-	None-None
FM	-	None-None
GM	-	None-None
HM	-	None-None
IM	-	None-None
JM	-	None-None
KM	-	None-None
LM	-	None-None
MM	-	None-None
NM	-	None-None
OM	-	None-None
PM	-	None-None
QM	-	None-None
RM	-	None-None
SM	-	None-None
TM	-	None-None
UM	-	None-None
VM	-	None-None
WM	-	None-None
XM	-	None-None
YM	-	None-None
ZM	-	None-None
AN	-	None-None
BN	-	None-None
CN	-	None-None
DN	-	None-None
EN	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
FN	-	None-None
GN	-	None-None
HN	-	None-None
IN	-	None-None
JN	-	None-None
KN	-	None-None
LN	-	None-None
MN	-	None-None
NN	-	None-None
ON	-	None-None
PN	-	None-None
QN	-	None-None
RN	-	None-None
SN	-	None-None
TN	-	None-None
UN	-	None-None
VN	-	None-None
WN	-	None-None
XN	-	None-None
YN	-	None-None
ZN	-	None-None
AO	-	None-None
BO	-	None-None
CO	-	None-None
DO	-	None-None
EO	-	None-None
FO	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
GO	-	None-None
HO	-	None-None
IO	-	None-None
JO	-	None-None
KO	-	None-None
LO	-	None-None
MO	-	None-None
NO	-	None-None
OO	-	None-None
PO	-	None-None
QO	-	None-None
RO	-	None-None
SO	-	None-None
TO	-	None-None
UO	-	None-None
VO	-	None-None
WO	-	None-None
XO	-	None-None
YO	-	None-None
ZO	-	None-None
AP	-	None-None
BP	-	None-None
CP	-	None-None
DP	-	None-None
EP	-	None-None
FP	-	None-None
GP	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
HP	-	None-None
IP	-	None-None
JP	-	None-None
KP	-	None-None
LP	-	None-None
MP	-	None-None
NP	-	None-None
OP	-	None-None
PP	-	None-None
QP	-	None-None
RP	-	None-None
SP	-	None-None
TP	-	None-None
UP	-	None-None
VP	-	None-None
WP	-	None-None
XP	-	None-None
YP	-	None-None
ZP	-	None-None
AQ	-	None-None
BQ	-	None-None
CQ	-	None-None
DQ	-	None-None
EQ	-	None-None
FQ	-	None-None
GQ	-	None-None
HQ	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
IQ	-	None-None
JQ	-	None-None
KQ	-	None-None
LQ	-	None-None
MQ	-	None-None
NQ	-	None-None
OQ	-	None-None
PQ	-	None-None
QQ	-	None-None
RQ	-	None-None
SQ	-	None-None
TQ	-	None-None
UQ	-	None-None
VQ	-	None-None
WQ	-	None-None
XQ	-	None-None
YQ	-	None-None
ZQ	-	None-None
AR	-	None-None
BR	-	None-None
CR	-	None-None
DR	-	None-None
ER	-	None-None
FR	-	None-None
GR	-	None-None
HR	-	None-None
IR	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
JR	-	None-None
KR	-	None-None
LR	-	None-None
MR	-	None-None
NR	-	None-None
OR	-	None-None
PR	-	None-None
QR	-	None-None
RR	-	None-None
SR	-	None-None
TR	-	None-None
UR	-	None-None
VR	-	None-None
WR	-	None-None
XR	-	None-None
YR	-	None-None
ZR	-	None-None
AS	-	None-None
BS	-	None-None
CS	-	None-None
DS	-	None-None
ES	-	None-None
FS	-	None-None
GS	-	None-None
HS	-	None-None
IS	-	None-None
JS	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
KS	-	None-None
LS	-	None-None
MS	-	None-None
NS	-	None-None
OS	-	None-None
PS	-	None-None
QS	-	None-None
RS	-	None-None
SS	-	None-None
TS	-	None-None
US	-	None-None
VS	-	None-None
WS	-	None-None
XS	-	None-None
YS	-	None-None
ZS	-	None-None
AT	-	None-None
BT	-	None-None
CT	-	None-None
DT	-	None-None
ET	-	None-None
FT	-	None-None
GT	-	None-None
HT	-	None-None
IT	-	None-None
JT	-	None-None
KT	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
LT	-	None-None
MT	-	None-None
NT	-	None-None
OT	-	None-None
PT	-	None-None
QT	-	None-None
RT	-	None-None
ST	-	None-None
TT	-	None-None
UT	-	None-None
VT	-	None-None
WT	-	None-None
XT	-	None-None
YT	-	None-None
ZT	-	None-None
AU	-	None-None
BU	-	None-None
CU	-	None-None
DU	-	None-None
EU	-	None-None
FU	-	None-None
GU	-	None-None
HU	-	None-None
IU	-	None-None
JU	-	None-None
KU	-	None-None
LU	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
MU	-	None-None
NU	-	None-None
OU	-	None-None
PU	-	None-None
QU	-	None-None
RU	-	None-None
SU	-	None-None
TU	-	None-None
UU	-	None-None
VU	-	None-None
WU	-	None-None
XU	-	None-None
YU	-	None-None
ZU	-	None-None
AV	-	None-None
BV	-	None-None
CV	-	None-None
DV	-	None-None
EV	-	None-None
FV	-	None-None
GV	-	None-None
HV	-	None-None
IV	-	None-None
JV	-	None-None
KV	-	None-None
LV	-	None-None
MV	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
NV	-	None-None
OV	-	None-None
PV	-	None-None
QV	-	None-None
RV	-	None-None
SV	-	None-None
TV	-	None-None
UV	-	None-None
VV	-	None-None
WV	-	None-None
XV	-	None-None
YV	-	None-None
ZV	-	None-None
AW	-	None-None
BW	-	None-None
CW	-	None-None
DW	-	None-None
EW	-	None-None
FW	-	None-None
GW	-	None-None
HW	-	None-None
IW	-	None-None
JW	-	None-None
KW	-	None-None
LW	-	None-None
MW	-	None-None
NW	-	None-None

Chain ID	Rigid bodies	Non-rigid segments
OW	-	None-None
PW	-	None-None
QW	-	None-None
RW	-	None-None
SW	-	None-None
TW	-	None-None
UW	-	None-None
VW	-	1-2
WW	-	1-4
XW	-	1-2
YW	-	1-2
ZW	-	1-45
AX	-	1-43
BX	-	1-17
CX	-	1-8
DX	-	1-4
EX	-	1-11
FX	-	1-41
GX	-	1-10
HX	-	1-47
IX	-	1-5
JX	-	1-54
KX	-	1-1
LX	-	1-8
MX	-	1-3
NX	-	1-10
OX	-	1-69

Chain ID	Rigid bodies	Non-rigid segments
PX	-	1-105
QX	-	1-4
RX	-	1-134
SX	-	1-16
TX	-	1-29
UX	-	1-21
VX	-	1-10
WX	-	1-25
XX	-	1-1
YX	-	1-61
ZX	-	1-22
AY	-	1-72
BY	-	1-97
CY	-	1-2
DY	-	1-241
EY	-	1-36
FY	-	1-19
GY	-	1-22
HY	-	1-2
IY	-	1-23
JY	-	1-11
KY	-	1-148
LY	-	1-6
MY	-	1-21
NY	-	1-20
OY	-	1-2
PY	-	1-7

Chain ID	Rigid bodies	Non-rigid segments
QY	-	1-2
RY	-	1-110
SY	-	1-47
TY	-	1-31
UY	-	1-5
VY	-	1-5
WY	-	1-41
XY	-	1-10
YY	-	1-1
ZY	-	1-10
AZ	-	1-29
BZ	-	1-1
CZ	-	1-10
DZ	-	1-9
EZ	-	1-20
FZ	-	1-1
GZ	-	1-251
HZ	-	1-4
IZ	-	1-1
JZ	-	1-29
KZ	-	1-147
LZ	-	1-3
MZ	-	1-3
NZ	-	1-13
OZ	-	1-13
PZ	-	1-3
QZ	-	1-12

