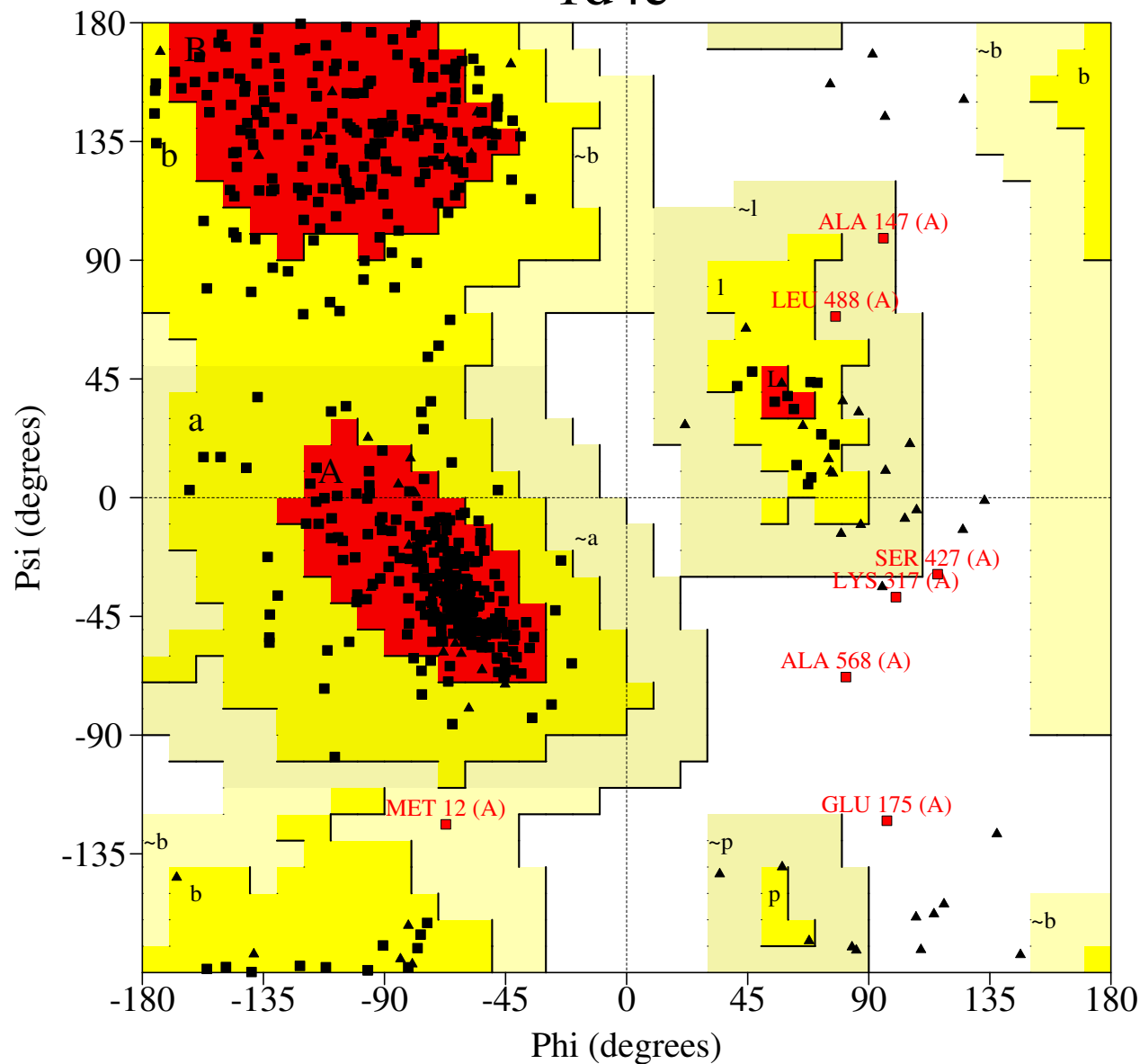


Ramachandran Plot

1d4e



Plot statistics

Residues in most favoured regions [A,B,L]	377	80.4%
Residues in additional allowed regions [a,b,l,p]	85	18.1%
Residues in generously allowed regions [-a,-b,-l,-p]	3	0.6%
Residues in disallowed regions	4	0.9%

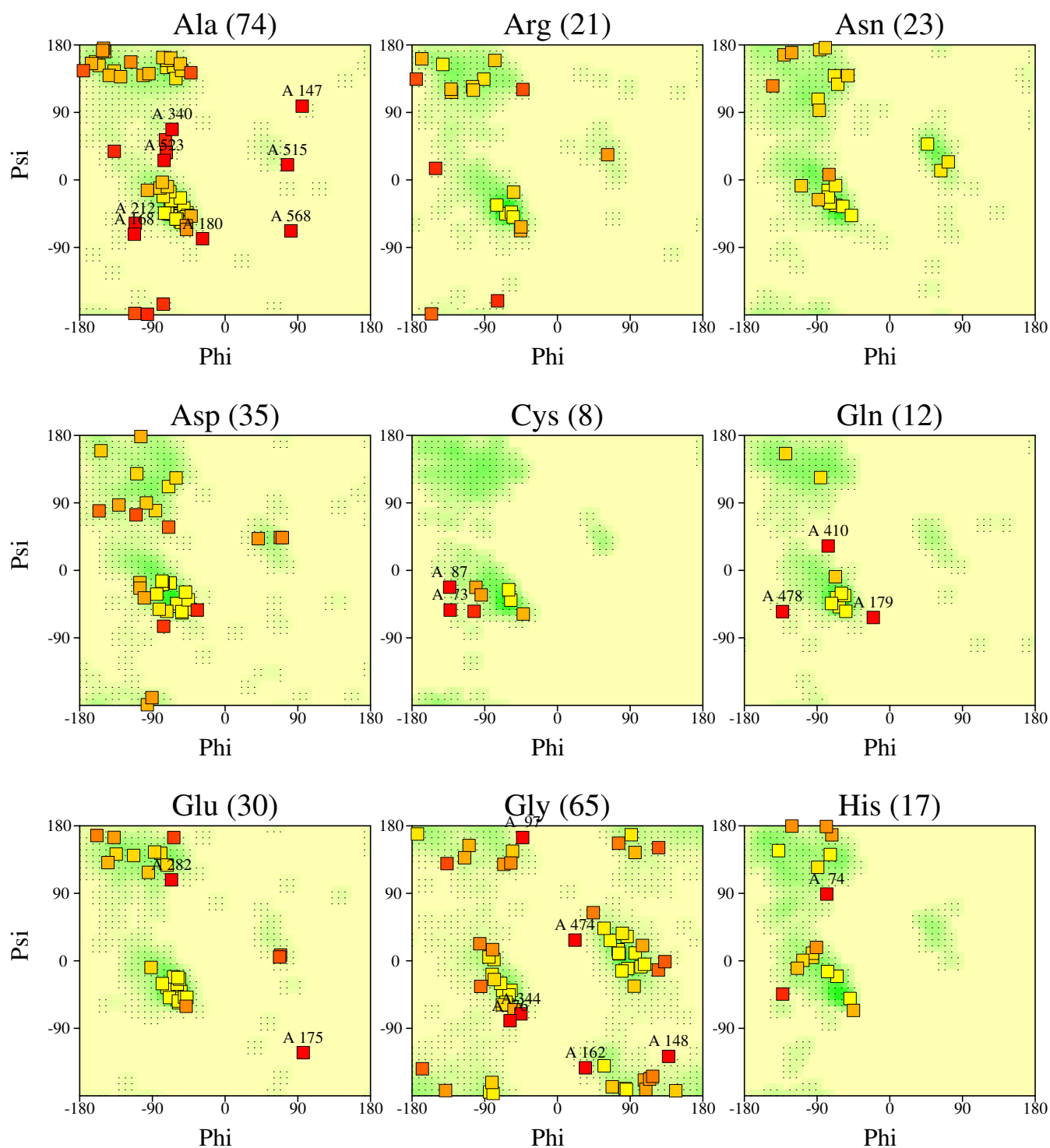
Number of non-glycine and non-proline residues	469	100.0%
Number of end-residues (excl. Gly and Pro)	6	
Number of glycine residues (shown as triangles)	66	
Number of proline residues	19	

