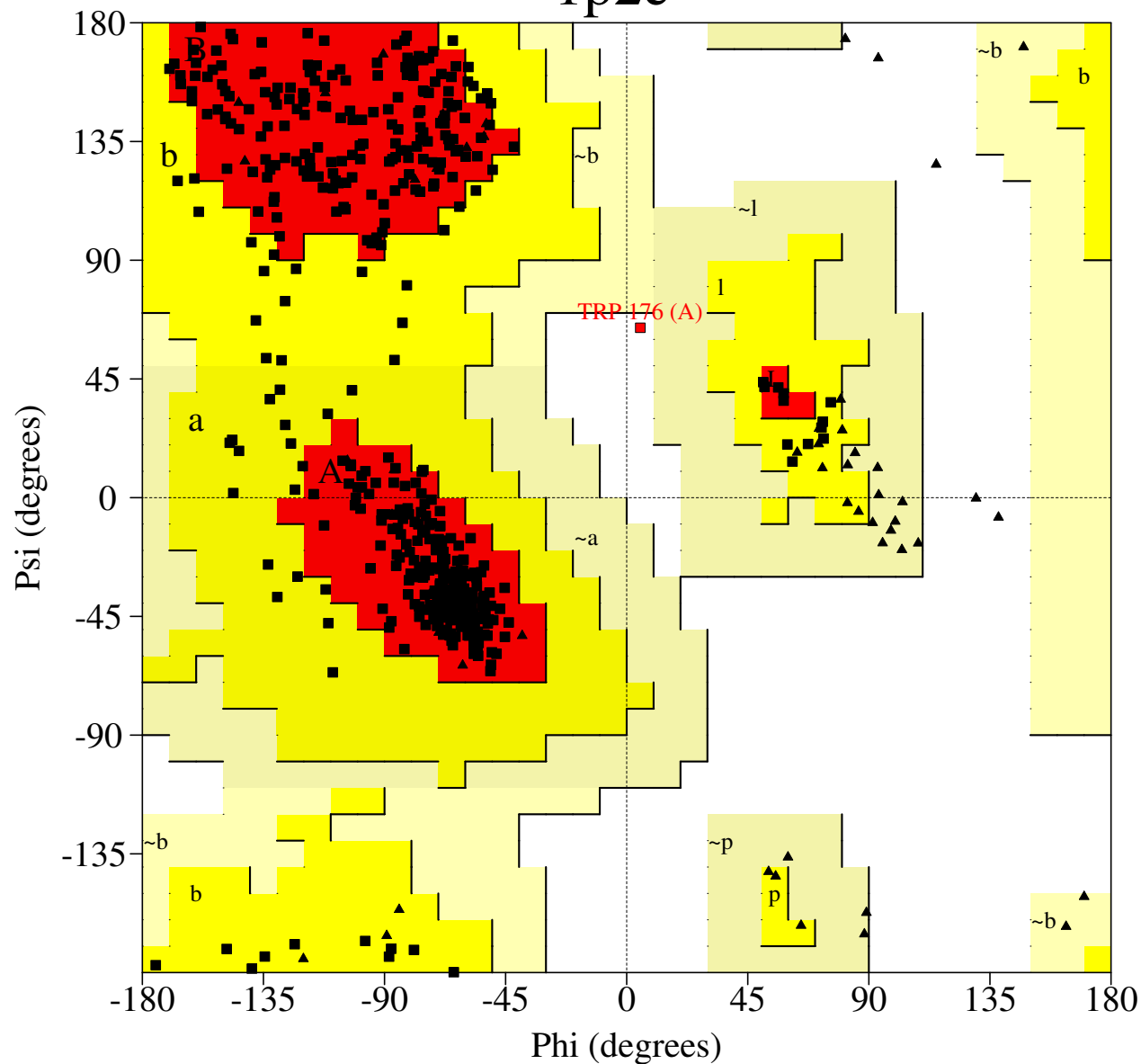


Ramachandran Plot

1p2e



Plot statistics

Residues in most favoured regions [A,B,L]	429	87.9%
Residues in additional allowed regions [a,b,l,p]	58	11.9%
Residues in generously allowed regions [-a,-b,-l,-p]	0	0.0%
Residues in disallowed regions	1	0.2%