Chain ID	Rigid bodies	Non-rigid segments
RZ	-	1-234
SZ	-	1-13
TZ	-	1-7
UZ	-	1-1
VZ	-	1-1
WZ	-	1-5
XZ	-	1-55
YZ	-	1-79
ZZ	-	1-8
AAA	-	1-2
BAA	-	1-40
CAA	-	1-68
DAA	-	1-2
EAA	-	1-13
FAA	-	1-9
GAA	-	1-100
HAA	-	1-6
IAA	-	1-9
JAA	-	1-2
KAA	-	1-15
LAA	-	1-50
MAA	-	1-5
NAA	-	1-1
OAA	-	1-6
PAA	-	1-14
QAA	-	1-5
RAA	-	1-263

Chain ID	Rigid bodies	Non-rigid segments
SAA	-	1-2
TAA	-	1-2
UAA	-	1-15

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	Molecular Placement of Cellulose, Xylan and Lignin	Initial Polymer Placement	None	None	False	False
2	1	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	Equilibration with Molecular Dynamics	None	None	False	False
3	1	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 analsis at https://doi.org/10.5281/zenodo.10179190	Production Simulations in the NVT ensemble	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	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	Proximity Calculations for Reproduction of ssNMR Observables	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	https://www.charmm.org/

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.

Standard geometry: bond outliers

There are 48665 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
O--H1	0.96	0.85	3305
O--H2	0.96	0.85	3305
O2--HO2	0.96	0.85	1500
O3--HO3	0.96	0.85	1500
O1--HO1	0.96	0.85	60
C2--H2	1.08	0.97	115
O4--HO4	0.98	0.85	230
C4--H4	1.11	0.97	7260
C3--H3	1.11	0.97	7260
C2--H2	1.11	0.97	7260
C1--H1	1.11	0.97	7260
C5--H5	1.11	0.97	6060
C5--H51	1.11	0.97	1200
C5--H52	1.11	0.97	1200
C2--H2	1.08	0.93	230
C5--H5	1.08	0.93	229
C6--H6	1.08	0.93	345
C3--H3	1.08	0.93	229
C8--H8	1.09	0.93	5
C8--H8	1.10	0.93	110
C5--H5	1.08	0.85	1
C3--H3	1.08	1.34	1

Standard geometry: angle outliers

There are 1276 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4-C5-O3	114.77	17.25	1
C4-C5-O3	114.77	17.27	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4-C5-O3	114.77	17.35	1
C4-C5-O3	114.77	17.37	1
C4-C5-O3	114.77	17.76	1
C4-C5-O3	114.77	17.81	1
C4-C5-O3	114.77	17.86	1
C4-C5-O3	114.77	17.90	1
C4-C5-O3	114.77	17.99	2
C4-C5-O3	114.77	18.04	1
C4-C5-O3	114.77	18.06	1
C4-C5-O3	114.77	18.08	1
C4-C5-O3	114.77	18.11	1
C4-C5-O3	114.77	18.16	1
C4-C5-O3	114.77	18.17	1
C4-C5-O3	114.77	18.19	1
C4-C5-O3	114.77	18.24	2
C4-C5-O3	114.77	18.26	1
C4-C5-O3	114.77	18.30	2
C4-C5-O3	114.77	18.39	1
C4-C5-O3	114.77	18.44	1
C4-C5-O3	114.77	18.53	1
C4-C5-O3	114.77	18.55	1
C4-C5-O3	114.77	18.57	1
C4-C5-O3	114.77	18.60	1
C4-C5-O3	114.77	18.62	2
C4-C5-O3	114.77	18.65	1
C4-C5-O3	114.77	18.69	1
C4-C5-O3	114.77	18.74	4

