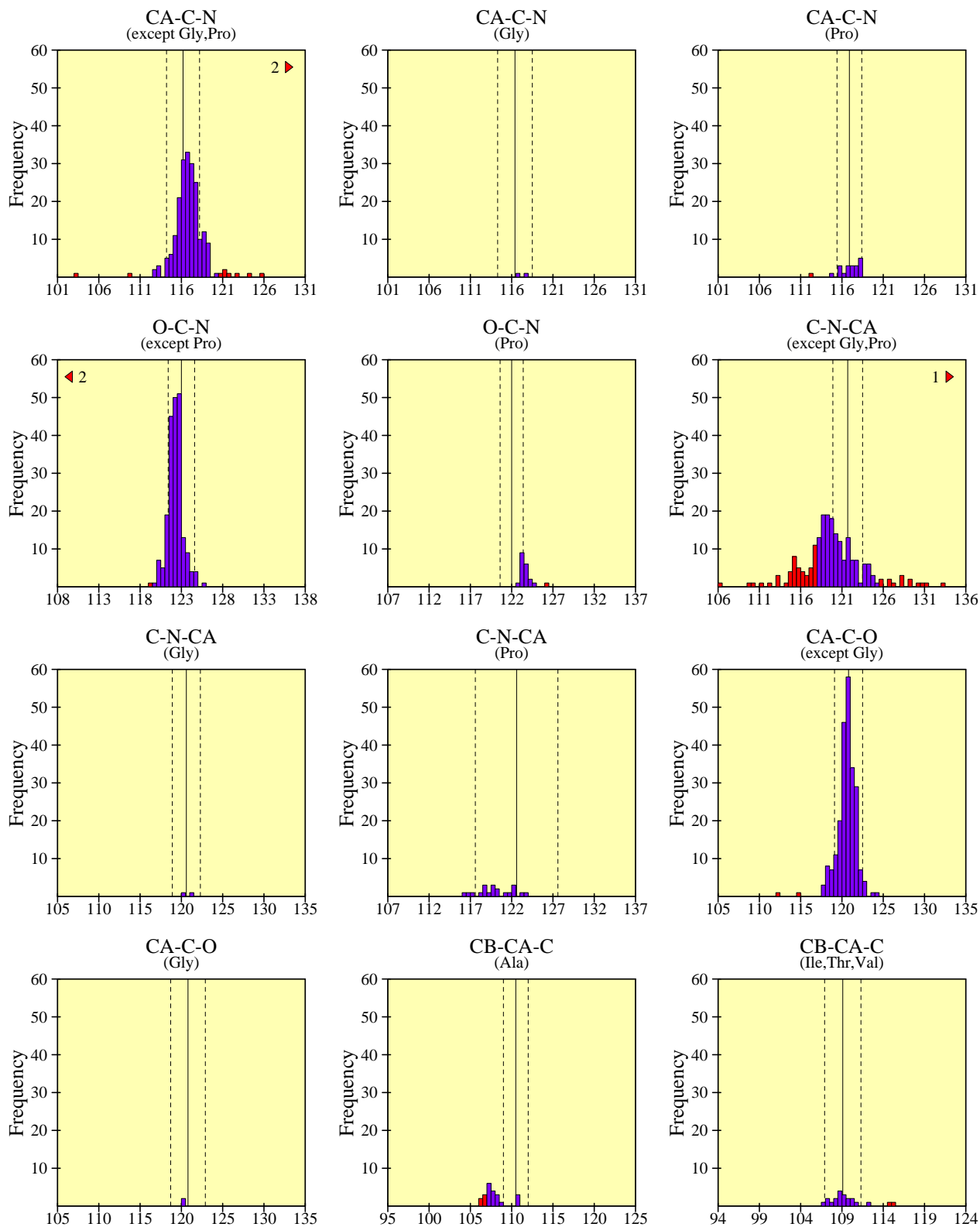


# Main-chain bond angles

## 23\_128\_72



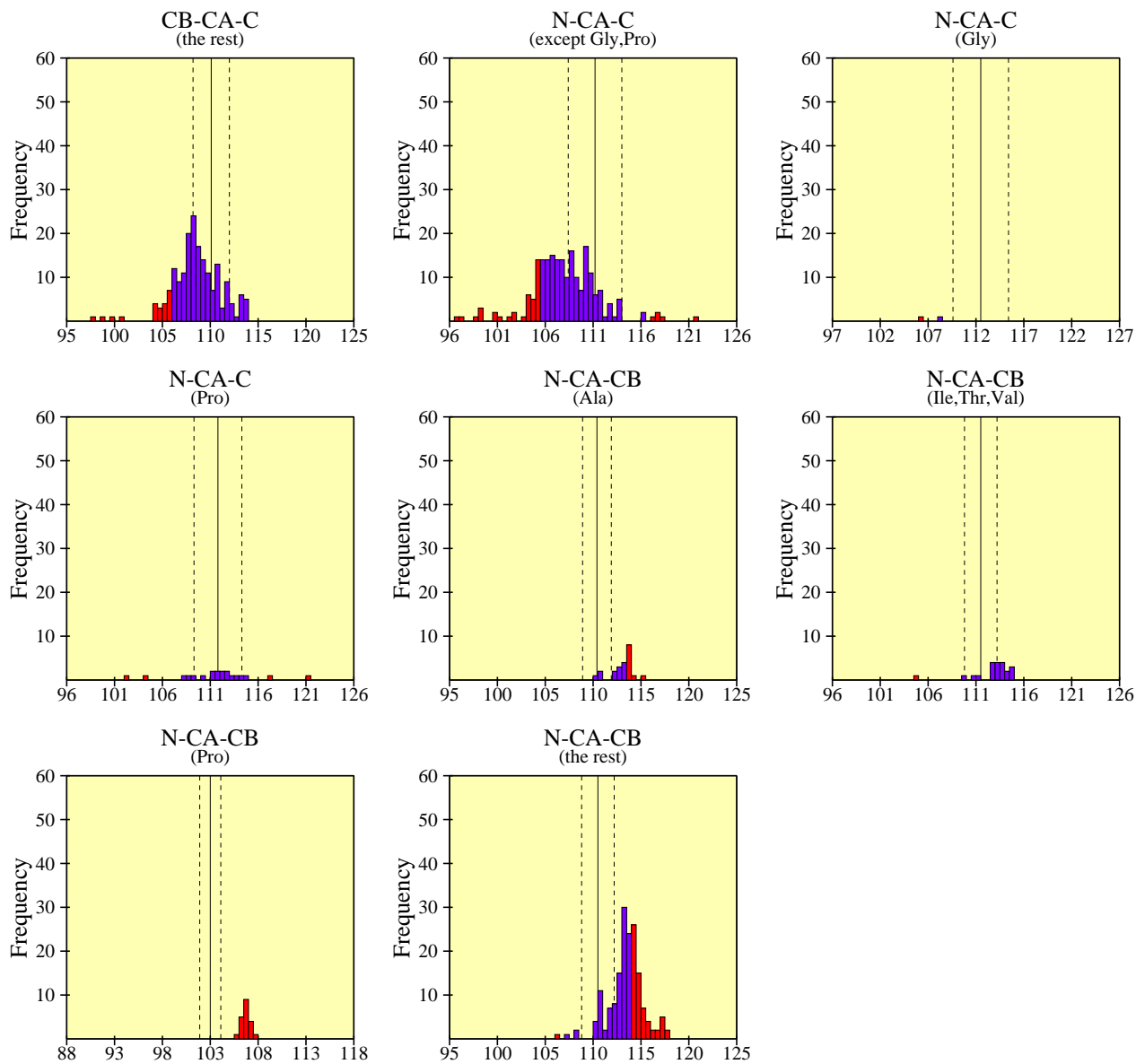
Black bars > 2.0 st. devs. from mean.

◀ or ▶ signifies data points off the graph in the direction shown.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain bond angles

