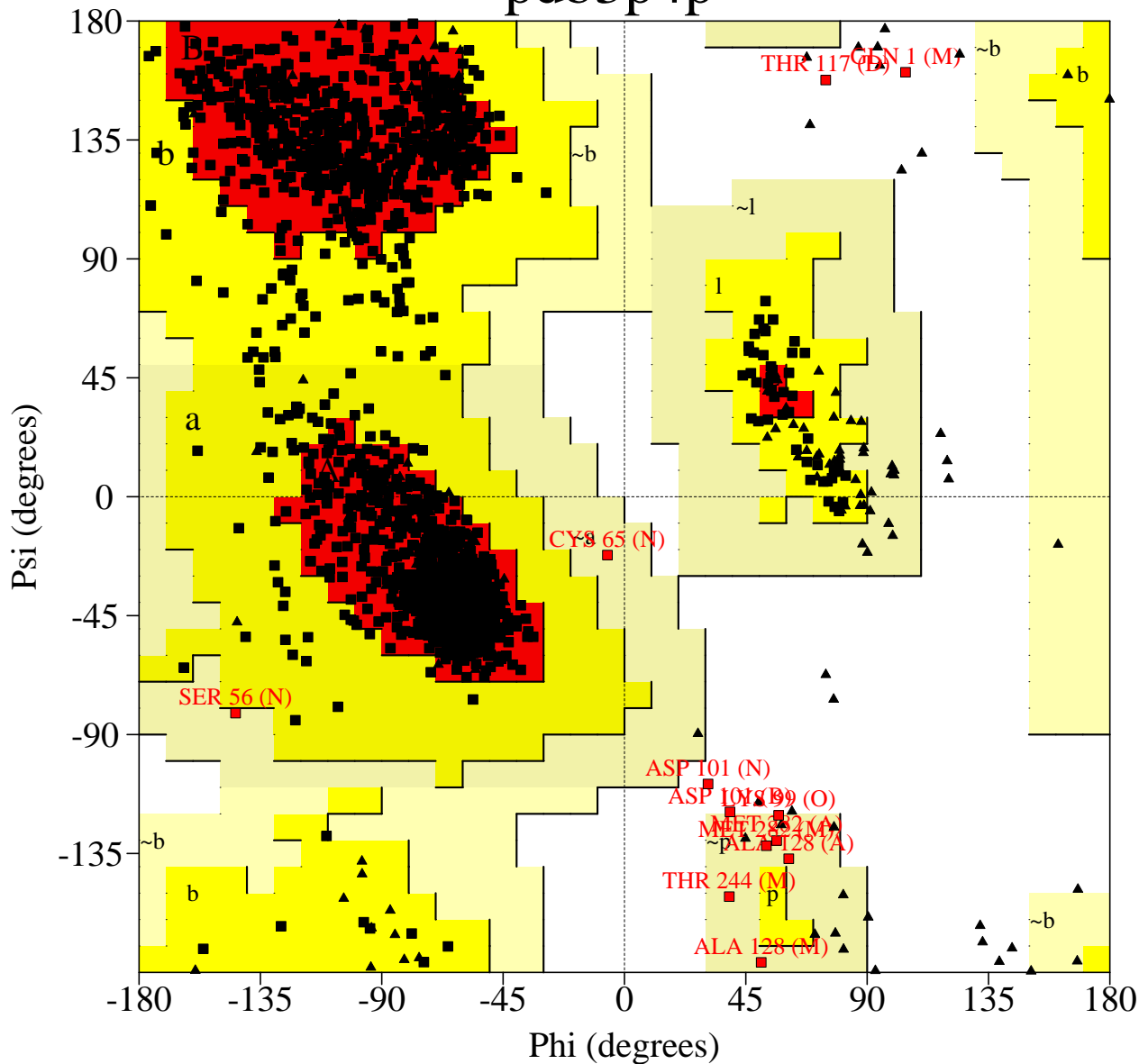


# Ramachandran Plot

pdb3p4p



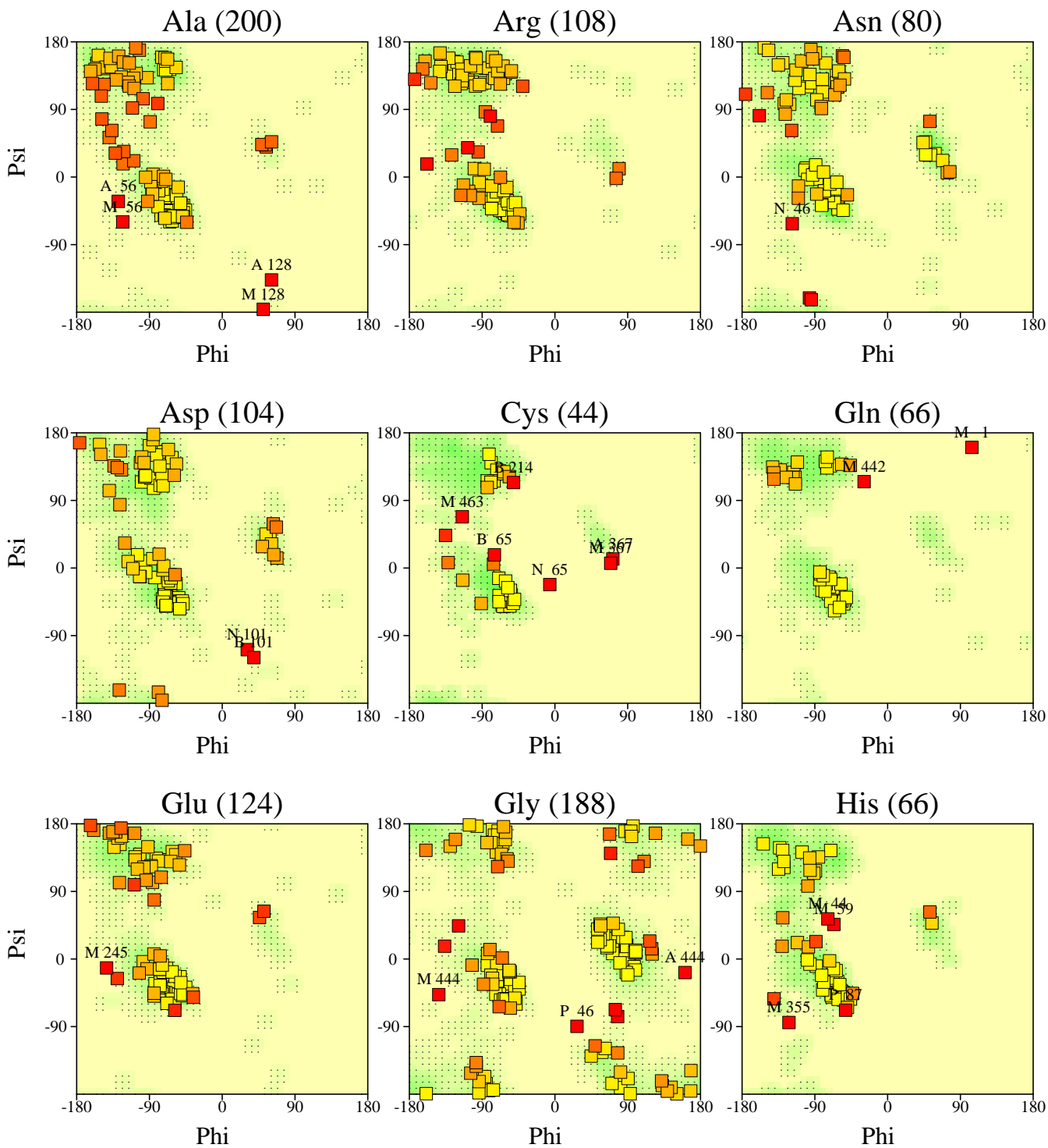
### Plot statistics

Residues in most favoured regions [A,B,L]	1656	90.6%
Residues in additional allowed regions [a,b,l,p]	160	8.8%
Residues in generously allowed regions [~a,~b,~l,~p]	8	0.4%
Residues in disallowed regions	4	0.2%
-----		
Number of non-glycine and non-proline residues	1828	100.0%
Number of end-residues (excl. Gly and Pro)	16	
Number of glycine residues (shown as triangles)	188	
Number of proline residues	106	
-----		
Total number of residues	2138	

