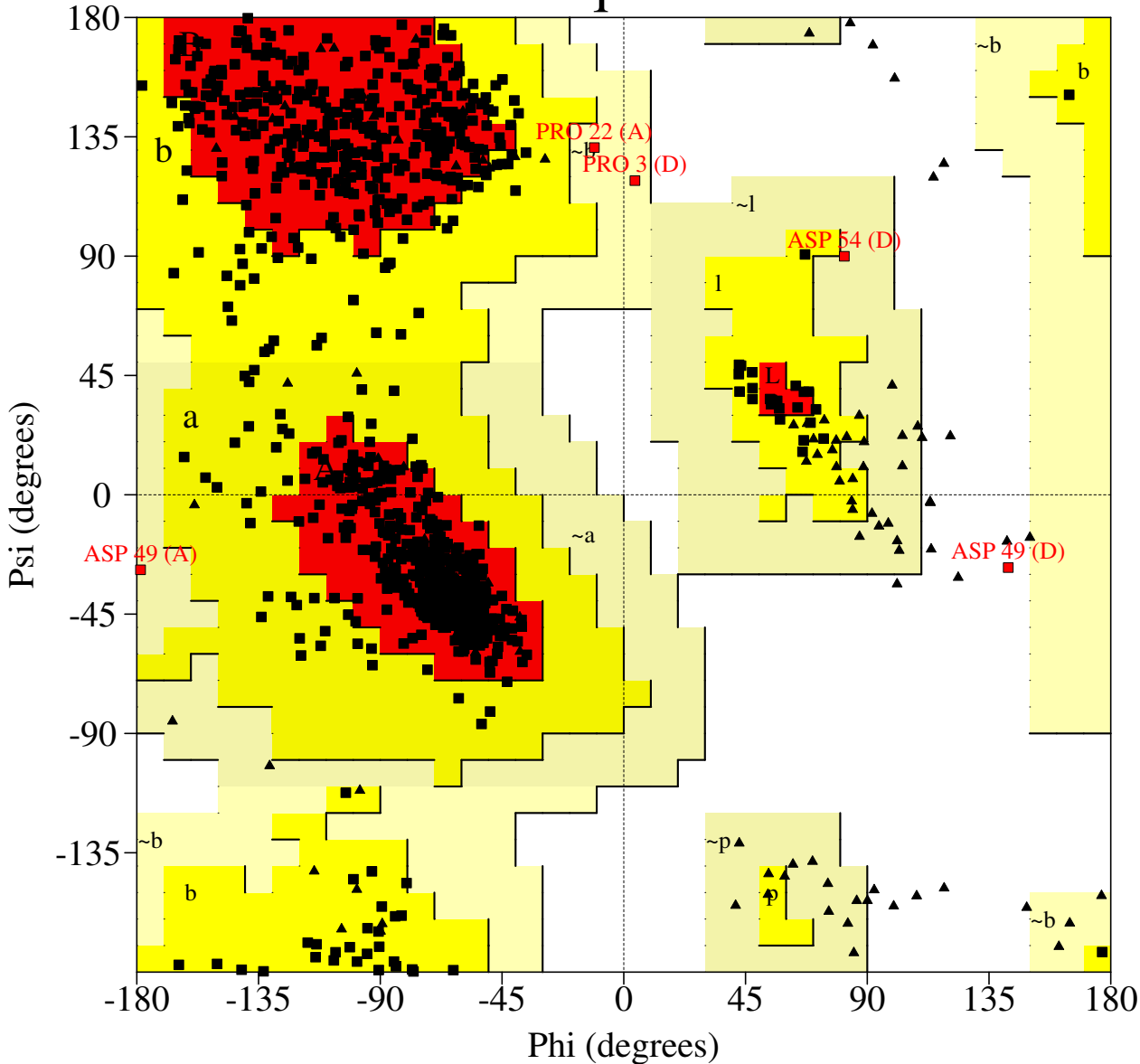


Ramachandran Plot

1qo8



Plot statistics

Residues in most favoured regions [A,B,L]	829	85.5%
Residues in additional allowed regions [a,b,l,p]	138	14.2%
Residues in generously allowed regions [-a,-b,-l,-p]	2	0.2%
Residues in disallowed regions	1	0.1%

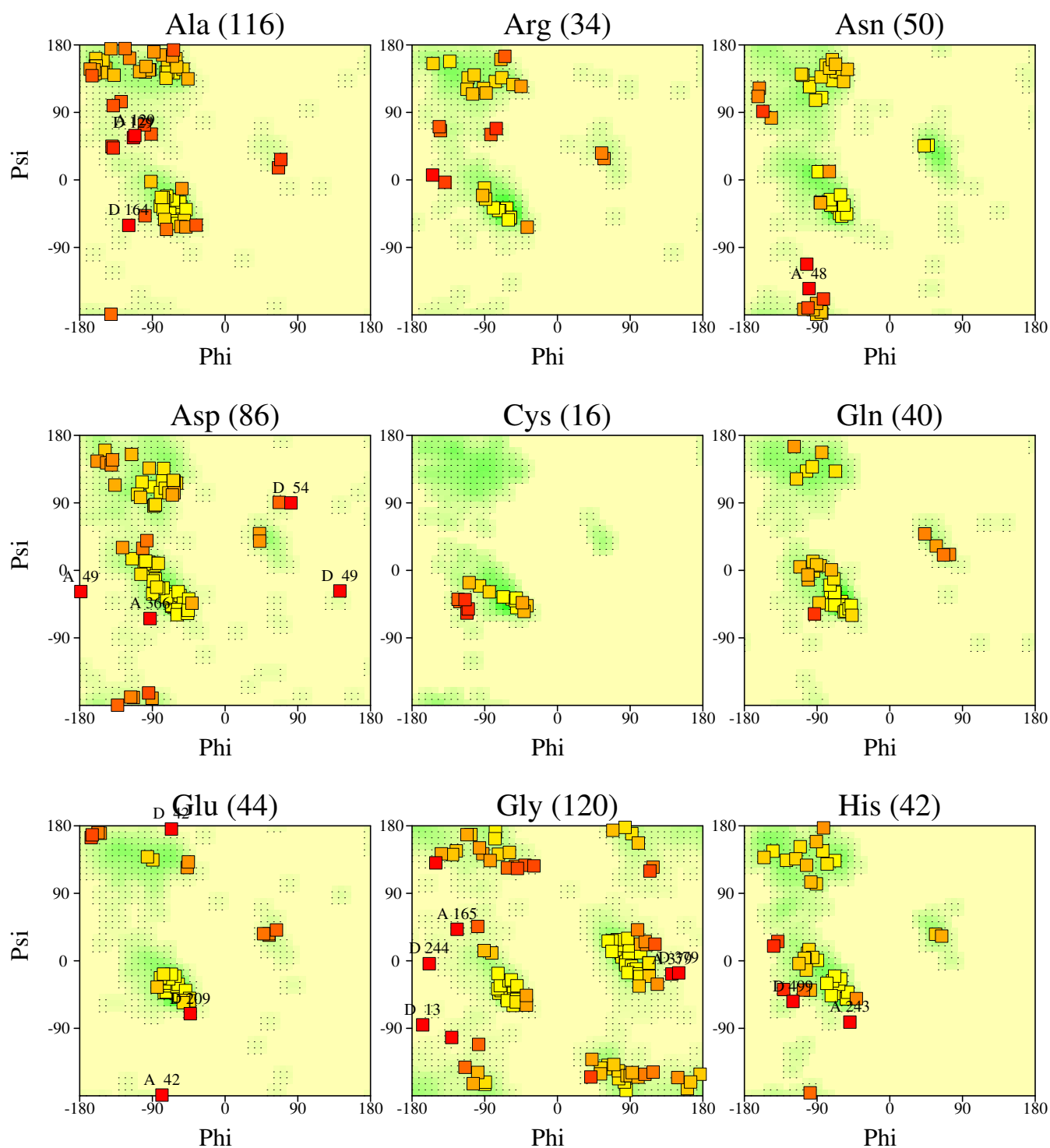
Number of non-glycine and non-proline residues	970	100.0%
Number of end-residues (excl. Gly and Pro)	4	
Number of glycine residues (shown as triangles)	120	
Number of proline residues	34	

Total number of residues	1128	

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.

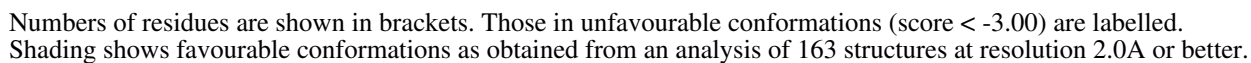
Ramachandran plots for all residue types

1qo8



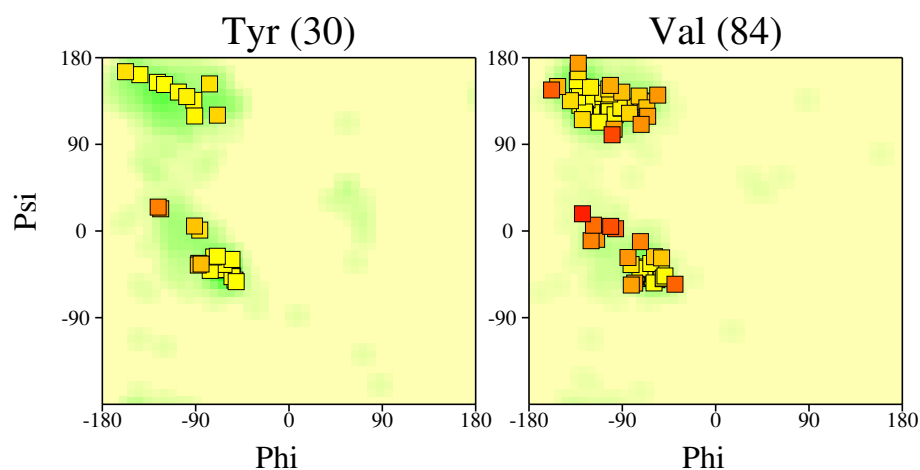
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