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4-C5-O3	114.77	18.76	1
C4-C5-O3	114.77	18.78	1
C4-C5-O3	114.77	18.79	1
C4-C5-O3	114.77	18.81	1
C4-C5-O3	114.77	18.83	1
C4-C5-O3	114.77	18.88	1
C4-C5-O3	114.77	18.89	1
C4-C5-O3	114.77	18.91	1
C4-C5-O3	114.77	18.93	1
C4-C5-O3	114.77	18.95	1
C4-C5-O3	114.77	18.98	1
C4-C5-O3	114.77	19.00	1
C4-C5-O3	114.77	19.03	2
C4-C5-O3	114.77	19.11	3
C4-C5-O3	114.77	19.14	1
C4-C5-O3	114.77	19.15	1
C4-C5-O3	114.77	19.26	1
C4-C5-O3	114.77	19.37	1
C4-C5-O3	114.77	19.38	2
C4-C5-O3	114.77	19.40	1
C4-C5-O3	114.77	19.45	1
C4-C5-O3	114.77	19.47	2
C4-C5-O3	114.77	19.48	2
C4-C5-O3	114.77	19.53	1
C4-C5-O3	114.77	19.61	1
C4-C5-O3	114.77	19.67	1
C4-C5-O3	114.77	19.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4-C5-O3	114.77	19.72	1
C4-C5-O3	114.77	19.73	2
C4-C5-O3	114.77	19.75	1
C4-C5-O3	114.77	19.77	1
C4-C5-O3	114.77	19.83	1
C4-C5-O3	114.77	19.84	1
C4-C5-O3	114.77	19.86	1
C4-C5-O3	114.77	19.90	2
C4-C5-O3	114.77	19.93	1
C4-C5-O3	114.77	19.94	1
C4-C5-O3	114.77	19.98	1
C4-C5-O3	114.77	20.04	1
C4-C5-O3	114.77	20.11	1
C4-C5-O3	114.77	20.12	1
C4-C5-O3	114.77	20.15	1
C4-C5-O3	114.77	20.16	1
C4-C5-O3	114.77	20.20	1
C4-C5-O3	114.77	20.28	1
C4-C5-O3	114.77	20.29	1
C4-C5-O3	114.77	20.30	1
C4-C5-O3	114.77	20.36	1
C4-C5-O3	114.77	20.56	1
C4-C5-O3	114.77	20.65	2
C4-C5-O3	114.77	20.66	1
C4-C5-O3	114.77	20.79	1
C4-C5-O3	114.77	20.80	1
C4-C5-O3	114.77	20.90	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C4-C5-O3	114.77	20.94	1
C4-C5-O3	114.77	20.97	1
C4-C5-O3	114.77	21.04	1
C4-C5-O3	114.77	21.06	1
C4-C5-O3	114.77	21.08	1
C4-C5-O3	114.77	21.10	1
C4-C5-O3	114.77	21.37	1
C4-C5-O3	114.77	21.40	1
C4-C5-O3	114.77	21.54	1
C4-C5-O3	114.77	21.62	1
C4-C5-O3	114.77	21.73	1
C4-C5-O3	114.77	21.74	1
C4-C5-O3	114.77	21.81	1
C1-C7-C6	118.23	25.49	1
C1-C7-C6	118.23	25.63	1
C4-C5-O3	114.77	22.28	1
C1-C7-C6	118.23	25.75	1
C4-C5-O3	114.77	22.43	1
C1-C7-C6	118.23	26.06	1
C1-C7-C6	118.23	26.14	1
C1-C7-C6	118.23	26.22	1
C1-C7-C6	118.23	26.33	1
C1-C7-C6	118.23	26.56	1
C1-C7-C6	118.23	26.61	1
C1-C7-C6	118.23	26.70	1
C4-C5-O3	114.77	23.28	1
C1-C7-C6	118.23	26.74	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C7-C6	118.23	26.78	1
C1-C7-C6	118.23	26.91	1
C1-C7-C6	118.23	26.93	1
C1-C7-C6	118.23	26.97	1
C1-C7-C6	118.23	27.16	1
C1-C7-C6	118.23	27.17	1
C1-C7-C6	118.23	27.25	1
C1-C7-C6	118.23	27.26	1
C1-C7-C6	118.23	27.27	1
C1-C7-C6	118.23	27.35	1
C1-C7-C6	118.23	27.42	1
C1-C7-C6	118.23	27.54	1
C1-C7-C6	118.23	27.68	1
C1-C7-C6	118.23	27.72	1
C1-C7-C6	118.23	27.79	1
C1-C7-C6	118.23	27.87	1
C1-C7-C6	118.23	27.89	1
C1-C7-C6	118.23	27.91	2
C1-C7-C6	118.23	27.92	1
C1-C7-C6	118.23	27.96	2
C1-C7-C6	118.23	27.98	1
C1-C7-C6	118.23	28.08	1
C1-C7-C6	118.23	28.13	1
C1-C7-C6	118.23	28.16	1
C1-C7-C6	118.23	28.21	1
C1-C7-C6	118.23	28.26	1
C1-C7-C6	118.23	28.37	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C7-C6	118.23	28.45	1
C1-C7-C6	118.23	28.46	2
C1-C7-C6	118.23	28.48	1
C1-C7-C6	118.23	28.50	1
C1-C7-C6	118.23	28.52	1
C1-C7-C6	118.23	28.56	1
C1-C7-C6	118.23	28.59	1
C1-C7-C6	118.23	28.67	1
C1-C7-C6	118.23	28.84	1
C1-C7-C6	118.23	28.89	1
C1-C7-C6	118.23	28.98	1
C1-C7-C6	118.23	28.99	1
C1-C7-C6	118.23	29.00	1
C1-C7-C6	118.23	29.01	1
C1-C7-C6	118.23	29.02	1
C1-C7-C6	118.23	29.11	1
C1-C7-C6	118.23	29.12	1
C1-C7-C6	118.23	29.20	1
C1-C7-C6	118.23	29.27	1
C1-C7-C6	118.23	29.28	1
C1-C7-C6	118.23	29.35	1
C1-C7-C6	118.23	29.45	1
C1-C7-C6	118.23	29.46	1
C1-C7-C6	118.23	29.54	1
C1-C7-C6	118.23	29.70	1
C1-C7-C6	118.23	29.74	1
C1-C7-C6	118.23	29.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C7-C6	118.23	29.89	1
C1-C7-C6	118.23	29.91	1
C1-C7-C6	118.23	29.92	1
C1-C7-C6	118.23	29.94	1
C10-C9-C8	123.29	35.03	1
C1-C7-C6	118.23	30.03	1
C1-C7-C6	118.23	30.04	2
C1-C7-C6	118.23	30.10	2
C1-C7-C6	118.23	30.14	1
C1-C7-C6	118.23	30.26	2
C1-C7-C6	118.23	30.31	1
C1-C7-C6	118.23	30.34	1
C1-C7-C6	118.23	30.41	1
C1-C7-C6	118.23	30.46	1
C1-C7-C6	118.23	30.47	1
C1-C7-C6	118.23	30.49	1
C1-C7-C6	118.23	30.52	1
C1-C7-C6	118.23	30.60	1
C1-C7-C6	118.23	30.67	2
C1-C7-C6	118.23	30.72	1
C1-C7-C6	118.23	30.83	1
C1-C7-C6	118.23	30.85	1
C1-C7-C6	118.23	30.88	1
C1-C7-C6	118.23	31.00	1
C1-C7-C6	118.23	31.10	1
C1-C7-C6	118.23	31.15	1
C1-C7-C6	118.23	31.17	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C7-C6	118.23	31.24	2
C1-C7-C6	118.23	31.25	1
C1-C7-C6	118.23	31.42	1
C1-C7-C6	118.23	31.44	1
C1-C7-C6	118.23	31.50	1
C10-C9-C8	123.29	36.59	1
C1-C7-C6	118.23	31.63	1
C1-C7-C6	118.23	31.87	1
C1-C7-C6	118.23	31.93	1
C1-C7-C6	118.23	31.97	1
C1-C7-C6	118.23	32.06	1
C10-C9-C8	123.29	37.40	1
C1-C7-C6	118.23	32.59	1
C1-C7-C6	118.23	32.68	1
C1-C7-C6	118.23	32.81	1
C10-C9-C8	123.29	38.03	1
C1-C7-C6	118.23	33.26	1
C1-C7-C6	118.23	33.42	1
C1-C7-C6	118.23	33.64	1
C10-C9-C8	123.29	40.45	1
C10-C9-C8	123.29	41.85	1
C10-C9-C8	123.29	42.26	1
C10-C9-C8	123.29	43.36	1
C10-C9-C8	123.29	43.47	1
C10-C9-C8	123.29	43.94	1
C10-C9-C8	123.29	44.66	1
C10-C9-C8	123.29	45.18	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C10-C9-C8	123.29	45.19	1