## 23\_128\_72

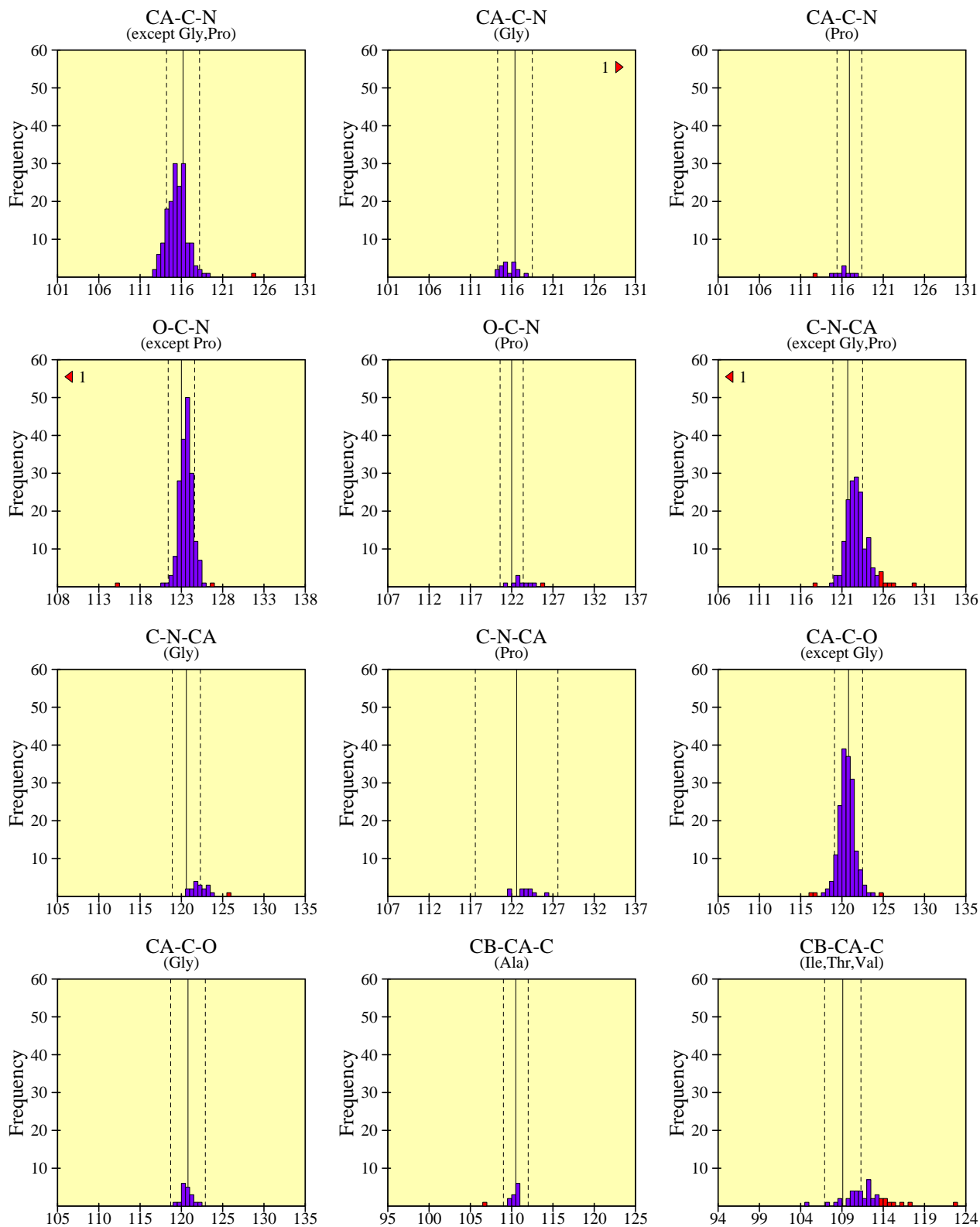


Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain bond angles

## Model\_12



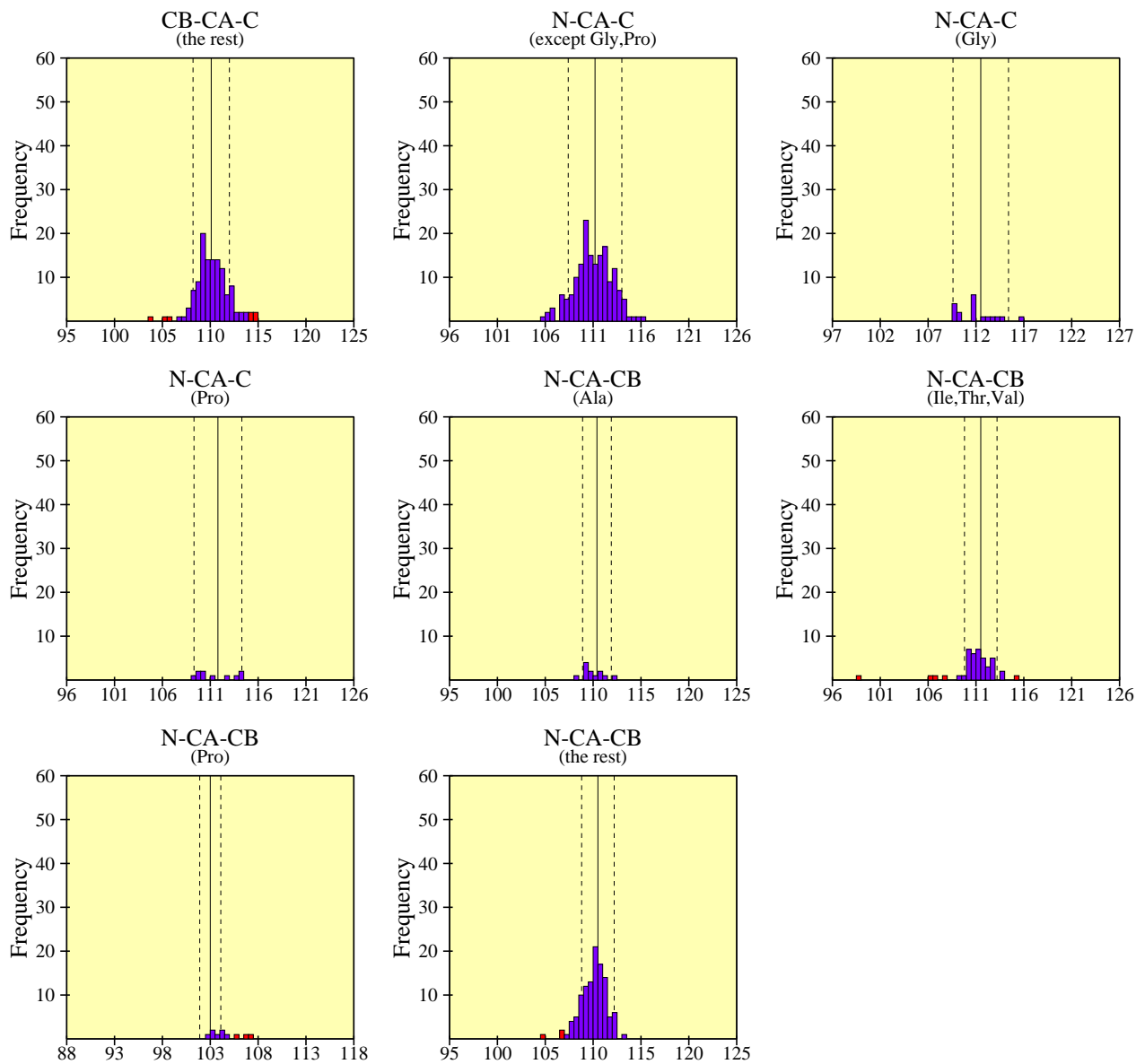
Black bars > 2.0 st. devs. from mean.

◀ or ▶ signifies data points off the graph in the direction shown.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain bond angles