1q08



Ramachandran plots for all residue types

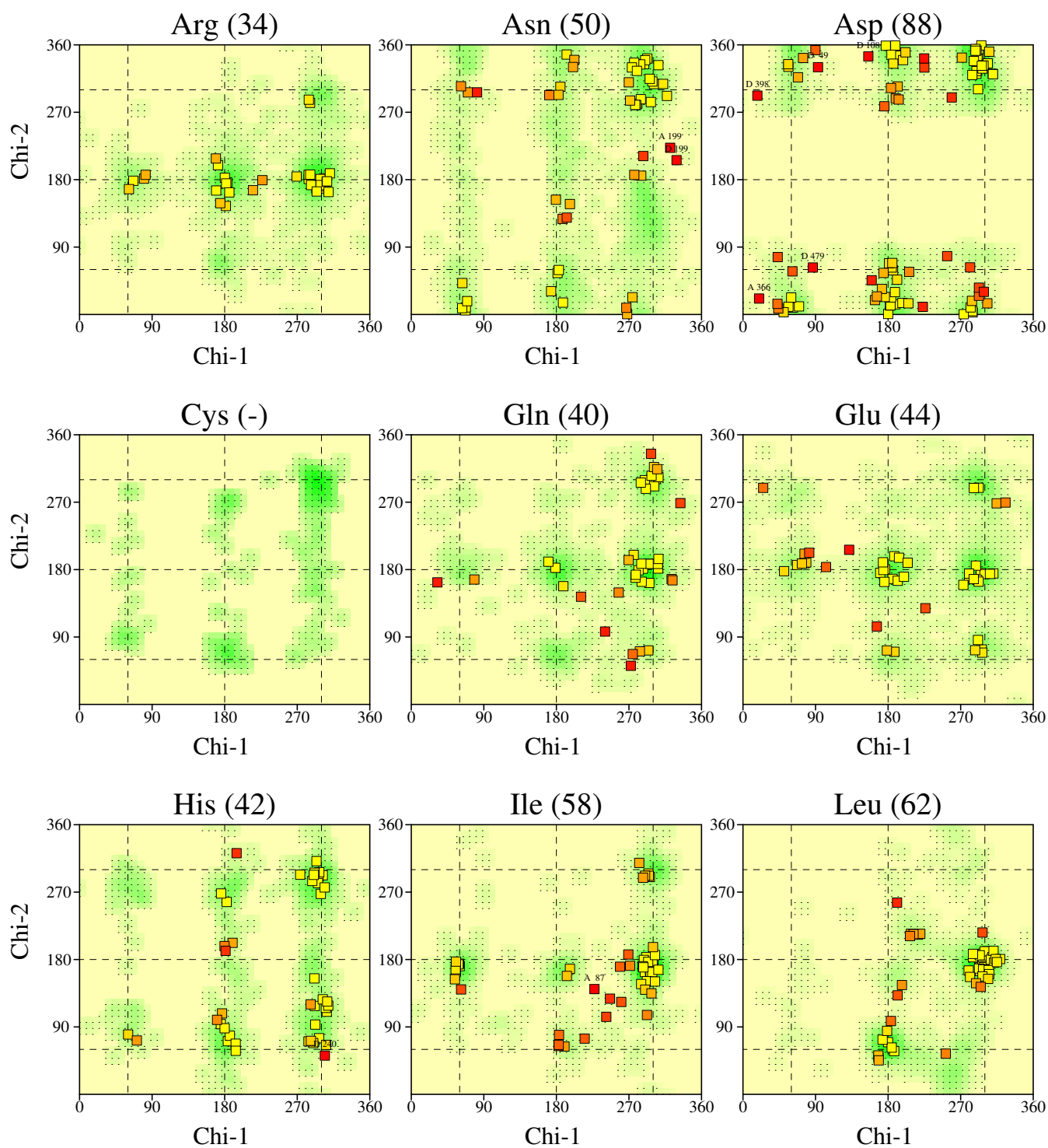
1qo8



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

Chi1-Chi2 plots

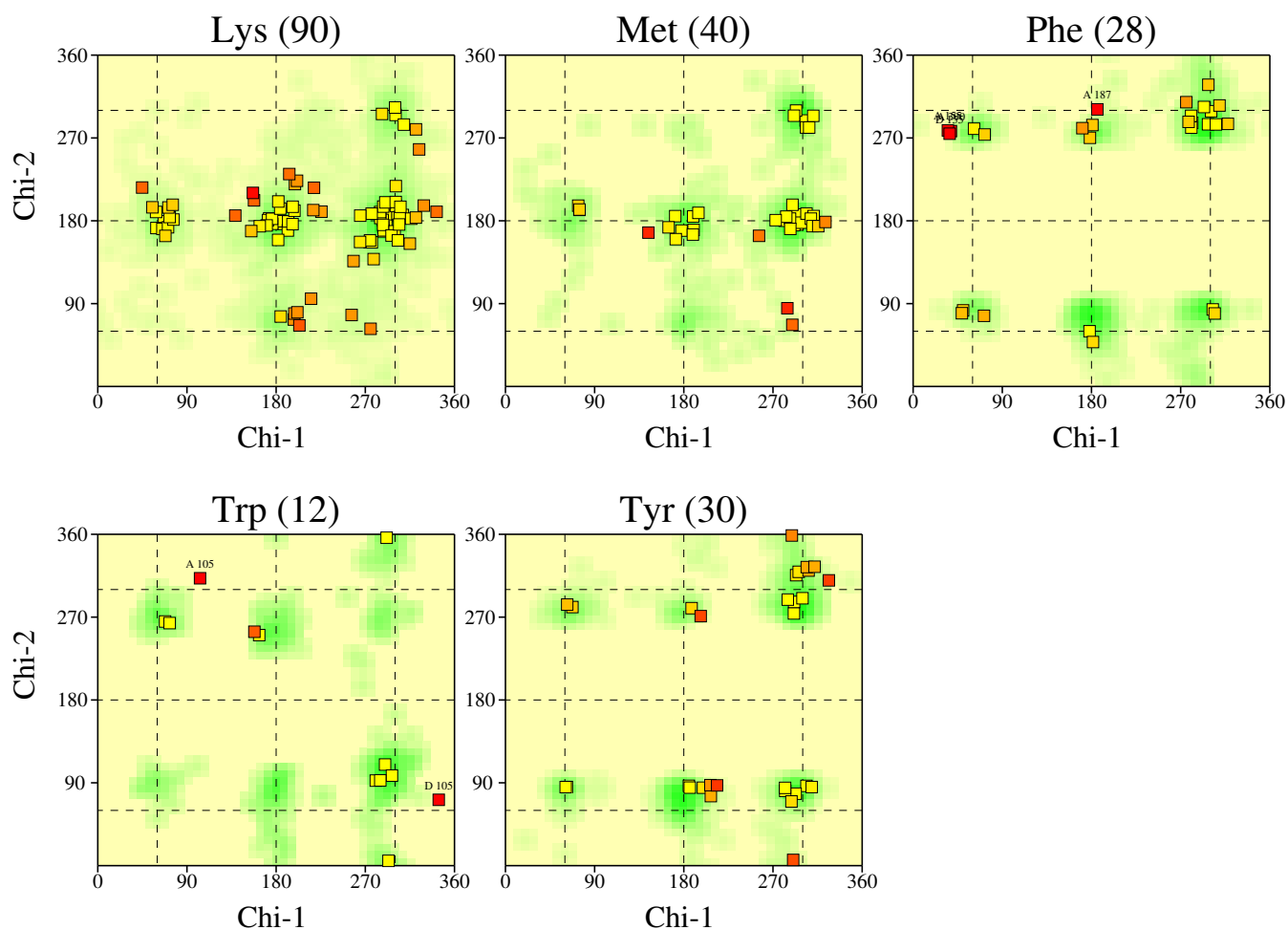
1qo8



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

Chi1-Chi2 plots

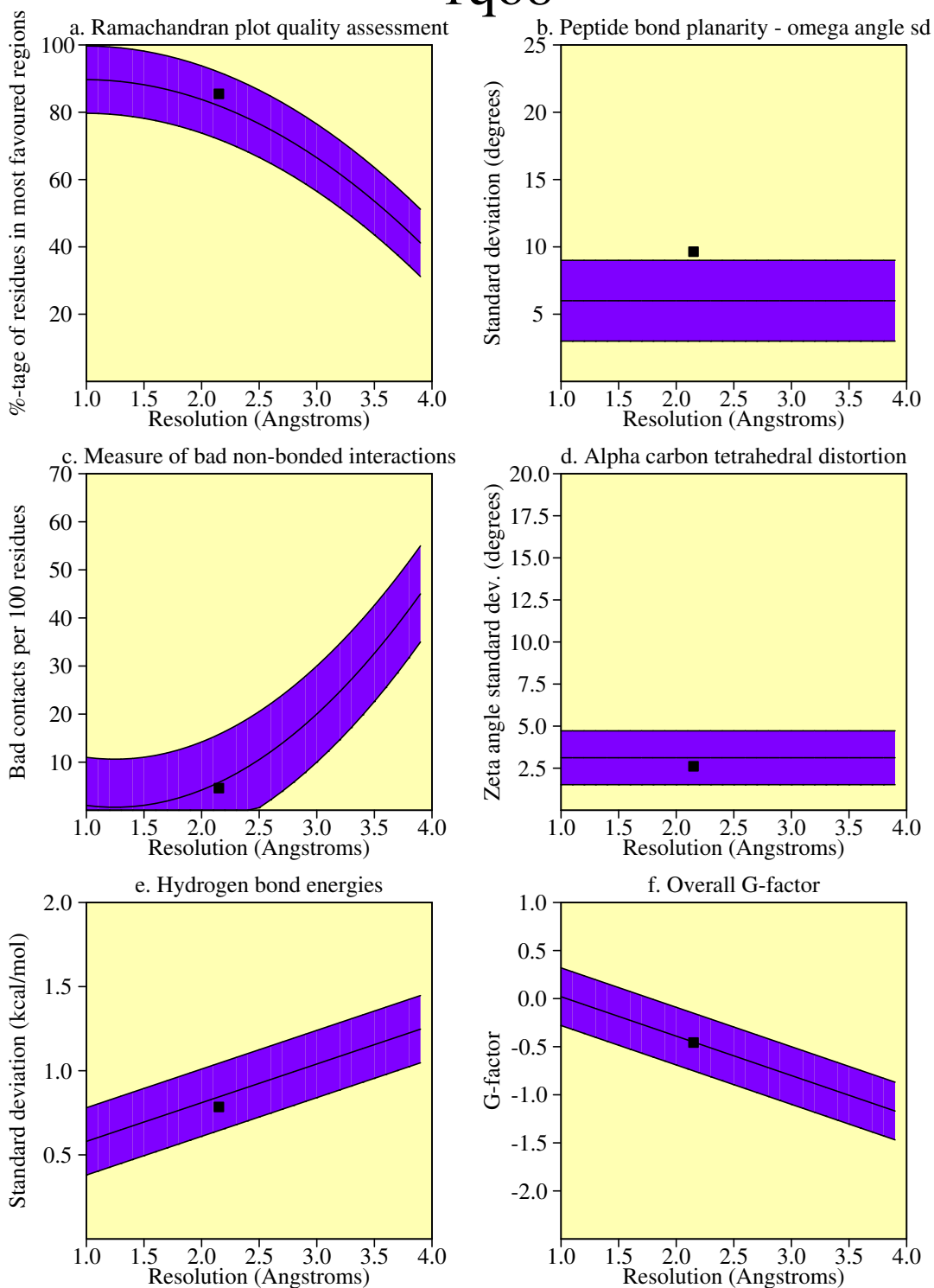
1qo8



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

1qo8

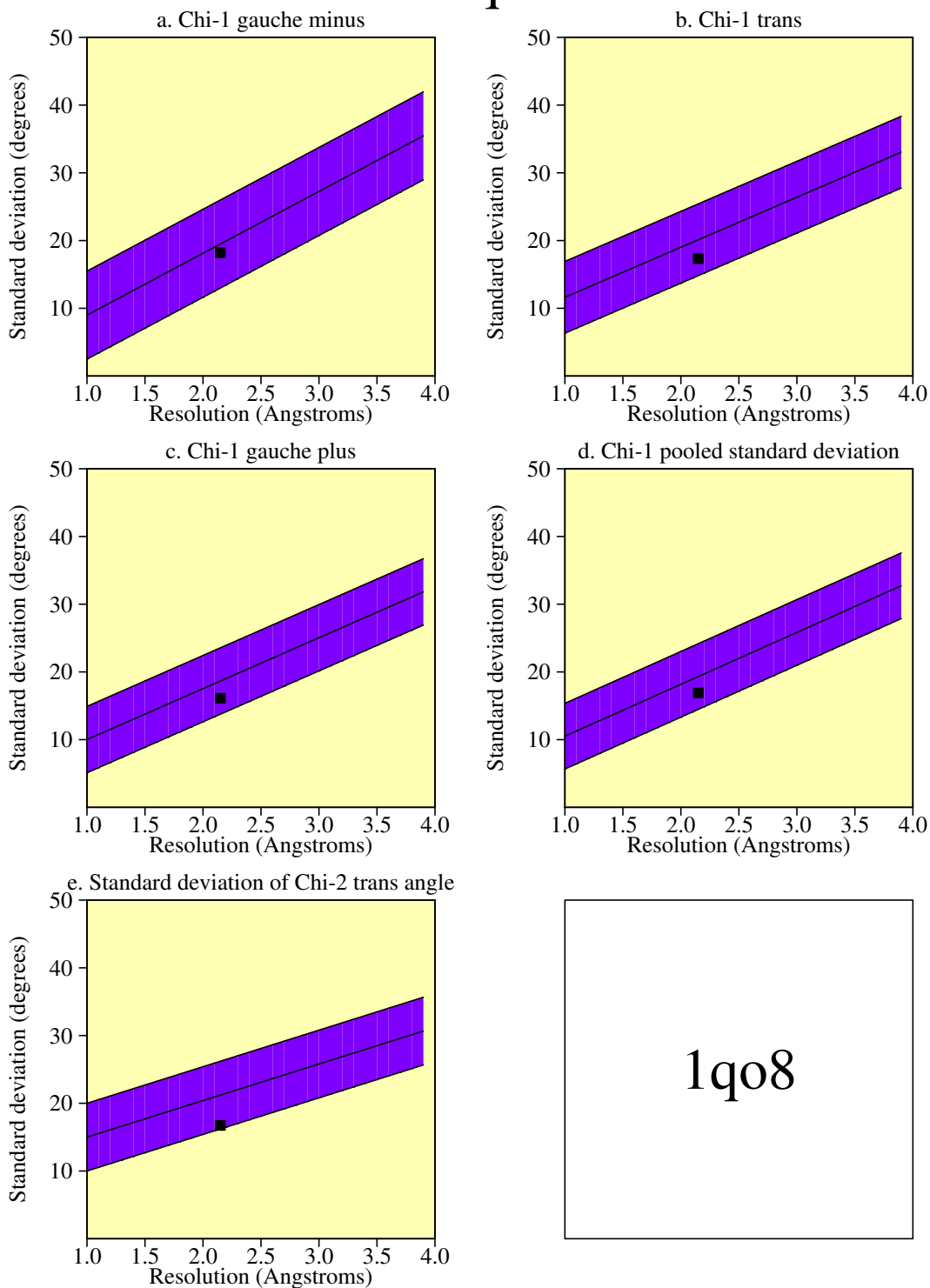


Plot statistics

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	970	85.5	81.9	10.0	0.4	Inside
b. Omega angle st dev	1126	9.6	6.0	3.0	1.2	WORSE
c. Bad contacts / 100 residues	52	4.6	5.8	10.0	-0.1	Inside
d. Zeta angle st dev	1008	2.6	3.1	1.6	-0.3	Inside
e. H-bond energy st dev	690	0.8	0.8	0.2	-0.3	Inside
f. Overall G-factor	1128	-0.5	-0.5	0.3	0.0	Inside

Side-chain parameters

1qo8



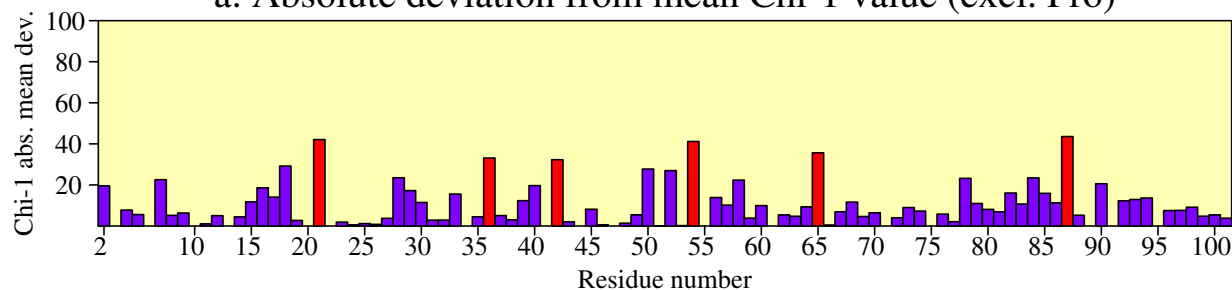
Plot statistics

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	157	18.2	19.5	6.5	-0.2	Inside
b. Chi-1 trans st dev	265	17.3	20.1	5.3	-0.5	Inside
c. Chi-1 gauche plus st dev	436	16.1	18.7	4.9	-0.5	Inside
d. Chi-1 pooled st dev	858	16.9	19.3	4.8	-0.5	Inside
e. Chi-2 trans st dev	291	16.7	21.2	5.0	-0.9	Inside

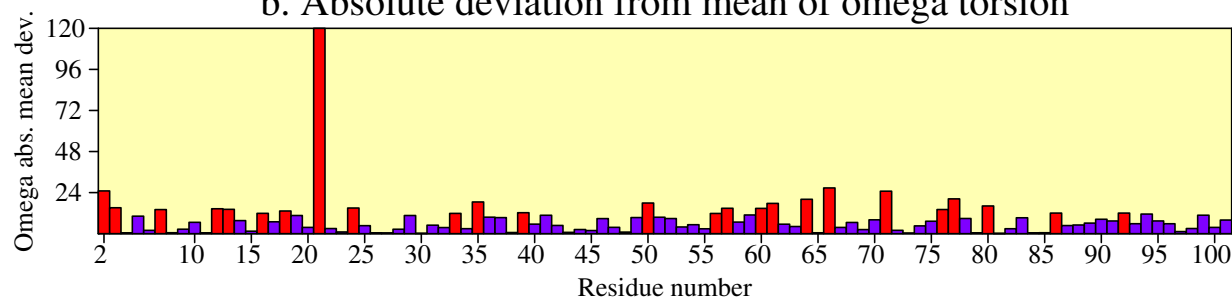
Residue properties

1qo8

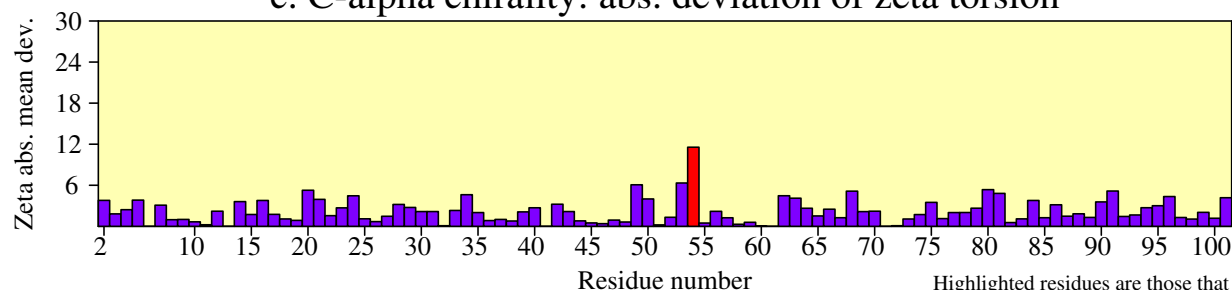
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

