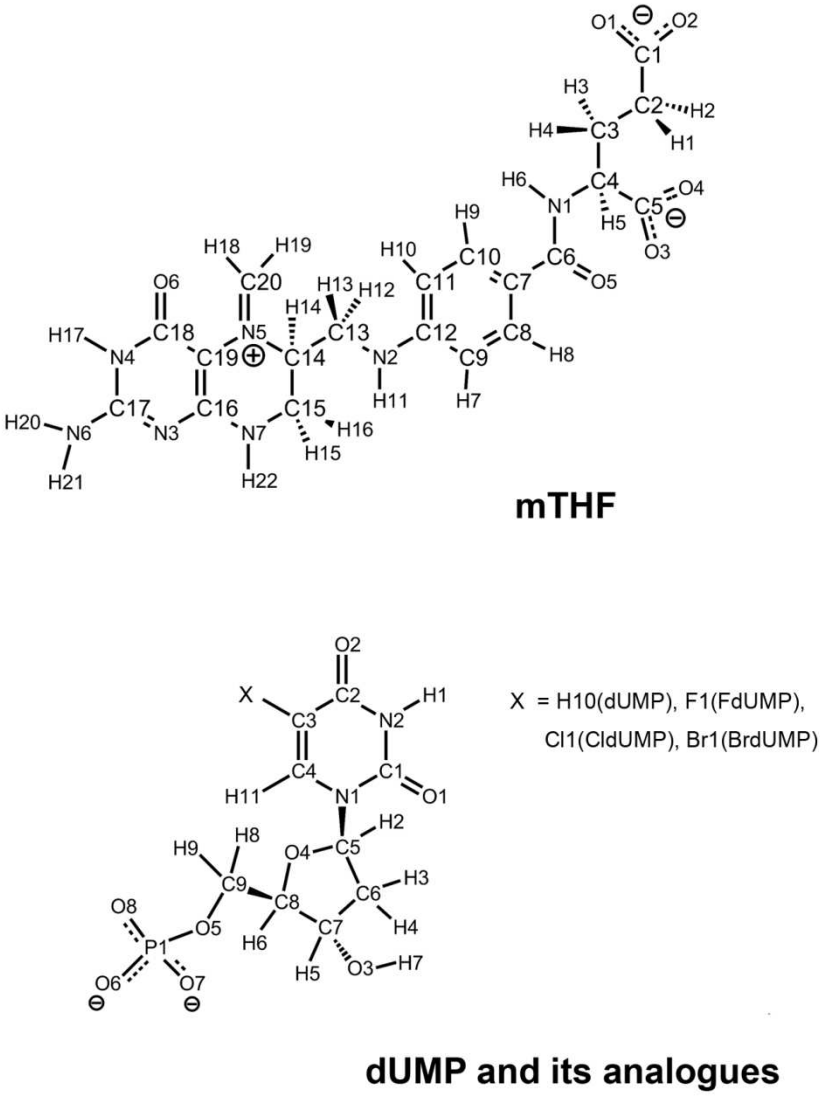

Figure S1 Chemical structures of mTHF and dUMP and its analogues

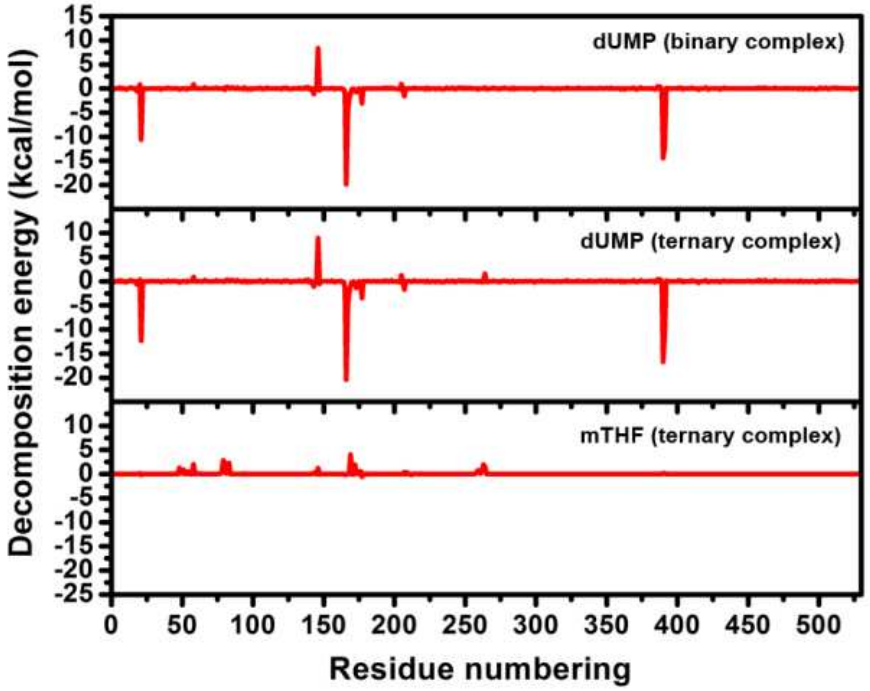

Figure S2. Decomposition energy on a pairwise per-residue basis for all the TS residues in the binding of dUMP and mTHF in the binary and ternary complexes

