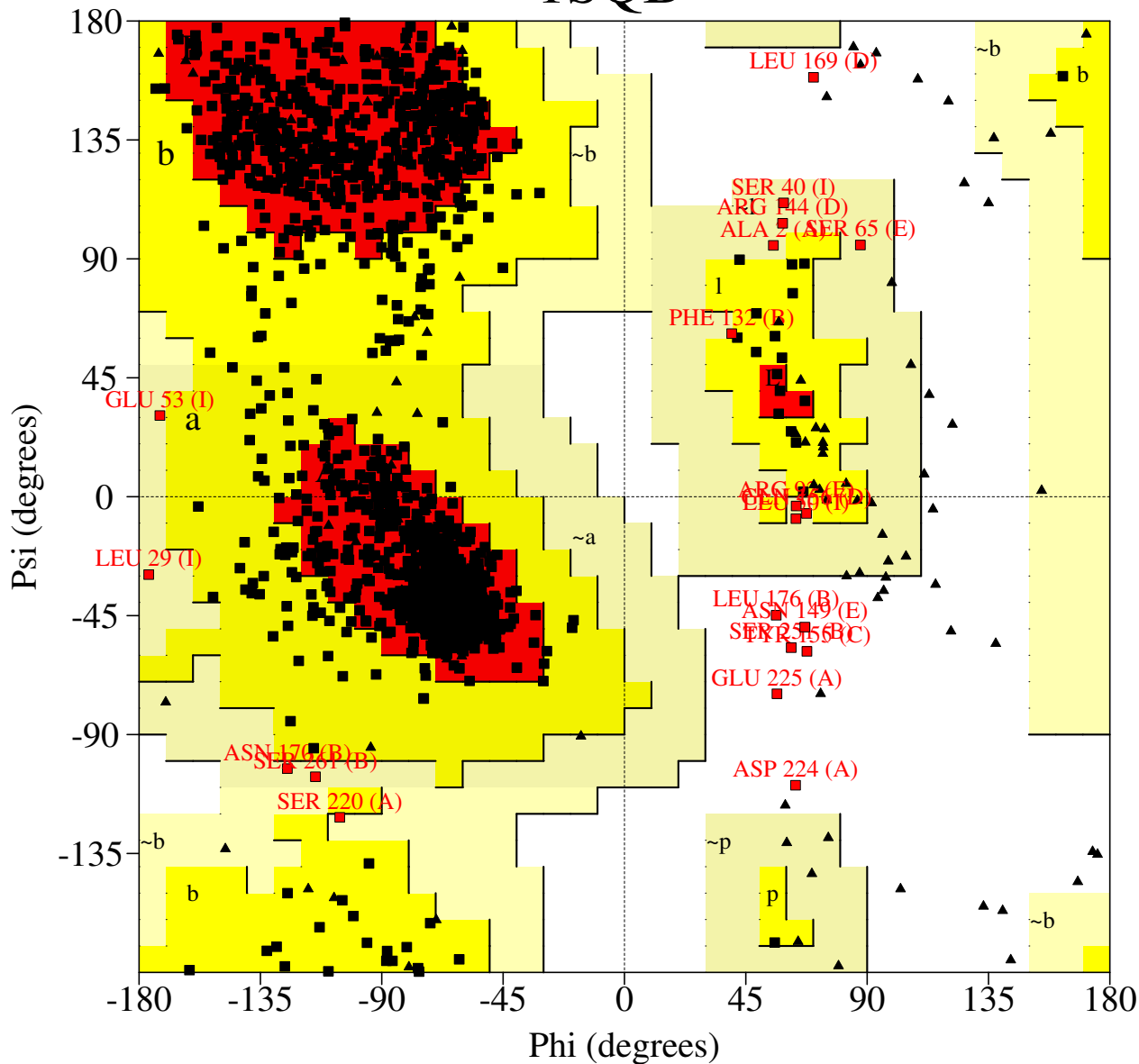


# Ramachandran Plot

## 1SQB



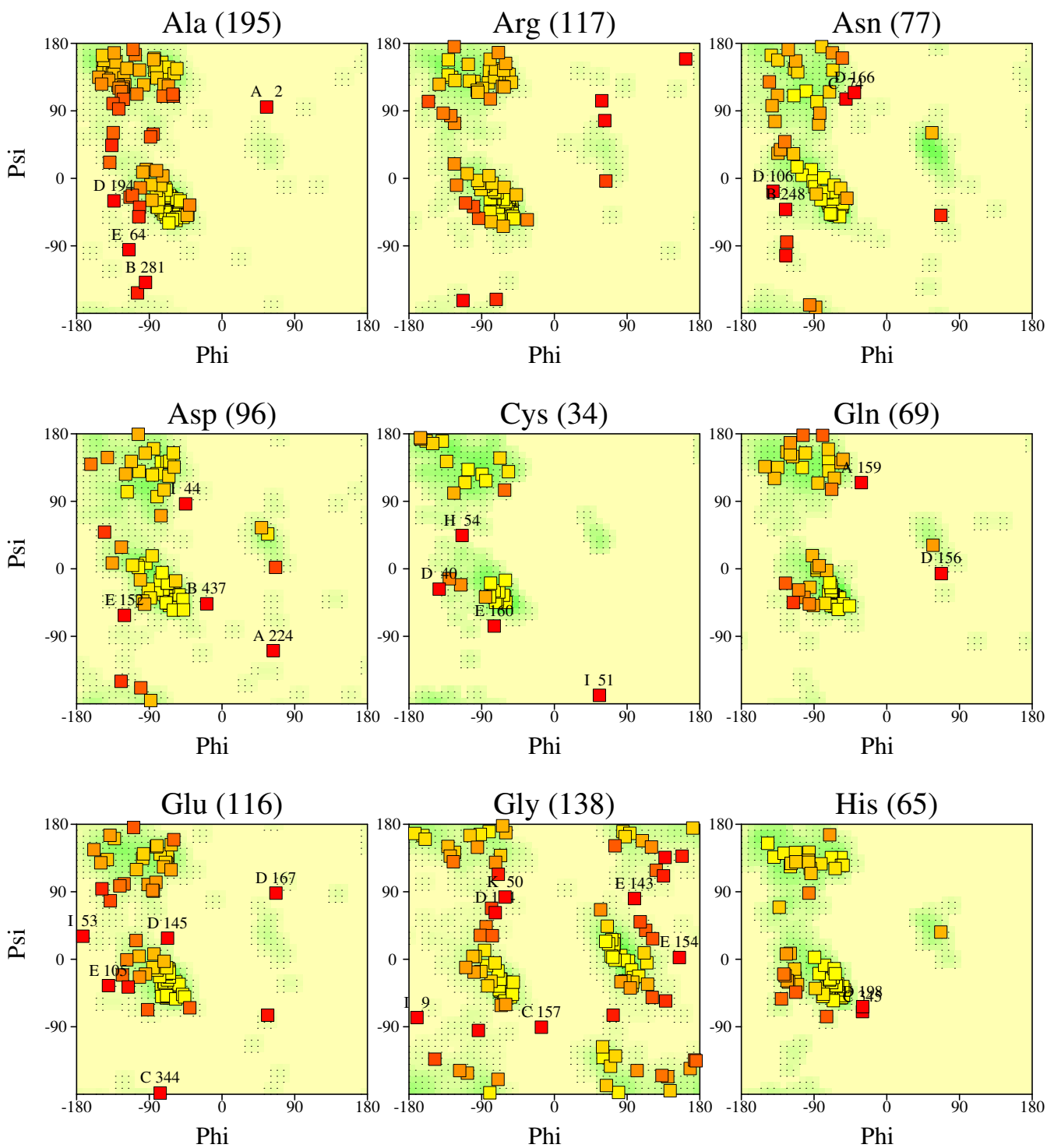
### Plot statistics

Residues in most favoured regions [A,B,L]	1652	90.1%
Residues in additional allowed regions [a,b,l,p]	162	8.8%
Residues in generously allowed regions [-a,-b,-l,-p]	13	0.7%
Residues in disallowed regions	7	0.4%
	----	-----
Number of non-glycine and non-proline residues	1834	100.0%
Number of end-residues (excl. Gly and Pro)	19	
Number of glycine residues (shown as triangles)	141	
Number of proline residues	109	
	----	
Total number of residues	2103	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

# Ramachandran plots for all residue types

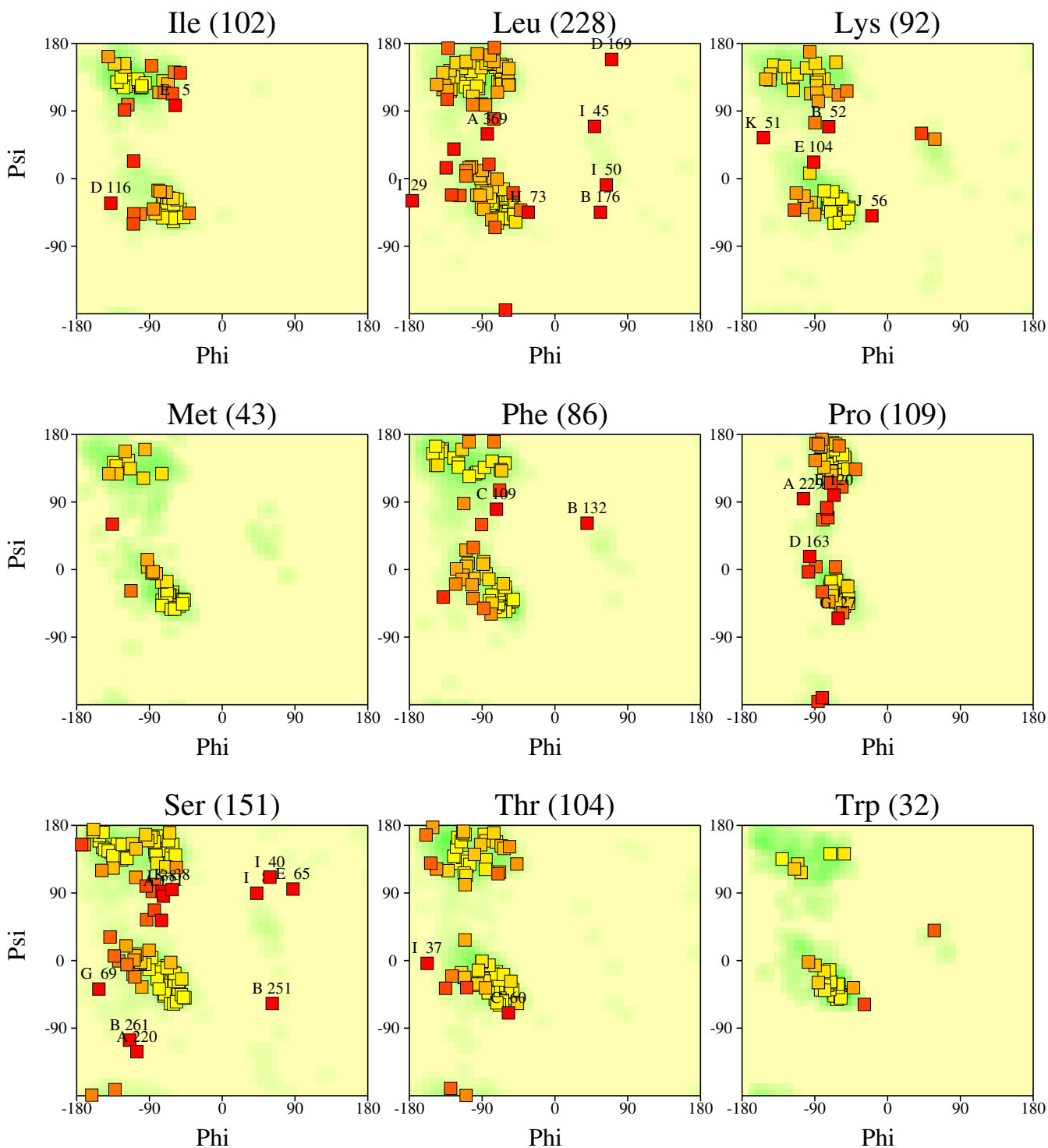
## 1SQB



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Ramachandran plots for all residue types

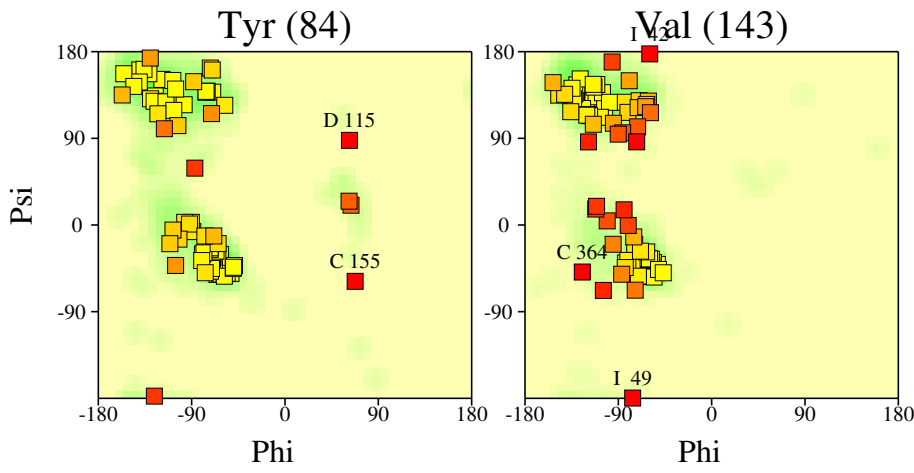
## 1SQB



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Ramachandran plots for all residue types