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

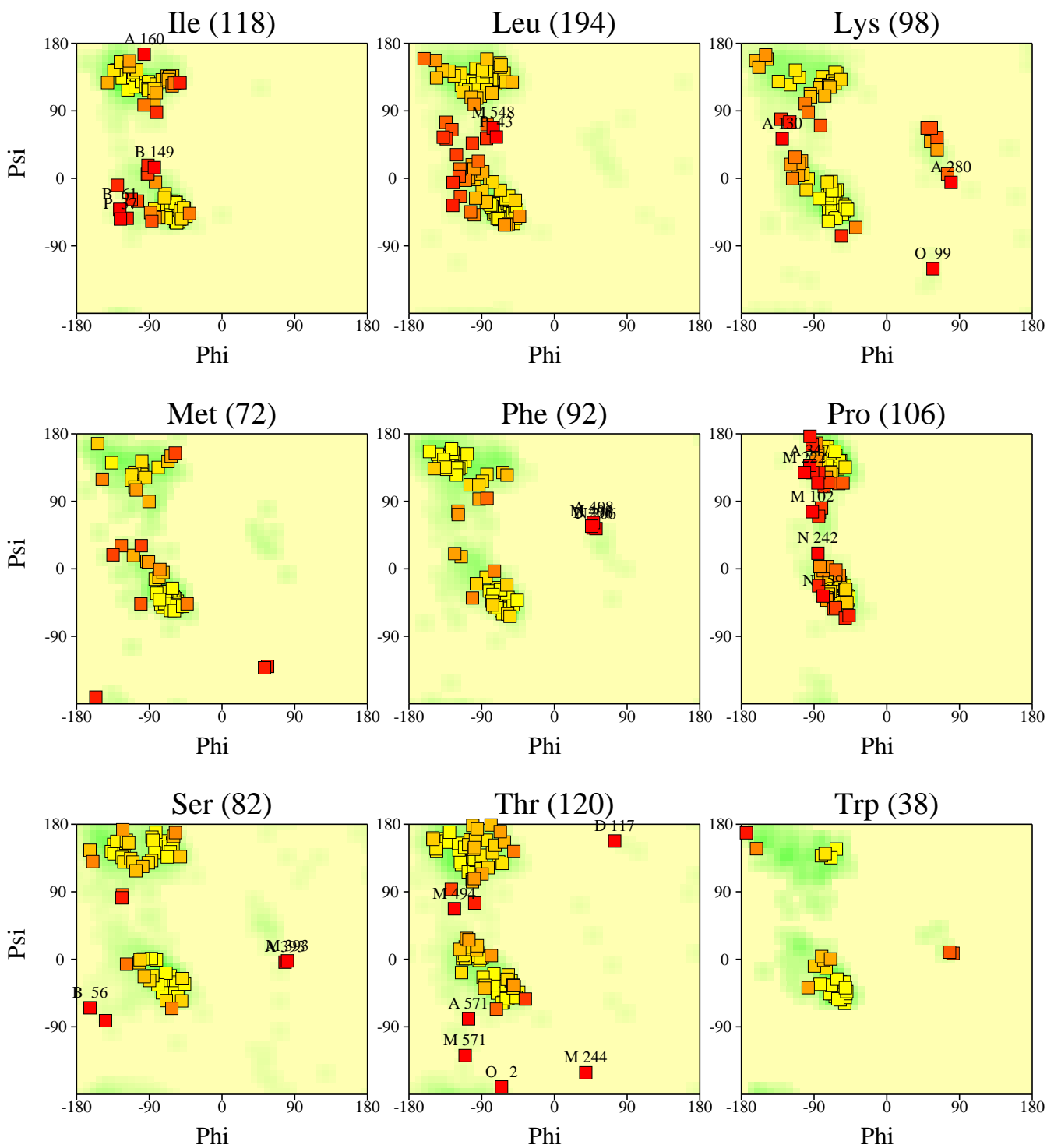
## pdb3p4p



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

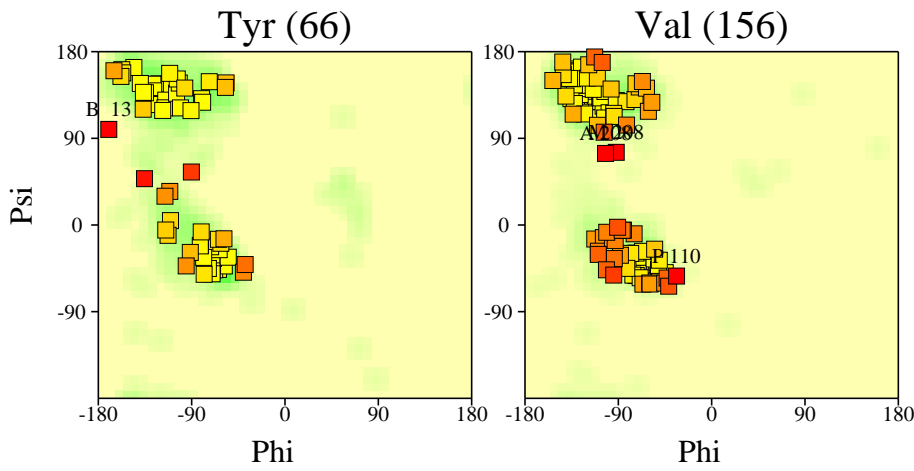
## pdb3p4p



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

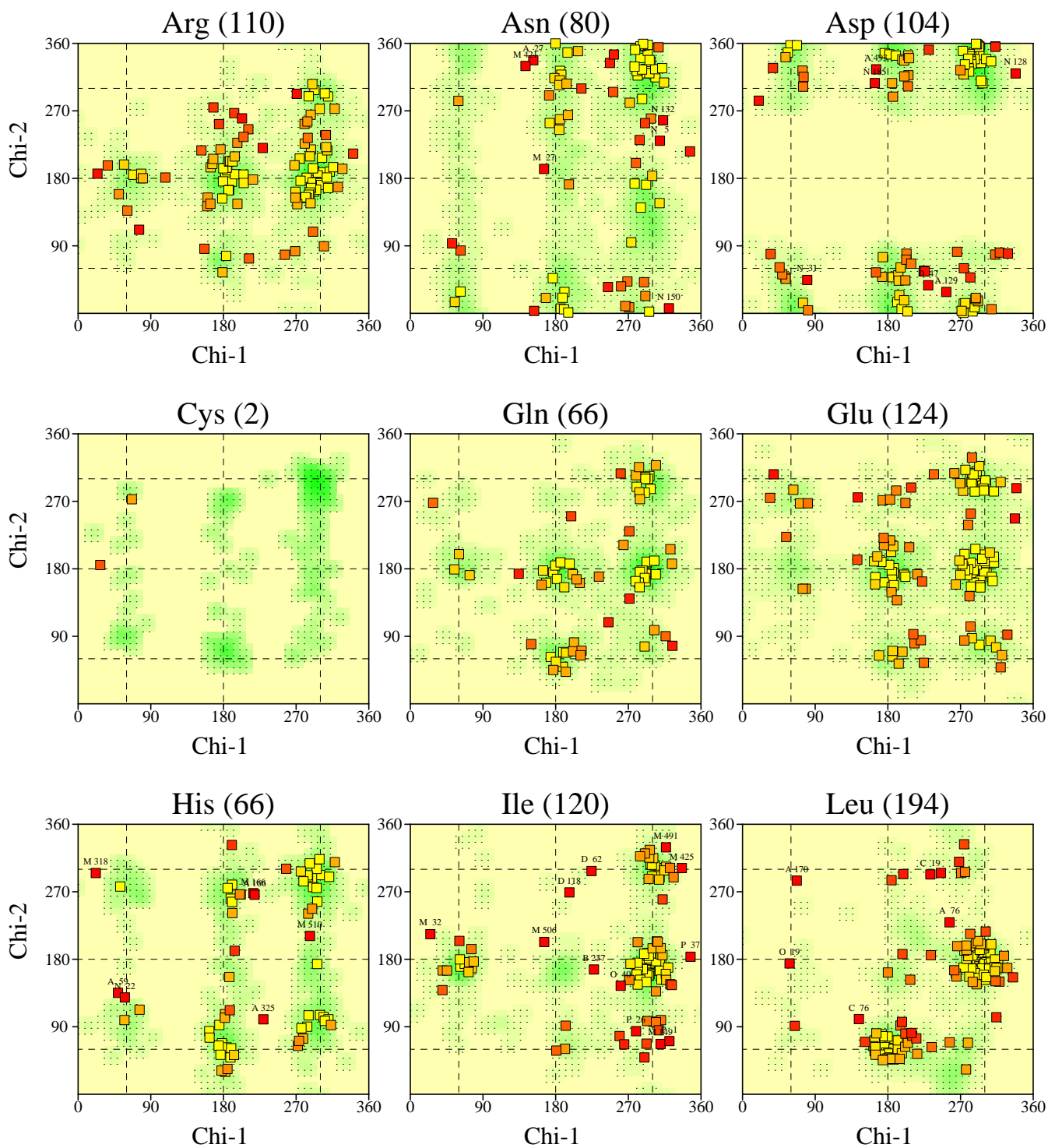
## pdb3p4p



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

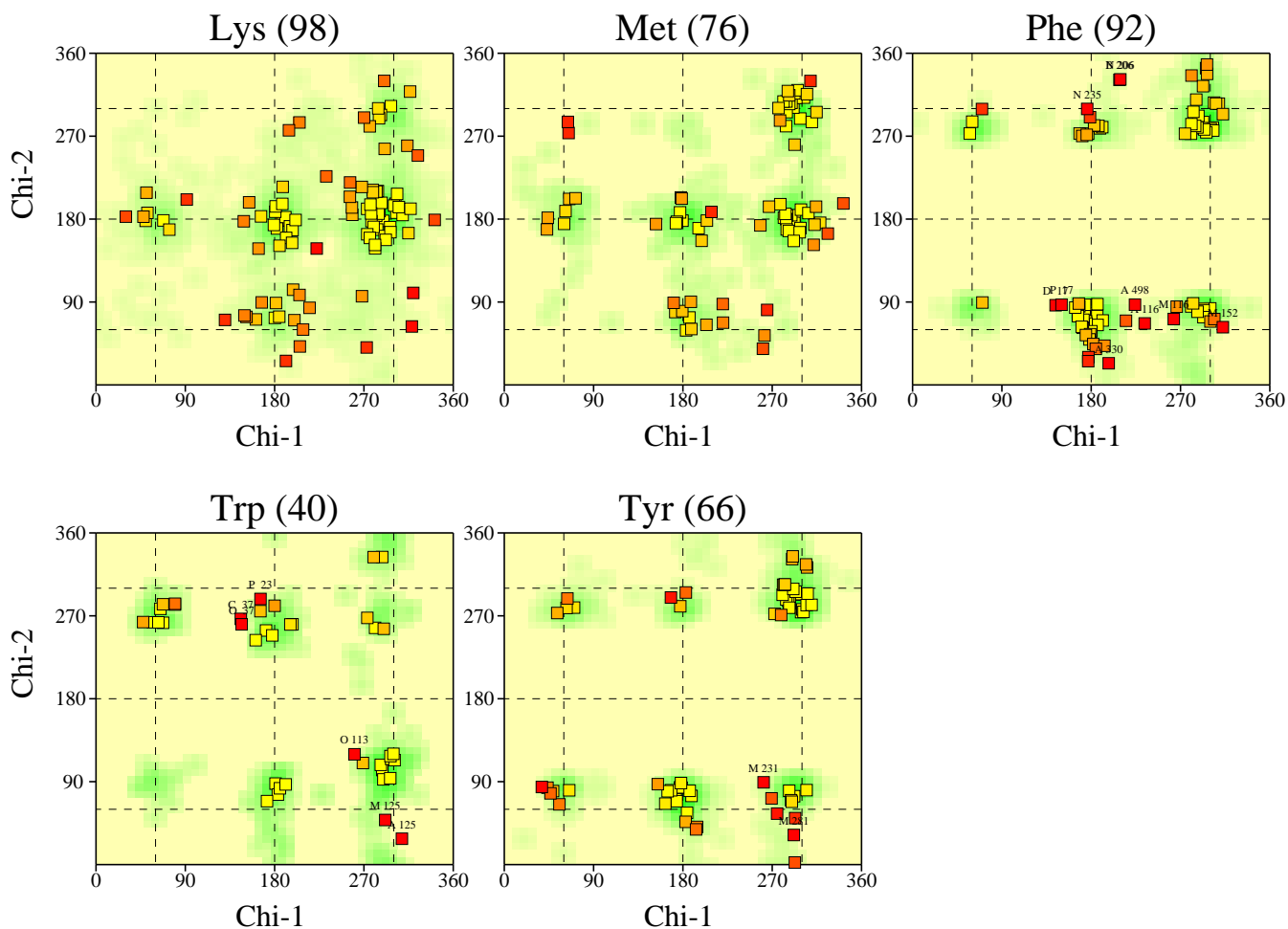
## pdb3p4p



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

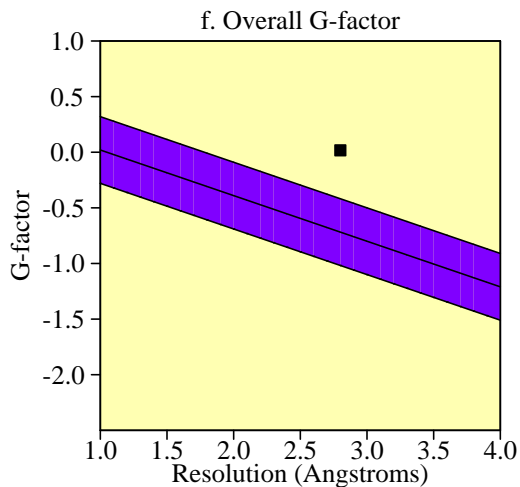
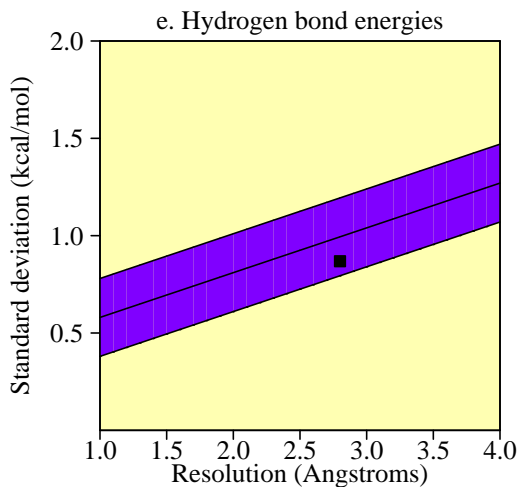
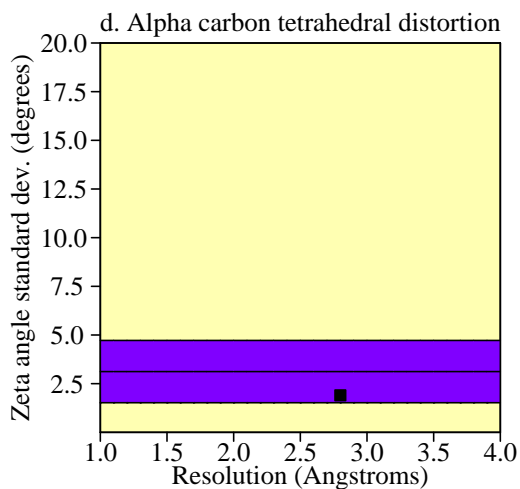
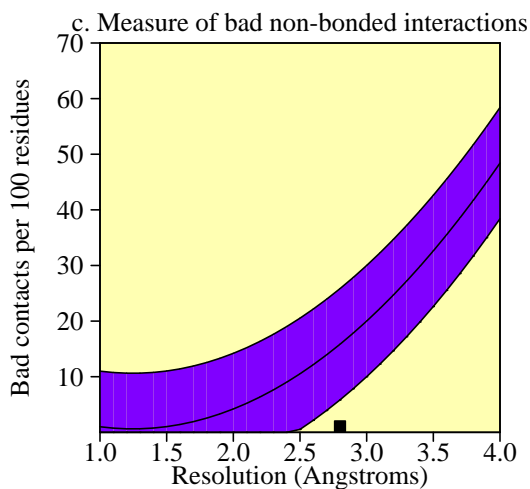
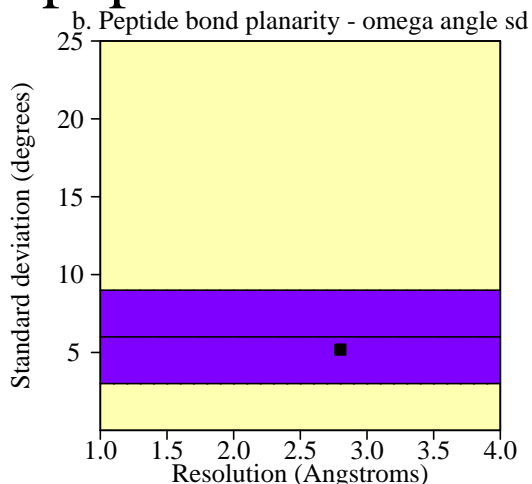
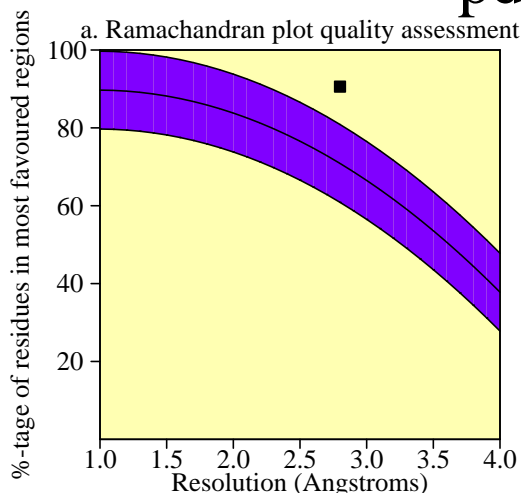
## pdb3p4p



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

## pdb3p4p

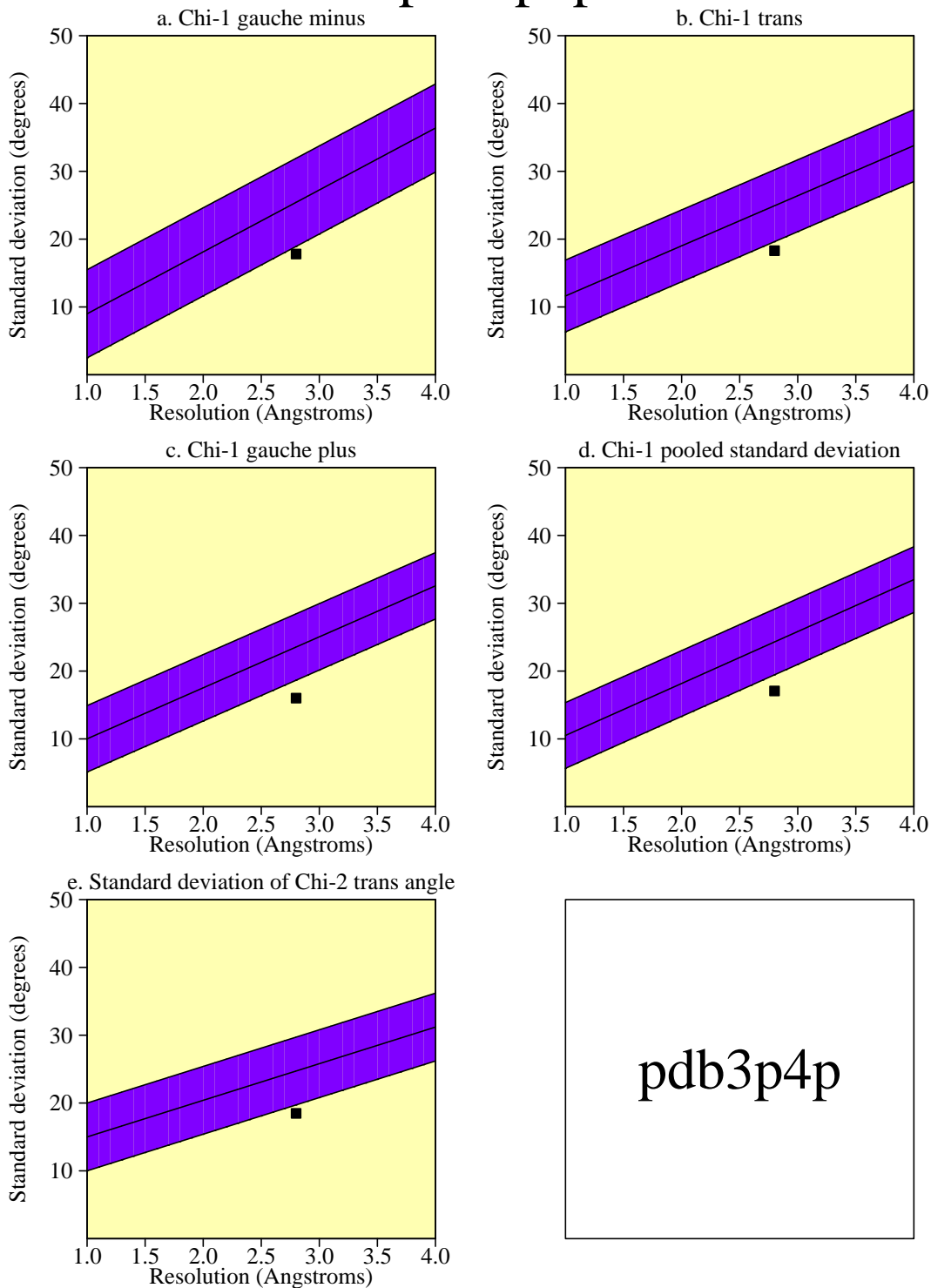


### Plot statistics

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	1828	90.6	70.9	10.0	2.0	BETTER
b. Omega angle st dev	2128	5.2	6.0	3.0	-0.3	Inside
c. Bad contacts / 100 residues	23	1.1	15.8	10.0	-1.5	BETTER
d. Zeta angle st dev	1950	1.9	3.1	1.6	-0.8	Inside
e. H-bond energy st dev	1393	0.9	1.0	0.2	-0.6	Inside
f. Overall G-factor	2138	0.0	-0.7	0.3	2.5	BETTER

# Side-chain parameters

## pdb3p4p



pdb3p4p

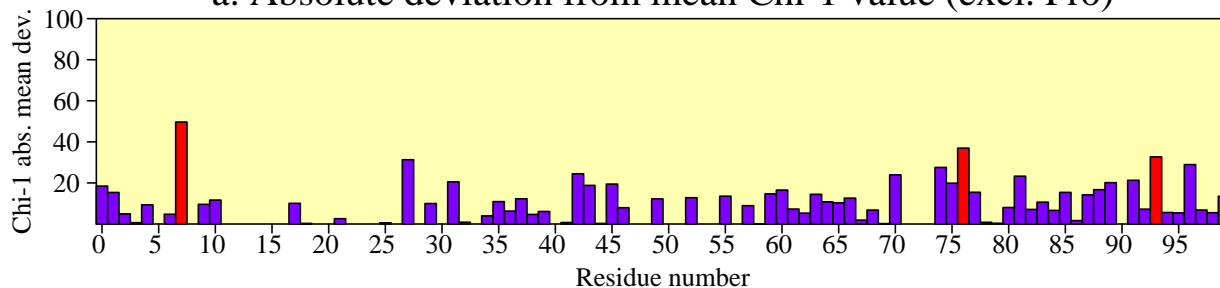
### Plot statistics

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	213	17.8	25.4	6.5	-1.2	BETTER
b. Chi-1 trans st dev	575	18.3	24.9	5.3	-1.2	BETTER
c. Chi-1 gauche plus st dev	852	16.0	23.5	4.9	-1.5	BETTER
d. Chi-1 pooled st dev	1640	17.1	24.3	4.8	-1.5	BETTER
e. Chi-2 trans st dev	496	18.5	24.7	5.0	-1.2	BETTER

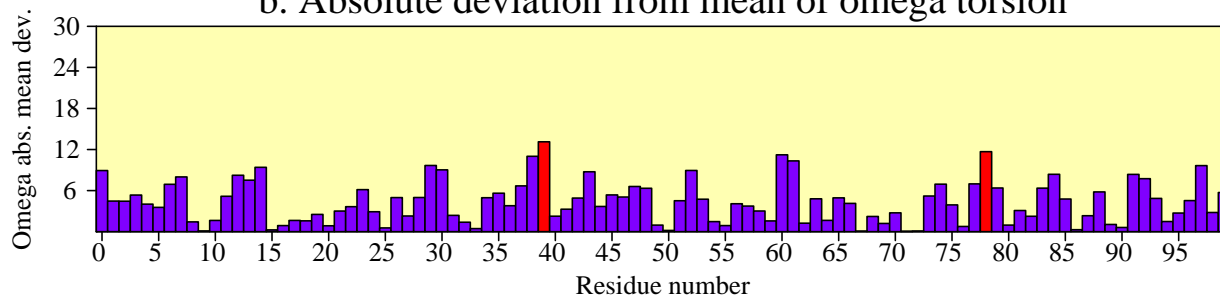


# Residue properties pdb3p4p

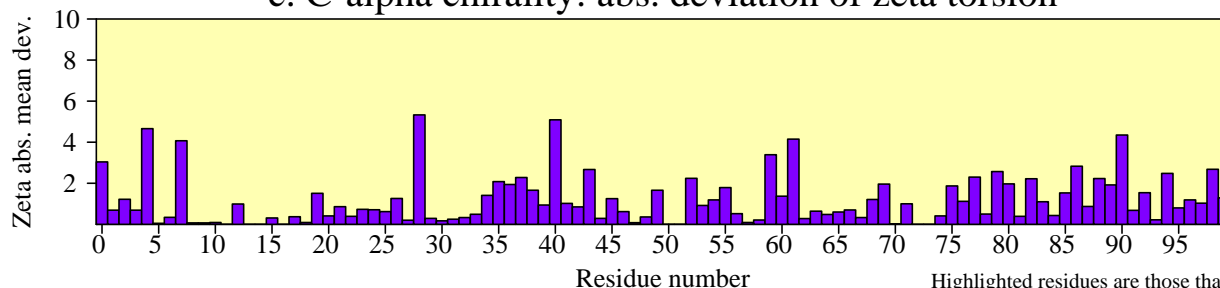
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

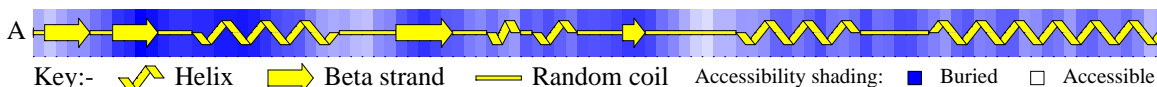


c. C-alpha chirality: abs. deviation of zeta torsion



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

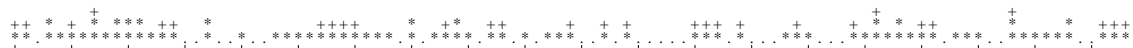
d. Secondary structure & estimated accessibility



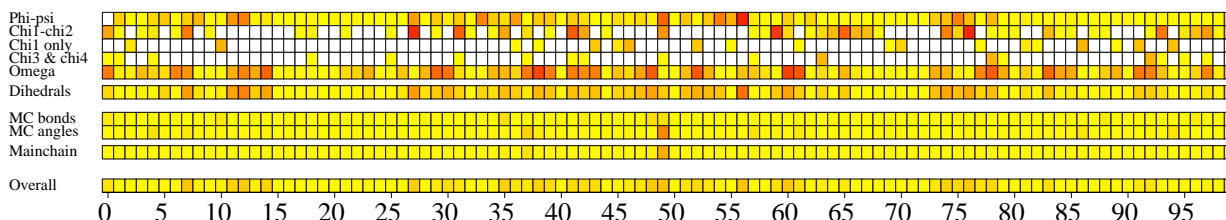
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

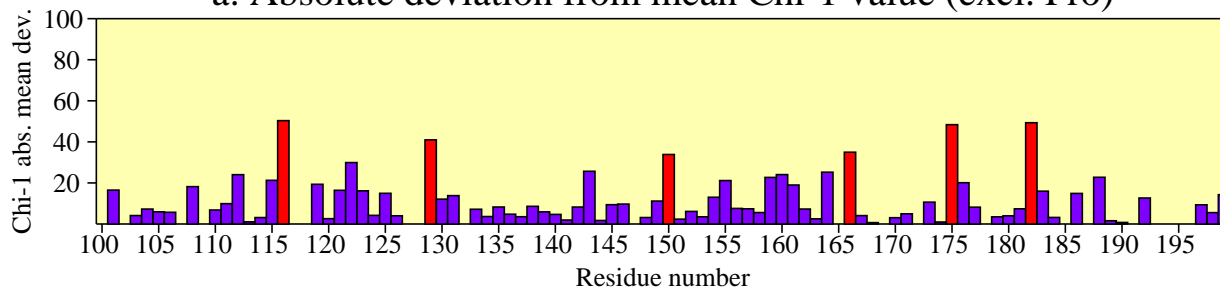


g. G-factors

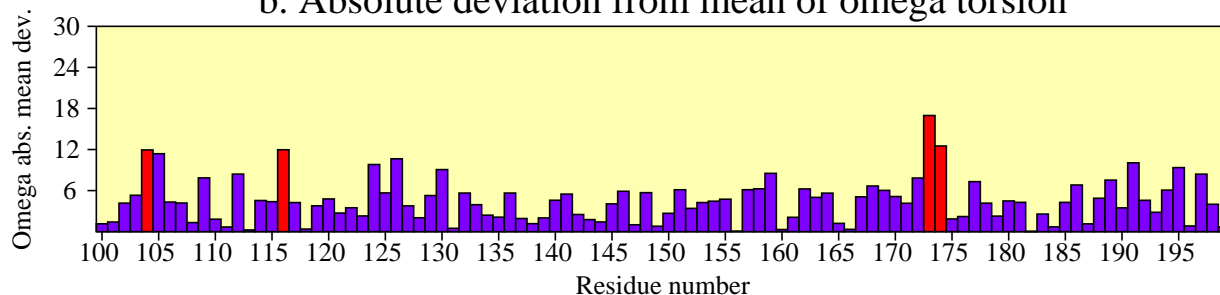


# Residue properties pdb3p4p

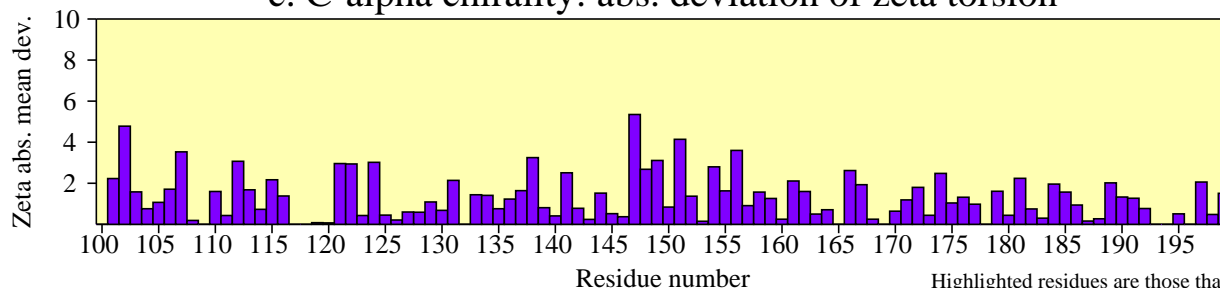
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### 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