Total number of residues	560	

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

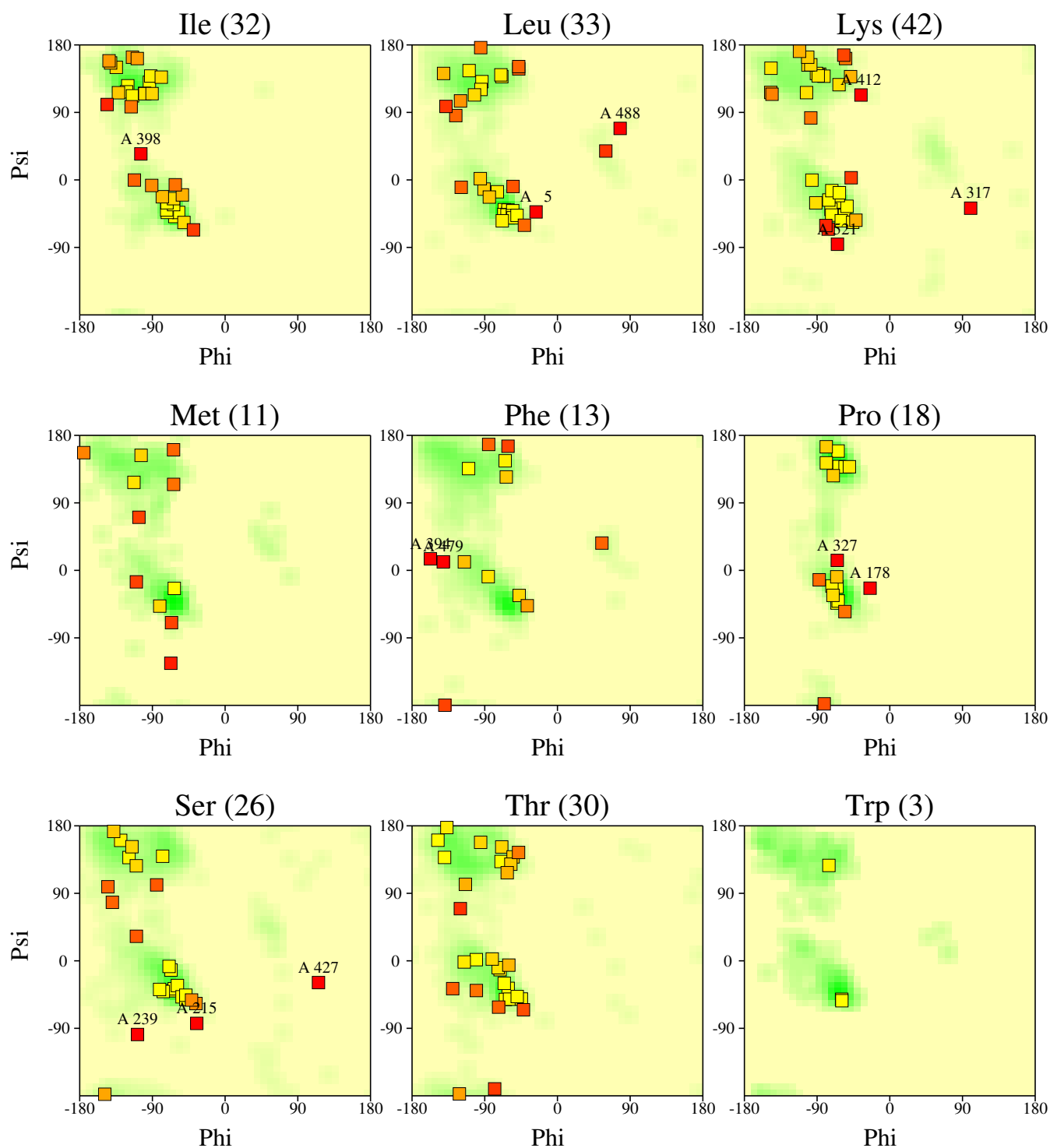
1d4e



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.

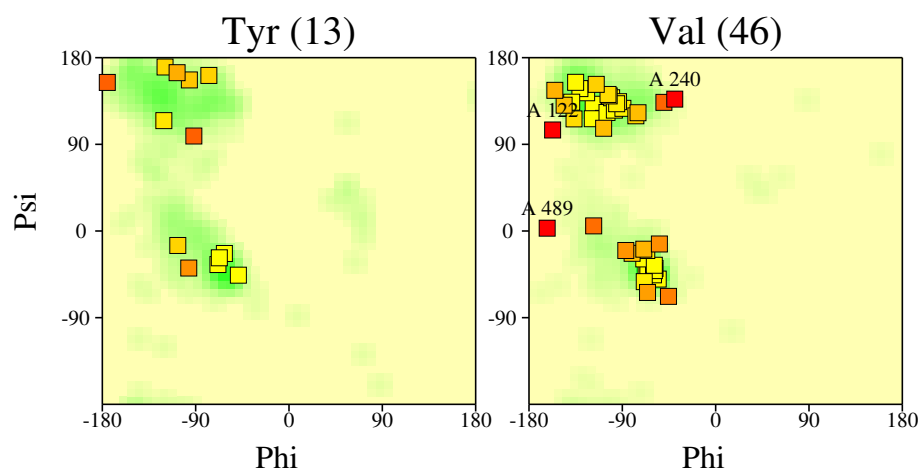
Ramachandran plots for all residue types