C10-C9-C8	123.29	45.97	1
C10-C9-C8	123.29	46.38	1
C10-C9-C8	123.29	46.66	1
C10-C9-C8	123.29	47.42	1
C10-C9-C8	123.29	47.56	1
C10-C9-C8	123.29	47.68	1
C10-C9-C8	123.29	47.93	1
C10-C9-C8	123.29	48.13	1
C10-C9-C8	123.29	48.17	1
C10-C9-C8	123.29	48.33	1
C10-C9-C8	123.29	48.42	1
C10-C9-C8	123.29	48.74	1
C10-C9-C8	123.29	49.67	1
C10-C9-C8	123.29	51.56	1
C10-C9-C8	123.29	51.63	1
C10-C9-C8	123.29	52.60	1
C2-O3-C5	118.67	48.07	1
C10-C9-C8	123.29	52.95	1
C2-O3-C5	118.67	48.44	1
C2-O3-C5	118.67	48.64	1
C2-O3-C5	118.67	48.67	1
C2-O3-C5	118.67	48.72	1
C2-O3-C5	118.67	48.94	1
C2-O3-C5	118.67	48.95	1
C2-O3-C5	118.67	49.00	1
C2-O3-C5	118.67	49.02	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C10-C9-C8	123.29	53.70	1
C2-O3-C5	118.67	49.11	1
C2-O3-C5	118.67	49.18	2
C2-O3-C5	118.67	49.21	2
C2-O3-C5	118.67	49.28	2
C2-O3-C5	118.67	49.30	1
C2-O3-C5	118.67	49.32	1
C2-O3-C5	118.67	49.34	1
C2-O3-C5	118.67	49.36	1
C2-O3-C5	118.67	49.38	1
C2-O3-C5	118.67	49.44	1
C2-O3-C5	118.67	49.50	1
C2-O3-C5	118.67	49.51	1
C2-O3-C5	118.67	49.52	1
C2-O3-C5	118.67	49.53	1
C2-O3-C5	118.67	49.54	1
C2-O3-C5	118.67	49.56	1
C2-O3-C5	118.67	49.57	2
C2-O3-C5	118.67	49.59	1
C2-O3-C5	118.67	49.60	2
C10-C9-C8	123.29	54.24	1
C2-O3-C5	118.67	49.63	1
C2-O3-C5	118.67	49.64	1
C2-O3-C5	118.67	49.66	3
C2-O3-C5	118.67	49.67	1
C2-O3-C5	118.67	49.68	1
C2-O3-C5	118.67	49.69	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-O3-C5	118.67	49.70	1
C2-O3-C5	118.67	49.71	1
C2-O3-C5	118.67	49.72	1
C2-O3-C5	118.67	49.75	2
C2-O3-C5	118.67	49.76	1
C2-O3-C5	118.67	49.78	1
C2-O3-C5	118.67	49.79	2
C2-O3-C5	118.67	49.80	1
C2-O3-C5	118.67	49.81	1
C2-O3-C5	118.67	49.82	2
C2-O3-C5	118.67	49.83	4
C2-O3-C5	118.67	49.84	1
C2-O3-C5	118.67	49.85	3
C2-O3-C5	118.67	49.87	1
C2-O3-C5	118.67	49.88	1
C2-O3-C5	118.67	49.90	3
C2-O3-C5	118.67	49.91	1
C2-O3-C5	118.67	49.92	1
C2-O3-C5	118.67	49.94	2
C2-O3-C5	118.67	49.95	7
C2-O3-C5	118.67	49.96	2
C2-O3-C5	118.67	49.98	1
C2-O3-C5	118.67	49.99	1
C2-O3-C5	118.67	50.01	1
C2-O3-C5	118.67	50.02	1
C2-O3-C5	118.67	50.03	1
C2-O3-C5	118.67	50.04	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C2-O3-C5	118.67	50.07	1
C2-O3-C5	118.67	50.08	2
C2-O3-C5	118.67	50.09	2
C2-O3-C5	118.67	50.10	1
C2-O3-C5	118.67	50.11	1
C2-O3-C5	118.67	50.12	1
C2-O3-C5	118.67	50.18	1
C2-O3-C5	118.67	50.20	1
C2-O3-C5	118.67	50.22	1
C10-C9-C8	123.29	54.87	1
C2-O3-C5	118.67	50.25	1
C2-O3-C5	118.67	50.28	1
C10-C9-C8	123.29	54.90	1
C2-O3-C5	118.67	50.29	2
C2-O3-C5	118.67	50.31	1
C2-O3-C5	118.67	50.32	1
C2-O3-C5	118.67	50.34	1
C2-O3-C5	118.67	50.35	1
C2-O3-C5	118.67	50.37	1
C2-O3-C5	118.67	50.38	3
C2-O3-C5	118.67	50.40	1
C2-O3-C5	118.67	50.58	2
C2-O3-C5	118.67	50.67	1
C2-O3-C5	118.67	50.89	1
C10-C9-C8	123.29	55.80	1
C10-C9-C8	123.29	55.84	1
C10-C9-C8	123.29	56.20	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C10-C9-C8	123.29	56.27	1
C2-O3-C5	118.67	51.76	1
C10-C9-C8	123.29	56.79	1
C10-C9-C8	123.29	56.96	1
C10-C9-C8	123.29	57.58	1
C10-C9-C8	123.29	58.56	1
C10-C9-C8	123.29	59.27	1
C10-C9-C8	123.29	59.41	1
C10-C9-C8	123.29	60.00	1
C10-C9-C8	123.29	60.29	1
C10-C9-C8	123.29	60.88	1
C10-C9-C8	123.29	61.37	1
C10-C9-C8	123.29	62.34	1
C10-C9-C8	123.29	63.44	1
C10-C9-C8	123.29	63.58	1
C10-C9-C8	123.29	63.83	1
C10-C9-C8	123.29	64.61	1
C10-C9-C8	123.29	64.85	1
C10-C9-C8	123.29	66.42	1
C10-C9-C8	123.29	66.56	1
C6-C7-C8	118.28	174.22	1
C10-C9-C8	123.29	68.26	1
C10-C9-C8	123.29	68.70	1
C10-C9-C8	123.29	69.00	1
C10-C9-C8	123.29	69.10	1
C10-C9-C8	123.29	69.36	1
C10-C9-C8	123.29	71.37	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C10-C9-C8	123.29	71.76	1
C6-C7-C8	118.28	169.20	1
C6-C7-C8	118.28	166.45	1
C6-C7-C8	118.28	165.38	1
C6-C7-C8	118.28	162.99	1
C10-C9-C8	123.29	78.83	1
C6-C7-C8	118.28	162.38	1
C10-C9-C8	123.29	79.59	1
C6-C7-C8	118.28	161.77	1
C6-C7-C8	118.28	161.57	1
C6-C7-C8	118.28	161.22	1
C6-C7-C8	118.28	160.81	1
C10-C9-C8	123.29	81.18	1
C6-C7-C8	118.28	160.34	1
C6-C7-C8	118.28	160.25	1
C6-C7-C8	118.28	159.63	1
C10-C9-C8	123.29	82.39	1
C6-C7-C8	118.28	159.10	1
C6-C7-C8	118.28	158.47	1
C10-C9-C8	123.29	83.85	1
C6-C7-C8	118.28	157.65	1
C10-C9-C8	123.29	83.93	1
C6-C7-C8	118.28	157.09	1
C6-C7-C8	118.28	156.93	1
C6-C7-C8	118.28	156.50	1
C3-C1-C7	120.82	158.42	1
C6-C7-C8	118.28	155.68	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3-C1-C7	120.82	157.54	1
C3-C1-C7	120.82	157.47	1
C10-C9-C8	123.29	87.15	1
C6-C7-C8	118.28	154.22	1
C6-C7-C8	118.28	153.97	1
C5-C6-C7	121.27	156.95	1
C5-C6-C7	121.27	156.41	1
C3-C1-C7	120.82	155.89	1
C5-C6-C7	121.27	156.28	1
C10-C9-C8	123.29	88.48	1
C10-C9-C8	123.29	88.61	1
C3-C1-C7	120.82	155.50	1
C10-C9-C8	123.29	88.64	1
C3-C1-C7	120.82	155.31	1
C5-C6-C7	121.27	155.64	1
C3-C1-C7	120.82	155.04	1
C6-C7-C8	118.28	152.18	1
C3-C1-C7	120.82	154.70	1
C6-C7-C8	118.28	152.13	1
C3-C1-C7	120.82	154.63	1
C5-C6-C7	121.27	155.00	1
C5-C6-C7	121.27	154.99	1
C6-C7-C8	118.28	151.75	1
C3-C1-C7	120.82	154.14	1
C6-C7-C8	118.28	151.54	1
C5-C6-C7	121.27	154.46	1