## Model\_12

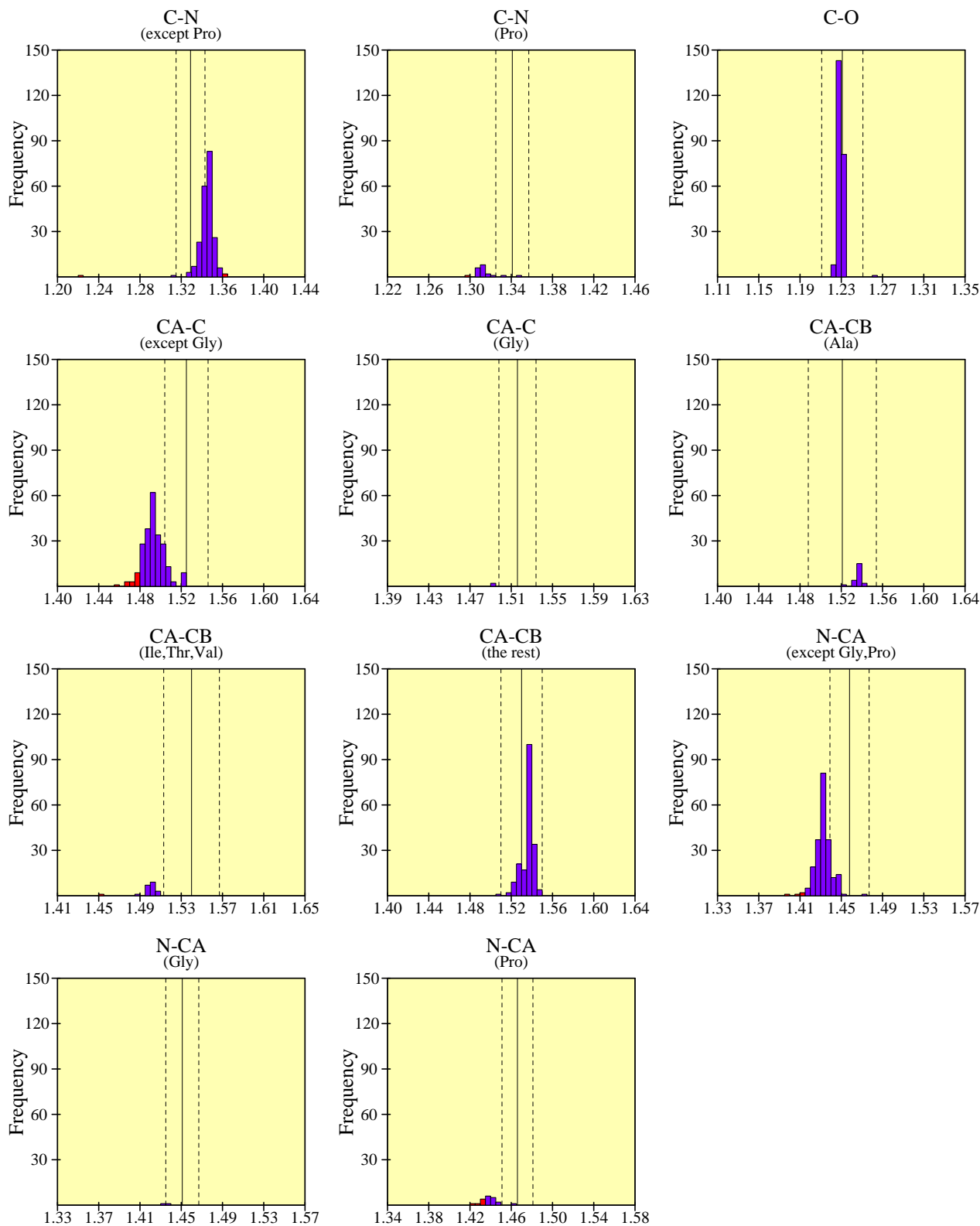


Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain bond lengths

## 23\_128\_72

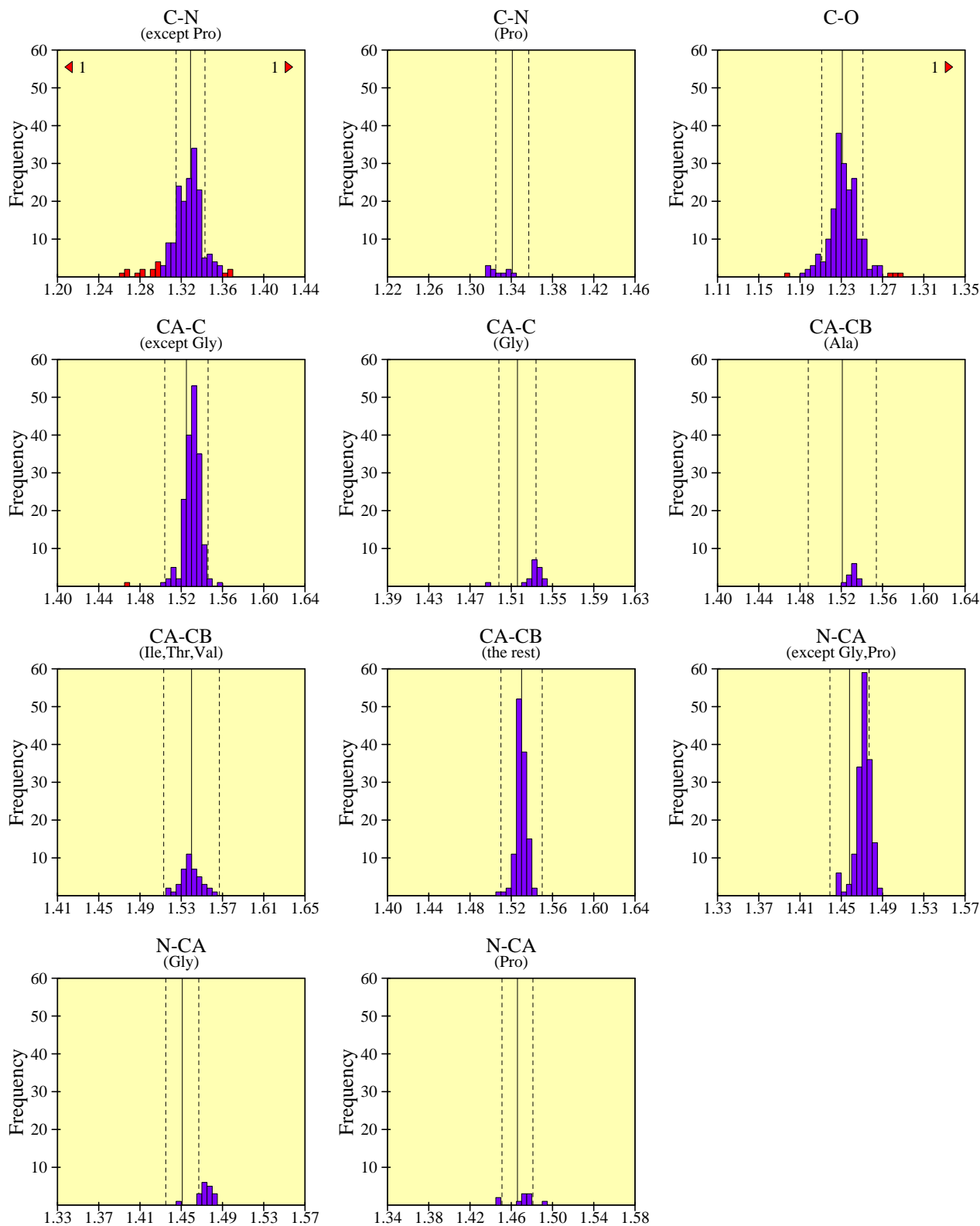


Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain bond lengths

## Model\_12



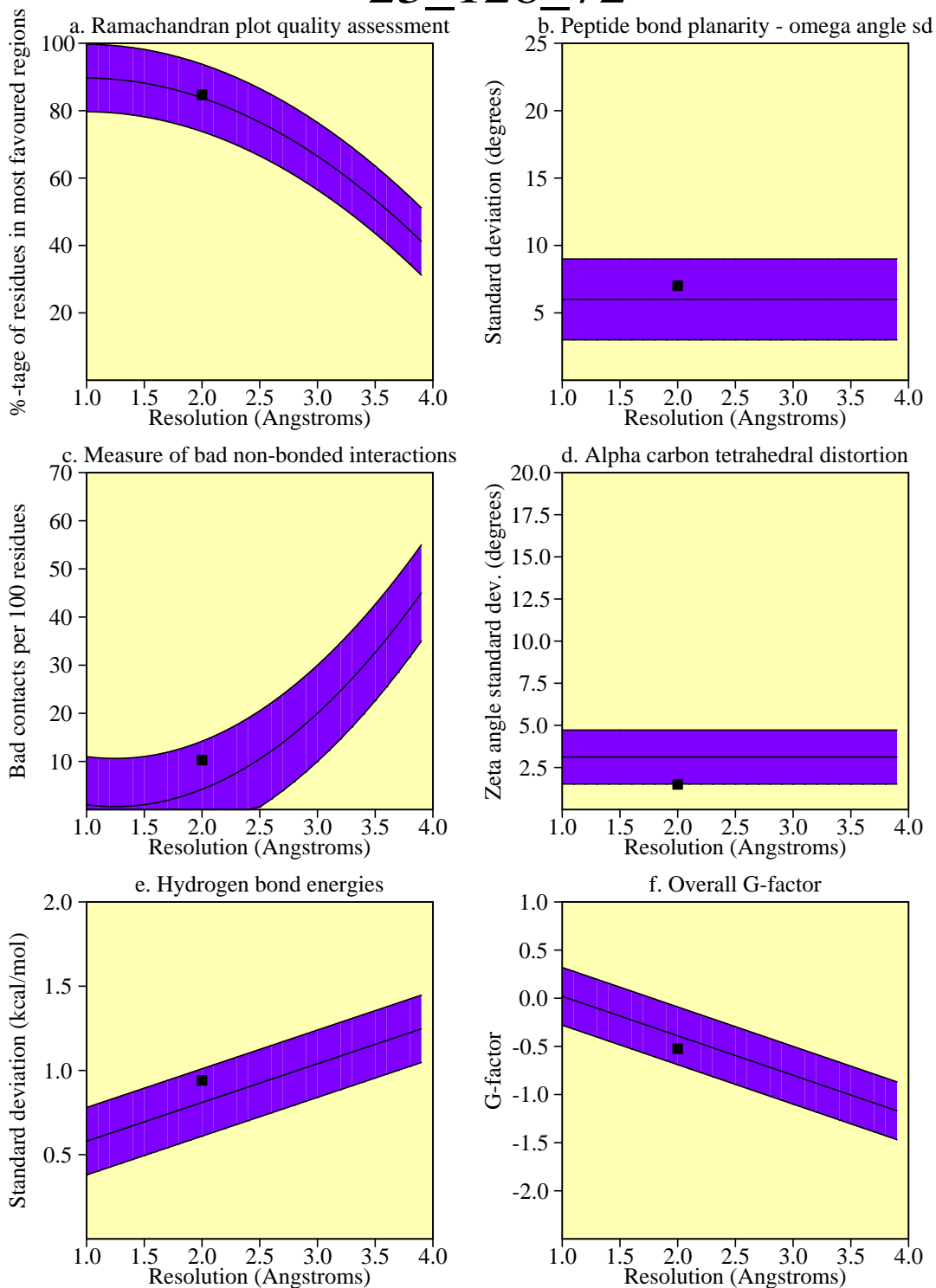
Black bars > 2.0 st. devs. from mean.

◀ or ▶ signifies data points off the graph in the direction shown.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain parameters