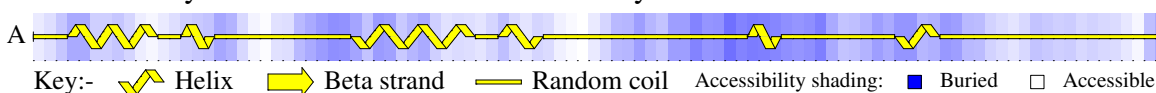


c. C-alpha chirality: abs. deviation of zeta torsion



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

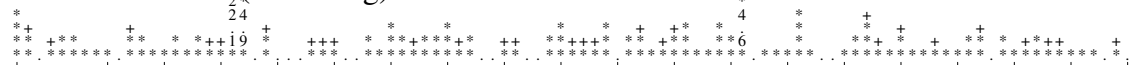
d. Secondary structure & estimated accessibility



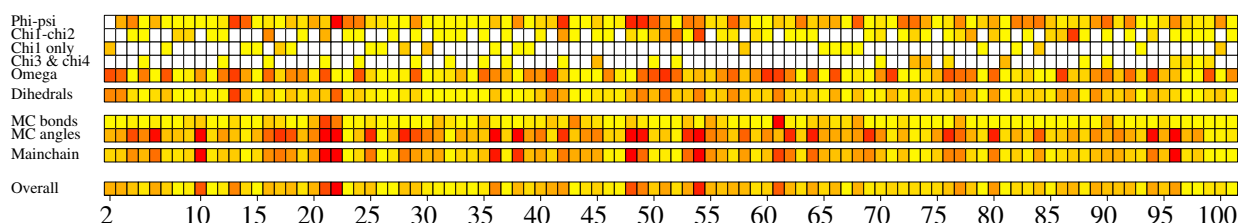
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

TPDMGSFHADMGSCQSCHAKP1KVTDSETHENAQCKSCHGEYAE LANDKLQFDPHNSHLGDI NCTSCHKGHEEPKFYCNECHSFDIKPMPFSDAKKKKSW

f. Max. deviation (see listing)



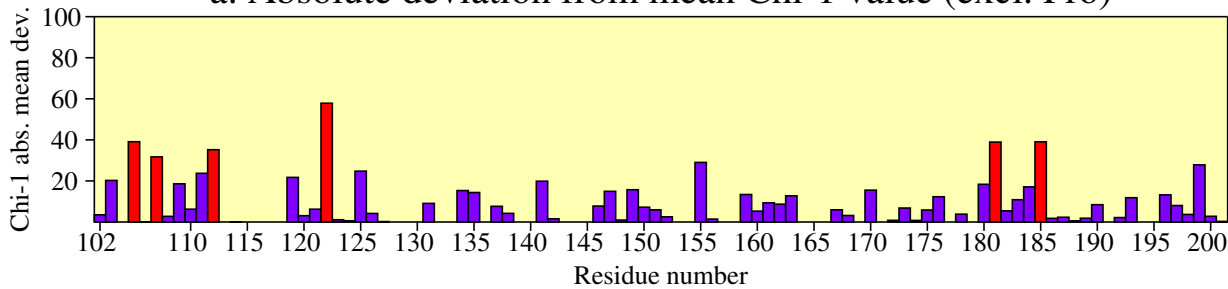
g. G-factors



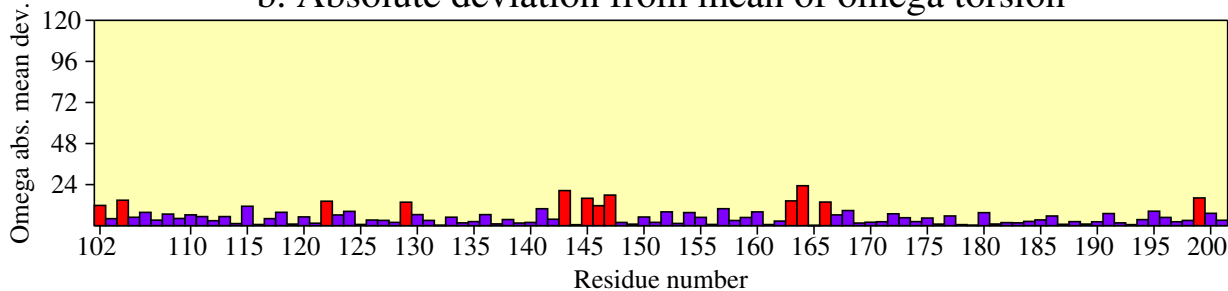
Residue properties

1qo8

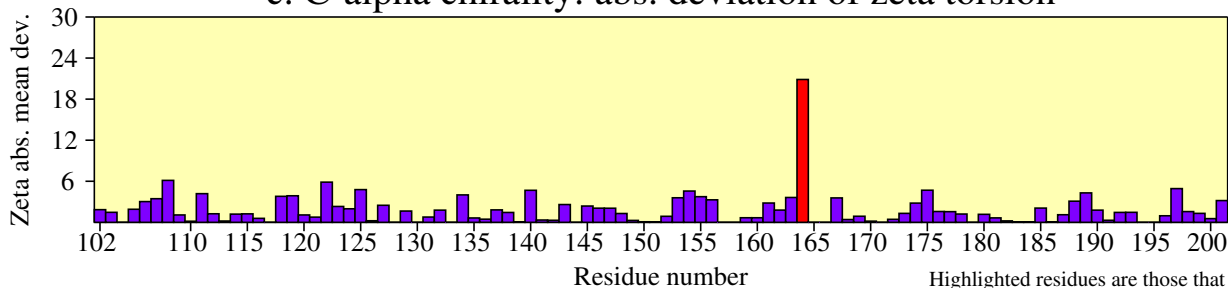
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

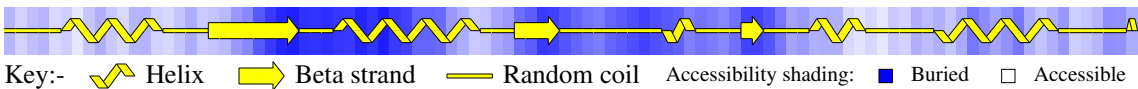


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



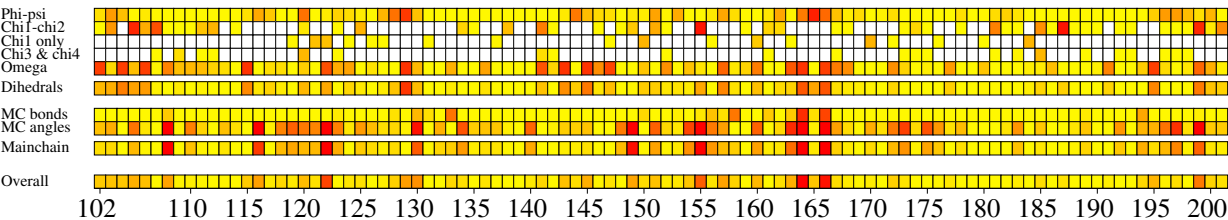
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



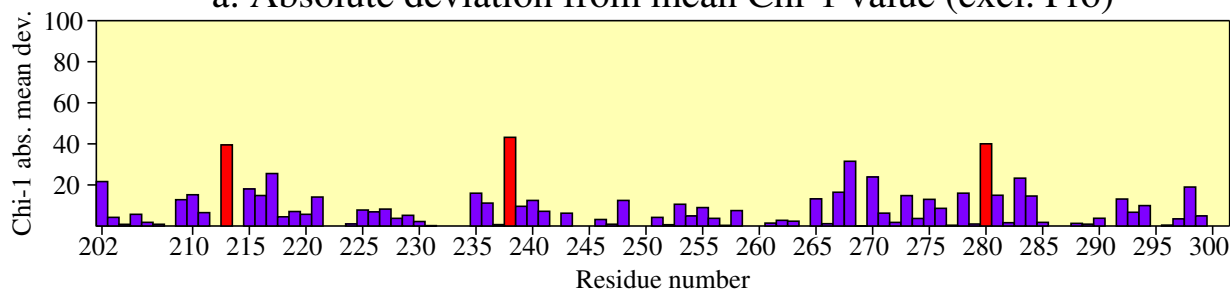
g. G-factors



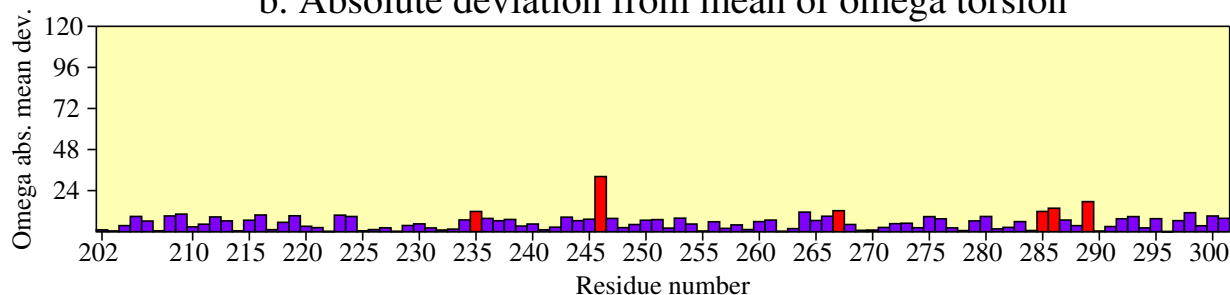
Residue properties

1qo8

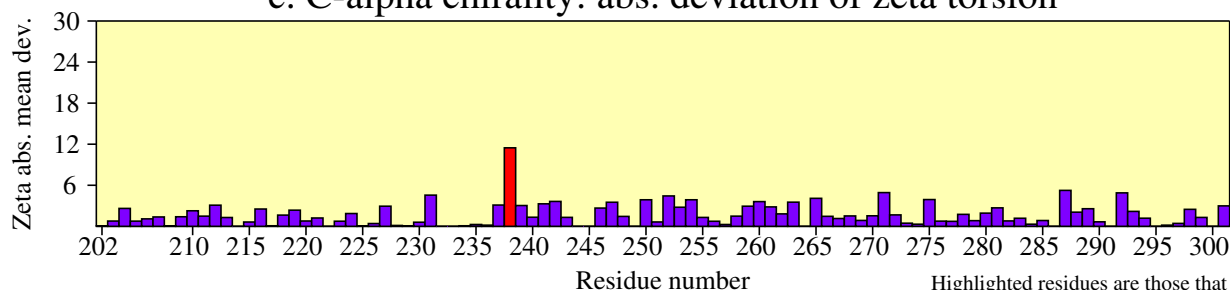
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

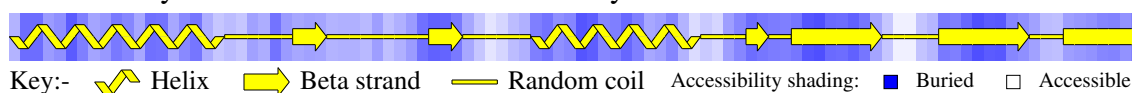


c. C-alpha chirality: abs. deviation of zeta torsion

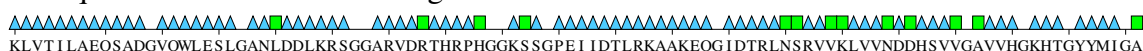


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

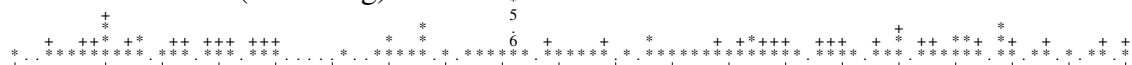
d. Secondary structure & estimated accessibility



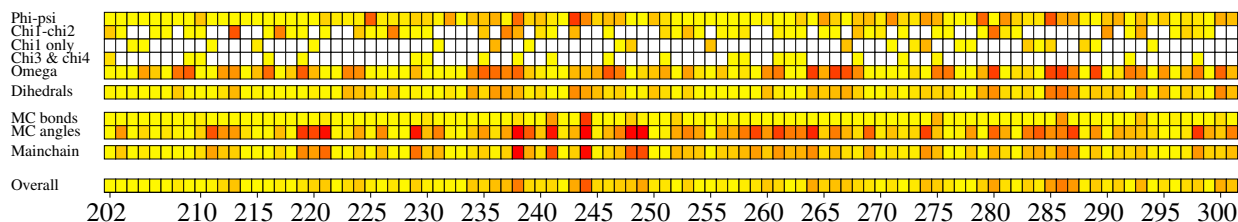
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