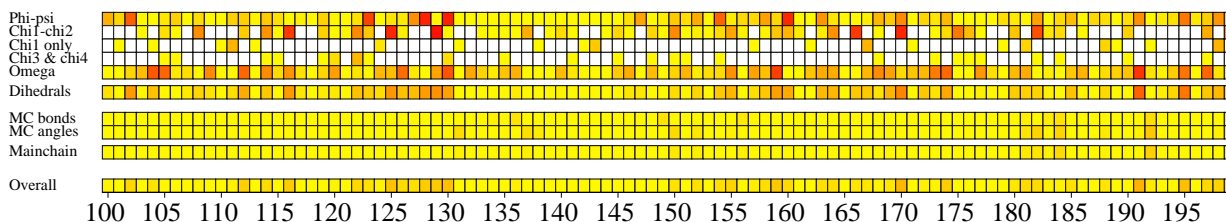
### e. Sequence & Ramachandran regions



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

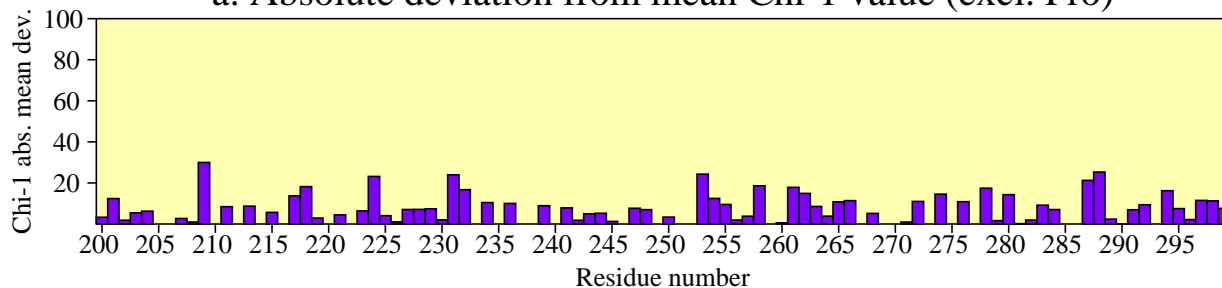


### g. G-factors

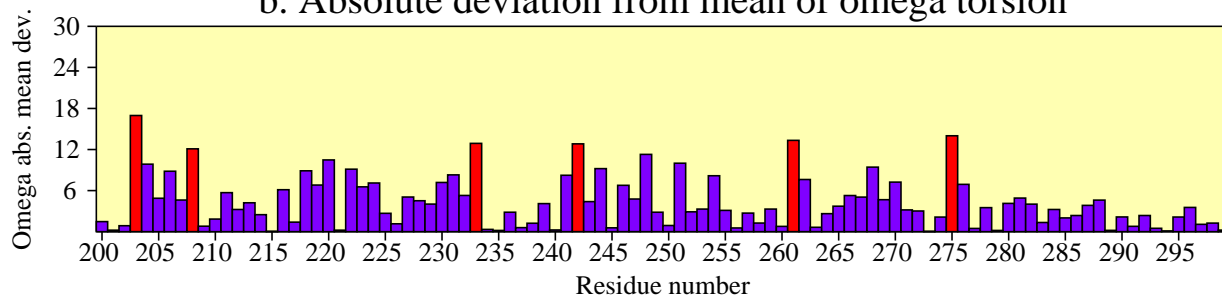


# Residue properties pdb3p4p

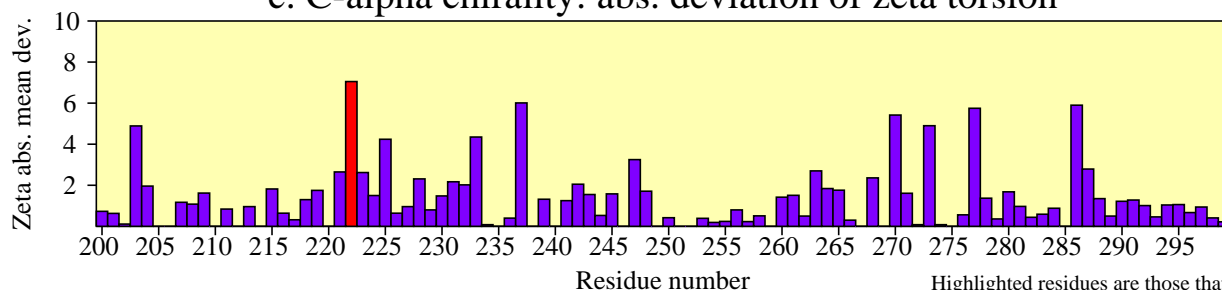
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

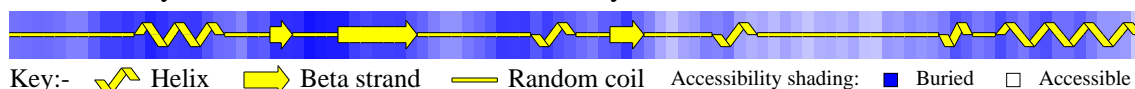


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



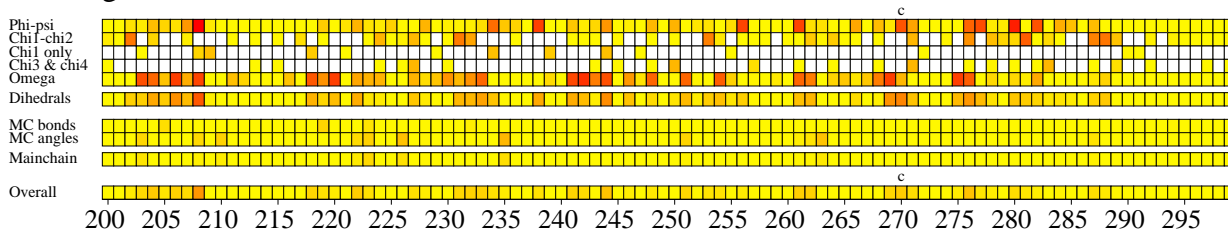
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



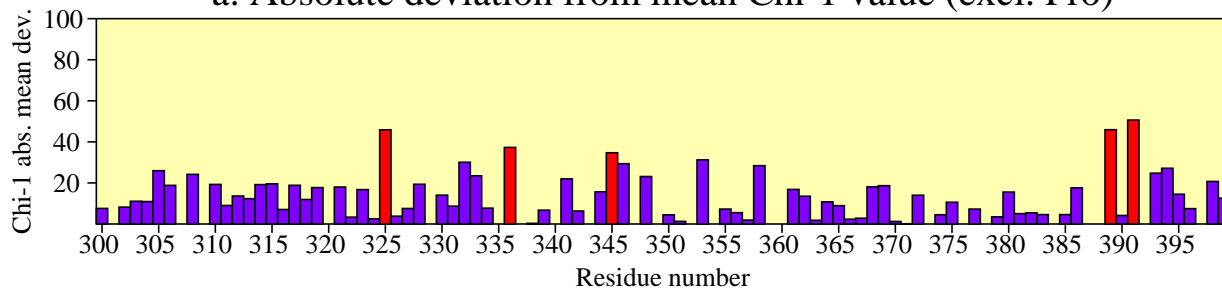
g. G-factors



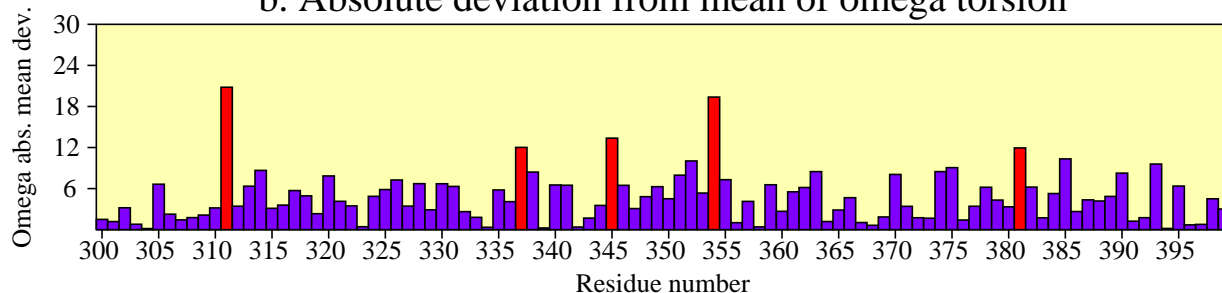
c = cis-peptide

# Residue properties pdb3p4p

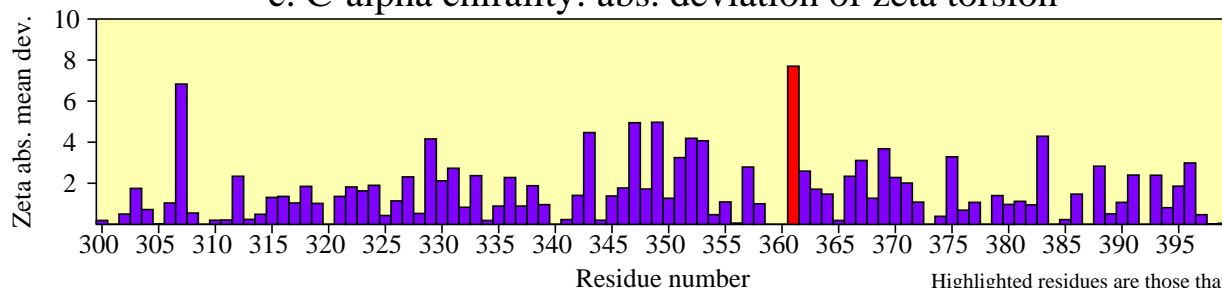
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### 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



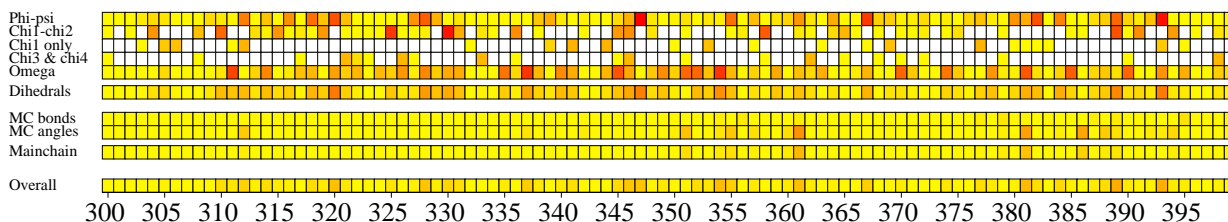
### e. Sequence & Ramachandran regions



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

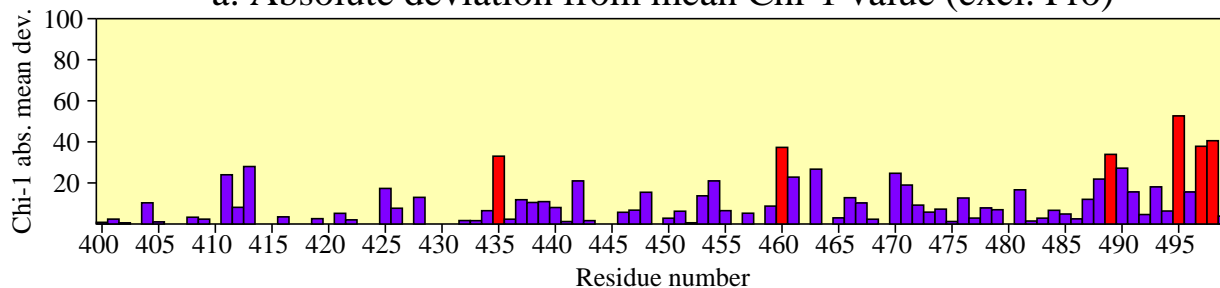


### g. G-factors

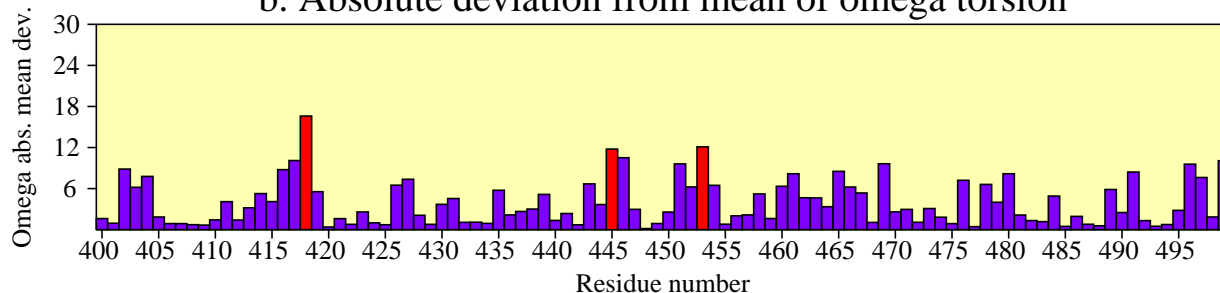


# Residue properties pdb3p4p

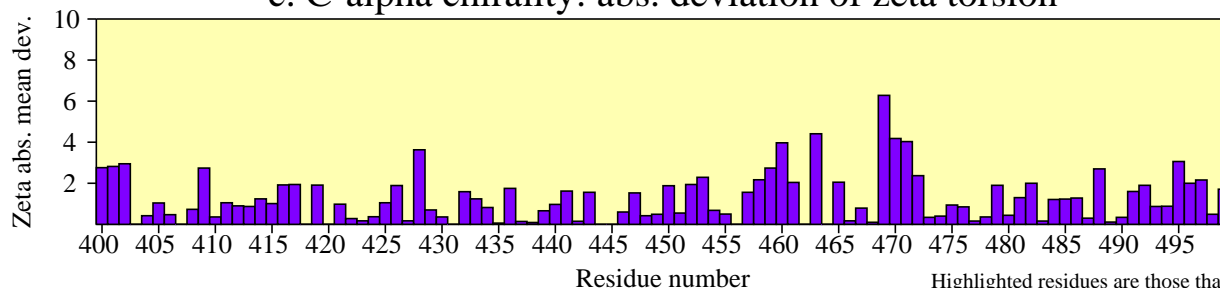
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

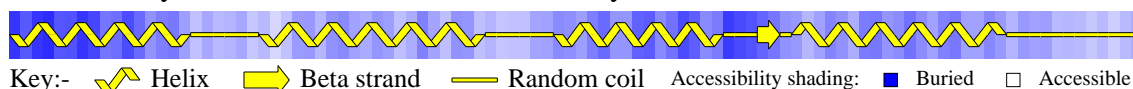


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



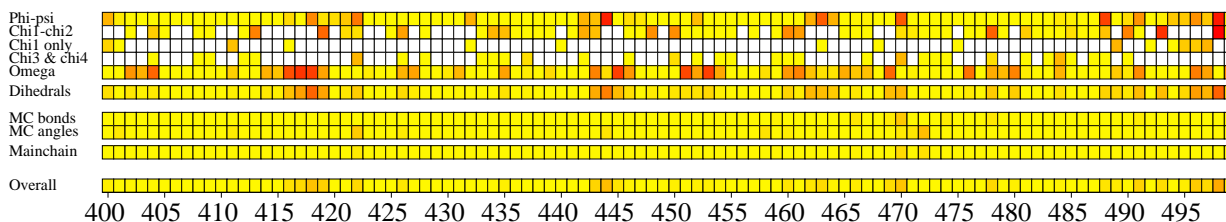
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

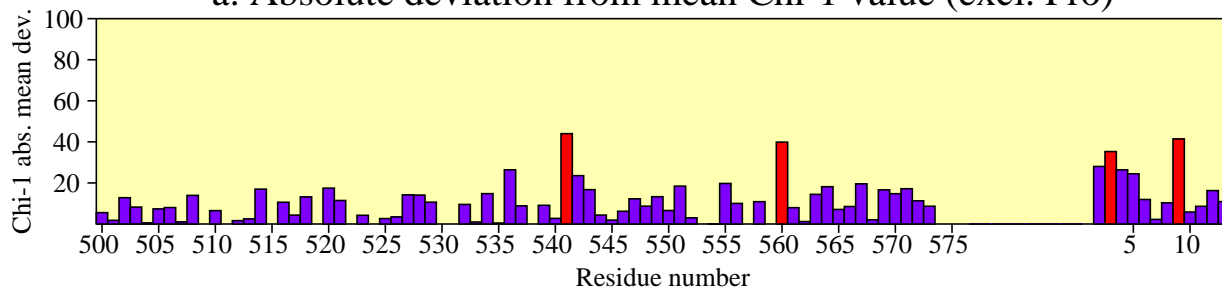


g. G-factors

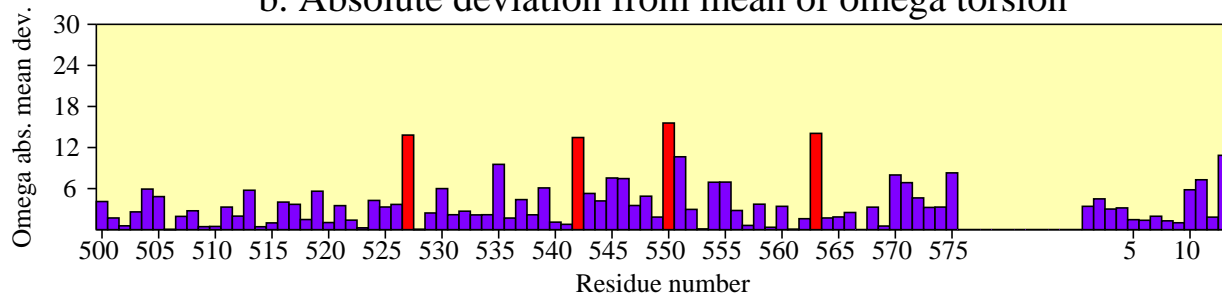


# Residue properties pdb3p4p

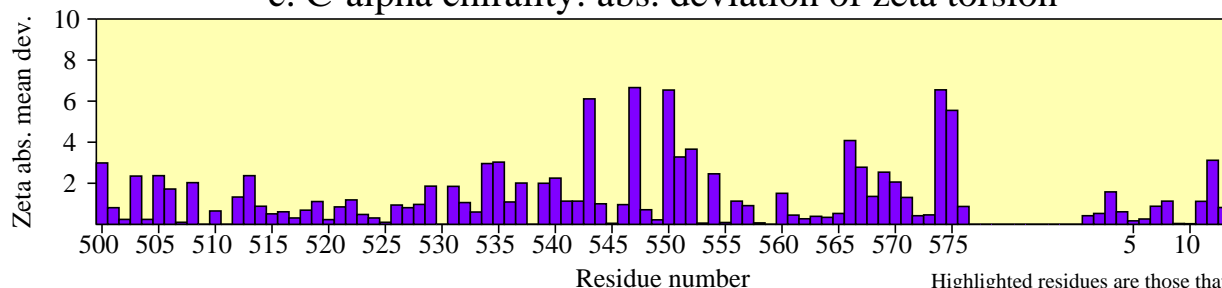
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

