

Using a Conformationally-Dependent Stereochemical Library Improves Crystallographic Refinement of Proteins – Supplemental Information

Table 1. *List of protein chains used in Figure 1.* 35 protein chains in each 0.1 Å resolution bin were selected from the PDBselect 25 list of Protein Databank entries. A chain name of “_” indicates the chain name was blank in the entry. Each column contains the indicated resolution bin.

1.0	1.1	1.2	1.3	1.4	1.5	1.6
1a6m	_	1bkr	A	1bx7	_	1cy5
1c7k	A	1c5e	A	1cse	I	1dcs
1eb6	A	1ctj	_	1fy6	A	1dg6
1g2y	B	1f86	A	1i24	A	1es9
1ga6	A	1gmx	A	1j98	A	1f9v
1gkm	A	1h4g	B	1knm	A	1flm
1jfb	A	1kt6	A	1lf7	A	1g61
1lkk	A	1l3k	A	1m15	A	1gk9
1lni	A	1ls1	A	1me4	A	1gk9
1mn8	D	1oh0	A	1nww	B	1hyo
1ms0	B	1qj4	A	1nz0	D	1i0d
1nqj	A	1ql0	A	1o08	A	1jcd
1o7j	A	1qlw	B	1o7i	B	1jhg
1oai	A	1qv1	A	1obo	A	1jl1
1od3	A	1r0r	I	1qu9	A	1ka1
1q6z	A	1rg8	A	1r5y	A	1lq9
1tt8	A	1su8	A	1ryo	A	1nxm
1y55	X	1t2d	A	1sen	A	1o2d
1zk4	A	1t8k	A	1tqw	A	1o7q
2a6z	A	1uz3	B	1tu9	A	1o8x
2chh	A	1yfq	A	1ucr	B	1oqv
2cnq	A	1ys1	X	1usm	A	1qdd
2cws	A	1z2u	A	1v8h	A	1qwy
2erl	_	1zl0	A	1vk1	A	1r29
2ggc	A	2abs	A	1vr7	B	1rut
2h3l	B	2agy	D	1w6s	B	1tjy
2i4a	A	2aib	A	1wc2	A	1ucd
2iim	A	2bhu	A	1wm3	A	1use
1cc8	A	2cal	A	1wn2	A	1v70
1cxq	A	2igd	_	1wxc	A	1w2l
1i27	A	1jm1	A	1wxc	B	1wew
1mfm	A	1g2b	A	1xdn	A	1wvf
1qtw	A	1jf8	A	1ymt	A	1xeo
1rw1	A	1k7c	A	1z0w	A	1yg9
1kqp	A	1lu4	A	1z2n	X	1zce

1.7		1.8		1.9		2.0		2.1		2.2		2.3	
1aqz	A	1a92	D	1alu	-	1aly	-	1c28	C	1b4u	A	1a2x	B
1ay7	B	1bb1	A	1at0	-	1aol	-	1cq	A	1b4u	B	1aux	A
1ddw	A	1dow	B	1b0n	B	1bbp	A	1d7k	A	1bg8	A	1b33	N
1ecs	A	1dqe	A	1dfn	A	1bys	A	1ehy	A	1c9k	C	1byl	A
1f3u	D	1fs1	A	1ef1	C	1clv	I	1fjm	A	1cty	-	1cr5	C
1flt	X	1g55	A	1emu	A	1d2z	D	1g3j	C	1de5	B	1ea3	A
1fvk	A	1gbg	-	1f08	B	1d3b	C	1gp4	A	1del	A	1f3m	A
1h03	P	1h7c	A	1fip	A	1d3b	L	1i4z	A	1dev	B	1f6f	A
1h6f	B	1her	A	1fle	I	1dqt	A	1j1v	A	1dku	A	1fjr	A
1h75	A	1jid	A	1gl2	A	1dtj	B	1k61	A	1dp5	B	1g2c	B
1hz6	B	1kp6	A	1gl2	C	1dvo	A	1l1n	B	1em2	A	1g2c	O
1j2l	A	1kvd	A	1gl2	D	1eq2	H	1ngn	A	1leys	C	1gtq	A
1j8f	A	1kvd	B	1jdh	B	1ezi	A	1otg	A	1leys	H	1gzs	D
1jos	A	1lbu	-	1jhs	A	1fc3	A	1qqh	A	1fl1	B	1h3o	A
1k94	A	1lc7	A	1jyo	A	1h6k	Z	1rmd	-	1fro	A	1iad	-
1m9x	D	1luz	A	1k3s	B	1h8e	I	1rp1	-	1fuj	A	1iar	B
1mxi	A	1lxj	A	1lsl	A	1hbk	A	1rz4	A	1g43	A	1ik7	A
1n0w	B	1m4d	A	1neu	-	1hjl	A	1s3t	B	1grj	-	1jlk	A
1nep	A	1mwp	A	1nh2	C	1hyb	A	1s7m	D	1hf2	A	1jsu	C
1nrj	A	1nkp	E	1q8b	A	1i7w	D	1t4w	A	1i8n	A	1kil	E
1osy	B	1no5	B	1q8r	B	1jeo	A	1tue	A	1igu	B	1kr2	F
1p3q	Q	1ojh	J	1qa7	A	1ku0	B	1un1	B	1im3	D	1l1s	A
1pby	C	1q8d	A	1qou	B	1lld	A	1vf6	B	1iwn	A	1l6l	8
1pfv	A	1qkq	A	1qqp	4	1lhv	A	1vf6	D	1jc5	F	1mhm	B
1q2h	A	1qpa	A	1qr0	A	1m5i	A	1vj7	A	1jlx	A	1n0l	D
1qst	A	1ro7	A	1qzm	A	1mbm	D	1vjh	A	1jmt	A	1n9w	A
1rh6	B	1sc3	B	1r8h	C	1mby	A	1vjq	A	1jyb	A	1o5l	A
1s5u	G	1tf1	D	1reg	Y	1mi8	A	1vk0	A	1k1f	A	1p19	D
1t0b	G	1v54	G	1rk8	C	1mki	A	1w3n	A	1n69	B	1pv1	A
1t1j	B	1v54	H	1ryp	L	1mzg	B	1wy9	A	1nf2	A	1q67	B
1t2b	A	1v54	I	1sfp	-	1mzw	B	1xeq	B	1nmp	A	1qdn	C
1t82	D	1v54	J	1sq9	A	1n2d	C	1xg8	A	1o6b	A	1r1v	A
1tsf	A	1v54	K	1ta9	B	1ni9	A	1zmq	A	1ohz	B	1r4a	E
1u5d	B	1v54	L	1u0s	A	1nkz	A	1zx2	B	1png	-	1r5x	A
1ub4	A	1vm0	A	1ua8	A	1nlw	D	2a06	I	1pug	A	1ro5	A

