

**SUPPLEMENT 1          PDBID-LIST OF 72  
CRYSTAL STRUCTURES OF THE N37S MUTANT  
OF HIV-1 PROTEASE**

1upj  
2zga  
1ajv  
1ajx  
1c70  
1d4h  
1d4i  
1d4j  
1dif  
1ebw  
1ebz  
1ec0  
1ec1  
1ec2  
1ec3  
1g2k  
1g35  
1gno  
1hbv  
1hfh  
1hos  
1hps  
1hpx  
1hpx  
1hsg  
1htf  
1htg  
1hvi  
1hvj  
1hvk  
1hvl  
1hxb  
1iiq  
1m0b  
1nh0  
1npa  
1npv  
1npw  
1ohr  
1sp5  
1t7k  
1u8g  
1w5v  
1w5w  
1w5x  
1w5y  
1wbk  
1wbm  
1x12  
1x15  
2a4f  
2bb9

2bbb  
2bpv  
2bpy  
2bpz  
2bqv  
2cej  
2cem  
2cen  
2pqz  
2pwc  
2pwr  
2qnn  
2qnp  
2qnp  
2qnx  
2uy0  
3bgb  
3bgc  
3bhe  
7upj

**SUPPLEMENT 2      STATISTICAL ANALYSIS  
OF REPRESENTATIVE 60 PAIRS IDENTIFIED BY  
KOSLOFF AND KOLODNY (2008)**

ACC, SN, SP, and MCC computed against each of the three golden standards (the ANGL\_CORE, ANGL, and ANGL\_SUPP regions).

**Table S1.** Accuracy (ACC)

Golden Standards	D <sup>2</sup> coding (%)	PB coding (%)	DSSP coding (%)
ANGL_CORE	88.7	86.4	86.0
ANGL	86.4	85.1	84.5
ANGL_SUPP	57.6	59.7	58.3

**Table S2.** Sensitivity (SN)

Golden Standards	D <sup>2</sup> coding (%)	PB coding (%)	DSSP coding (%)
ANGL_CORE	65.6	78.2	63.1
ANGL	52.3	59.9	52.3
ANGL_SUPP	24.1	29.0	26.8

**Table S3.** Specificity (SP)

Golden Standards	D <sup>2</sup> coding (%)	PB coding (%)	DSSP coding (%)
ANGL_CORE	90.3	86.4	87.4
ANGL	92.8	88.7	89.9
ANGL_SUPP	95.4	91.3	92.7

**Table S4.** Matthews correlation coefficient (MCC)

Golden Standards	D <sup>2</sup> coding (%)	PB coding (%)	DSSP coding (%)
ANGL_CORE	42.9	43.7	36.8
ANGL	44.9	43.6	40.5
ANGL_SUPP	24.5	23.9	24.