1d4e



Ramachandran plots for all residue types

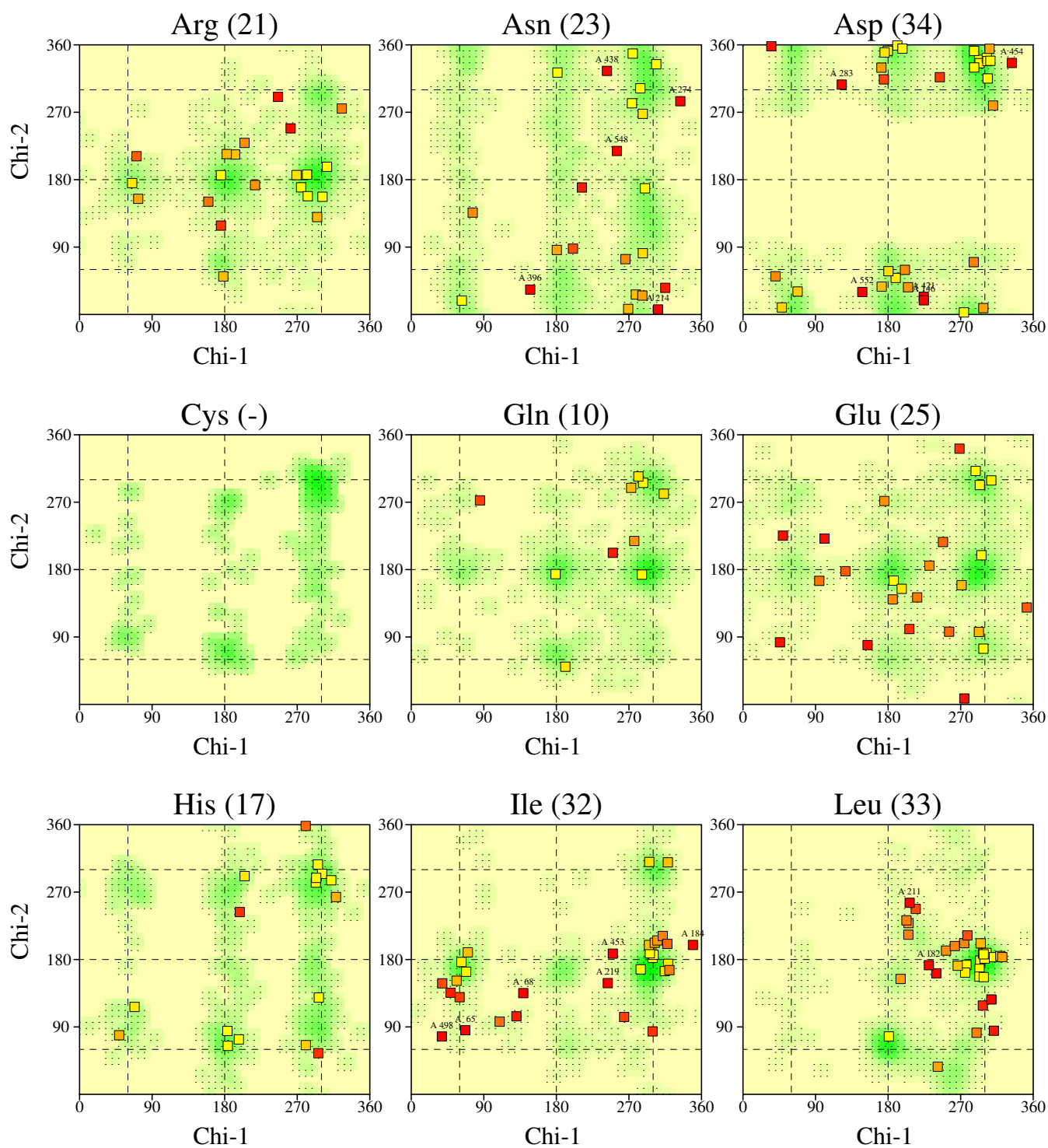
1d4e



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

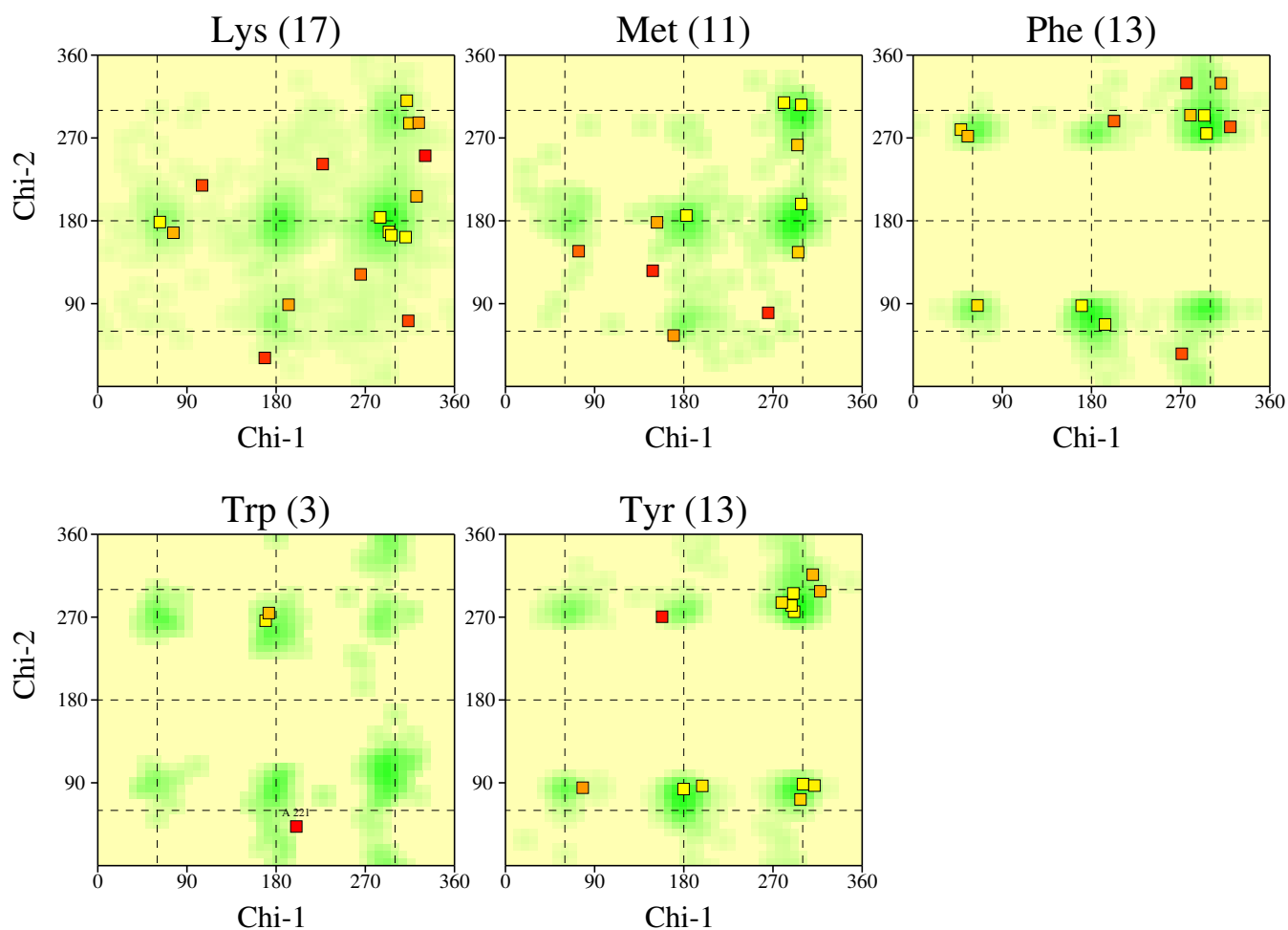
1d4e



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

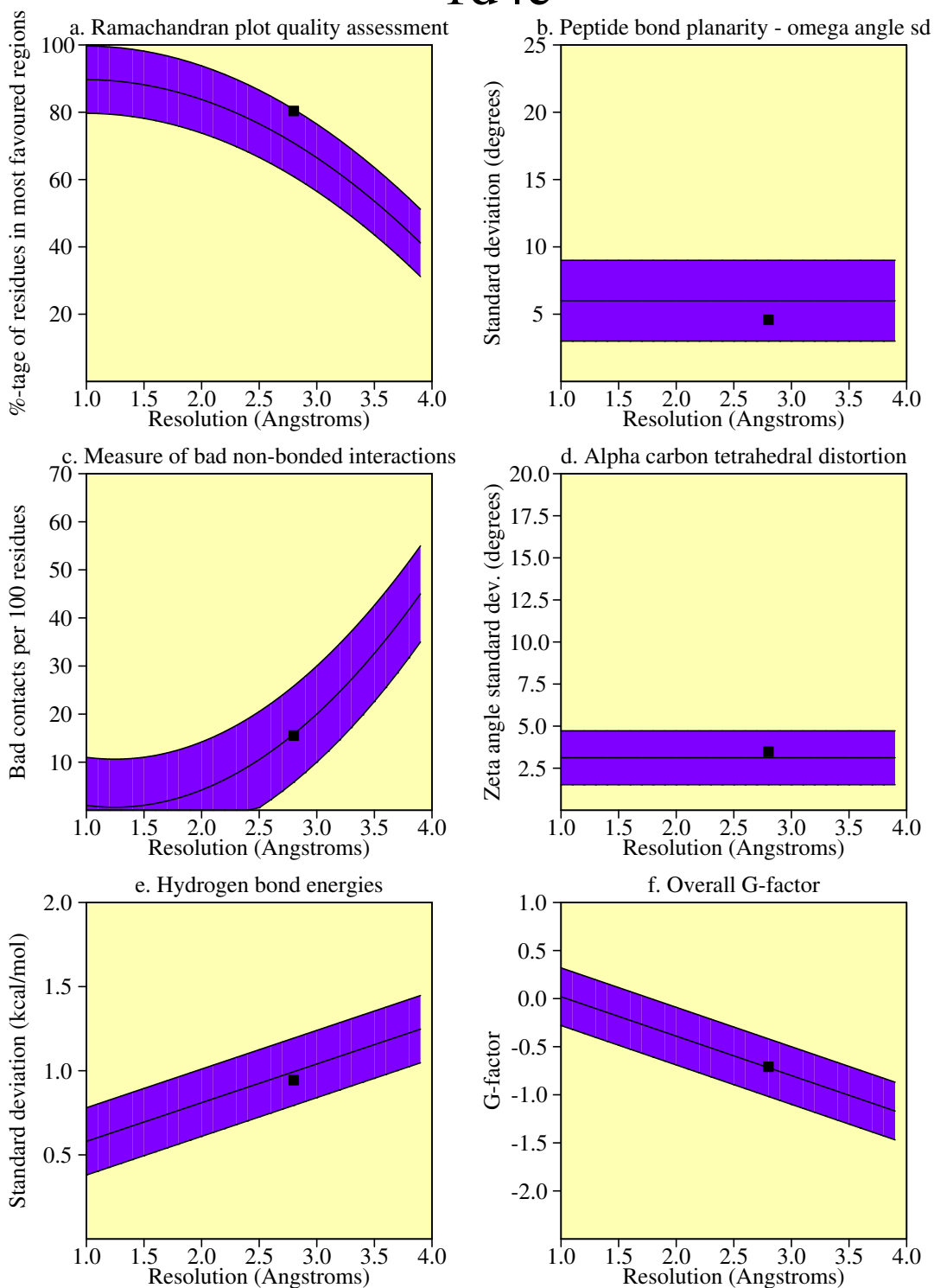
1d4e



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.

Main-chain parameters

1d4e

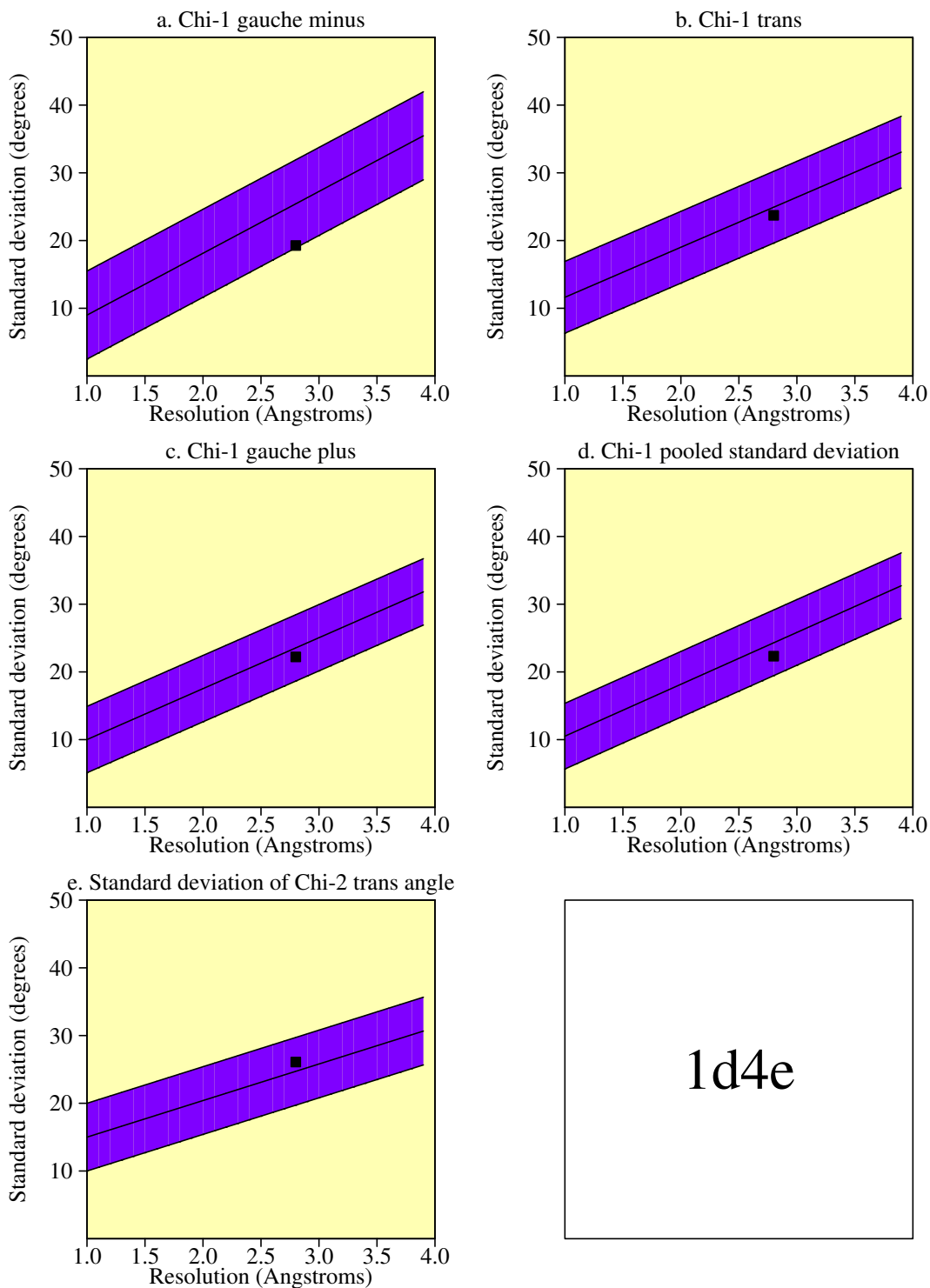


Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	469	80.4	70.9	10.0	1.0	Inside
b. Omega angle st dev	555	4.6	6.0	3.0	-0.5	Inside
c. Bad contacts / 100 residues	87	15.5	15.8	10.0	0.0	Inside
d. Zeta angle st dev	490	3.5	3.1	1.6	0.2	Inside
e. H-bond energy st dev	336	0.9	1.0	0.2	-0.3	Inside
f. Overall G-factor	560	-0.7	-0.7	0.3	0.0	Inside