2.4	2.5	2.6	2.7	2.8	2.9	3.0							
1avq	C	1a5o	A	1avg	I	1a02	F	1ao0	A	1bnl	A	1adu	A
1b35	A	1a7j	-	1bh9	A	1b87	A	1avo	A	1c9i	B	1b26	A
1b35	D	1aih	B	1c4r	A	1bxn	I	1avo	B	1cja	A	1b9x	A
1b55	A	1b4a	A	1c7z	A	1csg	A	1bqh	G	1cqj	B	1b9y	C
1bt6	A	1bcr	B	1cf7	A	1cui	-	1cid	-	1dfc	B	1bev	3
1cnt	2	1bdf	D	1cf7	B	1dml	B	1cma	A	1es7	B	1bh8	B
1eai	C	1byk	A	1dk4	A	1dt9	A	1f2n	C	1f02	T	1bu2	A
1ep2	B	1cc5	-	1i78	B	1ecx	A	1f45	A	1f7v	A	1c4t	A
1ern	B	1d2p	A	1jkw	-	1exc	A	1fhf	A	1fbv	A	1cjk	A
1f7c	A	1ewa	A	1kcg	C	1fbm	A	1g23	A	1fg9	C	1d2h	A
1gsq	-	1f5q	D	1ksj	B	1fuo	A	1gg3	A	1ft4	B	1d6m	A
1gyw	A	1fl9	A	1ltb	C	1gme	A	1gn1	D	1h6o	A	1dch	A
1h3q	A	1gk0	B	1ml8	A	1gxb	D	1gvm	D	1h79	A	1e0j	B
1hg4	C	1guo	C	1nay	B	1gxc	A	1i1a	C	1hlm	-	1equ	A
1hul	A	1hl6	D	1p65	A	1hcf	X	1is7	K	1hm7	B	1exj	A
1i1r	B	1hm8	A	1pd3	A	1hq6	A	1jik	A	1hwh	A	1f51	B
1iah	A	1hup	-	1q3i	A	1i3s	A	1jmu	A	1hwh	B	1f5t	A
1id1	A	1j0r	A	1r1i	A	1i4l	B	1jx7	A	1j4u	A	1f7	B
1ifq	A	1j9a	A	1r6a	A	1i69	A	1k3e	A	1j7v	R	1fq1	A
1jog	A	1jb0	I	1r8l	A	1i9b	A	1kqg	B	1jdn	A	1fze	C
1me5	C	1jb0	J	1sf8	H	1ioi	A	1l8o	A	1jk9	B	1fze	D
1mg3	D	1jb0	L	1sg3	B	1ipk	B	1lbum	A	1jwa	D	1g88	C
1no1	A	1jb0	M	1skv	B	1kf6	B	1lia	A	1kmi	Z	1gnh	A
1oq9	A	1jnz	B	1ss9	A	1kf6	C	1m3w	A	1l0a	A	1gqw	B
1pj5	A	1k4j	A	1tex	C	1kf6	D	1m6x	A	1l0o	A	1grc	B
1qmt	A	1luj	B	1w0c	D	1kp0	A	1mdy	A	1l0o	C	1gtp	A
1qzq	B	1lzw	A	1wpr	A	1mhz	B	1mhd	A	1l9a	A	1h56	A
1rty	A	1lzw	B	1wv4	B	1mhz	G	1mpy	A	1ln2	A	1h6v	C
1sfj	A	1m3e	B	1ww1	B	1ncn	A	1n0f	C	1n8b	A	1he8	A
1t94	A	1nf1	A	1xl4	A	1nlt	A	1n7i	B	1nbq	A	1hlg	A
1u10	C	1o51	A	1xpq	D	1ns1	C	1nlx	A	1nen	D	1hux	A
1u5z	A	1ofh	G	1ymf	A	1o7d	E	1nsk	L	1nrx	A	1t83	C
1umi	A	1oo5	A	1ymy	A	1ofq	B	1nub	A	1ocz	E	1ijd	B
1vp7	F	1oqe	K	1z9h	A	1p73	C	1nwn	A	1ocz	M	1io4	A
1vyq	A	1p5c	A	2a41	C	1pex	-	1nxh	A	1oft	A	1ism	A

Fig. 1. **Agreement of existing model's main chain bond lengths with the CSD-X library and the CDL as a function of resolution.** The median rmsd of main chain bond lengths from the CSD-X library (blue squares) and the CDL (red circles) for 35 protein chains in each 0.1 Å resolution shell are plotted as a function of resolution.

All Backbone Bonds