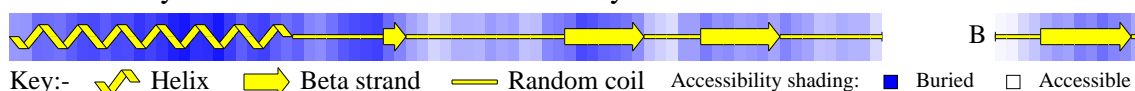


### c. C-alpha chirality: abs. deviation of zeta torsion

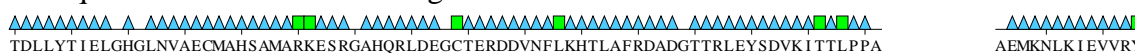


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



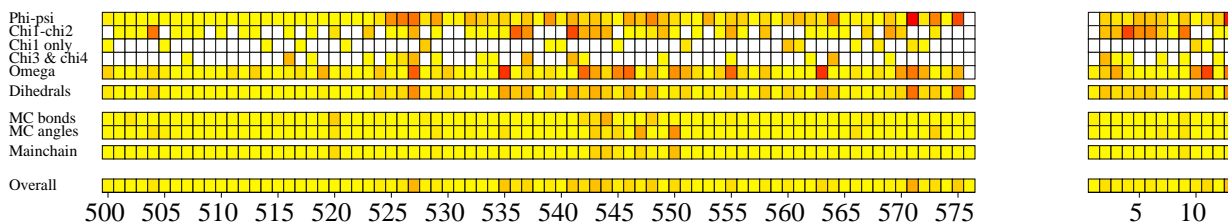
### e. Sequence & Ramachandran regions



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



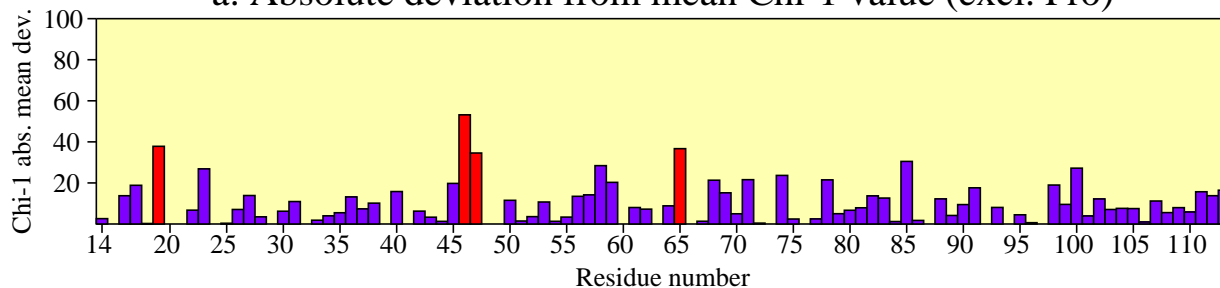
### g. G-factors



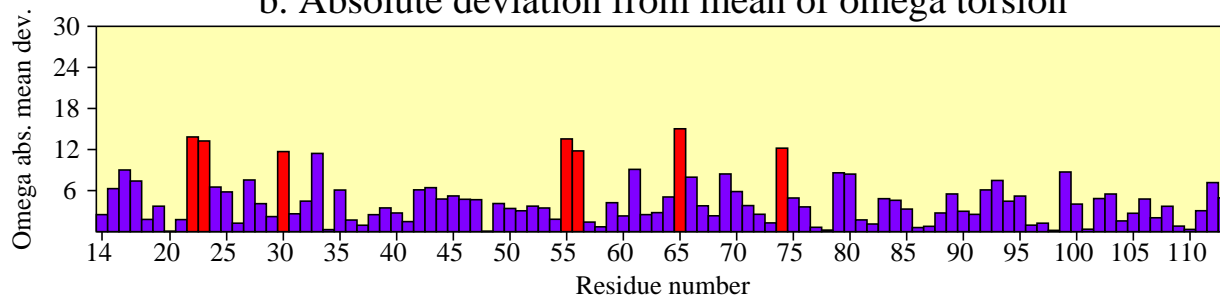
# Residue properties

## pdb3p4p

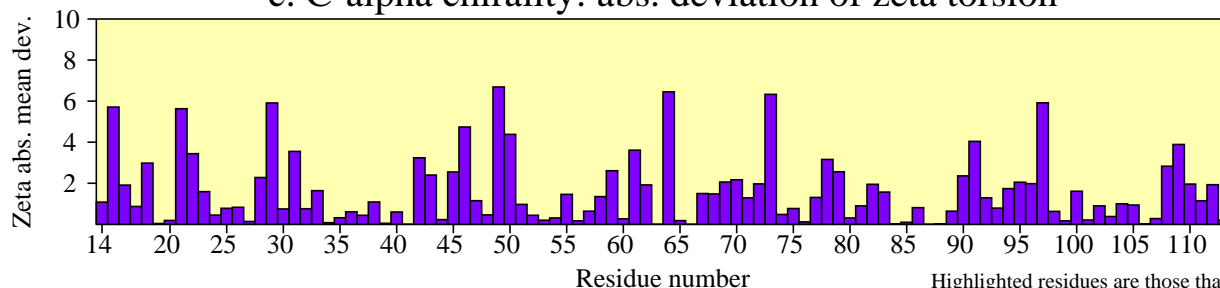
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

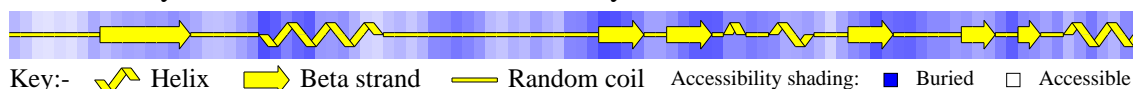


c. C-alpha chirality: abs. deviation of zeta torsion



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

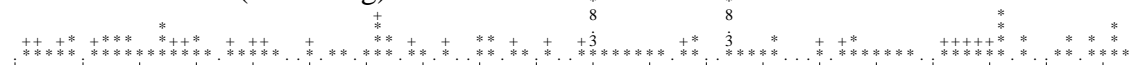
d. Secondary structure & estimated accessibility



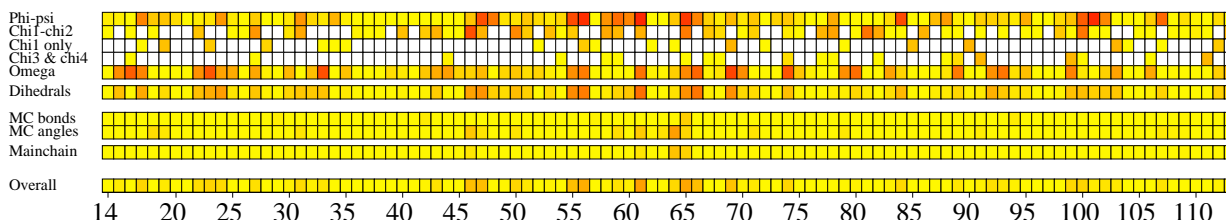
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



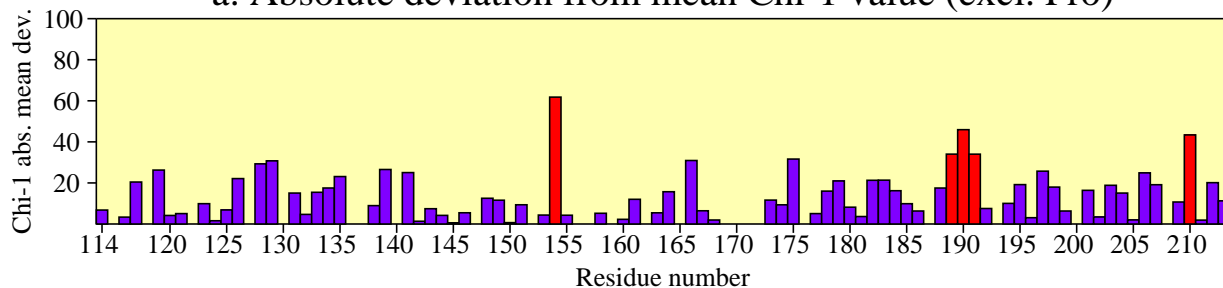
g. G-factors



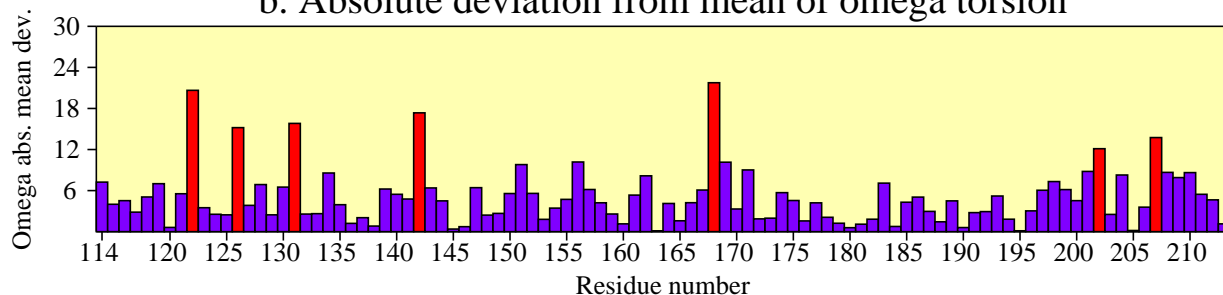
# Residue properties

## pdb3p4p

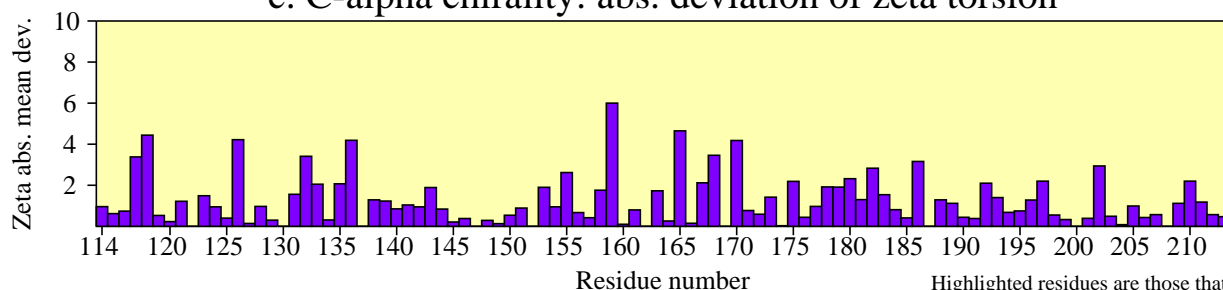
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

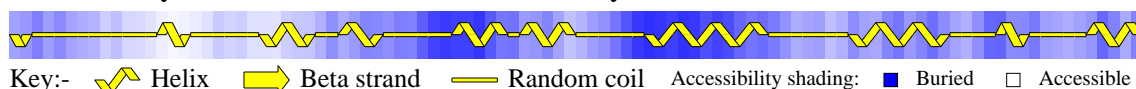


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



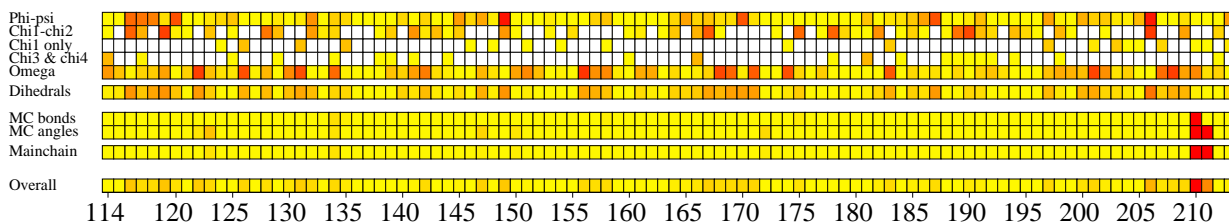
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

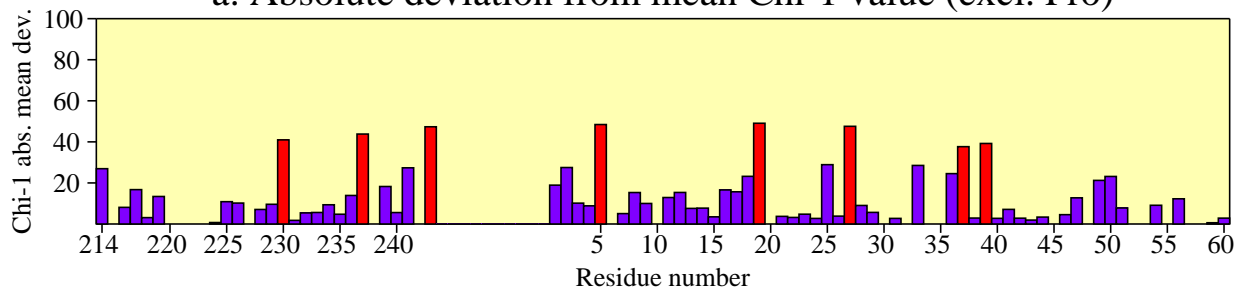




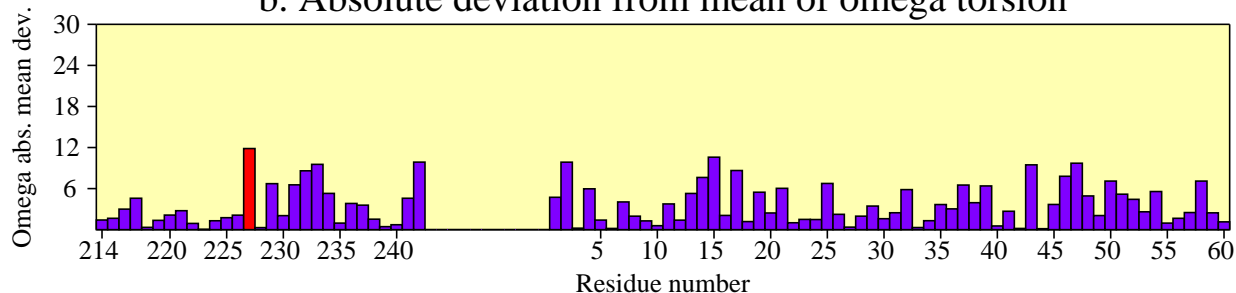
# Residue properties

## pdb3p4p

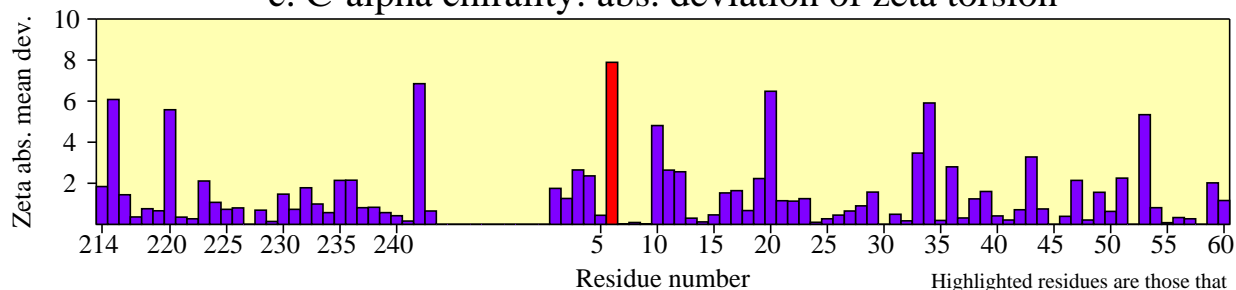
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

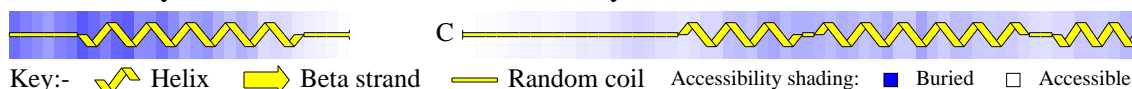


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



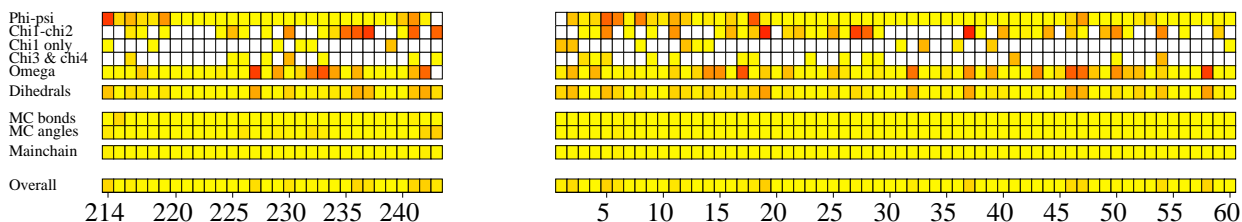
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

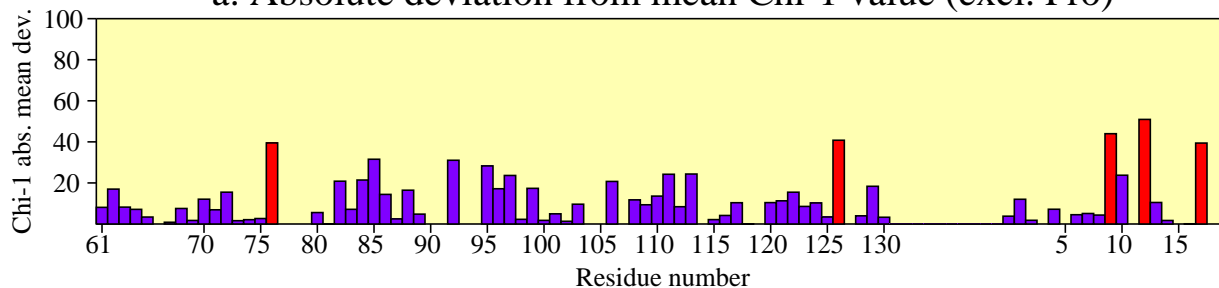


g. G-factors

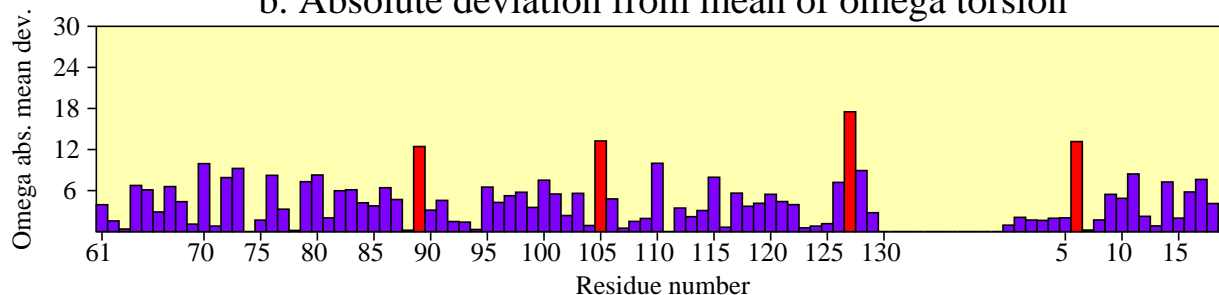


# Residue properties pdb3p4p

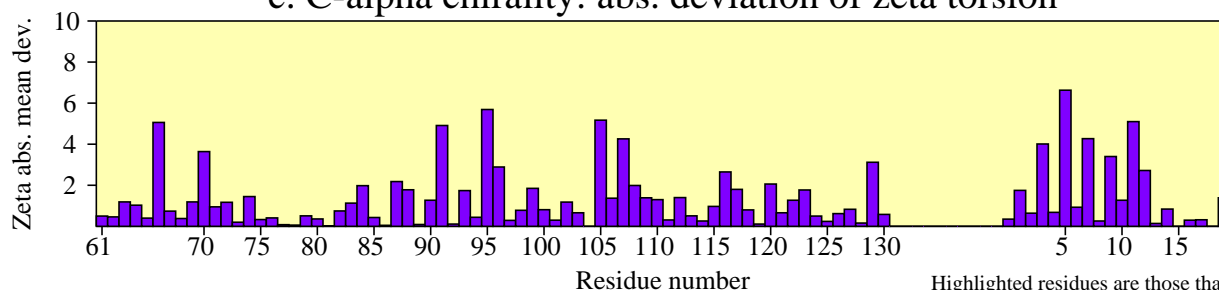
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