Side-chain parameters

1d4e



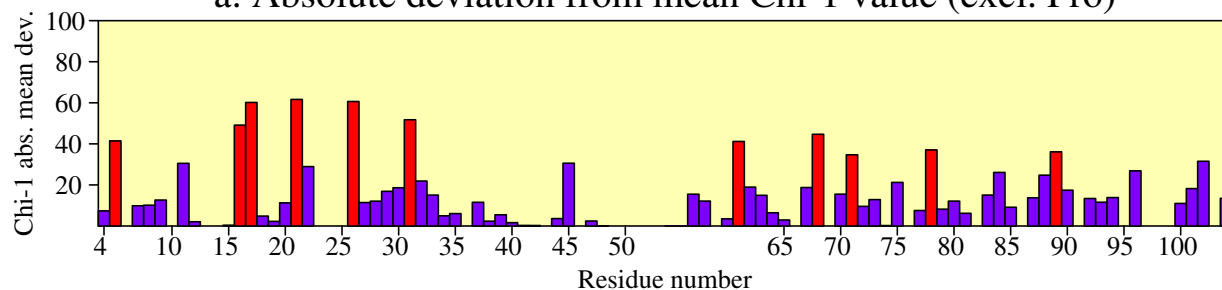
Plot statistics

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	62	19.3	25.4	6.5	-0.9	Inside
b. Chi-1 trans st dev	120	23.7	24.9	5.3	-0.2	Inside
c. Chi-1 gauche plus st dev	176	22.2	23.5	4.9	-0.3	Inside
d. Chi-1 pooled st dev	358	22.3	24.3	4.8	-0.4	Inside
e. Chi-2 trans st dev	98	26.1	24.7	5.0	0.3	Inside

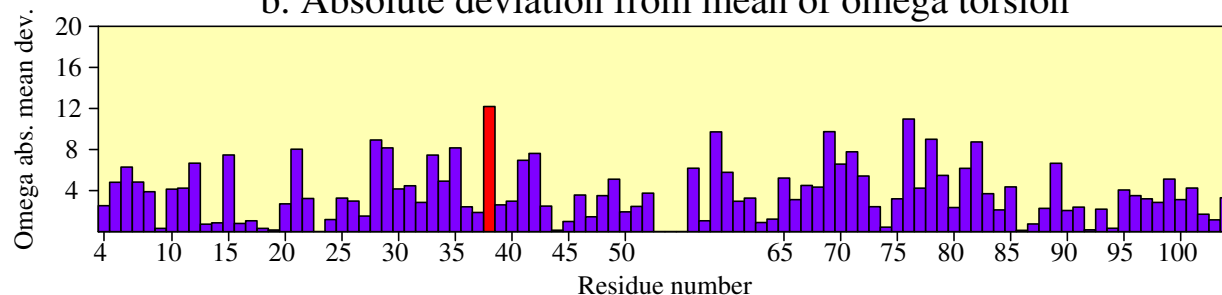
Residue properties

1d4e

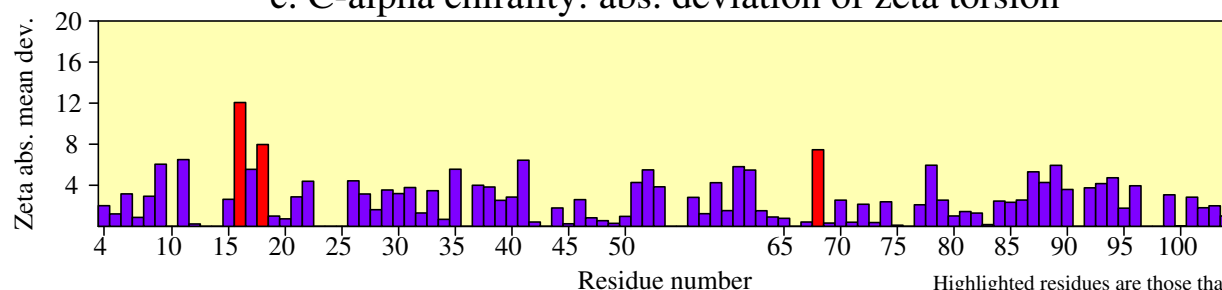
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

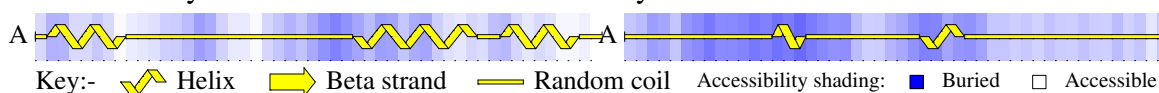


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



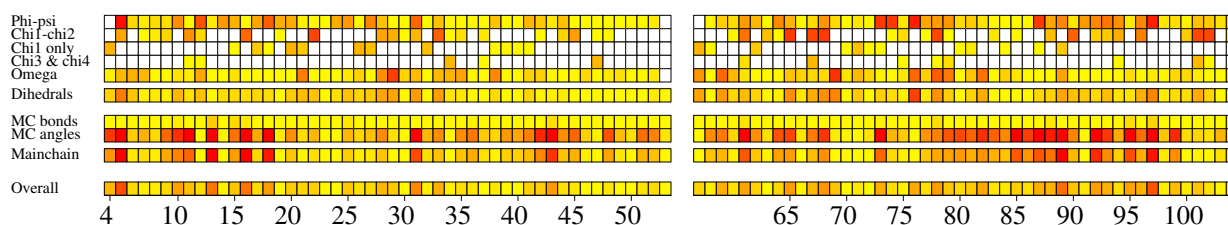
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



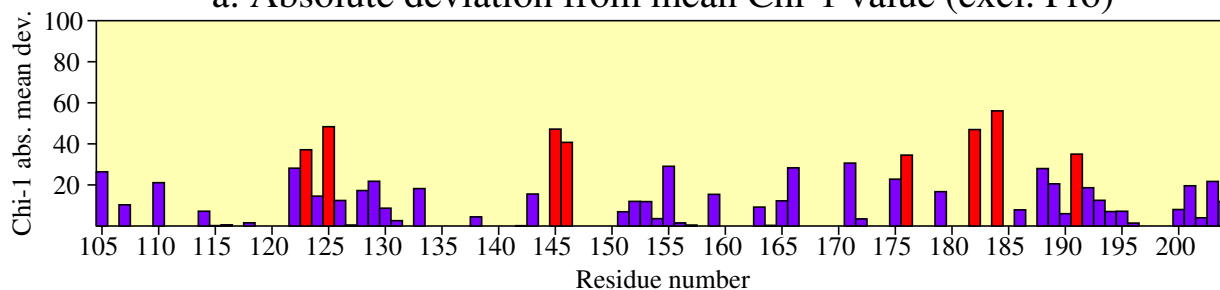
g. G-factors



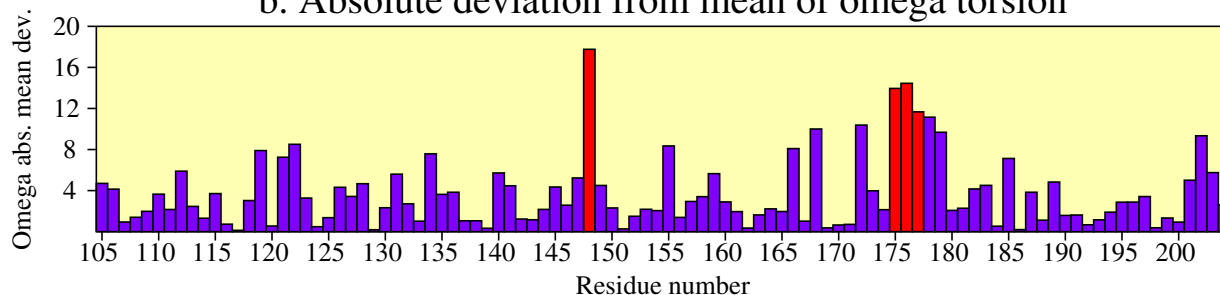
Residue properties

1d4e

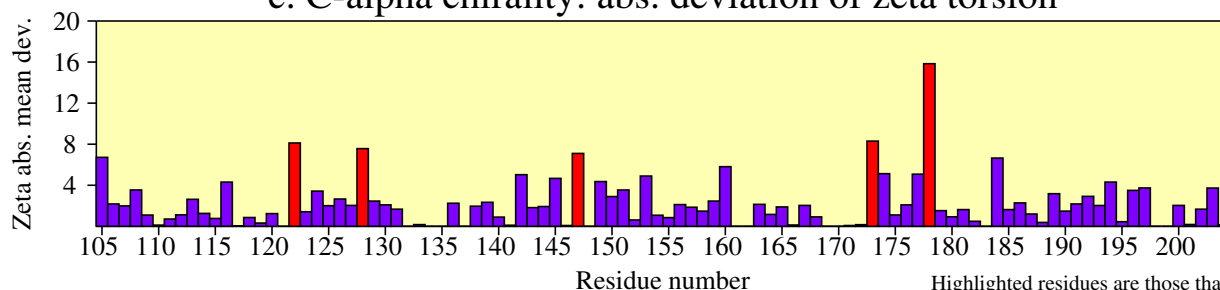
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

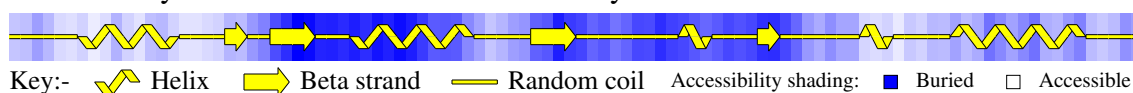


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



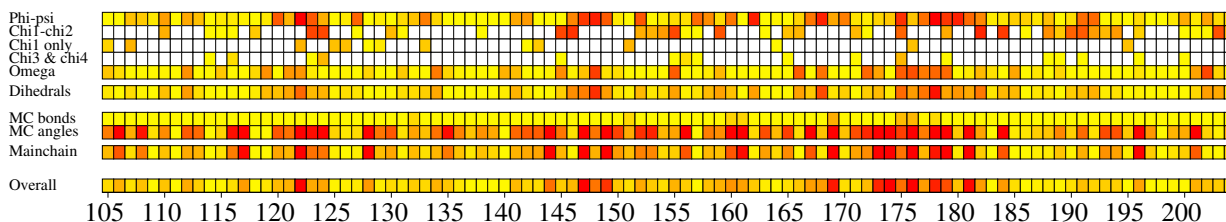
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