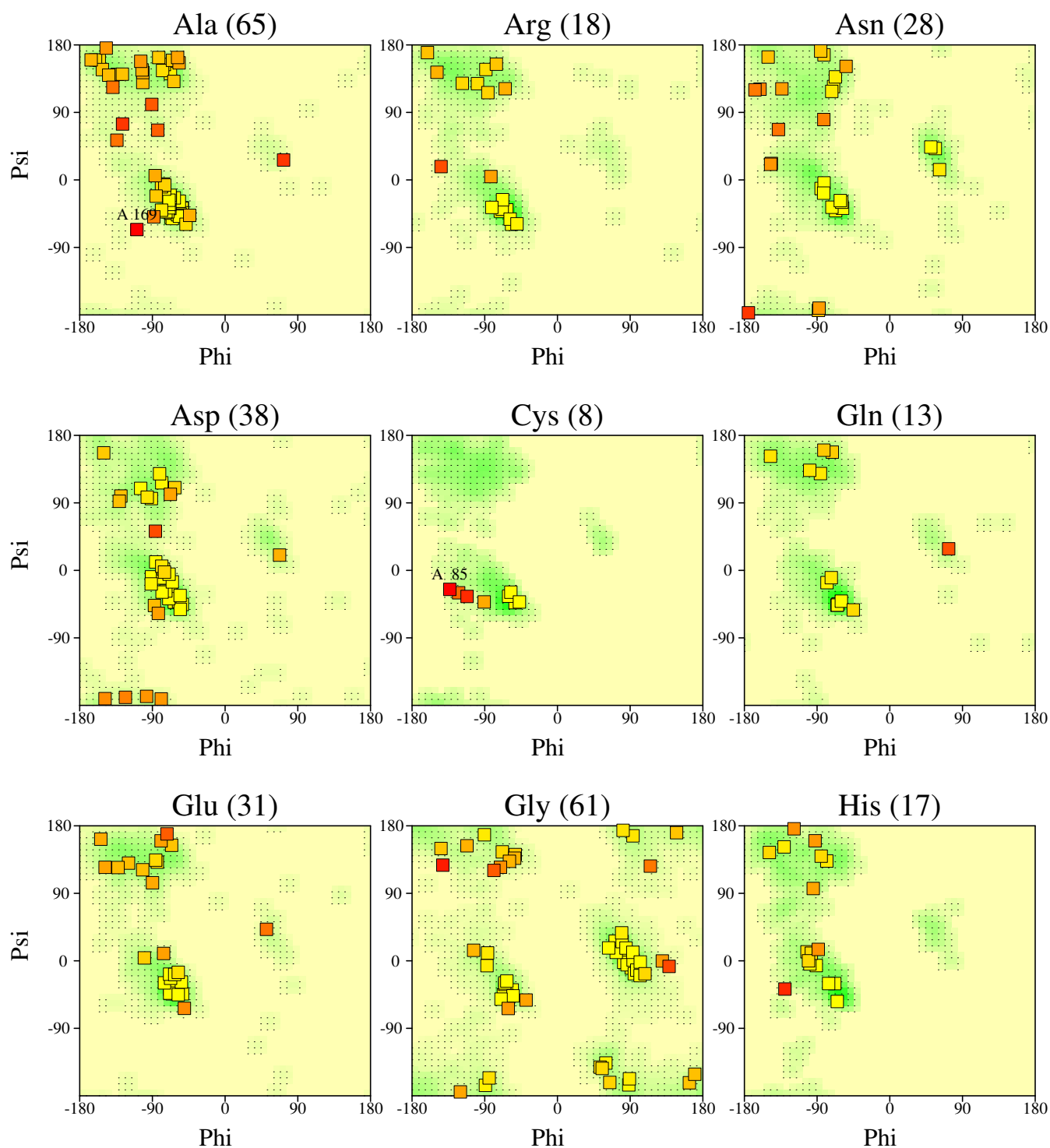
Number of non-glycine and non-proline residues	488	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	61	
Number of proline residues	17	