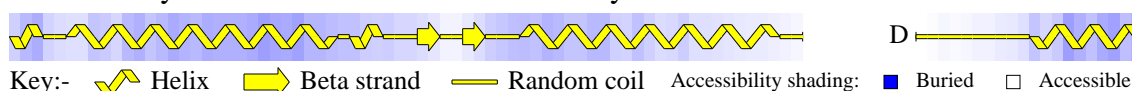


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



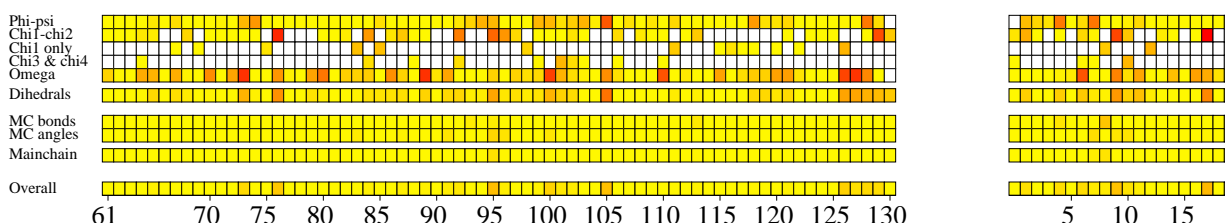
### e. Sequence & Ramachandran regions



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

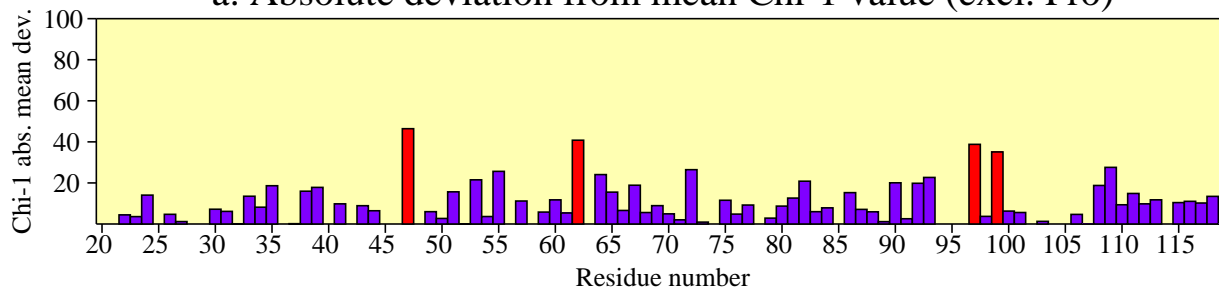


### g. G-factors

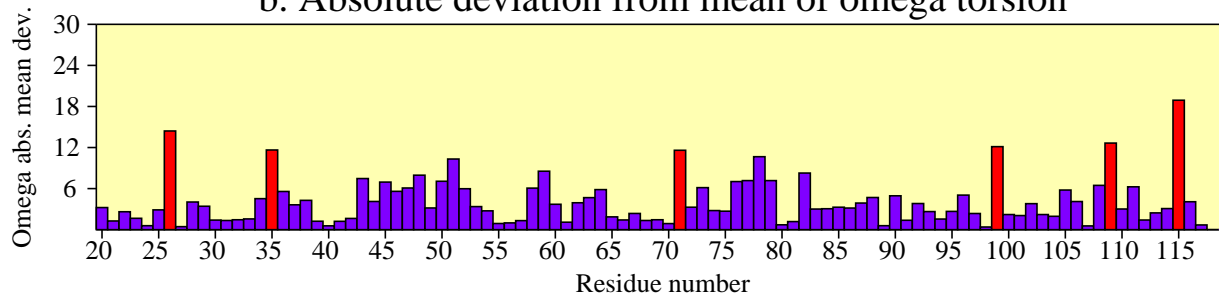


# Residue properties pdb3p4p

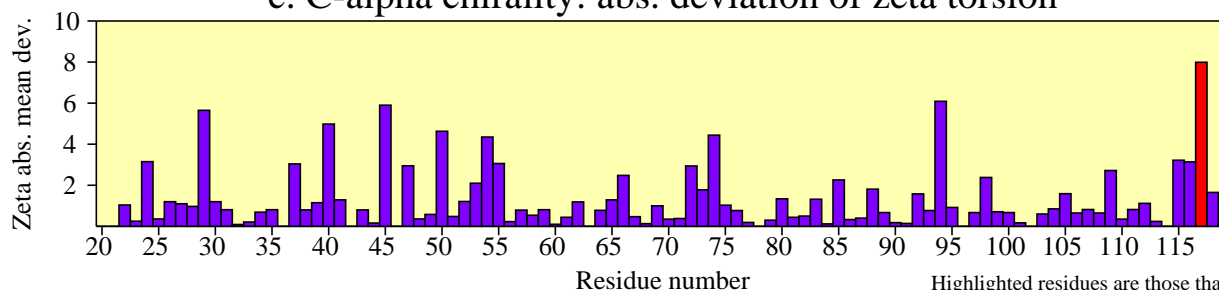
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

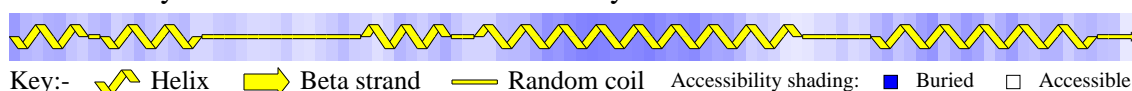


### c. C-alpha chirality: abs. deviation of zeta torsion

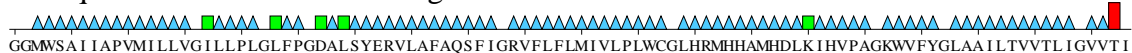


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



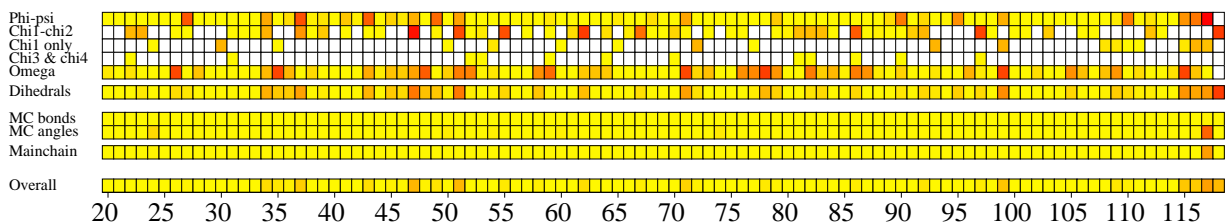
### e. Sequence & Ramachandran regions



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

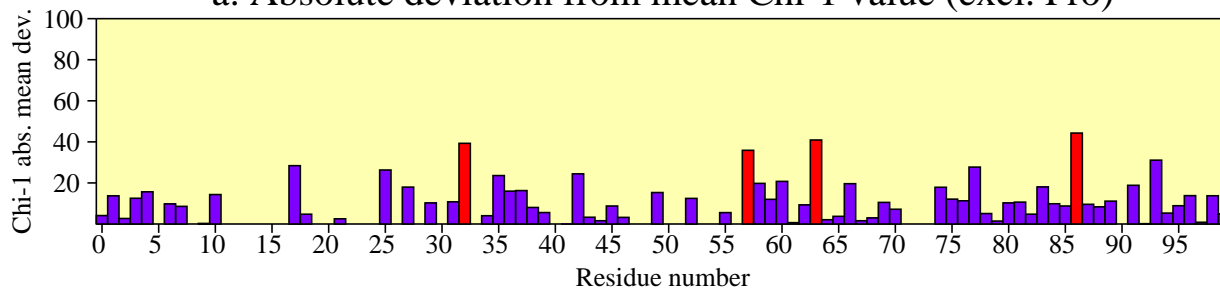


### g. G-factors

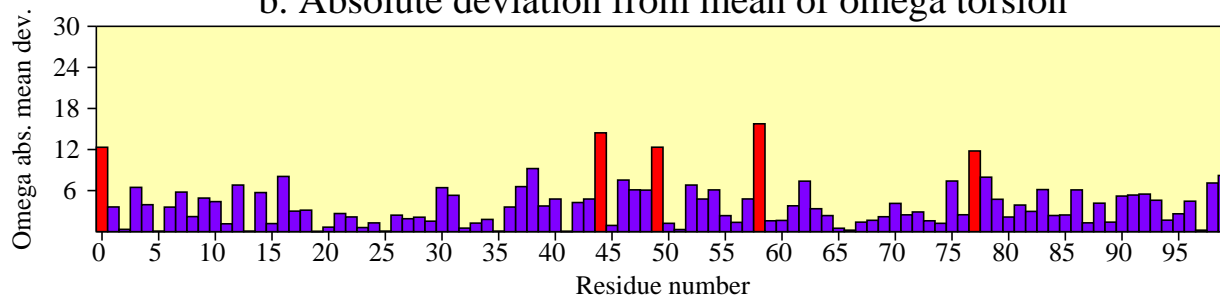


# Residue properties pdb3p4p

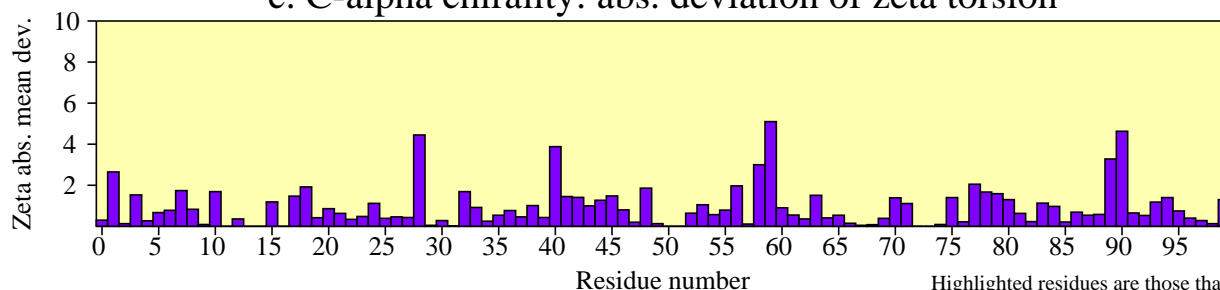
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

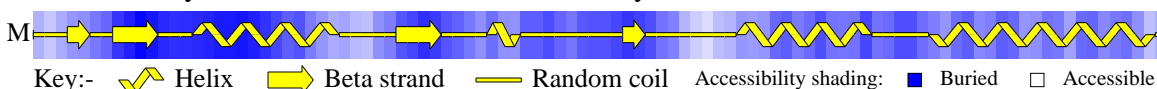


c. C-alpha chirality: abs. deviation of zeta torsion

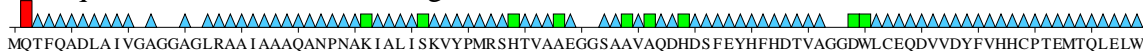


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

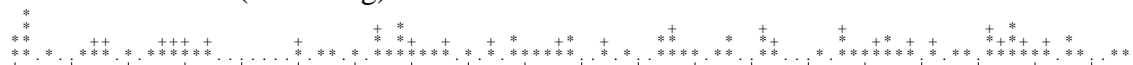
d. Secondary structure & estimated accessibility



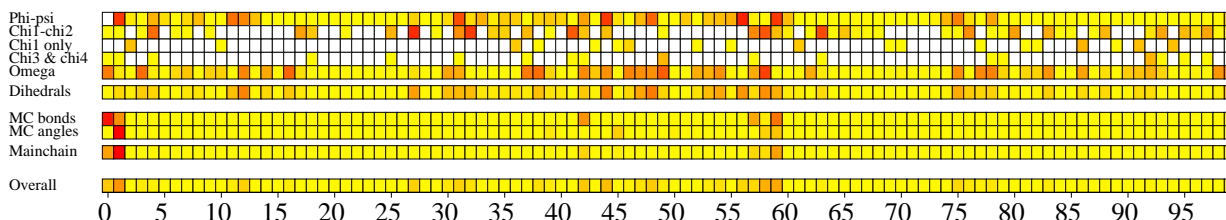
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

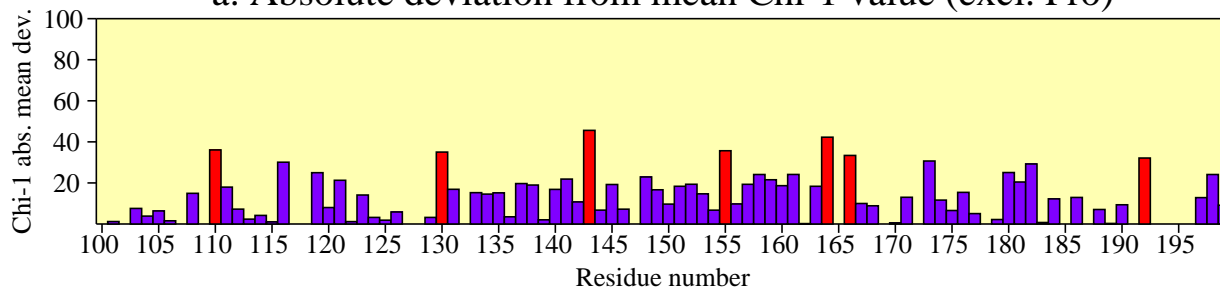


g. G-factors

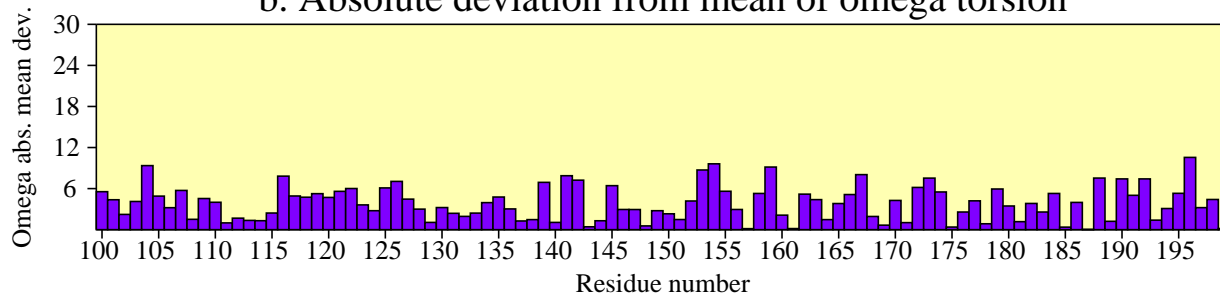


# Residue properties pdb3p4p

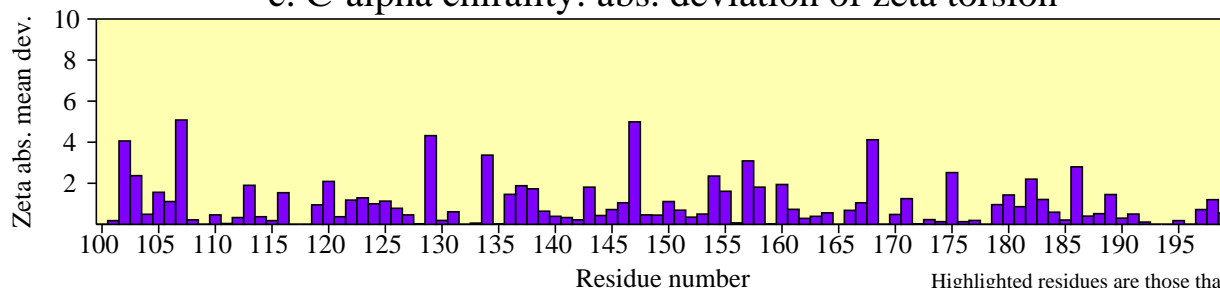
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

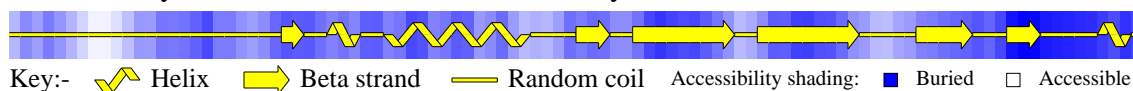


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



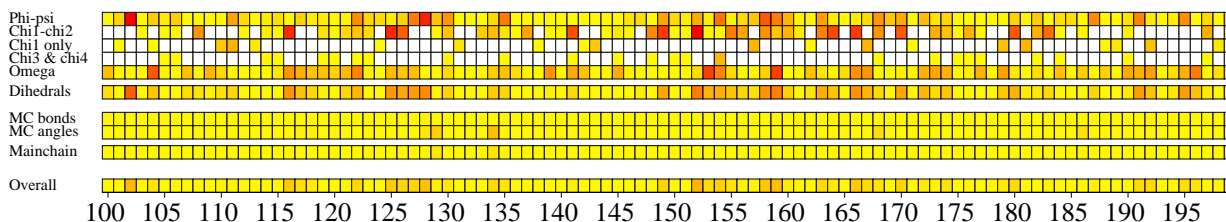
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



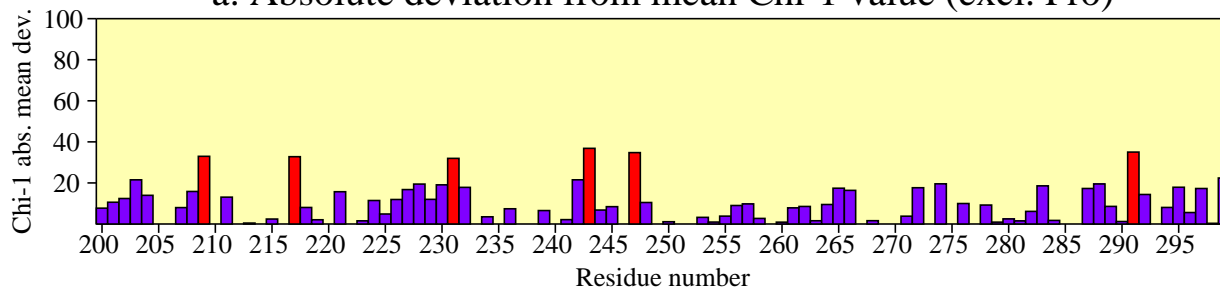
g. G-factors



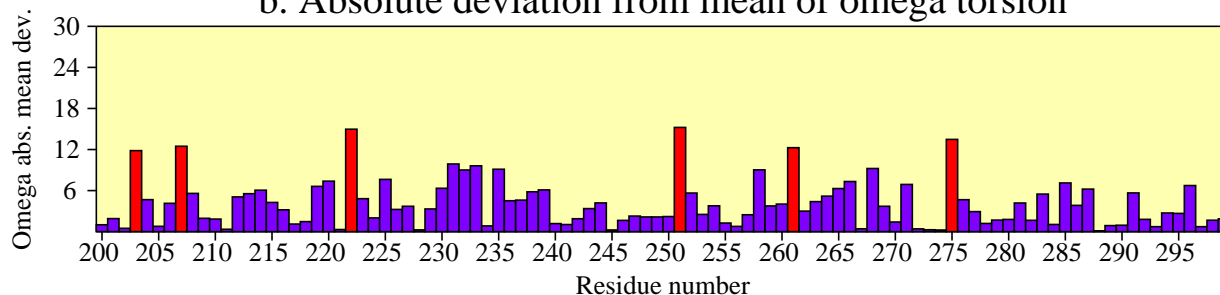
# Residue properties

## pdb3p4p

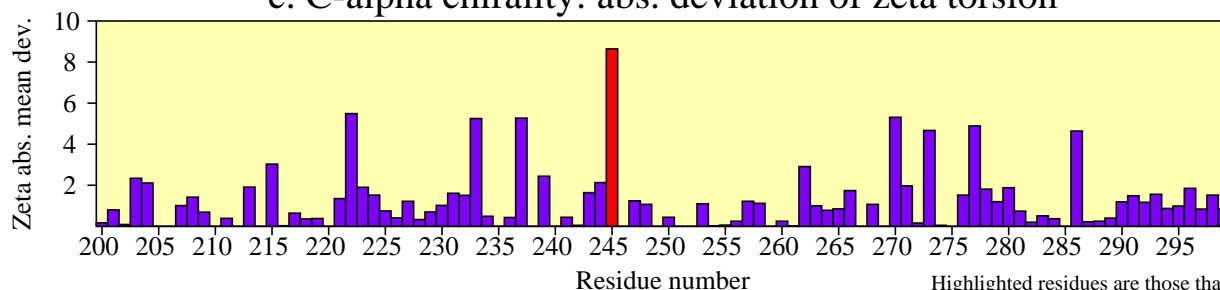
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

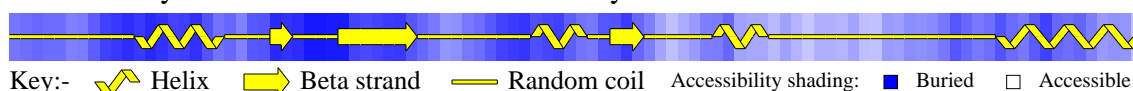


c. C-alpha chirality: abs. deviation of zeta torsion



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

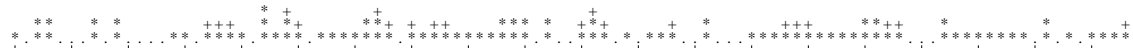
d. Secondary structure & estimated accessibility