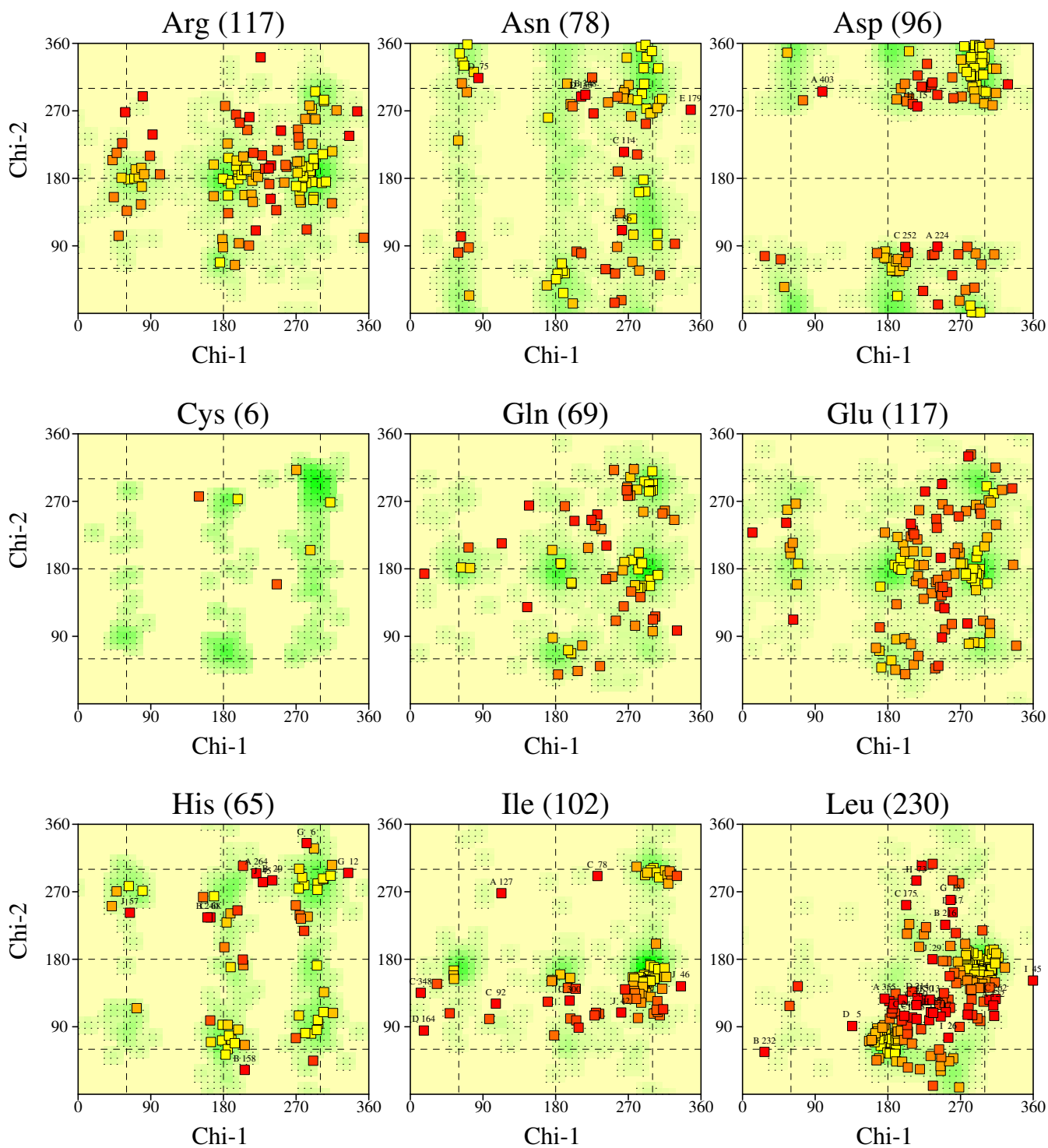
## 1SQB



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

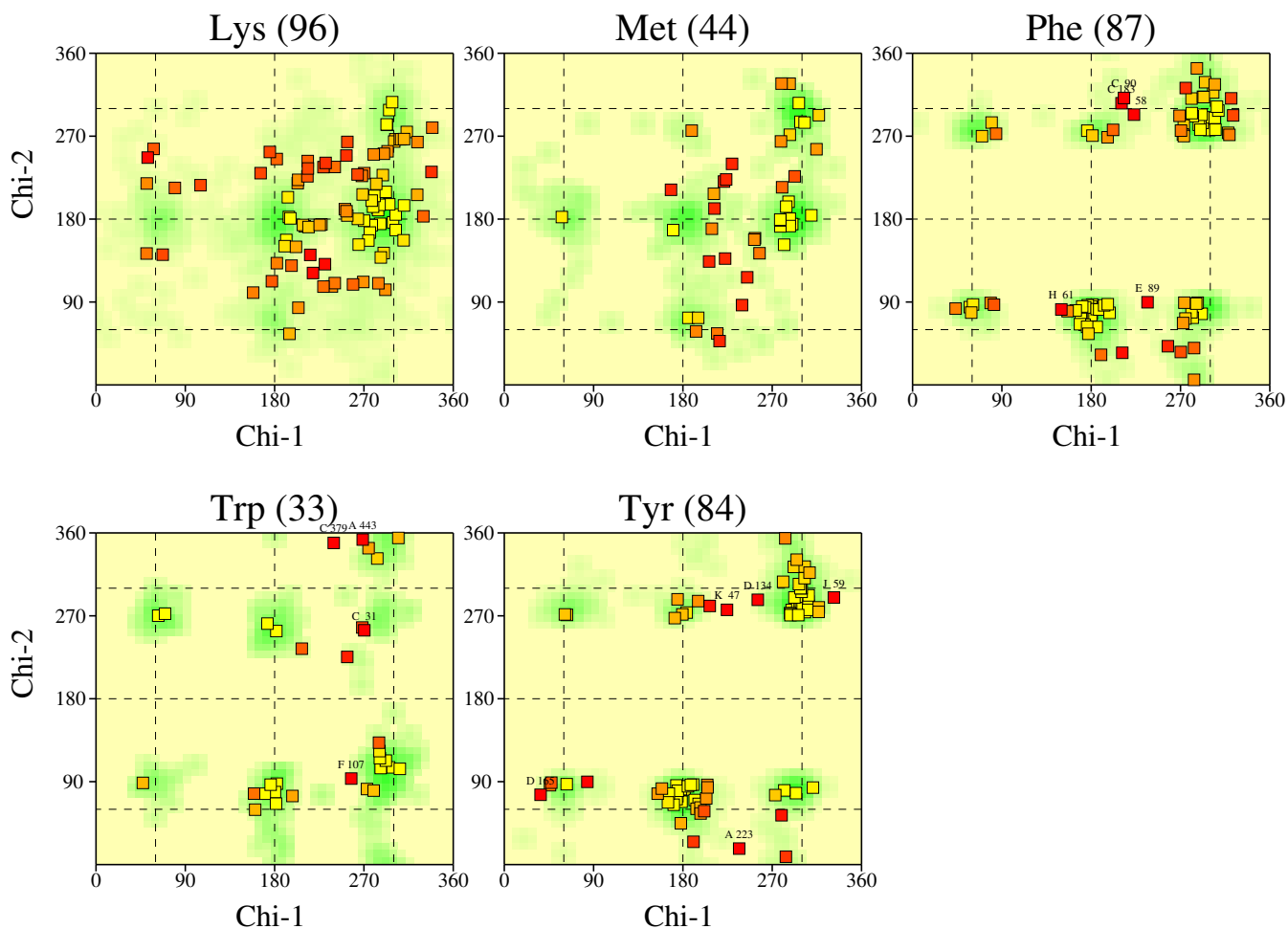
# Chi1-Chi2 plots

## 1SQB



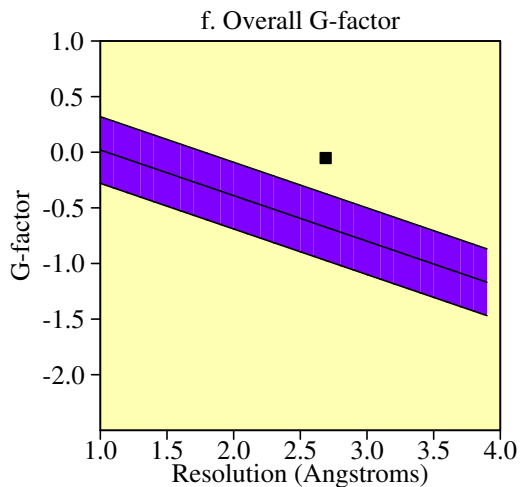
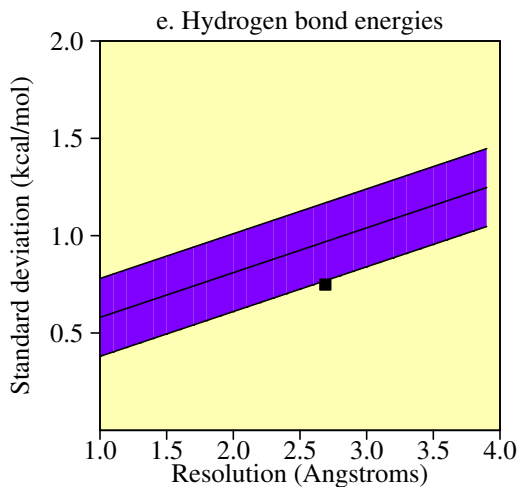
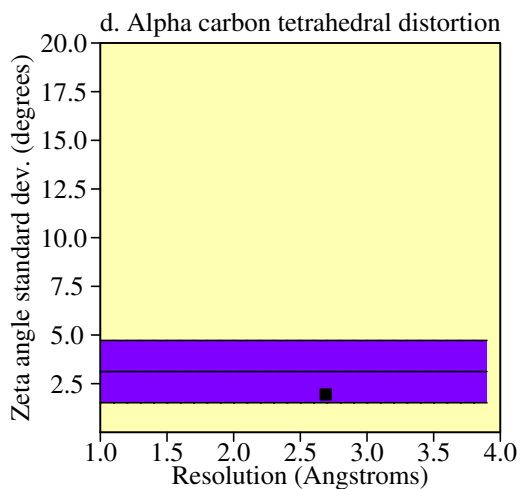
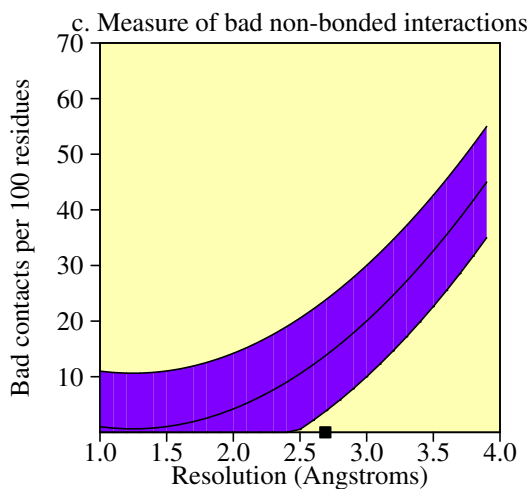
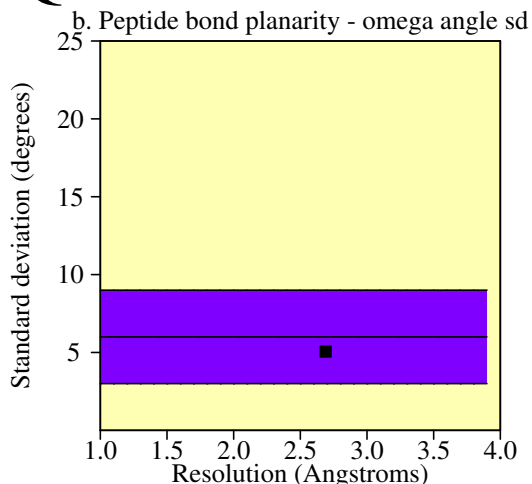
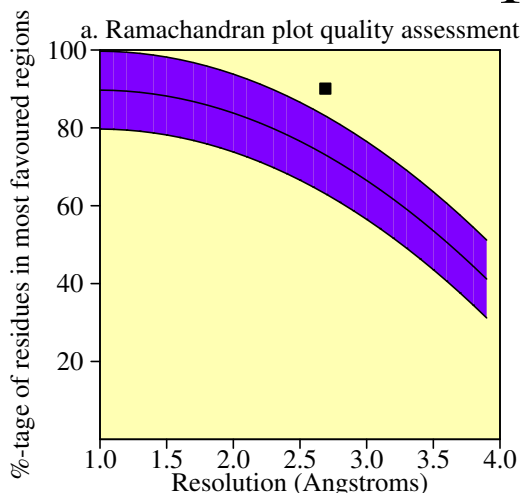
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0Å or better.

# Chi1-Chi2 plots 1SQB



Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

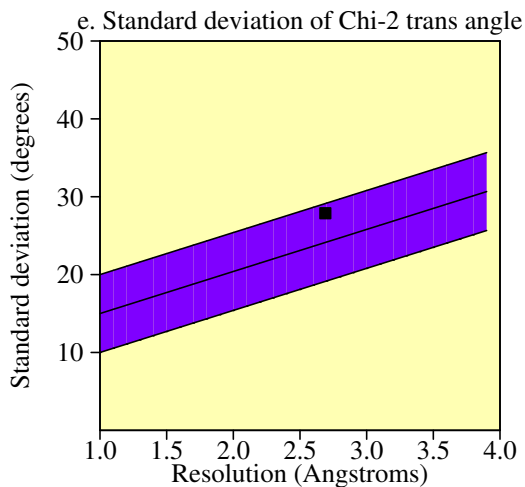
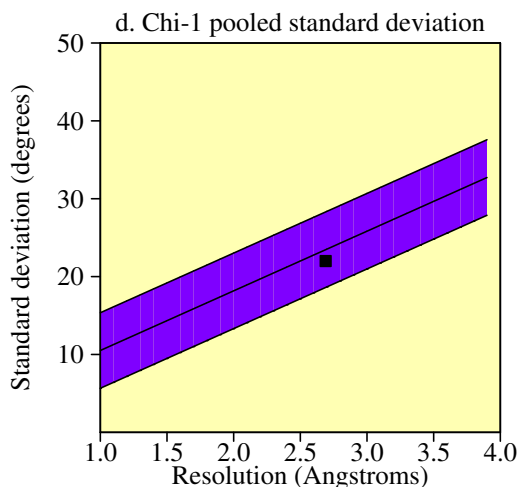
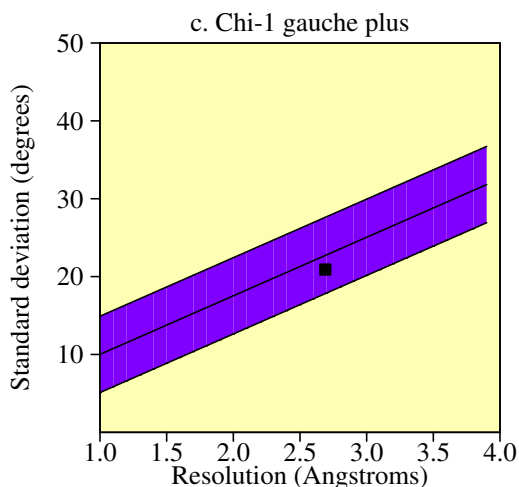
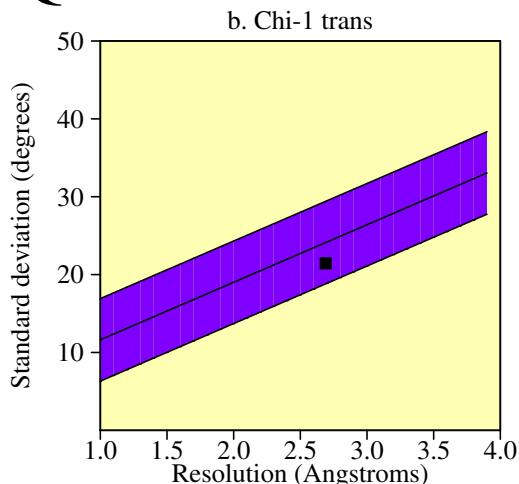
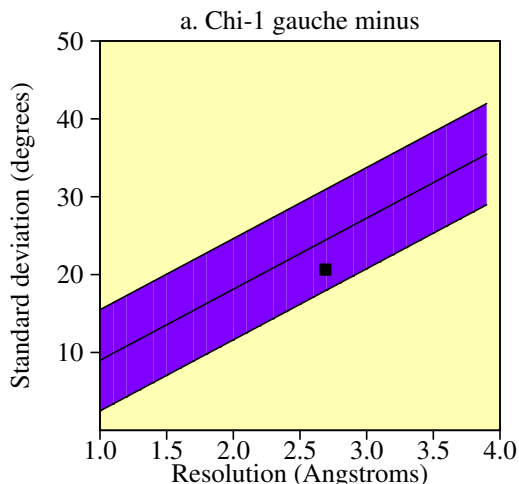
# Main-chain parameters 1SQB



### 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	1834	90.1	73.1	10.0	1.7	BETTER
b. Omega angle st dev	2091	5.1	6.0	3.0	-0.3	Inside
c. Bad contacts / 100 residues	0	0.0	13.8	10.0	-1.4	BETTER
d. Zeta angle st dev	1962	1.9	3.1	1.6	-0.7	Inside
e. H-bond energy st dev	1358	0.7	1.0	0.2	-1.1	BETTER
f. Overall G-factor	2103	-0.1	-0.7	0.3	2.1	BETTER

# Side-chain parameters 1SQB



1SQB

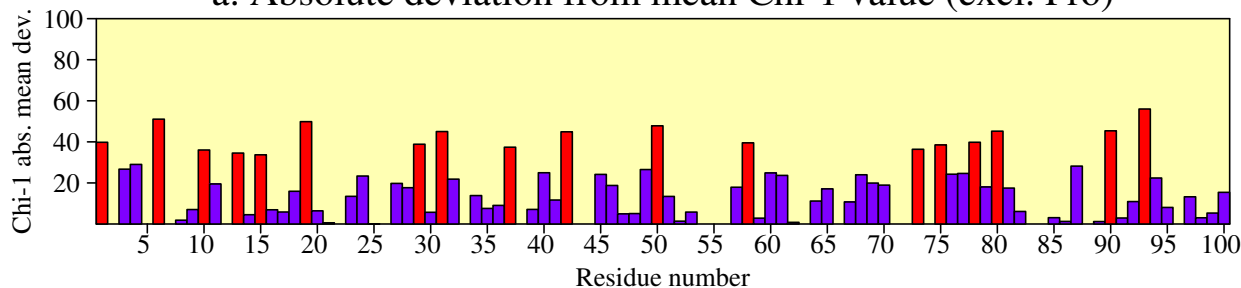
### Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean
			Typical value	Band width	
a. Chi-1 gauche minus st dev	235	20.6	24.4	6.5	-0.6 Inside
b. Chi-1 trans st dev	578	21.5	24.1	5.3	-0.5 Inside
c. Chi-1 gauche plus st dev	843	20.9	22.7	4.9	-0.4 Inside
d. Chi-1 pooled st dev	1656	22.0	23.5	4.8	-0.3 Inside
e. Chi-2 trans st dev	482	27.9	24.1	5.0	0.8 Inside

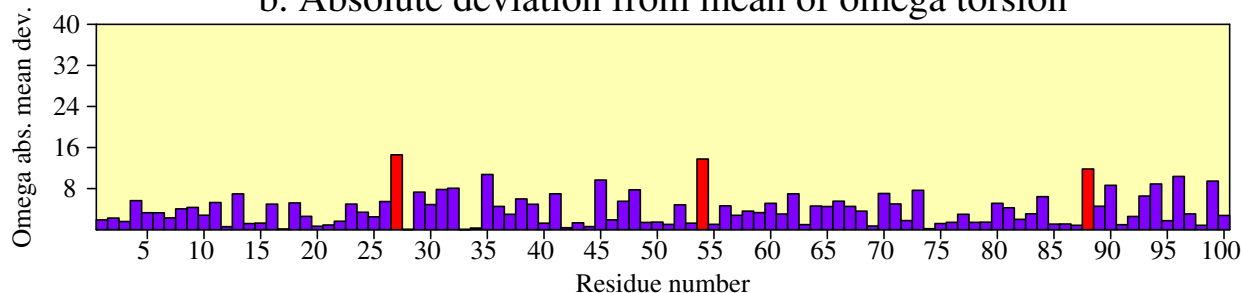


# Residue properties 1SQB

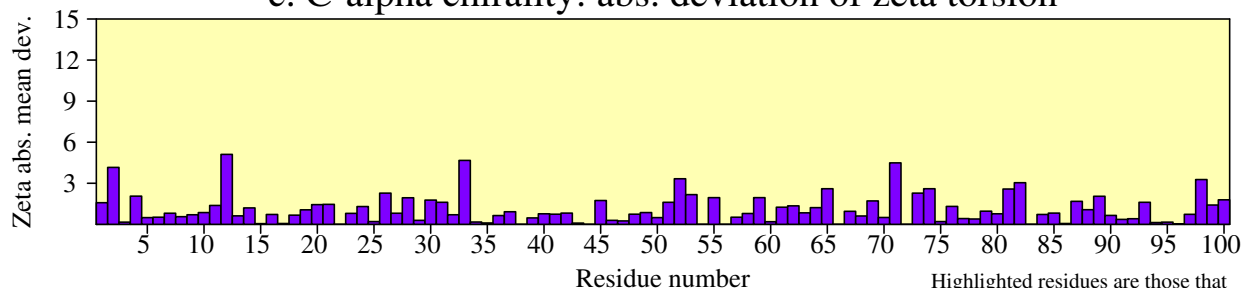
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

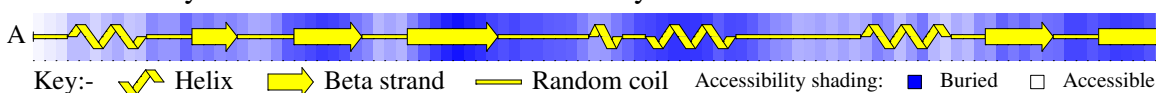


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

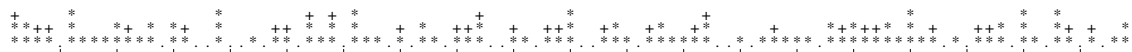
d. Secondary structure & estimated accessibility



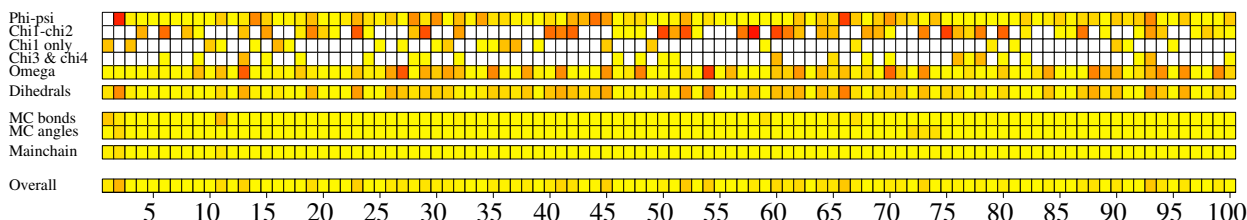
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

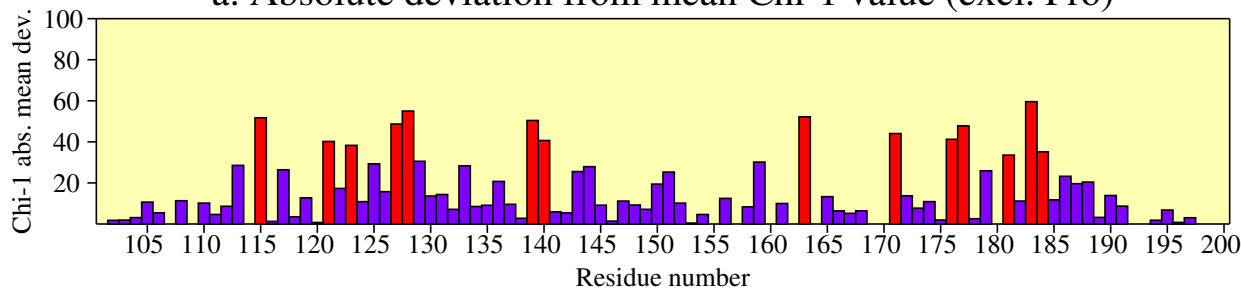


g. G-factors

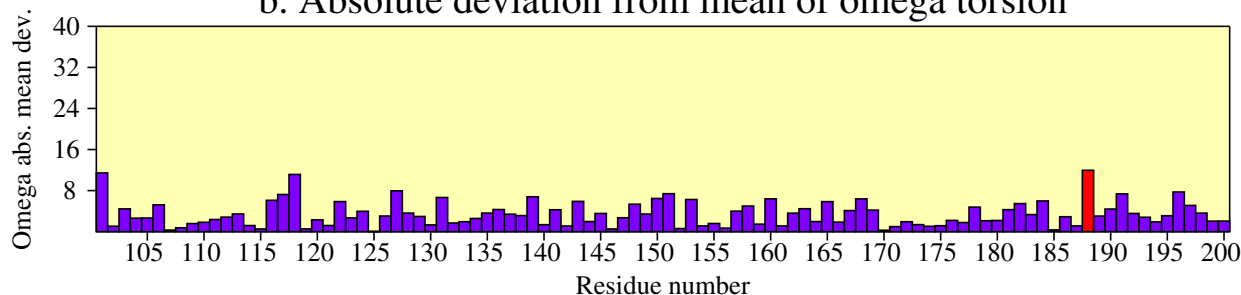


# Residue properties 1SQB

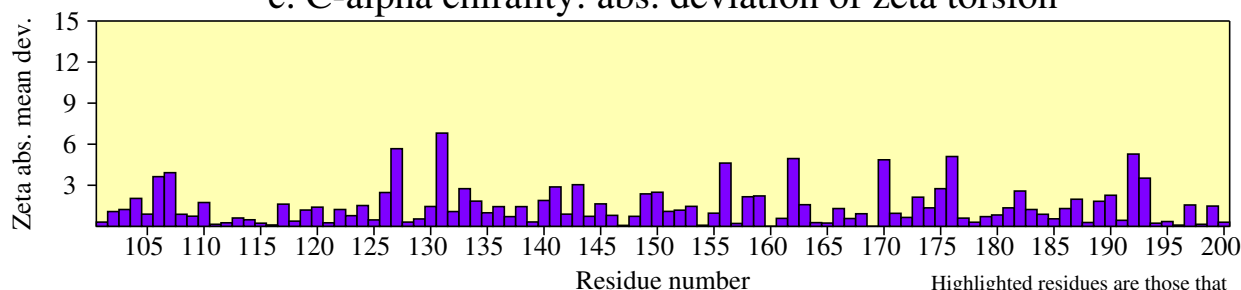
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

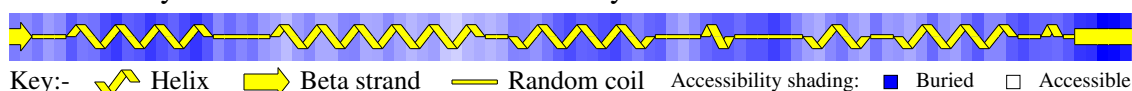


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

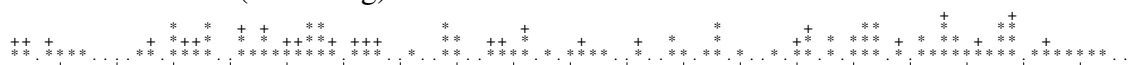
d. Secondary structure & estimated accessibility



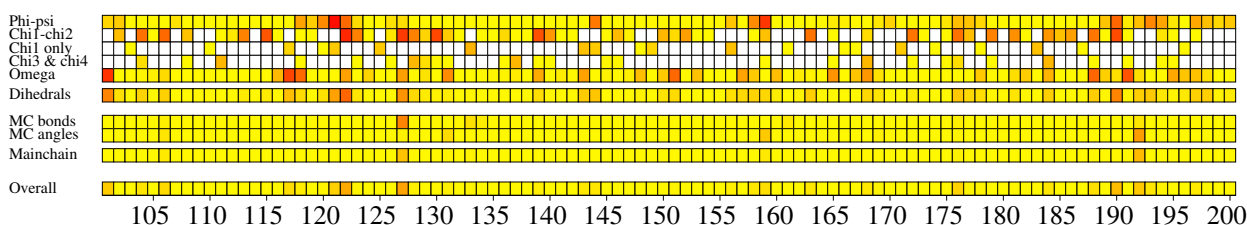
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