Total number of residues	568	

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

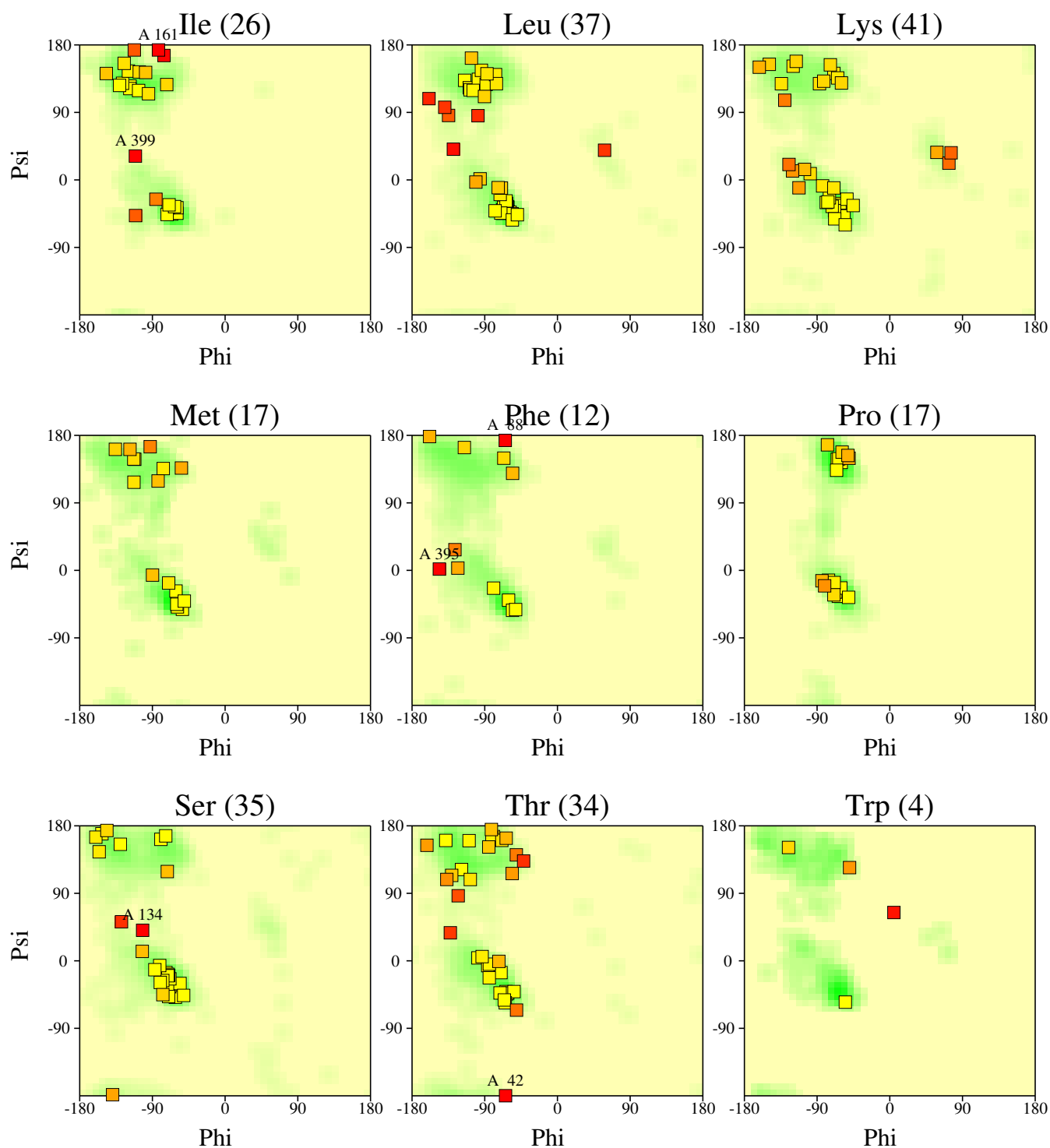
1p2e



