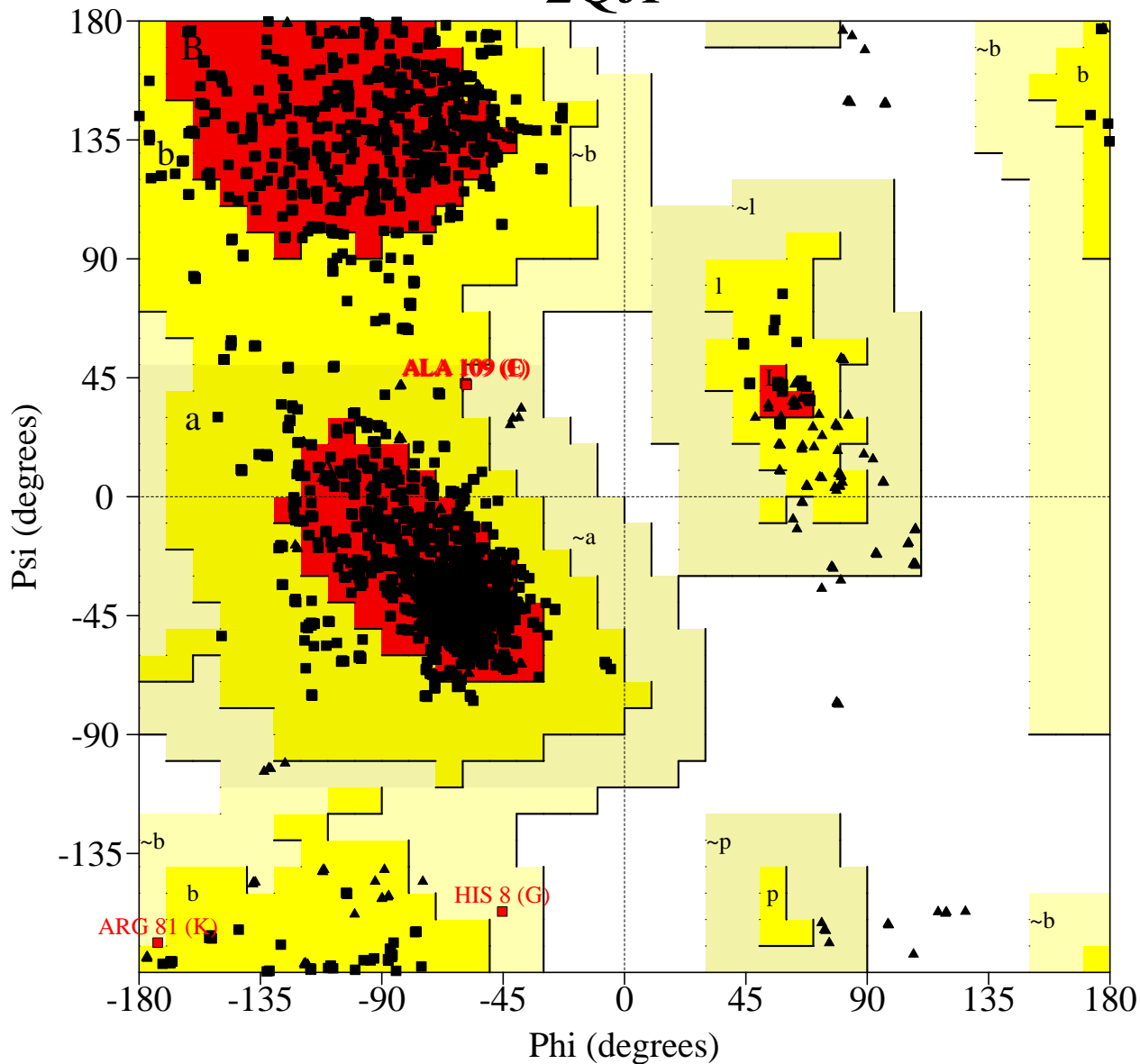


# Ramachandran Plot

## 2QJP



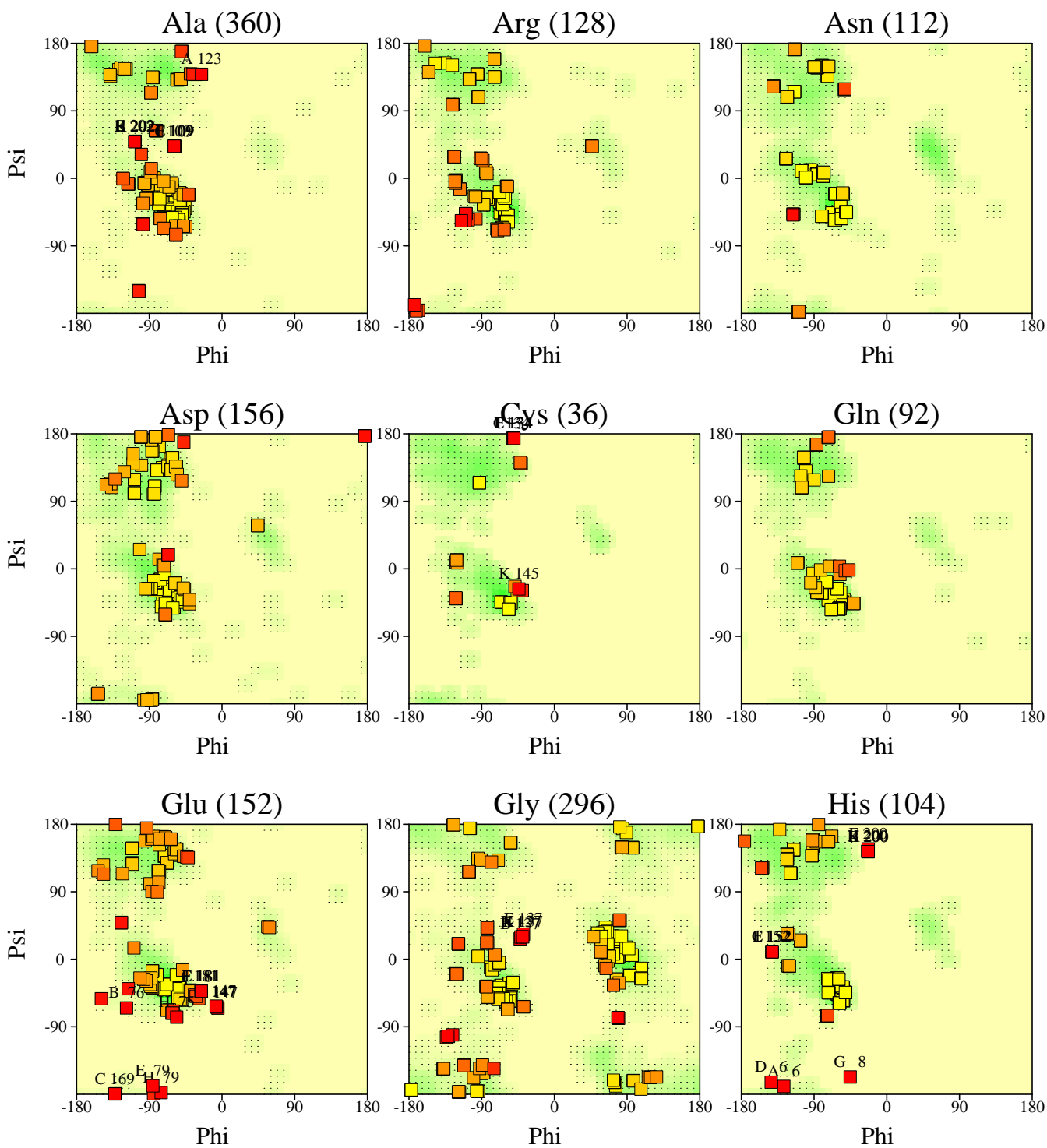
### Plot statistics

Residues in most favoured regions [A,B,L]	2502	86.3%
Residues in additional allowed regions [a,b,l,p]	392	13.5%
Residues in generously allowed regions [-~a,-~b,-~l,-~p]	6	0.2%
Residues in disallowed regions	0	0.0%
----		
Number of non-glycine and non-proline residues	2900	100.0%
Number of end-residues (excl. Gly and Pro)	12	
Number of glycine residues (shown as triangles)	308	
Number of proline residues	232	
----		
Total number of residues	3452	

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

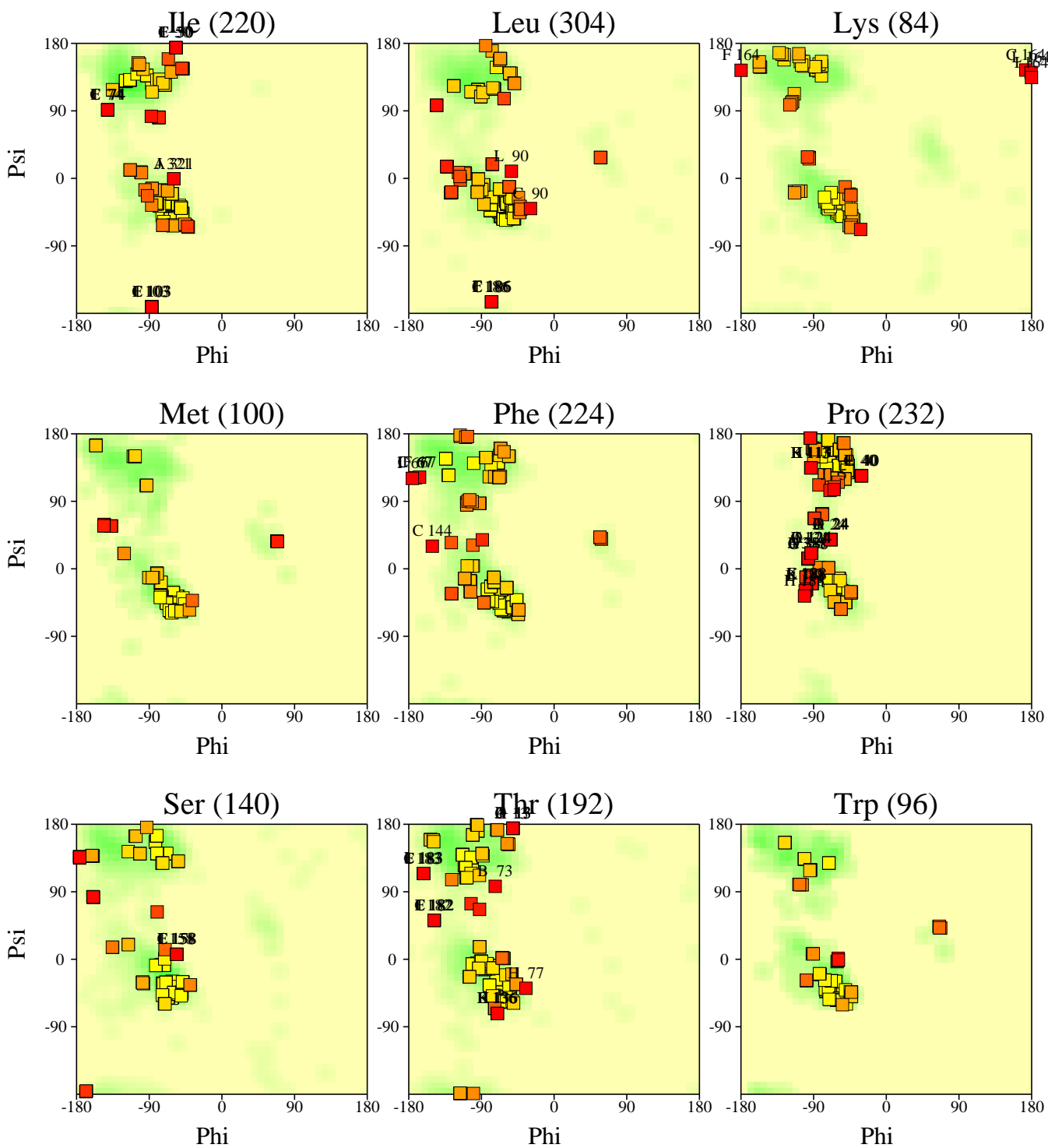
## 2QJP



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

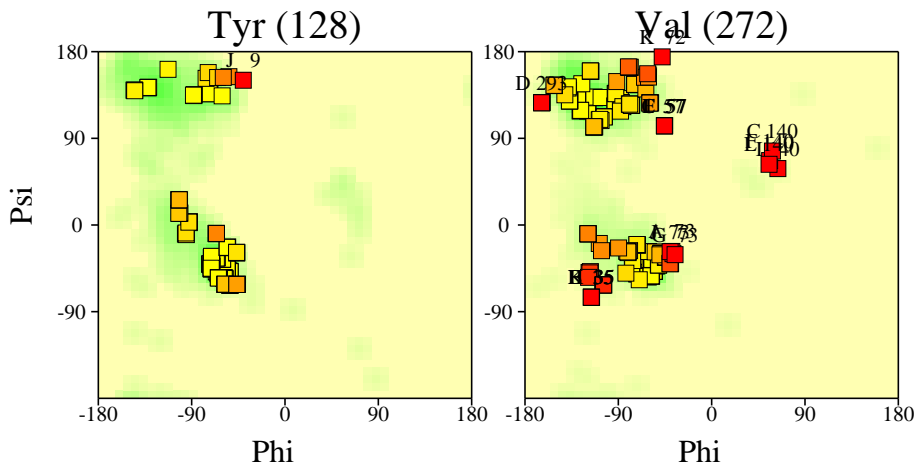
## 2QJP



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

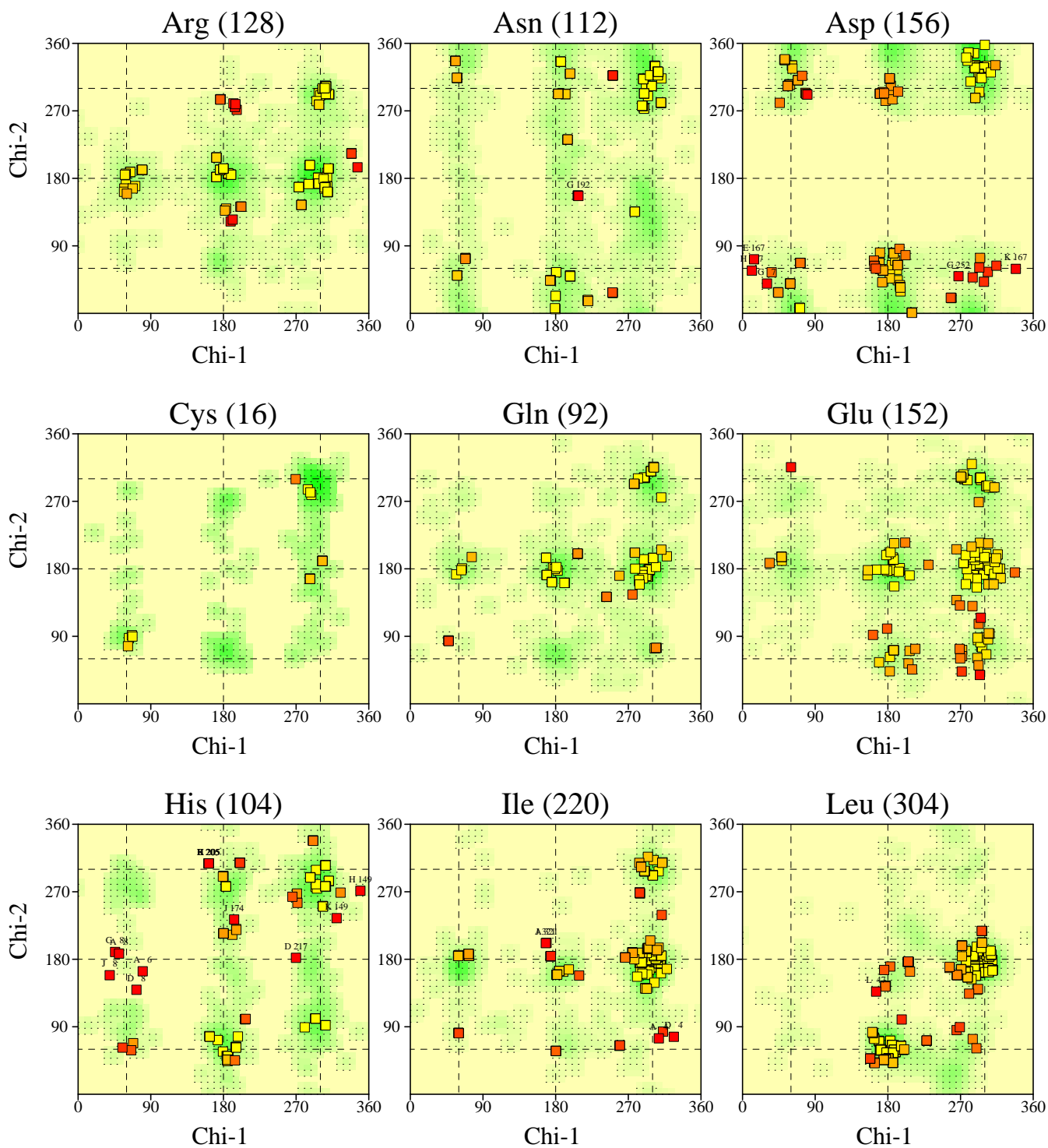
## 2QJP



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.

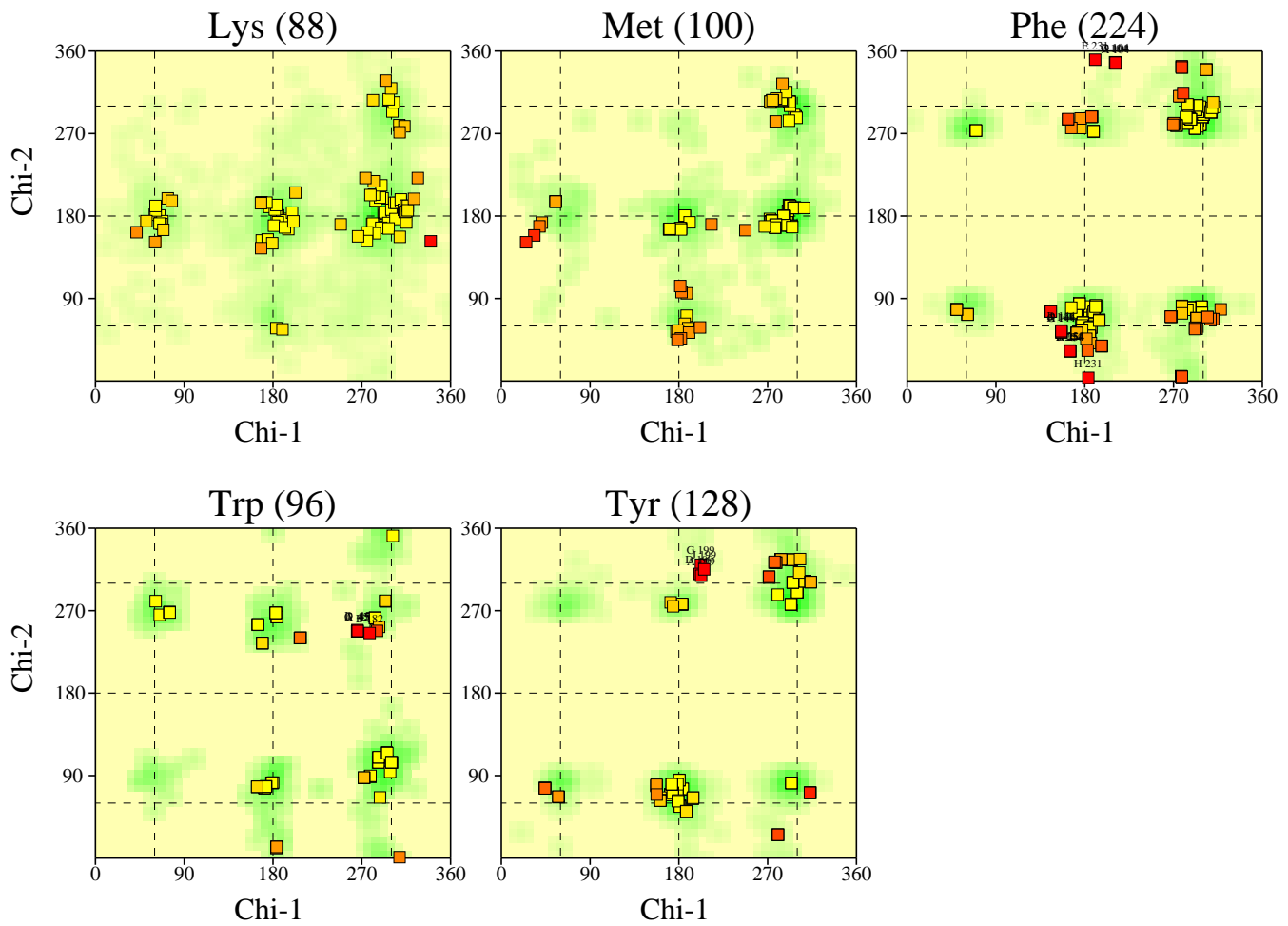
# Chi1-Chi2 plots

## 2QJP



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.

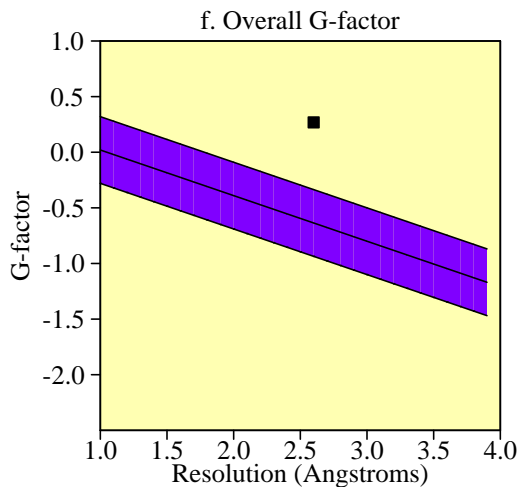
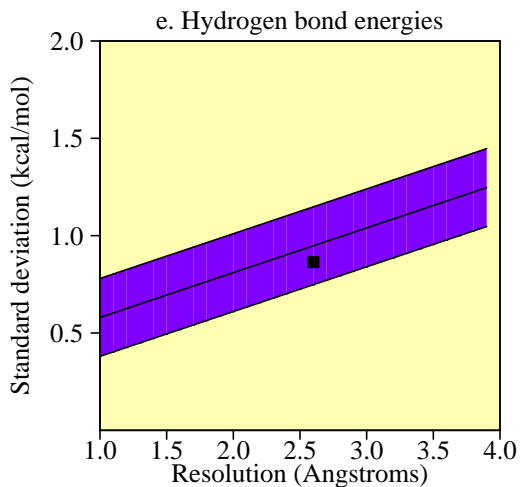
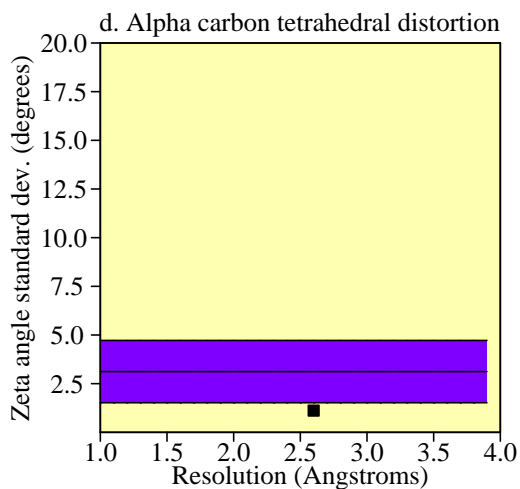
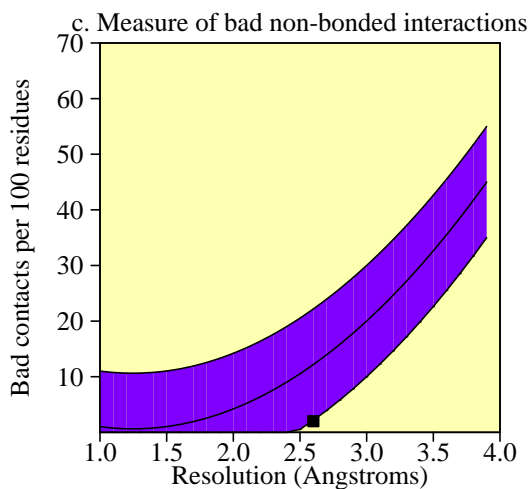
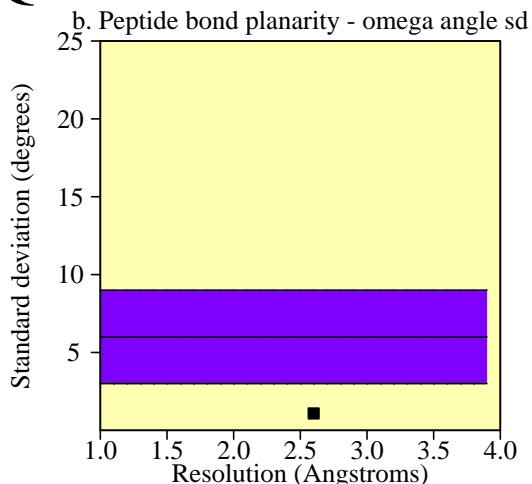
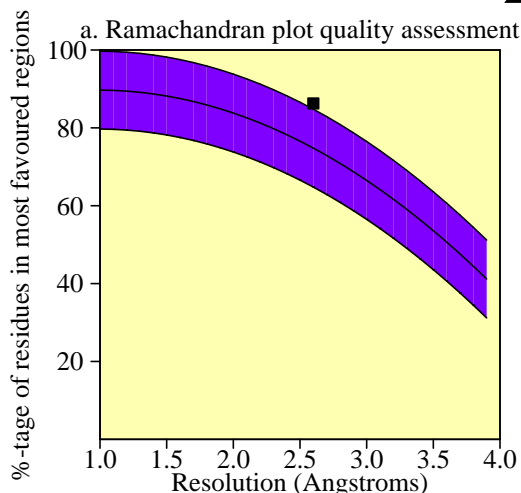
# Chi1-Chi2 plots 2QJP



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

## 2QJP

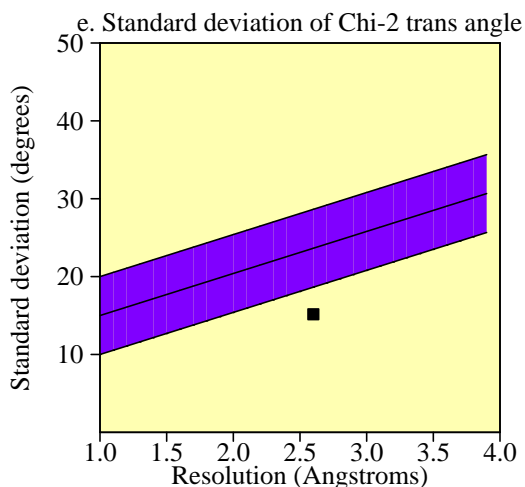
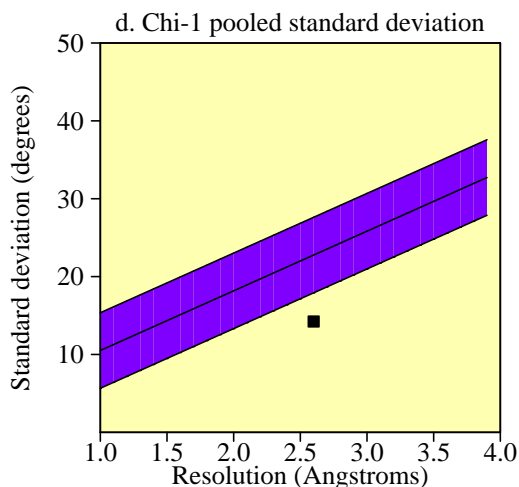
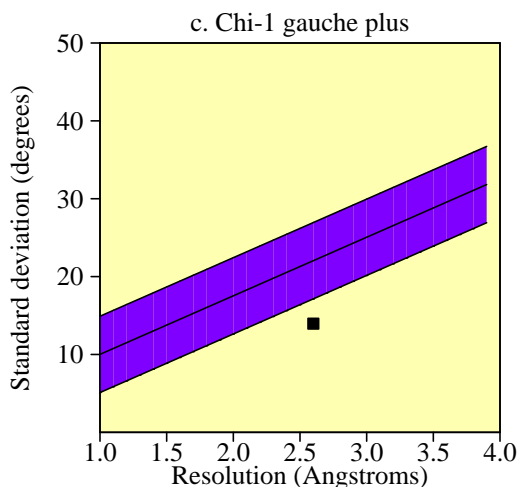
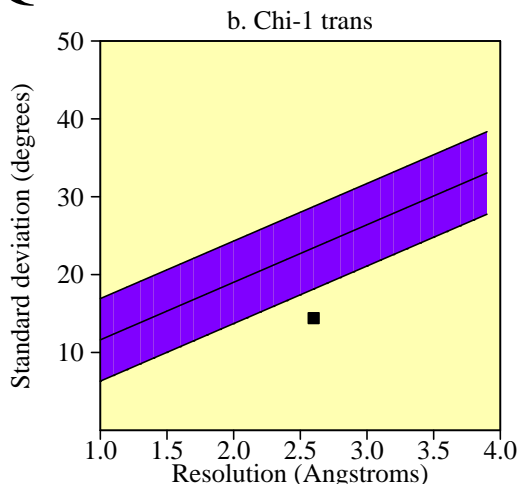
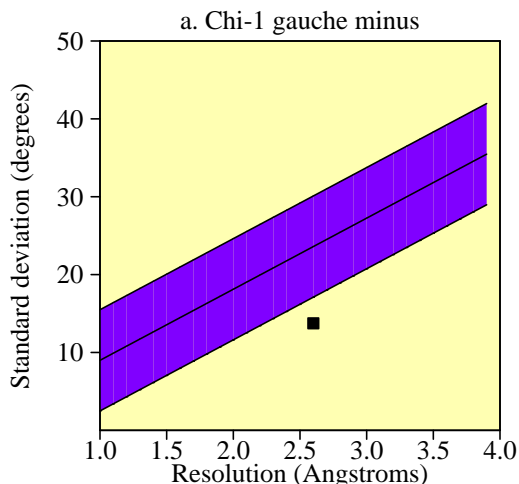


