



$$\Delta G_F = \Delta H - T\Delta S$$

$$\left(\Delta H_{\text{COVAL}} + \Delta H_{\text{COUL}} + \Delta H_{\text{H-BOND}} + \Delta H_{\text{VDW}} \right) - T(\Delta S_{\text{PROT}} + \Delta S_{\text{H}_2\text{O}})$$

ENTHALPY

TYPE	NATURE	H (CO-TERMS)	Fx. BROKE
COVALENT		400	1/10 ²⁰
IONIC		50	1/10 ⁹
H-BOND		20	1/3000
VDW		1	4/10
DISTORT		~0	NA

AT ROOM TEMP, HOW FAVORABLE WOULD ΔG HAVE TO BE TO BE FOLDED 99% OF THE TIME?

LOAD UP...

(RES 10 121) \rightarrow 22 kJ/mol \rightarrow IF NOT FORMED IN UNFOLDED STATE, $\Delta H = H_F - \emptyset$

CAN WRITE TERMS FOR OTHER INTERACTIONS:

SHOW SLIDE FROM VH

ENTROPY

$$\Delta S = R \ln(N_F/N_U) \leftarrow \text{REALLY HARD TO ESTIMATE "N" ABSOLUTELY. SOMETIMES CAN GET RELATIVE RATIOS}$$

EXAMPLE:

FOLD ARG \rightarrow 81 $R \ln(1/81) = 0.0087 \rightarrow -2.6 \text{ kJ/mol}$
 LYS
 HIS
 ASN
 GLN
 DISFAVORS FOLDING.

WHAT DRIVES FOLDING, ENTROPY OR ENTHALPY?

$$-40 = \sim \phi - 298(0.13) \leftarrow \text{NULL}$$

- 1) WATER FORMS HBONDS, VDW AND COMPETES TO FORM HBONDS TO IONS
- 2) WATER IS SS M.

INTERACTIONS VERY SIMILAR BETWEEN F AND U (OR BOUND/UNBOUND),

$$\Delta H \sim \phi$$

FOR ENTALPY -