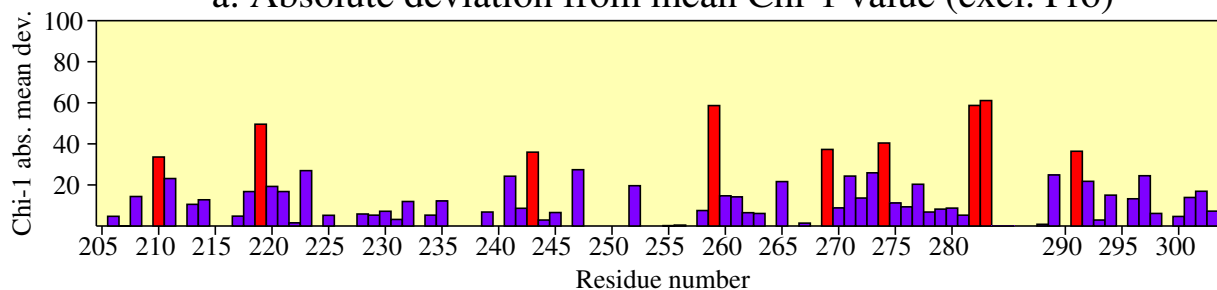
g. G-factors



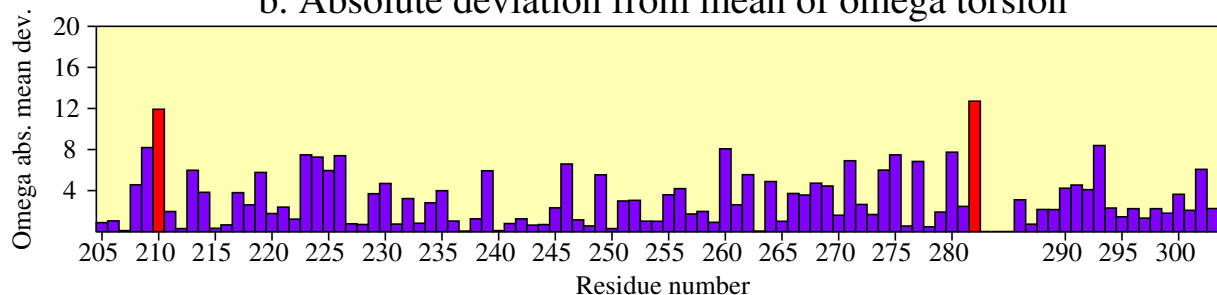
Residue properties

1d4e

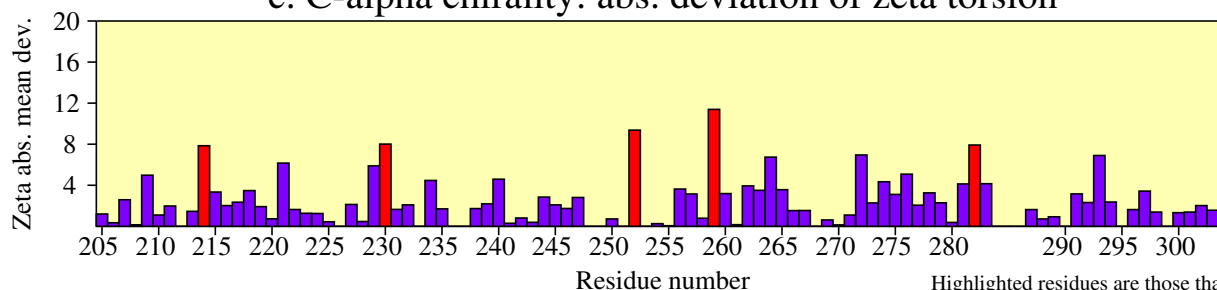
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

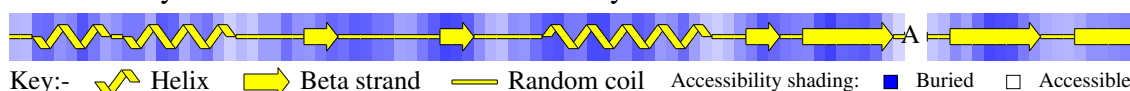


c. C-alpha chirality: abs. deviation of zeta torsion



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

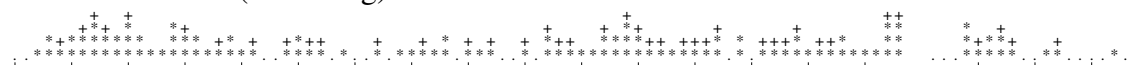
d. Secondary structure & estimated accessibility



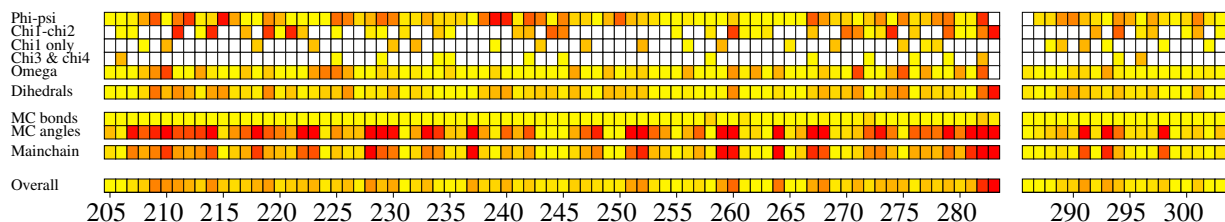
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



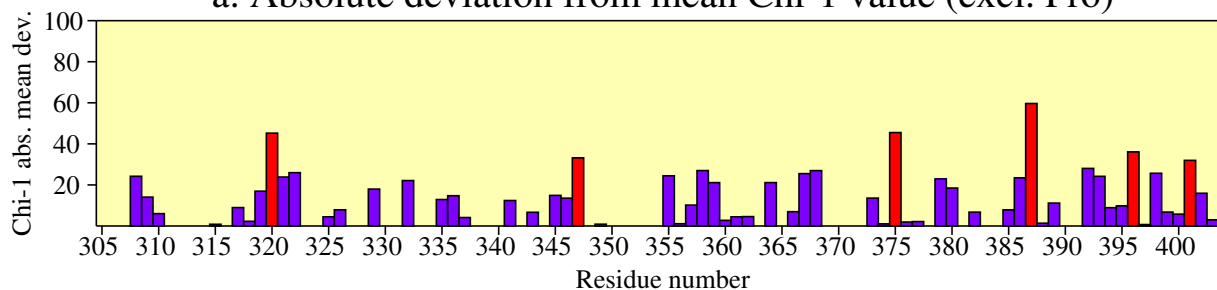
g. G-factors



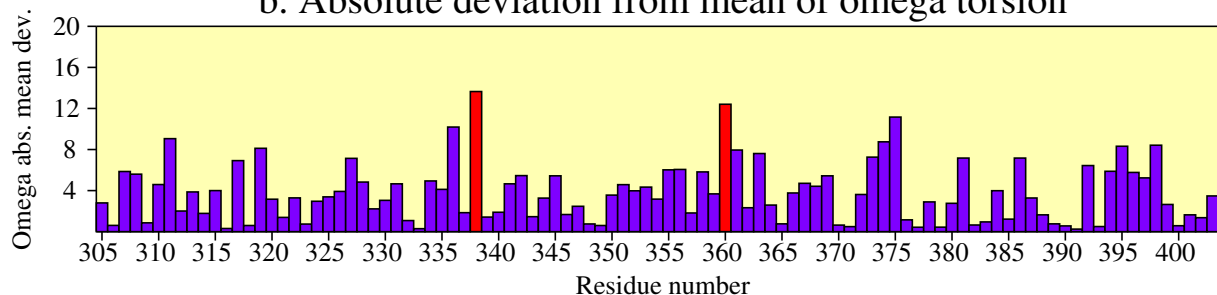
Residue properties

1d4e

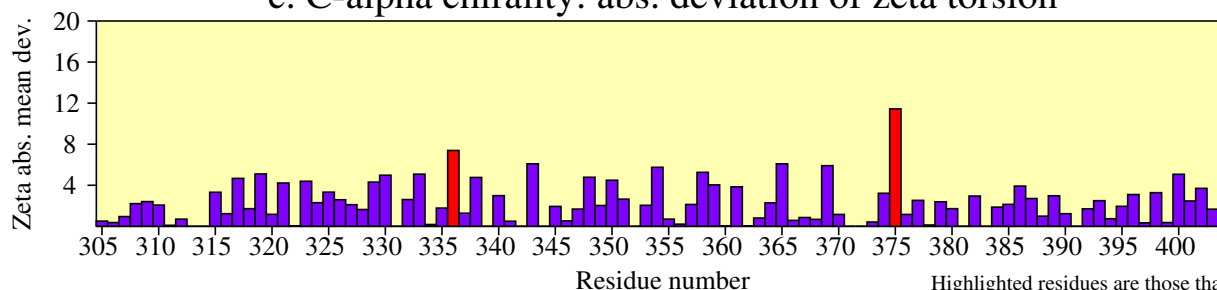
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

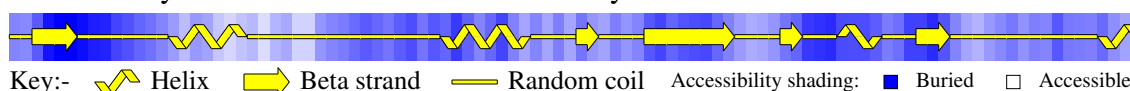


c. C-alpha chirality: abs. deviation of zeta torsion



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

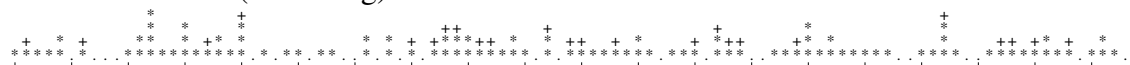
d. Secondary structure & estimated accessibility



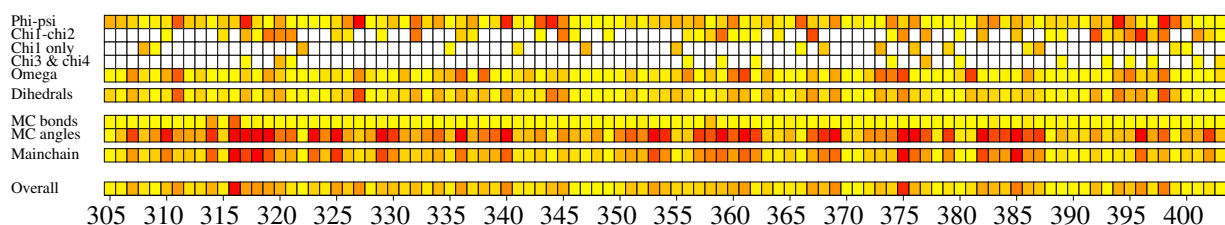
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