C10-C9-C8	123.29	90.11	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3-C1-C7	120.82	153.93	1
C5-C6-C7	121.27	154.34	1
C5-C6-C7	121.27	154.32	1
C5-C6-C7	121.27	154.29	1
C1-C3-C4	120.78	87.77	1
C5-C6-C7	121.27	154.28	1
C5-C6-C7	121.27	154.22	1
C3-C1-C7	120.82	153.76	1
C3-C1-C7	120.82	153.73	1
C10-C9-C8	123.29	90.40	1
C10-C9-C8	123.29	90.46	1
C3-C1-C7	120.82	153.62	1
C1-C3-C4	120.78	87.99	1
C3-C1-C7	120.82	153.59	1
C5-C6-C7	121.27	153.99	1
C3-C1-C7	120.82	153.44	1
C3-C1-C7	120.82	153.43	1
C3-C1-C7	120.82	153.42	1
C5-C6-C7	121.27	153.83	1
C1-C3-C4	120.78	88.28	1
C1-C3-C4	120.78	88.34	1
C1-C3-C4	120.78	88.35	1
C1-C3-C4	120.78	88.39	2
C1-C3-C4	120.78	88.43	1
C5-C6-C7	121.27	153.57	2
C3-C1-C7	120.82	153.11	1
C1-C3-C4	120.78	88.49	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C3-C4	120.78	88.50	1
C1-C3-C4	120.78	88.53	1
C6-C7-C8	118.28	150.50	1
C10-C9-C8	123.29	91.08	1
C5-C6-C7	121.27	153.47	1
C10-C9-C8	123.29	91.15	1
C1-C3-C4	120.78	88.64	1
C5-C6-C7	121.27	153.41	1
C1-C3-C4	120.78	88.66	1
C1-C3-C4	120.78	88.68	1
C1-C3-C4	120.78	88.72	2
C1-C3-C4	120.78	88.74	1
C1-C3-C4	120.78	88.75	1
C3-C1-C7	120.82	152.83	1
C1-C3-C4	120.78	88.77	1
C5-C6-C7	121.27	153.27	2
C3-C1-C7	120.82	152.82	1
C1-C3-C4	120.78	88.78	1
C3-C1-C7	120.82	152.79	1
C1-C3-C4	120.78	88.83	2
C3-C1-C7	120.82	152.75	1
C1-C3-C4	120.78	88.88	2
C5-C6-C7	121.27	153.15	1
C1-C3-C4	120.78	88.91	1
C1-C3-C4	120.78	88.93	1
C1-C3-C4	120.78	88.94	3
C1-C3-C4	120.78	89.01	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C6-C7	121.27	153.02	1
C3-C1-C7	120.82	152.57	1
C5-C6-C7	121.27	153.01	1
C1-C3-C4	120.78	89.04	1
C1-C3-C4	120.78	89.07	2
C1-C3-C4	120.78	89.09	2
C5-C6-C7	121.27	152.96	1
C1-C3-C4	120.78	89.11	2
C1-C3-C4	120.78	89.13	1
C1-C3-C4	120.78	89.14	1
C1-C3-C4	120.78	89.15	1
C5-C6-C7	121.27	152.90	1
C1-C3-C4	120.78	89.17	1
C5-C6-C7	121.27	152.85	1
C5-C6-C7	121.27	152.84	1
C1-C3-C4	120.78	89.21	1
C3-C1-C7	120.82	152.38	1
C1-C3-C4	120.78	89.23	1
C1-C3-C4	120.78	89.24	1
C1-C3-C4	120.78	89.25	2
C1-C3-C4	120.78	89.26	2
C1-C3-C4	120.78	89.29	1
C1-C3-C4	120.78	89.30	1
C1-C3-C4	120.78	89.32	1
C1-C3-C4	120.78	89.33	1
C5-C6-C7	121.27	152.71	1
C1-C3-C4	120.78	89.36	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C3-C4	120.78	89.37	2
C1-C3-C4	120.78	89.38	3
C3-C1-C7	120.82	152.21	1
C1-C3-C4	120.78	89.40	1
C5-C6-C7	121.27	152.65	1
C1-C3-C4	120.78	89.41	1
C1-C3-C4	120.78	89.42	1
C1-C3-C4	120.78	89.43	2
C1-C3-C4	120.78	89.44	1
C3-C1-C7	120.82	152.14	2
C1-C3-C4	120.78	89.47	2
C1-C3-C4	120.78	89.48	2
C1-C3-C4	120.78	89.49	1
C1-C3-C4	120.78	89.51	1
C1-C3-C4	120.78	89.52	1
C1-C3-C4	120.78	89.53	1
C1-C3-C4	120.78	89.54	1
C1-C3-C4	120.78	89.62	1
C1-C3-C4	120.78	89.63	1
C10-C9-C8	123.29	92.15	1
C1-C3-C4	120.78	89.66	2
C5-C6-C7	121.27	152.37	1
C10-C9-C8	123.29	92.19	1
C1-C3-C4	120.78	89.69	1
C5-C6-C7	121.27	152.36	1
C1-C3-C4	120.78	89.70	2
C1-C3-C4	120.78	89.71	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C3-C4	120.78	89.74	2
C5-C6-C7	121.27	152.30	1
C3-C1-C7	120.82	151.84	1
C1-C3-C4	120.78	89.82	1
C5-C6-C7	121.27	152.22	1
C1-C3-C4	120.78	89.85	2
C5-C6-C7	121.27	152.18	2
C5-C6-C7	121.27	152.16	1
C1-C3-C4	120.78	89.91	1
C1-C3-C4	120.78	89.93	3
C5-C6-C7	121.27	152.11	1
C1-C3-C4	120.78	89.94	1
C5-C6-C7	121.27	152.09	1
C1-C3-C4	120.78	89.97	2
C3-C1-C7	120.82	151.63	1
C1-C3-C4	120.78	90.05	2
C1-C3-C4	120.78	90.07	1
C5-C6-C7	121.27	151.97	1
C5-C6-C7	121.27	151.95	1
C1-C3-C4	120.78	90.14	2
C5-C6-C7	121.27	151.90	1
C5-C6-C7	121.27	151.86	1
C5-C6-C7	121.27	151.85	1
C1-C3-C4	120.78	90.23	1
C1-C3-C4	120.78	90.24	1
C1-C3-C4	120.78	90.25	3
C3-C1-C7	120.82	151.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C3-C4	120.78	90.28	1
C5-C6-C7	121.27	151.76	1
C1-C3-C4	120.78	90.35	1
C5-C6-C7	121.27	151.70	2
C1-C3-C4	120.78	90.37	1
C1-C3-C4	120.78	90.38	1
C5-C6-C7	121.27	151.67	1
C1-C3-C4	120.78	90.40	1
C1-C3-C4	120.78	90.43	1
C5-C6-C7	121.27	151.59	1
C5-C6-C7	121.27	151.56	1
C5-C6-C7	121.27	151.52	2
C1-C3-C4	120.78	90.56	1
C10-C9-C8	123.29	93.08	1
C3-C1-C7	120.82	150.97	1
C5-C6-C7	121.27	151.41	1
C1-C3-C4	120.78	90.64	1
C3-C1-C7	120.82	150.95	1
C5-C6-C7	121.27	151.40	1
C1-C3-C4	120.78	90.72	1
C3-C1-C7	120.82	150.86	1
C3-C1-C7	120.82	150.84	1
C6-C7-C8	118.28	148.29	1
C10-C9-C8	123.29	93.30	1
C3-C1-C7	120.82	150.79	1
C5-C6-C7	121.27	151.24	1
C3-C1-C7	120.82	150.73	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C3-C4	120.78	90.92	1
C3-C1-C7	120.82	150.68	1
C6-C7-C8	118.28	148.08	1
C5-C6-C7	121.27	151.07	1
C5-C6-C7	121.27	151.06	1
C5-C6-C7	121.27	150.94	1
C3-C1-C7	120.82	150.48	1
C1-C3-C4	120.78	91.19	1
C3-C1-C7	120.82	150.40	1
C5-C6-C7	121.27	150.84	1
C3-C1-C7	120.82	150.39	1
C5-C6-C7	121.27	150.83	1
C10-C9-C8	123.29	93.79	1
C5-C6-C7	121.27	150.75	2
C5-C6-C7	121.27	150.74	1
C5-C6-C7	121.27	150.73	1
C5-C6-C7	121.27	150.72	1
C1-C3-C4	120.78	91.45	1
C5-C6-C7	121.27	150.55	1
C3-C1-C7	120.82	150.09	1
C5-C6-C7	121.27	150.54	1
C5-C6-C7	121.27	150.50	1
C5-C6-C7	121.27	150.49	1
C5-C6-C7	121.27	150.39	1
C3-C1-C7	120.82	149.94	1
C5-C6-C7	121.27	150.37	1