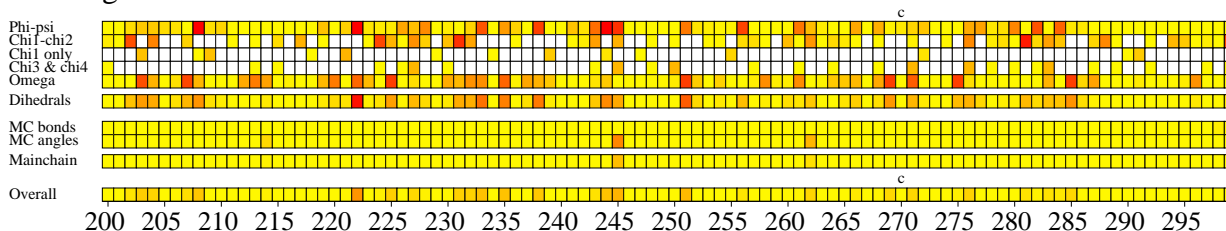
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



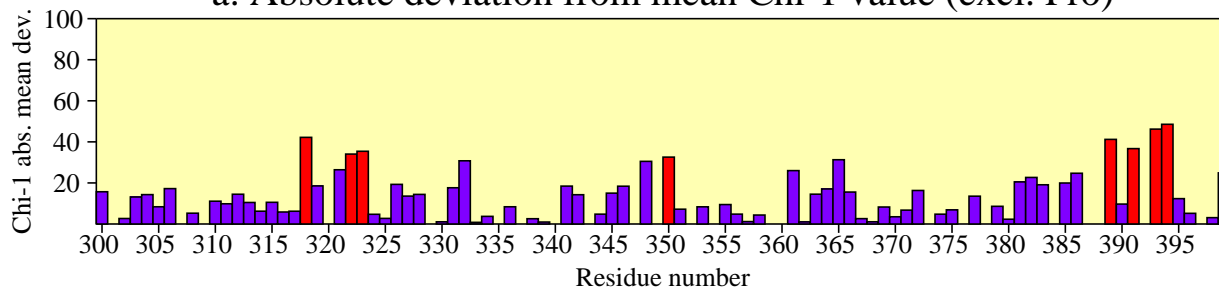
g. G-factors



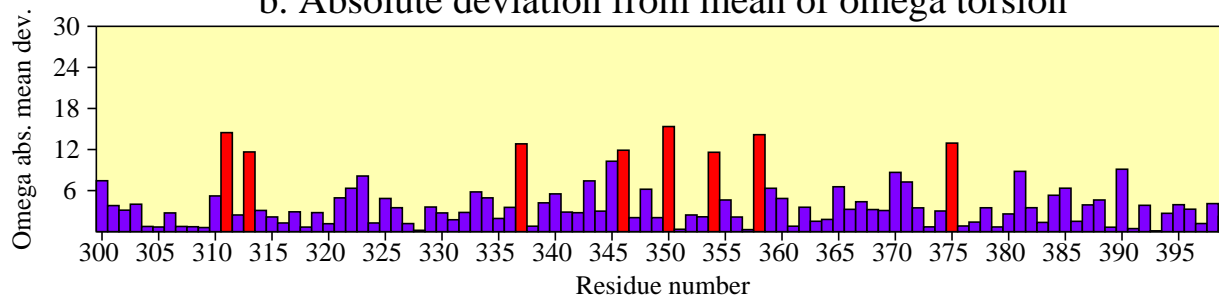
c = cis-peptide

# Residue properties pdb3p4p

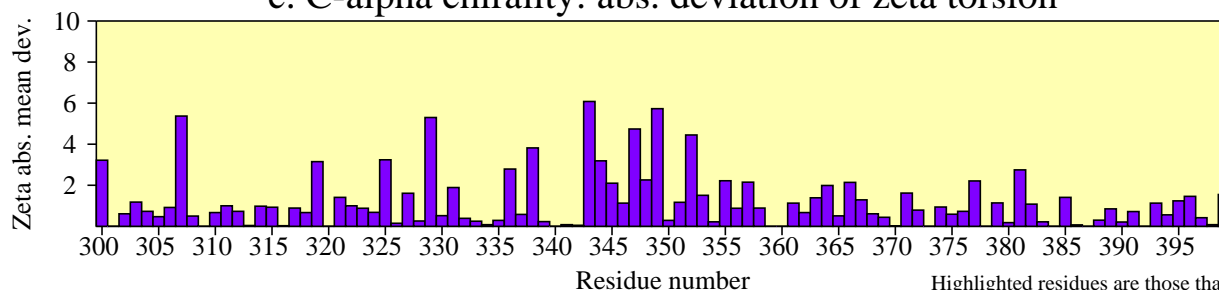
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

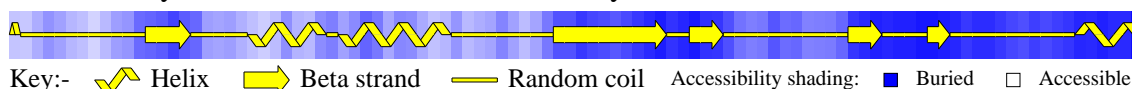


c. C-alpha chirality: abs. deviation of zeta torsion



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

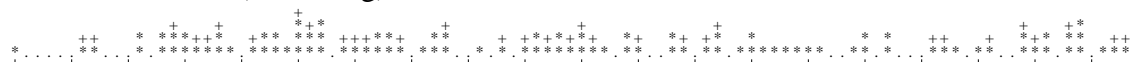
d. Secondary structure & estimated accessibility



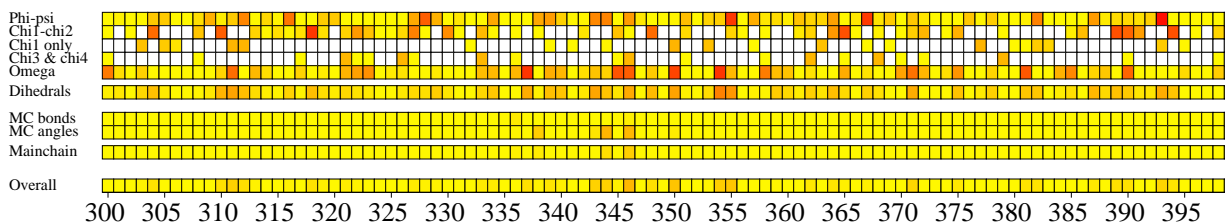
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

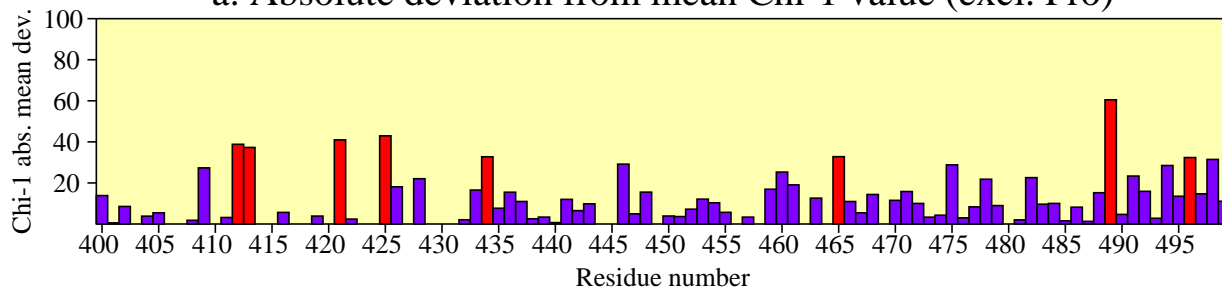


g. G-factors

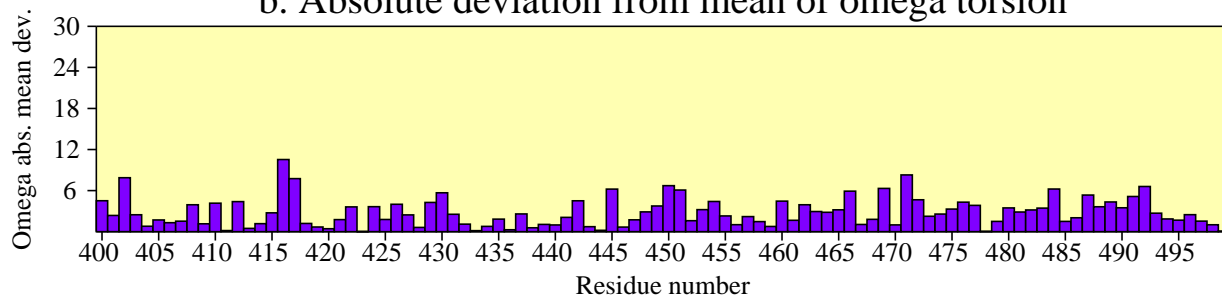


# Residue properties pdb3p4p

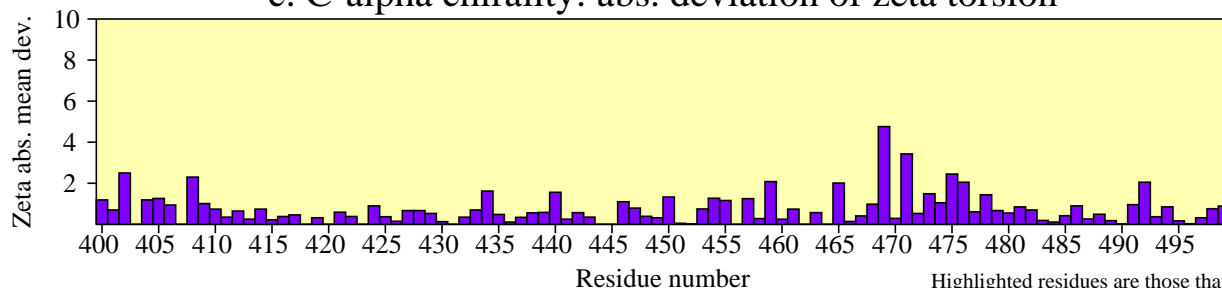
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

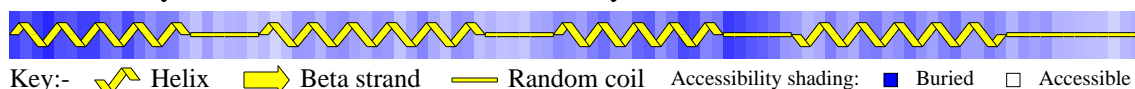


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



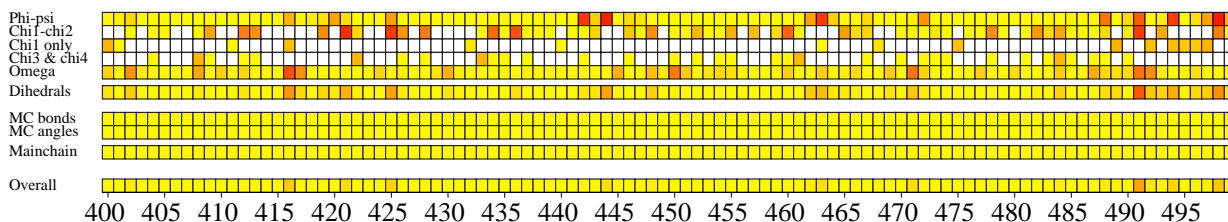
### e. Sequence & Ramachandran regions



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



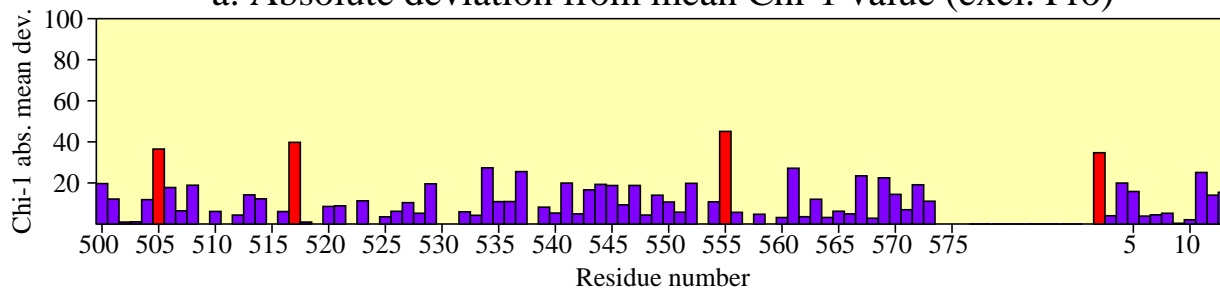
### g. G-factors



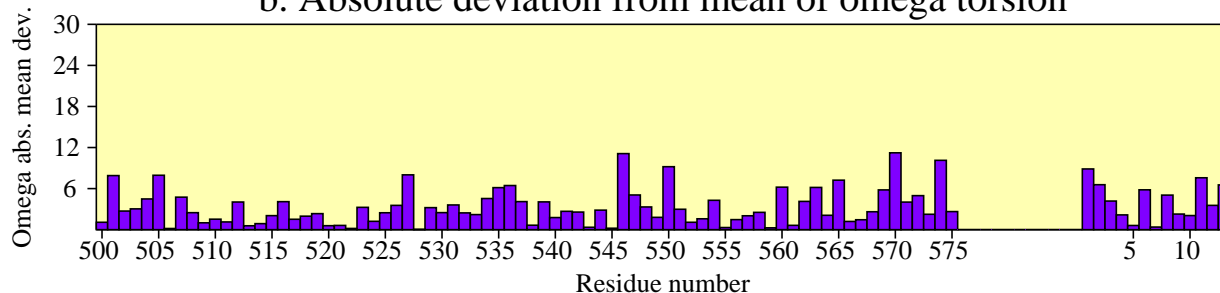


# Residue properties pdb3p4p

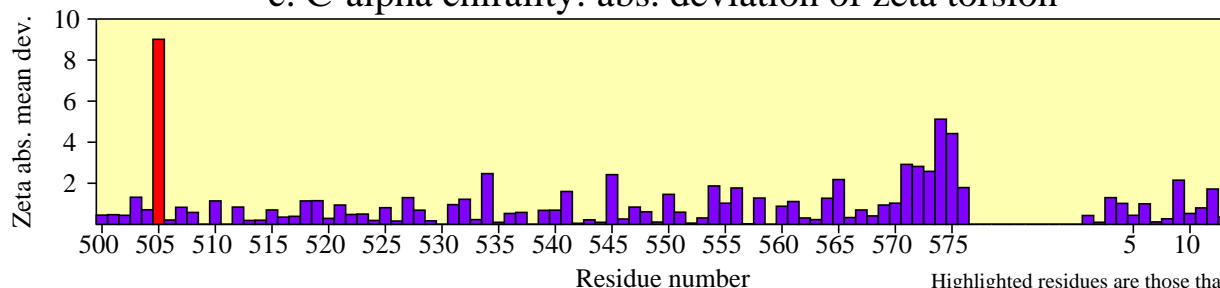
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

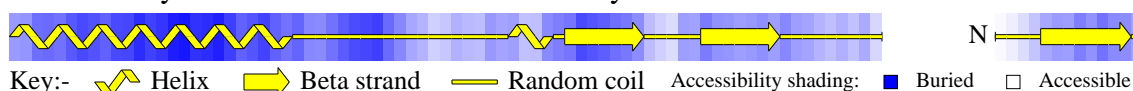


### c. C-alpha chirality: abs. deviation of zeta torsion

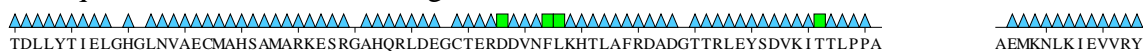


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

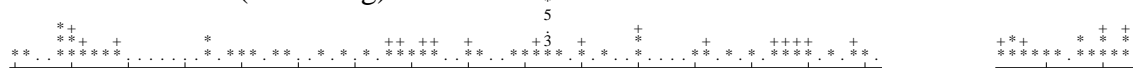
### d. Secondary structure & estimated accessibility



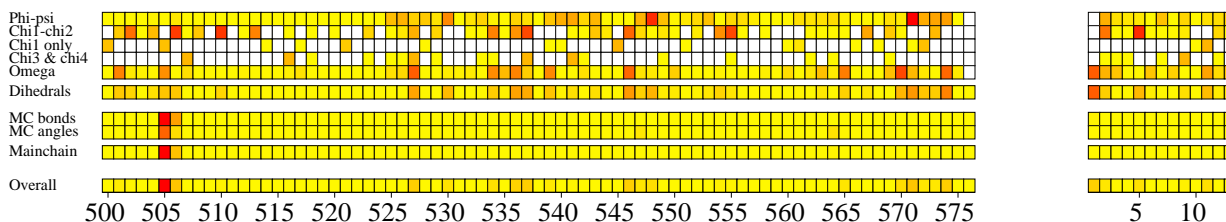
### e. Sequence & Ramachandran regions



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

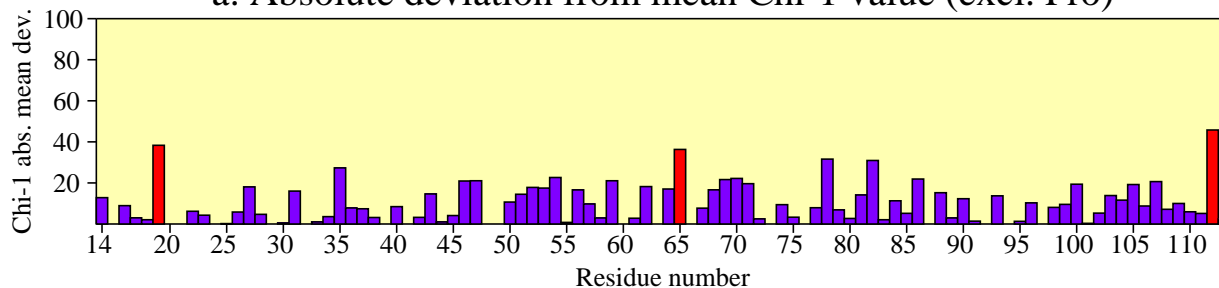


### g. G-factors

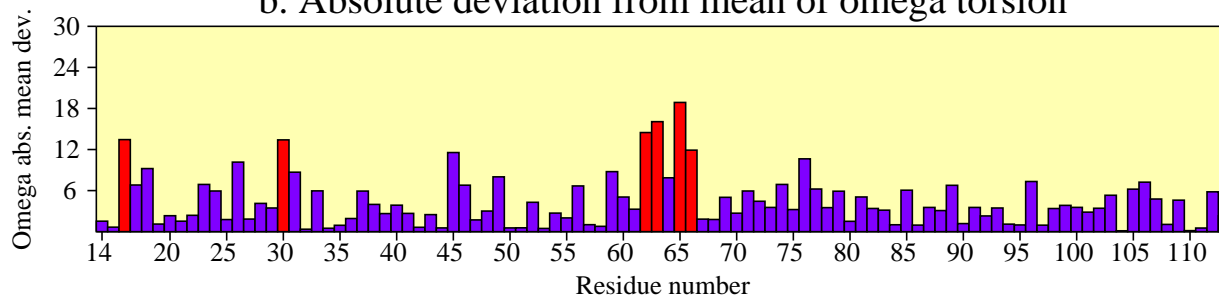


# Residue properties pdb3p4p

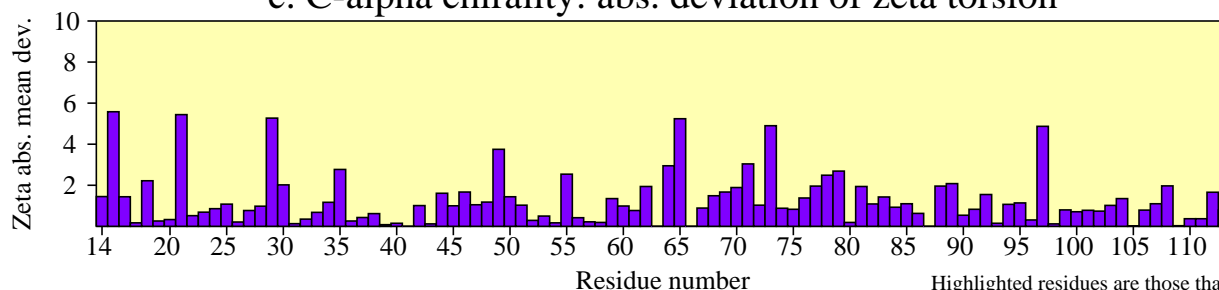
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