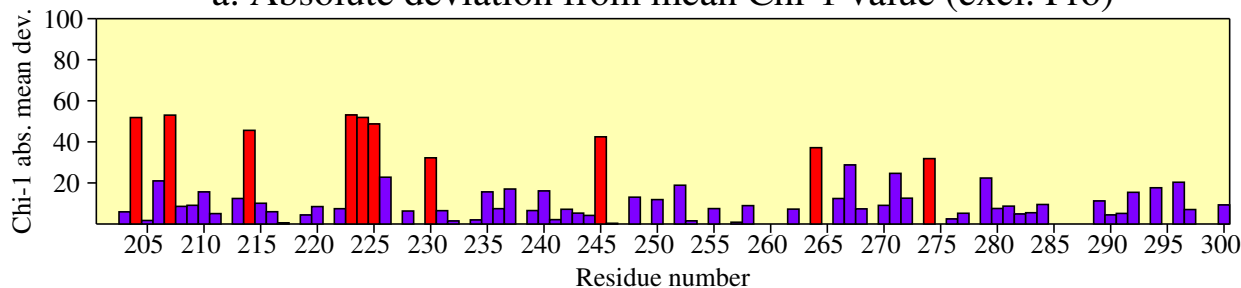


g. G-factors

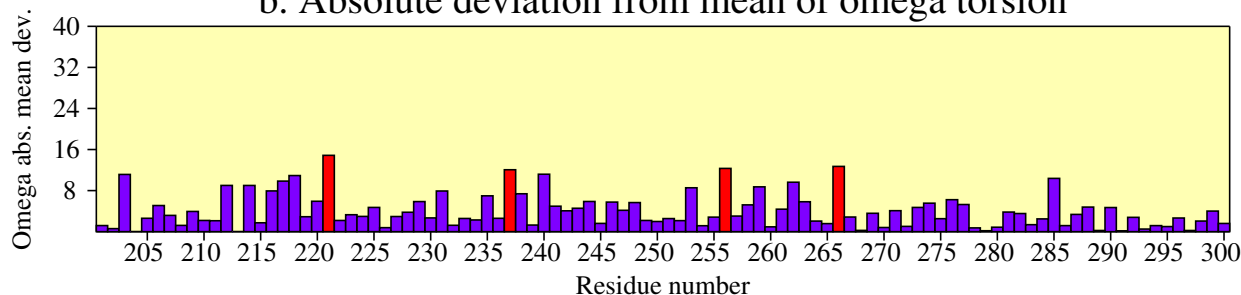


# Residue properties 1SQB

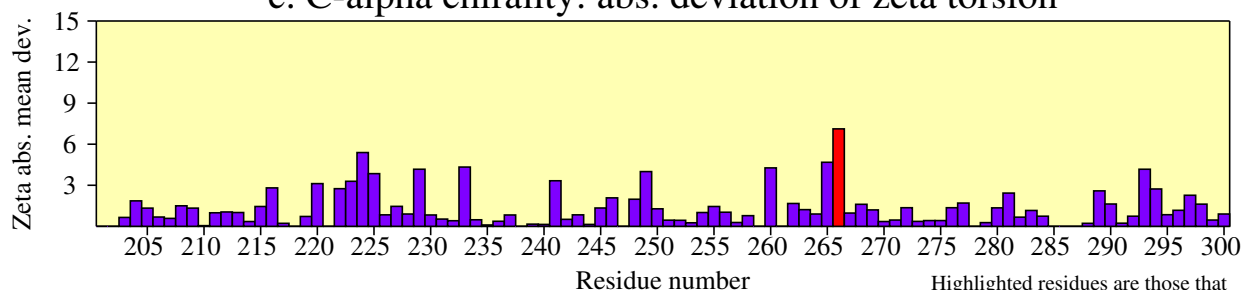
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

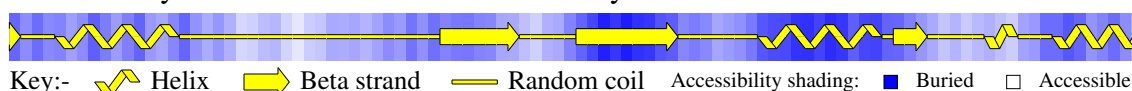


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



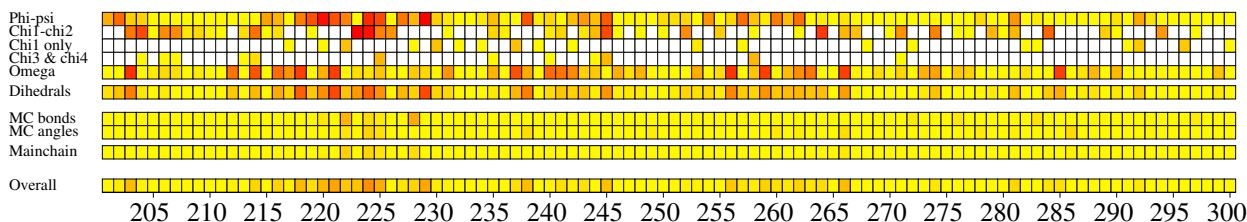
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

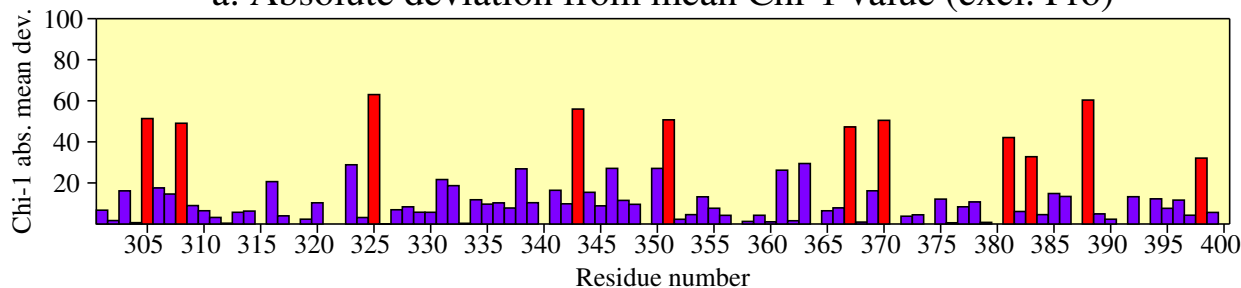


g. G-factors

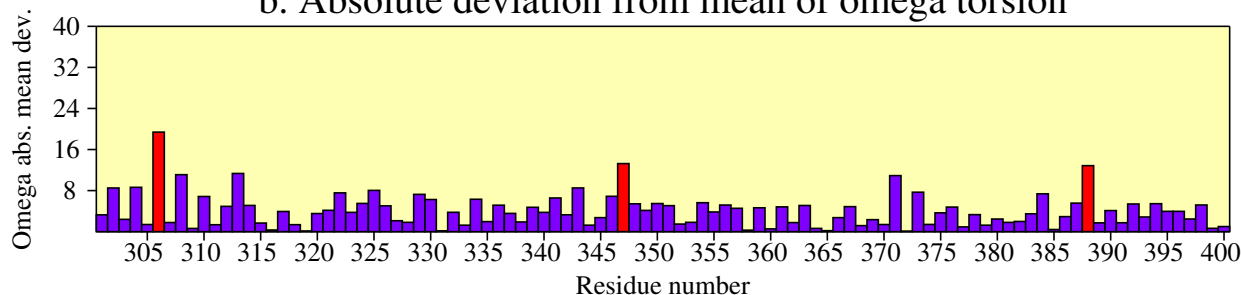


# Residue properties 1SQB

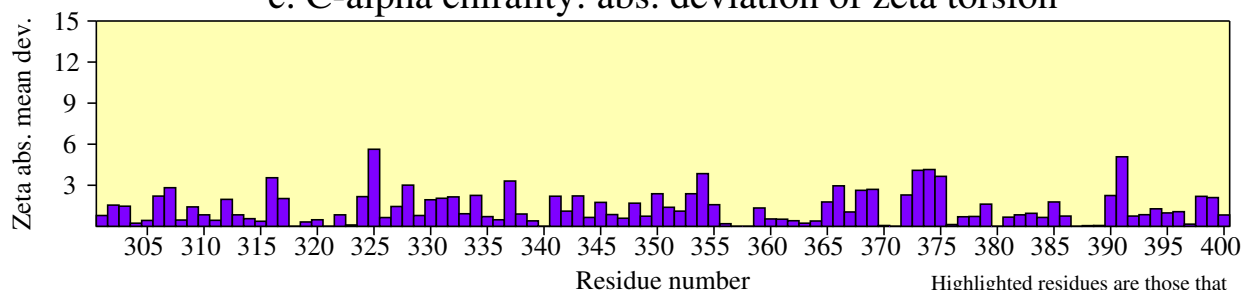
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

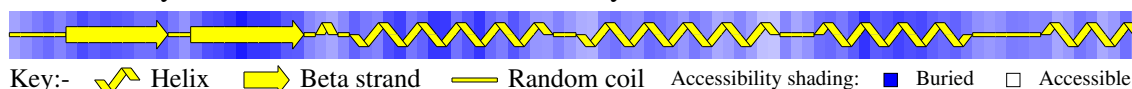


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

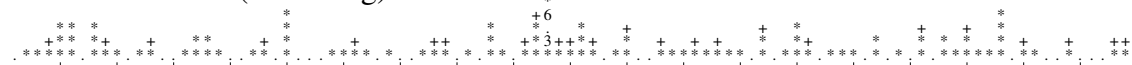
d. Secondary structure & estimated accessibility



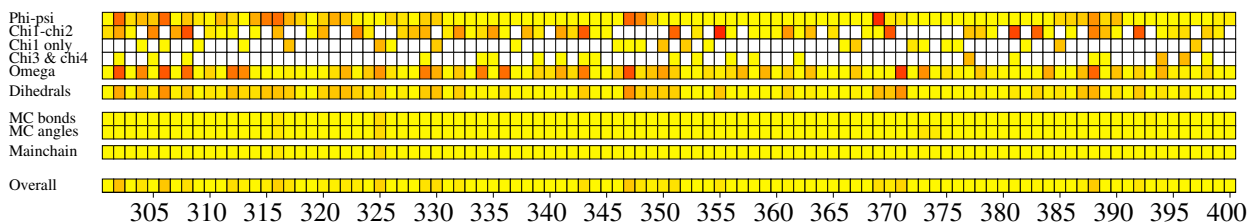
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

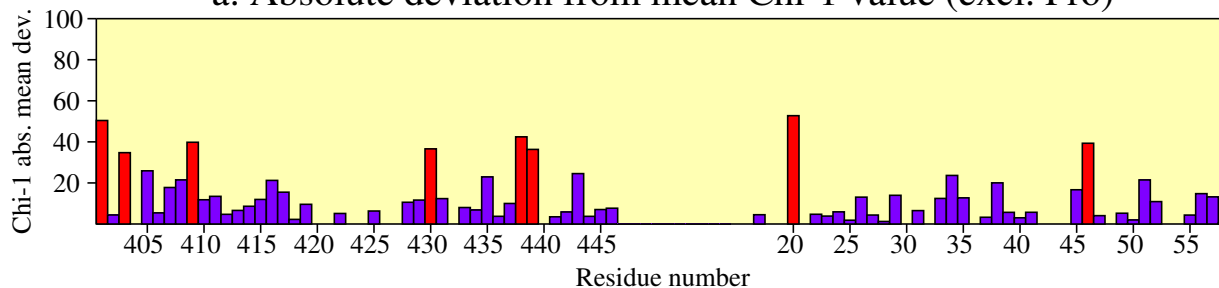


g. G-factors

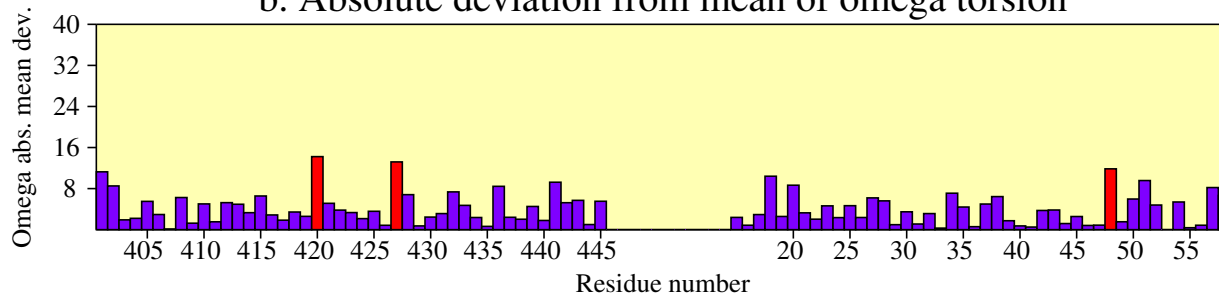


# Residue properties 1SQB

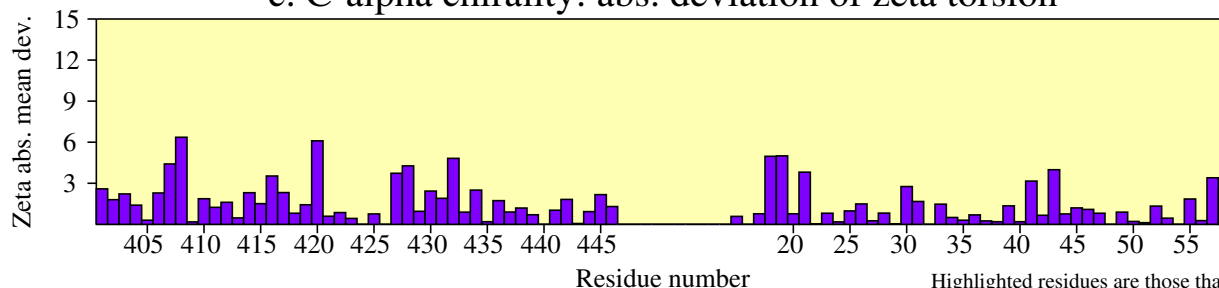
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

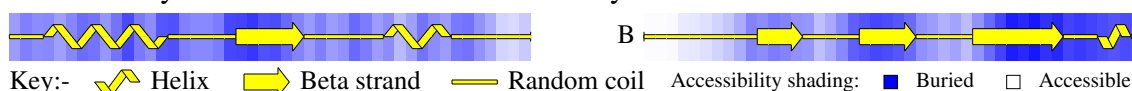


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

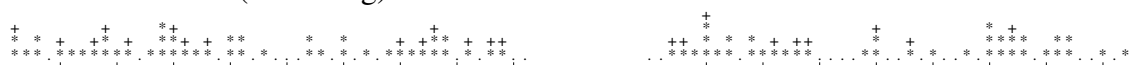
d. Secondary structure & estimated accessibility



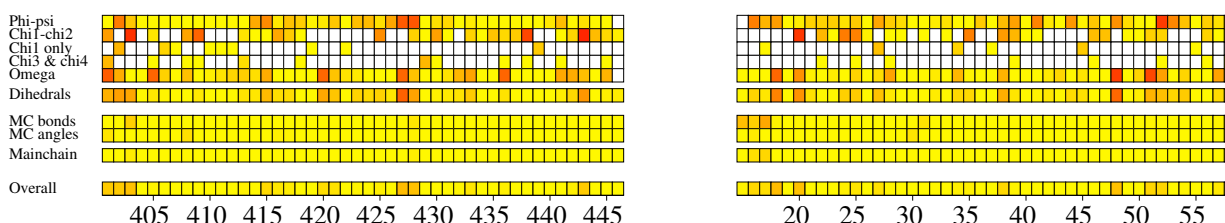
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

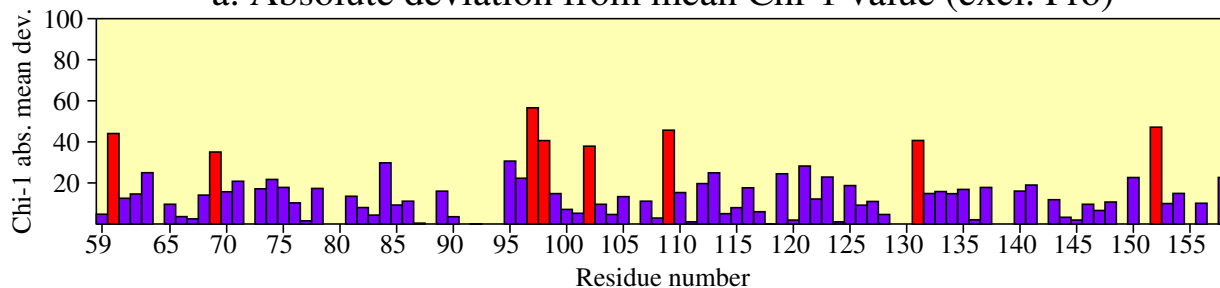


g. G-factors

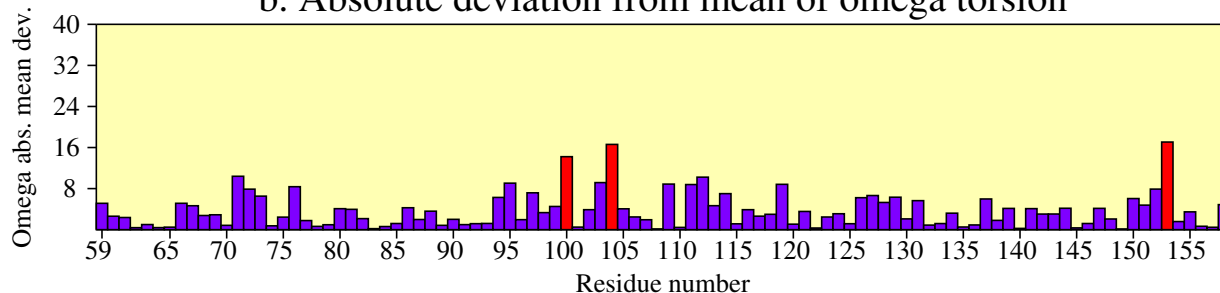


# Residue properties 1SQB

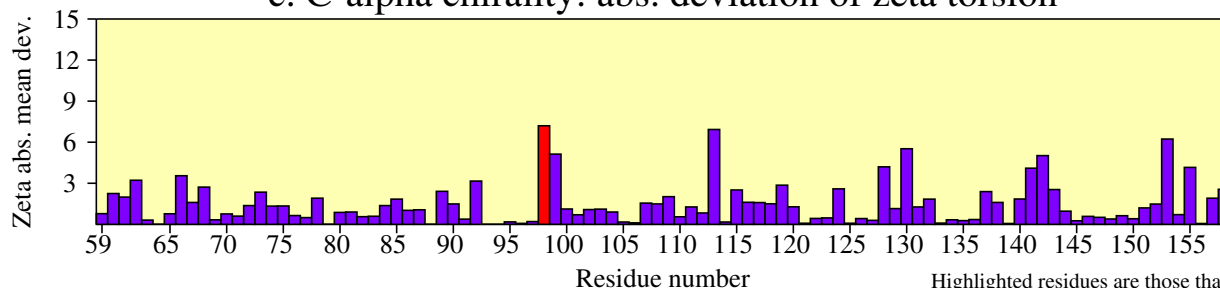
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

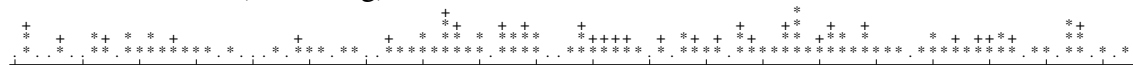
d. Secondary structure & estimated accessibility



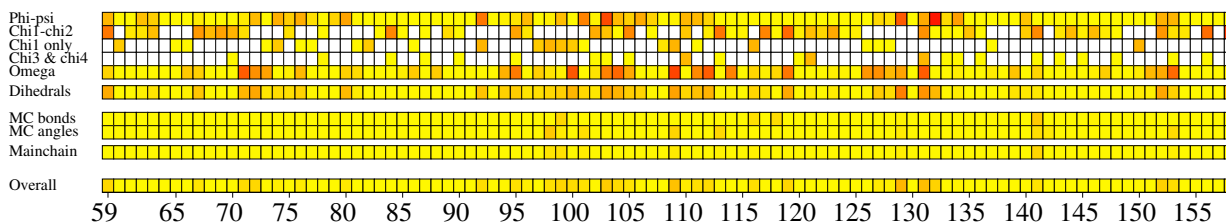
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

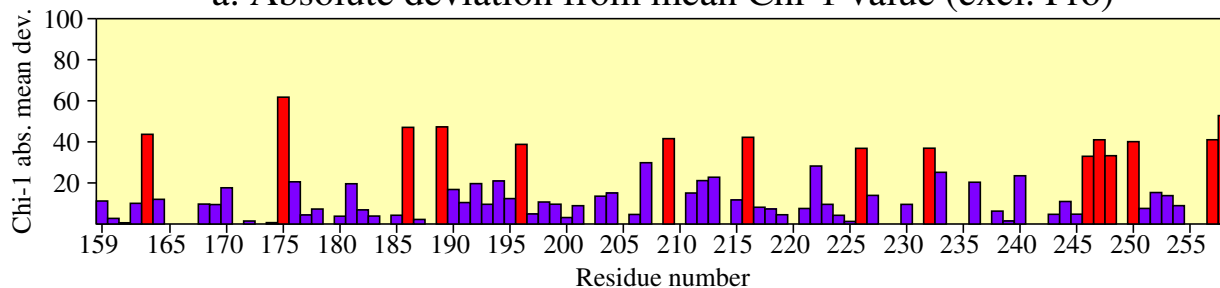


g. G-factors

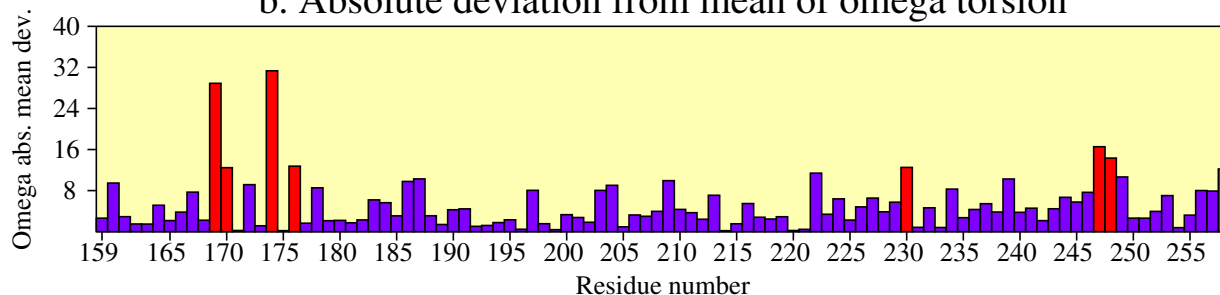


# Residue properties 1SQB

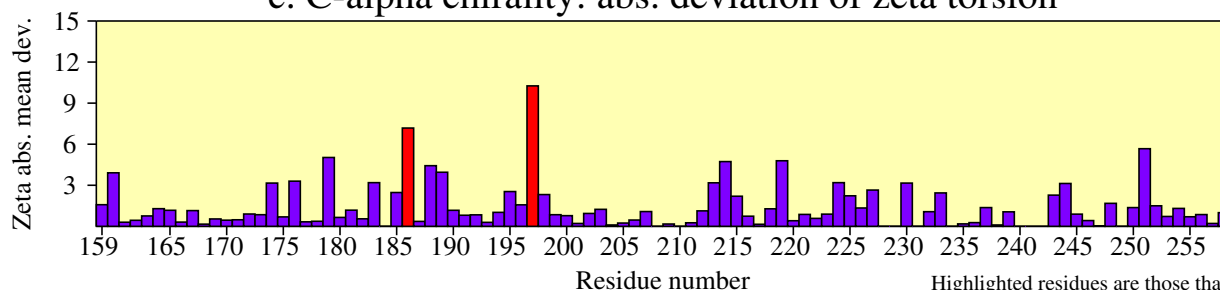
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