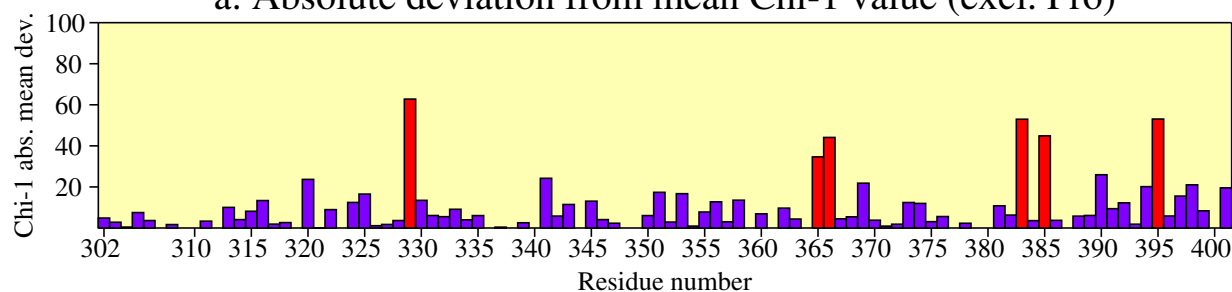
g. G-factors



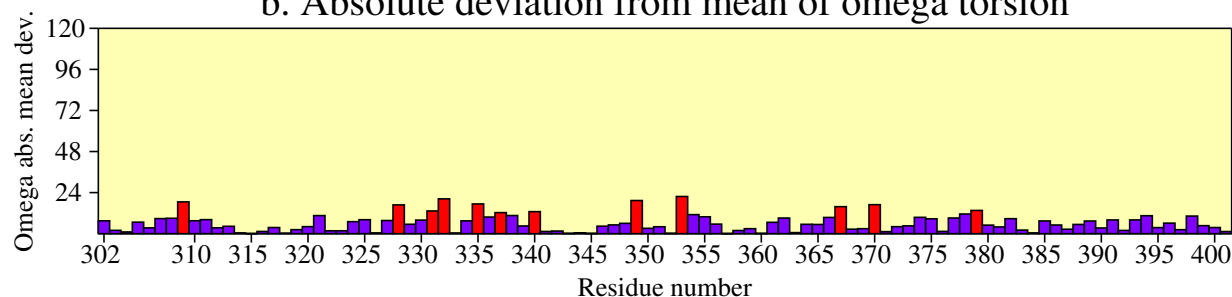
Residue properties

1qo8

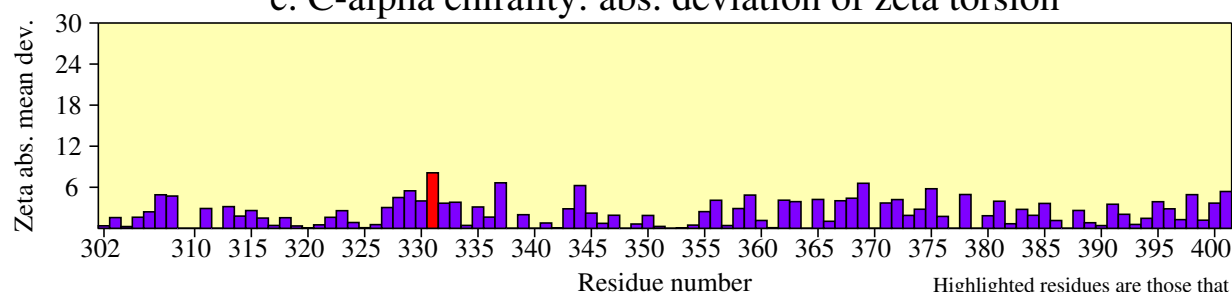
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

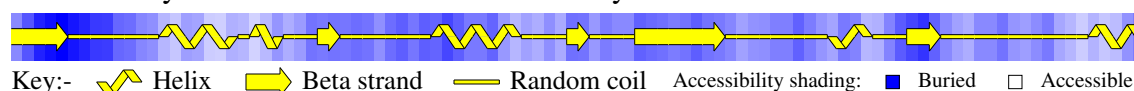


c. C-alpha chirality: abs. deviation of zeta torsion

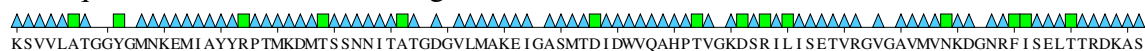


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



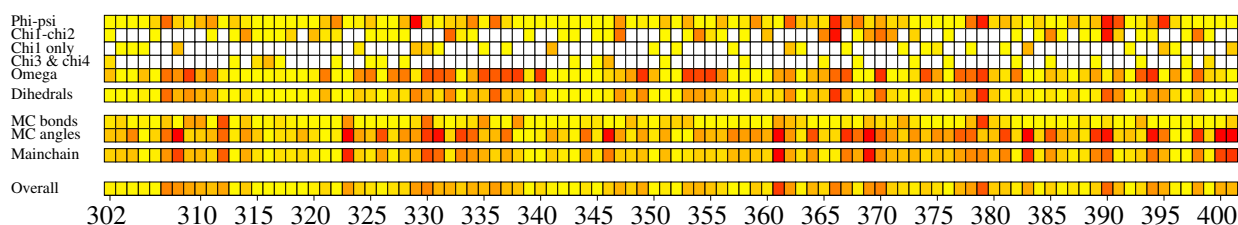
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



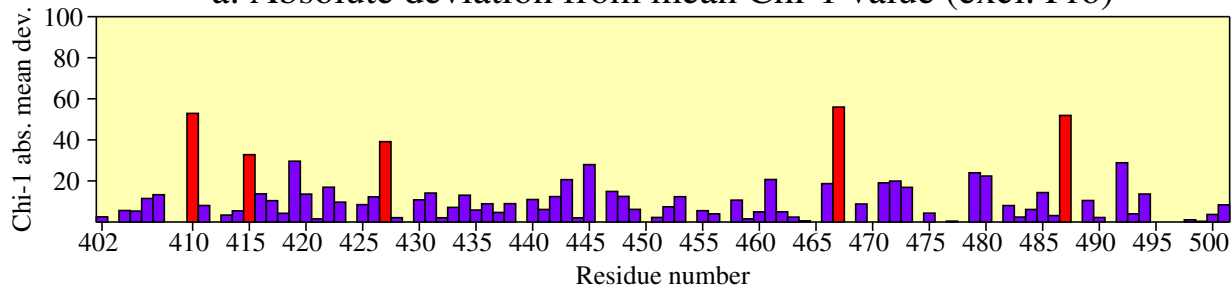
g. G-factors



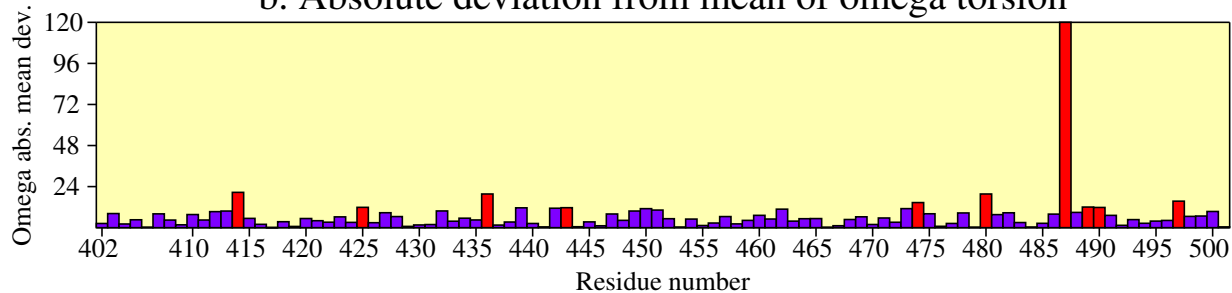
Residue properties

1qo8

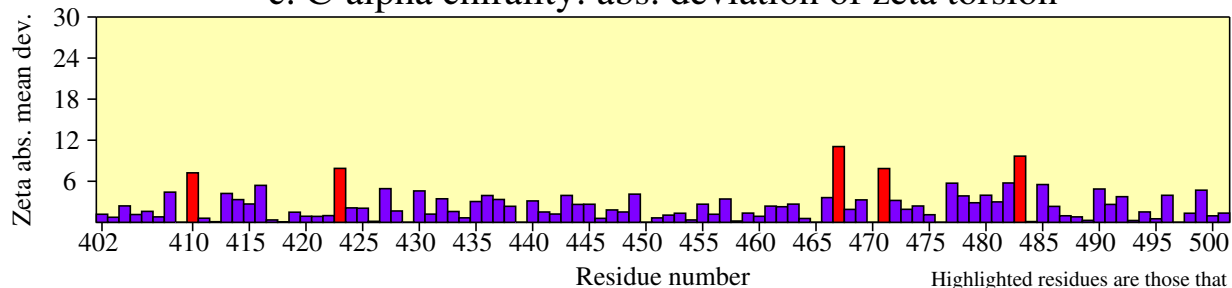
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

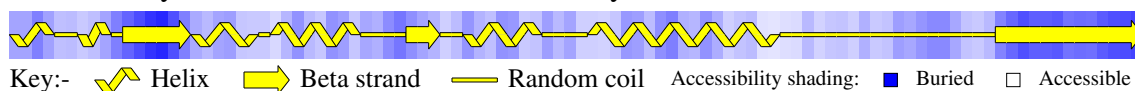


c. C-alpha chirality: abs. deviation of zeta torsion



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

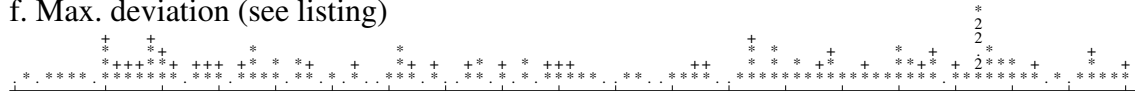
d. Secondary structure & estimated accessibility



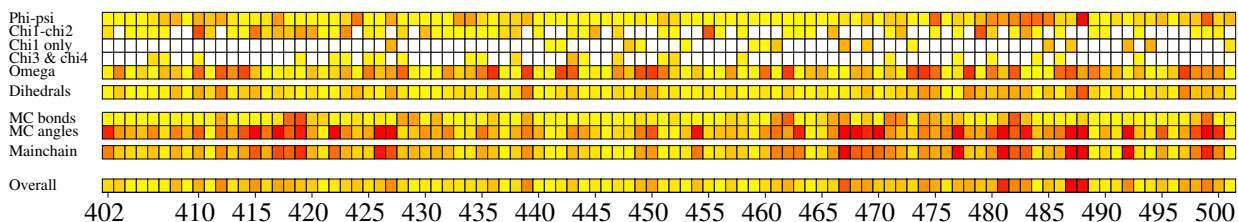
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



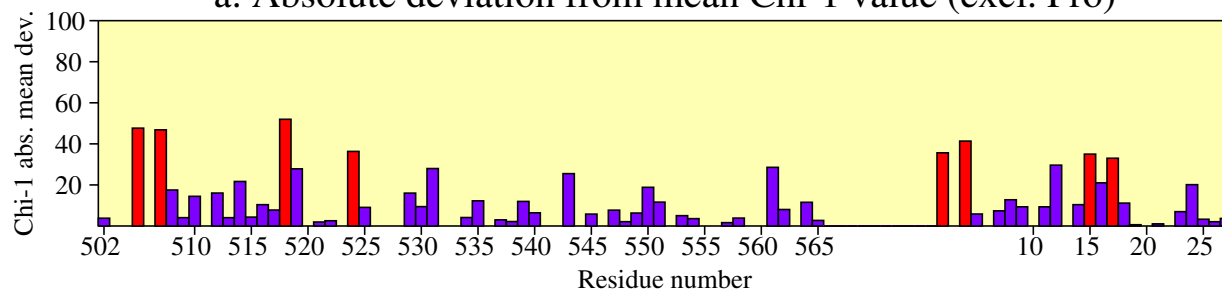
g. G-factors



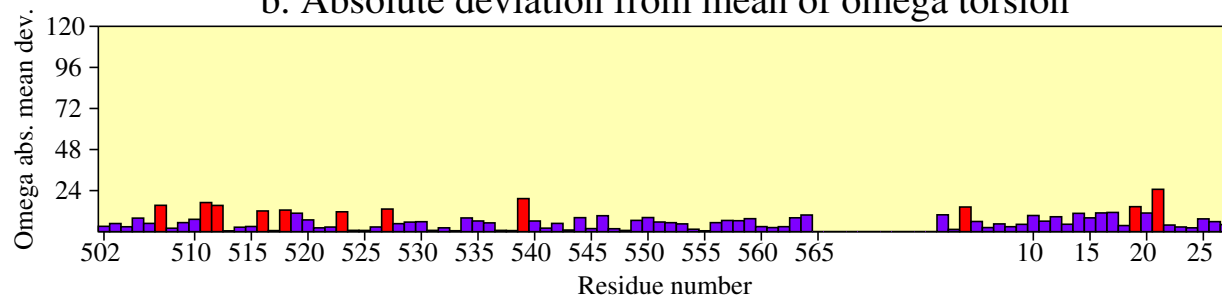
Residue properties

1qo8

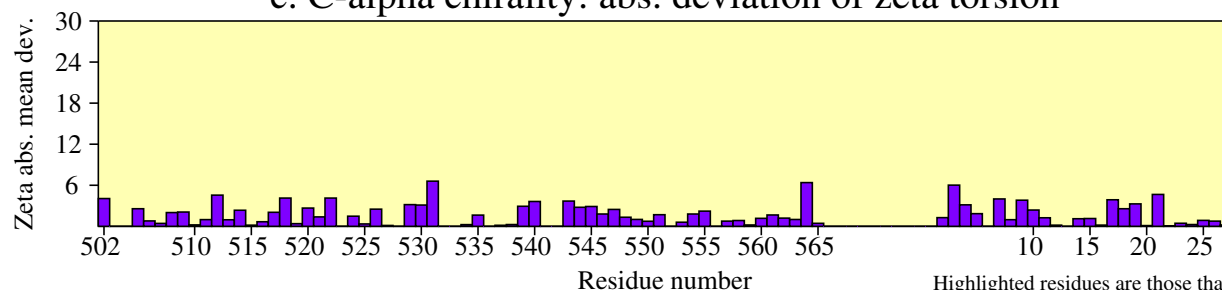
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

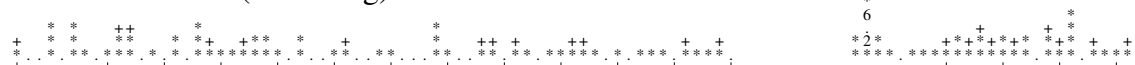
d. Secondary structure & estimated accessibility



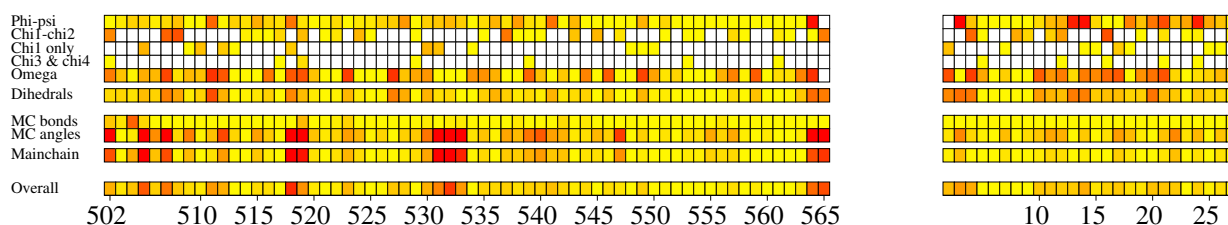
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