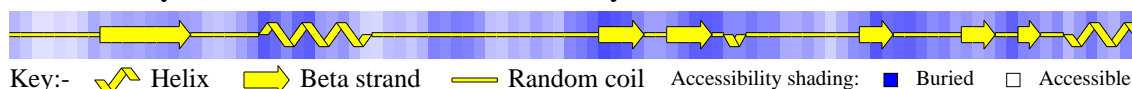


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



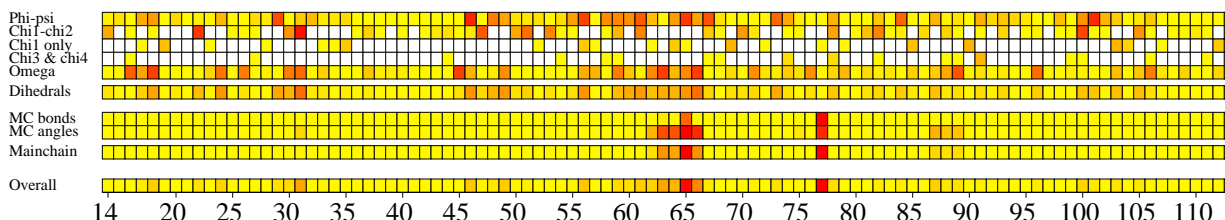
### e. Sequence & Ramachandran regions



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

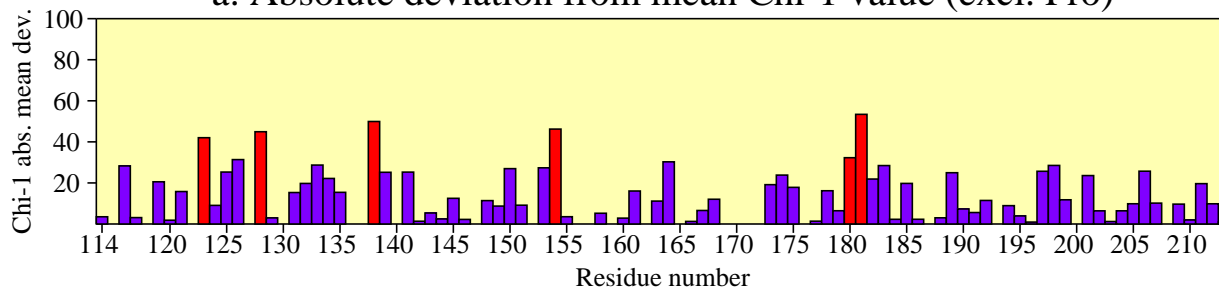


### g. G-factors

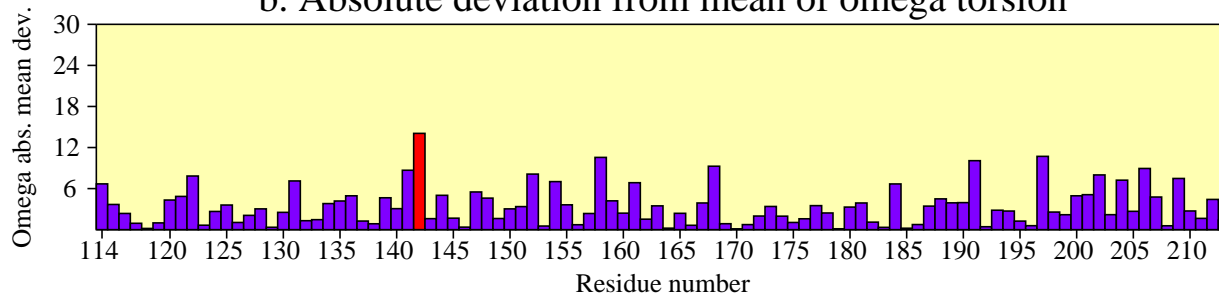


# Residue properties pdb3p4p

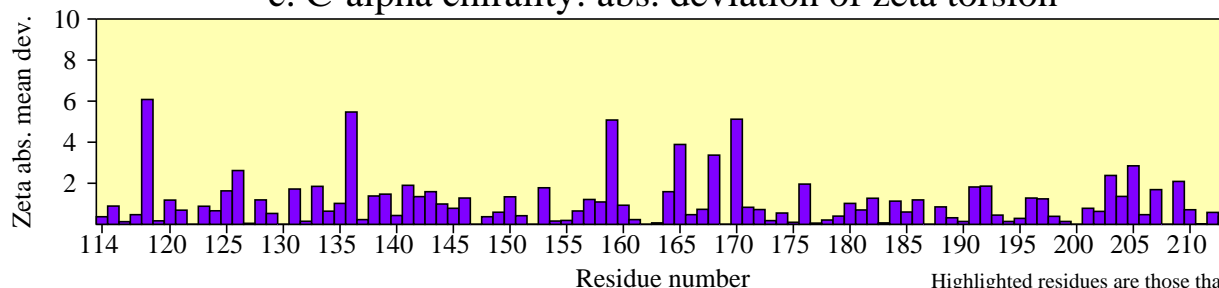
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

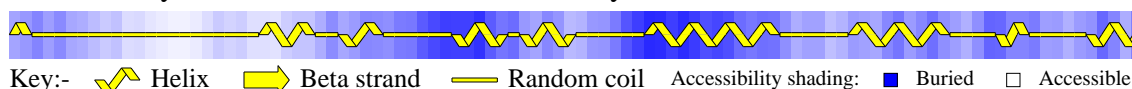


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



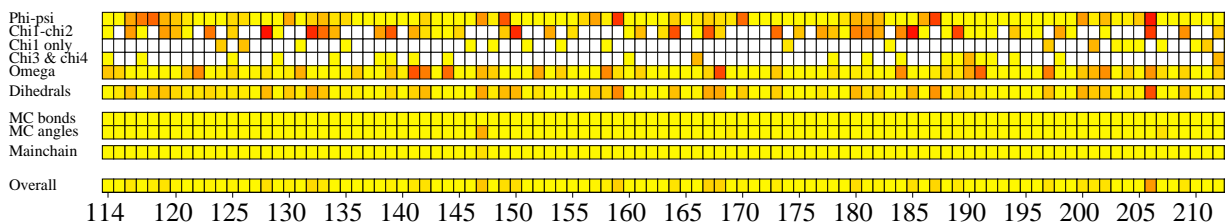
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

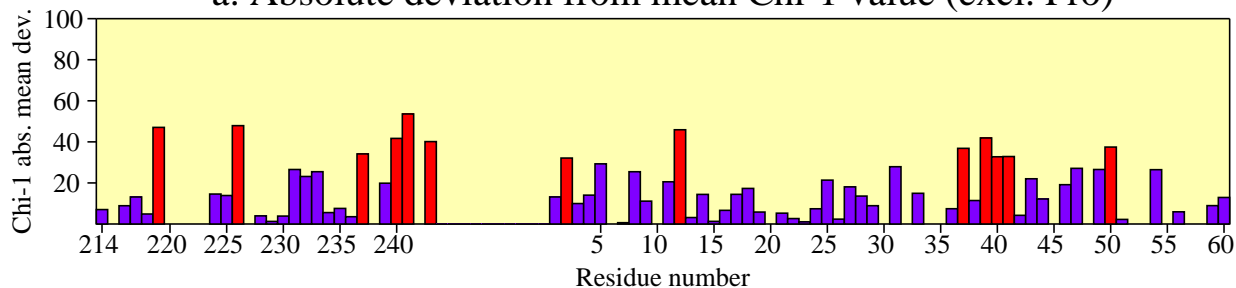


g. G-factors

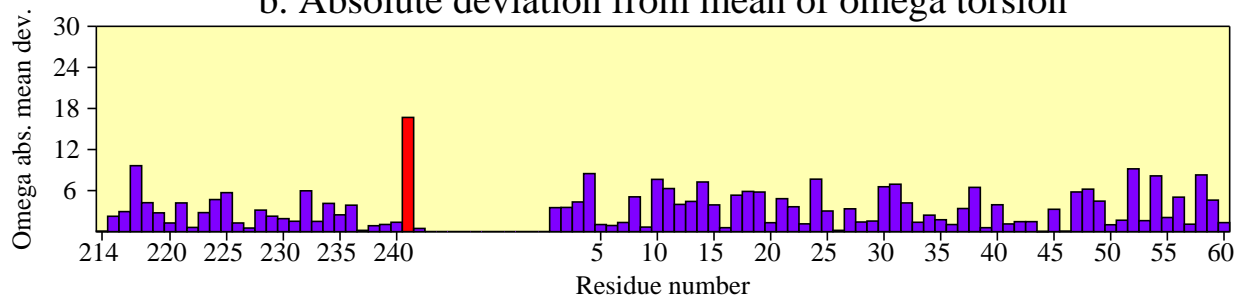


# Residue properties pdb3p4p

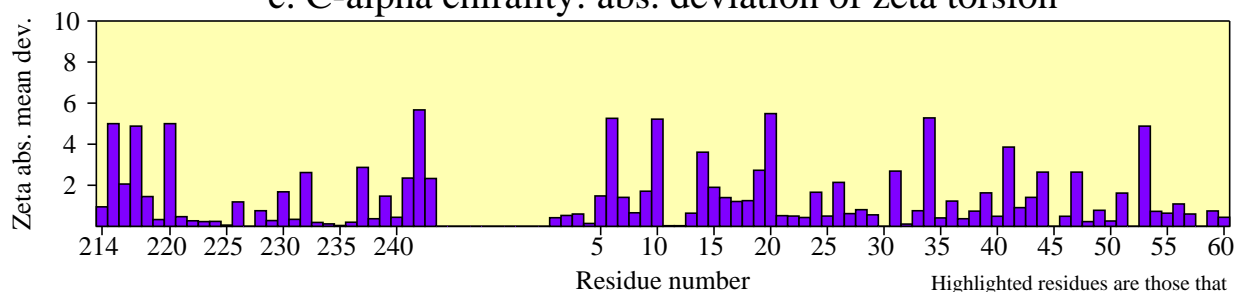
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

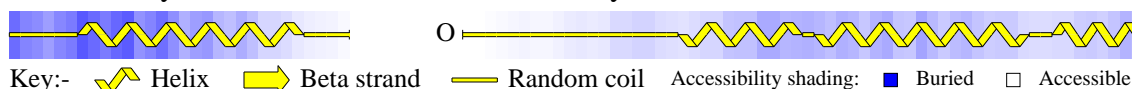


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



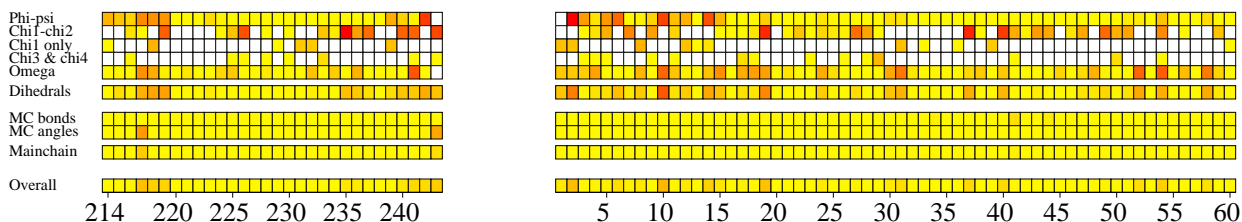
### e. Sequence & Ramachandran regions



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

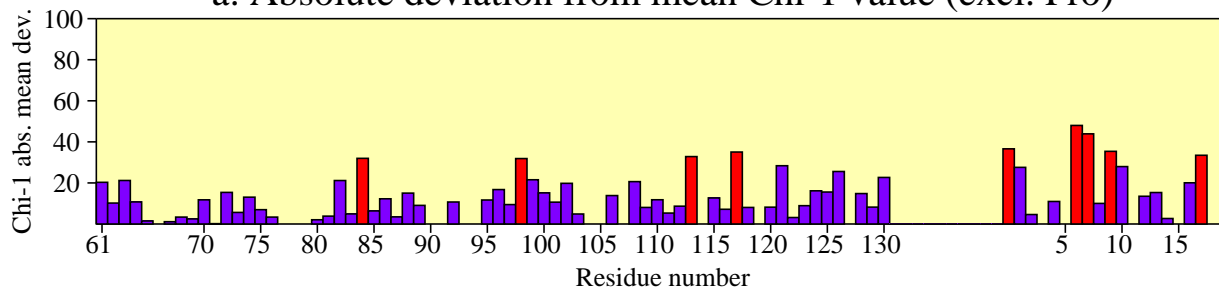


### g. G-factors

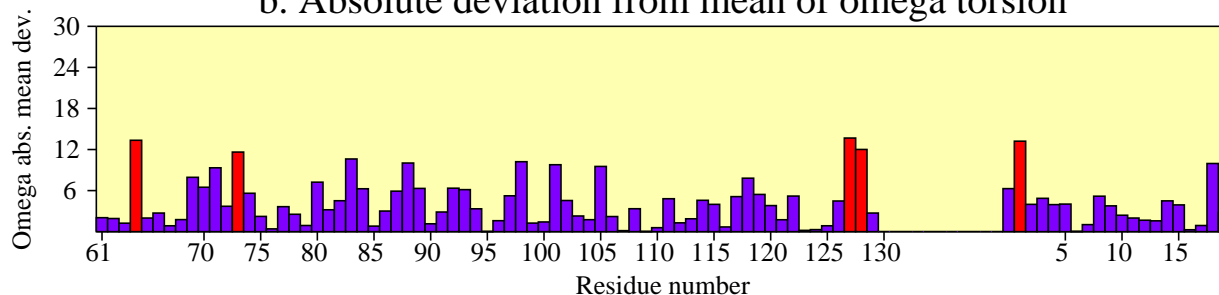


# Residue properties pdb3p4p

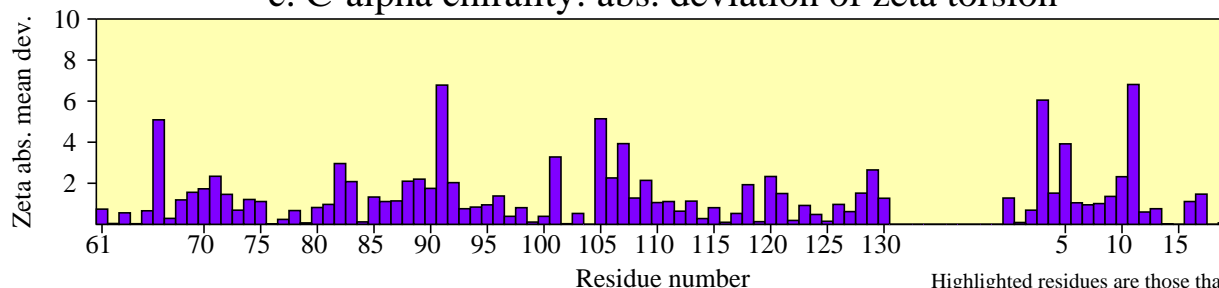
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

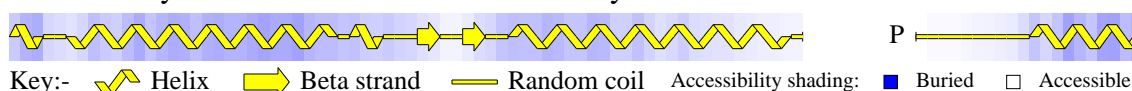


### c. C-alpha chirality: abs. deviation of zeta torsion

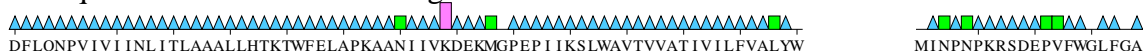


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



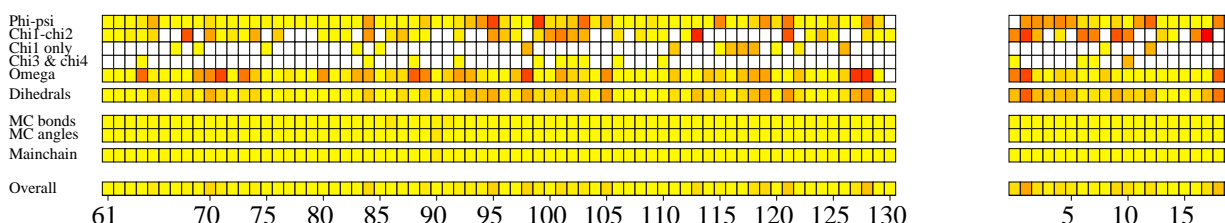
### e. Sequence & Ramachandran regions



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

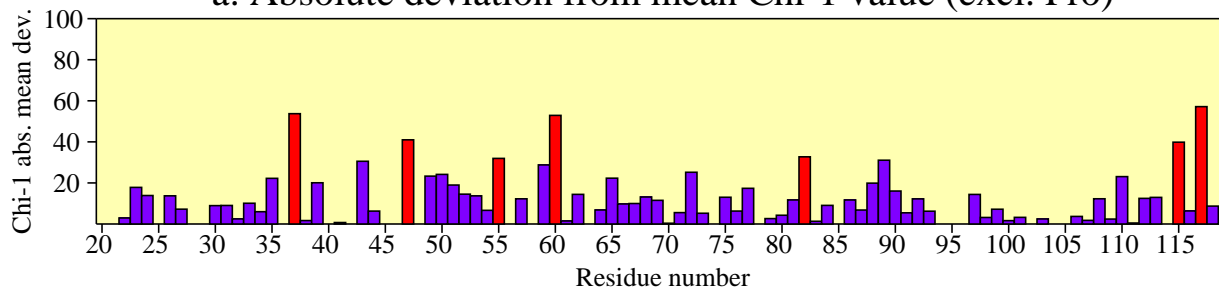


### g. G-factors

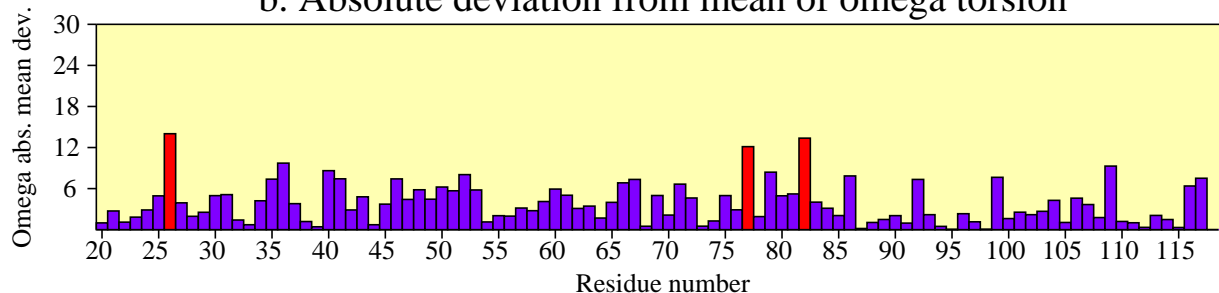


# Residue properties pdb3p4p

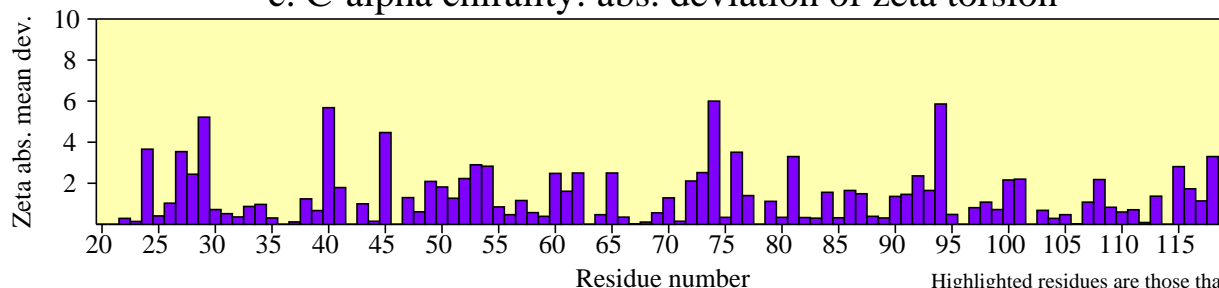
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