C5-C6-C7	121.27	150.29	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3-C1-C7	120.82	149.79	1
C5-C6-C7	121.27	150.20	1
C5-C6-C7	121.27	150.18	1
C5-C6-C7	121.27	150.14	1
C3-C1-C7	120.82	149.68	1
C5-C6-C7	121.27	150.12	1
C6-C7-C8	118.28	147.12	1
C3-C1-C7	120.82	149.64	1
C5-C6-C7	121.27	150.07	1
C3-C1-C7	120.82	149.61	1
C5-C6-C7	121.27	150.03	1
C5-C6-C7	121.27	150.01	1
C5-C6-C7	121.27	149.95	1
C5-C6-C7	121.27	149.83	1
C3-C1-C7	120.82	149.37	1
C3-C1-C7	120.82	149.36	1
C10-C9-C8	123.29	94.77	1
C5-C6-C7	121.27	149.70	1
C5-C6-C7	121.27	149.67	1
C5-C6-C7	121.27	149.66	1
C3-C1-C7	120.82	149.19	1
C5-C6-C7	121.27	149.61	1
C3-C1-C7	120.82	149.15	1
C5-C6-C7	121.27	149.57	1
C5-C6-C7	121.27	149.56	1
C3-C1-C7	120.82	149.08	2
C3-C1-C7	120.82	149.06	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C5-C6-C7	121.27	149.47	2
C3-C1-C7	120.82	149.00	1
C5-C6-C7	121.27	149.45	1
C3-C1-C7	120.82	148.97	1
C6-C5-O3	125.44	97.34	1
C3-C1-C7	120.82	148.89	1
C5-C6-C7	121.27	149.28	2
C3-C1-C7	120.82	148.81	1
C6-C5-O3	125.44	97.45	1
C5-C6-C7	121.27	149.25	2
C5-C6-C7	121.27	149.23	1
C3-C1-C7	120.82	148.72	1
C6-C7-C8	118.28	146.16	1
C5-C6-C7	121.27	149.13	1
C3-C1-C7	120.82	148.66	1
C6-C5-O3	125.44	97.65	1
C5-C6-C7	121.27	149.05	1
C5-C6-C7	121.27	149.04	1
C5-C6-C7	121.27	149.02	1
C3-C1-C7	120.82	148.56	1
C3-C1-C7	120.82	148.54	1
C6-C5-O3	125.44	97.76	1
C6-C5-O3	125.44	97.77	1
C5-C6-C7	121.27	148.88	1
C6-C5-O3	125.44	97.84	1
C10-C9-C8	123.29	95.71	1
C6-C7-C8	118.28	145.84	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3-C1-C7	120.82	148.37	1
C5-C6-C7	121.27	148.80	1
C5-C6-C7	121.27	148.79	1
C6-C7-C8	118.28	145.77	1
C6-C7-C8	118.28	145.73	1
C5-C6-C7	121.27	148.72	1
C5-C6-C7	121.27	148.71	1
C3-C1-C7	120.82	148.23	1
C5-C6-C7	121.27	148.67	1
C6-C5-O3	125.44	98.05	2
C3-C1-C7	120.82	148.15	1
C3-C1-C7	120.82	148.09	1
C6-C5-O3	125.44	98.23	1
C6-C5-O3	125.44	98.24	1
C6-C5-O3	125.44	98.25	1
C5-C6-C7	121.27	148.46	1
C6-C5-O3	125.44	98.32	1
C3-C1-C7	120.82	147.93	1
C6-C5-O3	125.44	98.34	2
C10-C9-C8	123.29	96.23	1
C5-C6-C7	121.27	148.32	1
C10-C9-C8	123.29	96.32	1
C5-C6-C7	121.27	148.23	1
C6-C5-O3	125.44	98.53	1
C3-C1-C7	120.82	147.72	1
C3-C1-C7	120.82	147.69	1
C6-C7-C8	118.28	145.09	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-C5-O3	125.44	98.66	1
C3-C1-C7	120.82	147.59	1
C3-C1-C7	120.82	147.57	1
C6-C5-O3	125.44	98.69	1
C6-C5-O3	125.44	98.74	1
C5-C6-C7	121.27	147.94	1
C5-C6-C7	121.27	147.93	1
C6-C5-O3	125.44	98.86	1
C6-C5-O3	125.44	98.88	2
C5-C6-C7	121.27	147.82	2
C3-C1-C7	120.82	147.34	1
C6-C5-O3	125.44	98.93	1
C10-C9-C8	123.29	96.81	1
C6-C5-O3	125.44	98.96	1
C6-C5-O3	125.44	98.97	1
C6-C5-O3	125.44	99.00	1
C6-C5-O3	125.44	99.01	1
C3-C1-C7	120.82	147.24	1
C6-C5-O3	125.44	99.05	1
C6-C5-O3	125.44	99.06	2
C3-C1-C7	120.82	147.19	1
C6-C5-O3	125.44	99.10	1
C10-C9-C8	123.29	97.05	1
C6-C5-O3	125.44	99.26	1
C6-C5-O3	125.44	99.27	2
C3-C1-C7	120.82	146.96	2
C6-C5-O3	125.44	99.34	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-C5-O3	125.44	99.35	1
C6-C5-O3	125.44	99.39	1
C5-C6-C7	121.27	147.30	1
C6-C5-O3	125.44	99.41	1
C3-C1-C7	120.82	146.84	1
C6-C5-O3	125.44	99.44	1
C6-C5-O3	125.44	99.45	1
C3-C1-C7	120.82	146.73	1
C6-C5-O3	125.44	99.53	2
C10-C9-C8	123.29	97.44	1
C6-C5-O3	125.44	99.61	1
C3-C1-C7	120.82	146.64	1
C6-C7-C8	118.28	144.07	1
C6-C5-O3	125.44	99.67	1
C6-C5-O3	125.44	99.69	1
C3-C1-C7	120.82	146.56	1
C6-C5-O3	125.44	99.72	1
C6-C5-O3	125.44	99.73	1
C6-C5-O3	125.44	99.75	1
C6-C5-O3	125.44	99.78	1
C6-C5-O3	125.44	99.81	2
C6-C5-O3	125.44	99.87	1
C6-C5-O3	125.44	99.88	1
C3-C1-C7	120.82	146.37	1
C3-C1-C7	120.82	146.36	1
C6-C5-O3	125.44	99.92	1
C6-C5-O3	125.44	99.99	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C10-C9-C8	123.29	97.86	1
C6-C5-O3	125.44	100.01	1
C6-C5-O3	125.44	100.02	2
C3-C1-C7	120.82	146.24	1
C6-C5-O3	125.44	100.03	1
C10-C9-C8	123.29	97.91	1
C6-C5-O3	125.44	100.08	2
C6-C5-O3	125.44	100.10	1
C6-C5-O3	125.44	100.12	1
C6-C5-O3	125.44	100.13	1
C6-C5-O3	125.44	100.14	1
C6-C5-O3	125.44	100.15	1
C6-C5-O3	125.44	100.16	1
C6-C5-O3	125.44	100.19	1
C6-C5-O3	125.44	100.21	1
C6-C5-O3	125.44	100.23	1
C6-C5-O3	125.44	100.24	2
C3-C1-C7	120.82	145.99	1
C6-C5-O3	125.44	100.27	1
C3-C1-C7	120.82	145.98	1
C6-C5-O3	125.44	100.31	1
C6-C7-C8	118.28	143.40	1
C6-C5-O3	125.44	100.32	1
C6-C5-O3	125.44	100.33	1
C3-C1-C7	120.82	145.92	1
C6-C5-O3	125.44	100.35	1
C3-C1-C7	120.82	145.89	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-C5-O3	125.44	100.37	1
C6-C5-O3	125.44	100.45	1
C6-C5-O3	125.44	100.46	2
C3-C1-C7	120.82	145.80	1
C6-C5-O3	125.44	100.49	1
C6-C5-O3	125.44	100.50	1
C3-C1-C7	120.82	145.75	1
C6-C5-O3	125.44	100.53	1
C3-C1-C7	120.82	145.72	1
C6-C5-O3	125.44	100.56	1
C6-C5-O3	125.44	100.57	1
C6-C5-O3	125.44	100.58	1
C3-C1-C7	120.82	145.62	2
C6-C5-O3	125.44	100.64	1
C6-C5-O3	125.44	100.66	1
C3-C1-C7	120.82	145.60	1
C6-C5-O3	125.44	100.67	3
C3-C1-C7	120.82	145.58	1
C6-C5-O3	125.44	100.70	1
C3-C1-C7	120.82	145.56	1
C6-C5-O3	125.44	100.71	2
C6-C5-O3	125.44	100.72	1
C6-C5-O3	125.44	100.73	1