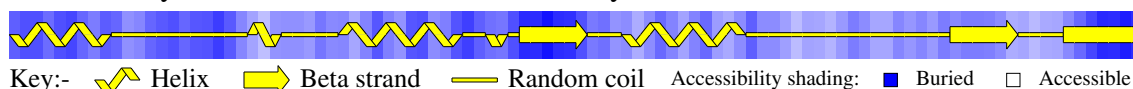


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



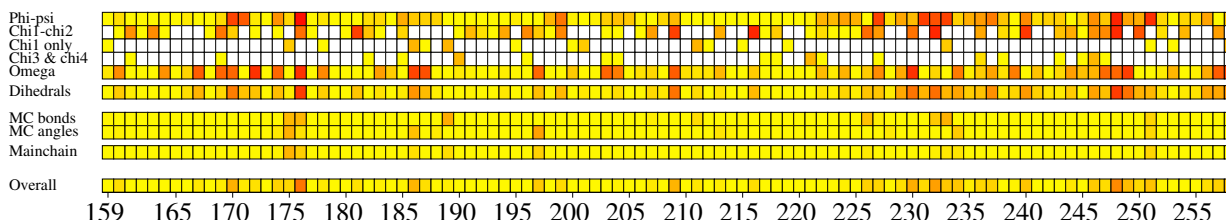
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

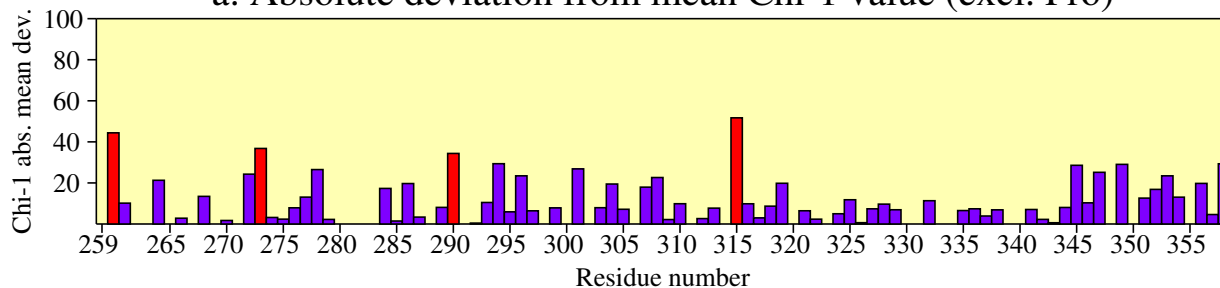


g. G-factors

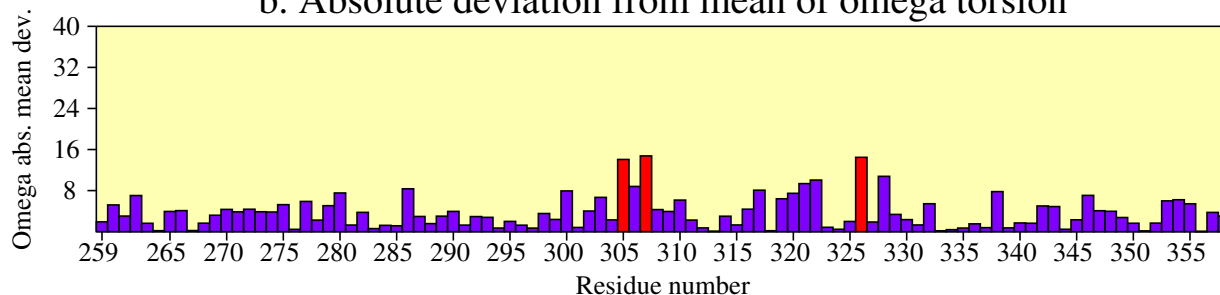


# Residue properties 1SQB

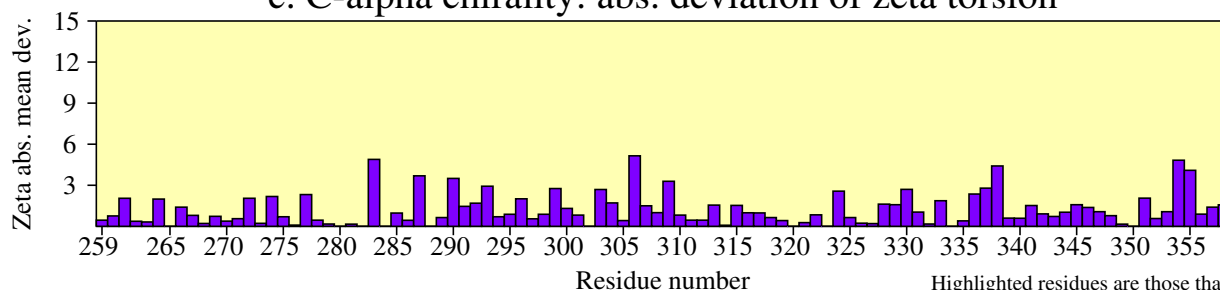
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

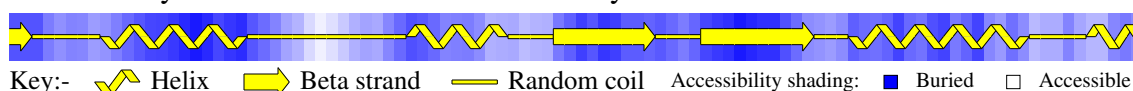


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



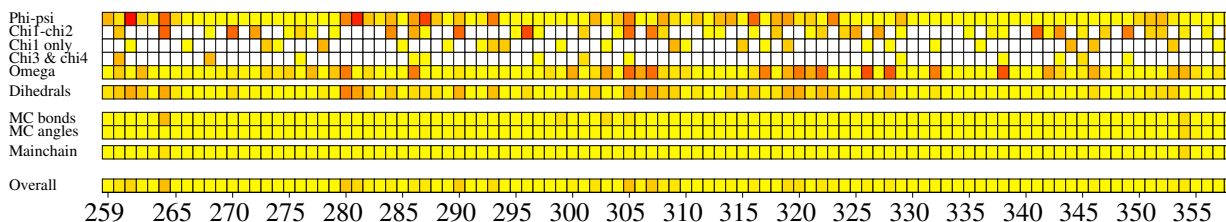
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



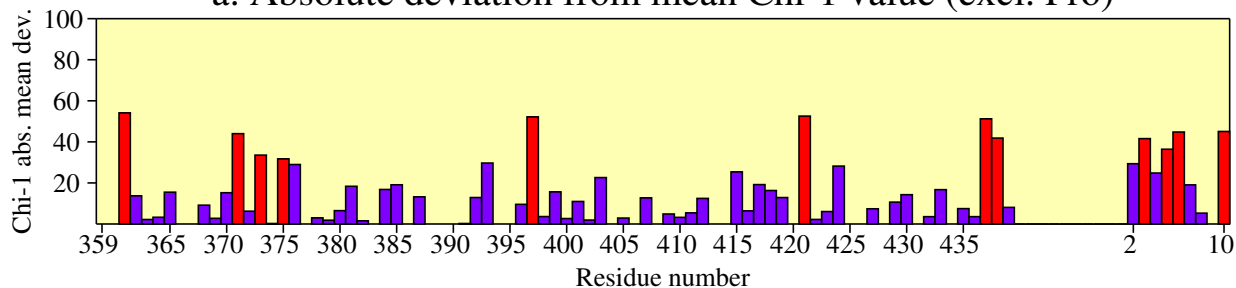
g. G-factors



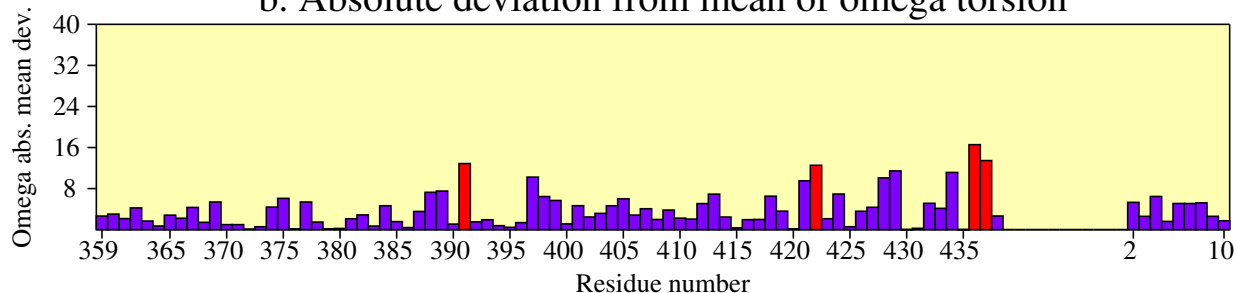


# Residue properties 1SQB

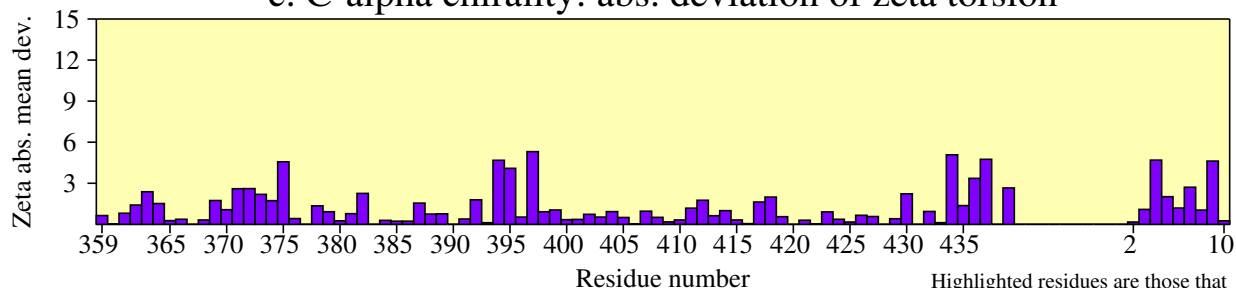
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

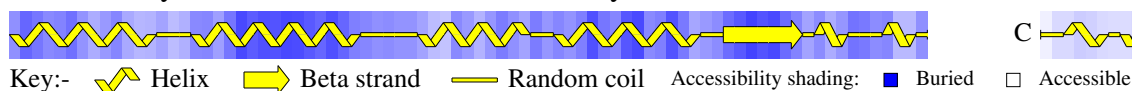


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

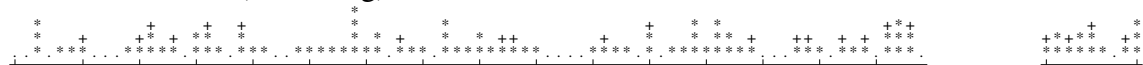
d. Secondary structure & estimated accessibility



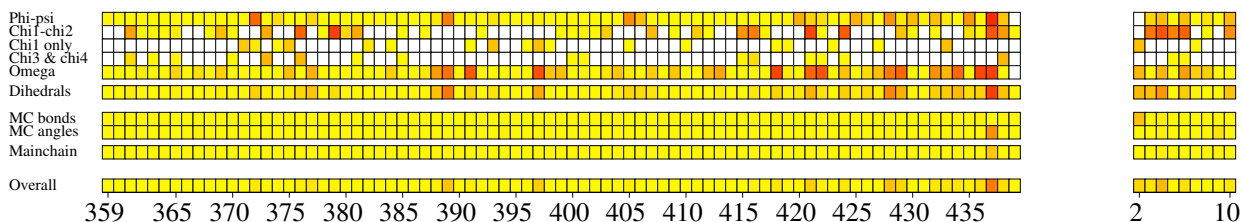
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

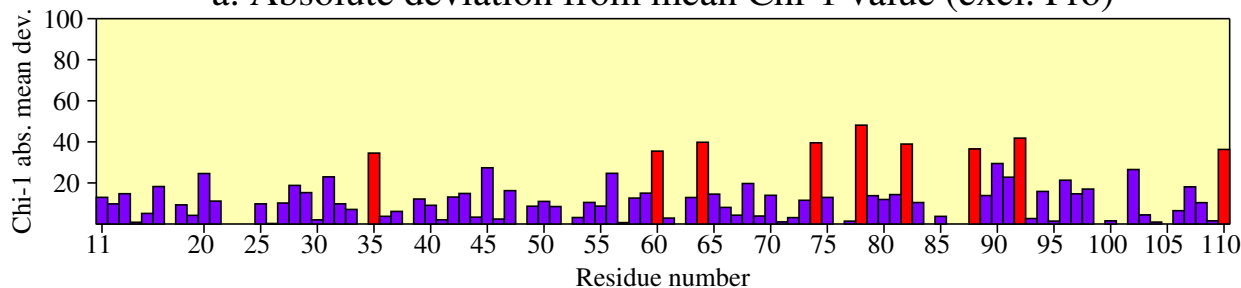


g. G-factors

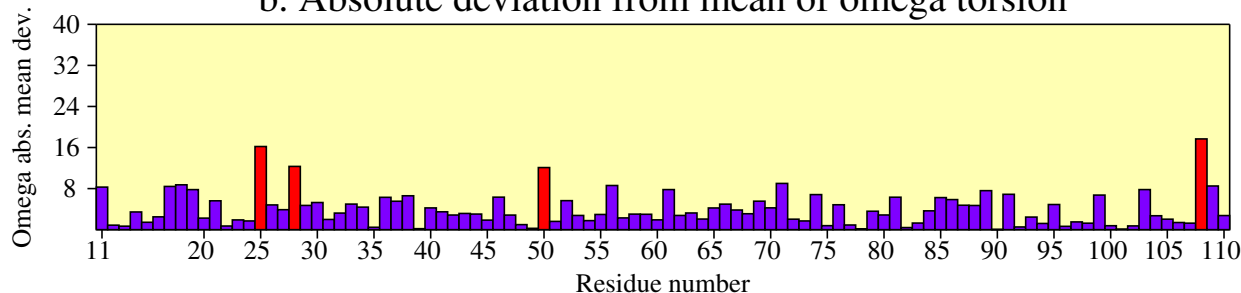


# Residue properties 1SQB

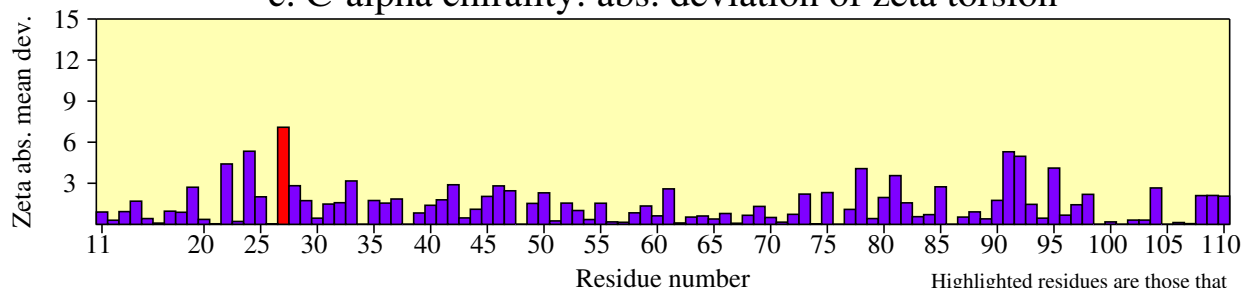
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

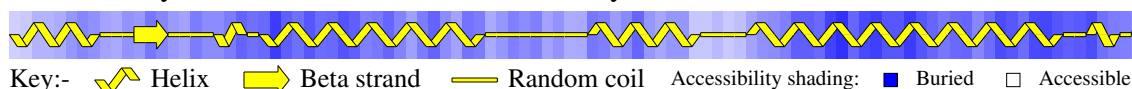


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



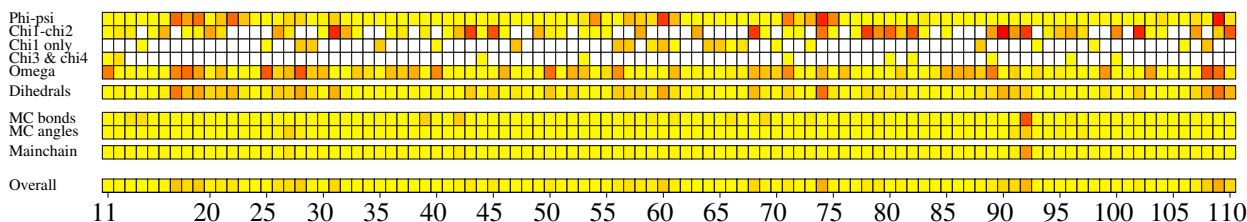
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

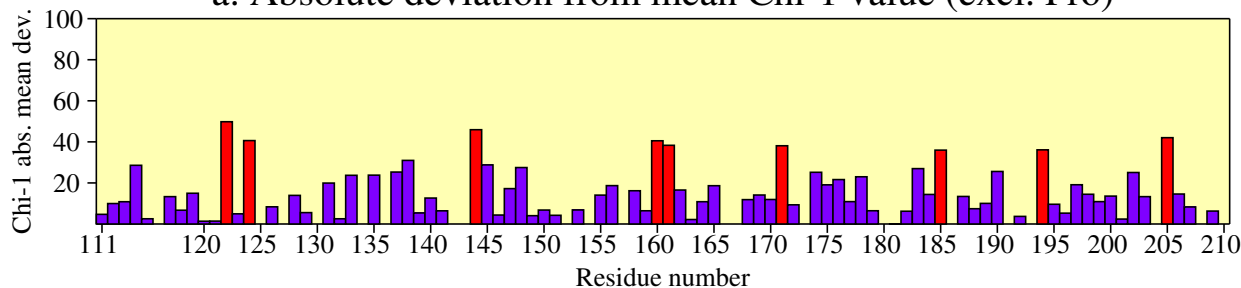


g. G-factors

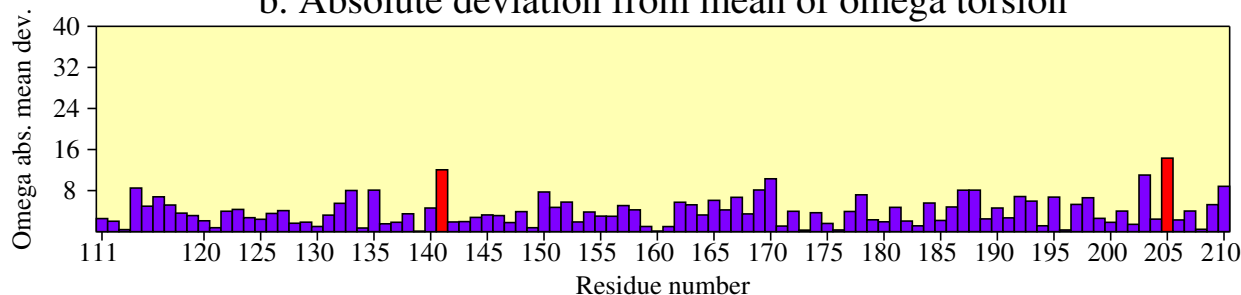


# Residue properties 1SQB

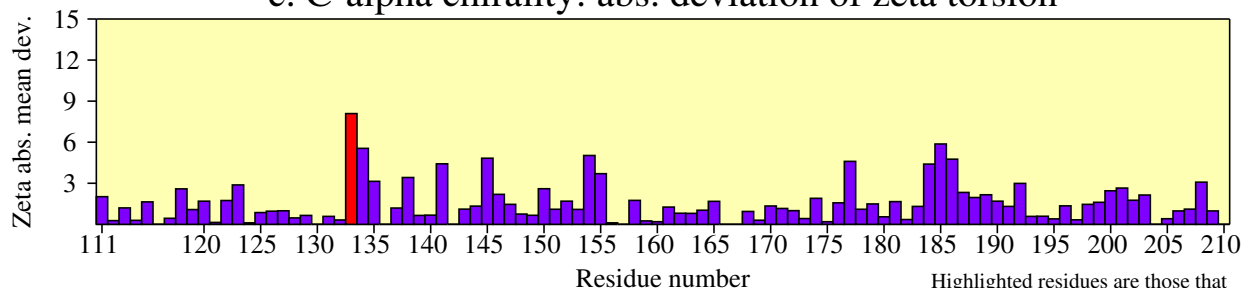
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

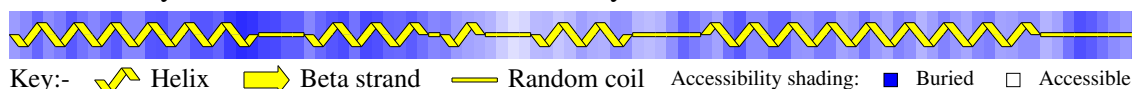


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

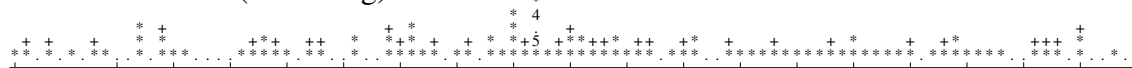
d. Secondary structure & estimated accessibility