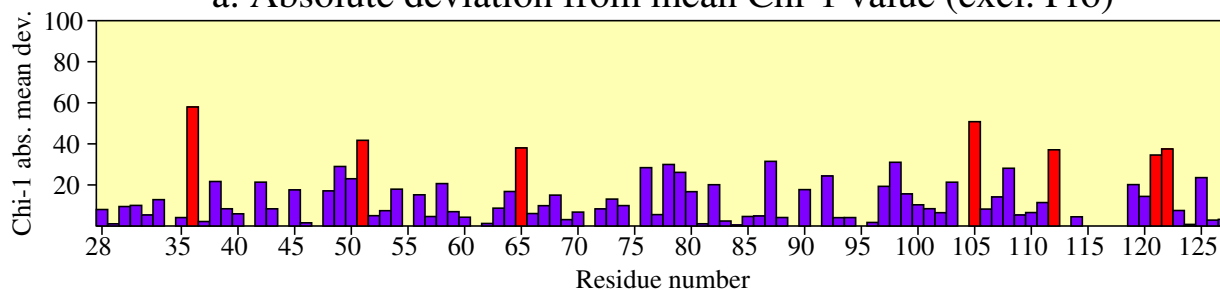
g. G-factors



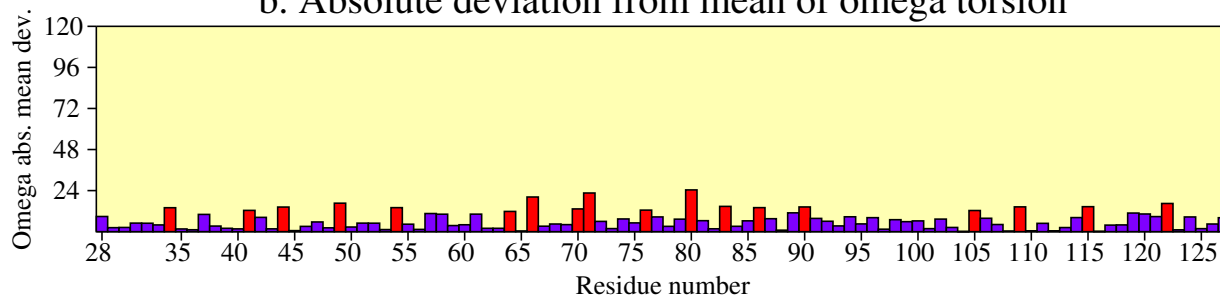
Residue properties

1qo8

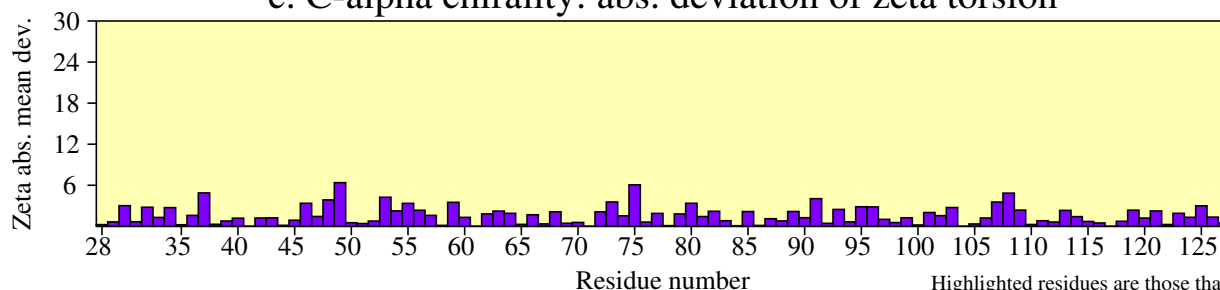
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

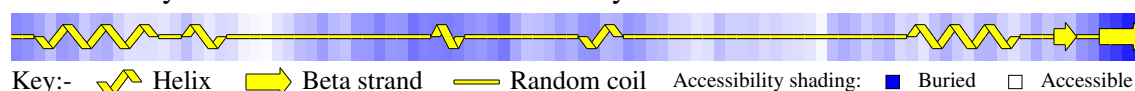


c. C-alpha chirality: abs. deviation of zeta torsion

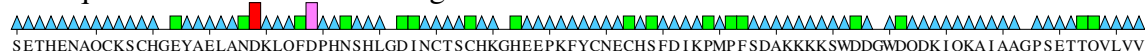


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

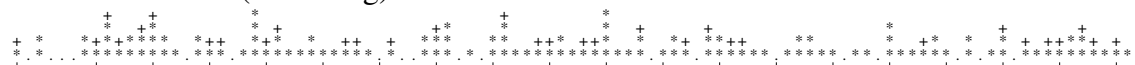
d. Secondary structure & estimated accessibility



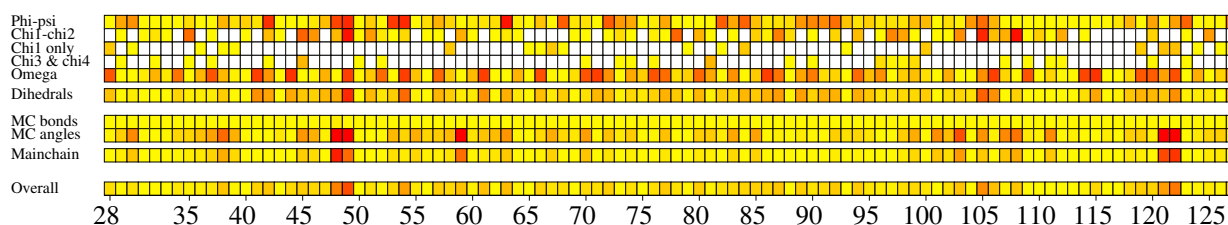
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



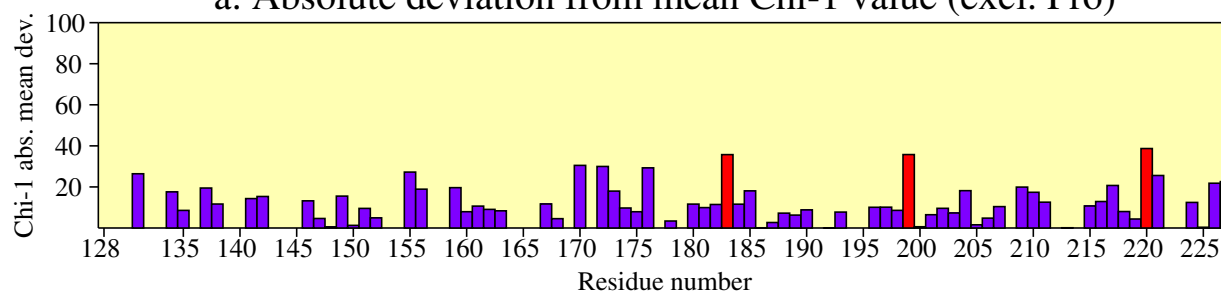
g. G-factors



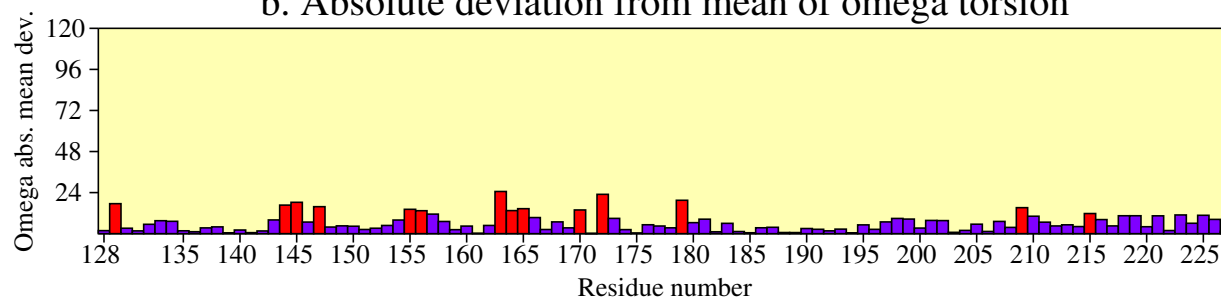
Residue properties

1qo8

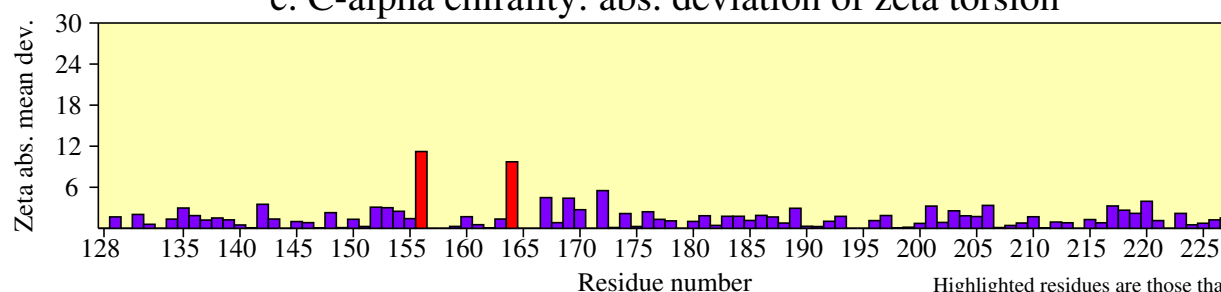
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

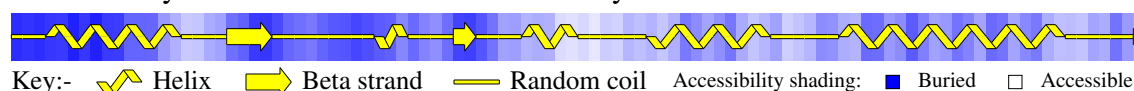


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



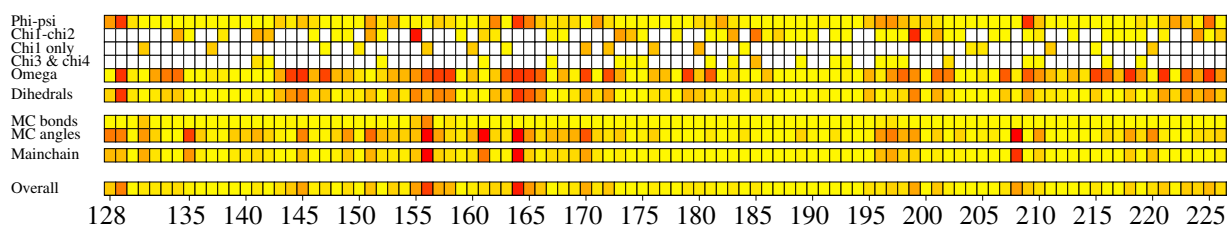
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



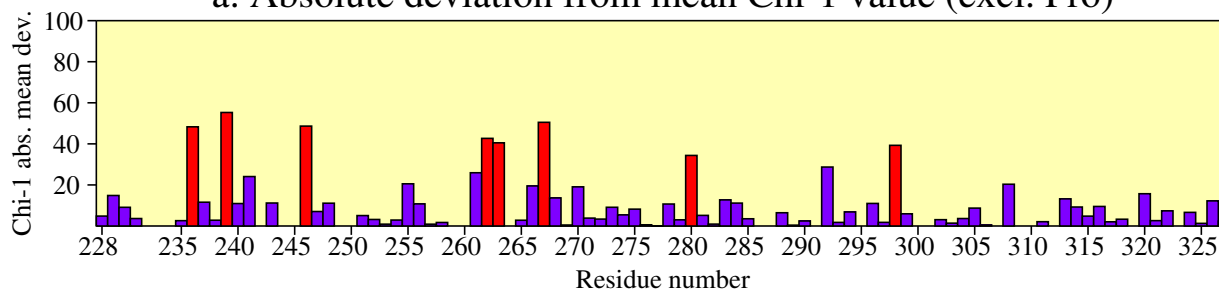
g. G-factors



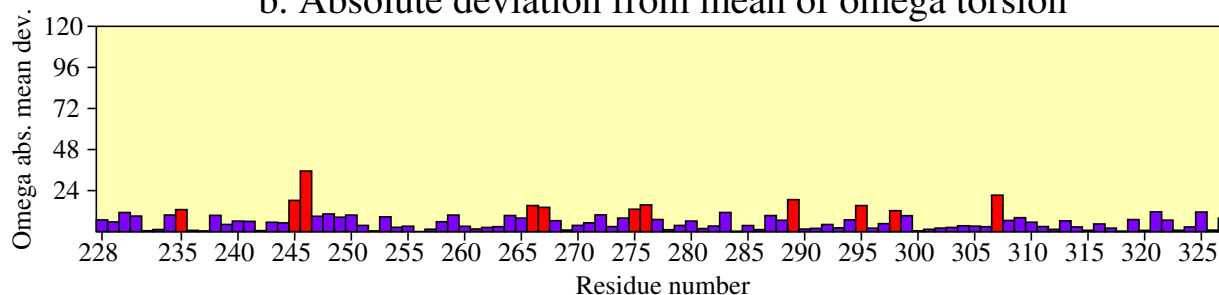
Residue properties

1qo8

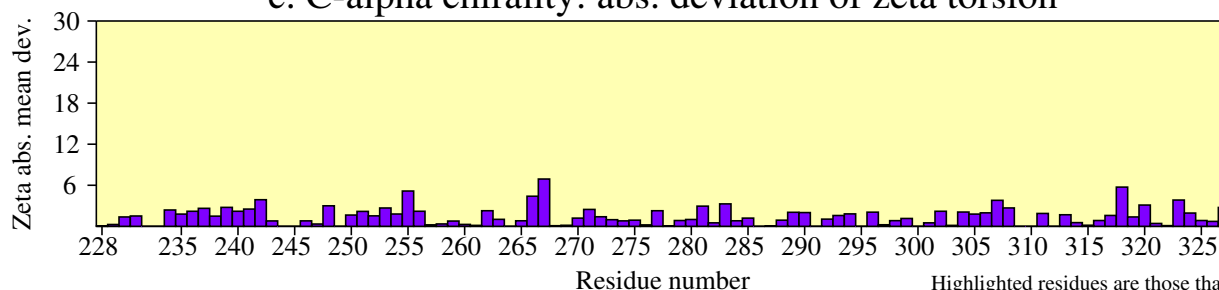
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