Table S1 Atom names, atom types, and partial atomic charges (q) of mTHF and dUMP and its analogues

mTHF			dUMP			FdUMP			CldUMP			BrdUMP		
Atom name	**Atom type**	**q**	**Atom name**	**Atom type**	**q**	**Atom name**	**Atom type**	**q**	**Atom name**	**Atom type**	**q**	**Atom name**	**Atom type**	**q**
O1	O2	-0.937	**O6**	O2	-0.852	**O6**	O2	-0.848	**O6**	O2	-0.849	**O6**	O2	-0.845
C1	C	1.042	**P1**	P	1.208	**P1**	P	1.205	**P1**	P	1.218	**P1**	P	1.211
O2	O2	-0.937	**O7**	O2	-0.852	**O7**	O2	-0.848	**O7**	O2	-0.849	**O7**	O2	-0.845
C2	CT	-0.300	**O8**	O2	-0.852	**O8**	O2	-0.848	**O8**	O2	-0.849	**O8**	O2	-0.845
H1	HC	0.045	**O5**	OS	-0.581	**O5**	OS	-0.589	**O5**	OS	-0.601	**O5**	OS	-0.601
H2	HC	0.045	**C9**	CT	0.151	**C9**	CT	0.174	**C9**	CT	0.174	**C9**	CT	0.187
C3	CT	0.296	**H8**	H1	0.027	**H8**	H1	0.022	**H8**	H1	0.023	**H8**	H1	0.024
H3	HC	-0.034	**H9**	H1	0.027	**H9**	H1	0.022	**H9**	H1	0.023	**H9**	H1	0.024
H4	HC	-0.034	**C8**	CT	0.080	**C8**	CT	0.084	**C8**	CT	0.080	**C8**	CT	0.086
C4	CT	-0.166	**O4**	OS	-0.552	**O4**	OS	-0.566	**O4**	OS	-0.566	**O4**	OS	-0.566
C5	C	1.109	**H6**	H1	0.054	**H6**	H1	0.048	**H6**	H1	0.049	**H6**	H1	0.051
O3	O2	-0.921	**C7**	CT	0.672	**C7**	CT	0.663	**C7**	CT	0.639	**C7**	CT	0.626
O4	O2	-0.921	**O3**	OH	-0.837	**O3**	OH	-0.830	**O3**	OH	-0.842	**O3**	OH	-0.826
H5	H1	0.084	**H7**	HO	0.457	**H7**	HO	0.451	**H7**	HO	0.457	**H7**	HO	0.445
N1	N	-0.833	**H5**	H1	-0.054	**H5**	H1	-0.051	**H5**	H1	-0.057	**H5**	H1	-0.055
H6	H	0.408	**C6**	CT	-0.343	**C6**	CT	-0.346	**C6**	CT	-0.311	**C6**	CT	-0.315
C6	C	1.031	**H3**	HC	0.072	**H3**	HC	0.069	**H3**	HC	0.070	**H3**	HC	0.068
O5	O	-0.748	**H4**	HC	0.072	**H4**	HC	0.069	**H4**	HC	0.070	**H4**	HC	0.068
C7	CA	-0.274	**C5**	CT	0.273	**C5**	CT	0.348	**C5**	CT	0.322	**C5**	CT	0.295
C10	CA	-0.023	**H2**	H2	0.098	**H2**	H2	0.080	**H2**	H2	0.104	**H2**	H2	0.102
H9	HA	0.153	**N1**	N*	-0.183	**N1**	N*	-0.207	**N1**	N*	-0.307	**N1**	N*	-0.307
C11	CA	-0.346	**C1**	C	0.762	**C1**	C	0.756	**C1**	C	0.756	**C1**	C	0.765
H10	HA	0.170	**O1**	O	-0.691	**O1**	O	-0.683	**O1**	O	-0.683	**O1**	O	-0.683
C8	CA	-0.023	**N2**	NA	-0.668	**N2**	NA	-0.676	**N2**	NA	-0.674	**N2**	NA	-0.664
H8	HA	0.153	**H1**	H	0.357	**H1**	H	0.375	**H1**	H	0.369	**H1**	H	0.358

mTHF			dUMP			FdUMP			CldUMP			BrdUMP		
Atom name	**Atom type**	**q**	**Atom name**	**Atom type**	**q**	**Atom name**	**Atom type**	**q**	**Atom name**	**Atom type**	**q**	**Atom name**	**Atom type**	**q**
C9	CA	-0.346	**C2**	C	0.846	**C2**	C	0.717	**C2**	C	0.773	**C2**	C	0.765
H7	HA	0.170	**O2**	O	-0.691	**O2**	O	-0.641	**O2**	O	-0.654	**O2**	O	-0.636
C12	CA	0.466	**C3**	CM	-0.612	**C3**	CM	-0.004	**C3**	CM	-0.303	**C3**	CM	-0.427
N2	N2	-0.773	**H10**	HA	0.224	**F1**	F	-0.202	**Cl1**	Cl	-0.040	**Br1**	Br	-0.043
H11	H	0.376	**C4**	CM	0.172	**C4**	CM	-0.043	**C4**	CM	0.265	**C4**	CM	0.320
C13	CT	-0.035	**H11**	H4	0.219	**H11**	H4	0.299	**H11**	H4	0.192	**H11**	H4	0.261
H12	H1	0.142												
H13	H1	0.142												
C14	CT	-0.019												
H14	H1	0.126												
C15	CT	-0.071												
H15	H1	0.114												
H16	H1	0.114												
N7	NT	-0.621												
H22	H	0.417												
C16	CM	0.781												
N3	NC	-0.916												
C17	CA	1.241												
N6	N2	-1.160												
H20	H	0.293												
H21	H	0.293												
N4	NA	-0.997												
H17	H	0.514												
C18	C	0.959												
O6	O	-0.687												
C19	CM	-0.492												
N5	NT	0.716												
C20	CM	-0.209												
H18	HA	0.212												
H19	HA	0.212												