Statistical Learning of Protein Elastic Network from Positional Covariance Matrix

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Table 1: List of protein structures in constructing homologous ensemble for RT. All structures in this work are solved by X-ray diffraction.

PDB ID	Chain	Resolution	Ligand
1a0h	B	3.2	0G6,NAG
1a0j	A	1.7	BEN,CA,SO4
1a0l	A	3	APA
1a5i	A	2.9	0GJ
1acb	E	2	
1ao5	A	2.6	NAG
1avw	A	1.75	CA
1azz	A	2.3	
1bda	A	3.35	2Z0
1bml	A	2.9	
1bqy	A	2.5	0GJ
1bru	P	2.3	1NB
1c1m	A	2.2	CA,SO4,XE
1dx5	M	2.3	0GJ,CA,FMT,NA,NAG
1ekb	B	2.3	0QE,LYK,ZN
1elt	A	1.61	CA
1euf	A	2.4	NAG,PO4
1fiz	A	2.9	BMA,FUL,NAG,NDG,PBZ,SO4
1fuj	A	2.2	FUC,NAG
1fxy	A	2.15	0G6
1npm	A	2.1	NAG
1o5e	H	1.75	132
1op2	A	2.1	NAG,SO4
1pfx	C	3	0G6,BHD,CGU
1pjp	A	2.2	0QE,HPH,NAG,ZN
1pyt	C	2.35	CA,ZN
1sgf	G	3.15	NAG,ZN
1spj	A	1.7	ACY,CA,NAG
1ton	A	1.8	ZN
1trn	A	2.2	ISP,PTR
1ym0	A	2.06	FUC,MAN,MG,NAG,PCA,SO4
2aip	A	1.65	ACT,GOL,NAG,SO4
2eek	A	1.85	BEN,CA,NA
2f91	A	1.2	CD,CL
2f9n	A	1.6	ACE,AR7,BU3,FUC,NAG
2psx	A	2.3	ACE,AR7,NAG
2pux	B	2	NAG

Table 1: Continued on the previous page.

PDB ID	Chain	Resolution	Ligand
2qxg	A	2.6	K7I
2tbs	A	1.8	BEN,CA
2vnt	A	2.2	QGG,SO4
2zch	P	2.83	CL,NDG,PO4
3bg8	A	1.6	BEN,G0R,SO4
3e0n	B	1.7	ARM,DPN,GOL,SO4
3ela	H	2.2	0Z6,CA,FUC,GLC
3qk1	A	2.08	BEN,CA,EDO,GOL,IMD,SO4
3s69	A	1.43	CA
3s9a	A	1.9	NAG
3tgi	E	1.8	CA,SO4
3uwi	A	1.43	ANH,CA,EDO,GOL,SO4
3w94	A	2	
4dg4	A	1.4	CA,SO4
4dgj	A	1.9	
4e7n	A	1.75	GOL,NAG
4gso	A	2.6	
4iw4	E	3.2	
4nfe	A	1.9	BEN,SO4
4niv	A	1	CA,GOL
5f8t	A	1.75	MRZ,SO4
5gvt	A	2.61	BMA,MAN
5jbb	S	1.56	0GJ,CA,DMS
5lhn	A	2.55	EDO,SO4
5lpe	A	2.65	SO4,ZN
5lyo	A	2.5	SO4
5ms3	A	2.3	CA
5zfh	A	1.93	
6pxj	B	1.7	GOL,MG
6qfg	A	1.68	GOL,J08

Table 2: List of protein structures in constructing homologous ensemble of DEDDh family of exonucleases. All structures in this work are solved by X-ray diffraction.

PDB ID	Chain	Resolution	Ligand
6a45	AB	1.9	PO4
1y97	AB	2.5	MSE
3mxj	BA	1.95	
5ywu	AB	3.4	MG
5yws	AB	2	MG
6w10	AB	1.8	
3mxi	BA	2.55	CA
2oa8	AB	2.1	CA,MSE
2ioc	BA	2.1	D5M,MN,MSE
3mxm	BA	1.75	CA,IOD
2o4i	AB	3.5	
3u6f	BA	2.3	BU1,MG
3u3y	BA	2.28	BU1,CA