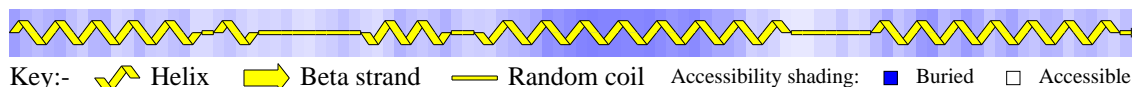


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



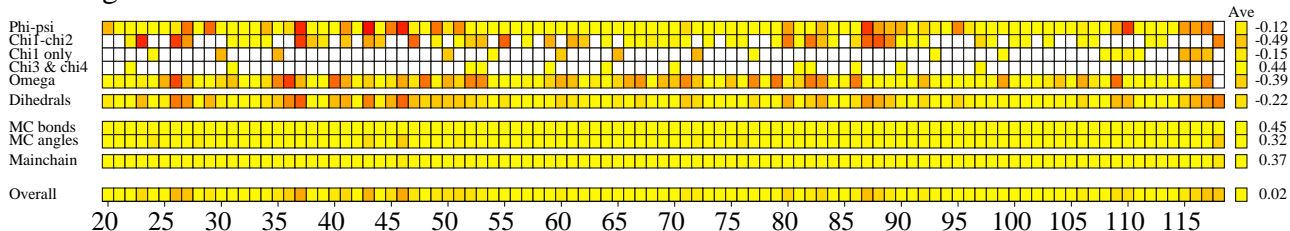
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

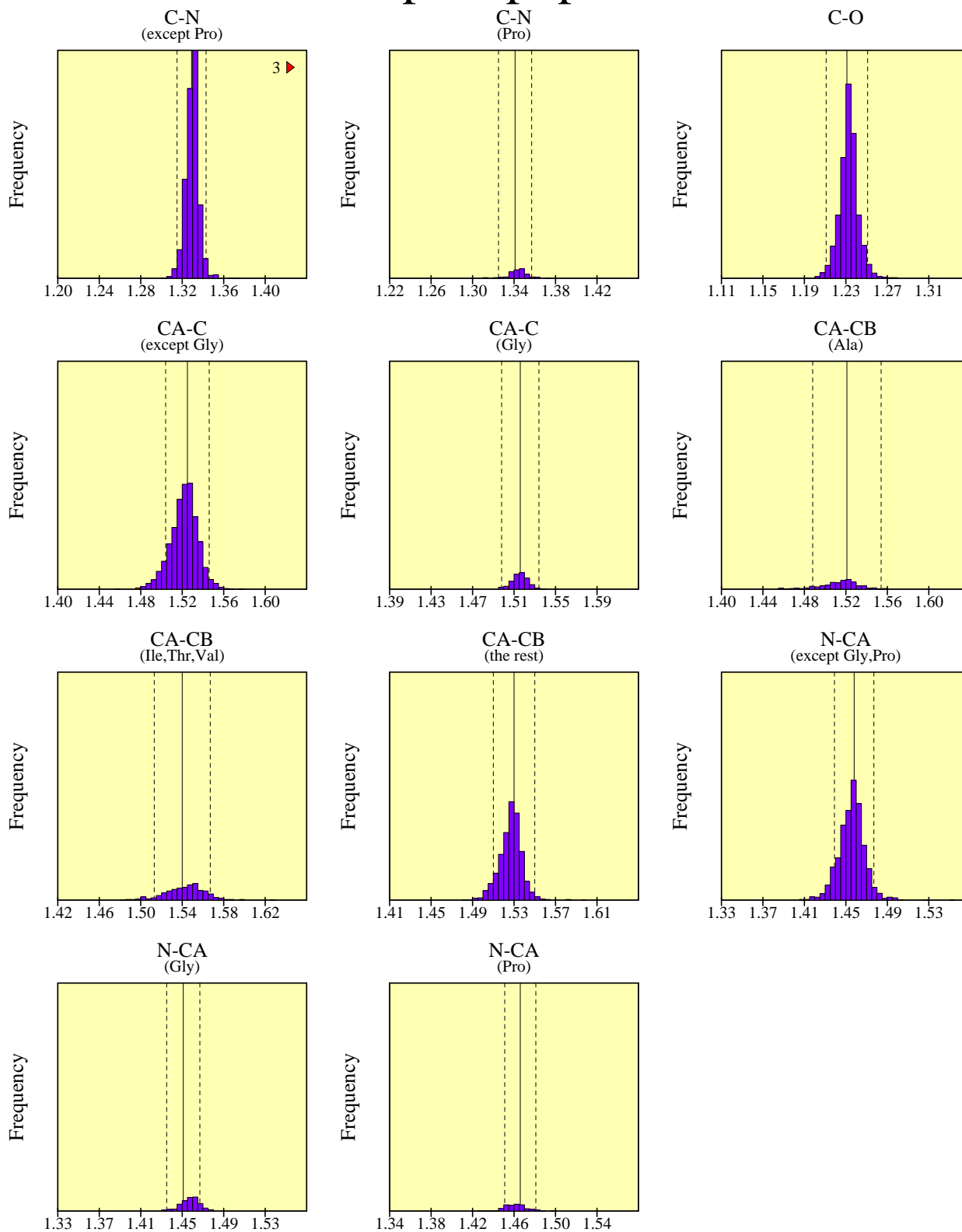


g. G-factors



# Main-chain bond lengths

## pdb3p4p



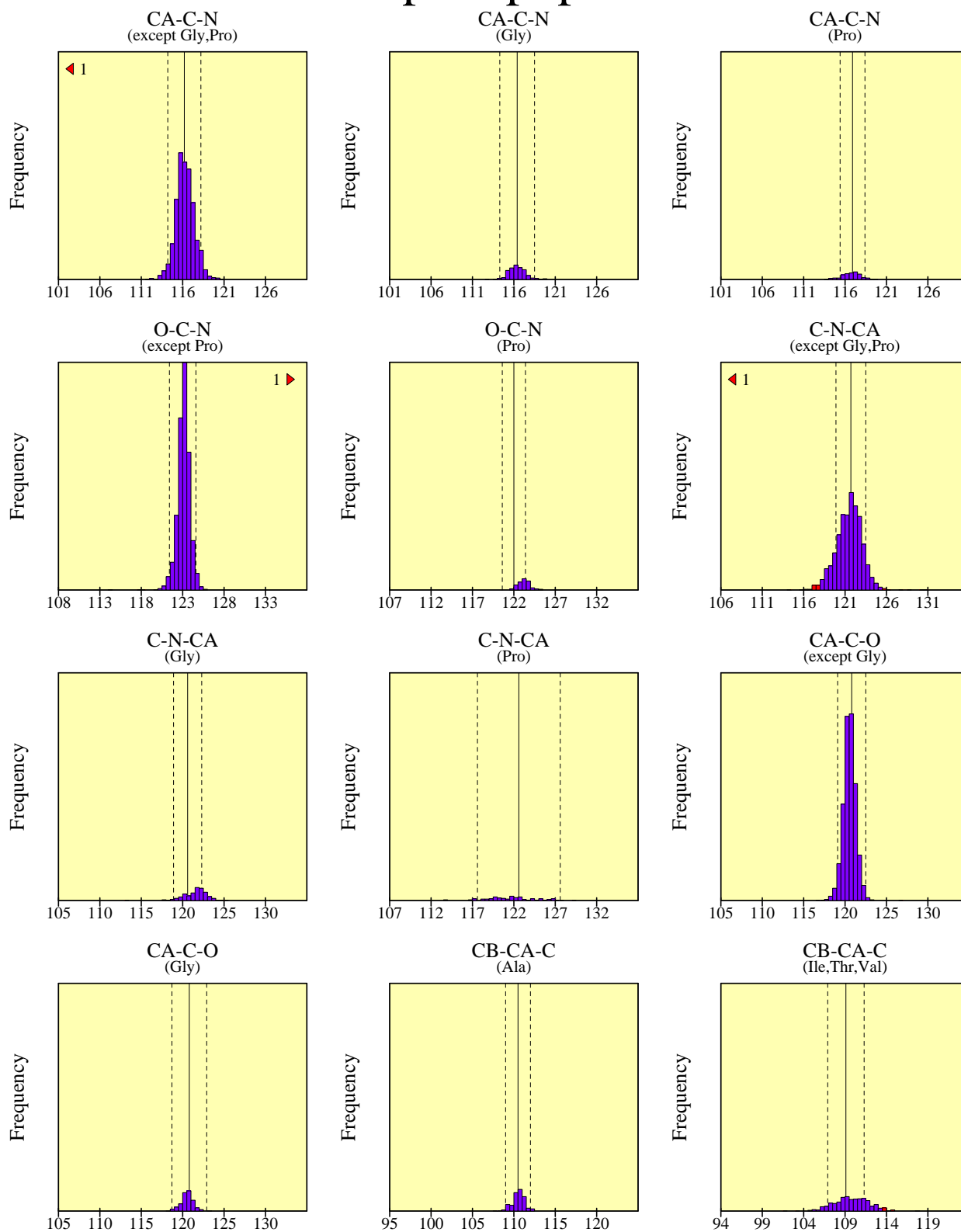
Black bars > 2.0 st. devs. from mean.

◀ 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

## pdb3p4p



Black bars > 2.0 st. devs. from mean.

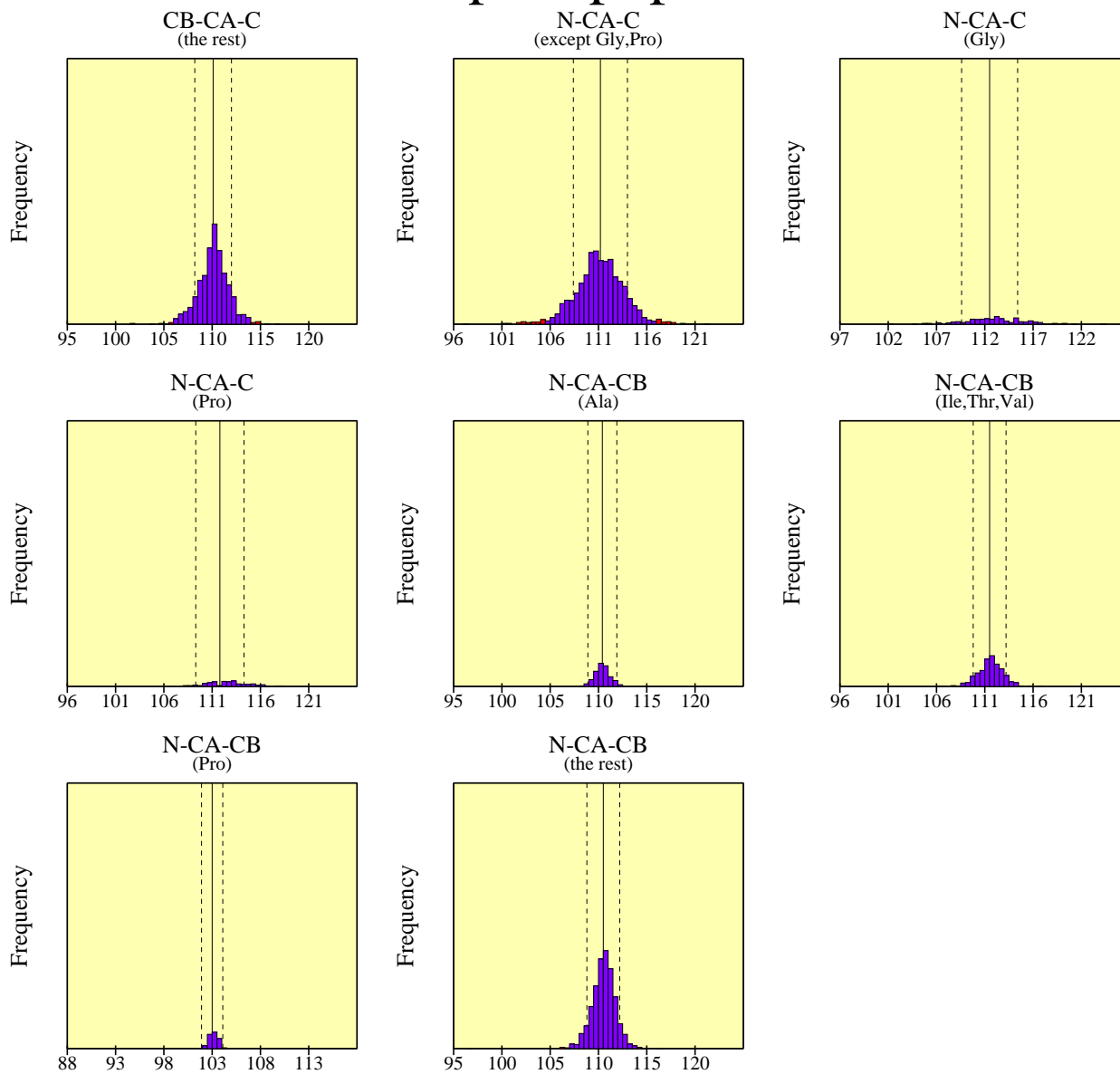
◀ or ▶ signifies data points off the graph in the direction shown.

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



# Main-chain bond angles

## pdb3p4p

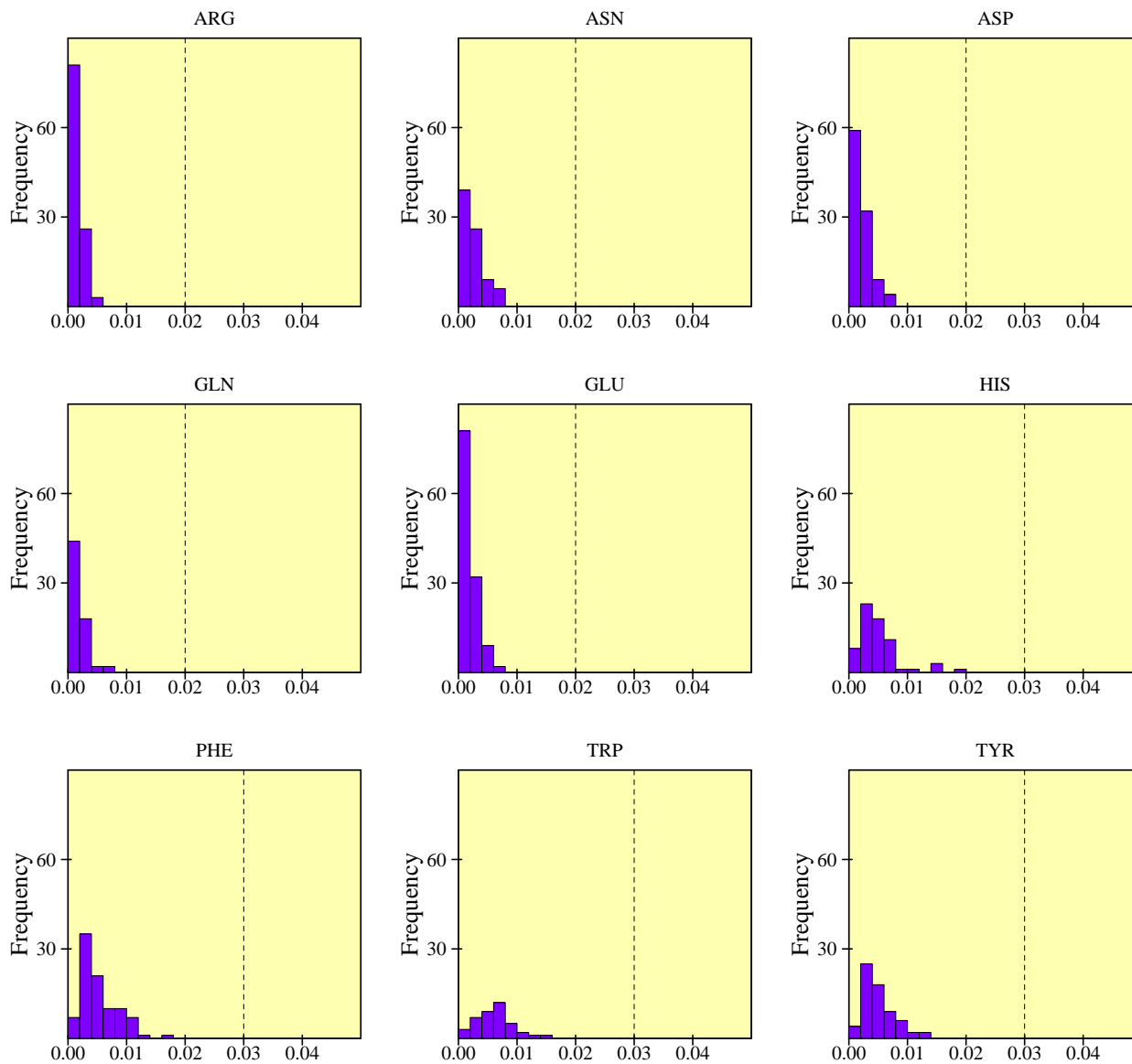


Black bars > 2.0 st. devs. from mean.

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

# RMS distances from planarity

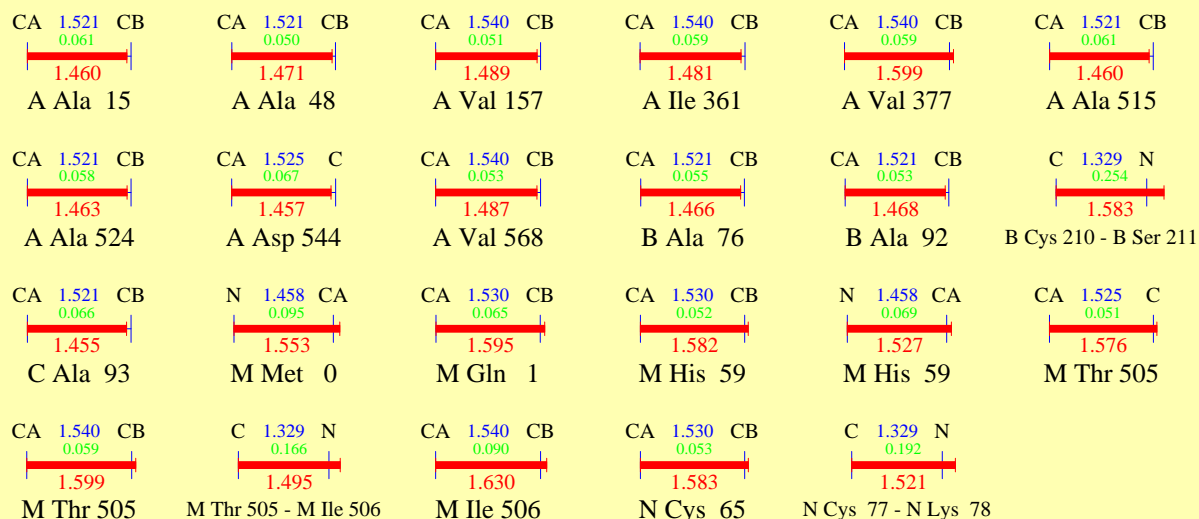
## pdb3p4p



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.

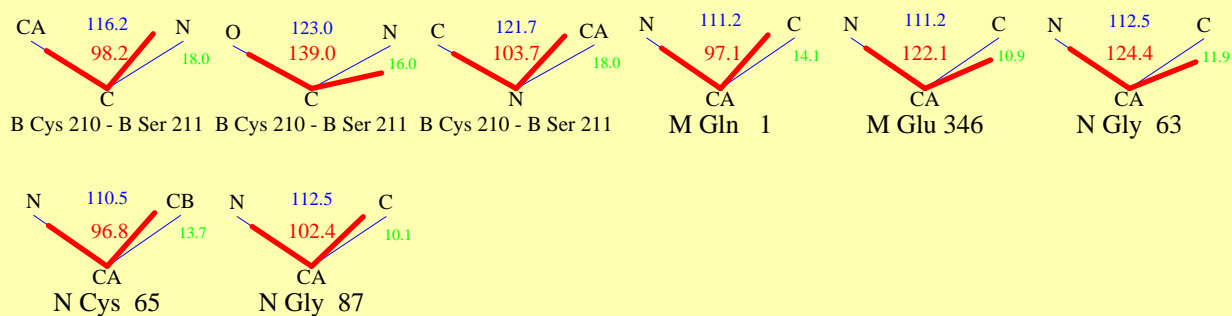
# Distorted geometry pdb3p4p

## Main-chain bond lengths



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

## Main-chain bond angles



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