## 23\_128\_72

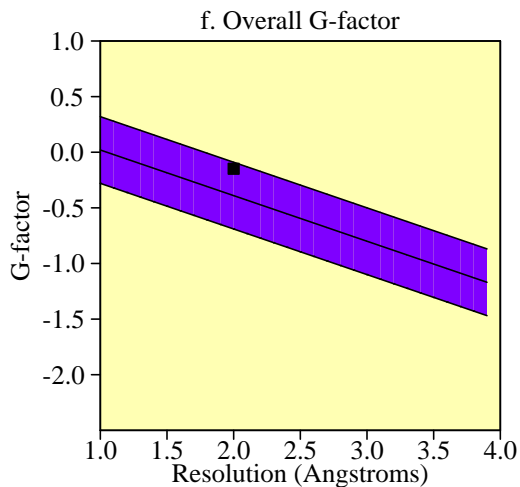
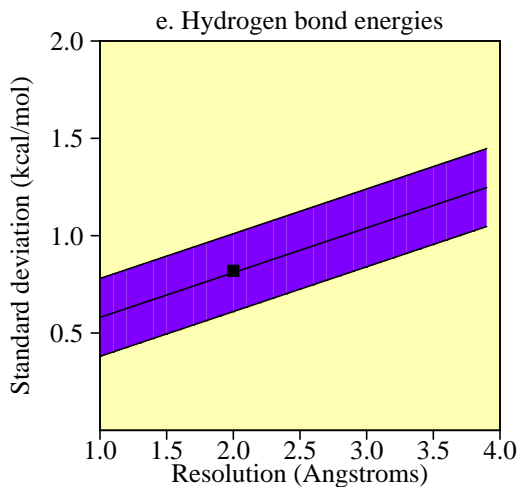
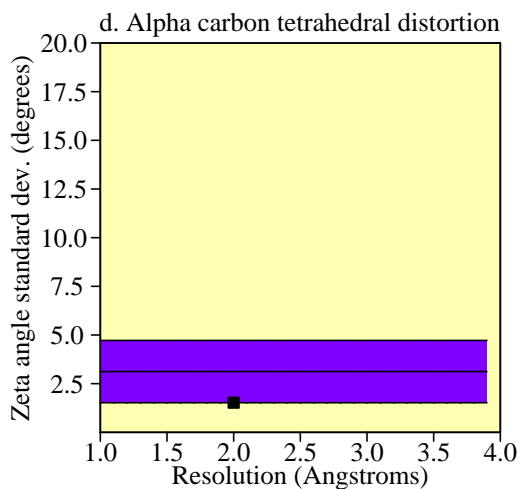
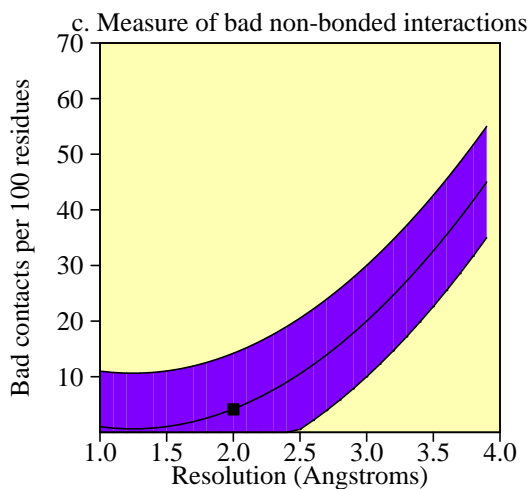
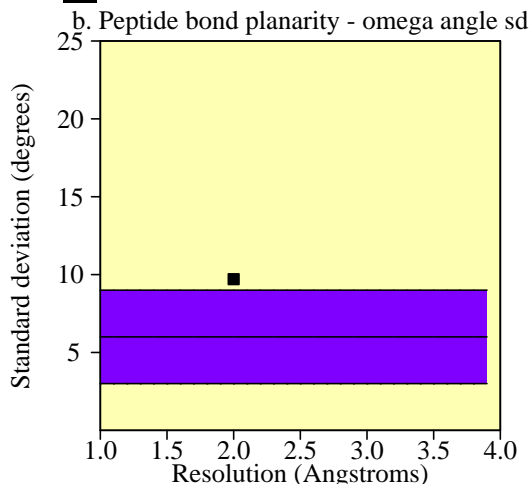
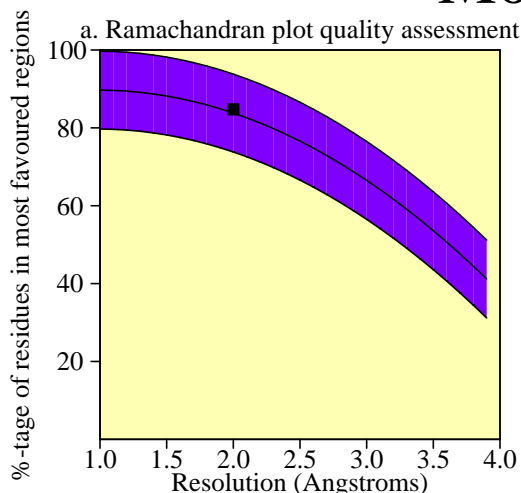


Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean
			Typical value	Band width	
a. %-tage residues in A, B, L	209	84.7	83.8	10.0	0.1 Inside
b. Omega angle st dev	232	7.0	6.0	3.0	0.3 Inside
c. Bad contacts / 100 residues	24	10.3	4.2	10.0	0.6 Inside
d. Zeta angle st dev	231	1.5	3.1	1.6	-1.0 BETTER
e. H-bond energy st dev	89	0.9	0.8	0.2	0.7 Inside
f. Overall G-factor	233	-0.5	-0.4	0.3	-0.5 Inside

# Main-chain parameters

## Model\_12



### Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. %-tage residues in A, B, L	164	84.8	83.8	10.0	0.1	Inside
b. Omega angle st dev	193	9.7	6.0	3.0	1.2	WORSE
c. Bad contacts / 100 residues	8	4.1	4.2	10.0	0.0	Inside
d. Zeta angle st dev	176	1.5	3.1	1.6	-1.0	Inside
e. H-bond energy st dev	118	0.8	0.8	0.2	0.0	Inside
f. Overall G-factor	194	-0.1	-0.4	0.3	0.8	Inside