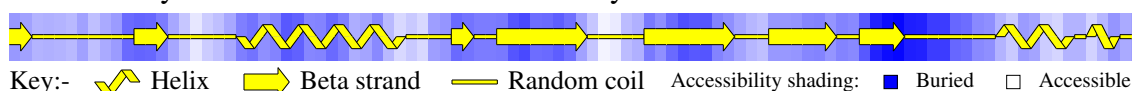


c. C-alpha chirality: abs. deviation of zeta torsion



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

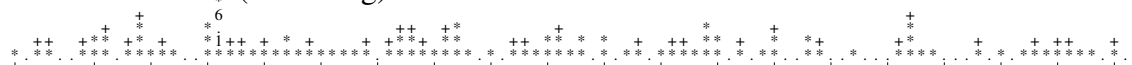
d. Secondary structure & estimated accessibility



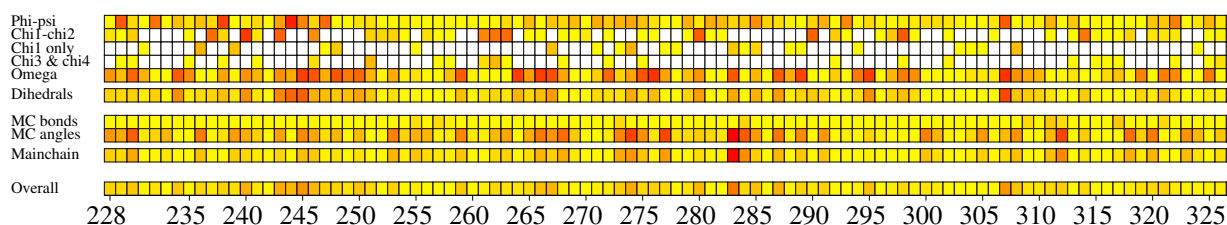
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



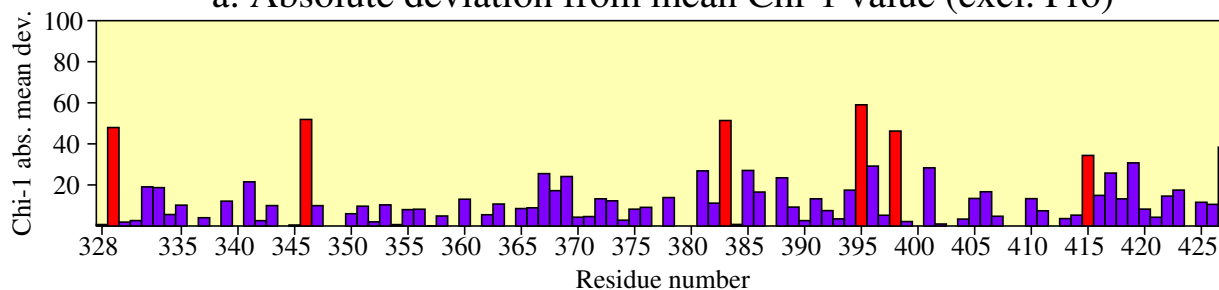
g. G-factors



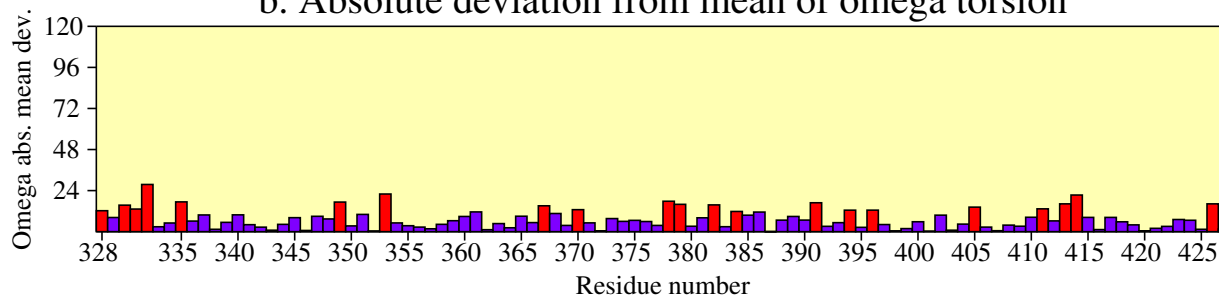
Residue properties

1qo8

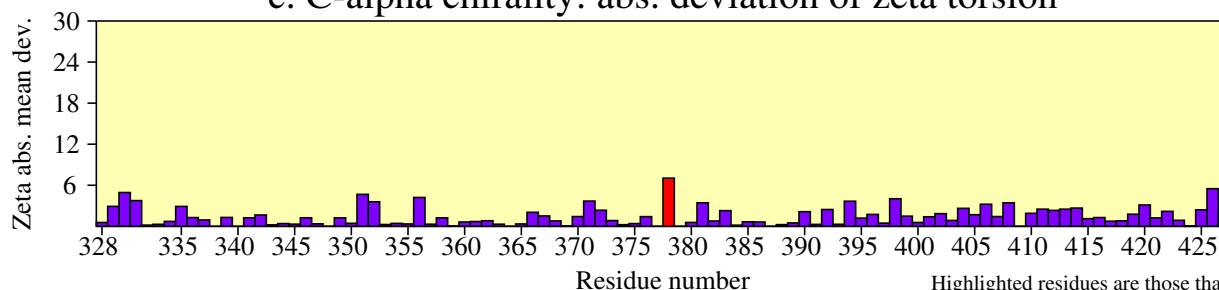
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

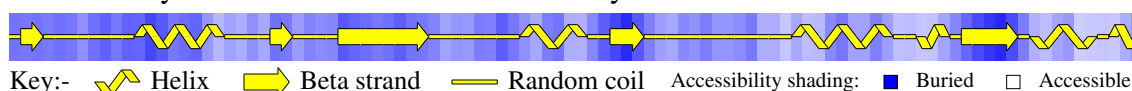


c. C-alpha chirality: abs. deviation of zeta torsion



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

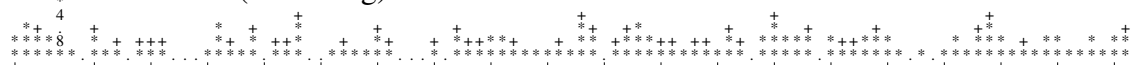
d. Secondary structure & estimated accessibility



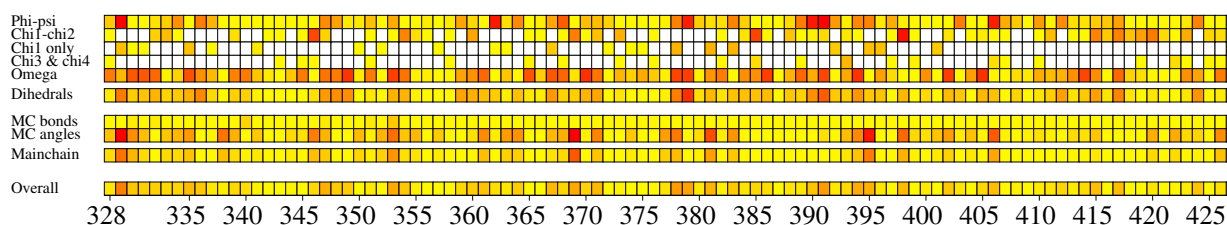
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



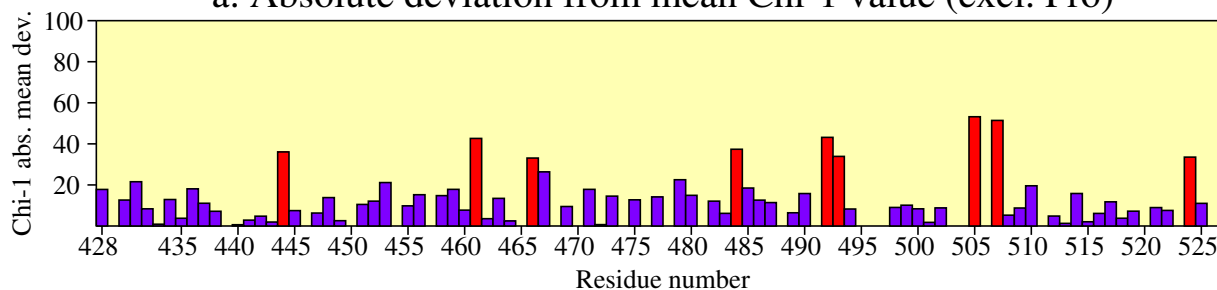
g. G-factors



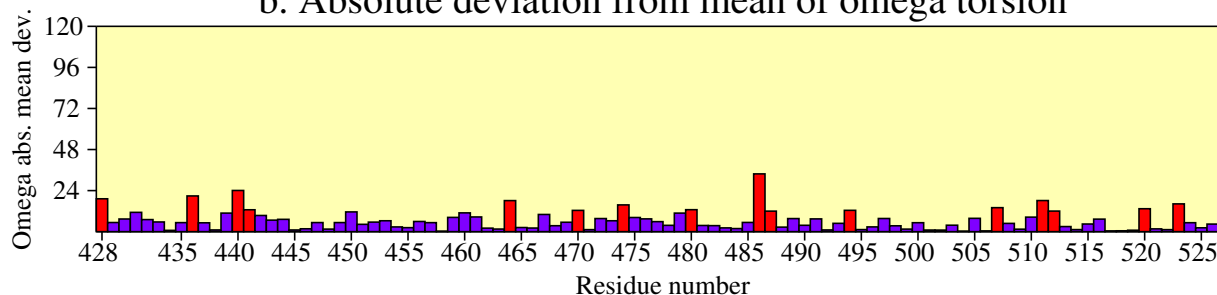
Residue properties

1qo8

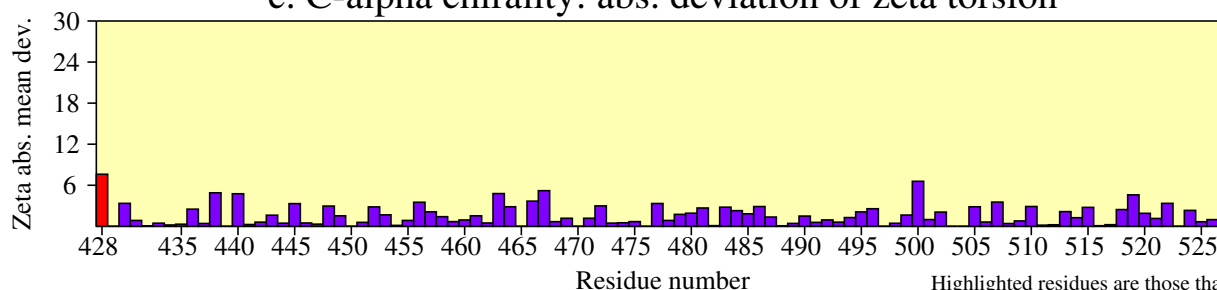
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

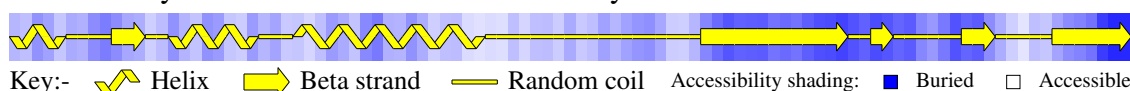


c. C-alpha chirality: abs. deviation of zeta torsion



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

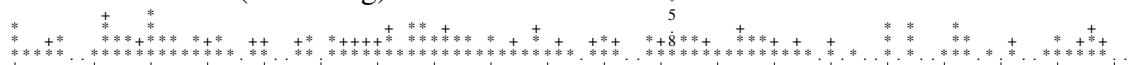
d. Secondary structure & estimated accessibility



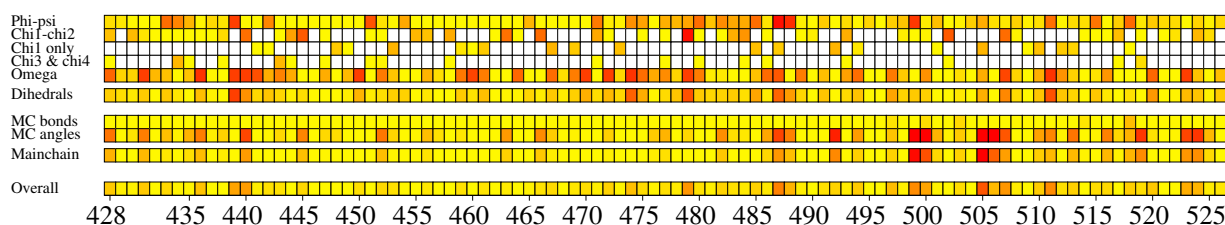
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