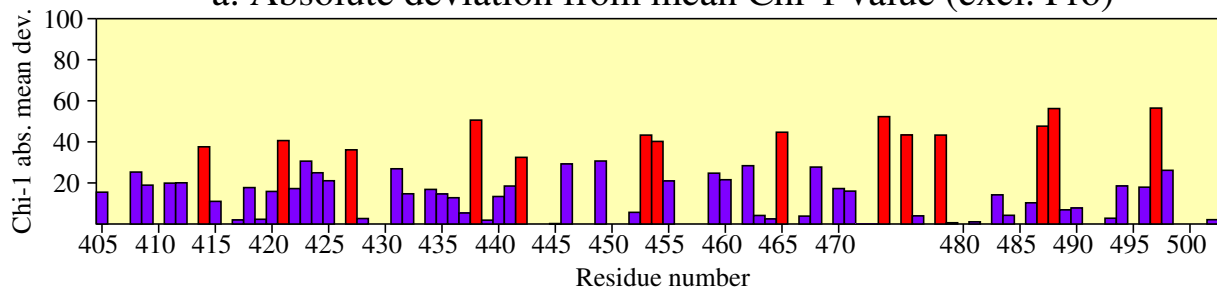
g. G-factors



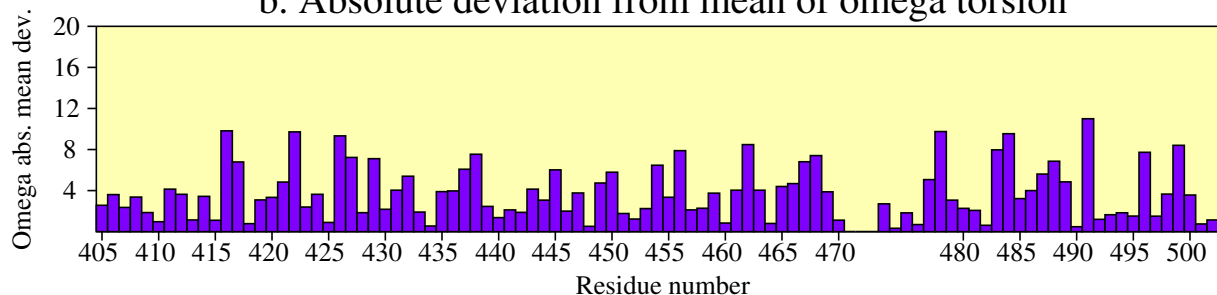
Residue properties

1d4e

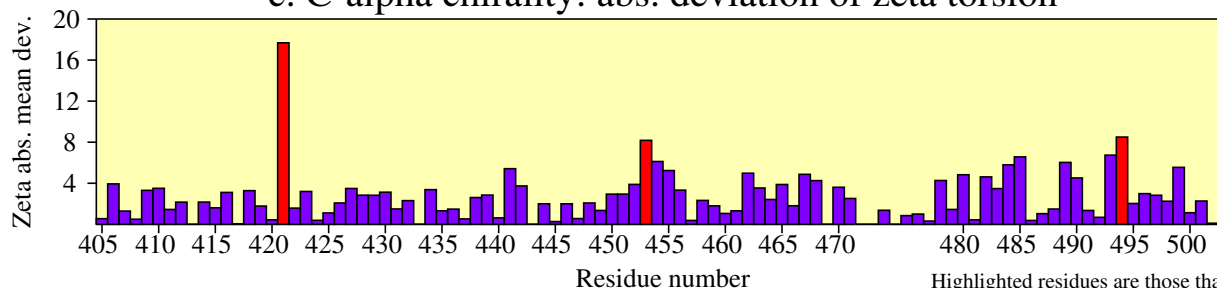
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

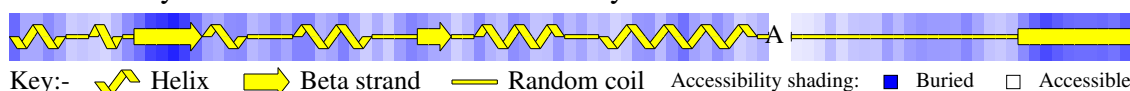


c. C-alpha chirality: abs. deviation of zeta torsion



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

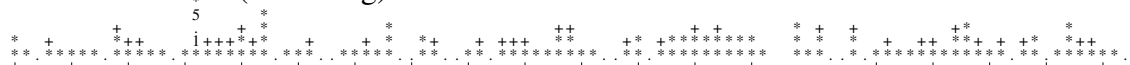
d. Secondary structure & estimated accessibility



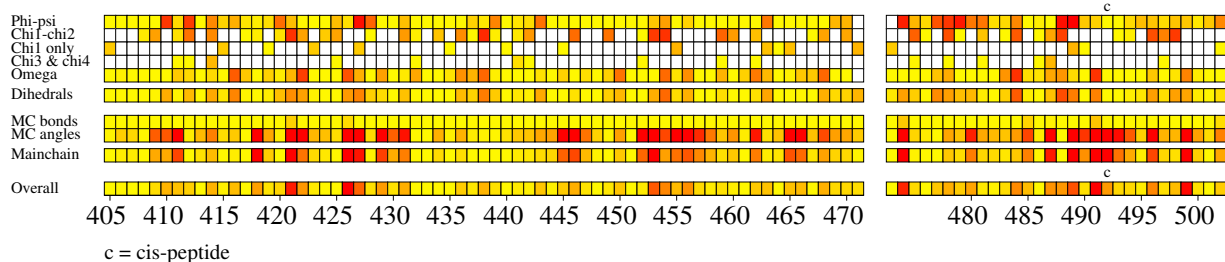
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



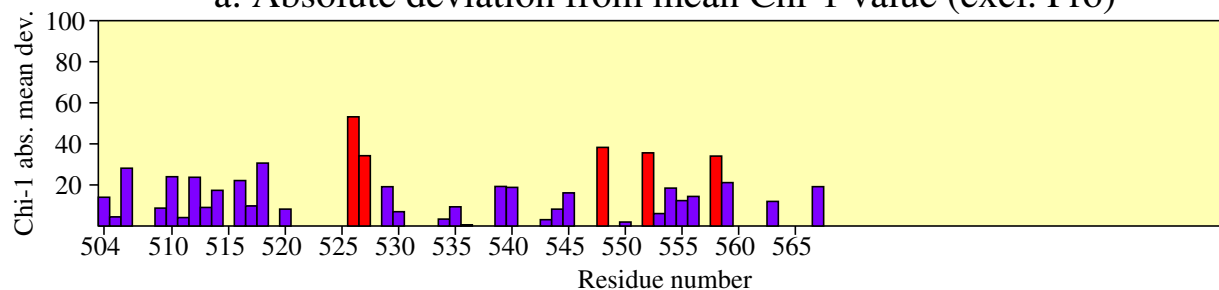
g. G-factors



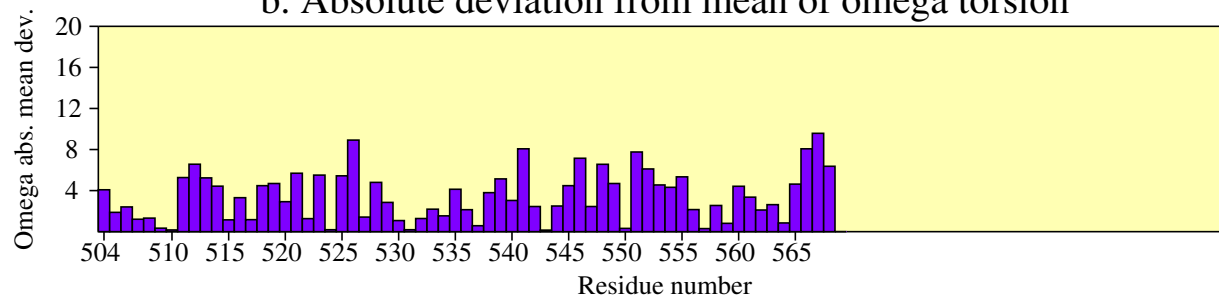
Residue properties

1d4e

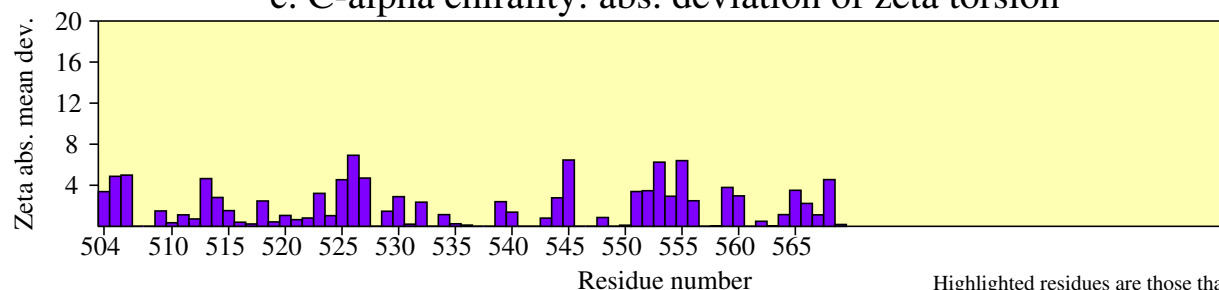
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

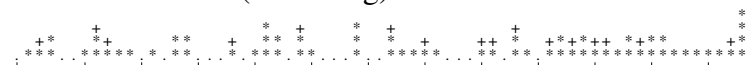


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

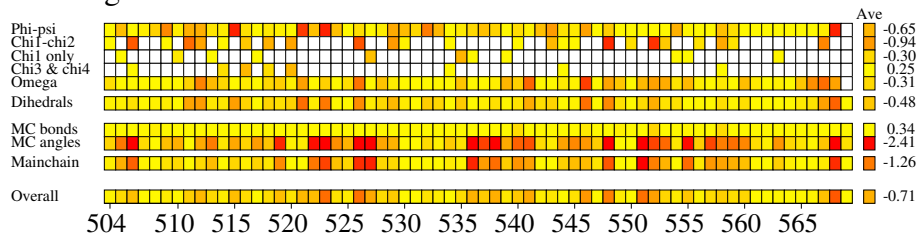
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