### Plot statistics

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	2900	86.3	74.8	10.0	1.1	BETTER
b. Omega angle st dev	3424	1.1	6.0	3.0	-1.6	BETTER
c. Bad contacts / 100 residues	69	2.0	12.2	10.0	-1.0	BETTER
d. Zeta angle st dev	3144	1.1	3.1	1.6	-1.3	BETTER
e. H-bond energy st dev	2203	0.9	0.9	0.2	-0.4	Inside
f. Overall G-factor	3452	0.3	-0.6	0.3	3.0	BETTER

# Side-chain parameters

## 2QJP



2QJP

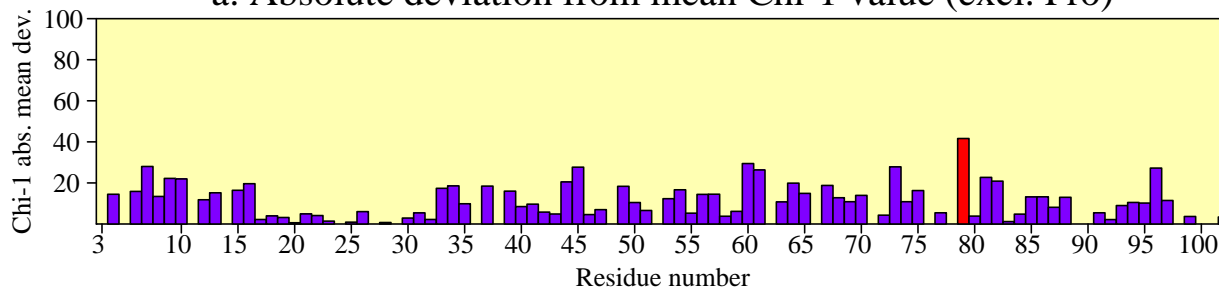
### Plot statistics

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	322	13.7	23.6	6.5	-1.5	BETTER
b. Chi-1 trans st dev	902	14.4	23.4	5.3	-1.7	BETTER
c. Chi-1 gauche plus st dev	1320	14.0	22.0	4.9	-1.7	BETTER
d. Chi-1 pooled st dev	2544	14.2	22.8	4.8	-1.8	BETTER
e. Chi-2 trans st dev	801	15.2	23.6	5.0	-1.7	BETTER

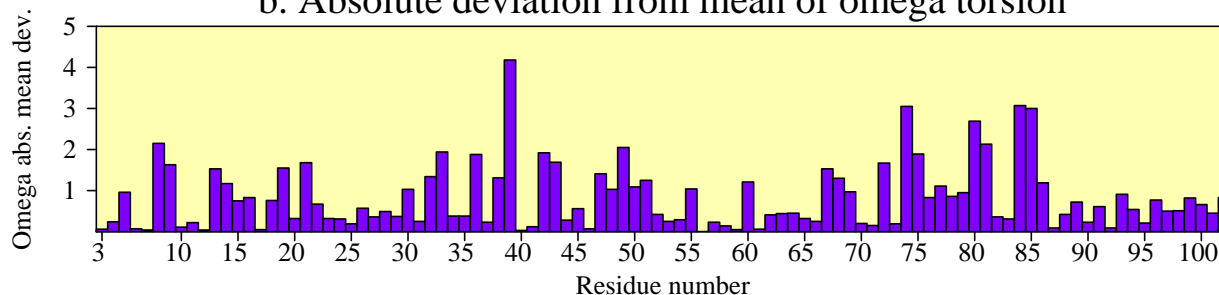


# Residue properties 2QJP

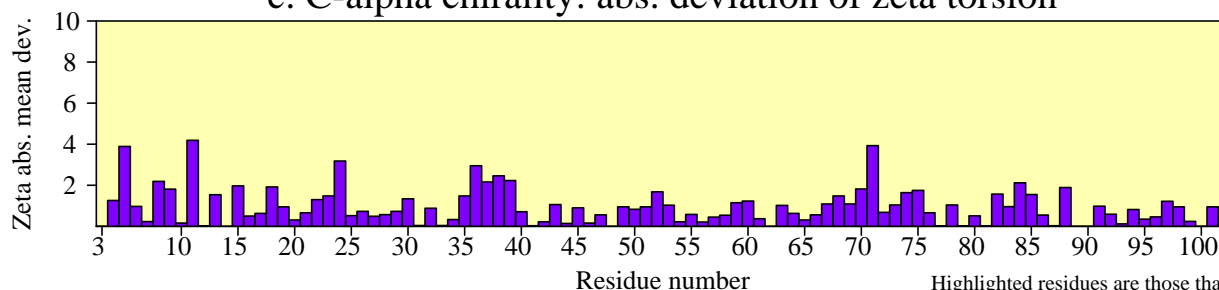
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

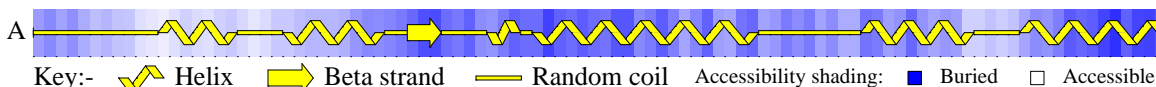


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



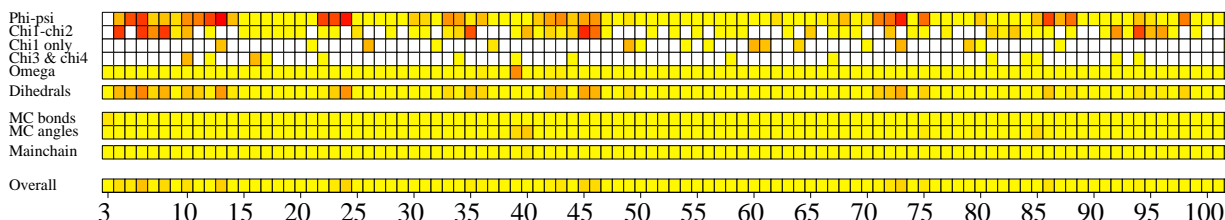
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

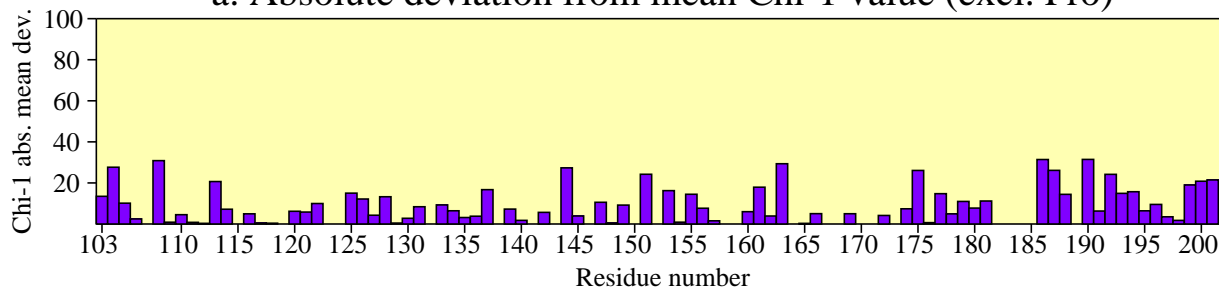


g. G-factors

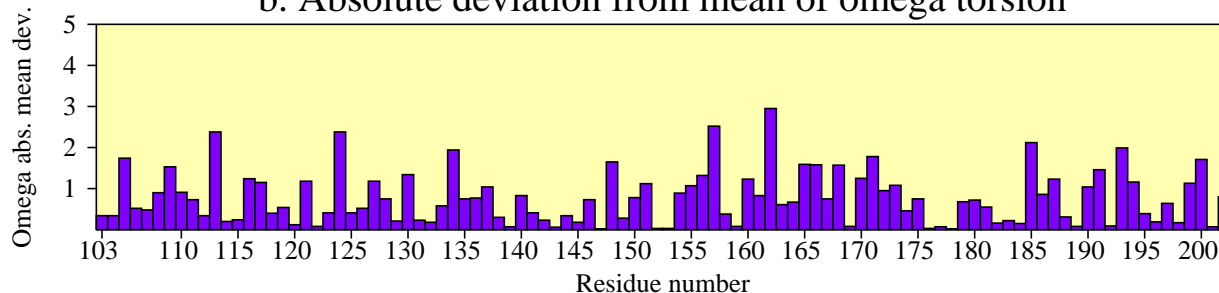


# Residue properties 2QJP

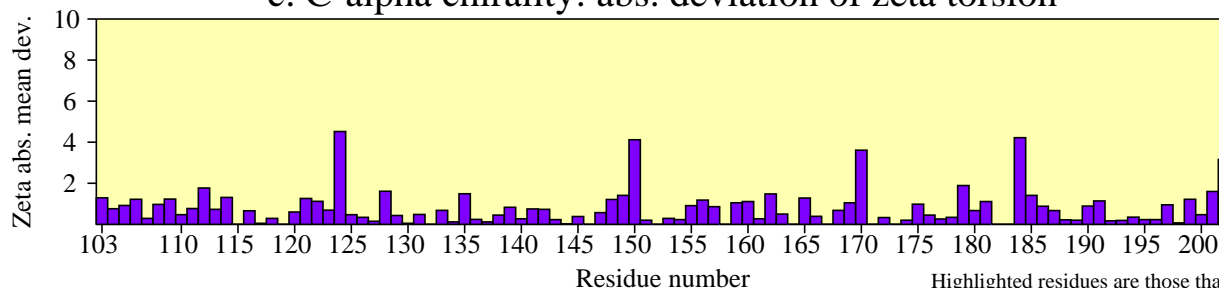
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

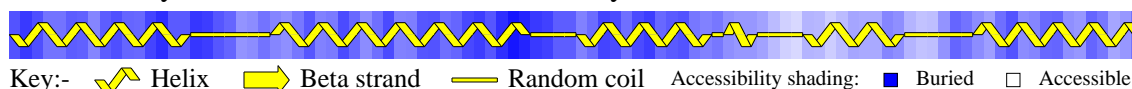


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



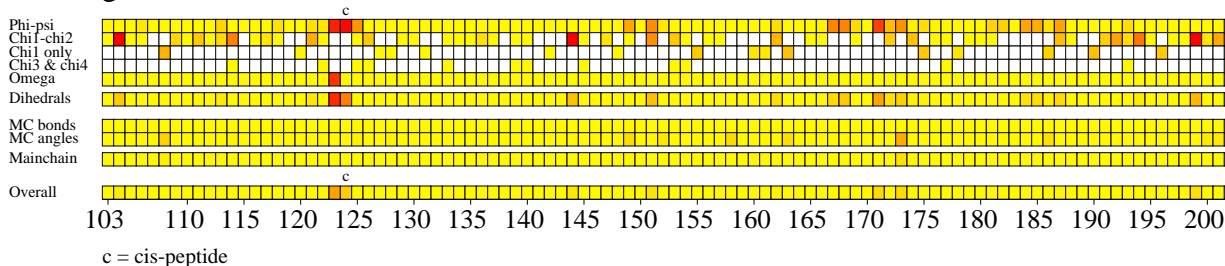
### e. Sequence & Ramachandran regions



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

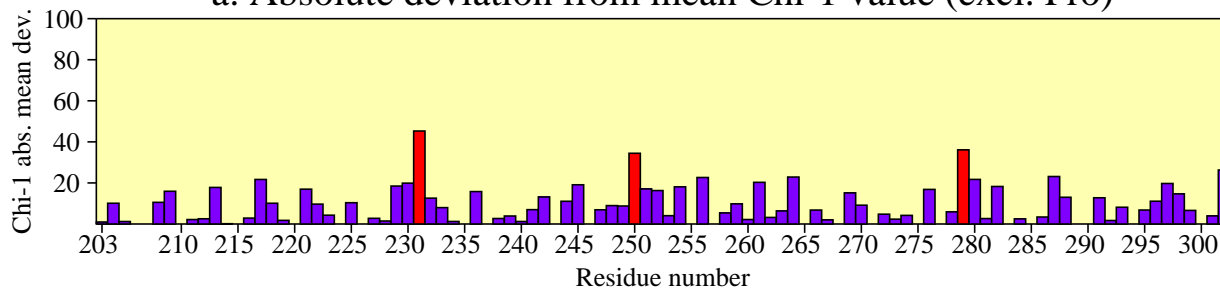


### g. G-factors

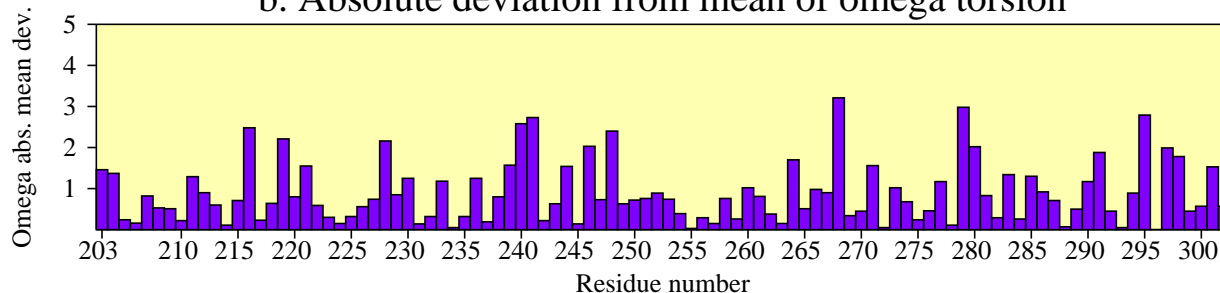


# Residue properties 2QJP

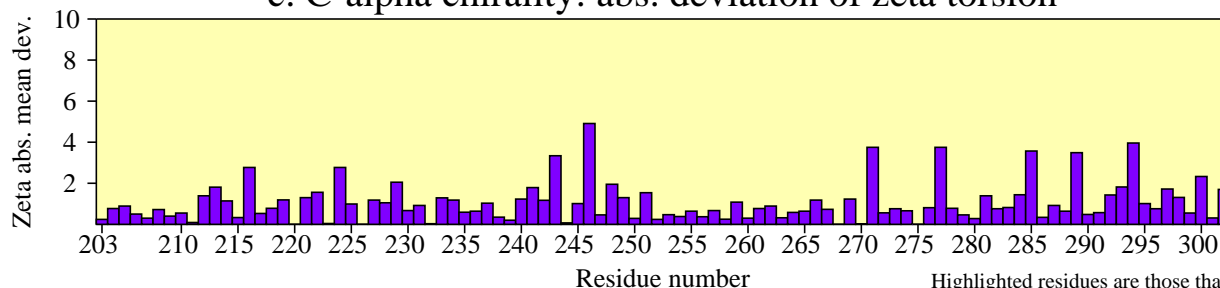
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



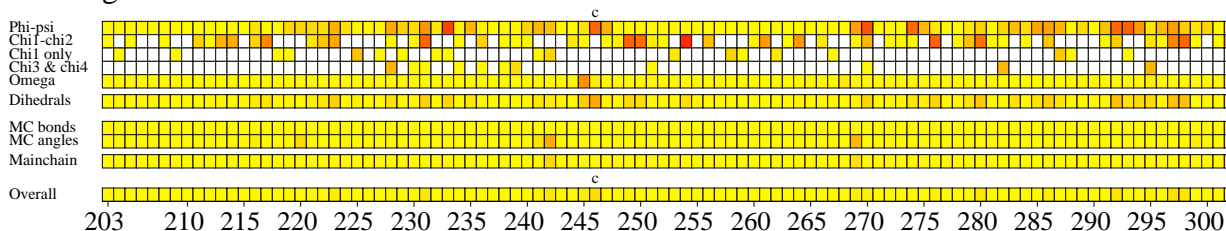
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



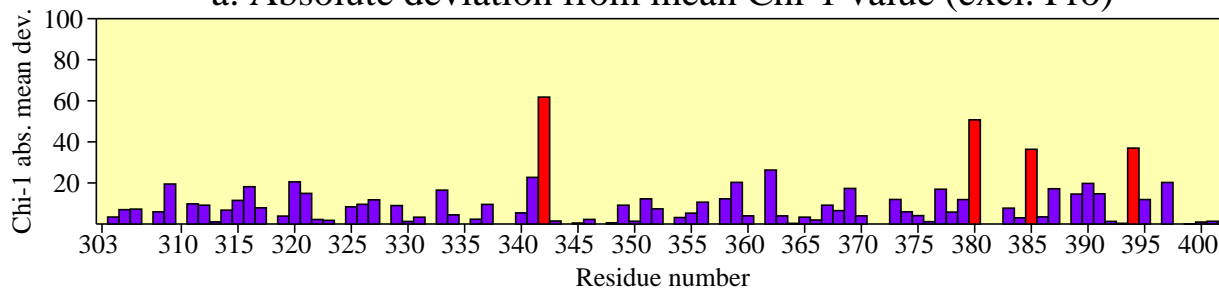
g. G-factors



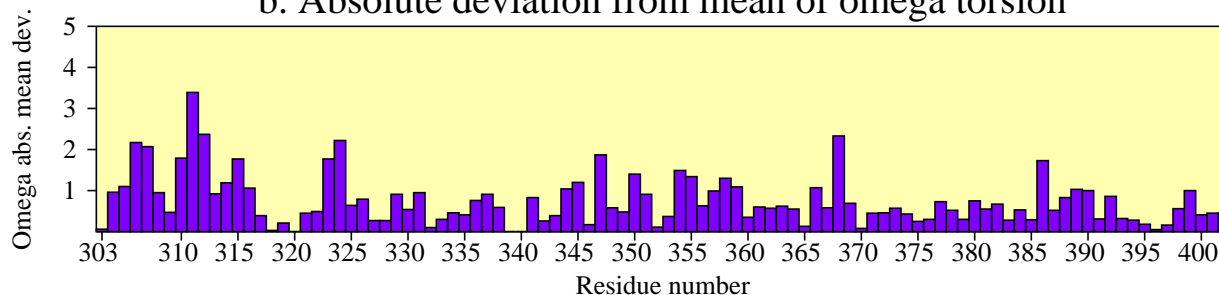
c = cis-peptide

# Residue properties 2QJP

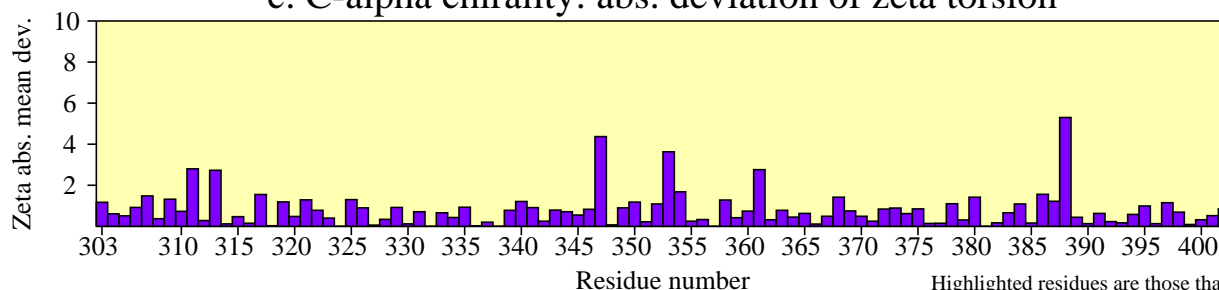
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

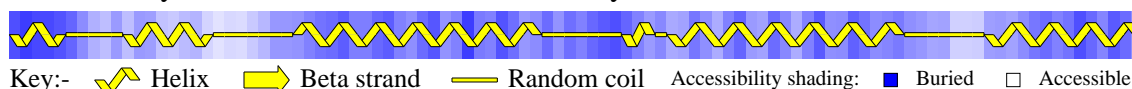


### c. C-alpha chirality: abs. deviation of zeta torsion



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

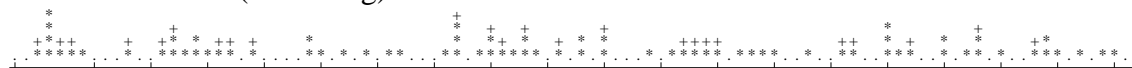
### d. Secondary structure & estimated accessibility



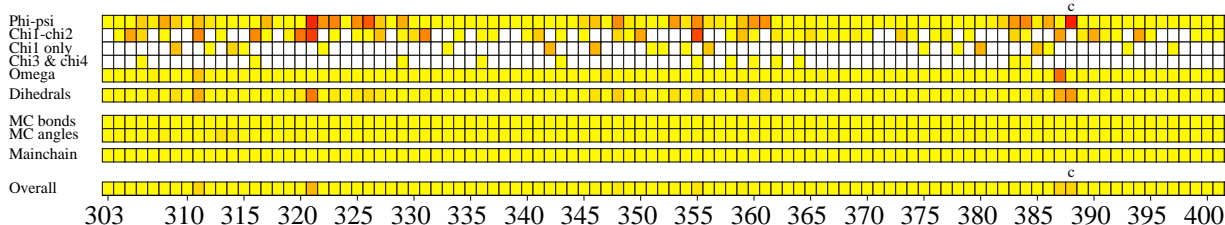
### e. Sequence & Ramachandran regions



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



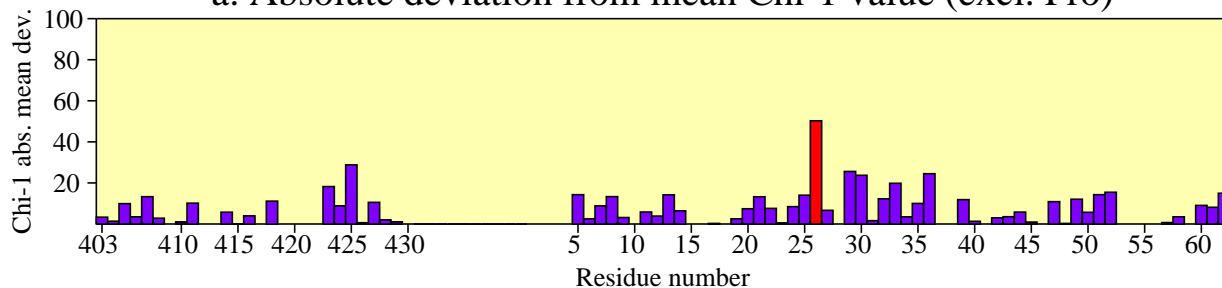
### g. G-factors



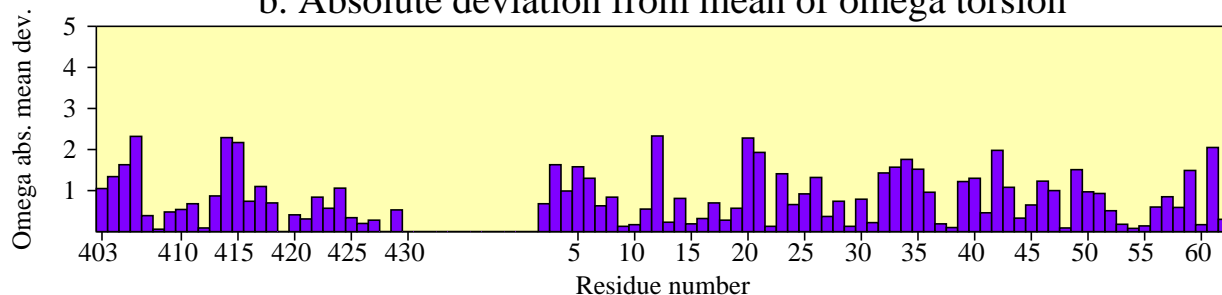
c = cis-peptide

# Residue properties 2QJP

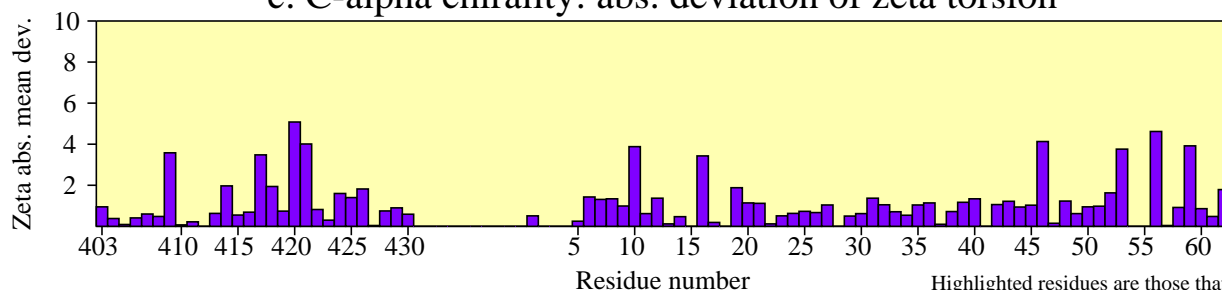
a. Absolute deviation from mean Chi-1 value (excl. Pro)



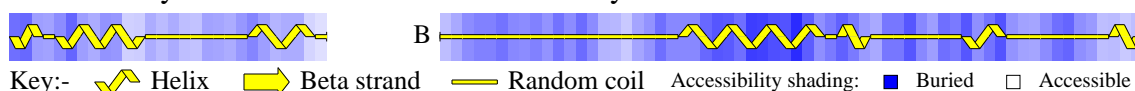
b. Absolute deviation from mean of omega torsion



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



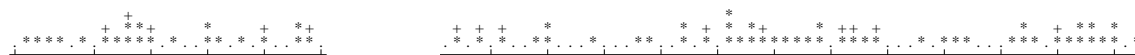
d. Secondary structure & estimated accessibility



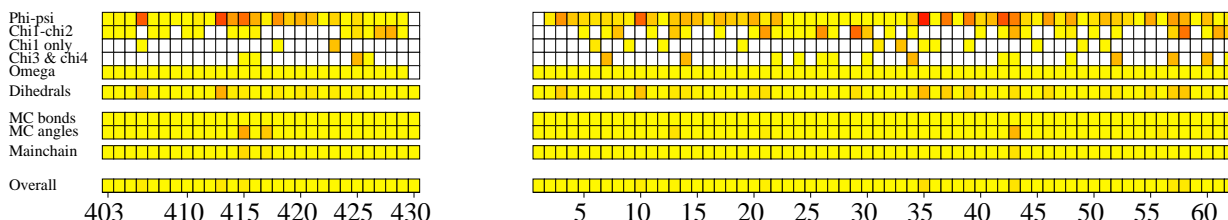
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

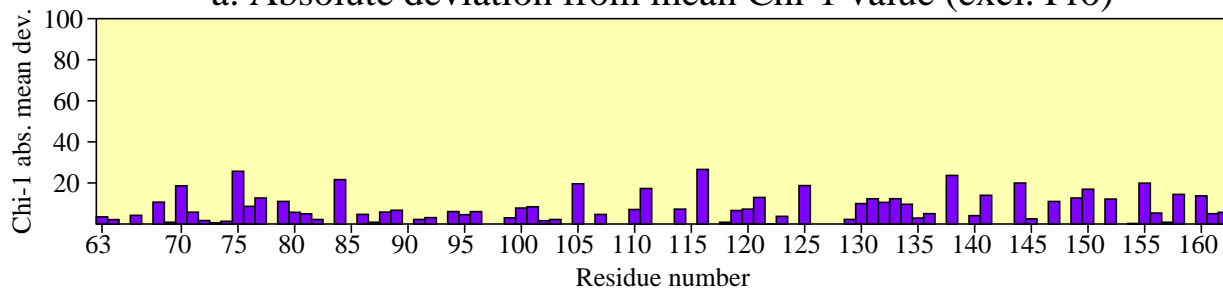


g. G-factors

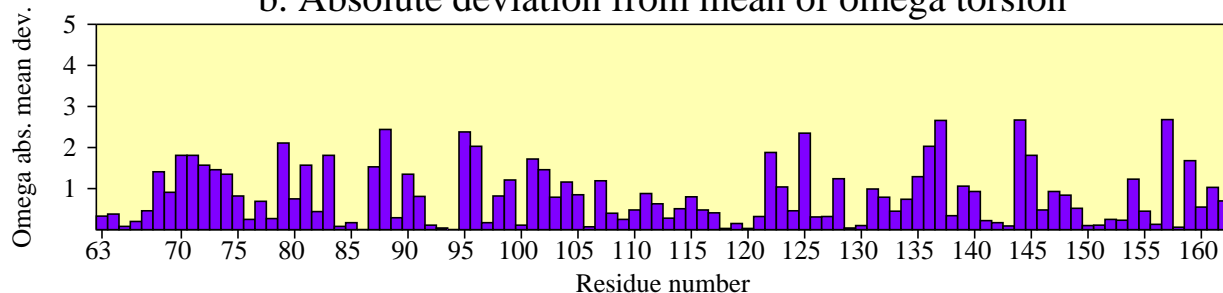


# Residue properties 2QJP

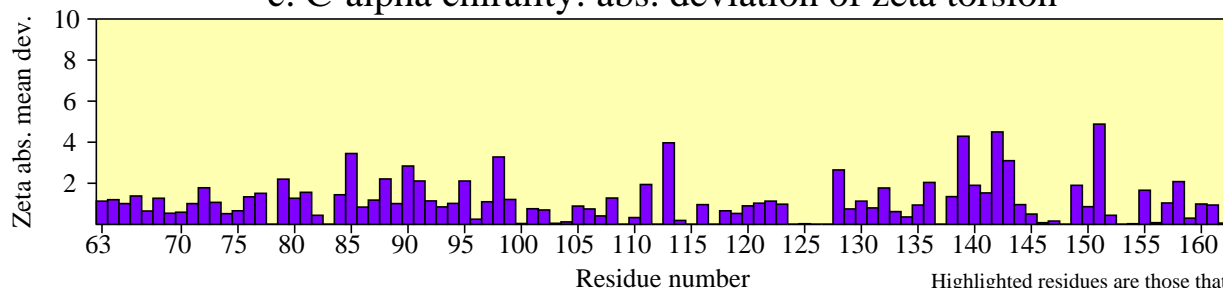
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