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

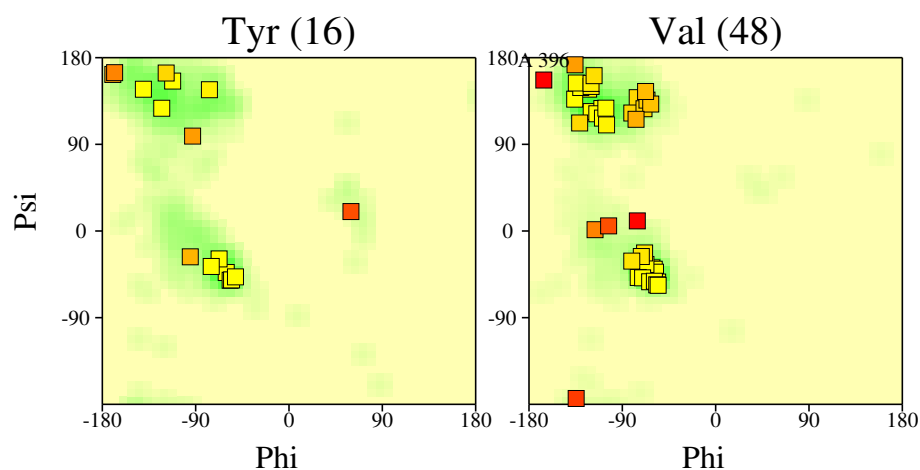
1p2e



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