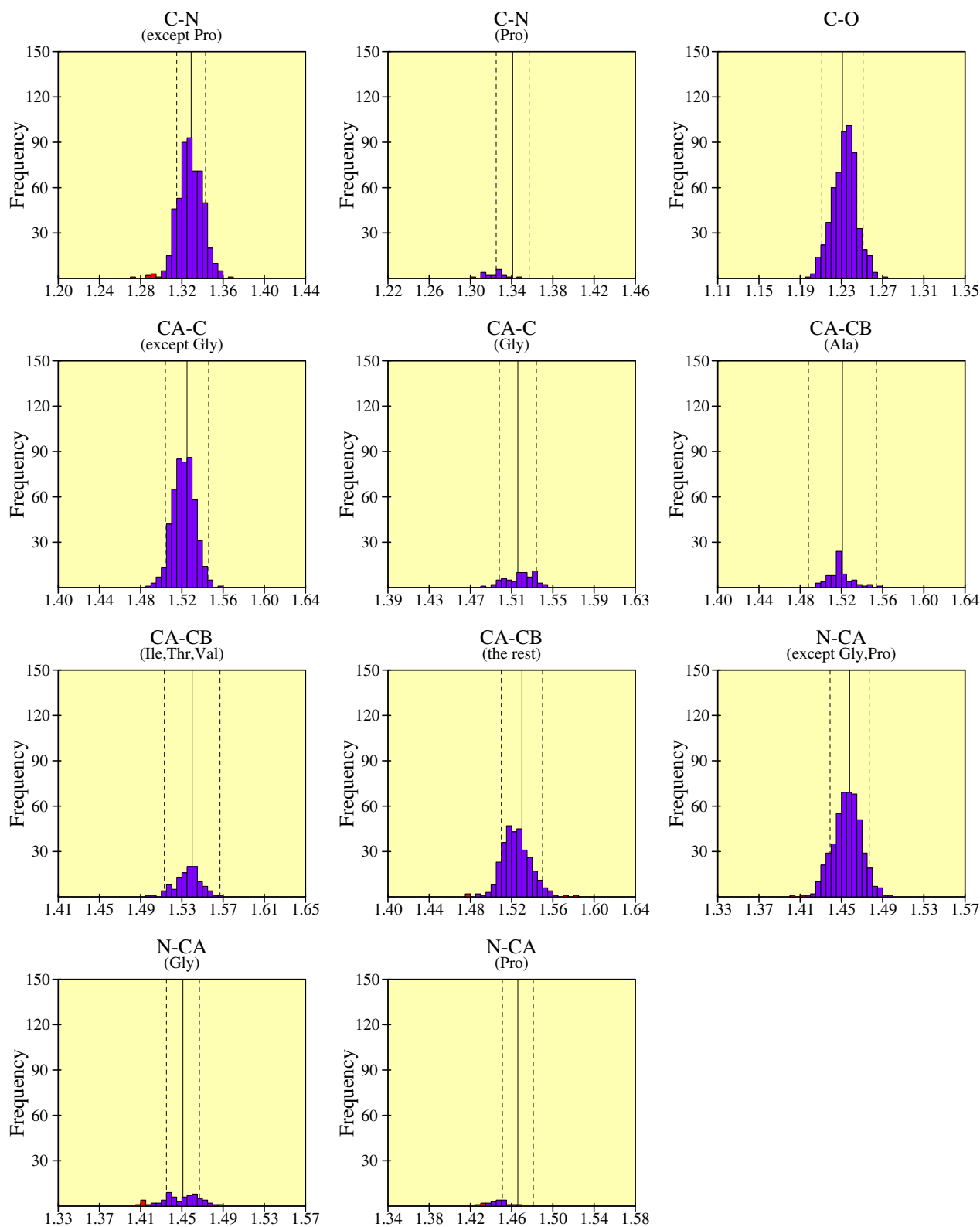


g. G-factors



Main-chain bond lengths

1d4e

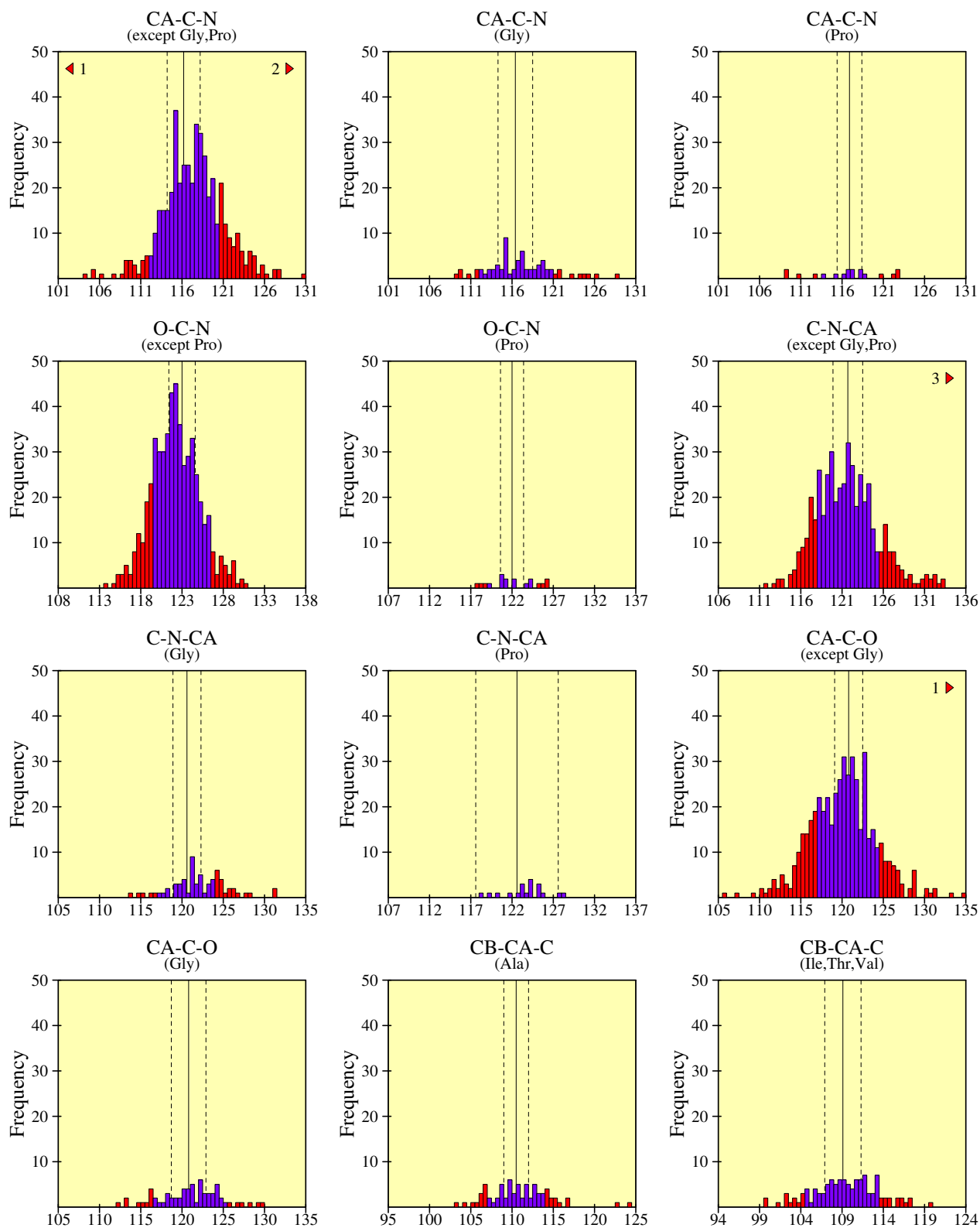


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

1d4e



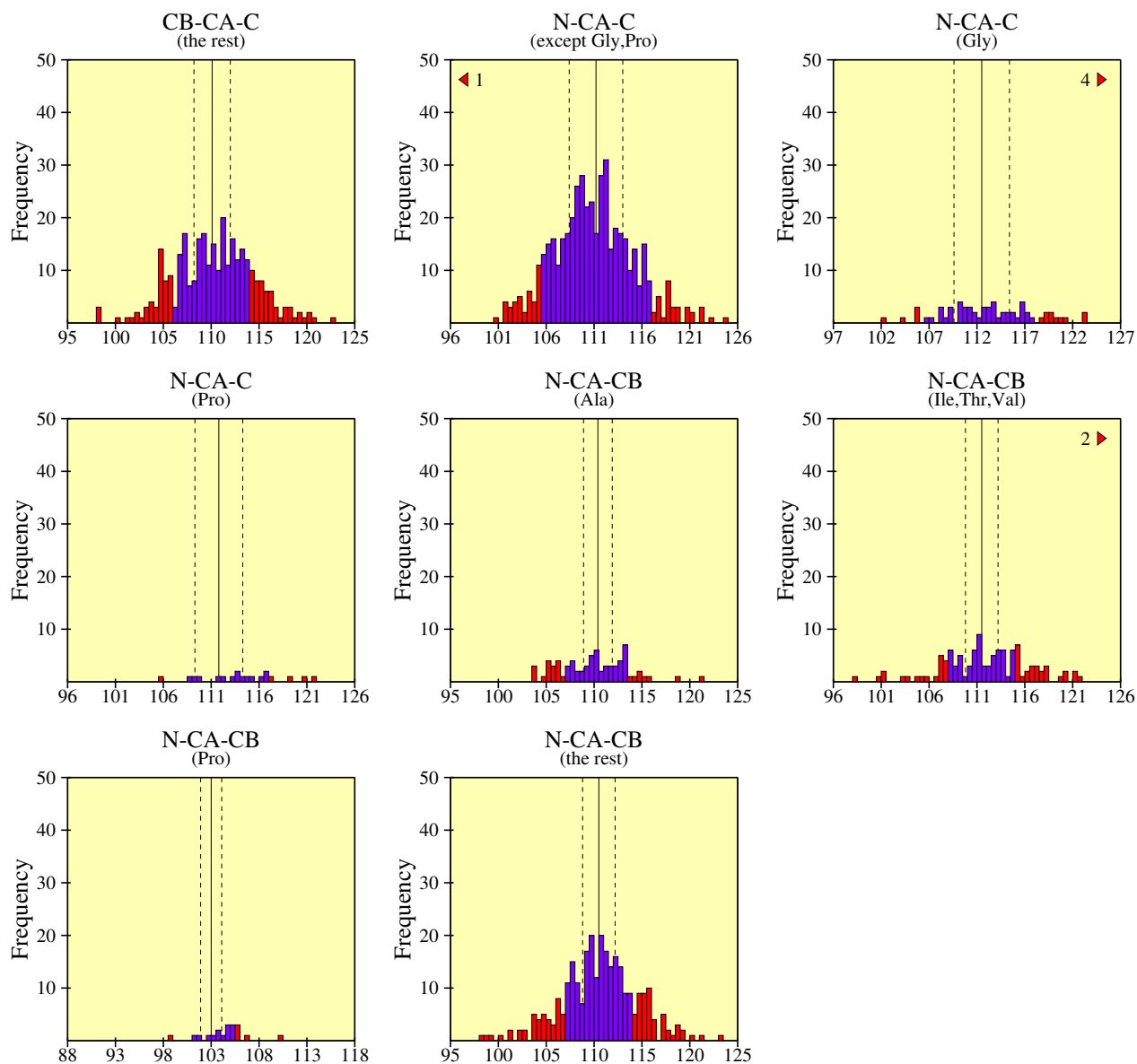
Black bars > 2.0 st. devs. from mean.