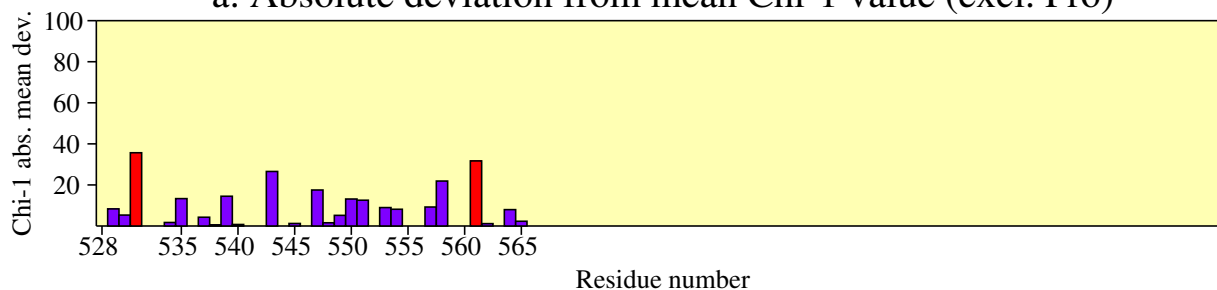
g. G-factors



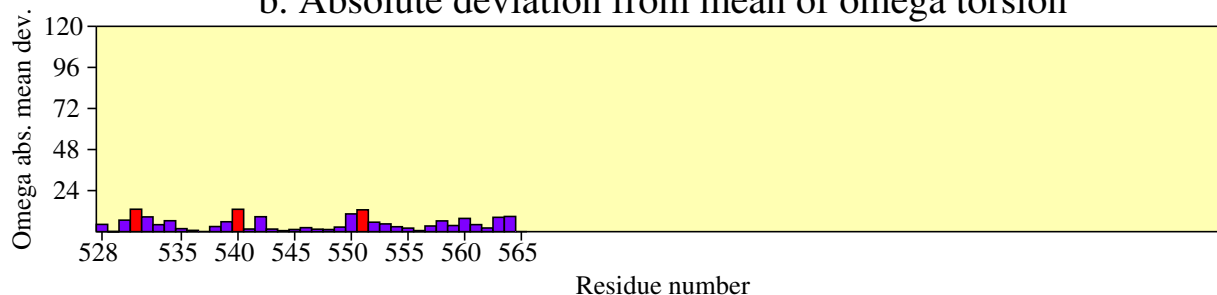
Residue properties

1qo8

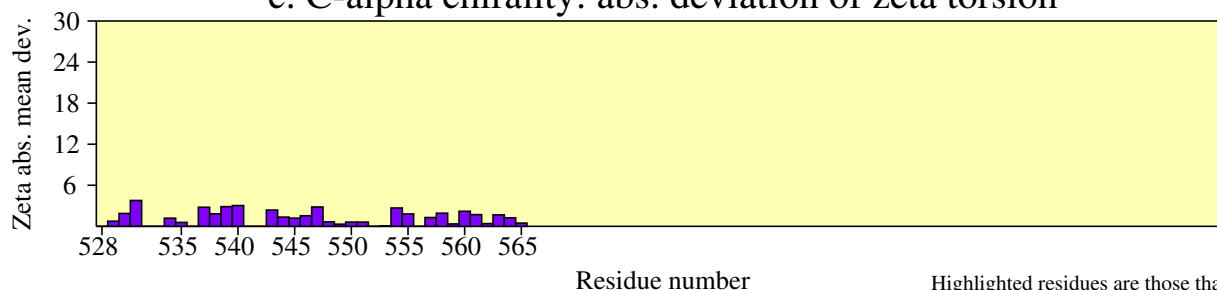
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

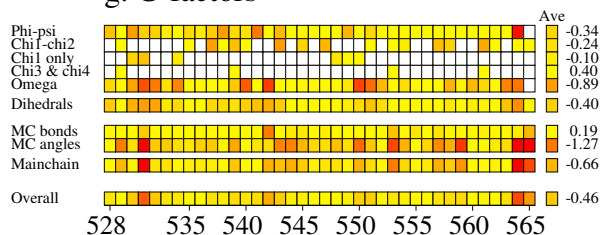
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

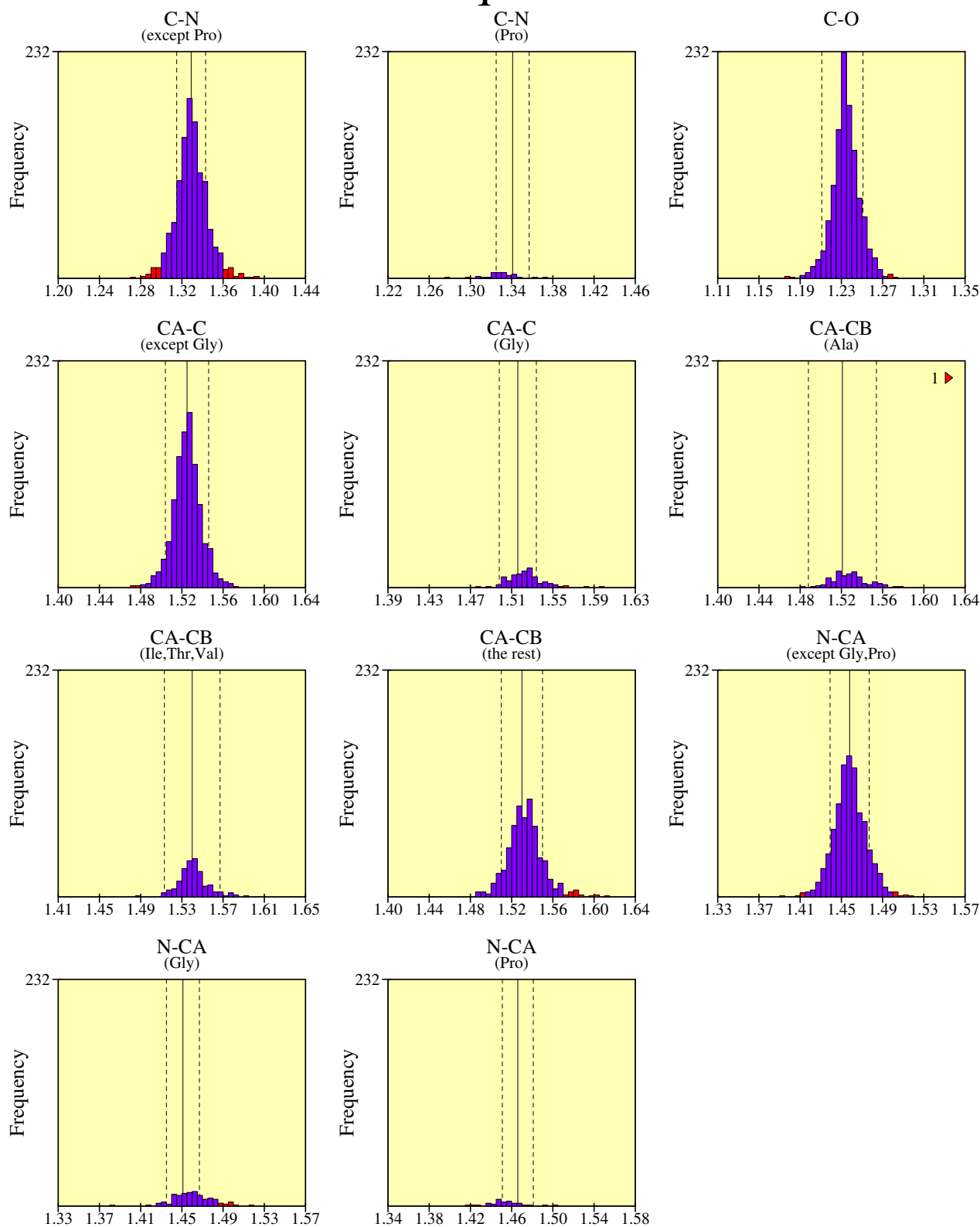


g. G-factors



Main-chain bond lengths

1qo8



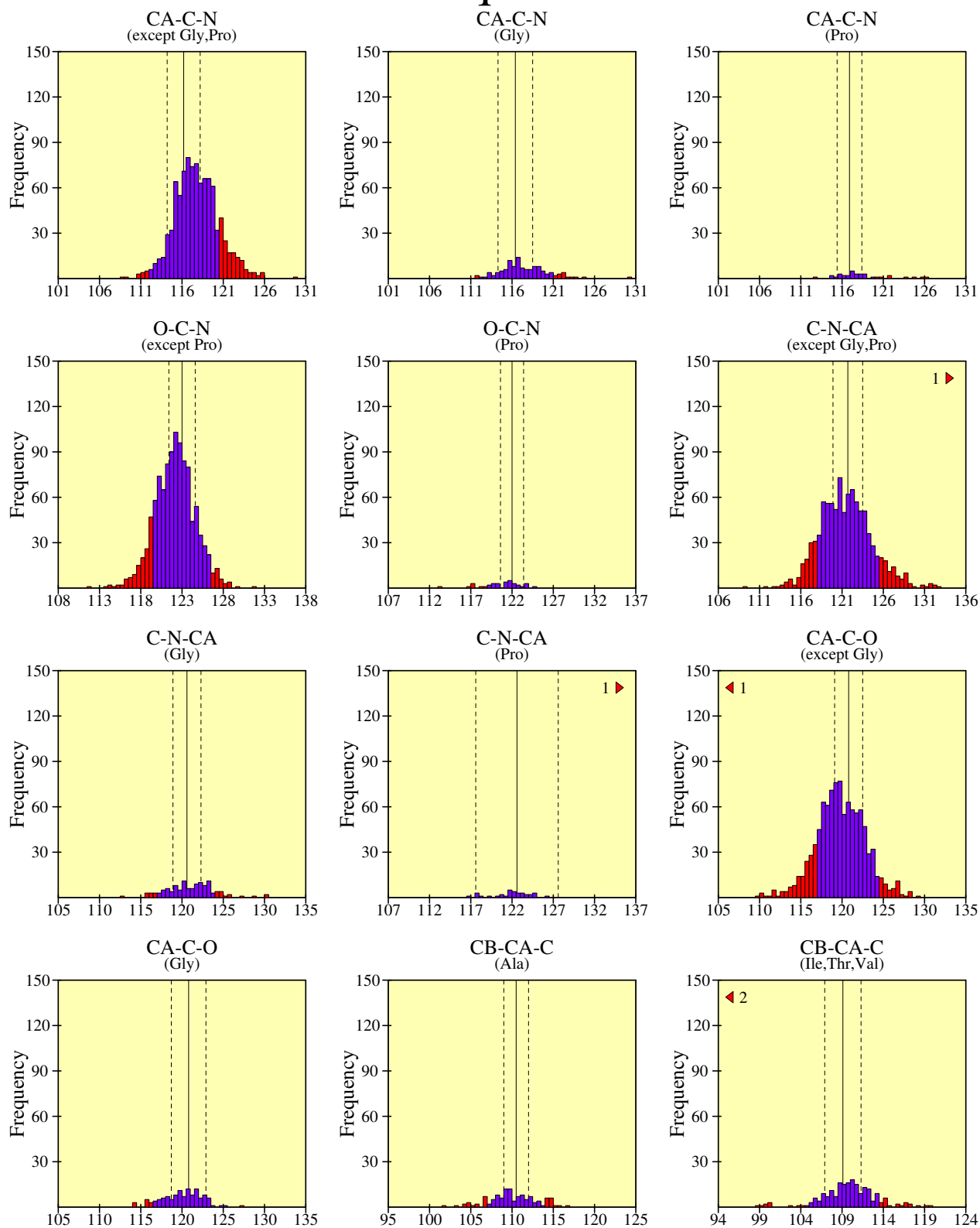
Black bars > 2.0 st. devs. from mean.

◀ 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

1qo8



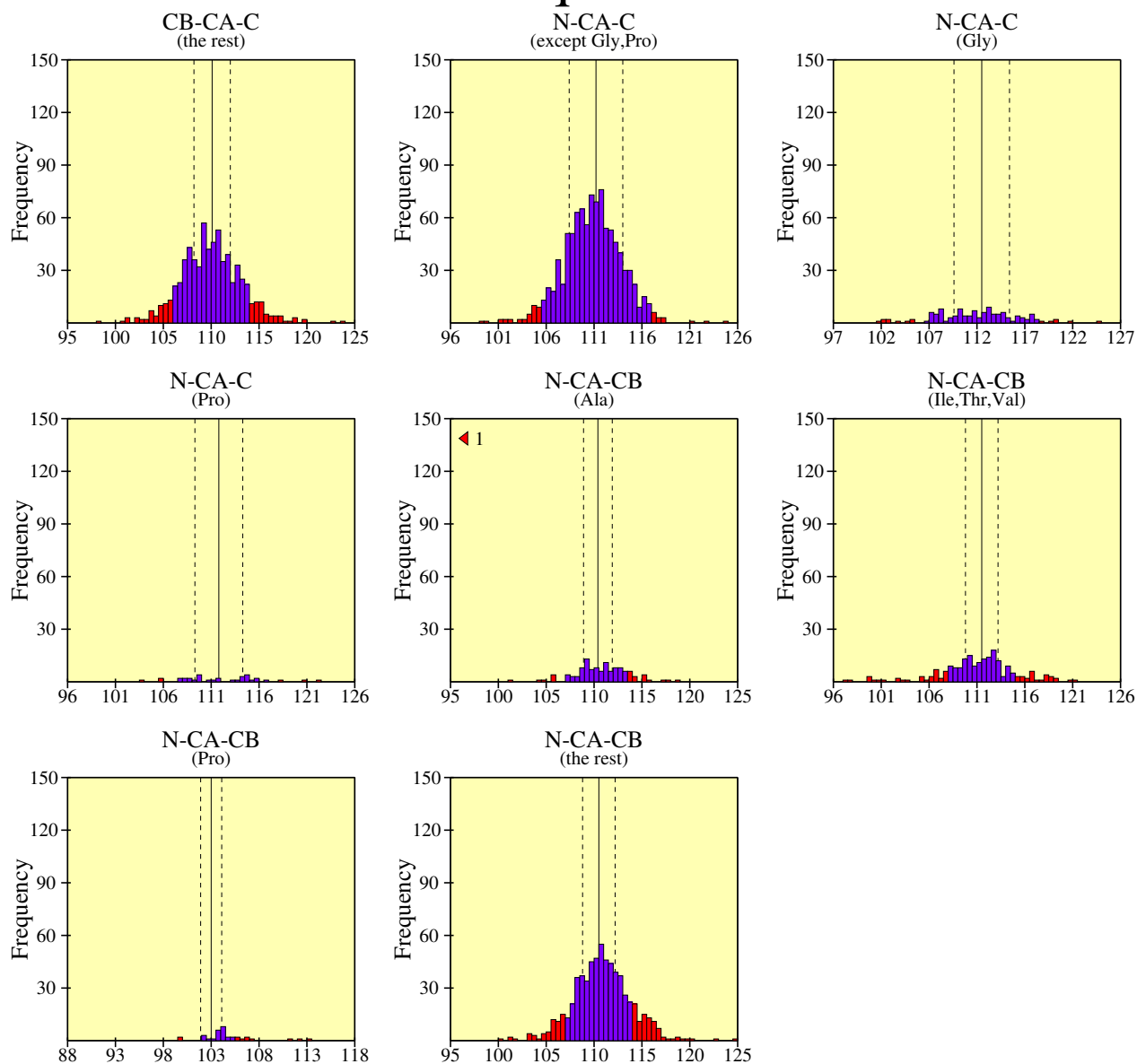
Black bars > 2.0 st. devs. from mean.