C6-C5-O3	125.44	100.77	1
C6-C5-O3	125.44	100.78	2
C3-C1-C7	120.82	145.46	1
C6-C5-O3	125.44	100.80	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-C5-O3	125.44	100.83	1
C3-C1-C7	120.82	145.38	1
C6-C5-O3	125.44	100.88	1
C6-C5-O3	125.44	100.90	1
C6-C5-O3	125.44	100.91	1
C6-C5-O3	125.44	100.96	1
C6-C5-O3	125.44	101.00	1
C6-C5-O3	125.44	101.04	1
C6-C5-O3	125.44	101.06	2
C5-C6-C7	121.27	145.63	1
C6-C7-C8	118.28	142.64	1
C3-C1-C7	120.82	145.12	1
C10-C9-C8	123.29	99.06	1
C3-C1-C7	120.82	145.04	1
C6-C5-O3	125.44	101.28	1
C5-C6-C7	121.27	145.37	1
C3-C1-C7	120.82	144.87	1
C6-C5-O3	125.44	101.40	1
C6-C5-O3	125.44	101.59	1
C6-C5-O3	125.44	101.60	1
C3-C1-C7	120.82	144.65	1
C10-C9-C8	123.29	99.48	1
C3-C1-C7	120.82	144.63	1
C6-C5-O3	125.44	101.72	1
C5-C6-C7	121.27	144.98	1
C3-C1-C7	120.82	144.18	1
C3-C1-C7	120.82	144.16	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C3-C1-C7	120.82	144.04	1
C3-C1-C7	120.82	143.72	1
C3-C1-C7	120.82	143.68	1
C3-C1-C7	120.82	143.62	1
C3-C1-C7	120.82	143.24	1
C3-C1-C7	120.82	142.98	1
C3-C1-C7	120.82	142.73	1
C6-C7-C8	118.28	139.69	1
C3-C1-C7	120.82	141.83	1
C10-C9-C8	123.29	102.70	1
C6-C7-C8	118.28	138.60	1
C6-C7-C8	118.28	138.46	1
C10-C9-C8	123.29	103.14	1
C6-C7-C8	118.28	138.29	1
C1-C7-C8	123.49	143.50	1
C3-C1-C7	120.82	140.63	1
C10-C9-C8	123.29	103.84	1
C6-C7-C8	118.28	137.69	1
C10-C9-C8	123.29	103.89	1
C1-C7-C8	123.49	142.61	1
C10-C9-C8	123.29	104.75	1
C3-C1-C7	120.82	139.23	1
C3-C1-C7	120.82	139.17	1
C10-C9-C8	123.29	105.84	2
C1-C7-C8	123.49	140.87	1
C6-C7-C8	118.28	135.65	1
C5-C4-O4	111.56	94.43	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C10-C9-C8	123.29	106.22	1
C6-C7-C8	118.28	101.46	1
C1-C7-C8	123.49	140.26	1
C10-C9-C8	123.29	106.54	1
C1-C7-C8	123.49	140.14	1
C10-C9-C8	123.29	106.65	1
C6-C7-C8	118.28	134.76	1
C6-C7-C8	118.28	134.74	1
C10-C9-C8	123.29	107.00	1
C1-C7-C8	123.49	139.76	1
C1-C7-C8	123.49	139.60	1
C3-C4-O4	107.92	123.54	1
C6-C7-C8	118.28	133.85	1
C3-C4-O4	107.92	123.35	1
C10-C9-C8	123.29	108.01	1
C10-C9-C8	123.29	108.03	2
C1-C7-C8	123.49	138.72	1
C3-C4-O4	107.92	122.99	1
C10-C9-C8	123.29	108.27	1
C4-C5-C6	111.30	126.25	1
C3-C4-O4	107.92	122.87	1
C6-C7-C8	118.28	103.71	1
C3-C4-O4	107.92	122.47	1
C3-C4-O4	111.32	125.82	1
C3-C4-O4	107.92	122.29	1
C3-C4-O4	107.92	122.22	1
C6-C7-C8	118.28	104.01	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C1-C7-C8	123.49	137.52	1
C3-C4-O4	107.92	121.93	1
C3-C4-O4	107.92	121.87	1
C3-C4-O4	107.92	121.83	1
C4-C5-O5	110.66	124.55	1
C1-C7-C8	123.49	137.31	1
C6-C5-O5	107.61	121.39	1
C3-C4-O4	107.92	121.64	1
C3-C4-O4	107.92	121.58	1
C3-C4-O4	107.92	121.52	1
C6-C5-O5	108.00	94.45	1
C1-C7-C8	123.49	137.01	1
C6-C7-C8	118.28	104.89	1
C4-C5-O5	109.55	122.90	1
C3-C4-O4	107.92	121.24	1
C1-C7-C8	123.49	136.79	2
C3-C4-O4	107.92	121.21	1
C10-C9-C8	123.29	110.01	1
C3-C4-O4	107.92	121.20	1
C3-C4-O4	107.92	121.19	1
C6-C5-O5	107.61	120.82	1
C6-C7-C8	118.28	105.13	1
C6-C5-O5	107.61	120.70	1
C2-C1-O5	109.74	96.70	1
C1-C7-C8	123.49	136.50	1
C3-C4-O4	107.92	120.88	1
C3-C4-O4	107.92	120.87	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-C7-C8	118.28	105.34	1
C6-C7-C8	118.28	105.40	1
C3-C4-O4	107.92	120.79	1
C3-C4-O4	107.92	120.72	1
C4-C5-O5	109.57	122.31	1
C3-C4-O4	107.92	120.64	1
C6-C7-C8	118.28	105.60	1
C1-C7-C8	123.49	136.14	1
C3-C4-O4	107.92	120.50	1
C5-C4-O4	111.56	98.98	1
C3-C4-O4	107.92	120.46	1
C3-C4-O4	107.92	120.43	1
C3-C4-O4	107.92	120.36	1
C3-C4-O4	107.92	120.30	1
C3-C4-O4	107.92	120.29	1
C3-C4-O4	107.92	120.27	1
C3-C4-O4	107.92	120.26	1
C3-C4-O4	107.92	120.25	1
C3-C4-O4	107.92	120.20	1
C2-C1-O5	109.74	97.46	1
C10-C9-C8	123.29	111.02	1
C5-C4-O4	111.56	99.29	1
C1-C7-C8	123.49	135.75	1
C3-C4-O4	107.92	120.18	2
C1-C2-C3	109.27	121.50	1
C3-C4-O4	107.92	120.14	1
C6-C7-C8	118.28	106.08	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C6-C7-C8	118.28	106.09	1
C6-C7-C8	118.28	130.46	1
C3-C4-O4	107.92	120.09	1
C6-C5-O5	108.00	95.87	1
C3-C4-O4	107.92	120.04	1
C1-C7-C8	123.49	135.57	1
C10-C9-C8	123.29	111.22	1
C6-C7-C8	118.28	106.21	1
C1-C7-C8	123.49	135.52	1
C3-C4-O4	107.92	119.95	1
C1-C7-C8	123.49	135.51	1
C3-C4-O4	107.92	119.94	1
O3-C2-H2	94.55	106.56	1
O3-C2-H2	94.51	106.56	1
O3-C2-H2	94.28	106.56	2
O3-C2-H2	94.25	106.56	1
O3-C2-H2	94.10	106.56	1
C2-O2-HO2	95.33	107.84	1
O3-C2-H2	94.01	106.56	1
O3-C2-H2	93.98	106.56	1
O3-C2-H2	93.97	106.56	1
O3-C2-H2	93.89	106.56	2
O3-C2-H2	93.88	106.56	1
O3-C2-H2	93.85	106.56	1
O3-C2-H2	93.81	106.56	1
O3-C2-H2	93.77	106.56	1
O3-C2-H2	93.75	106.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3-C2-H2	93.72	106.56	2
O3-C2-H2	93.67	106.56	1
O3-C2-H2	93.64	106.56	1
O3-C2-H2	93.61	106.56	1
O3-C2-H2	93.55	106.56	1
O3-C2-H2	93.41	106.56	1
O3-C2-H2	93.37	106.56	1
O3-C2-H2	93.36	106.56	1
O3-C2-H2	93.29	106.56	1
C6-C5-H5	96.02	109.32	1
O3-C2-H2	93.26	106.56	1
O3-C2-H2	93.23	106.56	1
O3-C2-H2	93.19	106.56	1
O3-C2-H2	93.17	106.56	1
O3-C2-H2	93.12	106.56	2
O3-C2-H2	93.04	106.56	1
O3-C2-H2	93.03	106.56	1
O3-C2-H2	93.02	106.56	1
O3-C2-H2	92.99	106.56	1