◀ 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

1d4e



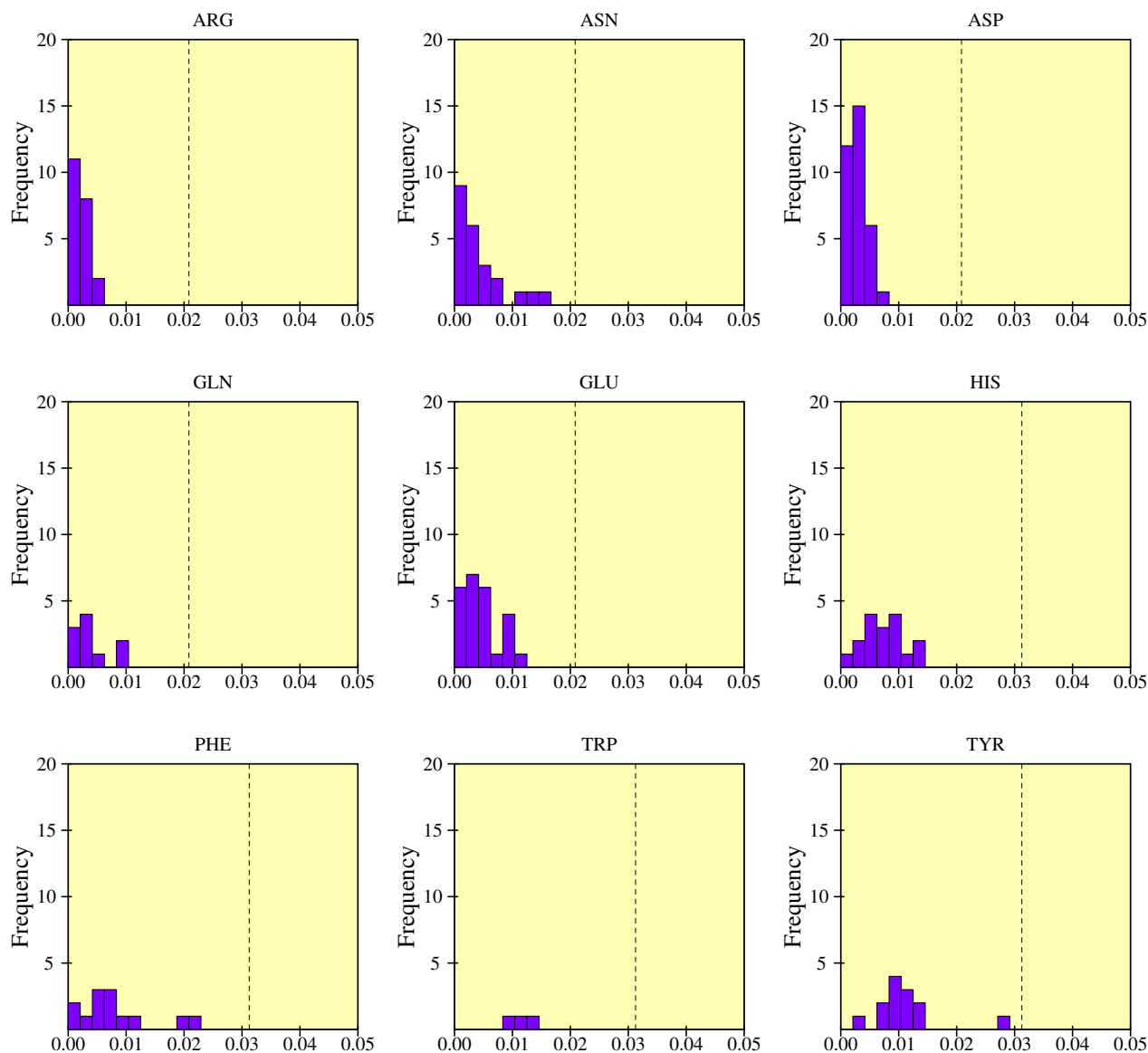
Black bars > 2.0 st. devs. from mean.

◀ 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

1d4e

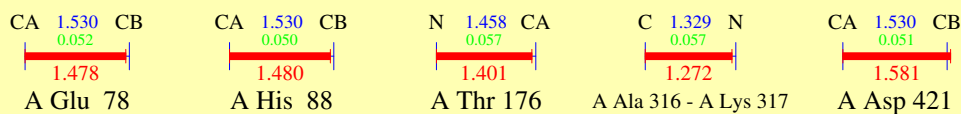


Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

Distorted geometry

1d4e

Main-chain bond lengths



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

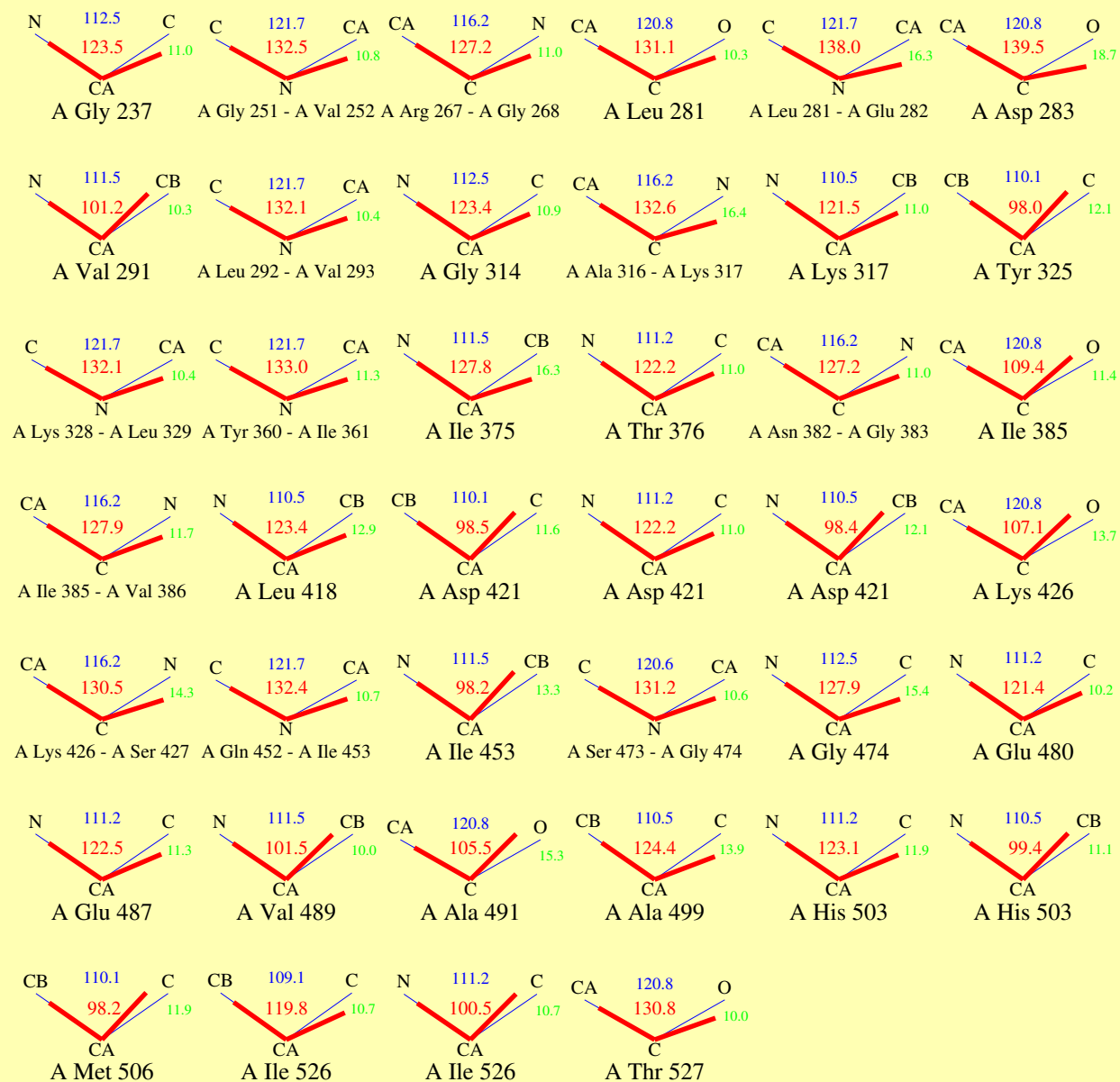
Main-chain bond angles



Distorted geometry

1d4e

Main-chain bond angles (contd)



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