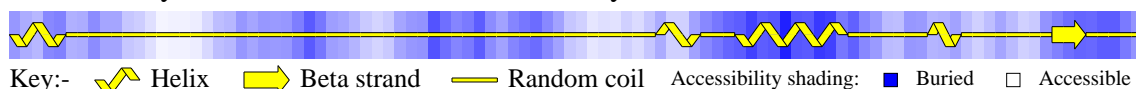


### c. C-alpha chirality: abs. deviation of zeta torsion



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

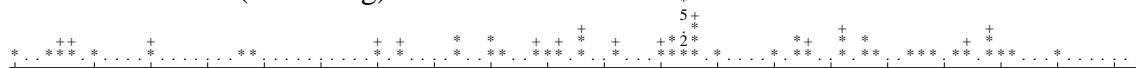
### d. Secondary structure & estimated accessibility



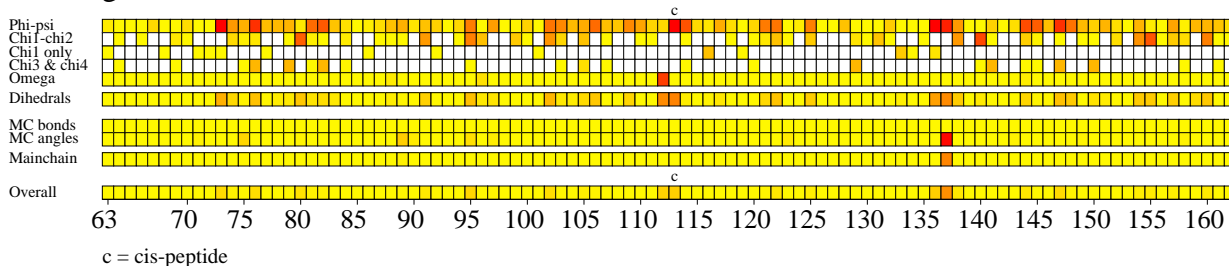
### e. Sequence & Ramachandran regions



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

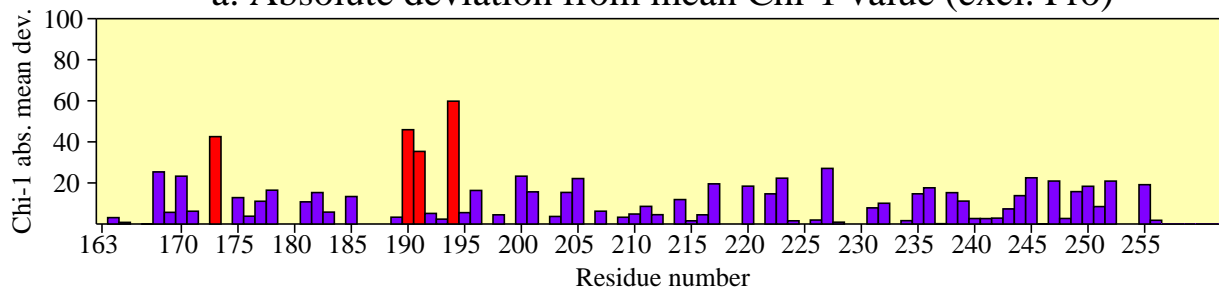


### g. G-factors

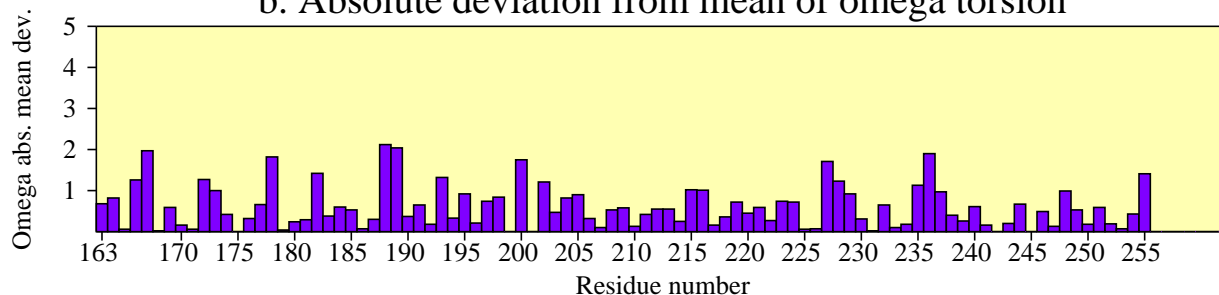


# Residue properties 2QJP

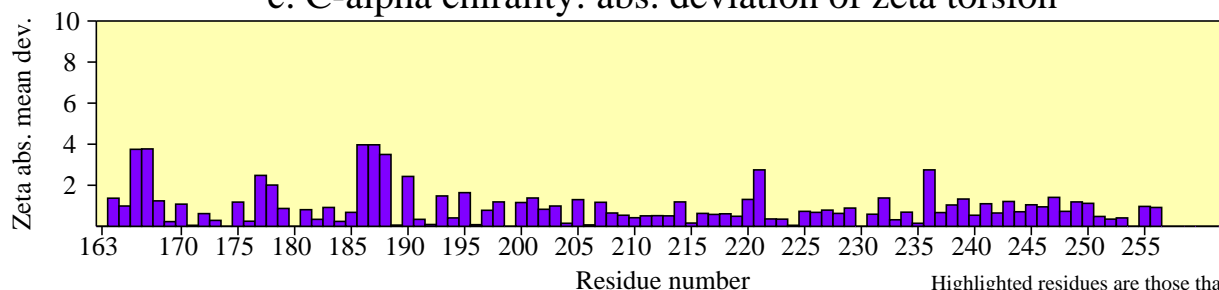
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



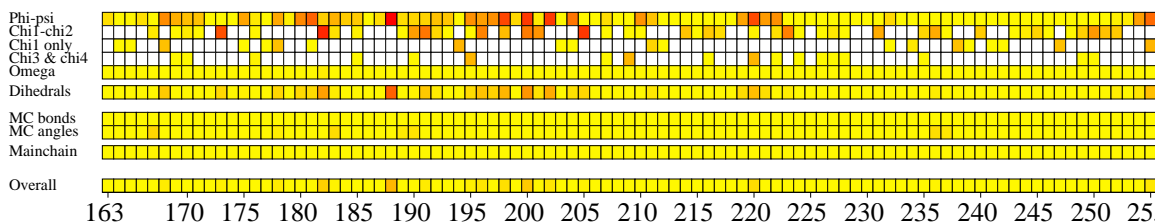
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

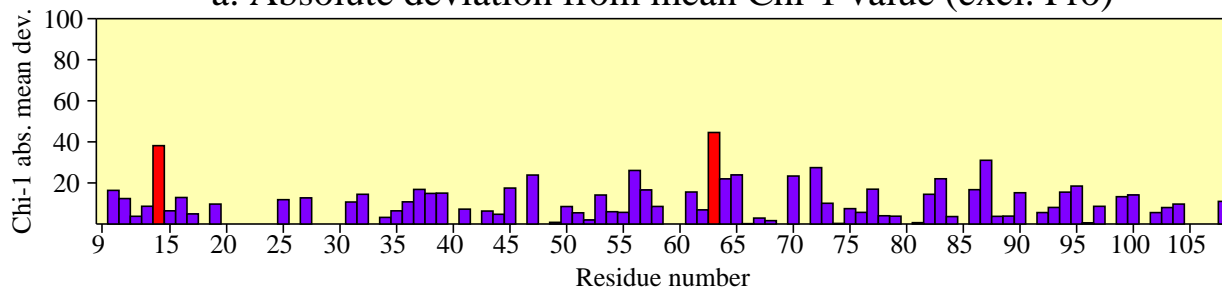


g. G-factors

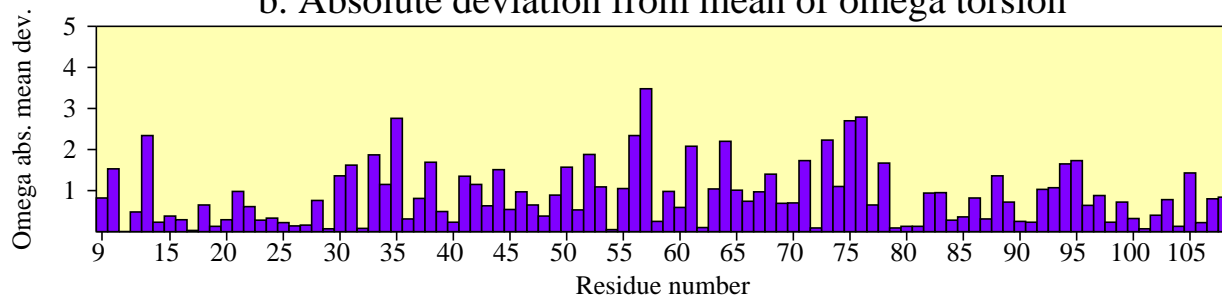


# Residue properties 2QJP

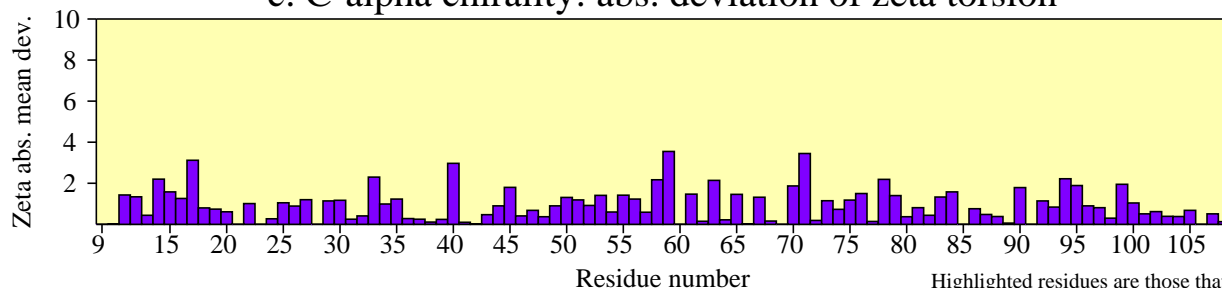
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

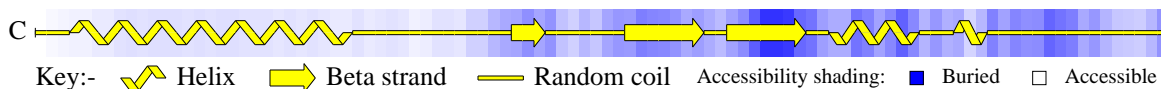


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



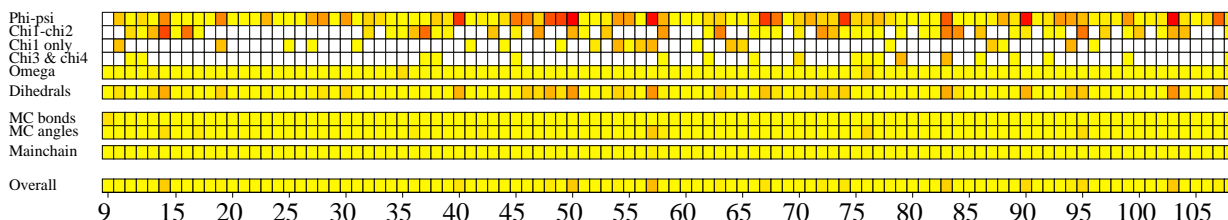
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



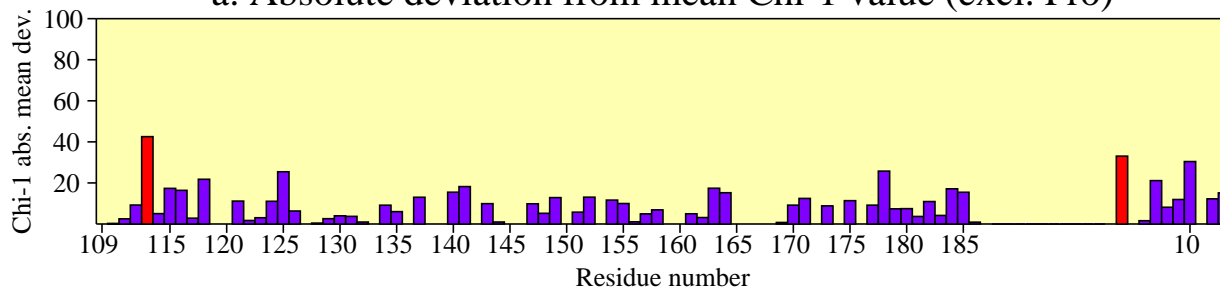
g. G-factors



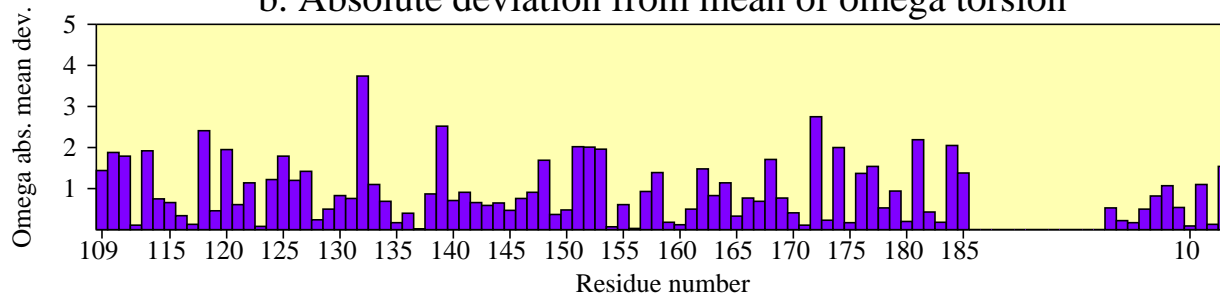


# Residue properties 2QJP

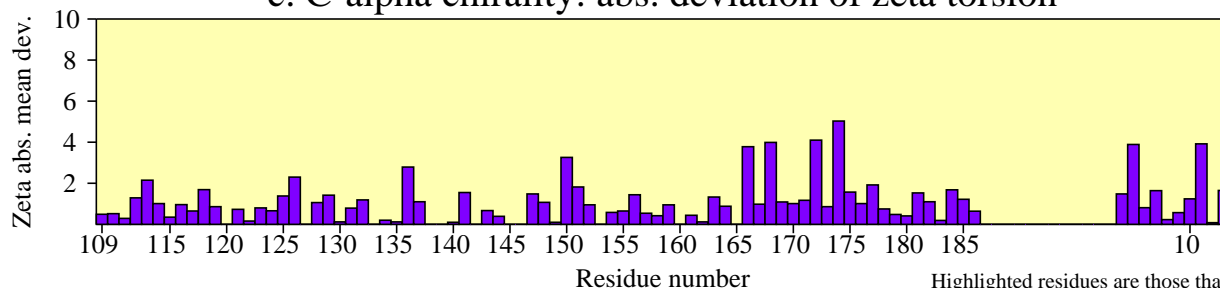
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

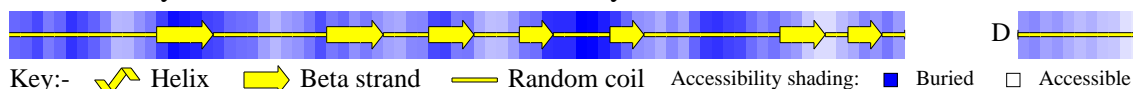


c. C-alpha chirality: abs. deviation of zeta torsion



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

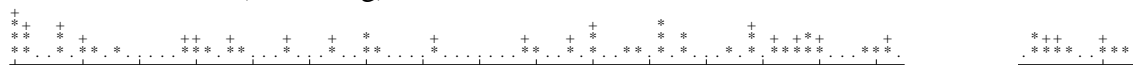
d. Secondary structure & estimated accessibility



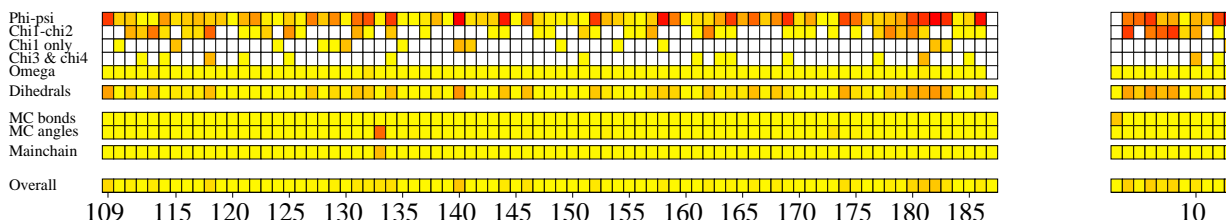
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

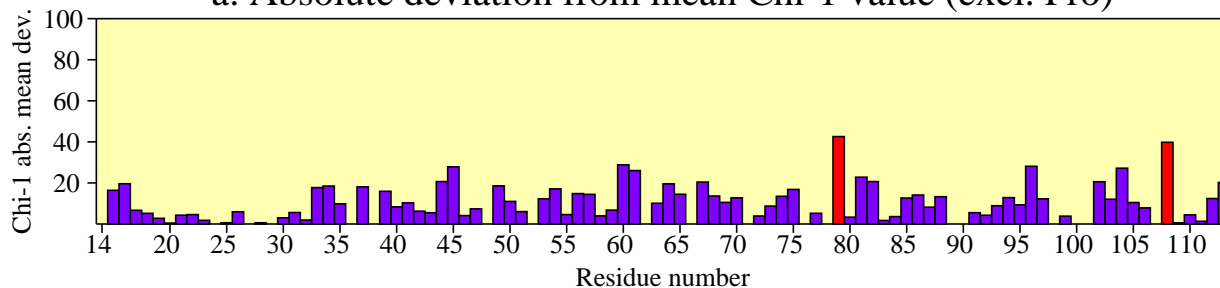


g. G-factors

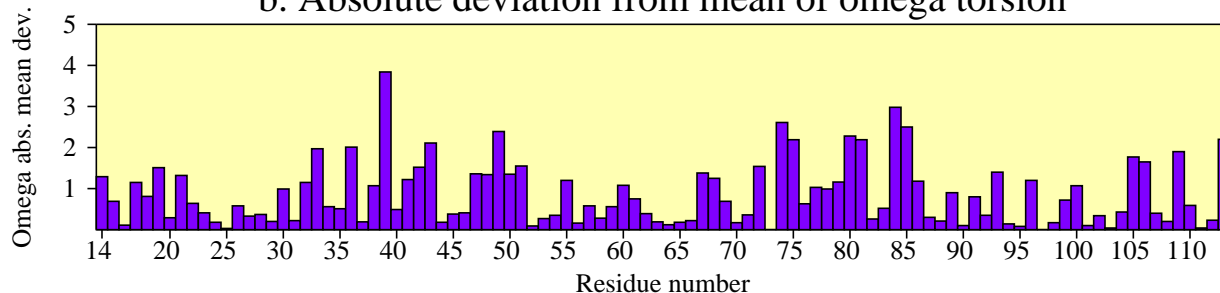


# Residue properties 2QJP

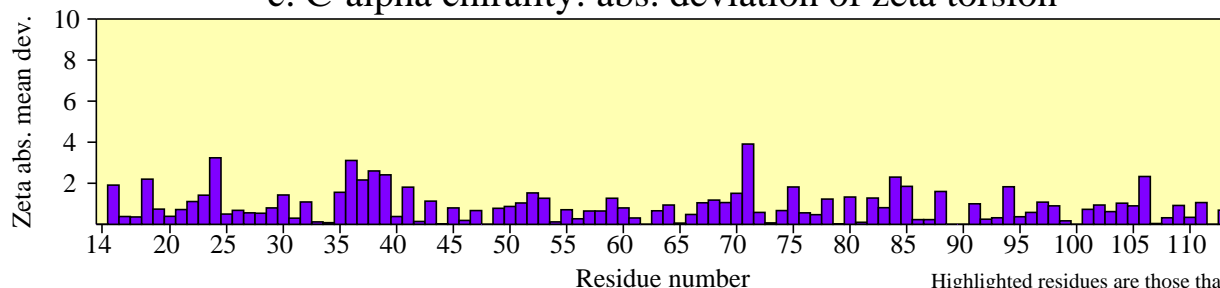
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



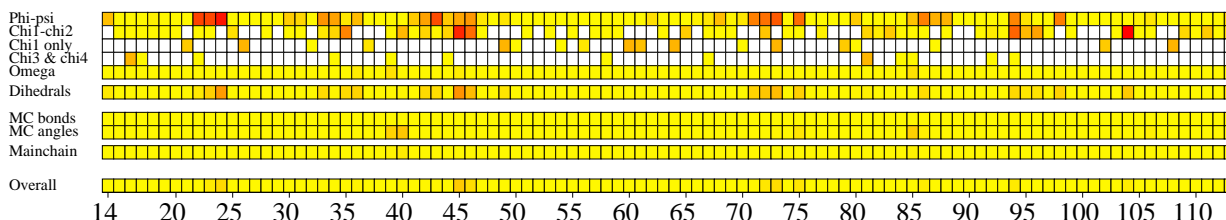
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

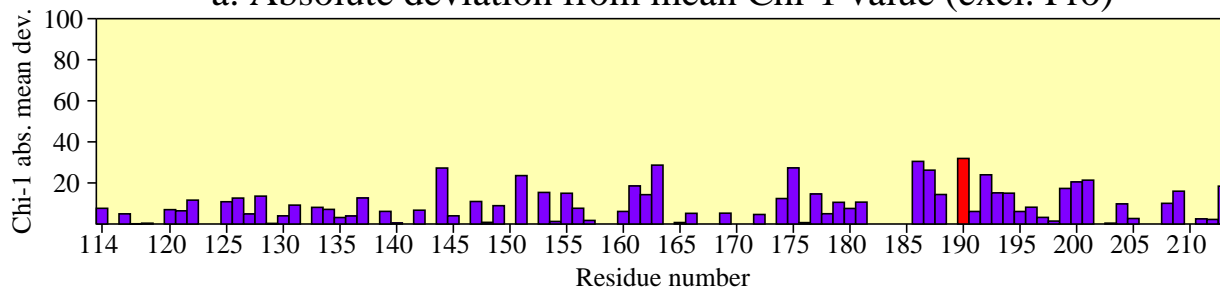


g. G-factors

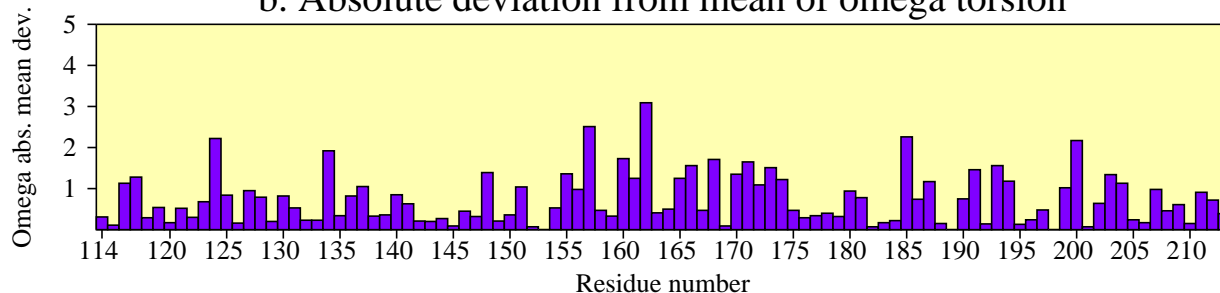


# Residue properties 2QJP

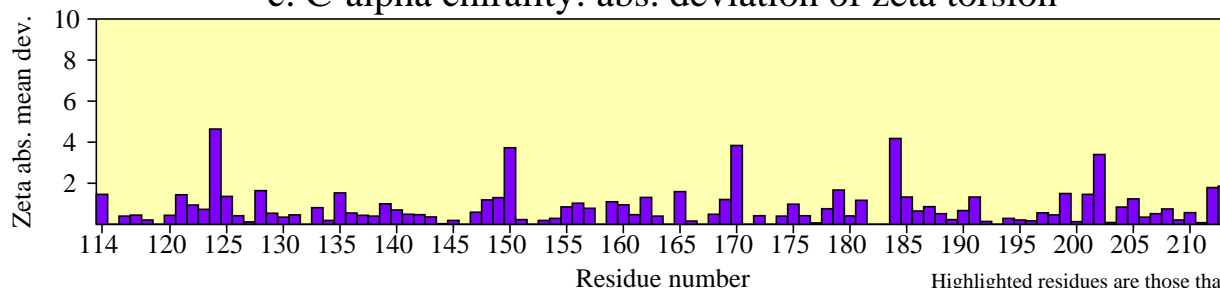
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

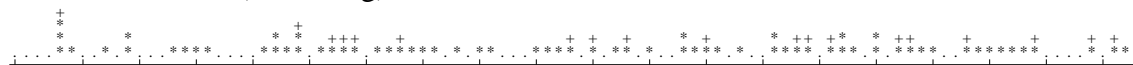
d. Secondary structure & estimated accessibility



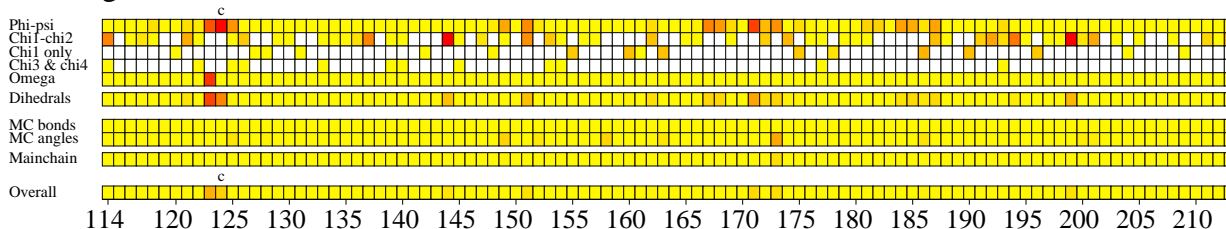
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



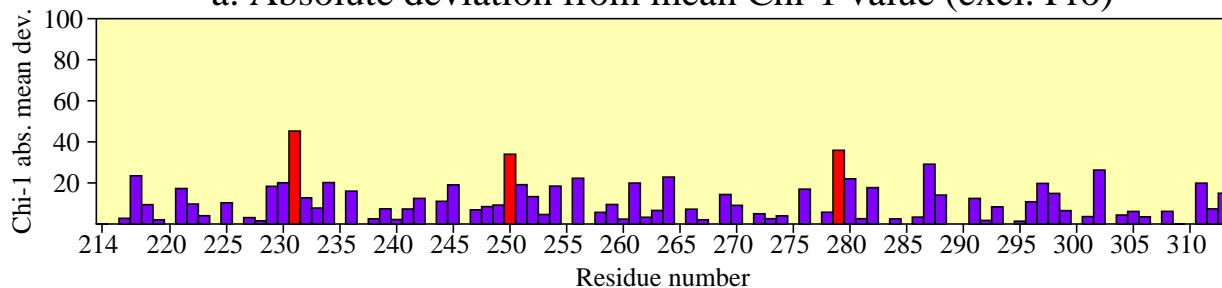
g. G-factors



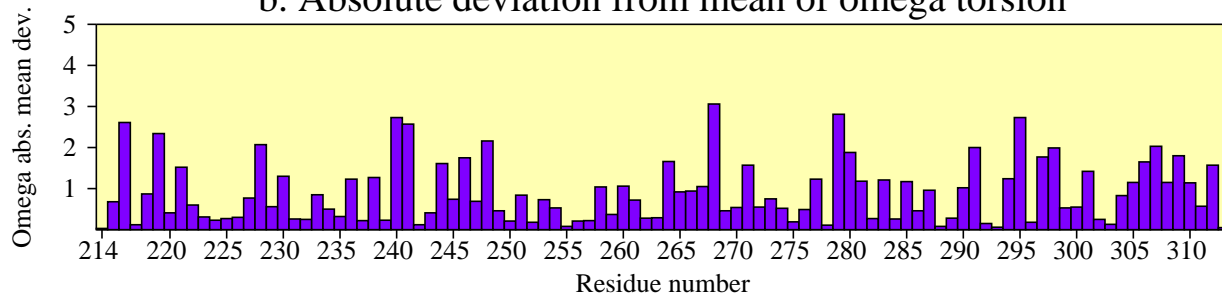
c = cis-peptide

# Residue properties 2QJP

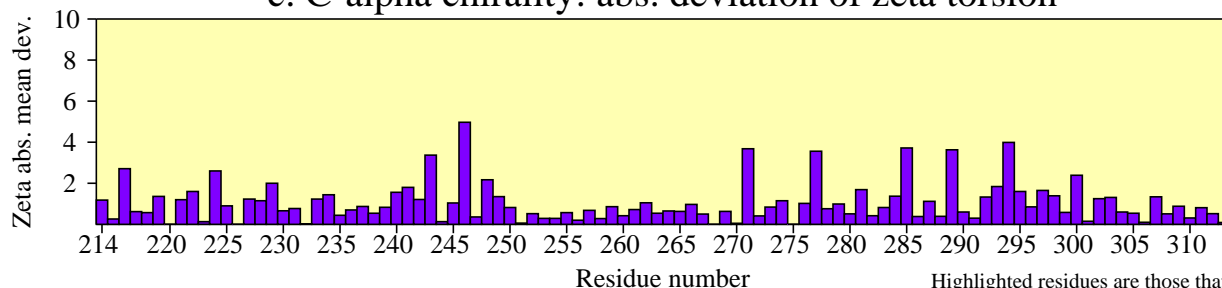
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

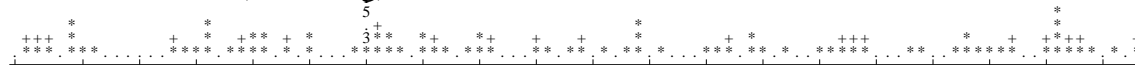
d. Secondary structure & estimated accessibility