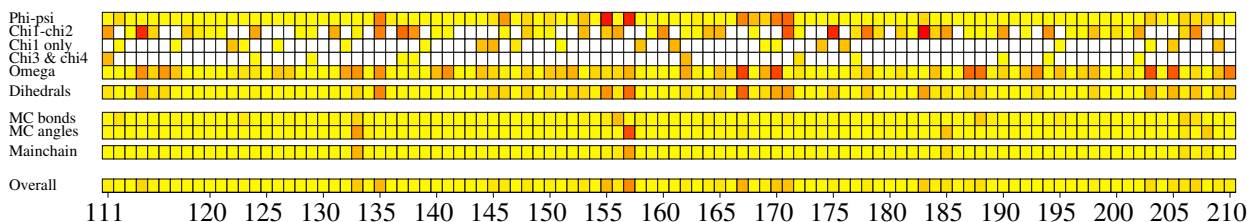
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

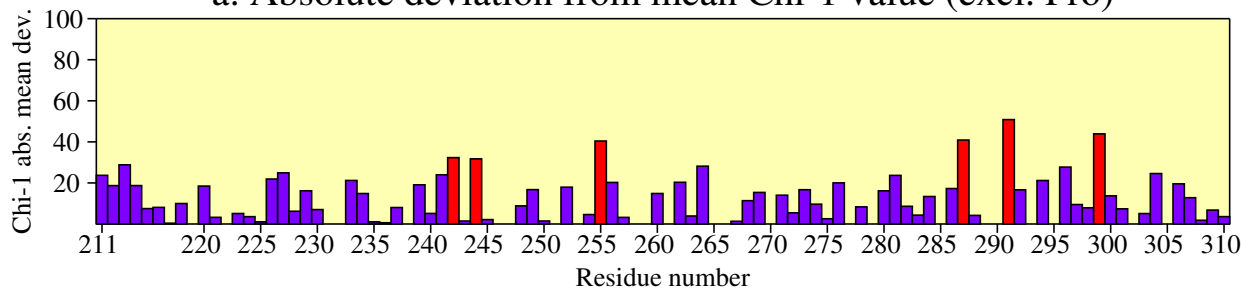


g. G-factors

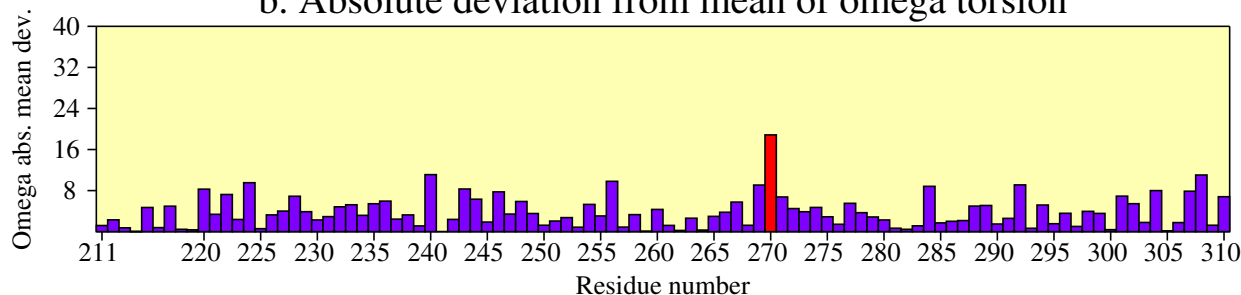


# Residue properties 1SQB

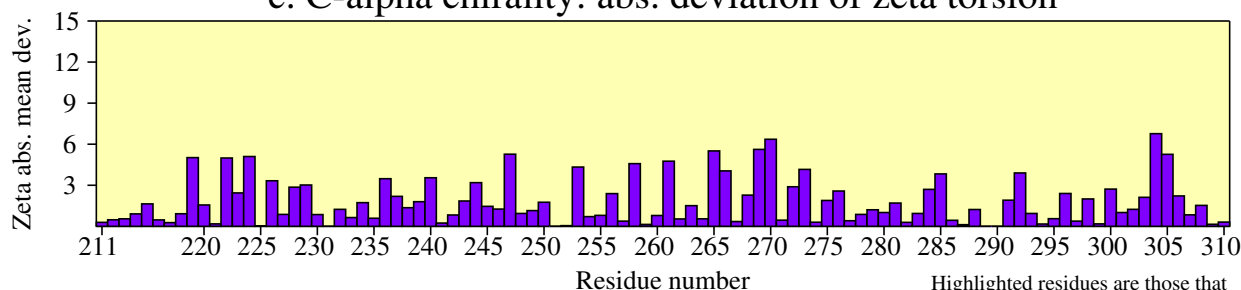
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

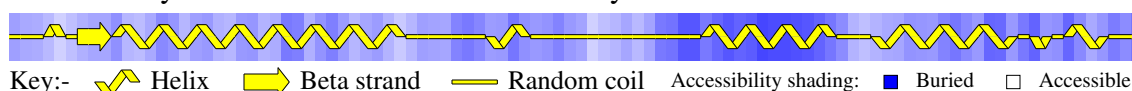


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

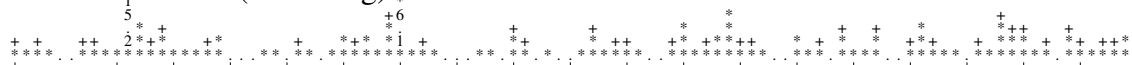


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

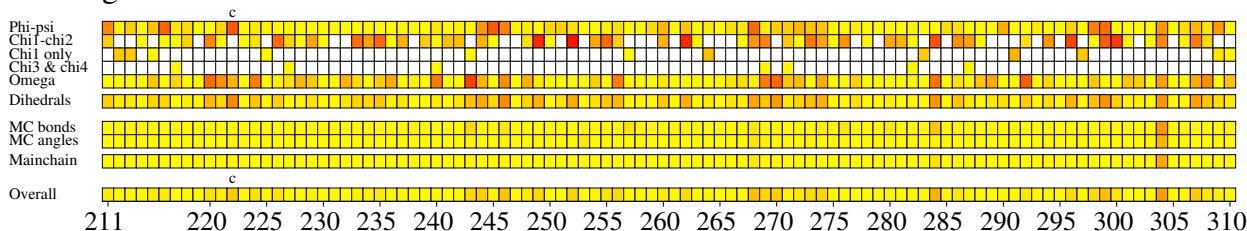
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



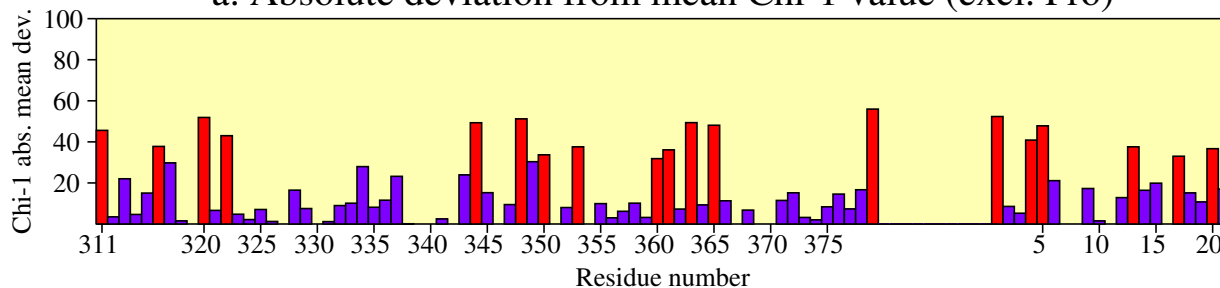
g. G-factors



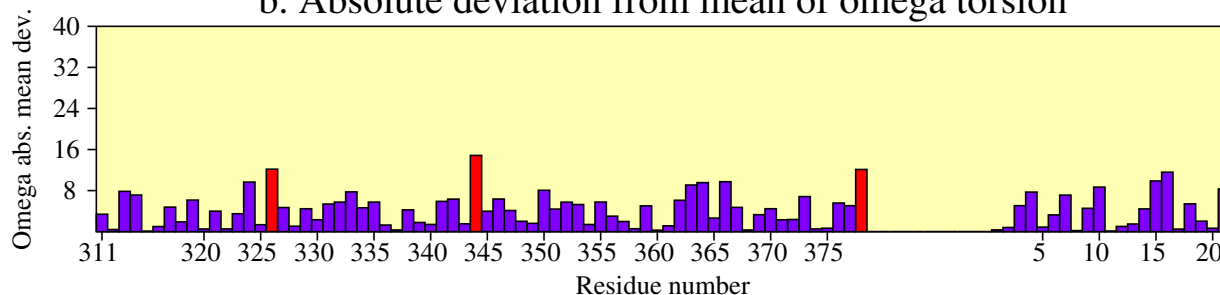
c = cis-peptide

# Residue properties 1SQB

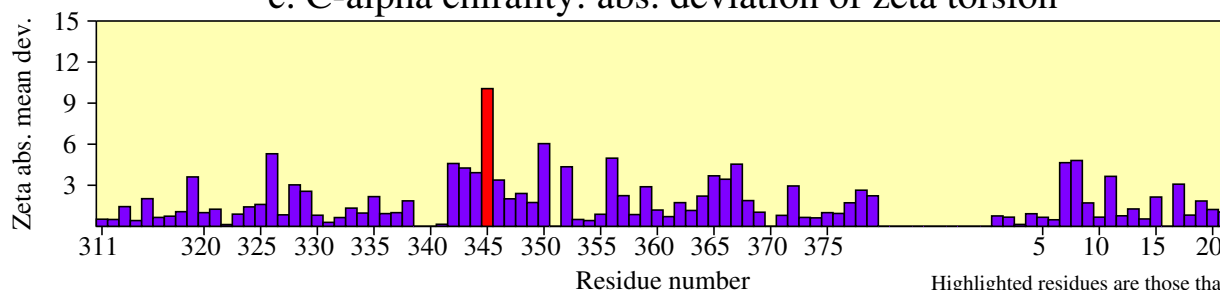
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

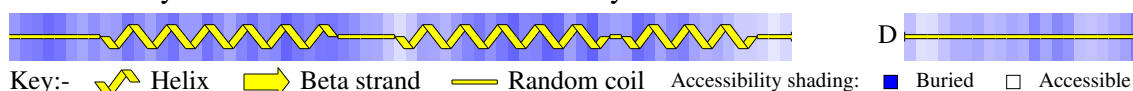


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



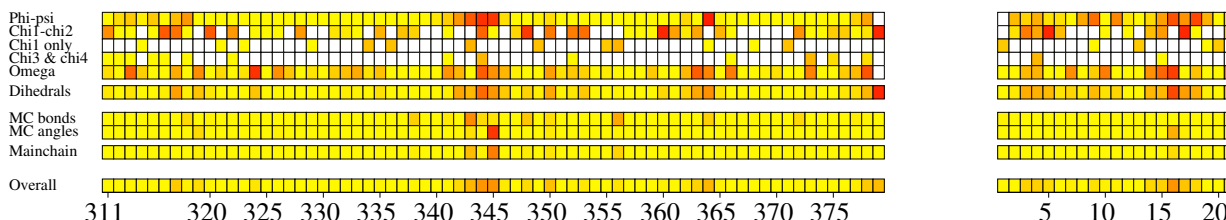
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

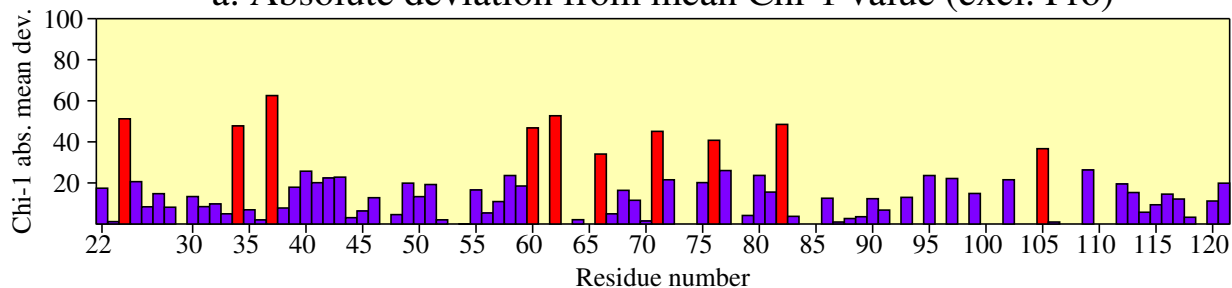


### g. G-factors

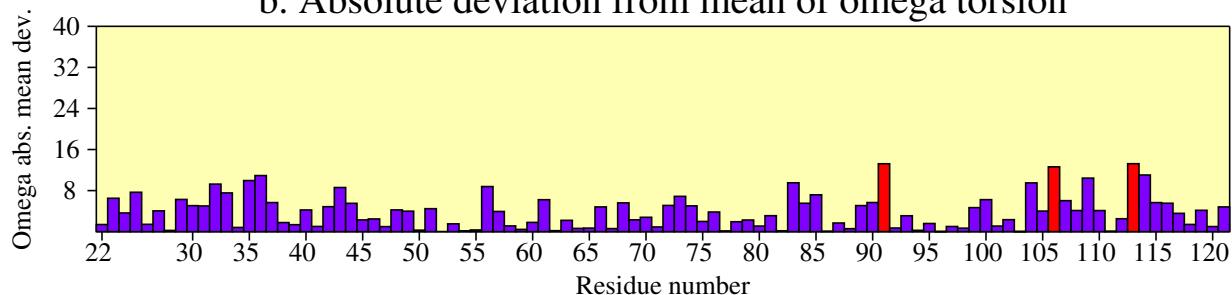


# Residue properties 1SQB

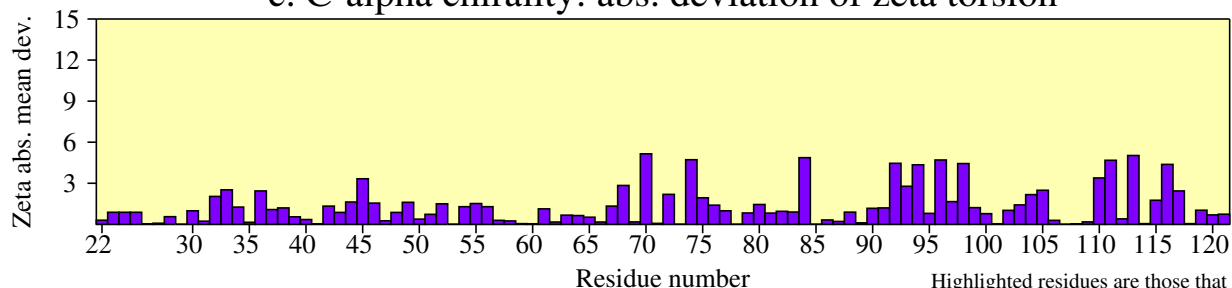
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

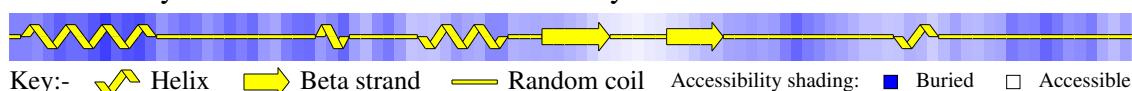


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



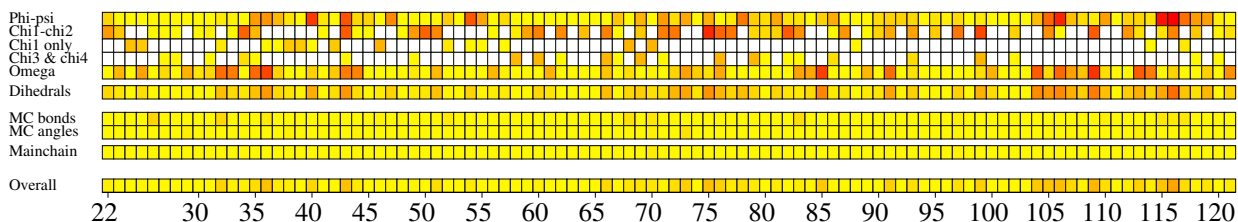
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

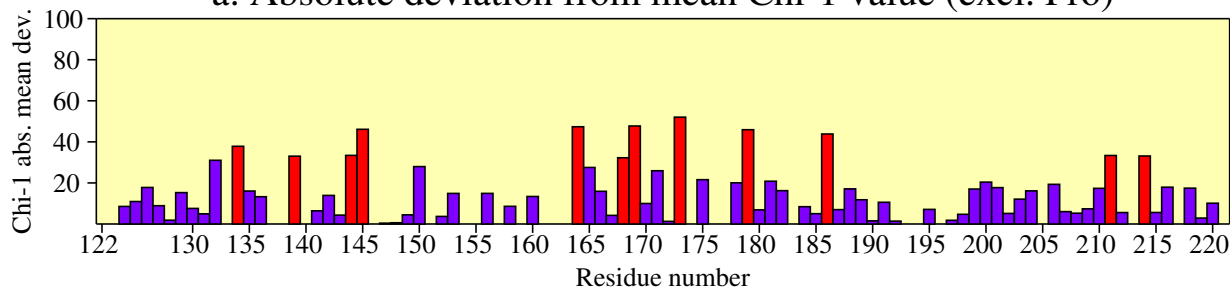


g. G-factors

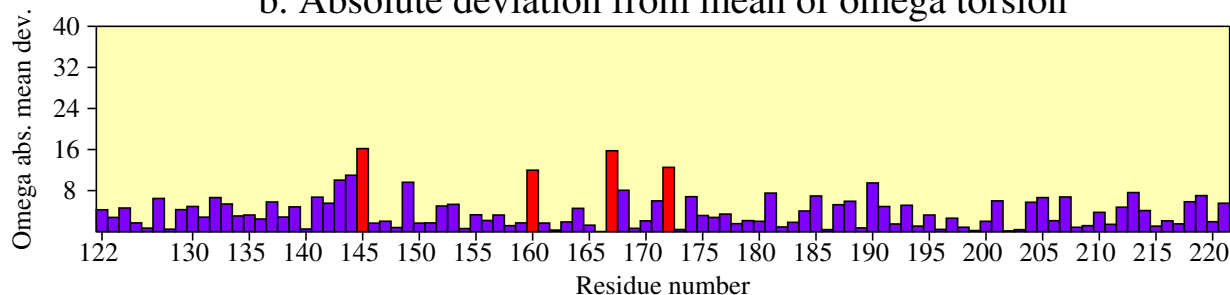


# Residue properties 1SQB

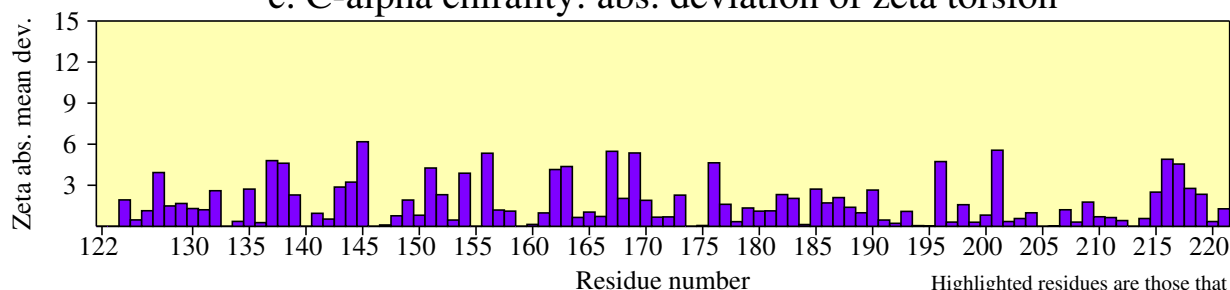
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

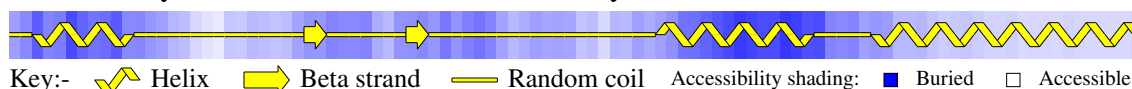


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



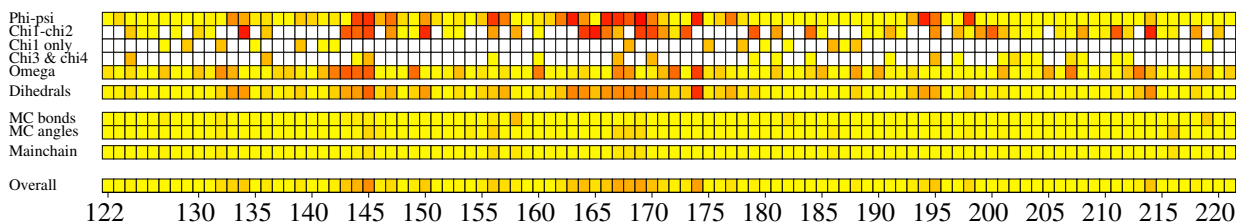
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