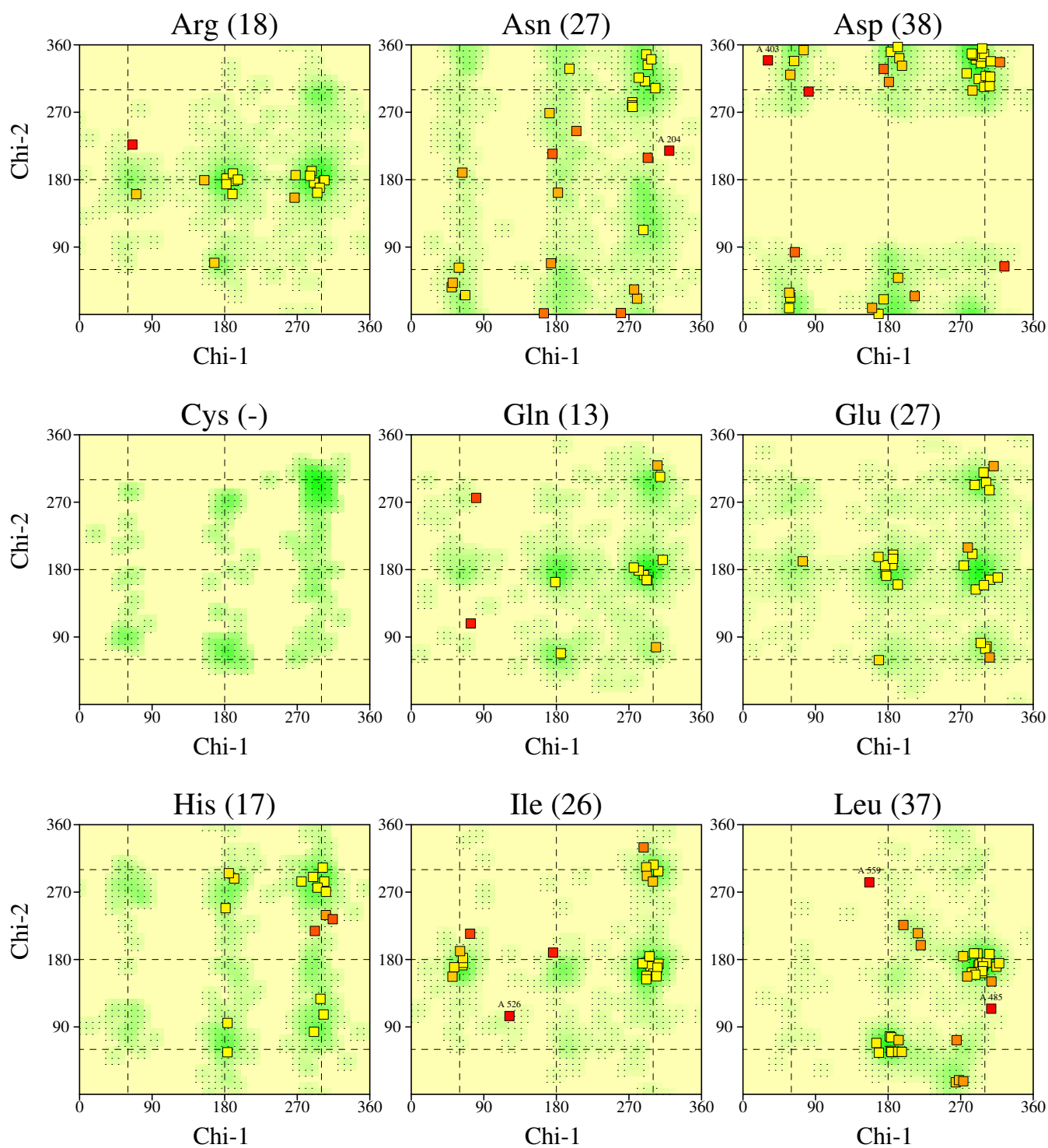
1p2e



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

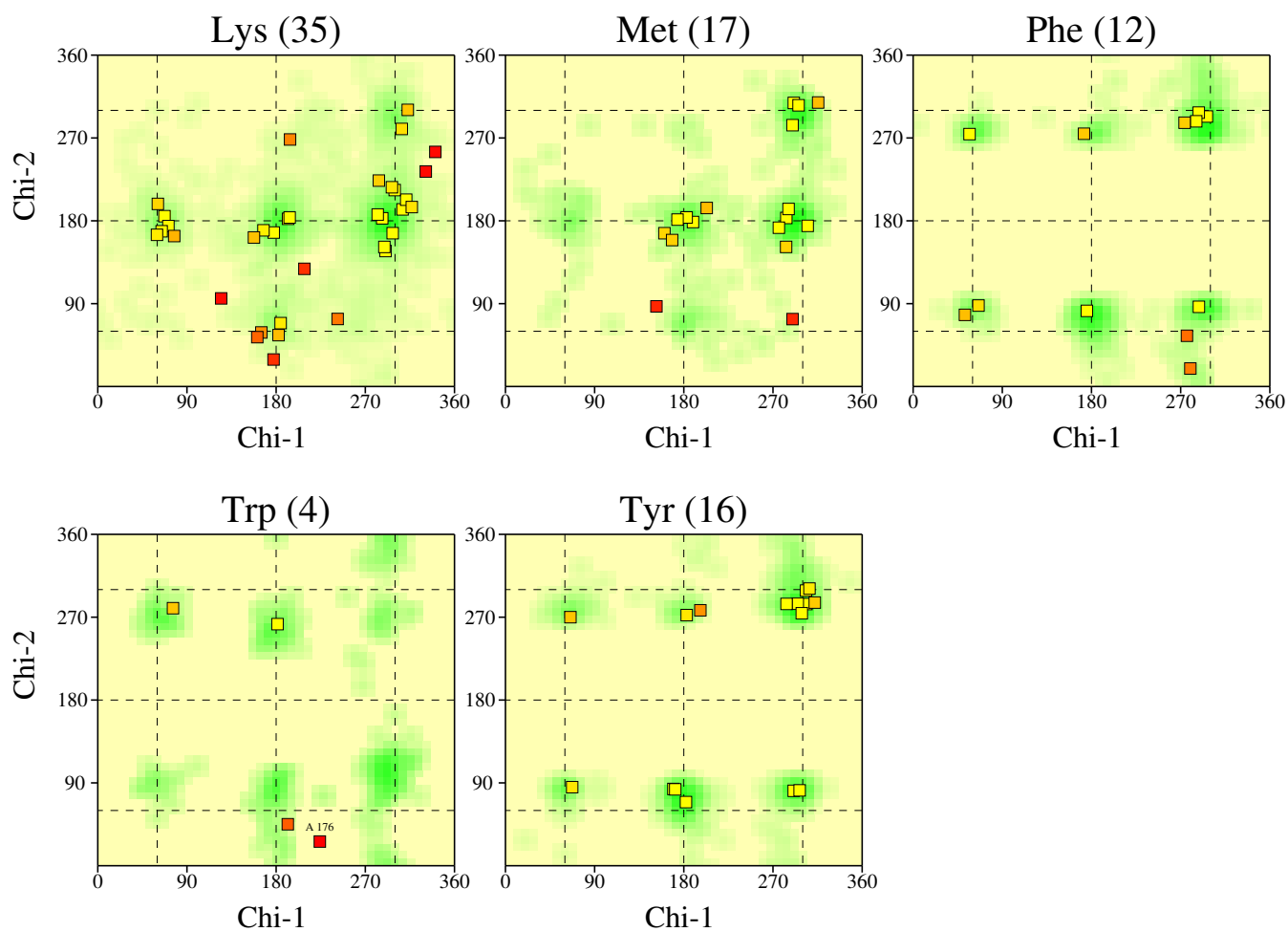
1p2e