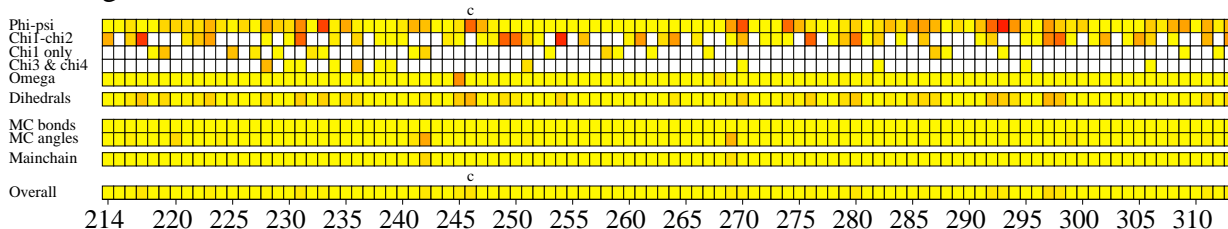
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



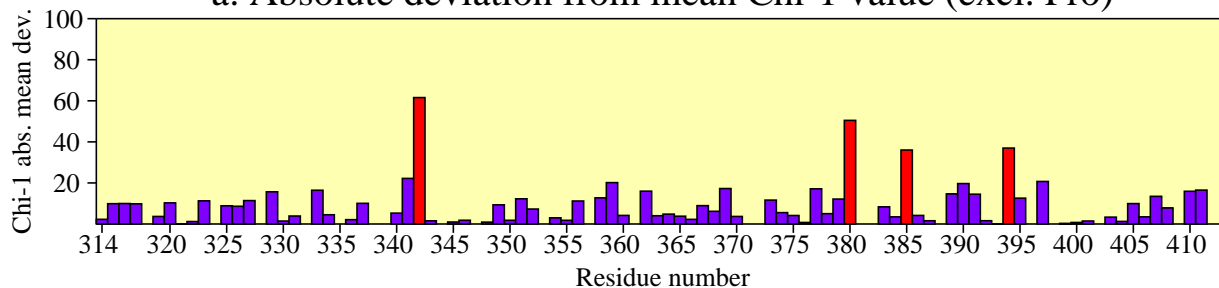
g. G-factors



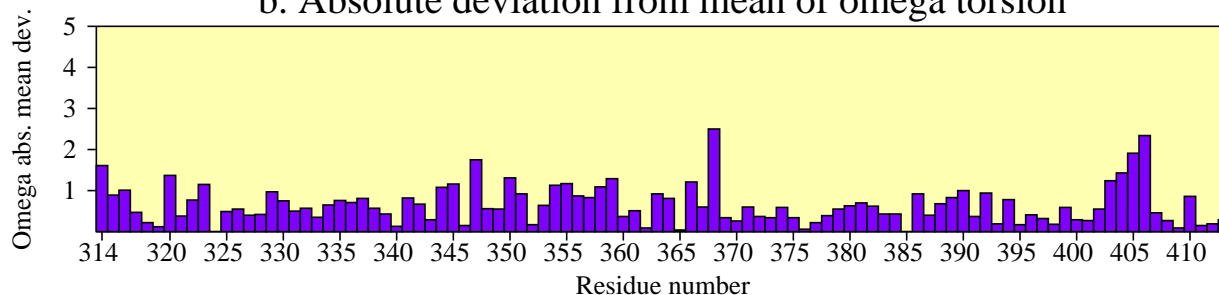
c = cis-peptide

# Residue properties 2QJP

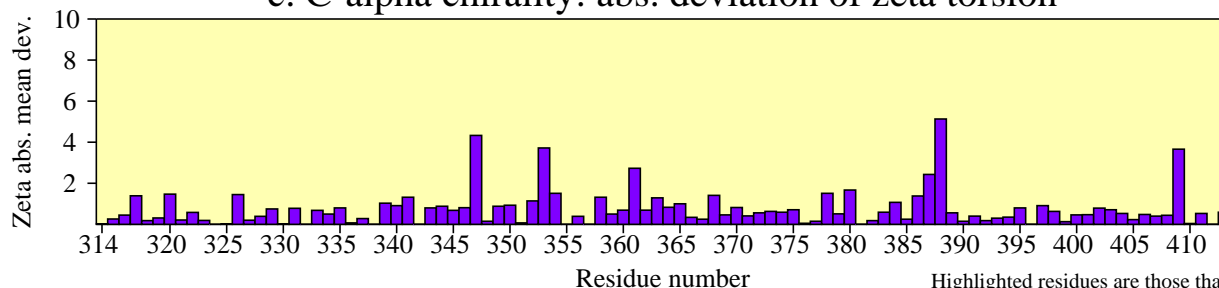
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

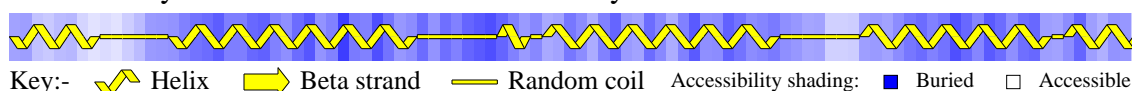


c. C-alpha chirality: abs. deviation of zeta torsion

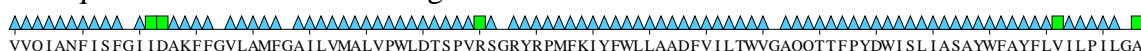


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



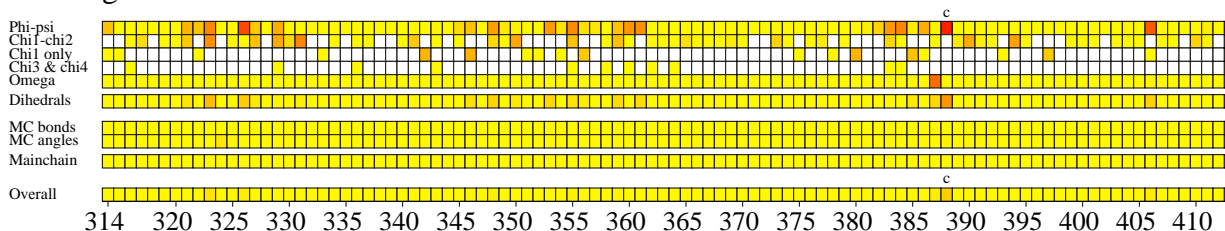
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



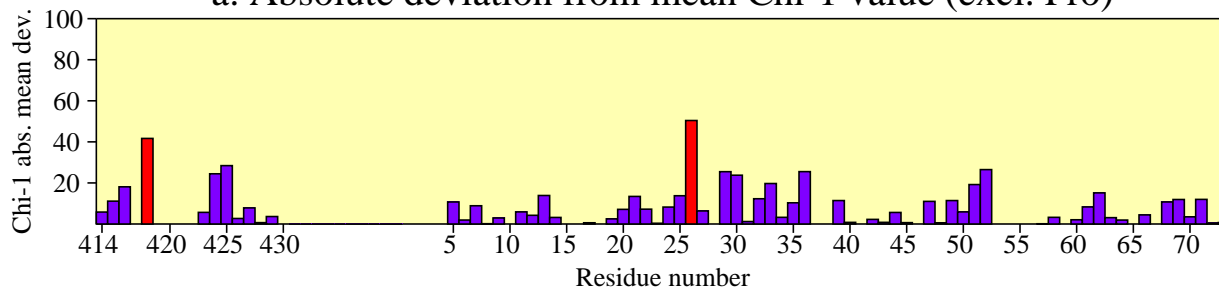
g. G-factors



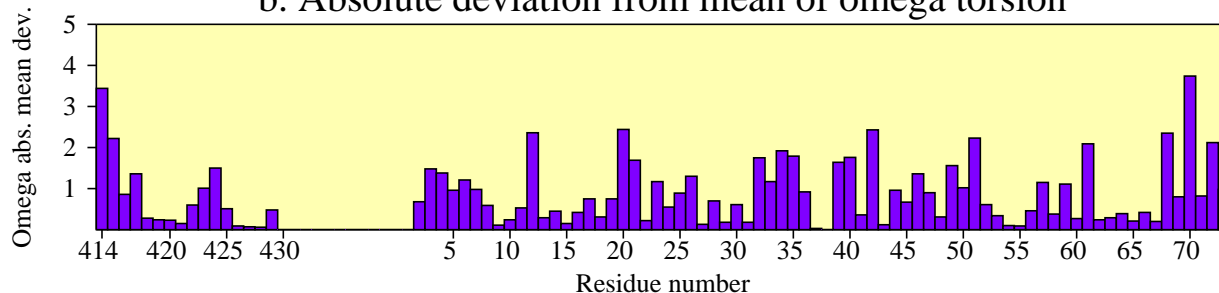
c = cis-peptide

# Residue properties 2QJP

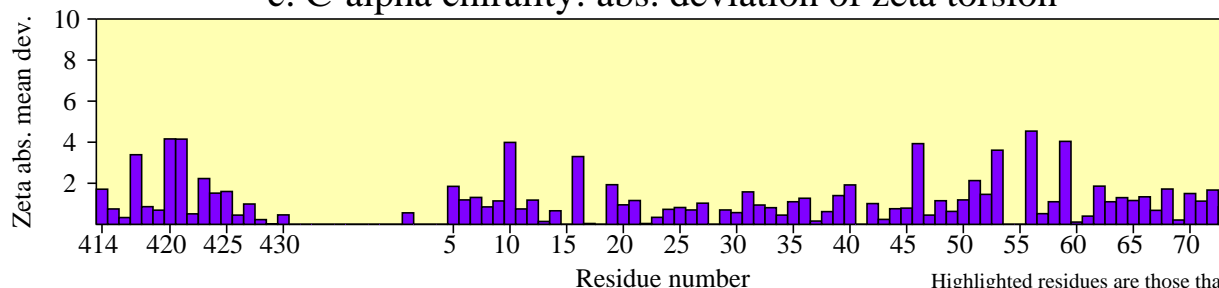
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

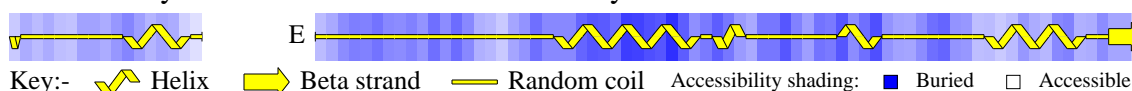


### c. C-alpha chirality: abs. deviation of zeta torsion



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

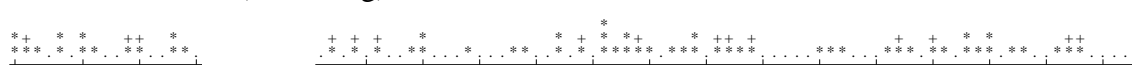
### d. Secondary structure & estimated accessibility



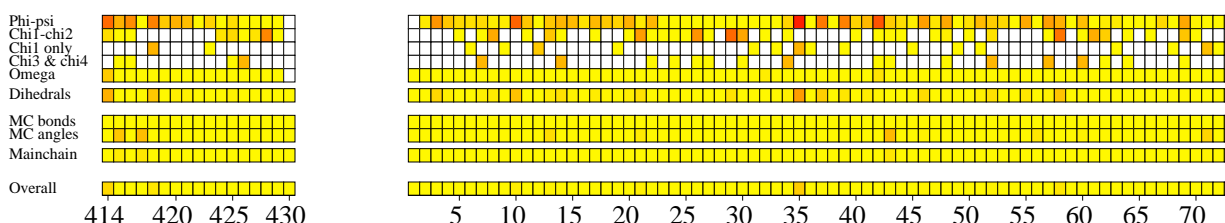
### e. Sequence & Ramachandran regions



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

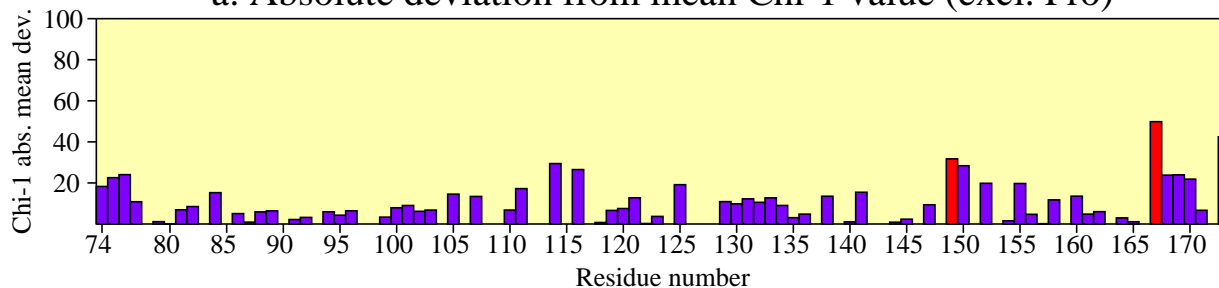


### g. G-factors

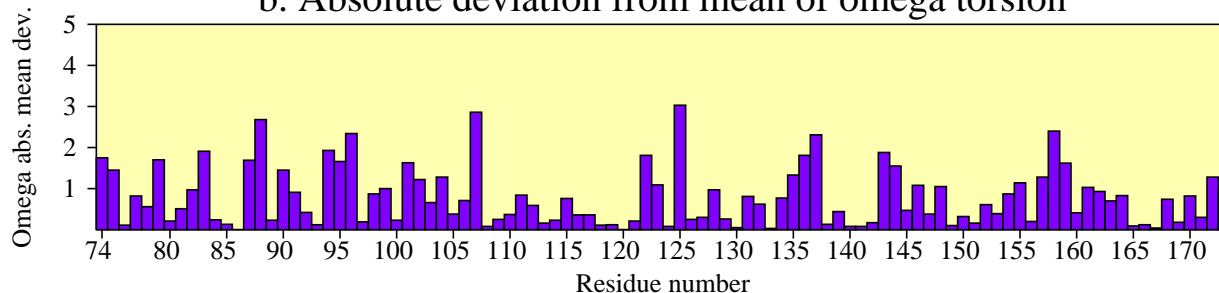


# Residue properties 2QJP

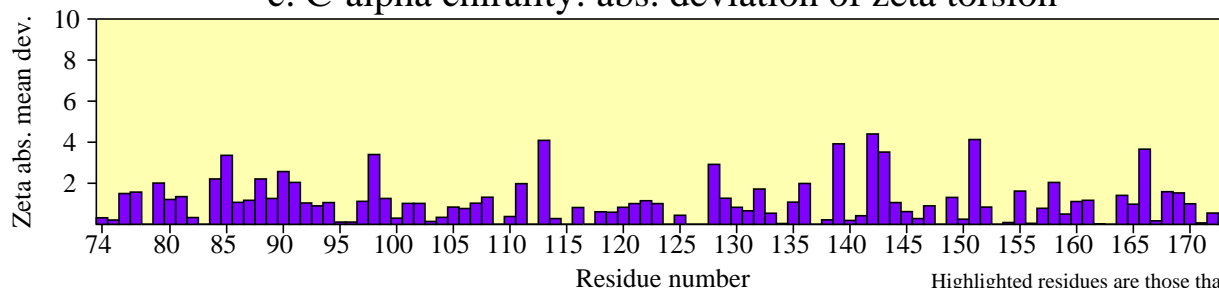
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

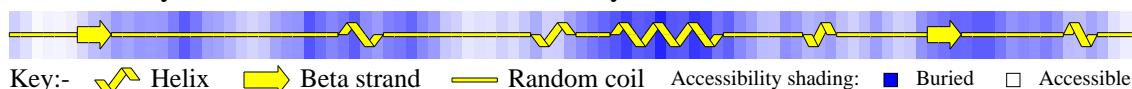


c. C-alpha chirality: abs. deviation of zeta torsion



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

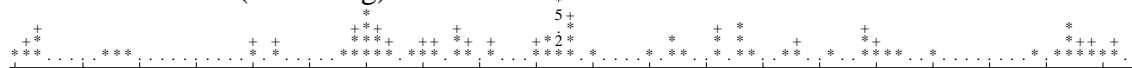
d. Secondary structure & estimated accessibility



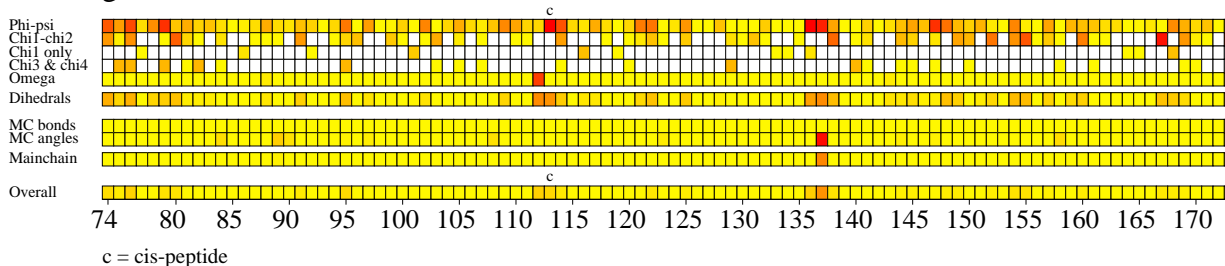
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

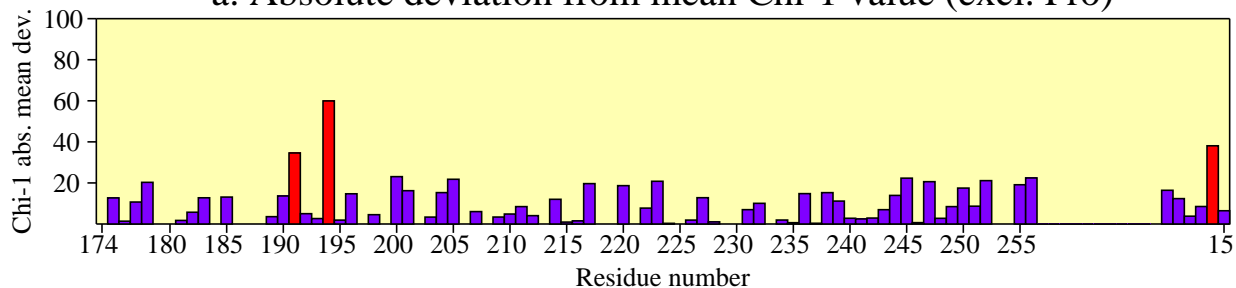


g. G-factors

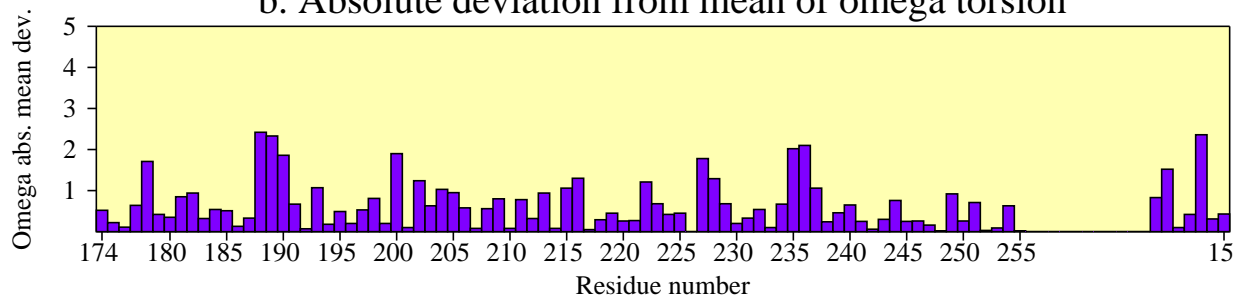


# Residue properties 2QJP

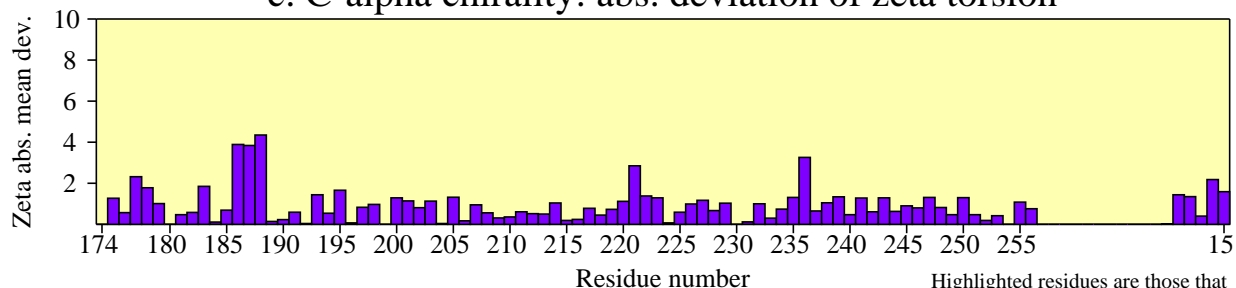
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

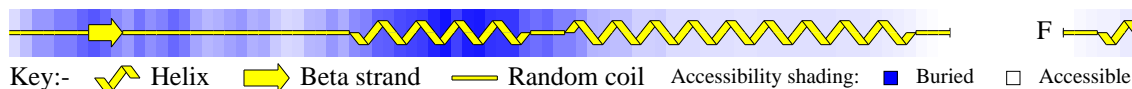


c. C-alpha chirality: abs. deviation of zeta torsion



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

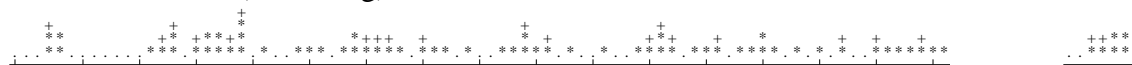
d. Secondary structure & estimated accessibility



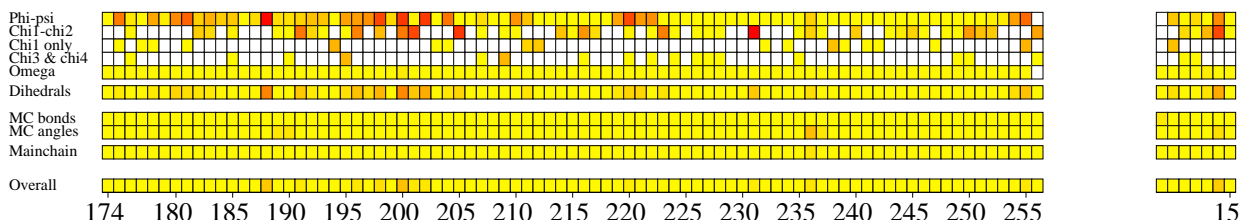
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



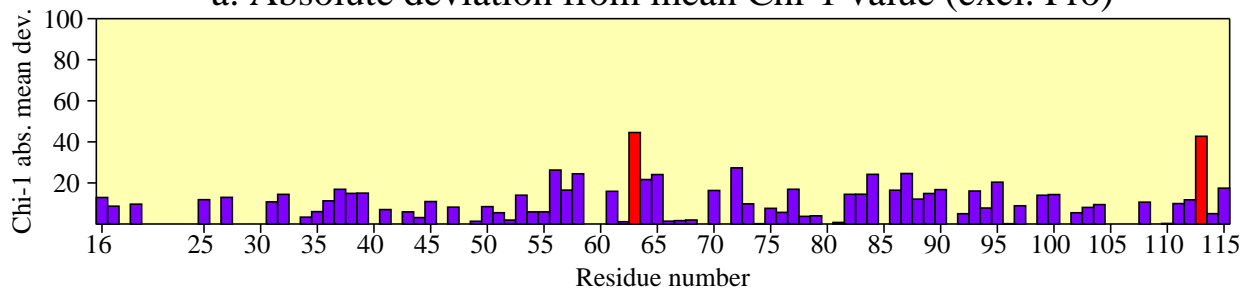
g. G-factors



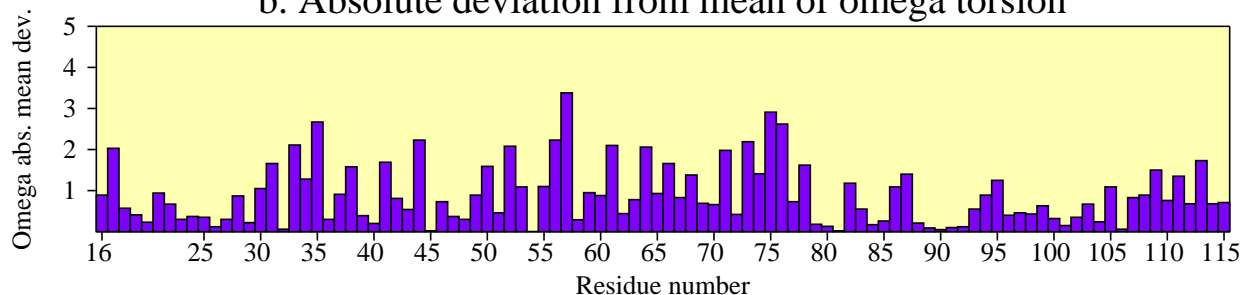


# Residue properties 2QJP

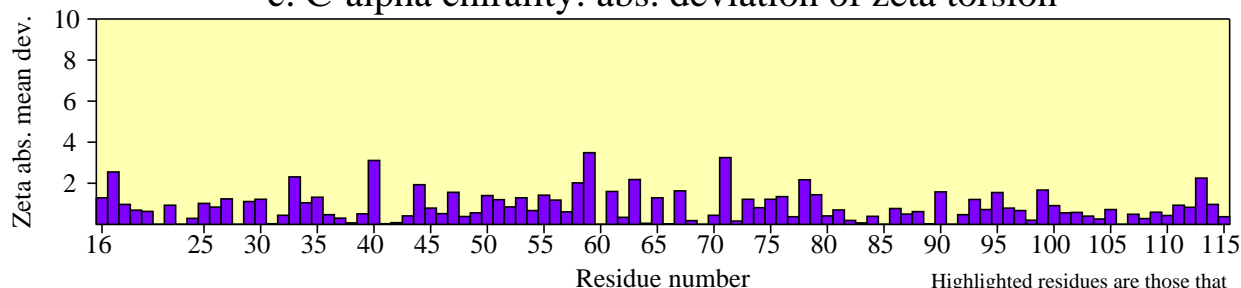
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

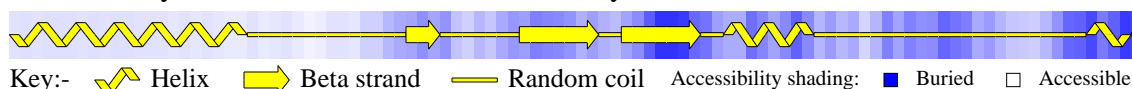


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



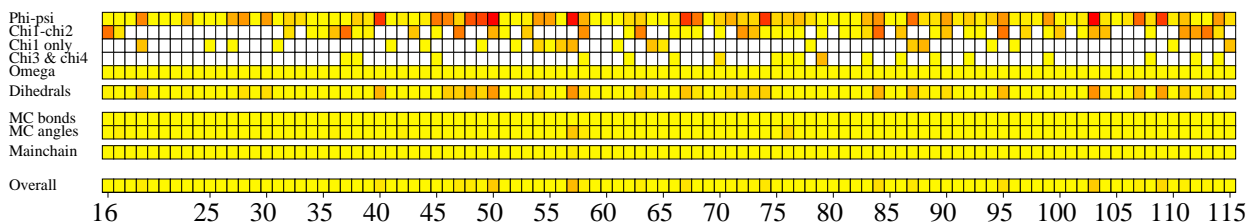
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

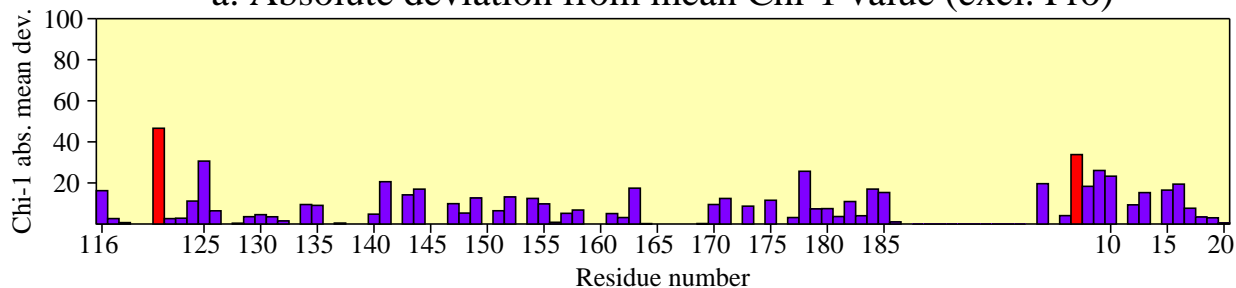


g. G-factors

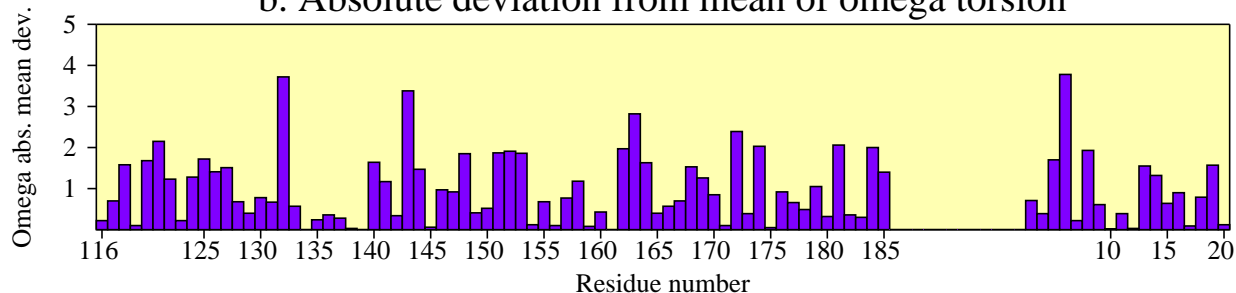


# Residue properties 2QJP

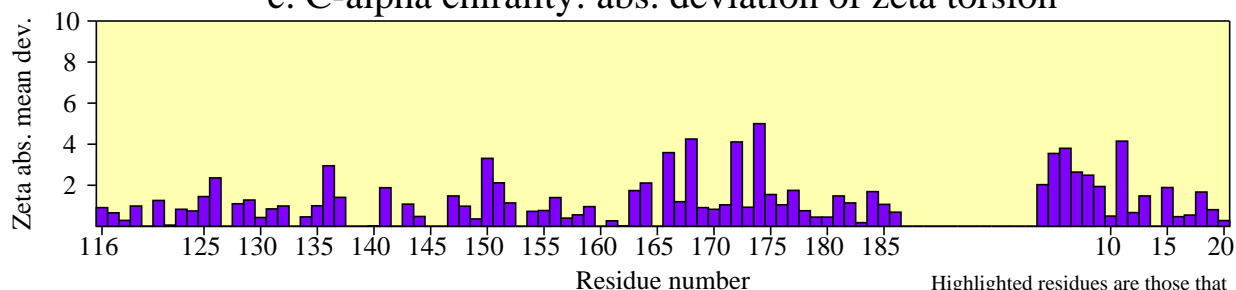
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