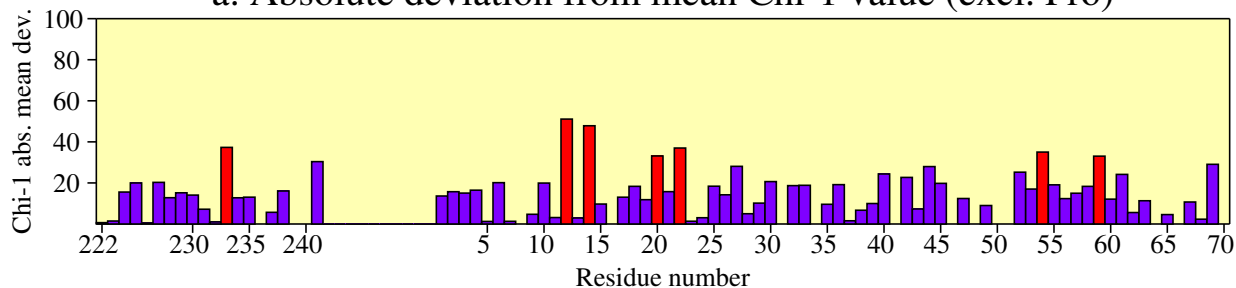


g. G-factors

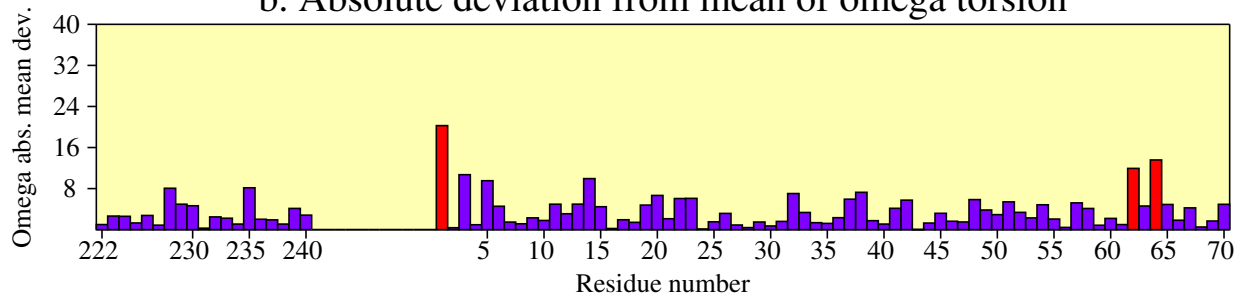


# Residue properties 1SQB

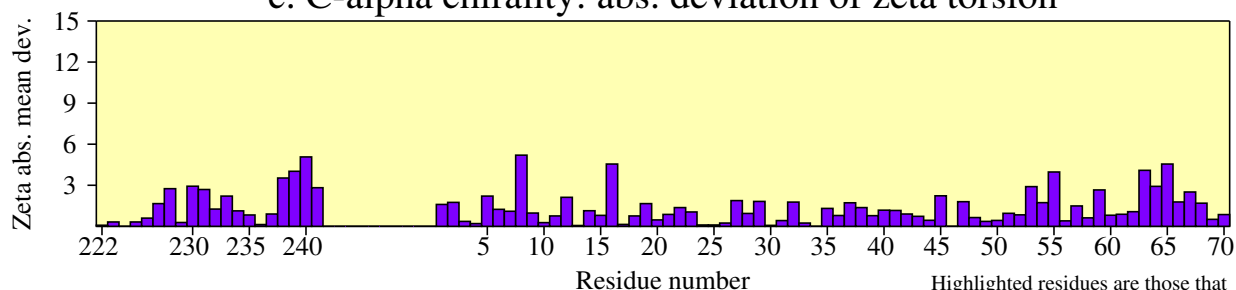
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

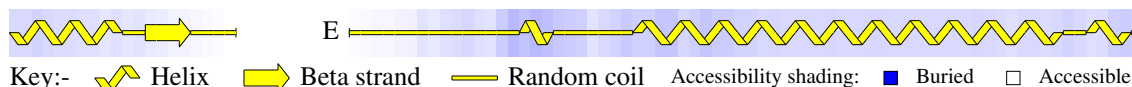


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

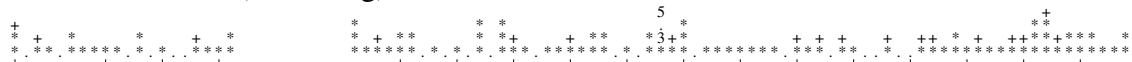
### d. Secondary structure & estimated accessibility



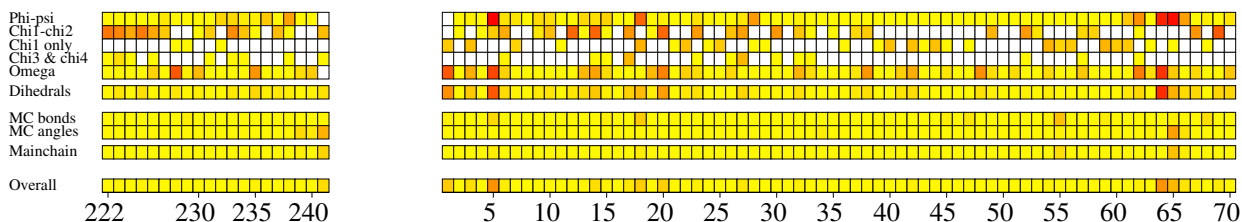
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)



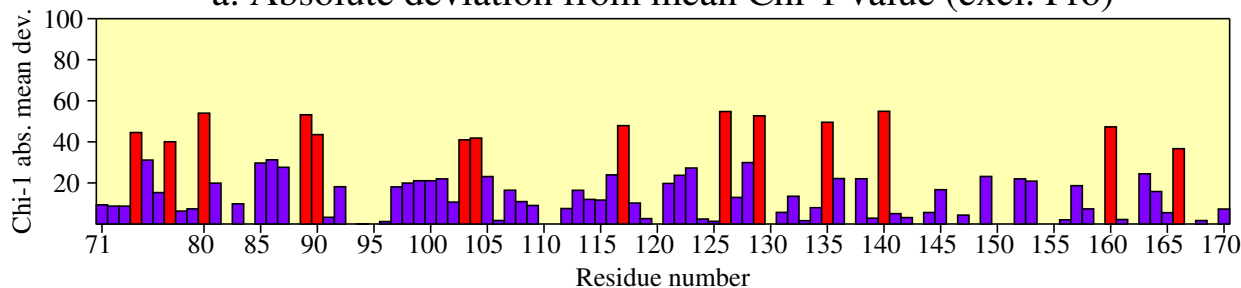
### g. G-factors



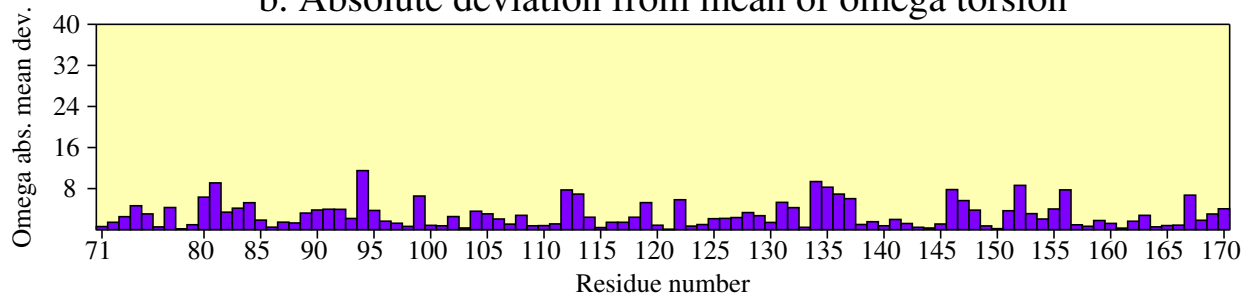


# Residue properties 1SQB

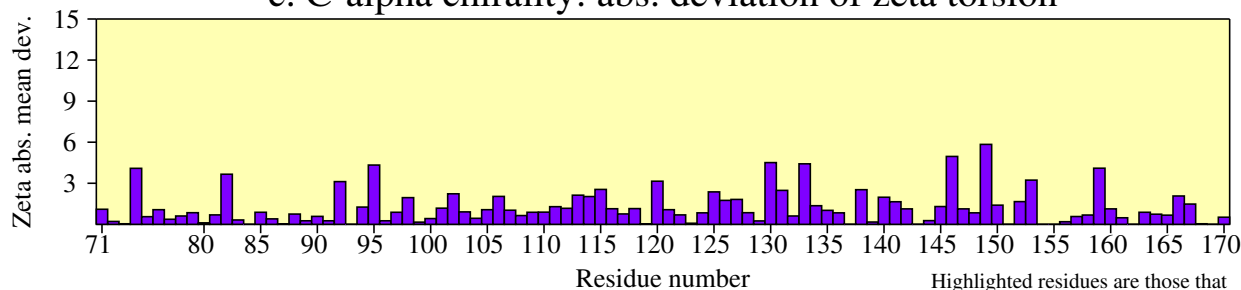
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

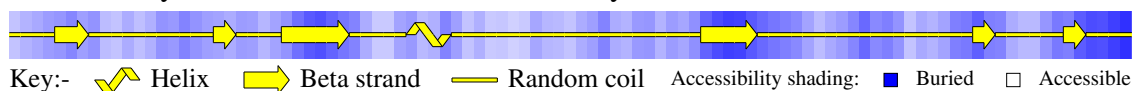


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



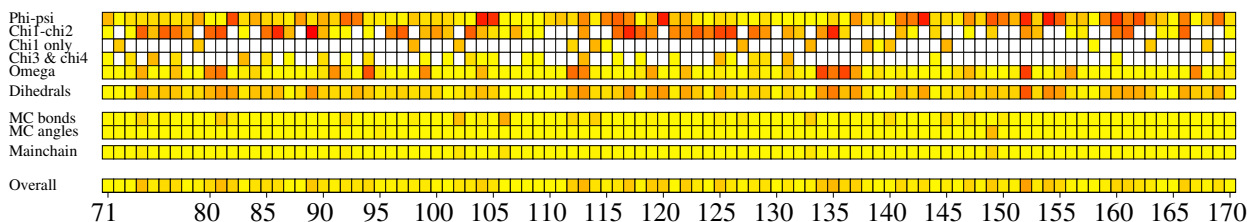
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

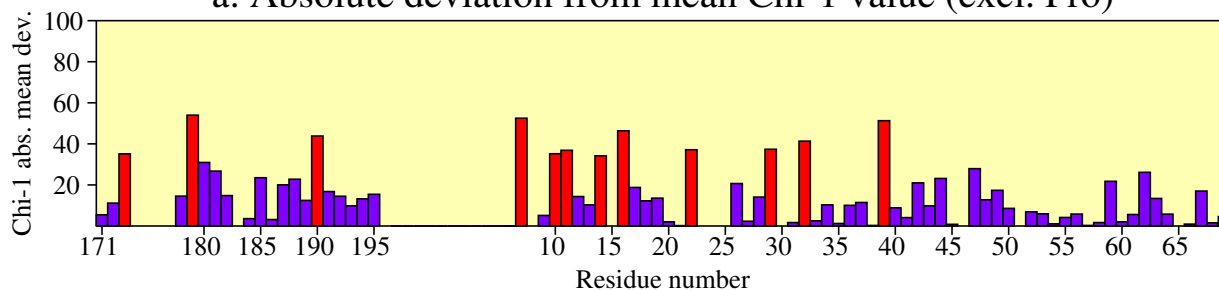


g. G-factors

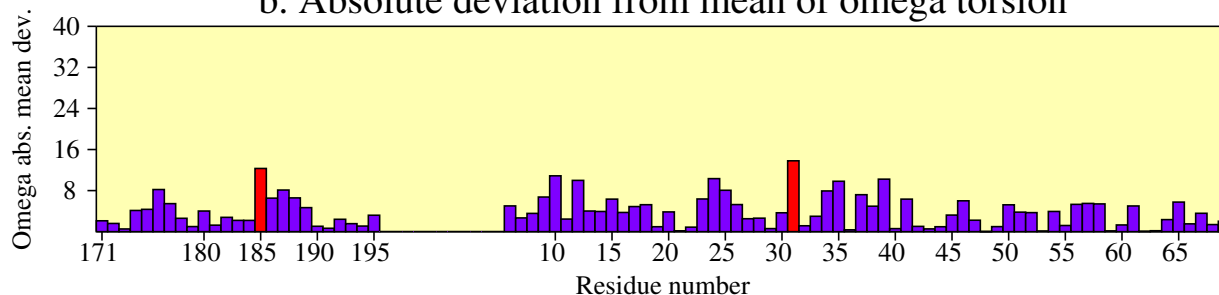


# Residue properties 1SQB

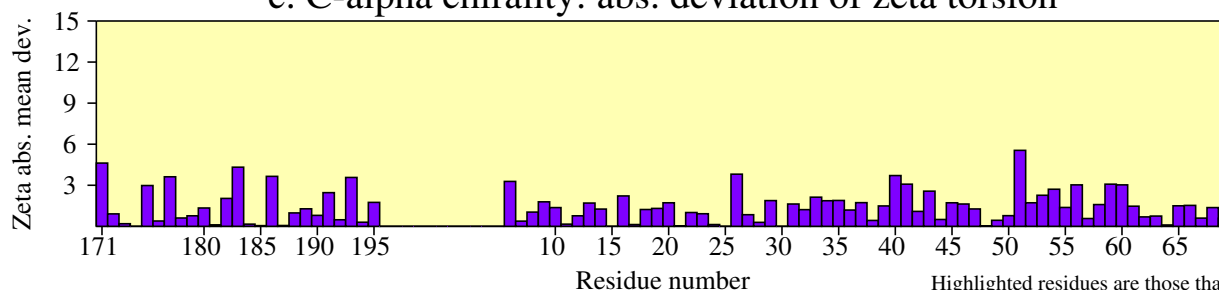
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

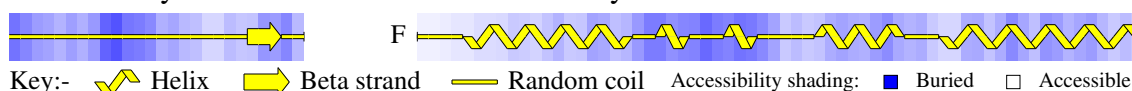


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

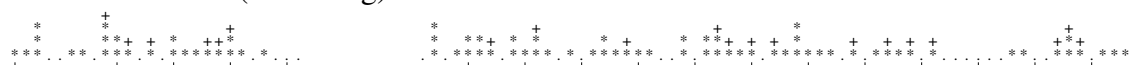
d. Secondary structure & estimated accessibility



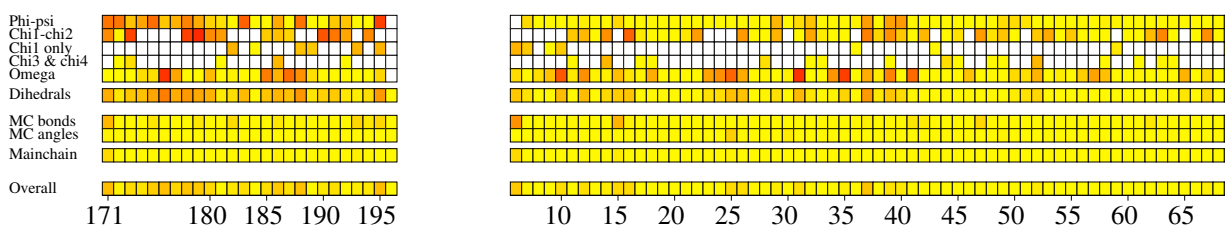
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

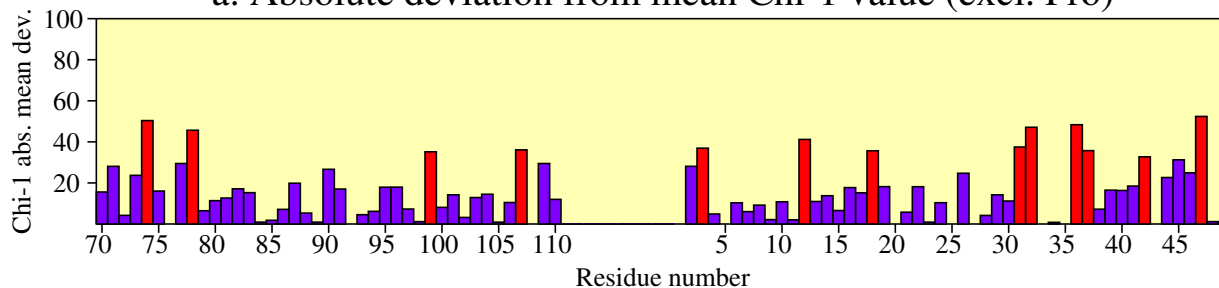


g. G-factors

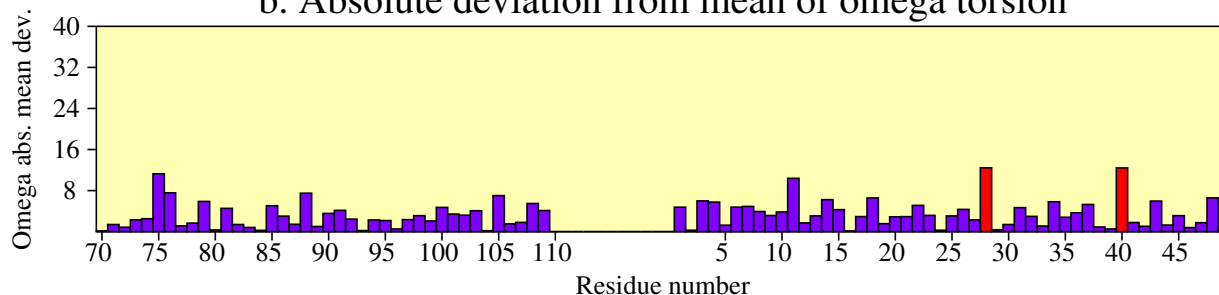


# Residue properties 1SQB

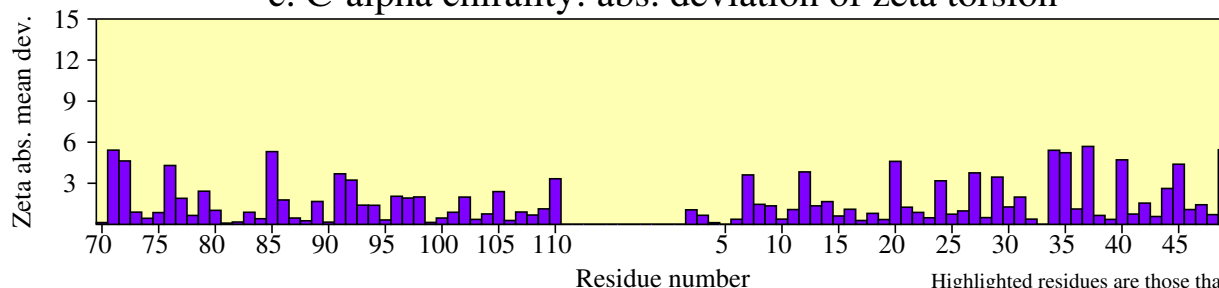
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

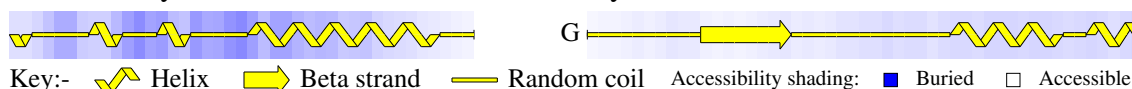


### c. C-alpha chirality: abs. deviation of zeta torsion

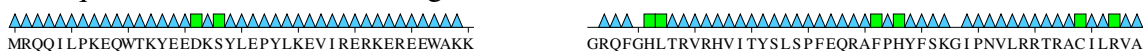


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



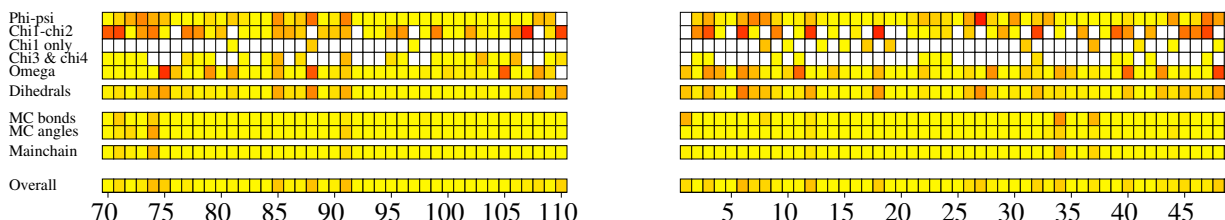
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

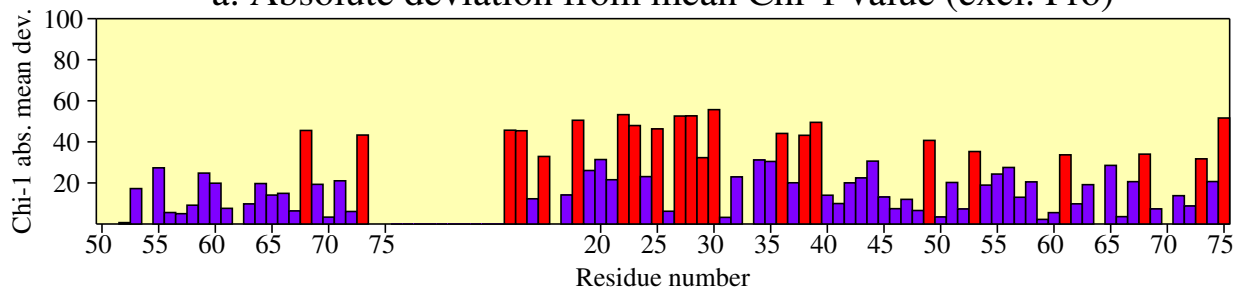


### g. G-factors

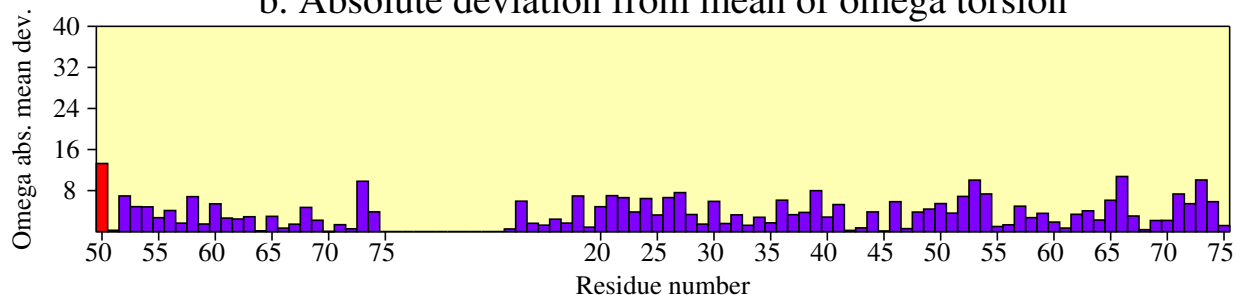


# Residue properties 1SQB

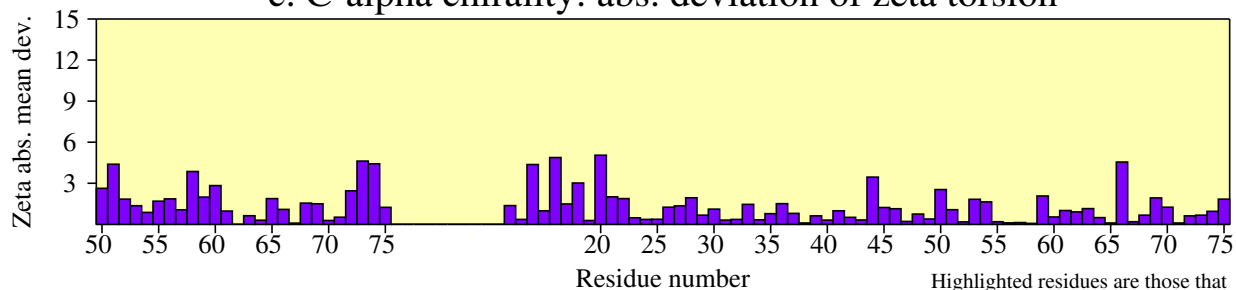
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