◀ 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

1qo8



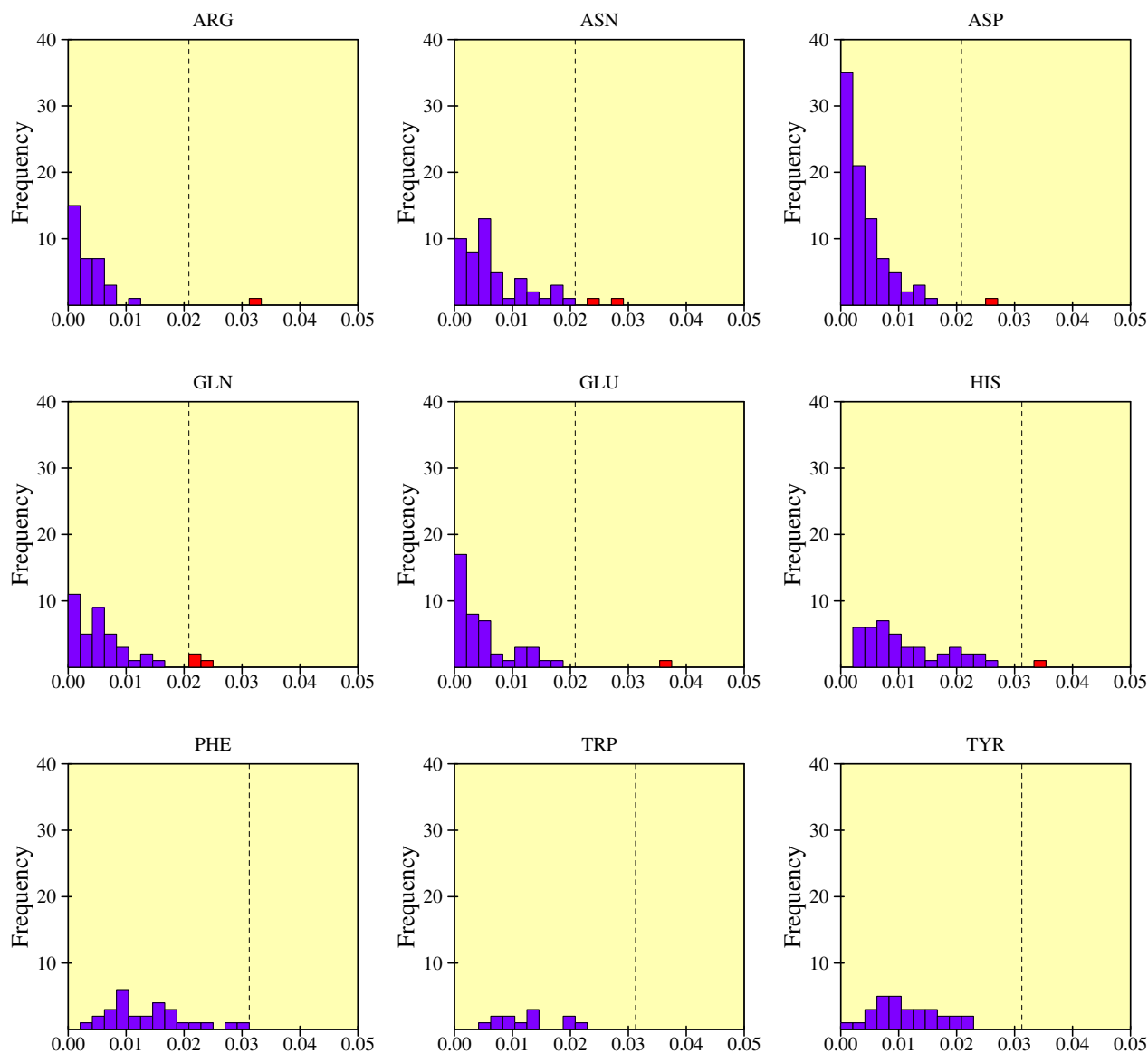
Black bars > 2.0 st. devs. from mean.

◄ 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

1qo8

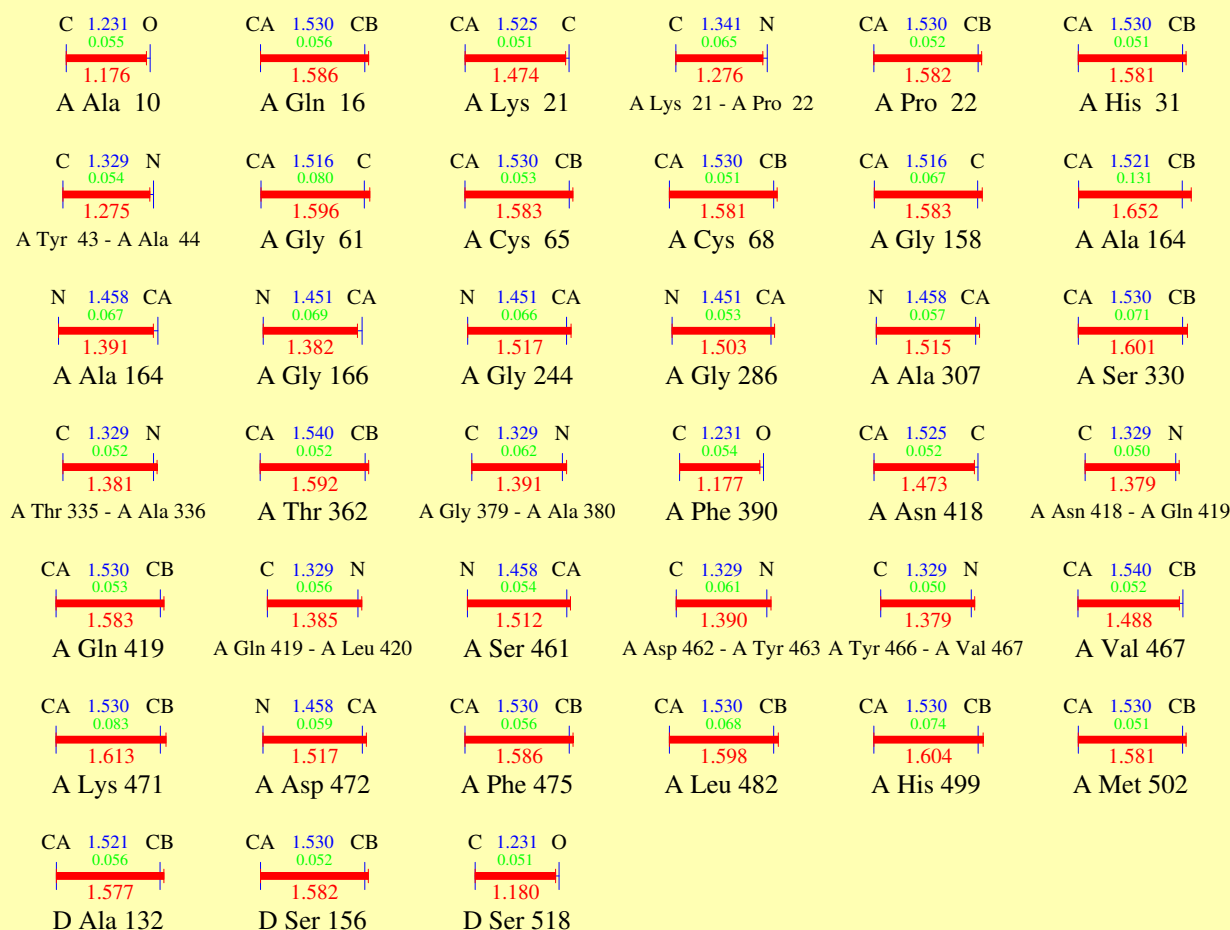


Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

Distorted geometry

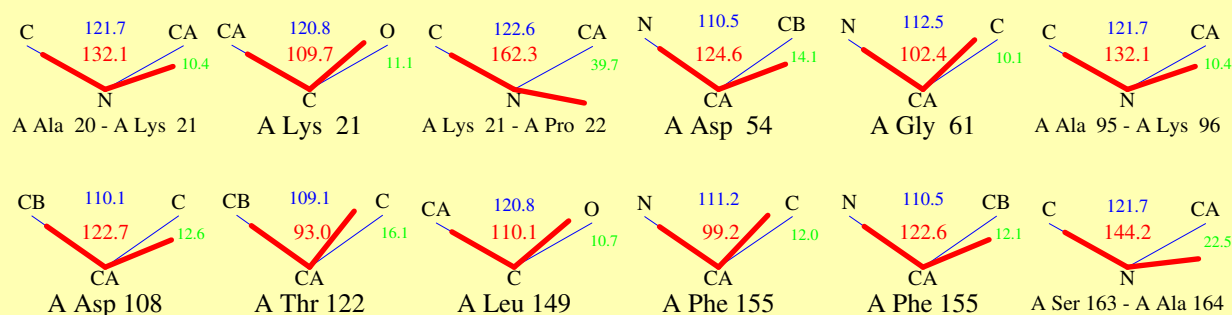
1qo8

Main-chain bond lengths



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

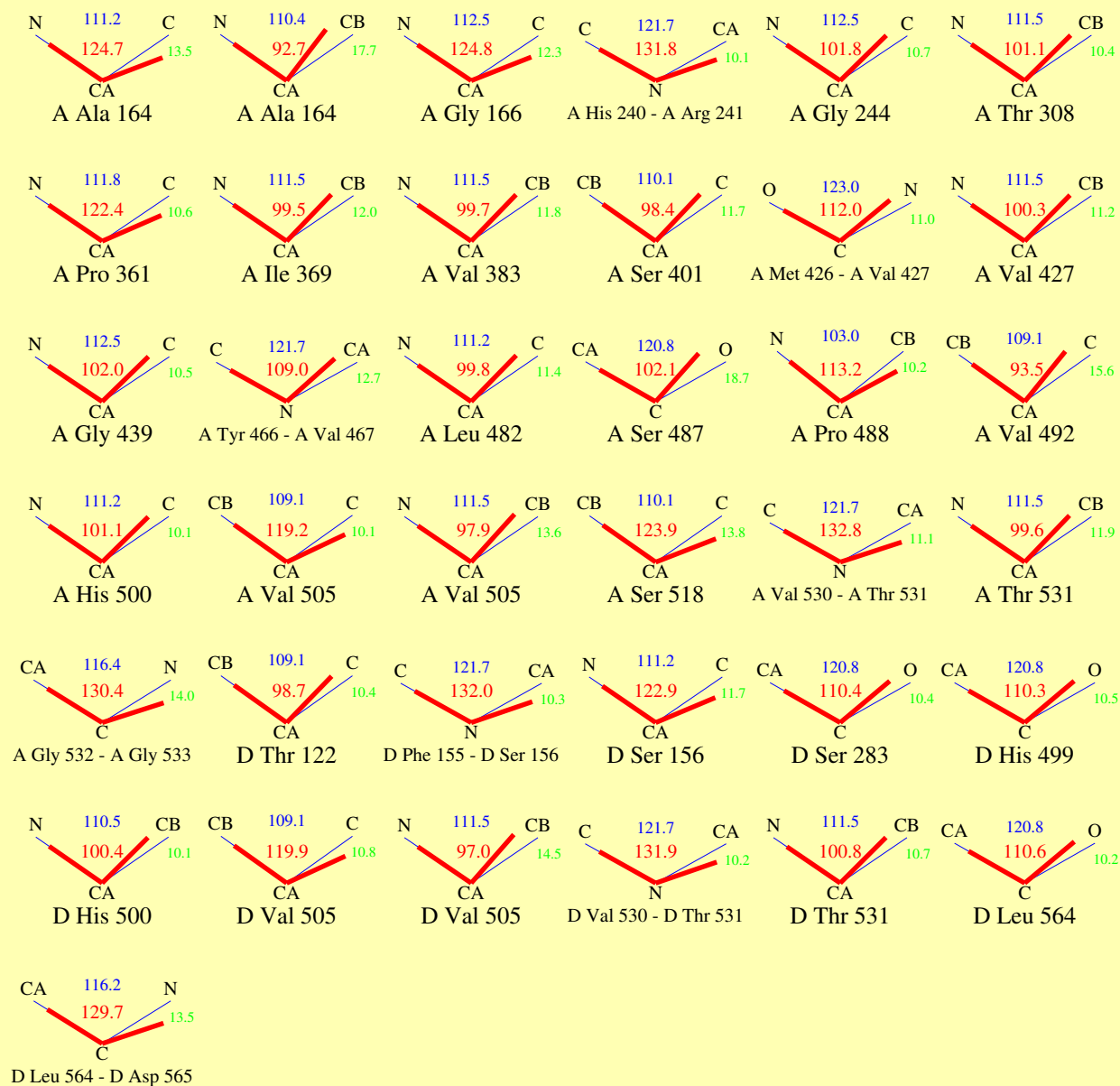
Main-chain bond angles



Distorted geometry

1qo8

Main-chain bond angles (contd)

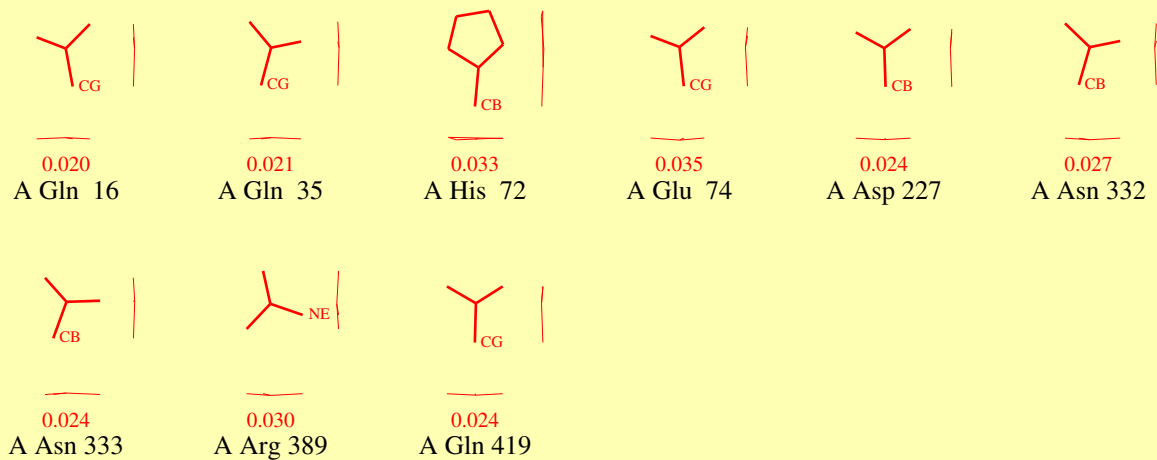


Bond angles differing by > 10.0 degrees from small-molec values. Values shown: "ideal", actual, diff.

Distorted geometry

1qo8

Planar groups



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