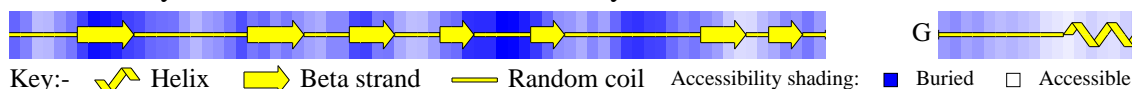


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



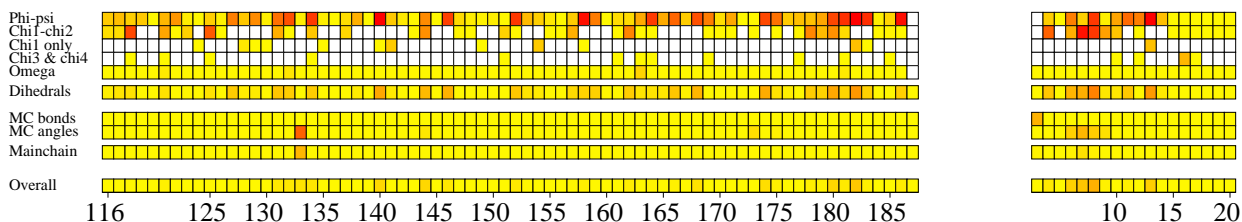
### e. Sequence & Ramachandran regions



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

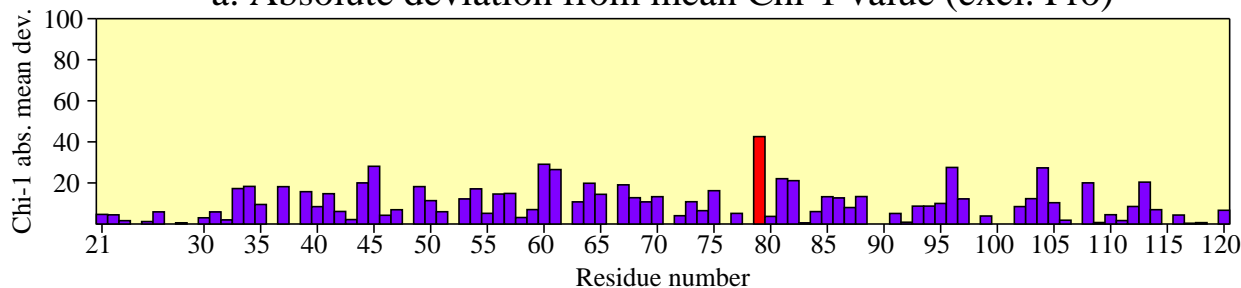


### g. G-factors

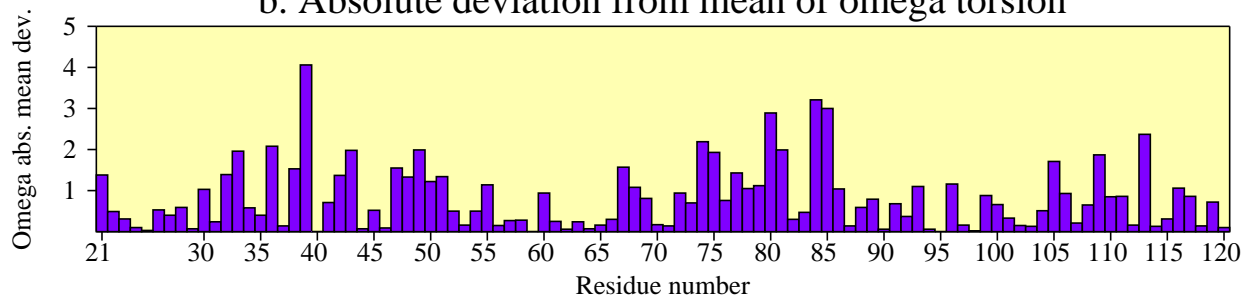


# Residue properties 2QJP

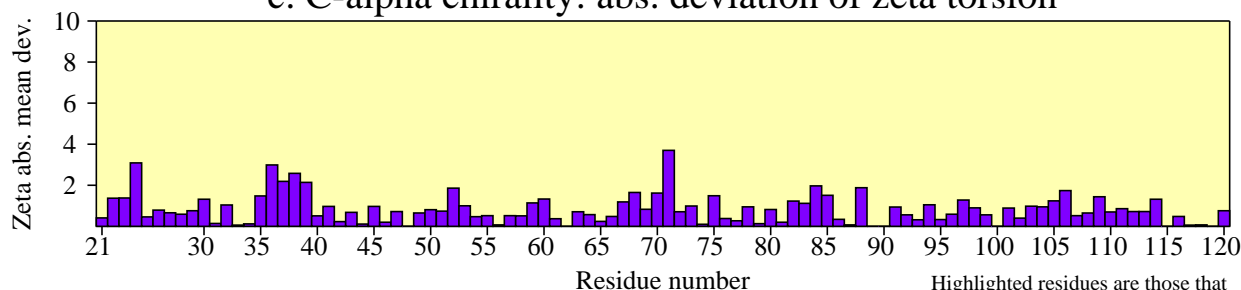
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

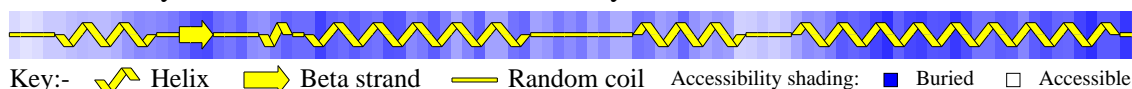


c. C-alpha chirality: abs. deviation of zeta torsion



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

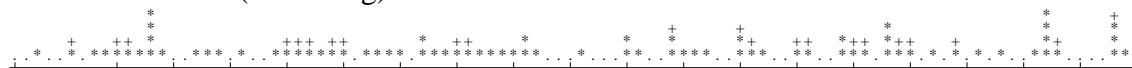
d. Secondary structure & estimated accessibility



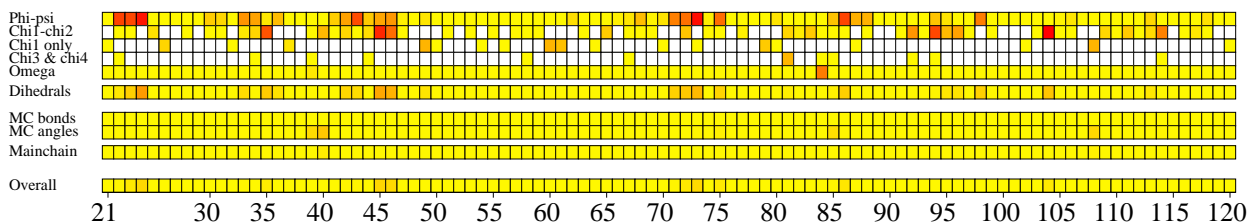
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

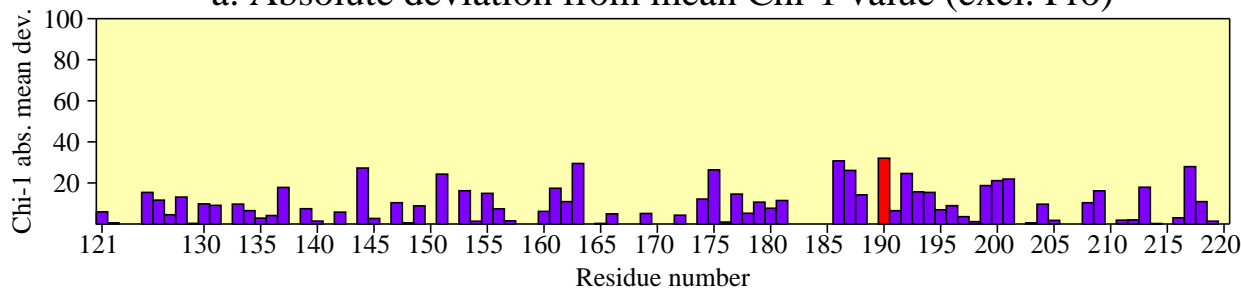


g. G-factors

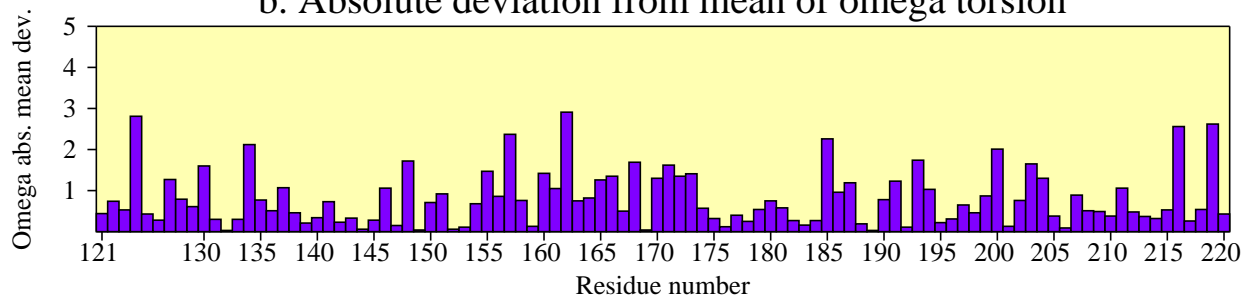


# Residue properties 2QJP

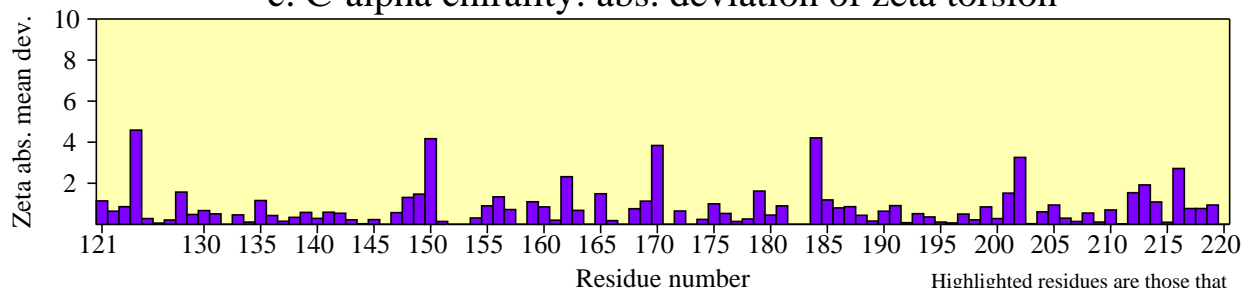
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

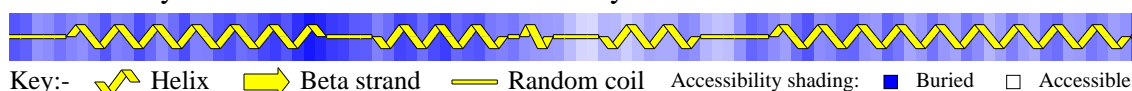


### c. C-alpha chirality: abs. deviation of zeta torsion



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

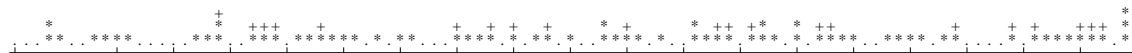
### d. Secondary structure & estimated accessibility



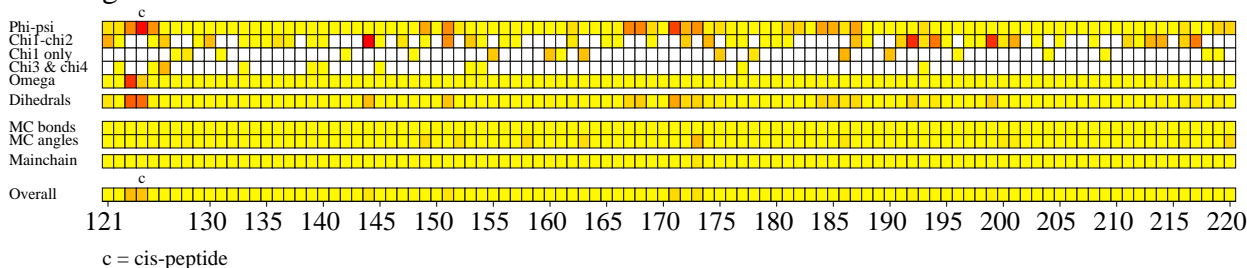
### e. Sequence & Ramachandran regions



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

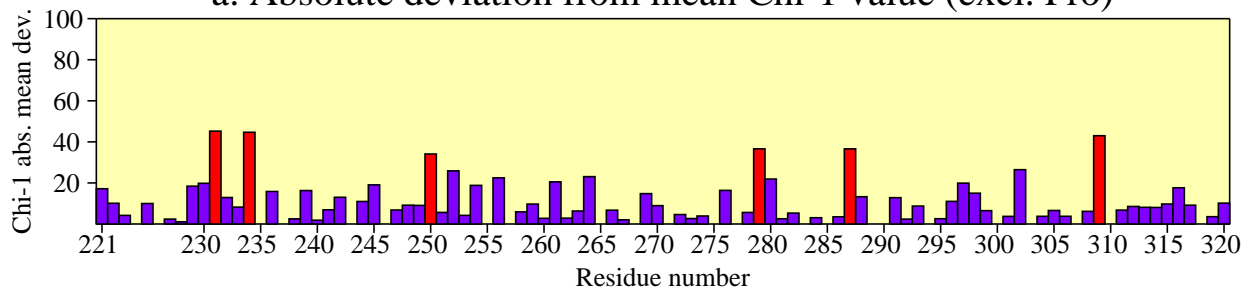


### g. G-factors

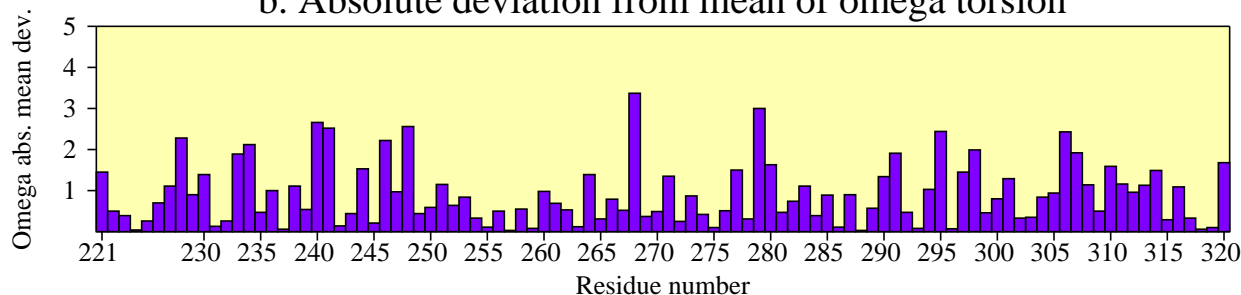


# Residue properties 2QJP

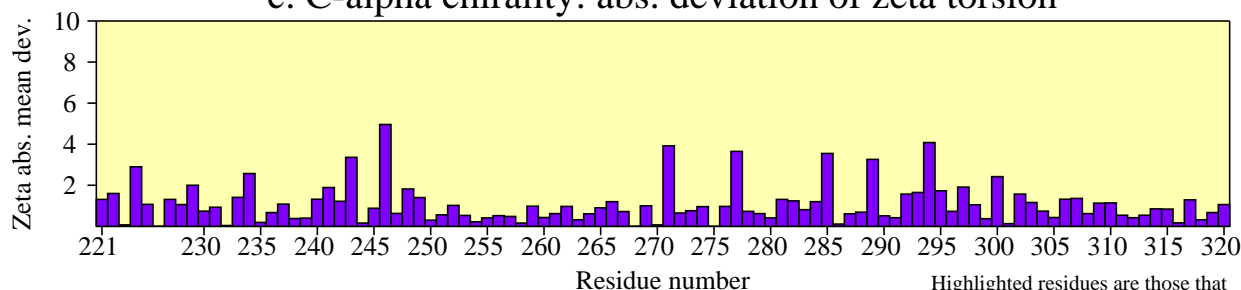
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

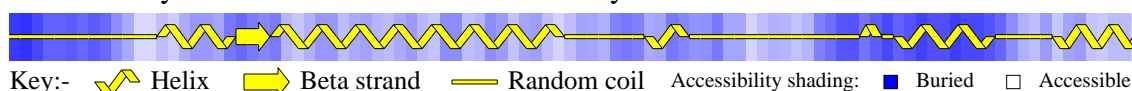


c. C-alpha chirality: abs. deviation of zeta torsion



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

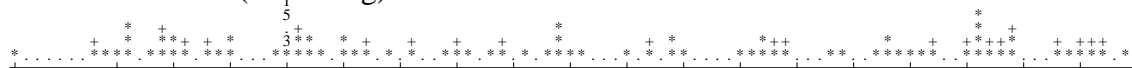
d. Secondary structure & estimated accessibility



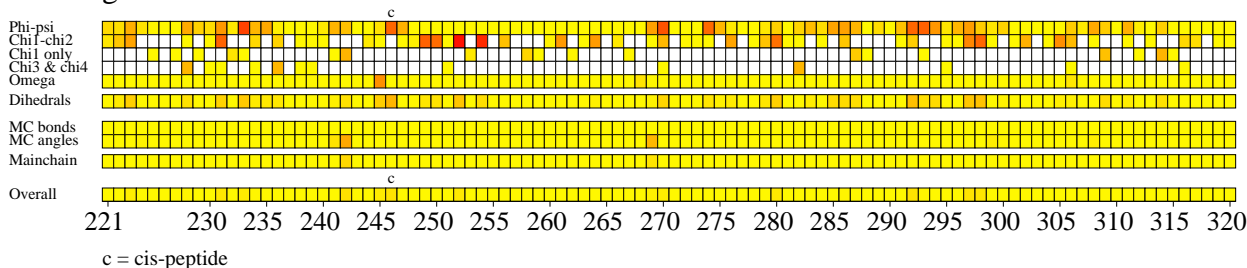
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

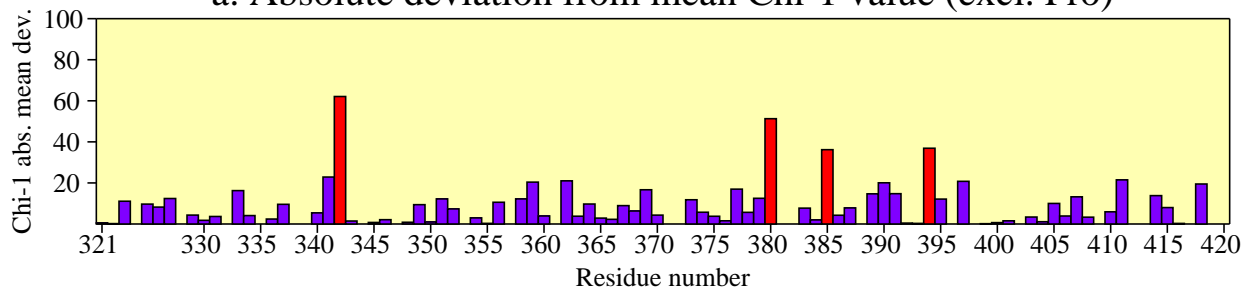


g. G-factors

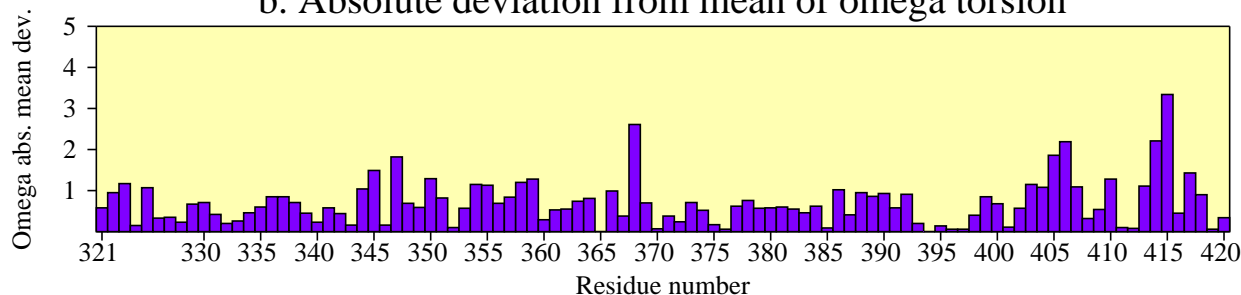


# Residue properties 2QJP

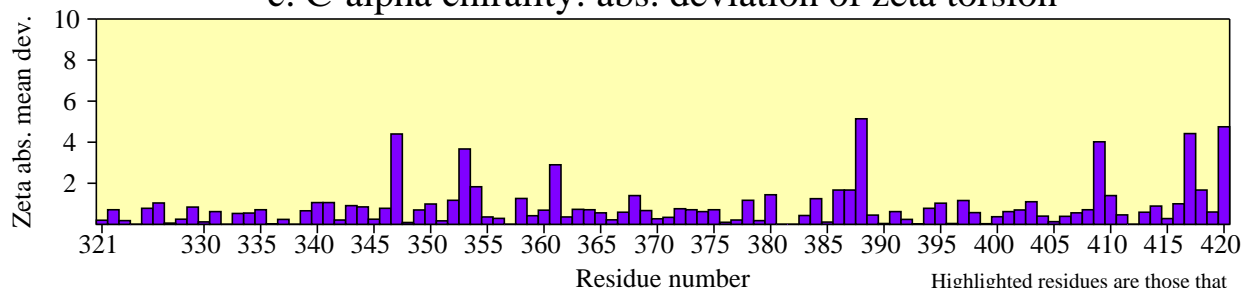
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

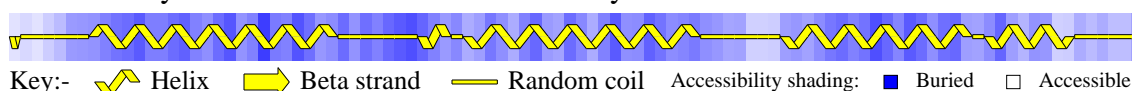


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



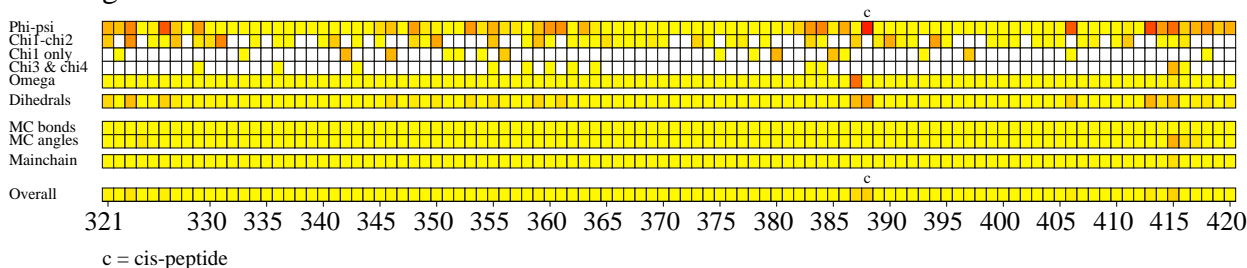
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

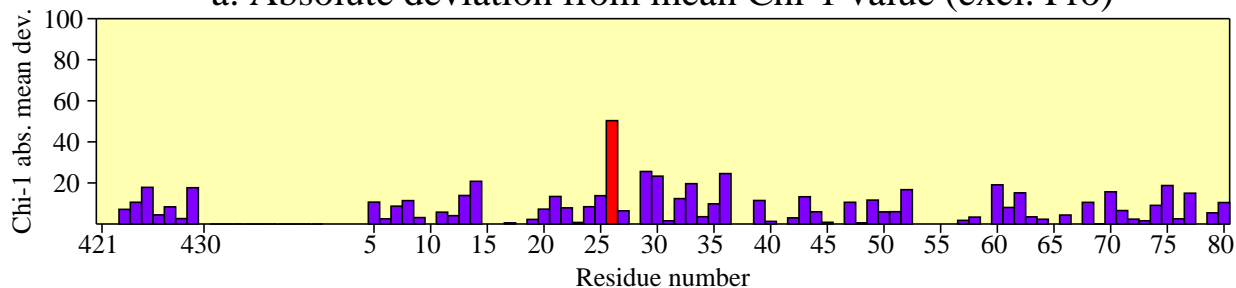


g. G-factors

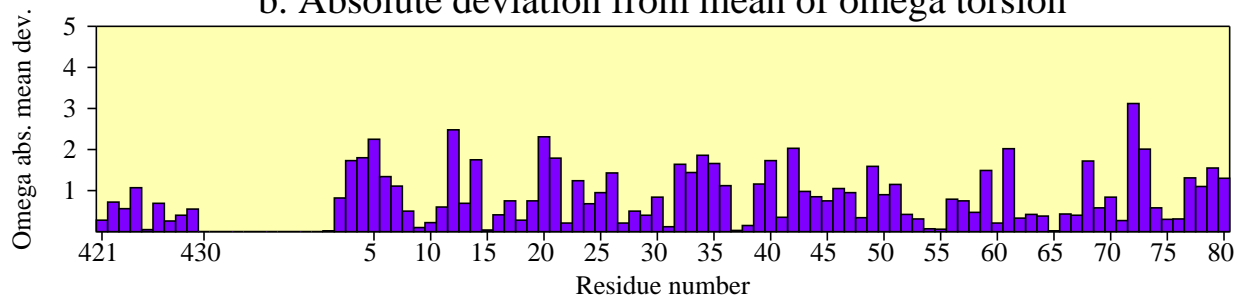


# Residue properties 2QJP

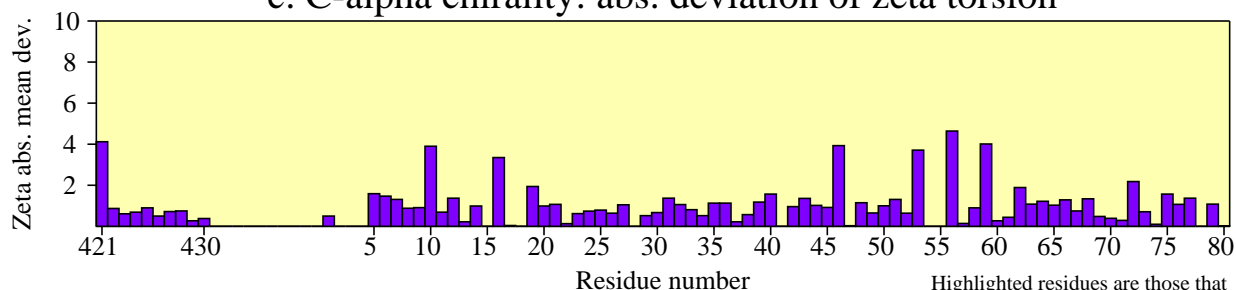
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



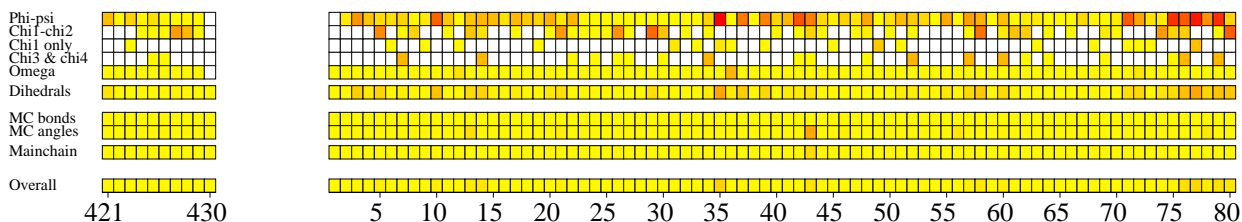
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