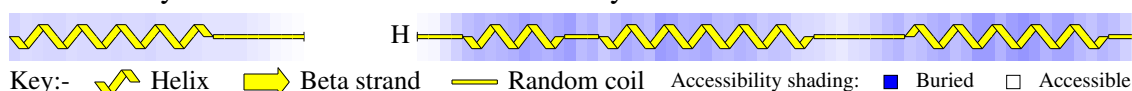


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

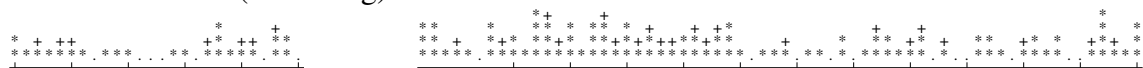
d. Secondary structure & estimated accessibility



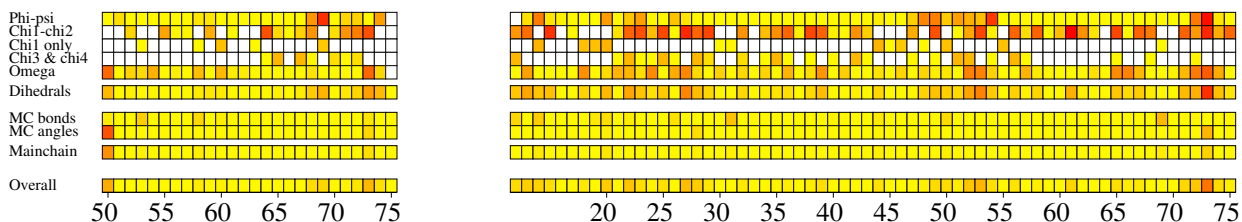
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

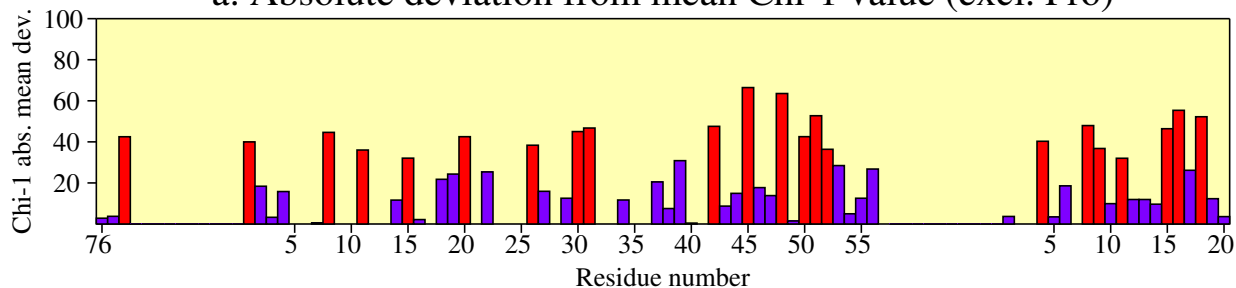


g. G-factors

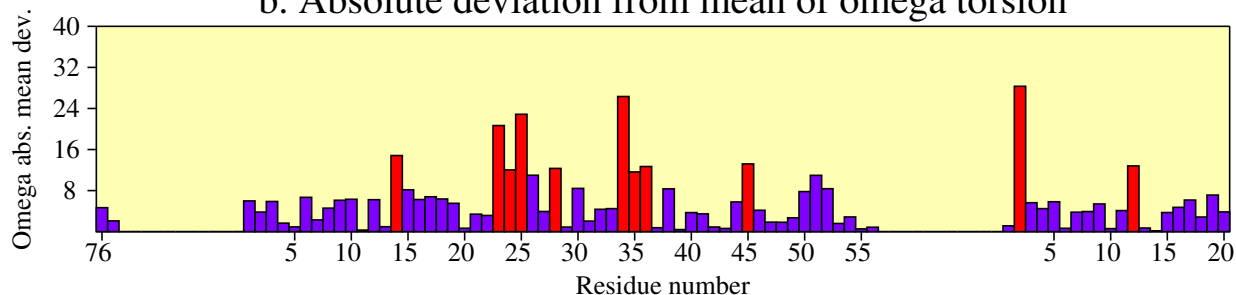


# Residue properties 1SQB

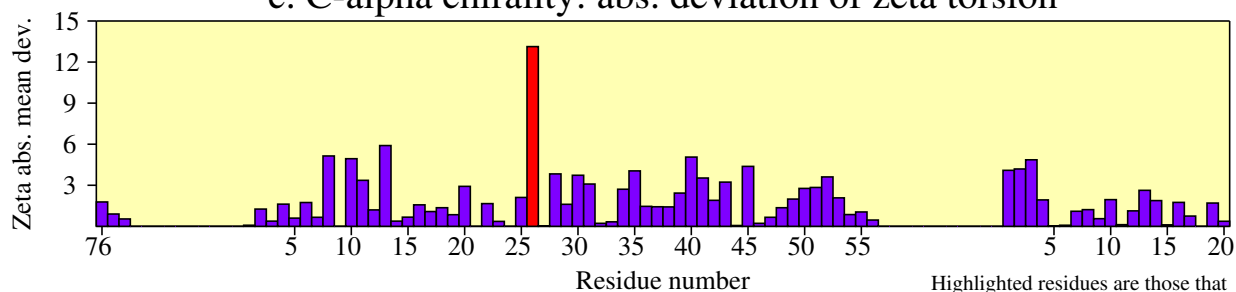
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

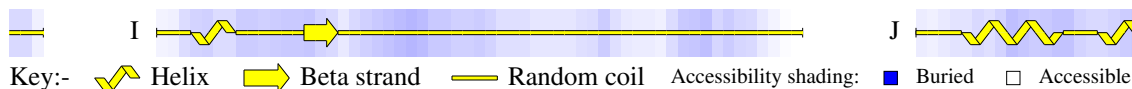


### c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

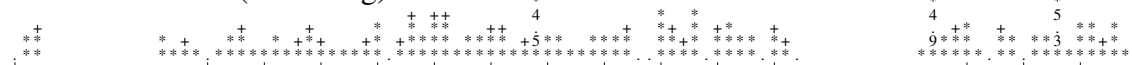
### d. Secondary structure & estimated accessibility



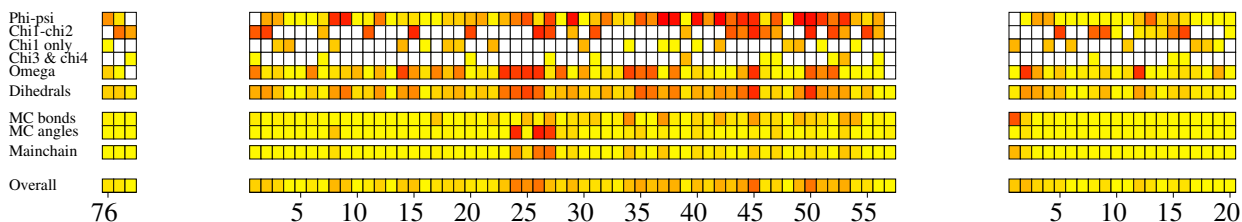
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

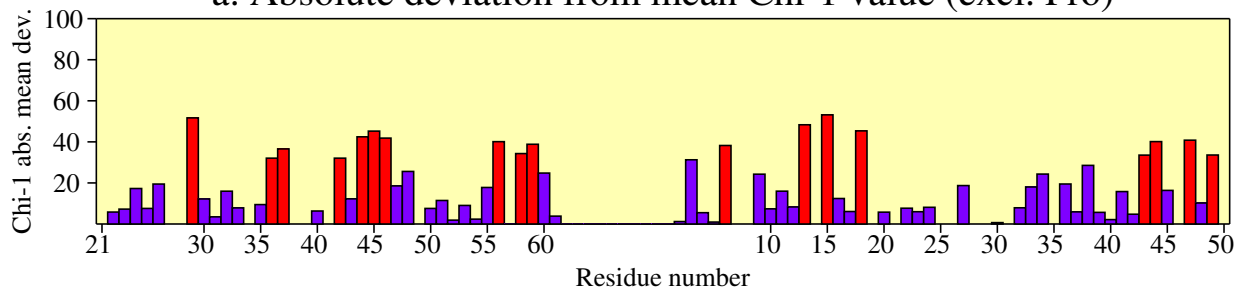


### g. G-factors

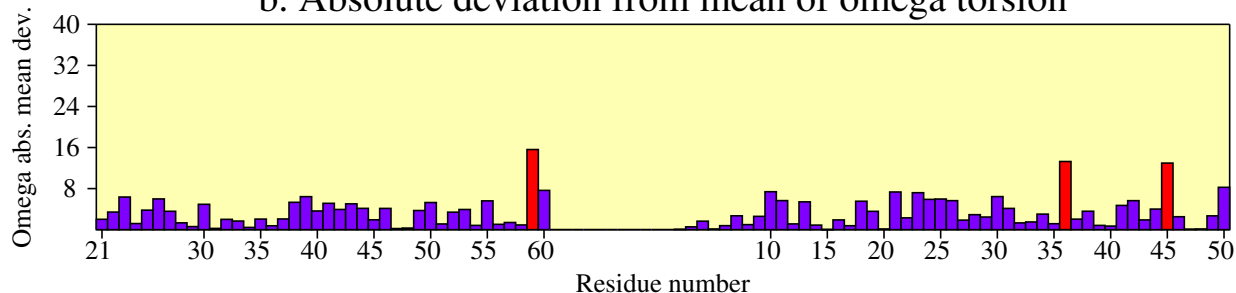


# Residue properties 1SQB

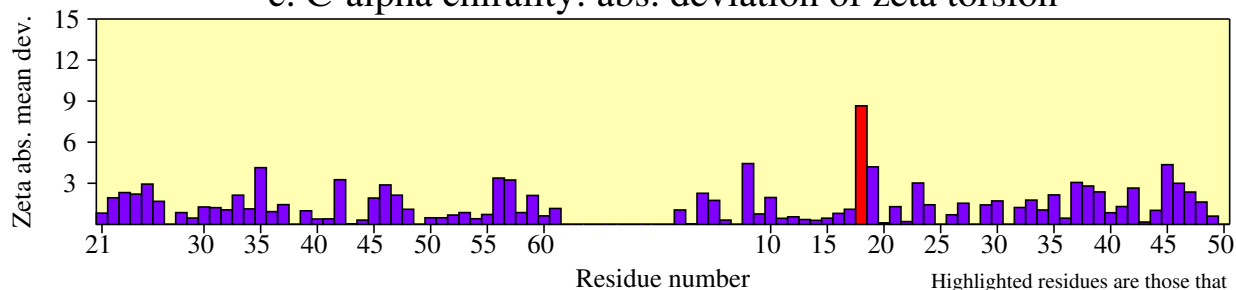
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

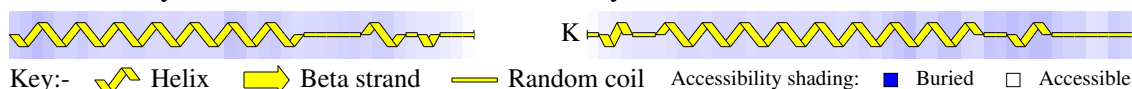


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



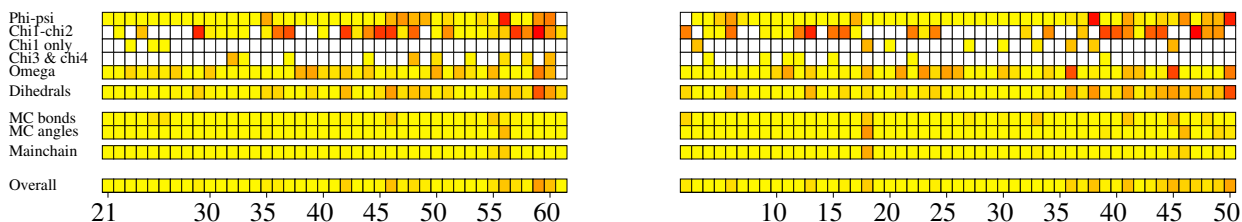
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

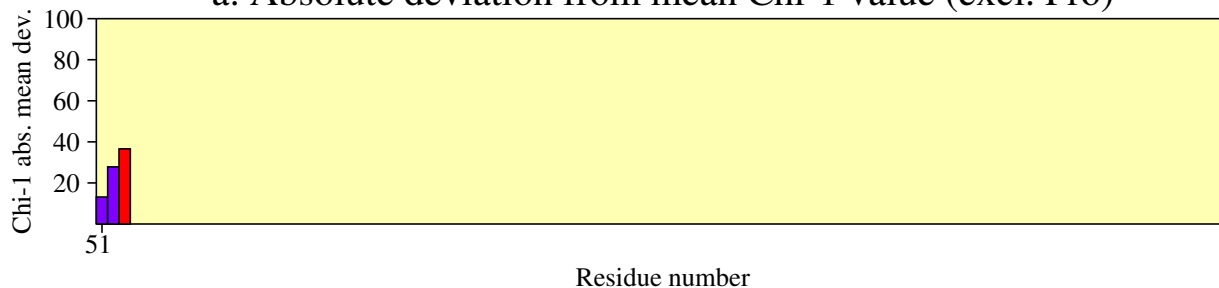


g. G-factors

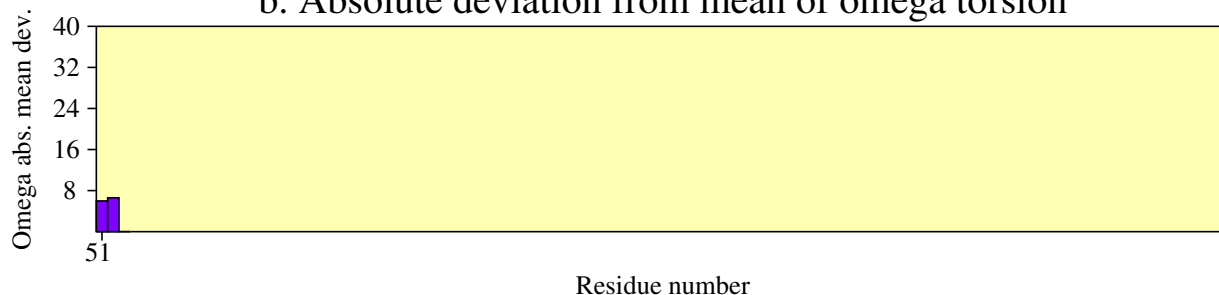


# Residue properties 1SQB

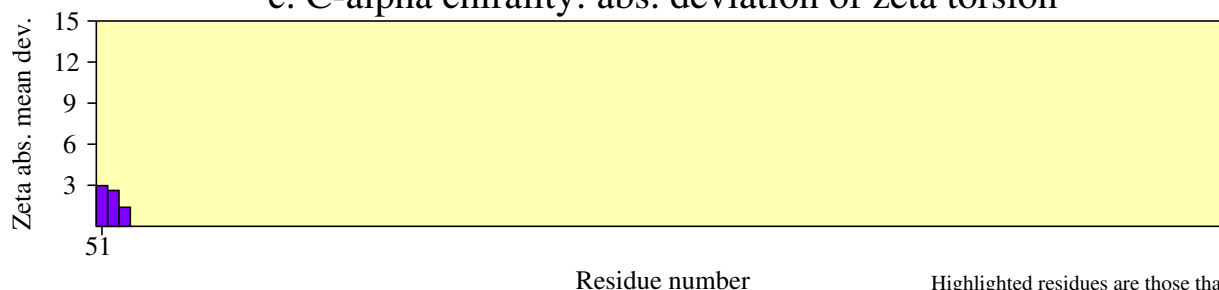
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

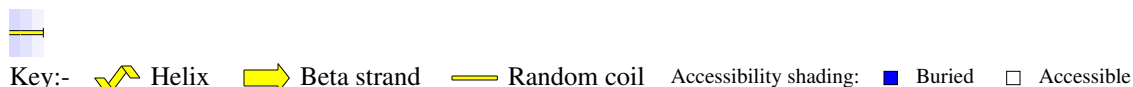


c. C-alpha chirality: abs. deviation of zeta torsion



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



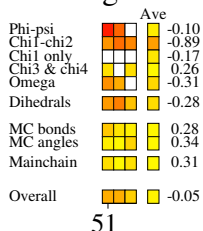
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

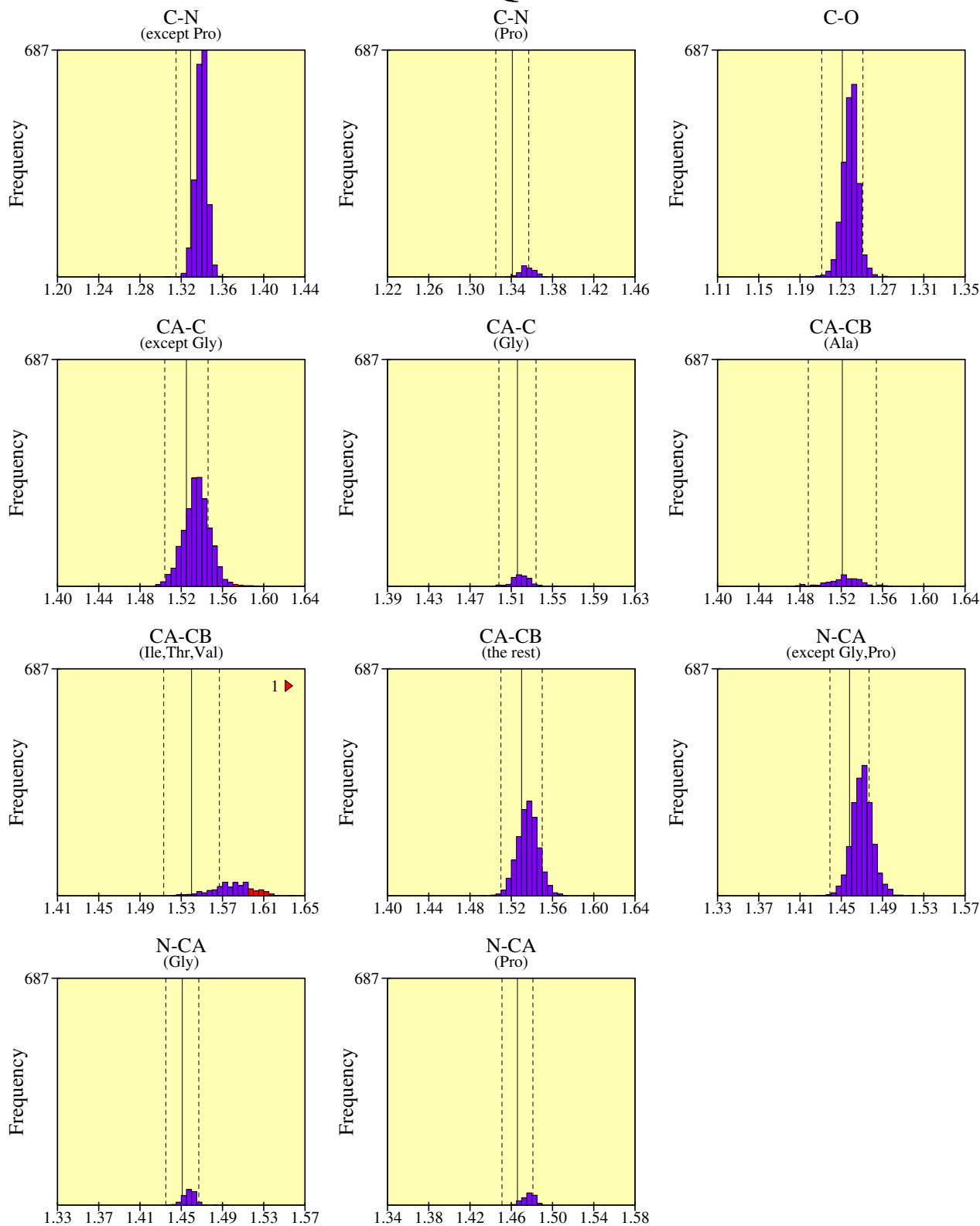


g. G-factors



# Main-chain bond lengths

## 1SQB



Black bars > 2.0 st. devs. from mean.