O3-C2-H2	92.95	106.56	1
O3-C2-H2	92.92	106.56	1
O3-C2-H2	92.69	106.56	1
O3-C2-H2	92.68	106.56	1
O3-C2-H2	92.67	106.56	1
O3-C2-H2	92.48	106.56	1
O3-C2-H2	92.43	106.56	2
O3-C2-H2	92.30	106.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3-C2-H2	92.26	106.56	1
O3-C2-H2	92.23	106.56	1
O3-C2-H2	92.19	106.56	1
O3-C2-H2	92.18	106.56	1
O3-C2-H2	92.06	106.56	2
O3-C2-H2	91.91	106.56	1
O3-C2-H2	91.87	106.56	1
O3-C2-H2	91.86	106.56	1
O3-C2-H2	91.78	106.56	1
O3-C2-H2	91.75	106.56	1
O3-C2-H2	91.57	106.56	1
O3-C2-H2	91.48	106.56	1
O3-C2-H2	91.46	106.56	1
O3-C2-H2	91.44	106.56	1
O3-C2-H2	91.28	106.56	1
O3-C2-H2	91.13	106.56	1
O3-C2-H2	90.94	106.56	1
O3-C2-H2	90.87	106.56	1
O3-C2-H2	90.51	106.56	1
O3-C2-H2	90.18	106.56	1
O3-C2-H2	90.07	106.56	1
O3-C2-H2	89.92	106.56	1
O3-C2-H2	89.79	106.56	1
O3-C2-H2	89.77	106.56	1
O3-C2-H2	89.68	106.56	1
O3-C2-H2	89.67	106.56	1
O3-C2-H2	89.64	106.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3-C2-H2	89.61	106.56	1
O3-C2-H2	89.38	106.56	1
O3-C2-H2	89.34	106.56	1
O3-C2-H2	89.17	106.56	1
O3-C2-H2	89.14	106.56	1
O3-C2-H2	89.13	106.56	1
O3-C2-H2	89.12	106.56	1
O3-C2-H2	89.08	106.56	1
O3-C2-H2	89.05	106.56	1
O3-C2-H2	88.91	106.56	1
O3-C2-H2	88.80	106.56	1
O3-C2-H2	88.63	106.56	1
O3-C2-H2	88.62	106.56	1
O3-C2-H2	88.56	106.56	1
O3-C2-H2	88.55	106.56	1
O3-C2-H2	88.40	106.56	1
O3-C2-H2	88.37	106.56	1
O3-C2-H2	88.33	106.56	1
O3-C2-H2	88.32	106.56	1
O3-C2-H2	88.31	106.56	1
O3-C2-H2	88.00	106.56	1
O3-C2-H2	87.68	106.56	1
O3-C2-H2	87.67	106.56	1
O3-C2-H2	87.22	106.56	1
O3-C2-H2	86.89	106.56	2
O3-C2-H2	86.85	106.56	1
O3-C2-H2	86.84	106.56	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
O3-C2-H2	86.80	106.56	1
O3-C2-H2	86.64	106.56	1
O3-C2-H2	85.68	106.56	1
O3-C2-H2	84.98	106.56	1
O3-C2-H2	84.95	106.56	1
O3-C2-H2	84.86	106.56	1
O3-C2-H2	84.35	106.56	1
C7-C6-H6	95.41	118.72	1
C7-C6-H6	95.25	118.72	1
C7-C6-H6	95.09	118.72	1
C7-C6-H6	94.70	118.72	1
C7-C6-H6	94.60	118.72	1
C7-C6-H6	94.39	118.72	1
C7-C6-H6	94.32	118.72	1
C7-C6-H6	94.00	118.72	1
C7-C6-H6	93.74	118.72	1
C7-C6-H6	93.56	118.72	1
C7-C6-H6	93.52	118.72	1
C7-C6-H6	93.39	118.72	1
C7-C6-H6	93.36	118.72	1
C7-C6-H6	93.31	118.72	1
C7-C6-H6	93.13	118.72	1
C7-C6-H6	93.06	118.72	1
C7-C6-H6	92.99	118.72	1
C7-C6-H6	92.86	118.72	1
C7-C6-H6	92.83	118.72	1
C7-C6-H6	92.80	118.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C7-C6-H6	92.78	118.72	1
C7-C6-H6	92.71	118.72	1
C7-C6-H6	92.69	118.72	1
C7-C6-H6	92.64	118.72	1
C7-C6-H6	92.60	118.72	1
C7-C6-H6	92.54	118.72	1
C7-C6-H6	92.48	118.72	1
C7-C6-H6	92.42	118.72	1
C7-C6-H6	92.33	118.72	1
C7-C6-H6	92.27	118.72	1
C7-C6-H6	92.15	118.72	2
C7-C6-H6	92.13	118.72	1
C7-C6-H6	91.85	118.72	1
C7-C6-H6	91.81	118.72	1
C7-C6-H6	91.69	118.72	1
C7-C6-H6	91.51	118.72	1
C7-C6-H6	91.49	118.72	1
C7-C6-H6	91.44	118.72	1
C7-C6-H6	91.37	118.72	1
C7-C6-H6	91.24	118.72	1
C7-C6-H6	91.06	118.72	2
C7-C6-H6	91.03	118.72	1
C7-C6-H6	90.87	118.72	1
C7-C6-H6	90.86	118.72	1
C7-C6-H6	90.77	118.72	1
C7-C6-H6	90.70	118.72	1
C7-C6-H6	90.65	118.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C7-C6-H6	90.62	118.72	1
C7-C6-H6	90.58	118.72	1
C7-C6-H6	90.55	118.72	2
C7-C6-H6	90.53	118.72	1
C7-C6-H6	90.50	118.72	1
C7-C6-H6	90.45	118.72	1
C7-C6-H6	90.43	118.72	1
C7-C6-H6	90.41	118.72	1
C7-C6-H6	90.34	118.72	1
C7-C6-H6	90.26	118.72	1
C7-C6-H6	90.23	118.72	1
C7-C6-H6	90.16	118.72	1
C7-C6-H6	90.14	118.72	1
C7-C6-H6	90.05	118.72	1
C7-C6-H6	90.01	118.72	1
C7-C6-H6	90.00	118.72	1
C7-C6-H6	89.91	118.72	1
C7-C6-H6	89.89	118.72	1
C7-C6-H6	89.80	118.72	1
C7-C6-H6	89.77	118.72	1
C7-C6-H6	89.72	118.72	1
C7-C6-H6	89.65	118.72	1
C7-C6-H6	89.62	118.72	1
C7-C6-H6	89.59	118.72	1
C7-C6-H6	89.57	118.72	1
C7-C6-H6	89.53	118.72	1
C7-C6-H6	89.46	118.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C7-C6-H6	89.45	118.72	1
C7-C6-H6	89.38	118.72	1
C7-C6-H6	89.37	118.72	1
C7-C6-H6	89.36	118.72	1
C7-C6-H6	89.27	118.72	1
C7-C6-H6	89.24	118.72	1
C7-C6-H6	89.22	118.72	1
C7-C6-H6	89.20	118.72	1
C7-C6-H6	89.13	118.72	2
C7-C6-H6	89.09	118.72	1
C7-C6-H6	88.95	118.72	1
C7-C6-H6	88.92	118.72	1
C7-C6-H6	88.82	118.72	1
C7-C6-H6	88.80	118.72	1
C7-C6-H6	88.78	118.72	1
C7-C6-H6	88.73	118.72	1
C7-C6-H6	88.71	118.72	2
C7-C6-H6	88.63	118.72	2
C7-C6-H6	88.60	118.72	1
C7-C6-H6	88.53	118.72	1
C7-C6-H6	88.45	118.72	1
C7-C6-H6	88.41	118.72	1
C7-C6-H6	88.40	118.72	1
C7-C6-H6	88.35	118.72	1
C7-C6-H6	88.31	118.72	1
C7-C6-H6	88.12	118.72	1
C7-C6-H6	87.93	118.72	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
C7-C6-H6	87.58	118.72	1
C7-C6-H6	87.21	118.72	1
C7-C6-H6	87.07	118.72	1
C7-C6-H6	86.28	118.72	1
C7-C6-H6	86.18	118.72	1
C7-C6-H6	85.71	118.72	1
C7-C6-H6	85.63	118.72	1
C7-C6-H6	84.74	118.72	1

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	0.0	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	0	0	0	0

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	0	0	0	0

Detailed list of outliers are tabulated below.

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.

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