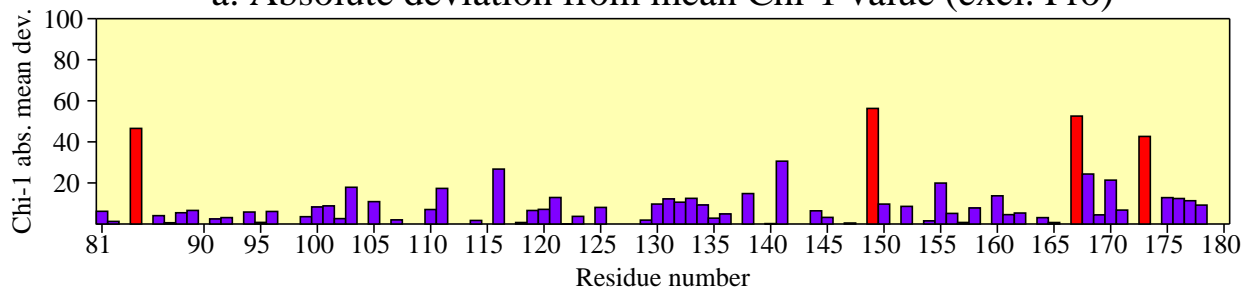


g. G-factors

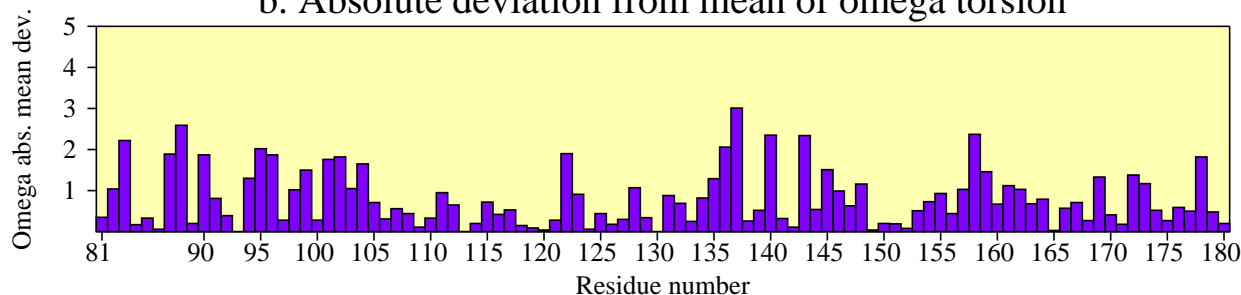


# Residue properties 2QJP

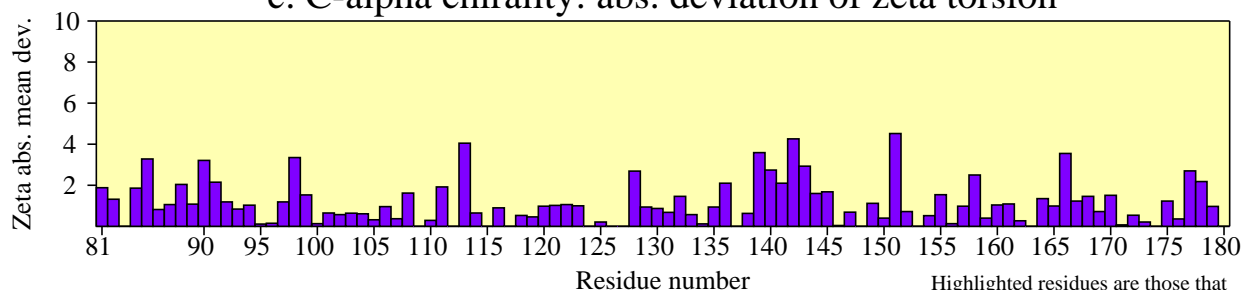
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

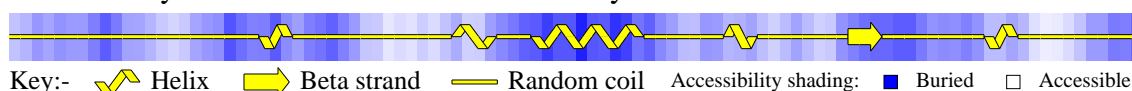


c. C-alpha chirality: abs. deviation of zeta torsion



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

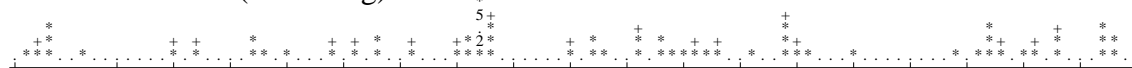
d. Secondary structure & estimated accessibility



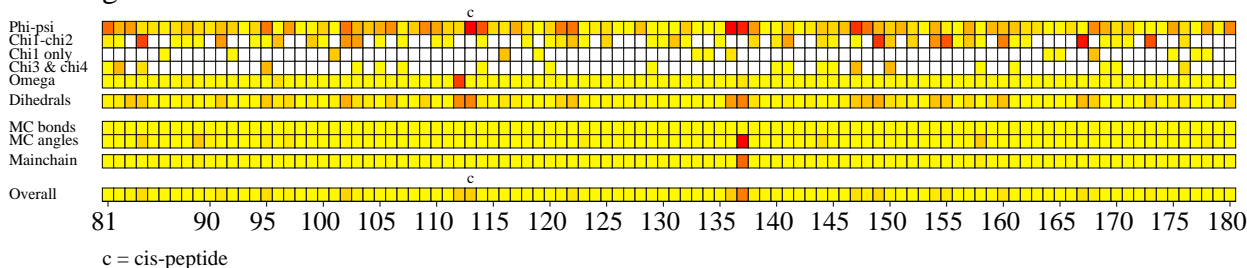
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

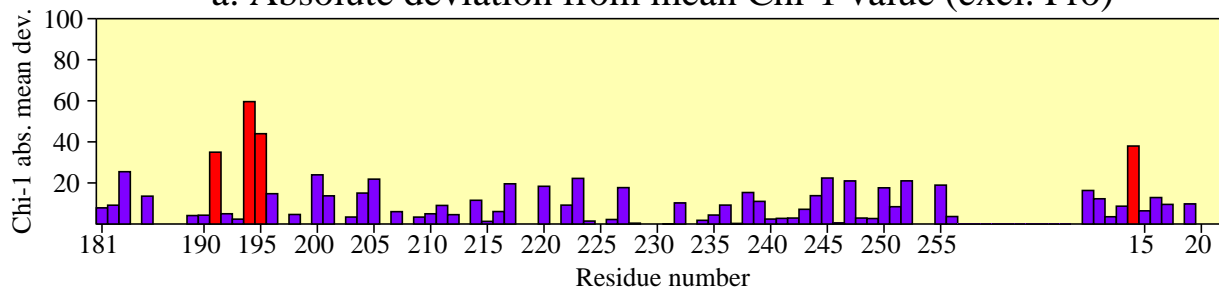


c = cis-peptide

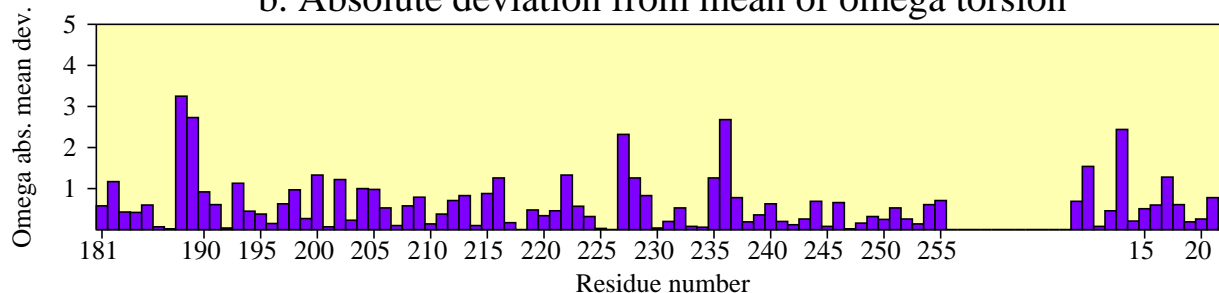


# Residue properties 2QJP

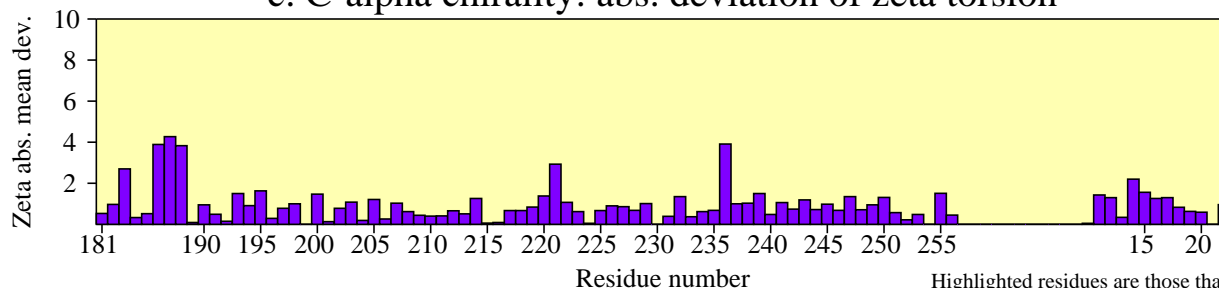
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

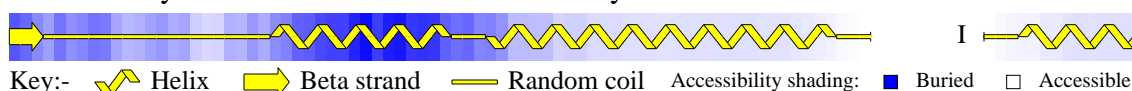


### c. C-alpha chirality: abs. deviation of zeta torsion

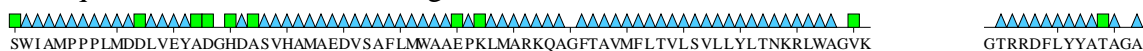


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

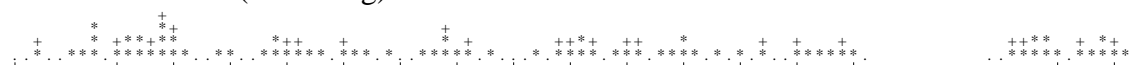
### d. Secondary structure & estimated accessibility



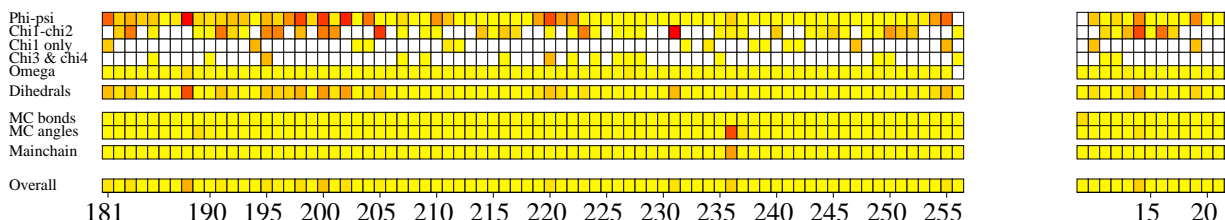
### e. Sequence & Ramachandran regions



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

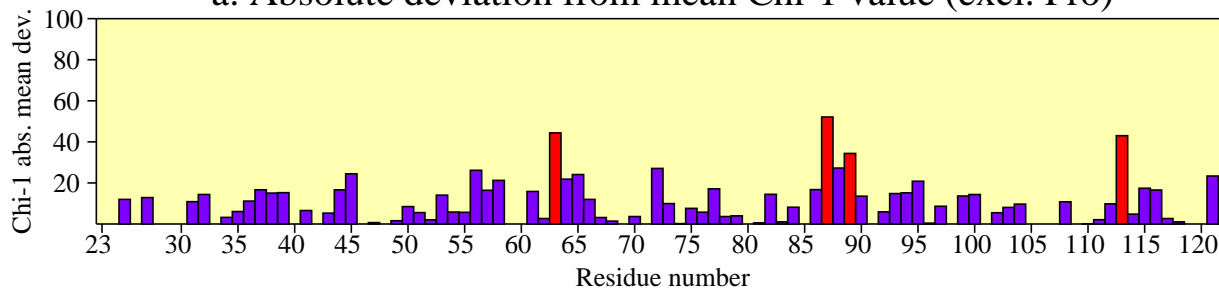


### g. G-factors

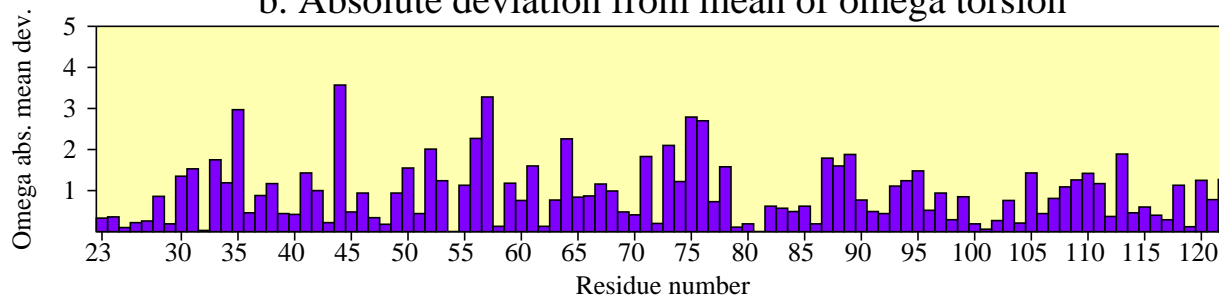


# Residue properties 2QJP

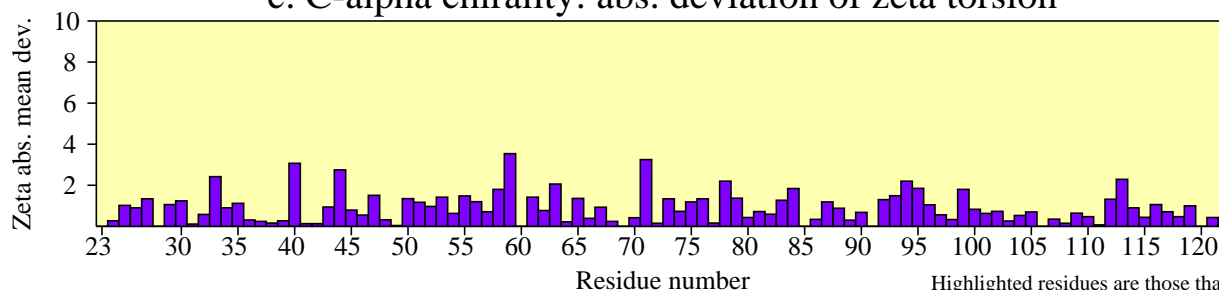
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

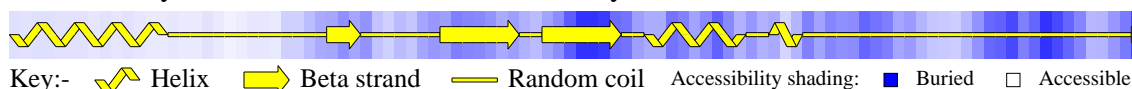


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



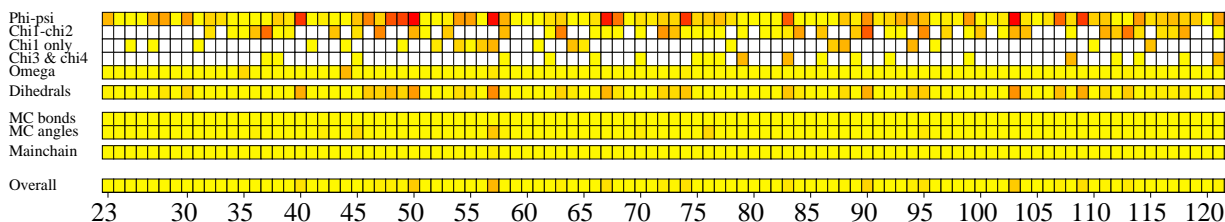
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

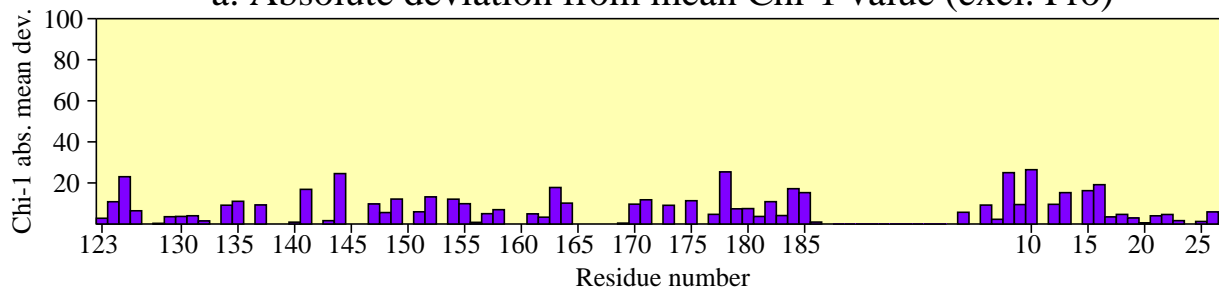


g. G-factors

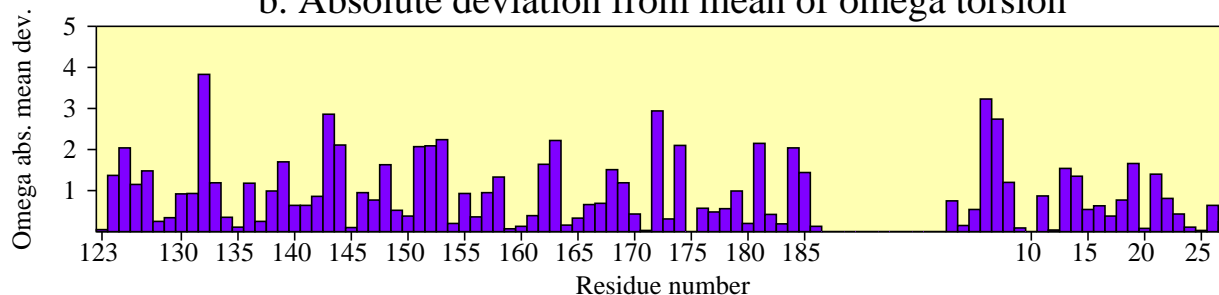


# Residue properties 2QJP

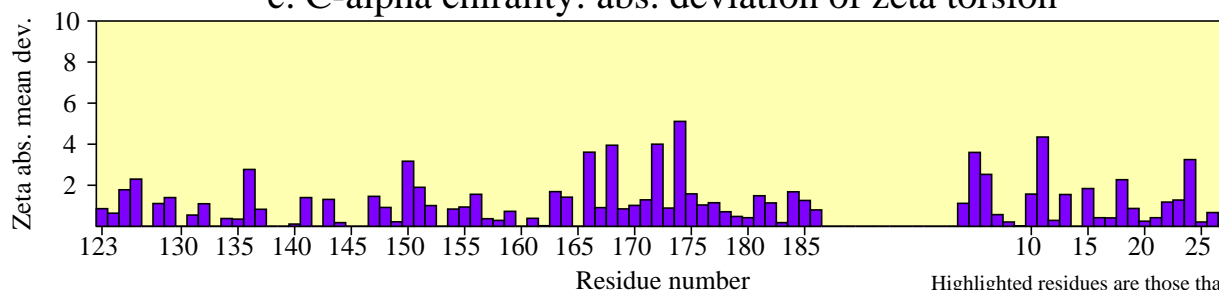
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

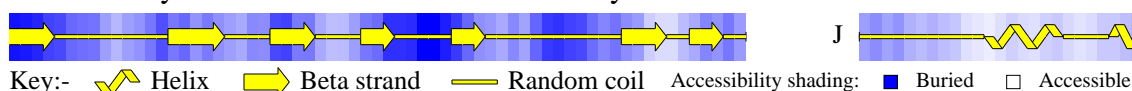


c. C-alpha chirality: abs. deviation of zeta torsion



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

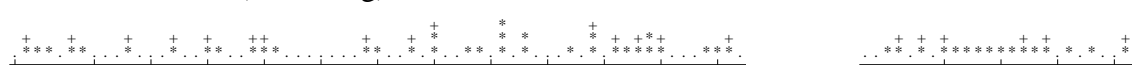
d. Secondary structure & estimated accessibility



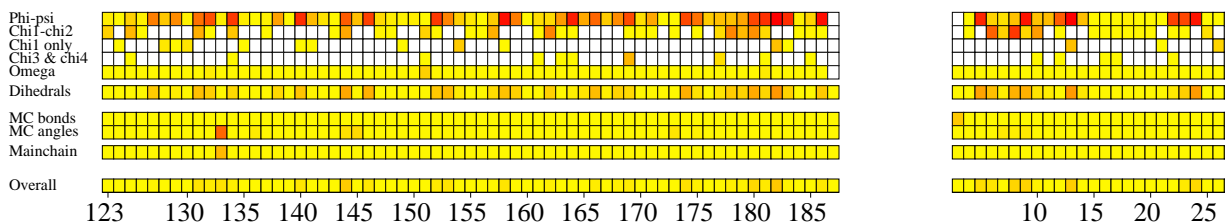
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

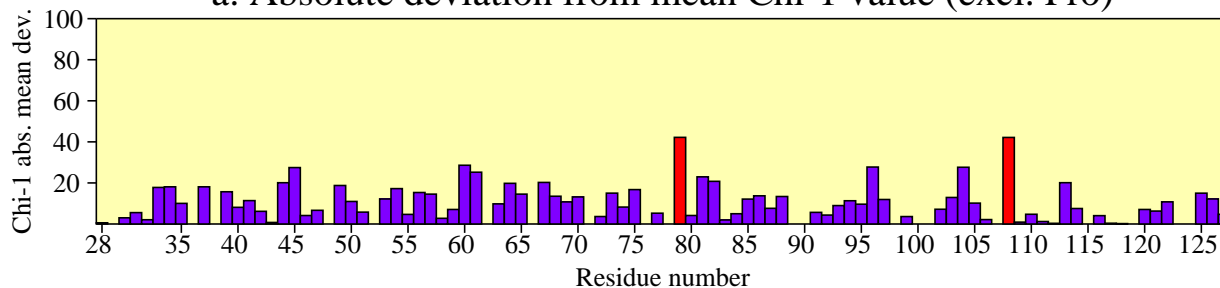


g. G-factors

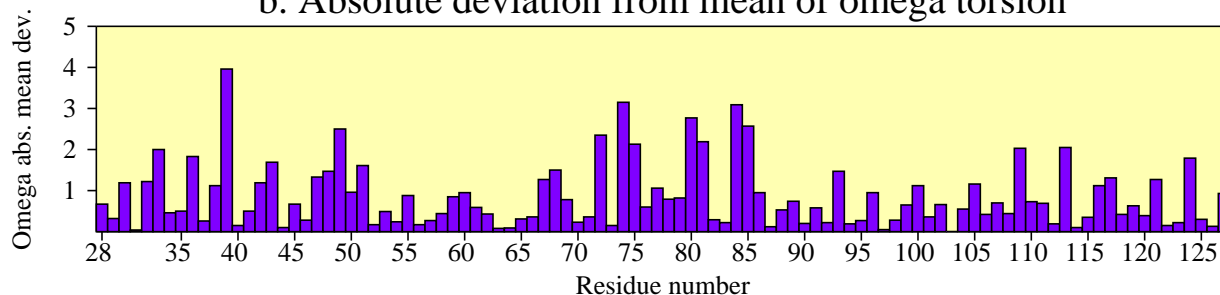


# Residue properties 2QJP

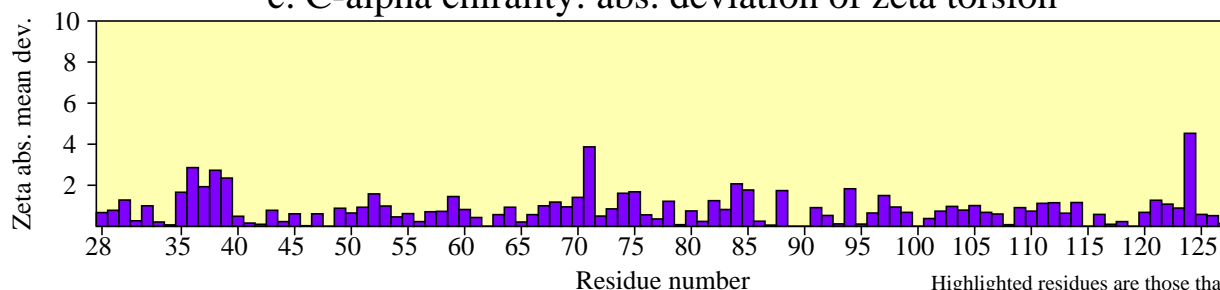
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

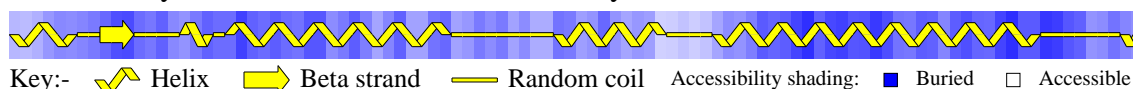


c. C-alpha chirality: abs. deviation of zeta torsion



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

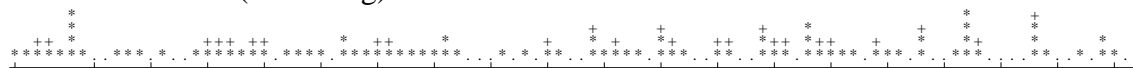
d. Secondary structure & estimated accessibility



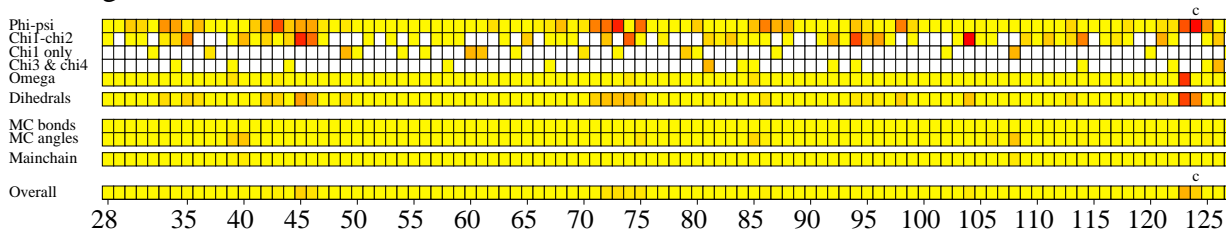
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



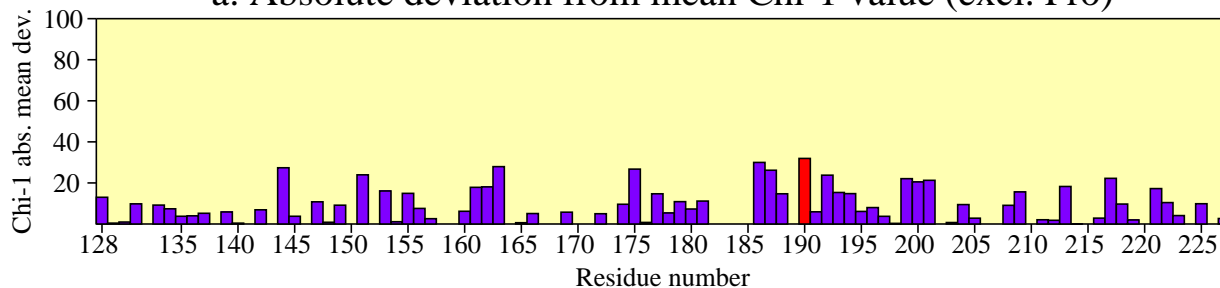
g. G-factors



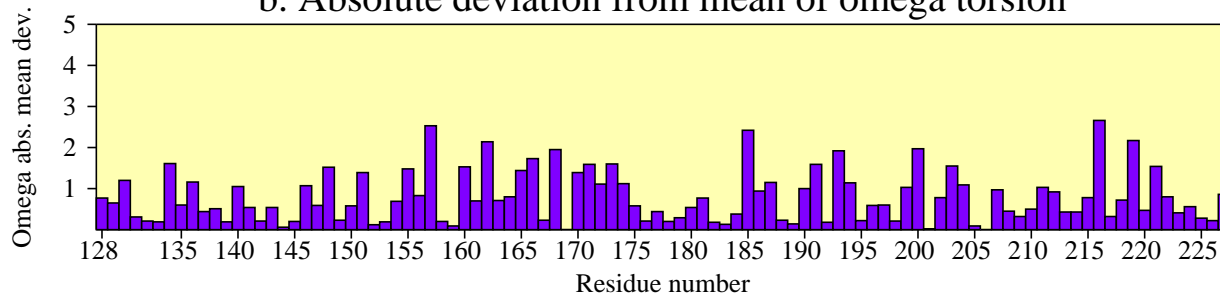
c = cis-peptide

# Residue properties 2QJP

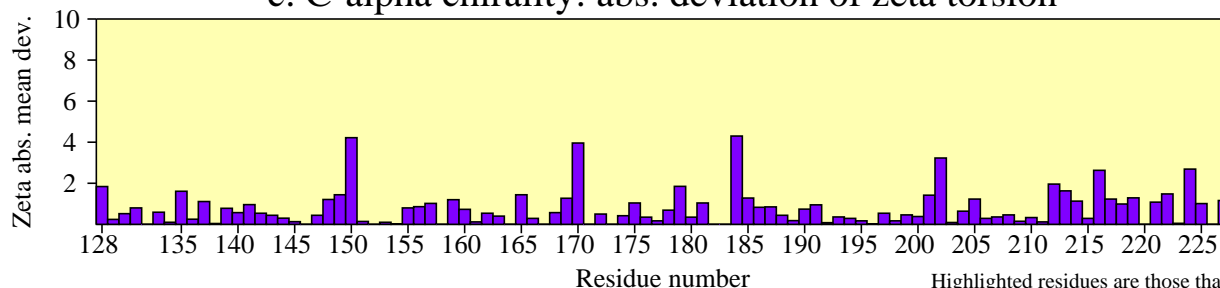
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

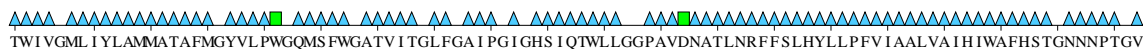


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

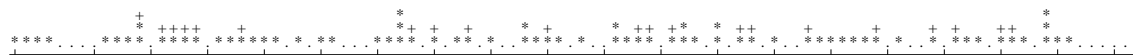
d. Secondary structure & estimated accessibility



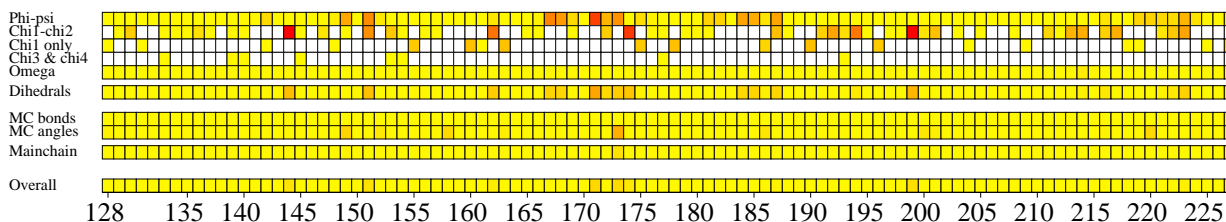
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