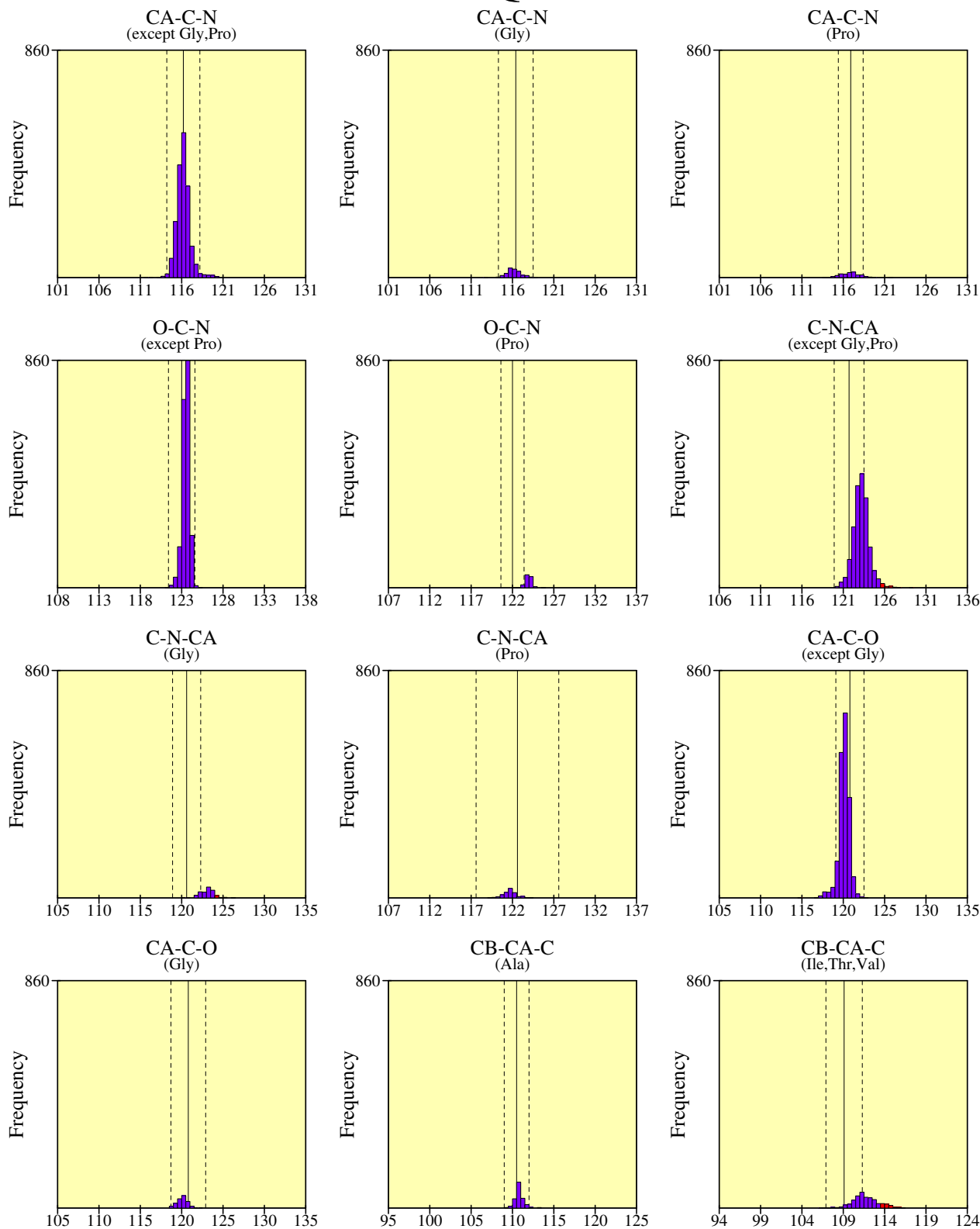
◀ or ▶ signifies data points off the graph in the direction shown.

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



# Main-chain bond angles

## 1SQB

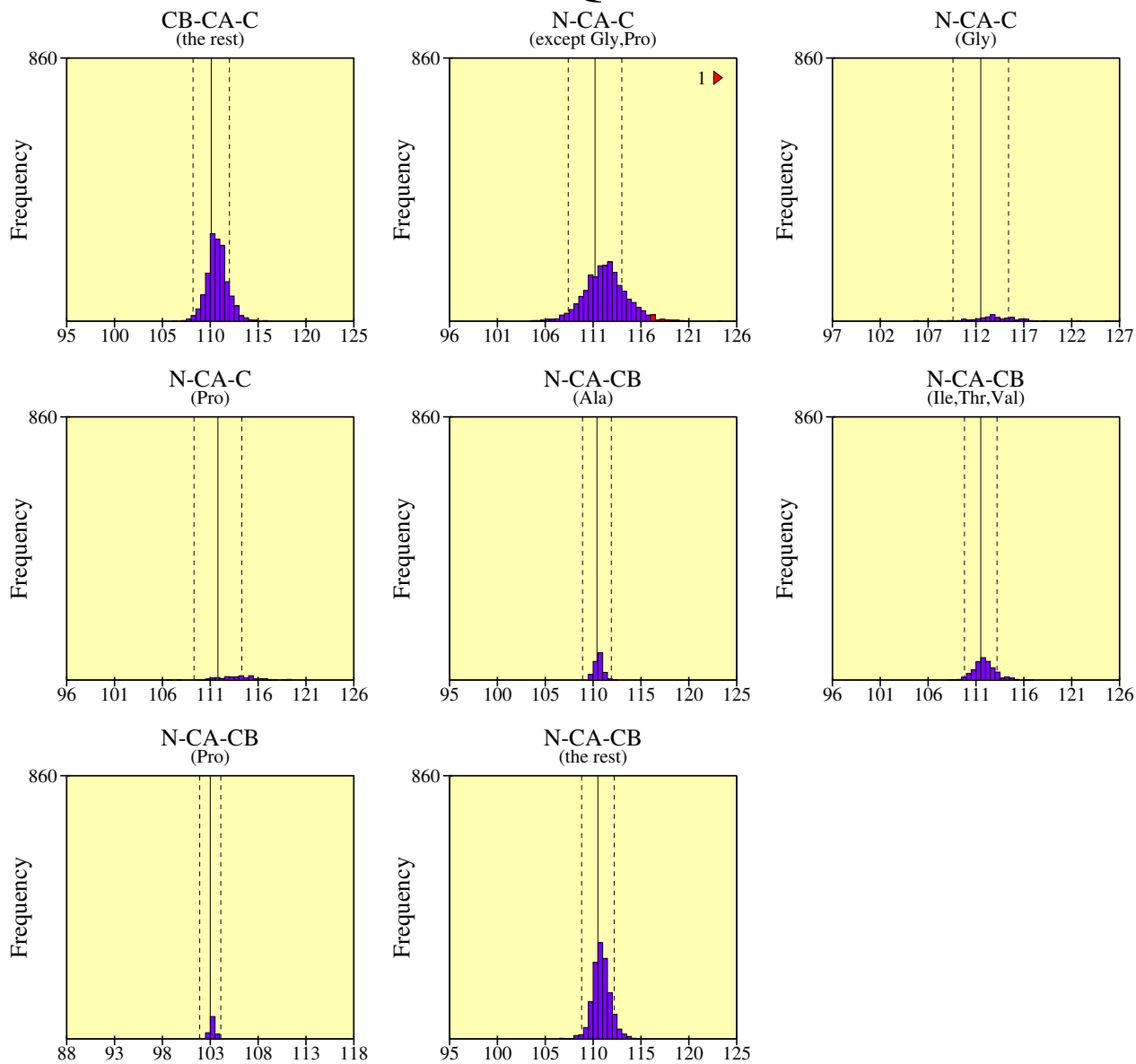


Black bars > 2.0 st. devs. from mean.

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

# Main-chain bond angles

## 1SQB



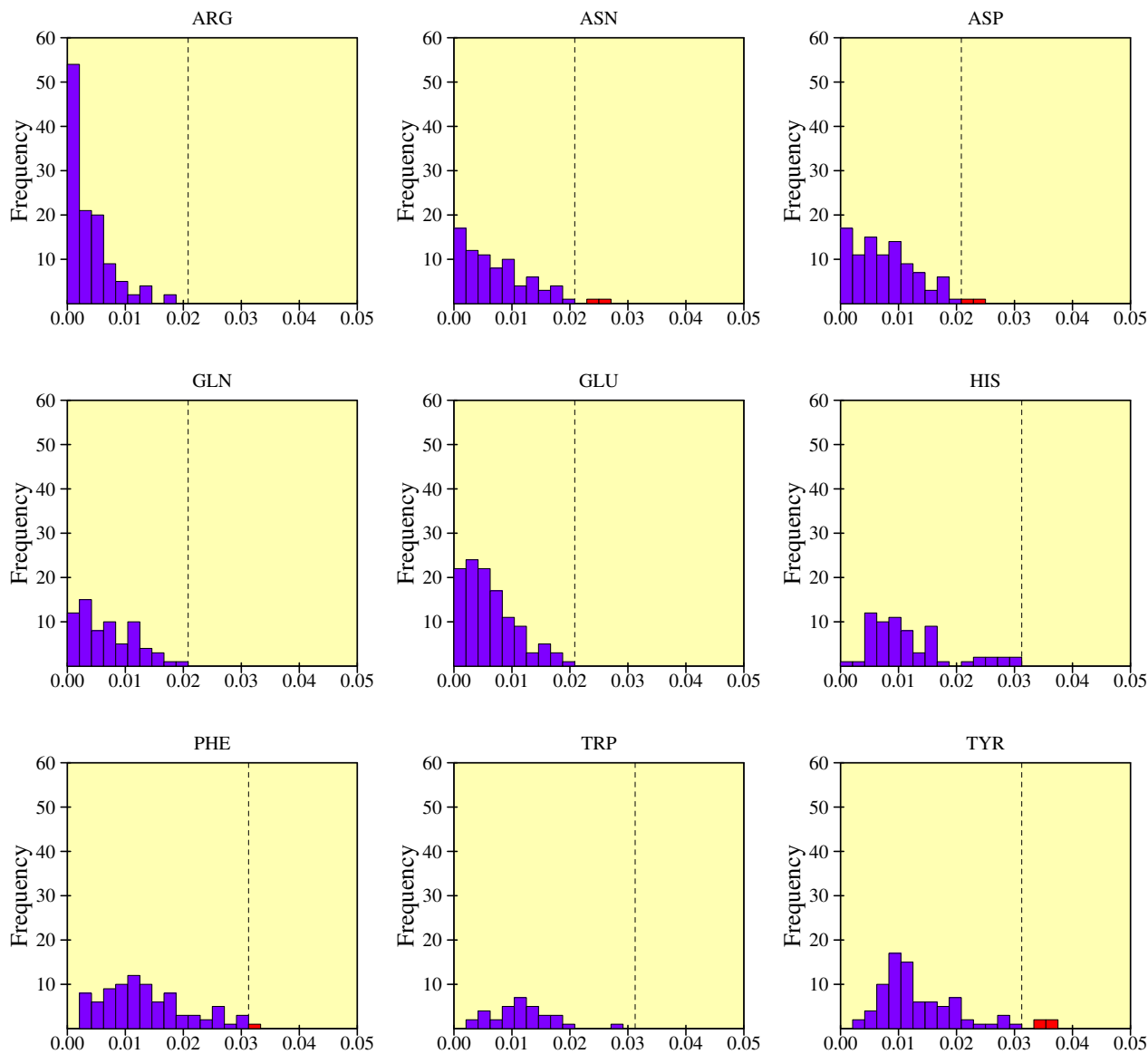
Black bars > 2.0 st. devs. from mean.

◀ 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.

# RMS distances from planarity

## 1SQB



Histograms showing RMS distances of planar atoms from best-fit plane.  
 Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

# Distorted geometry

## 1SQB

### Main-chain bond lengths

CA 1.540 CB 0.072 1.612 A Val 11	CA 1.540 CB 0.057 1.597 A Val 59	CA 1.540 CB 0.051 1.591 A Ile 99	CA 1.540 CB 0.097 1.637 A Ile 127	CA 1.540 CB 0.052 1.592 A Val 133	CA 1.540 CB 0.074 1.614 A Thr 222
CA 1.540 CB 0.073 1.613 A Val 228	CA 1.540 CB 0.058 1.598 A Val 253	CA 1.540 CB 0.056 1.596 A Val 272	CA 1.540 CB 0.076 1.616 A Val 325	CA 1.540 CB 0.066 1.606 B Val 17	CA 1.540 CB 0.051 1.591 B Ile 85
CA 1.540 CB 0.071 1.611 B Thr 99	CA 1.540 CB 0.056 1.596 B Ile 118	N 1.458 CA 0.060 1.518 B Leu 176	CA 1.540 CB 0.072 1.612 B Val 189	CA 1.540 CB 0.050 1.590 B Ile 207	CA 1.540 CB 0.051 1.591 B Val 211
CA 1.540 CB 0.051 1.591 B Val 215	CA 1.540 CB 0.076 1.616 B Ile 226	CA 1.540 CB 0.055 1.595 B Val 258	CA 1.540 CB 0.067 1.607 B Ile 264	CA 1.540 CB 0.052 1.592 B Val 303	CA 1.540 CB 0.052 1.592 B Ile 402
CA 1.540 CB 0.051 1.591 C Ile 4	CA 1.540 CB 0.064 1.604 C Ile 13	CA 1.540 CB 0.069 1.609 C Ile 39	CA 1.540 CB 0.074 1.614 C Ile 42	CA 1.540 CB 0.051 1.591 C Val 66	CA 1.540 CB 0.069 1.609 C Ile 69
CA 1.540 CB 0.055 1.595 C Ile 78	CA 1.540 CB 0.055 1.595 C Ile 79	CA 1.540 CB 0.116 1.656 C Ile 92	CA 1.540 CB 0.072 1.612 C Ile 156	CA 1.540 CB 0.050 1.590 C Val 170	CA 1.540 CB 0.056 1.596 C Ile 188
CA 1.540 CB 0.052 1.592 C Val 195	CA 1.540 CB 0.054 1.594 C Val 243	CA 1.540 CB 0.053 1.592 C Thr 257	CA 1.540 CB 0.064 1.604 C Ile 268	CA 1.540 CB 0.075 1.615 C Ile 284	CA 1.525 C 0.051 1.576 C Ile 304
CA 1.540 CB 0.059 1.599 C Ile 304	CA 1.525 C 0.051 1.576 C Arg 318	CA 1.540 CB 0.060 1.600 C Ile 338	CA 1.525 C 0.066 1.591 C Val 343	CA 1.540 CB 0.059 1.599 C Val 343	CA 1.540 CB 0.064 1.604 C Ile 348
CA 1.540 CB 0.068 1.608 C Ile 350	CA 1.540 CB 0.074 1.614 C Val 356	CA 1.540 CB 0.065 1.605 C Val 364	CA 1.540 CB 0.053 1.593 C Ile 372	CA 1.540 CB 0.063 1.603 D Ile 26	CA 1.540 CB 0.053 1.593 D Val 32
CA 1.540 CB 0.053 1.593 D Val 36	CA 1.540 CB 0.053 1.593 D Val 46	CA 1.540 CB 0.051 1.591 D Val 52	CA 1.540 CB 0.055 1.595 D Val 68	CA 1.540 CB 0.055 1.595 D Val 70	CA 1.540 CB 0.054 1.594 D Ile 116
CA 1.540 CB 0.051 1.591 D Val 117	CA 1.540 CB 0.079 1.619 D Ile 158	CA 1.540 CB 0.053 1.593 D Val 168	CA 1.540 CB 0.052 1.592 D Val 182	CA 1.540 CB 0.056 1.596 D Val 219	CA 1.540 CB 0.052 1.592 D Val 229

# Distorted geometry

## 1SQB

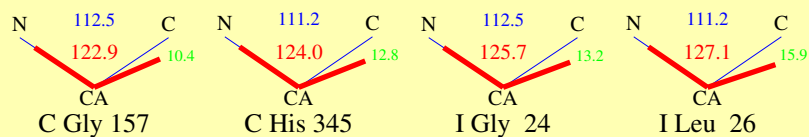
### Main-chain bond lengths (contd)

CA 1.540 CB 0.066 1.606 E Ile 5	CA 1.540 CB 0.060 1.600 E Val 18	CA 1.540 CB 0.052 1.592 E Val 39	CA 1.540 CB 0.053 1.593 E Val 45	CA 1.540 CB 0.056 1.595 E Val 47	CA 1.540 CB 0.069 1.609 E Val 55
CA 1.540 CB 0.056 1.596 E Val 59	CA 1.540 CB 0.051 1.591 E Val 68	CA 1.540 CB 0.062 1.602 E Ile 74	CA 1.540 CB 0.058 1.598 E Ile 81	CA 1.540 CB 0.056 1.596 E Val 98	CA 1.540 CB 0.065 1.605 E Thr 102
CA 1.540 CB 0.072 1.612 E Ile 106	CA 1.540 CB 0.051 1.591 E Val 112	CA 1.540 CB 0.060 1.600 E Val 114	CA 1.540 CB 0.067 1.607 E Val 133	CA 1.540 CB 0.054 1.594 E Ile 136	CA 1.540 CB 0.054 1.594 E Val 145
CA 1.540 CB 0.060 1.600 E Ile 147	CA 1.540 CB 0.078 1.618 E Ile 171	CA 1.540 CB 0.051 1.591 E Val 182	CA 1.540 CB 0.063 1.603 E Val 193	CA 1.540 CB 0.055 1.595 E Ile 194	CA 1.540 CB 0.062 1.602 E Val 195
CA 1.540 CB 0.071 1.611 F Val 6	CA 1.540 CB 0.053 1.593 F Ile 16	CA 1.540 CB 0.053 1.593 F Ile 47	CA 1.540 CB 0.060 1.600 F Ile 62	CA 1.540 CB 0.072 1.612 F Ile 74	CA 1.540 CB 0.051 1.591 F Ile 98
CA 1.540 CB 0.067 1.607 G Ile 34	CA 1.540 CB 0.080 1.620 G Val 37	CA 1.540 CB 0.067 1.607 G Val 53	CA 1.540 CB 0.059 1.599 G Val 58	CA 1.540 CB 0.058 1.598 H Val 14	CA 1.540 CB 0.068 1.608 H Val 31
CA 1.540 CB 0.052 1.592 H Thr 50	CA 1.540 CB 0.069 1.609 H Val 69	CA 1.540 CB 0.067 1.607 I Val 22	CA 1.525 C 0.062 1.587 I Ala 25	CA 1.525 C 0.062 1.587 I Arg 27	CA 1.540 CB 0.054 1.594 I Val 30
CA 1.525 C 0.057 1.582 I Val 34	CA 1.540 CB 0.065 1.605 I Thr 37	CA 1.540 CB 0.075 1.615 I Val 42	CA 1.525 C 0.057 1.582 I Leu 45	CA 1.540 CB 0.060 1.600 I Val 49	CA 1.525 C 0.051 1.576 I Ser 54
CA 1.540 CB 0.066 1.606 J Val 1	CA 1.540 CB 0.052 1.592 J Val 26	CA 1.540 CB 0.053 1.593 J Ile 42	CA 1.540 CB 0.062 1.602 J Ile 46	CA 1.540 CB 0.057 1.597 J Ile 55	CA 1.540 CB 0.063 1.603 K Val 18
CA 1.540 CB 0.051 1.591 K Val 30	CA 1.540 CB 0.060 1.600 K Val 33	CA 1.540 CB 0.065 1.605 K Ile 41	CA 1.540 CB 0.055 1.595 K Ile 48		

Bonds differing by > 0.05Å from small-molecule values. Values shown: "ideal", difference, actual

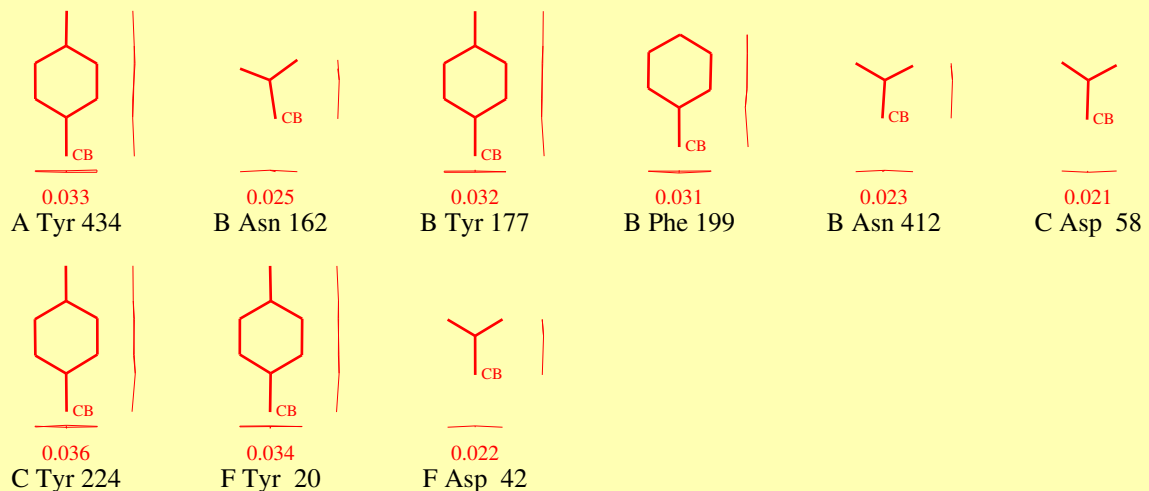
# Distorted geometry 1SQB

## Main-chain bond angles



Bond angles differing by > 10.0 degrees from small-molec values. Values shown: "ideal", actual, diff.

## Planar groups



Sidechains with RMS dist. from planarity > 0.03Å for rings, or > 0.02Å otherwise. Value shown is RMS dist.