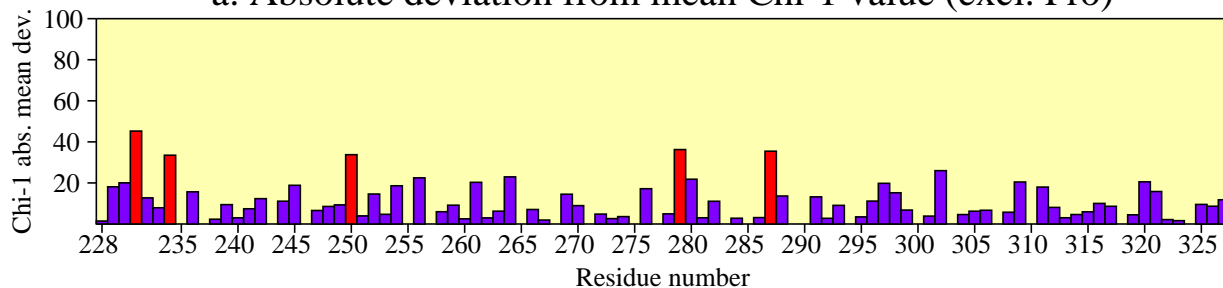


g. G-factors

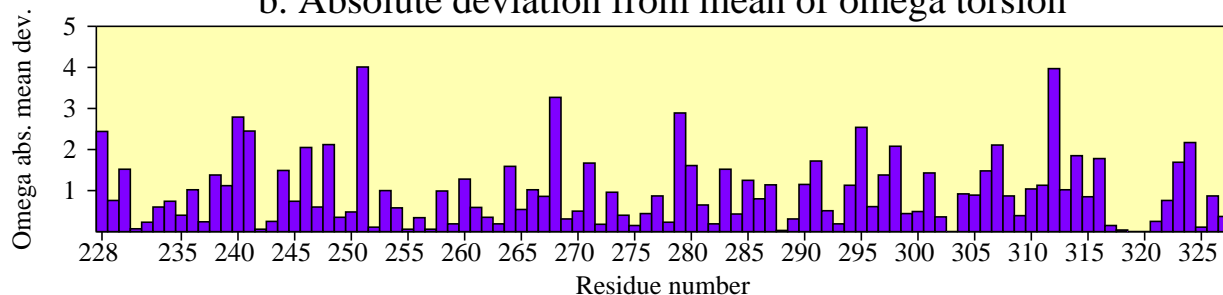


# Residue properties 2QJP

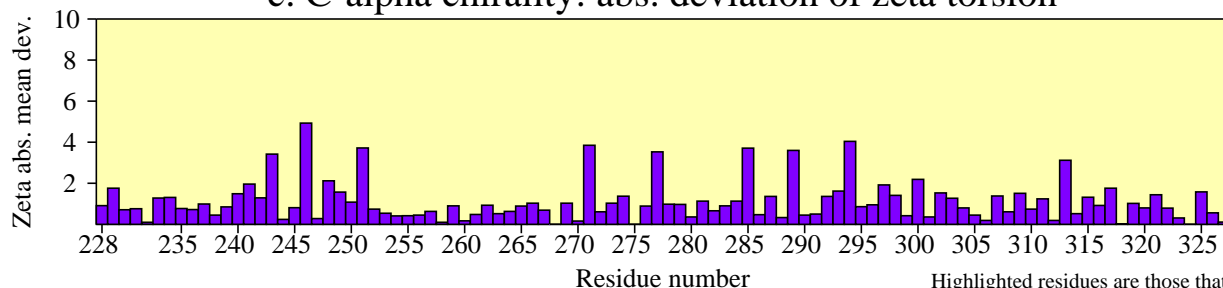
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

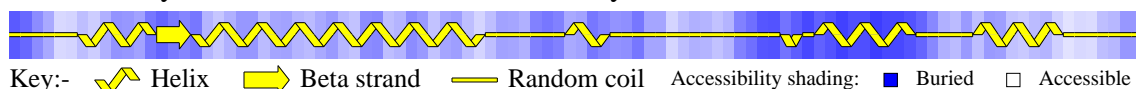


c. C-alpha chirality: abs. deviation of zeta torsion



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

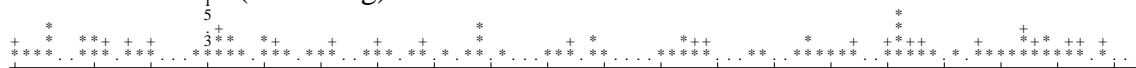
d. Secondary structure & estimated accessibility



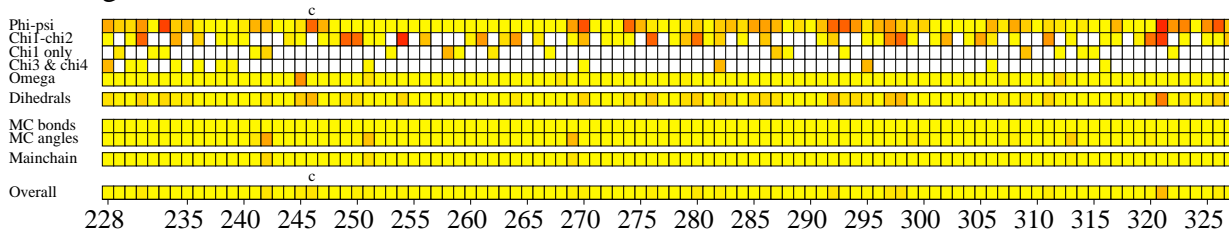
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



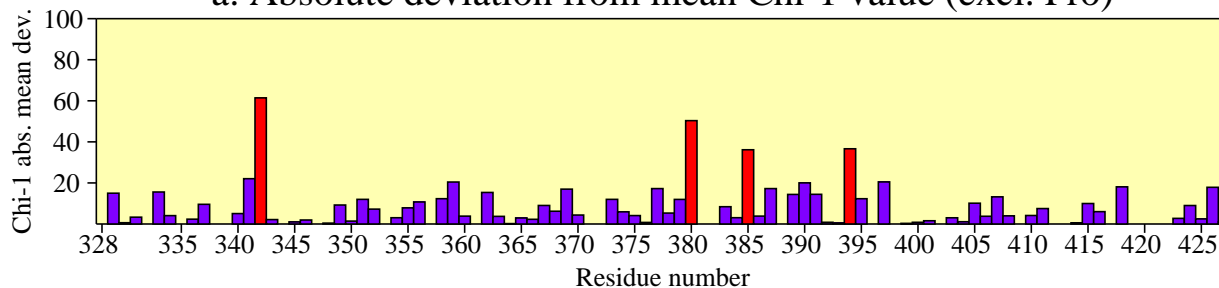
g. G-factors



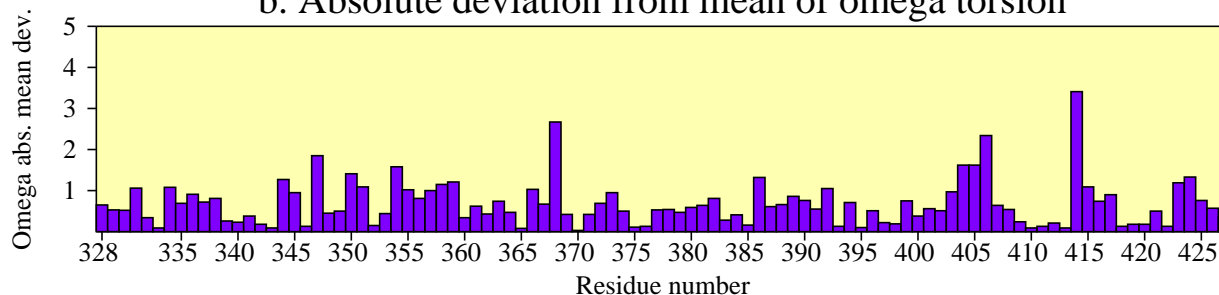
c = cis-peptide

# Residue properties 2QJP

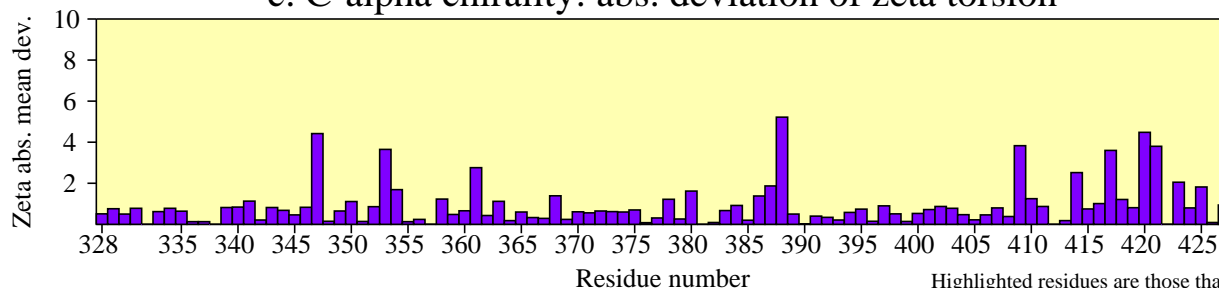
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



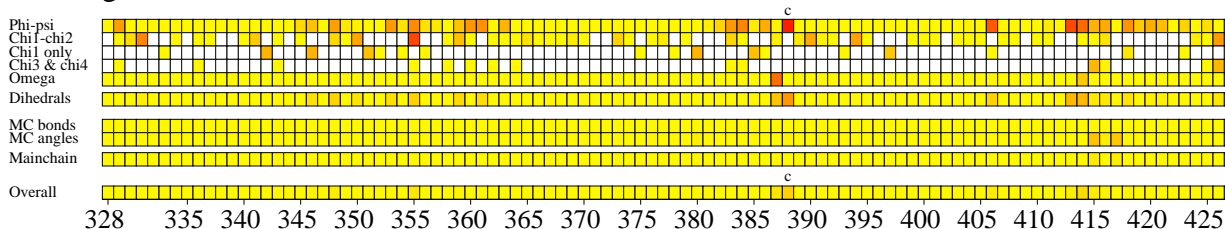
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



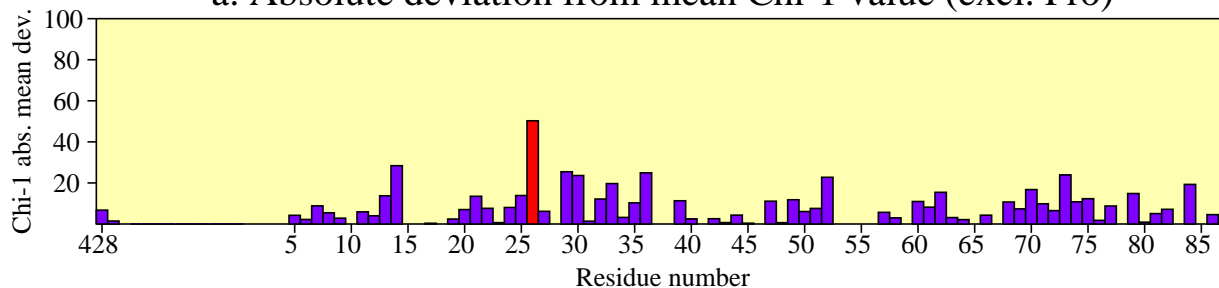
g. G-factors



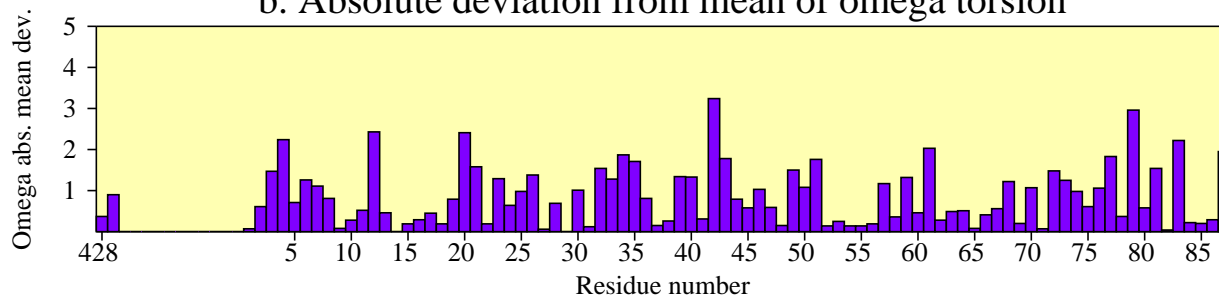
c = cis-peptide

# Residue properties 2QJP

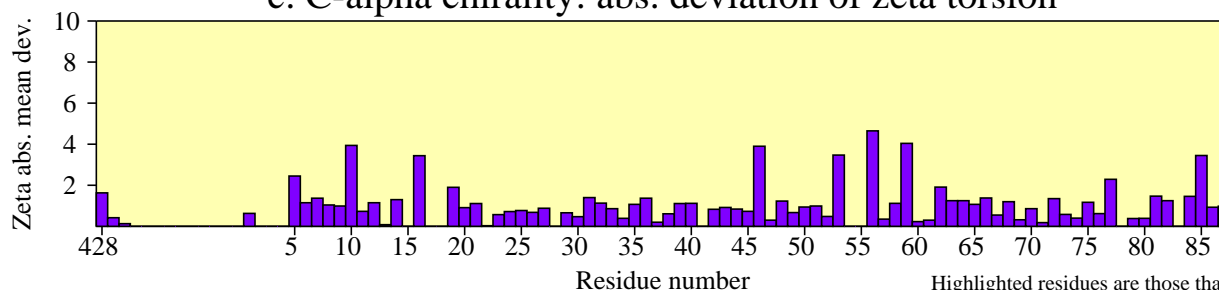
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

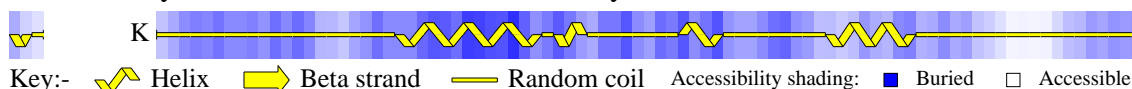


c. C-alpha chirality: abs. deviation of zeta torsion



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

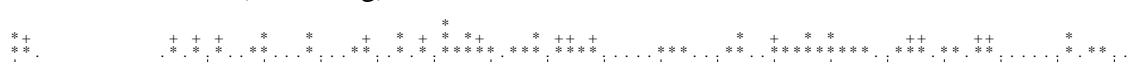
d. Secondary structure & estimated accessibility



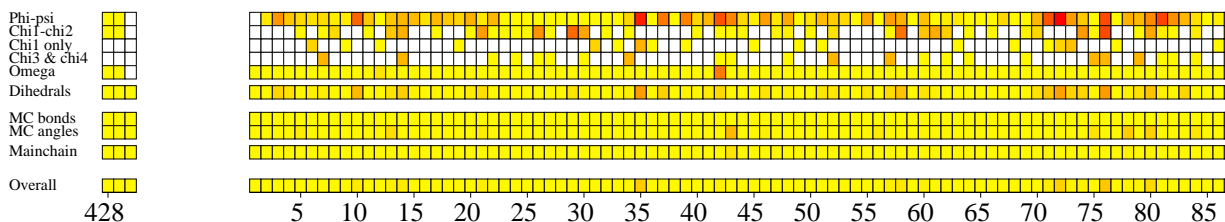
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



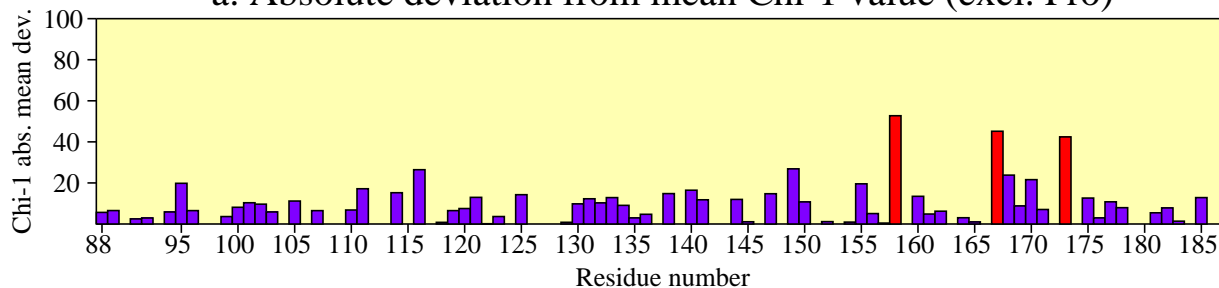
g. G-factors



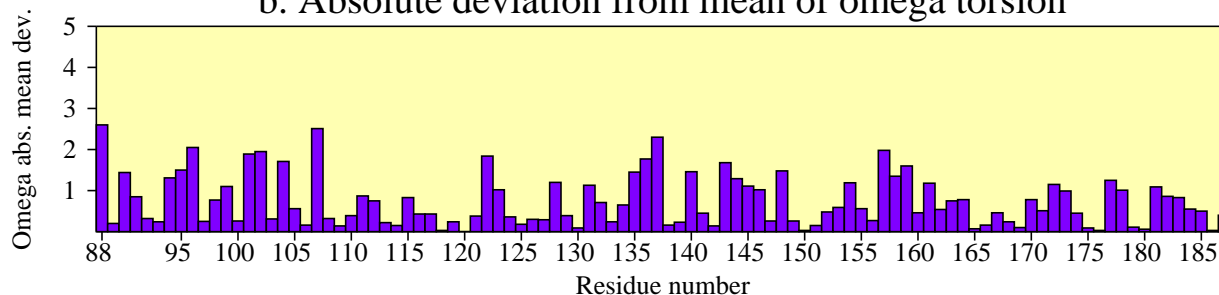


# Residue properties 2QJP

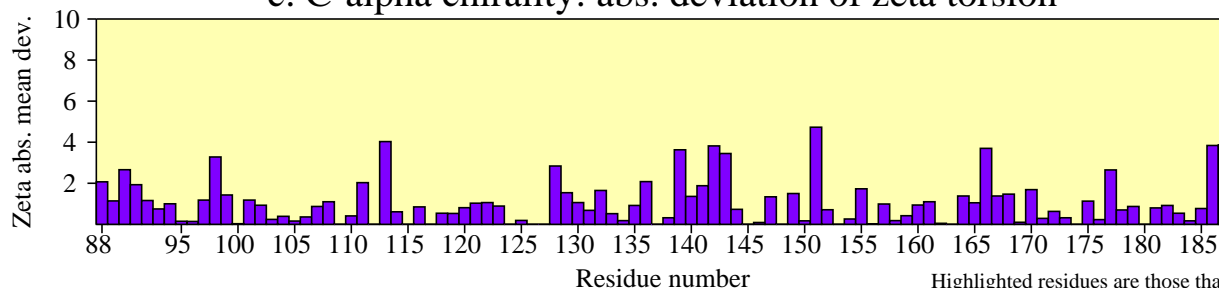
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

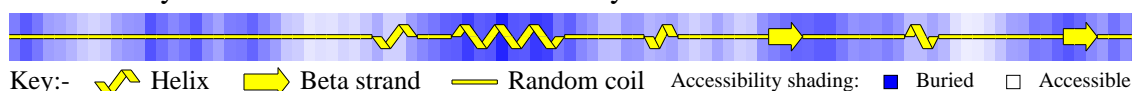


c. C-alpha chirality: abs. deviation of zeta torsion



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

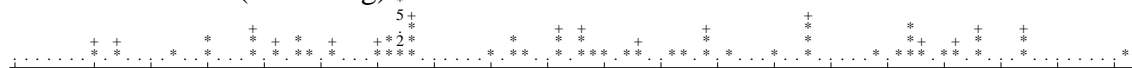
d. Secondary structure & estimated accessibility



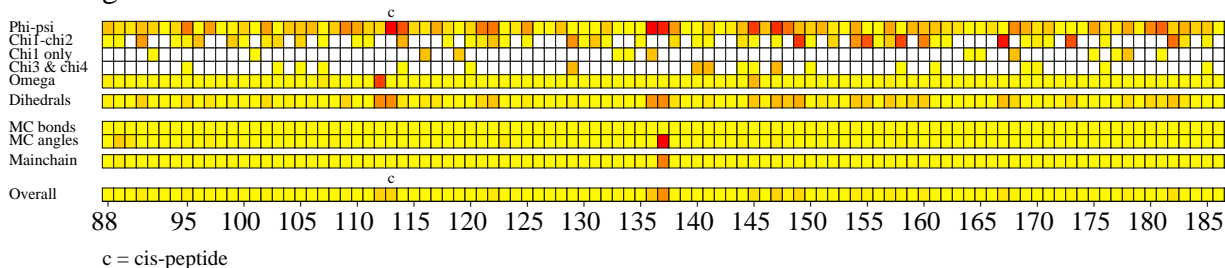
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

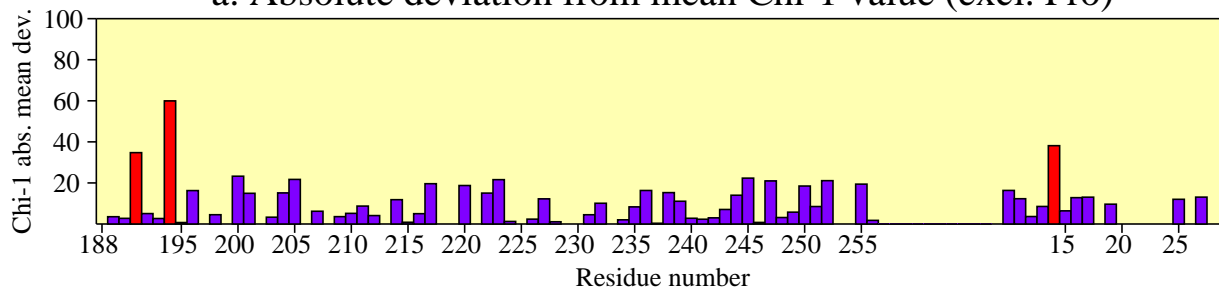


g. G-factors

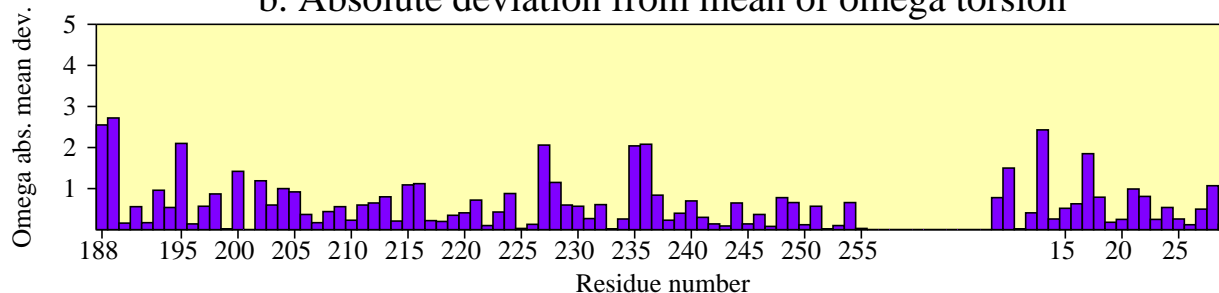


# Residue properties 2QJP

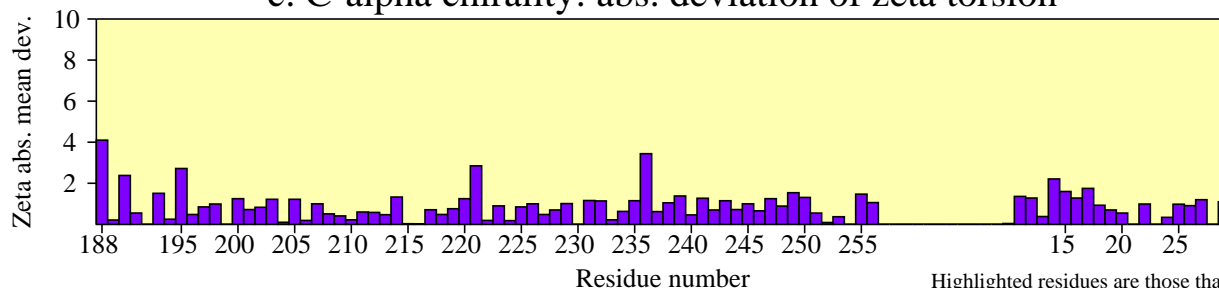
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

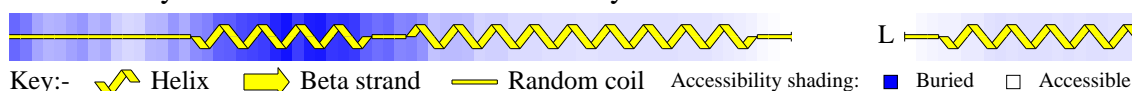


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



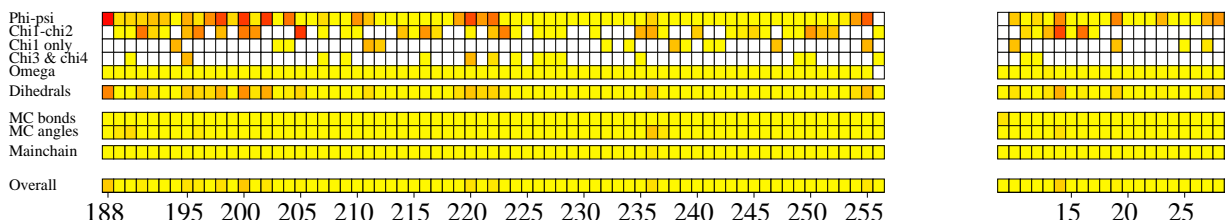
### e. Sequence & Ramachandran regions



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

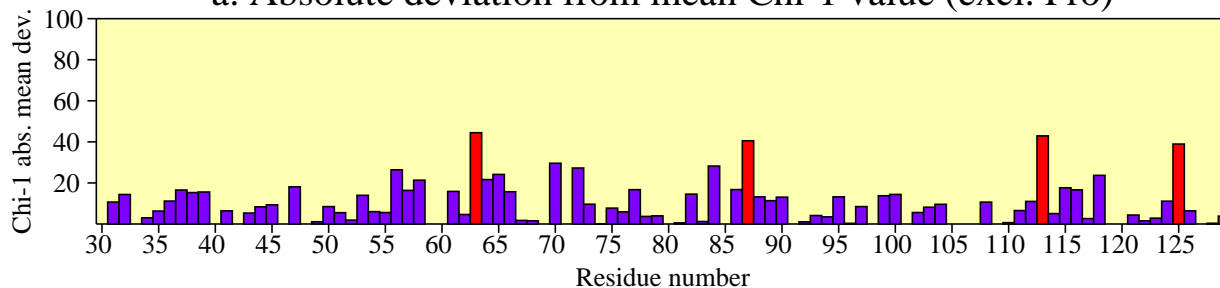


### g. G-factors

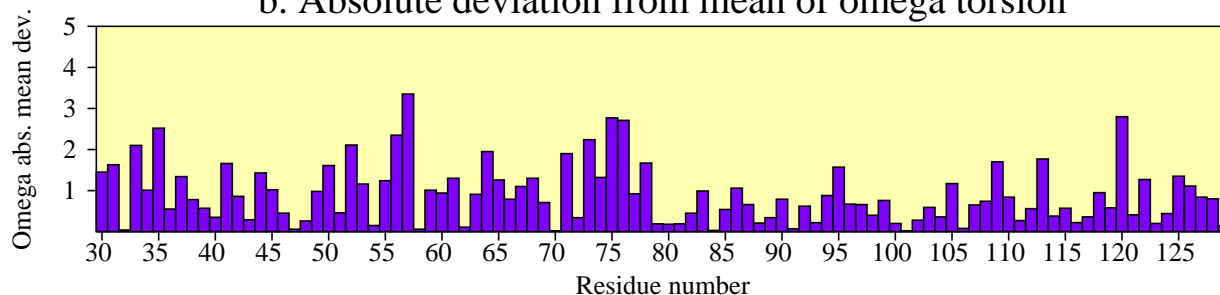


# Residue properties 2QJP

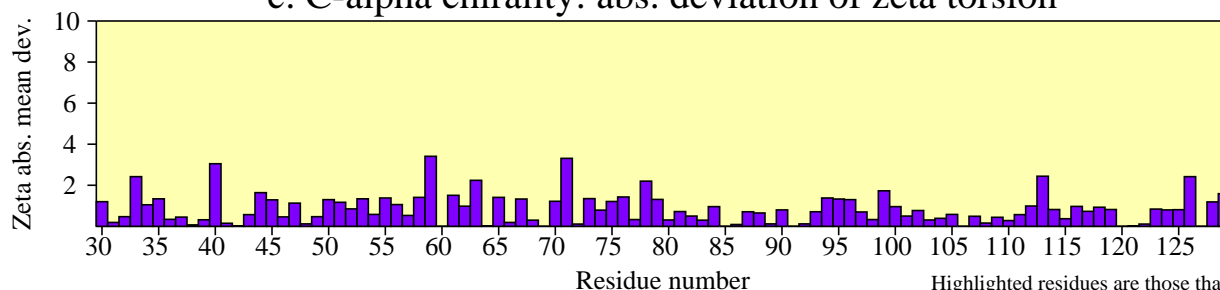
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

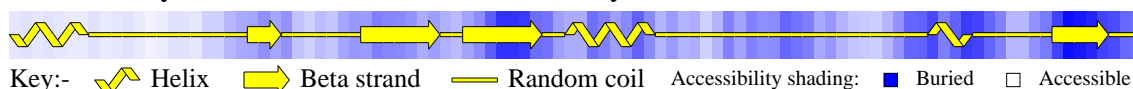


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



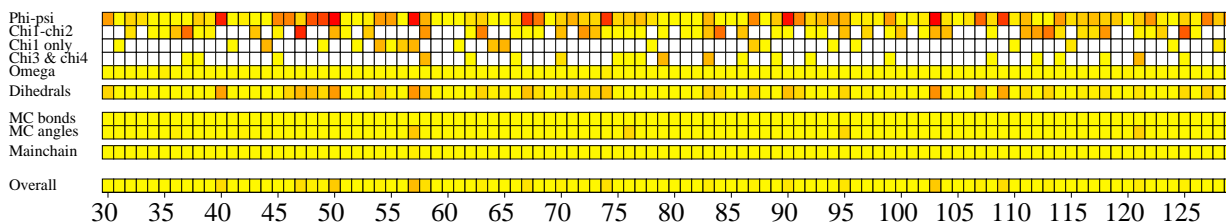
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

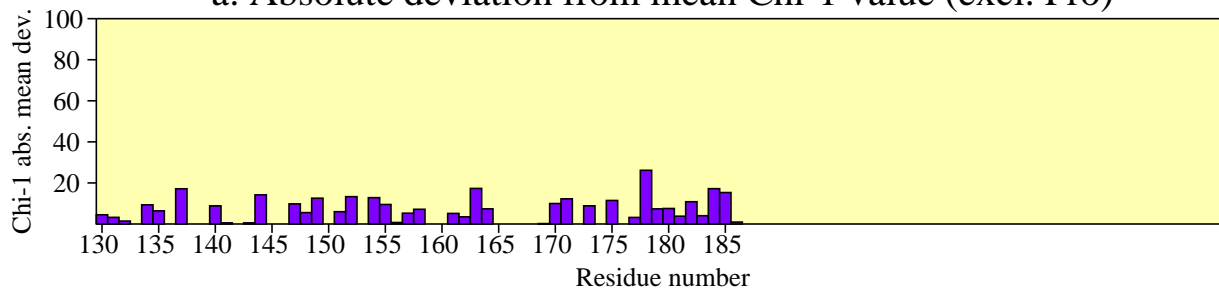


g. G-factors

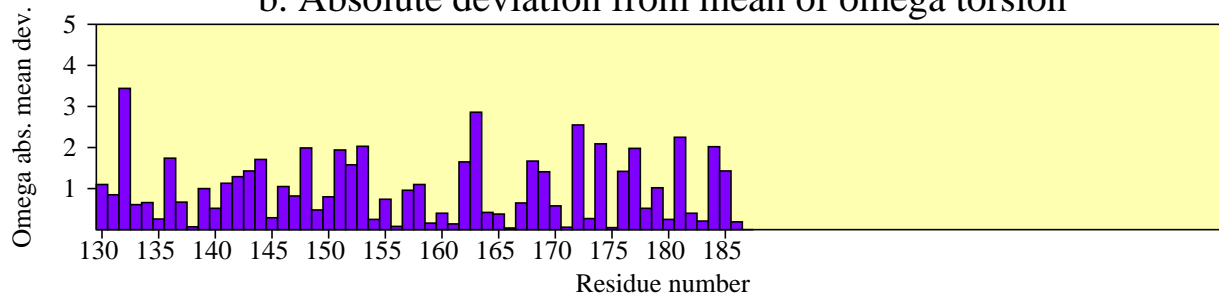


# Residue properties 2QJP

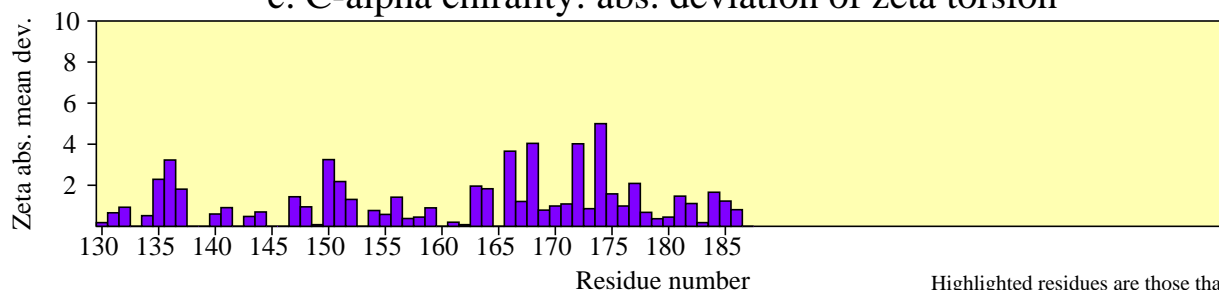
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

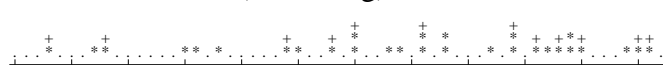


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

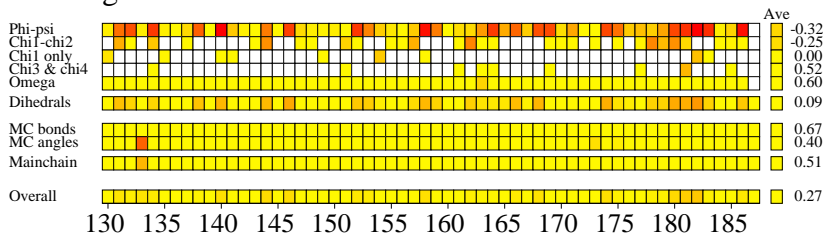
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

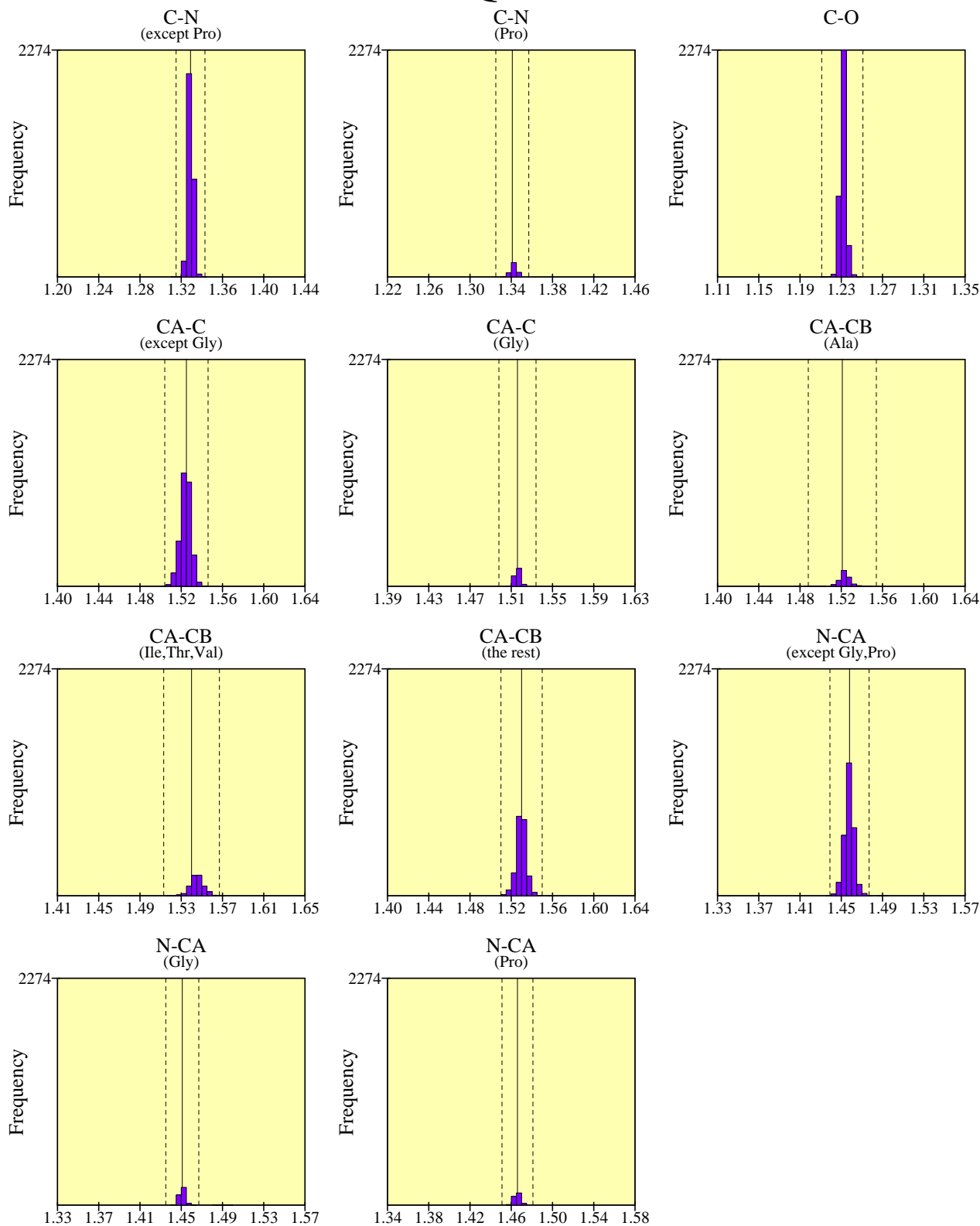


g. G-factors



# Main-chain bond lengths

## 2QJP

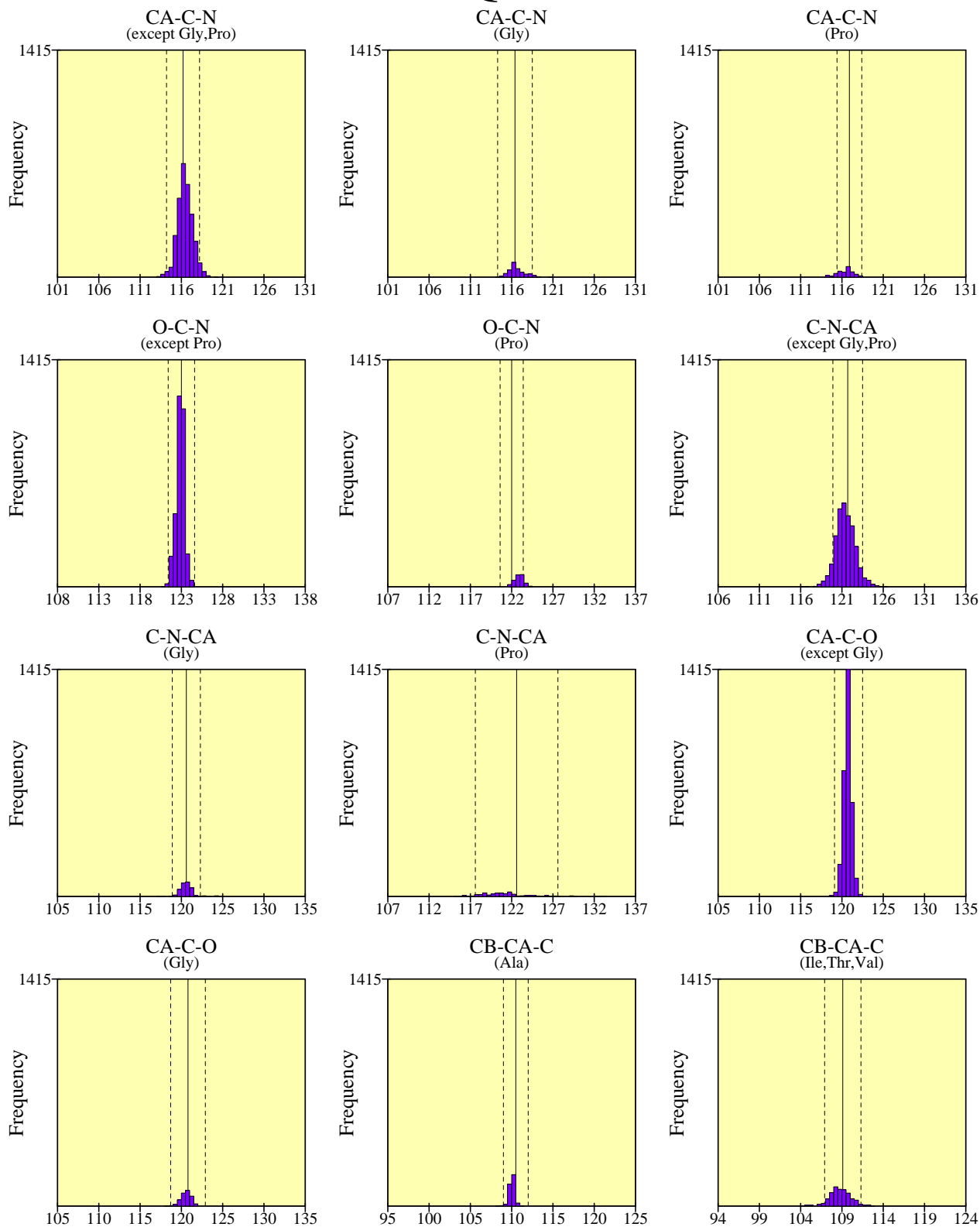


Black bars > 2.0 st. devs. from mean.

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

# Main-chain bond angles

## 2QJP

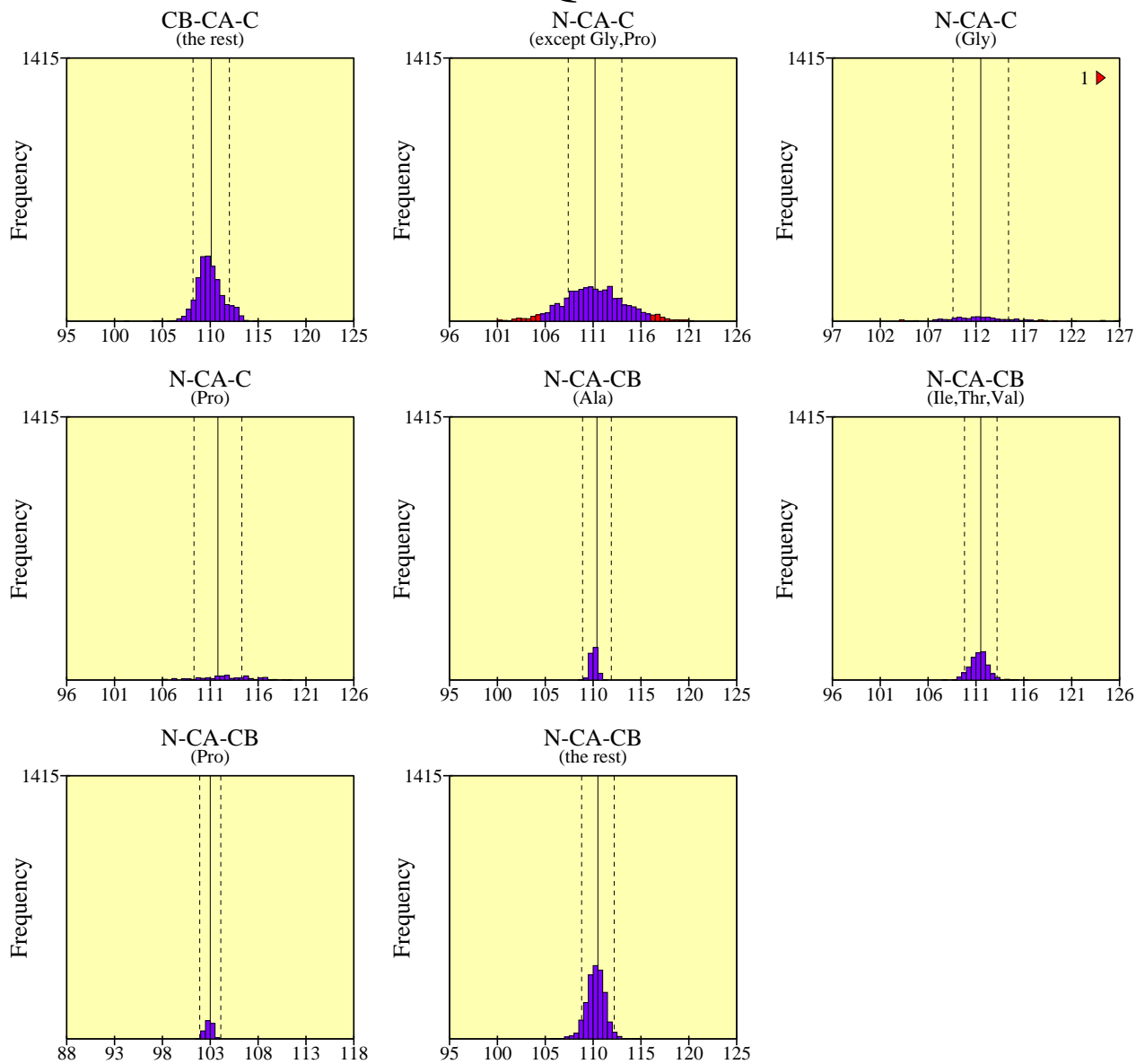


Black bars > 2.0 st. devs. from mean.

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

# Main-chain bond angles

## 2QJP



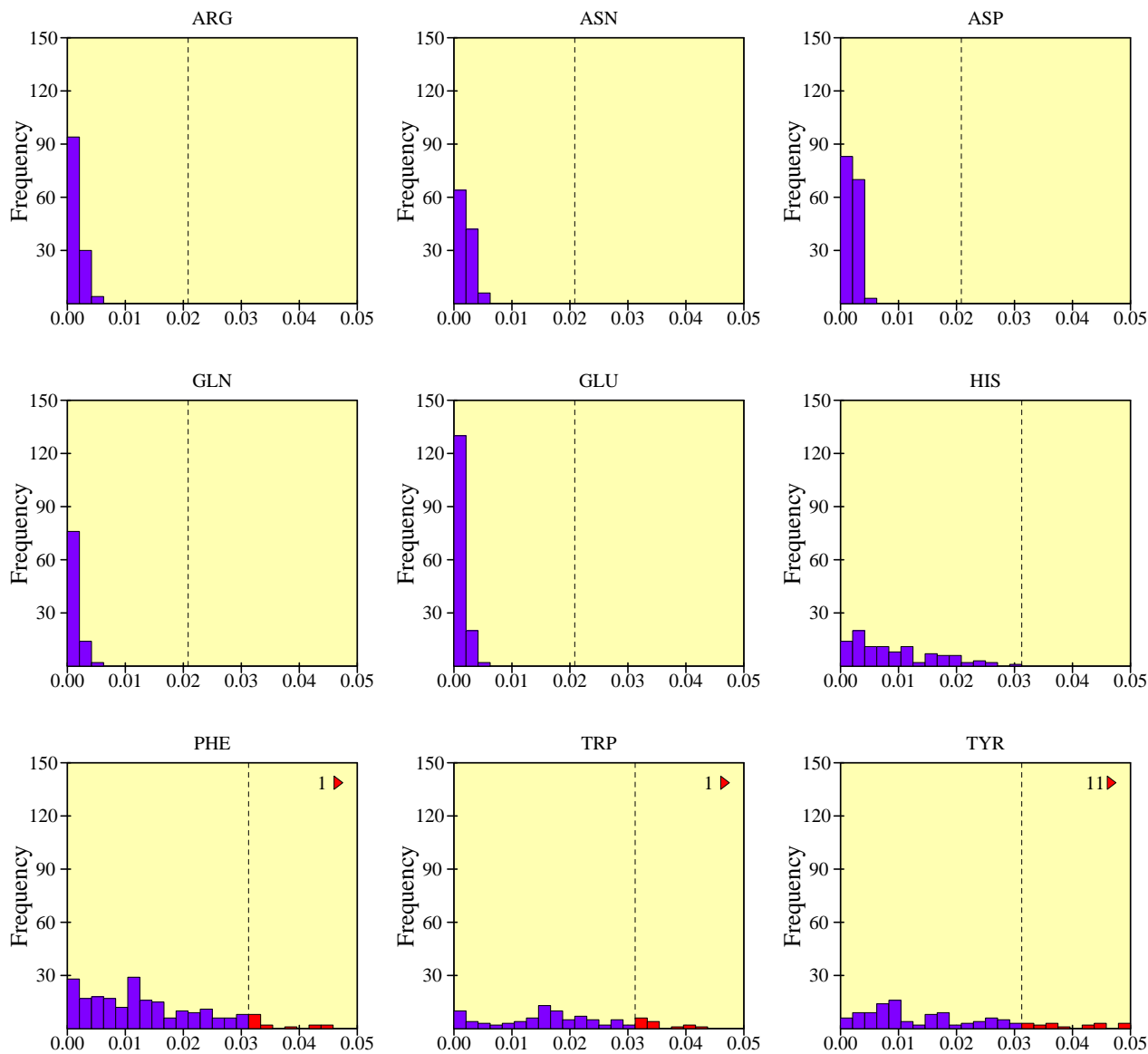
Black bars > 2.0 st. devs. from mean.

◀ 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

## 2QJP



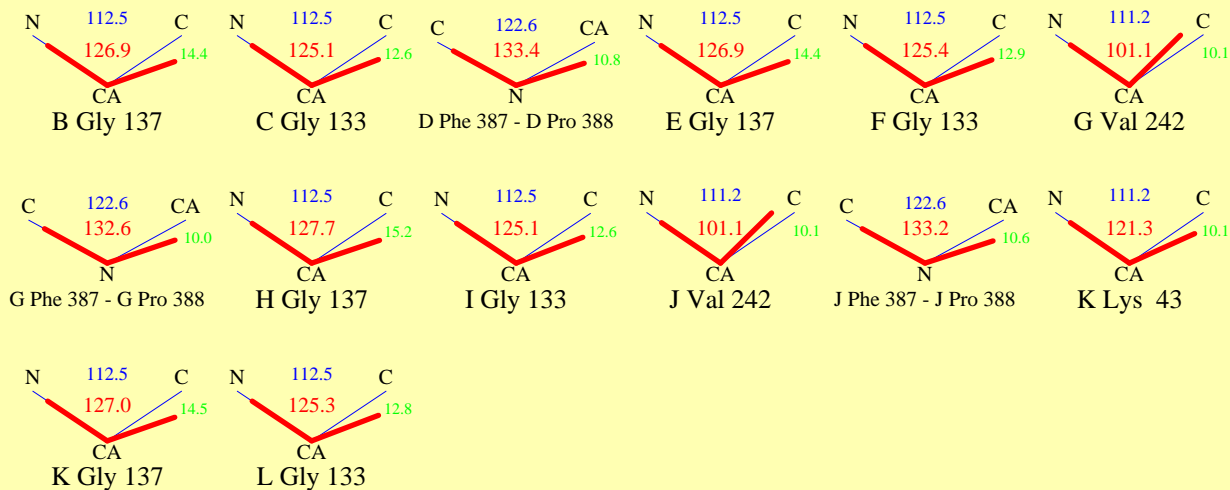
Histograms showing RMS distances of planar atoms from best-fit plane.  
 Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

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



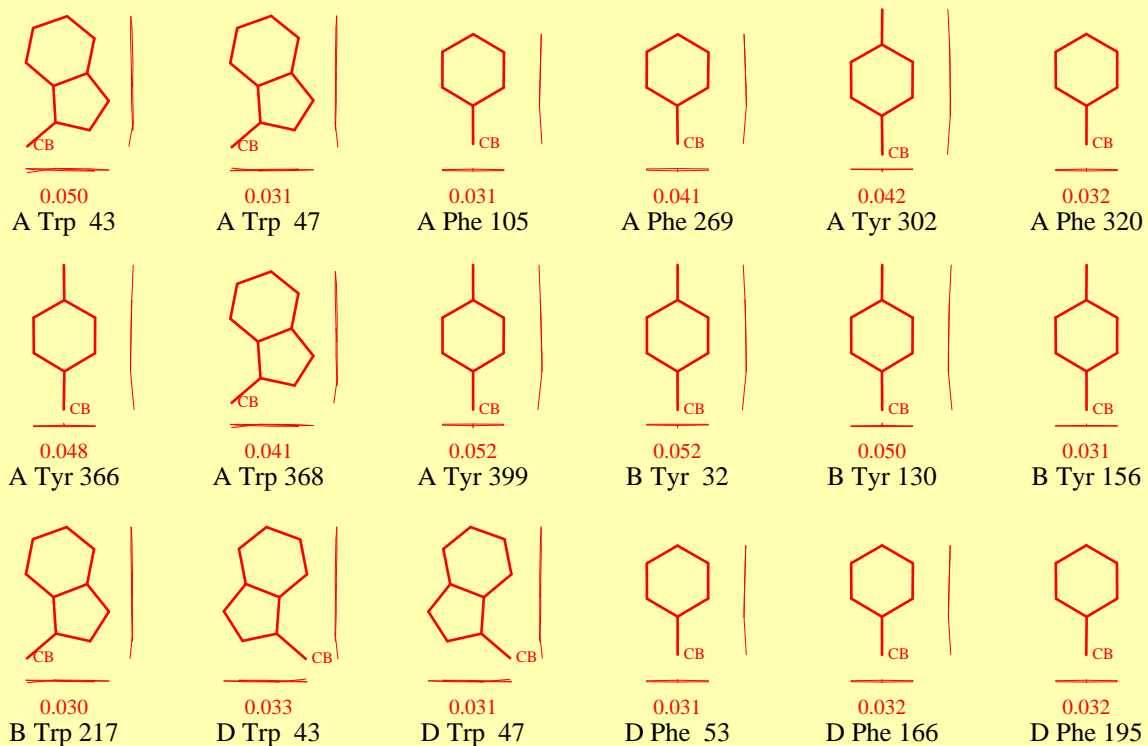
# Distorted geometry 2QJP

## Main-chain bond angles



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

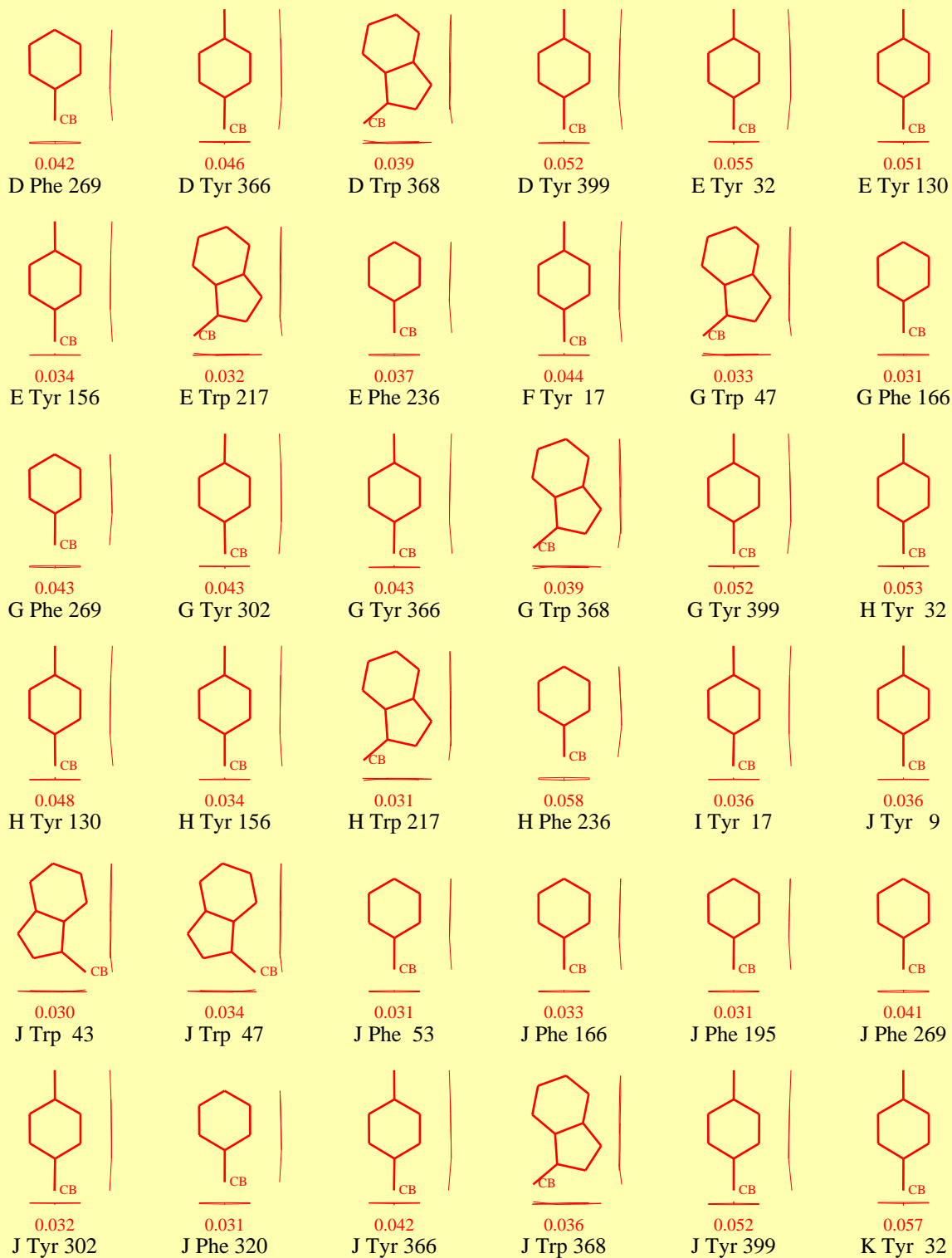
## Planar groups



# Distorted geometry

## 2QJP

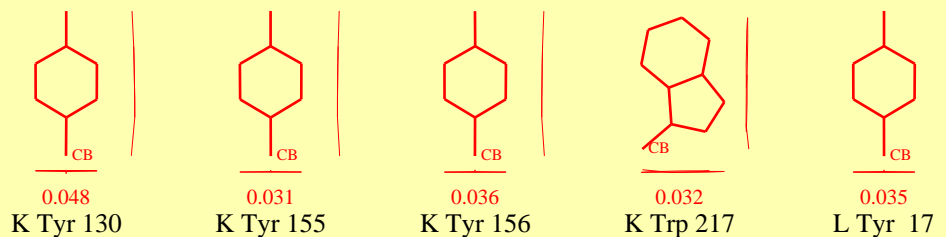
### Planar groups (contd)



# Distorted geometry

## 2QJP

### Planar groups (contd)



Sidechains with RMS dist. from planarity  $> 0.03\text{\AA}$  for rings, or  $> 0.02\text{\AA}$  otherwise. Value shown is RMS dist.