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

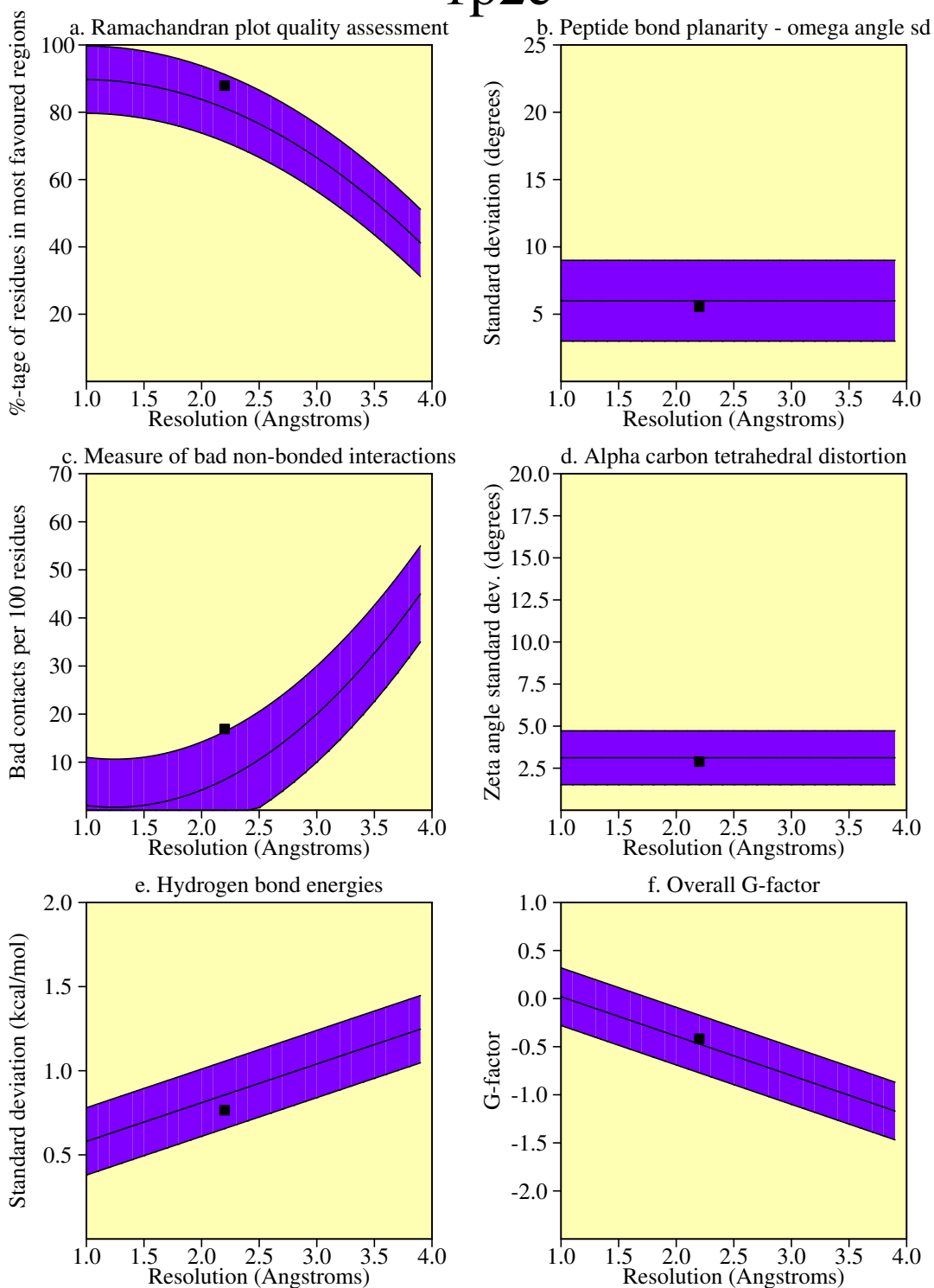
1p2e



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

1p2e

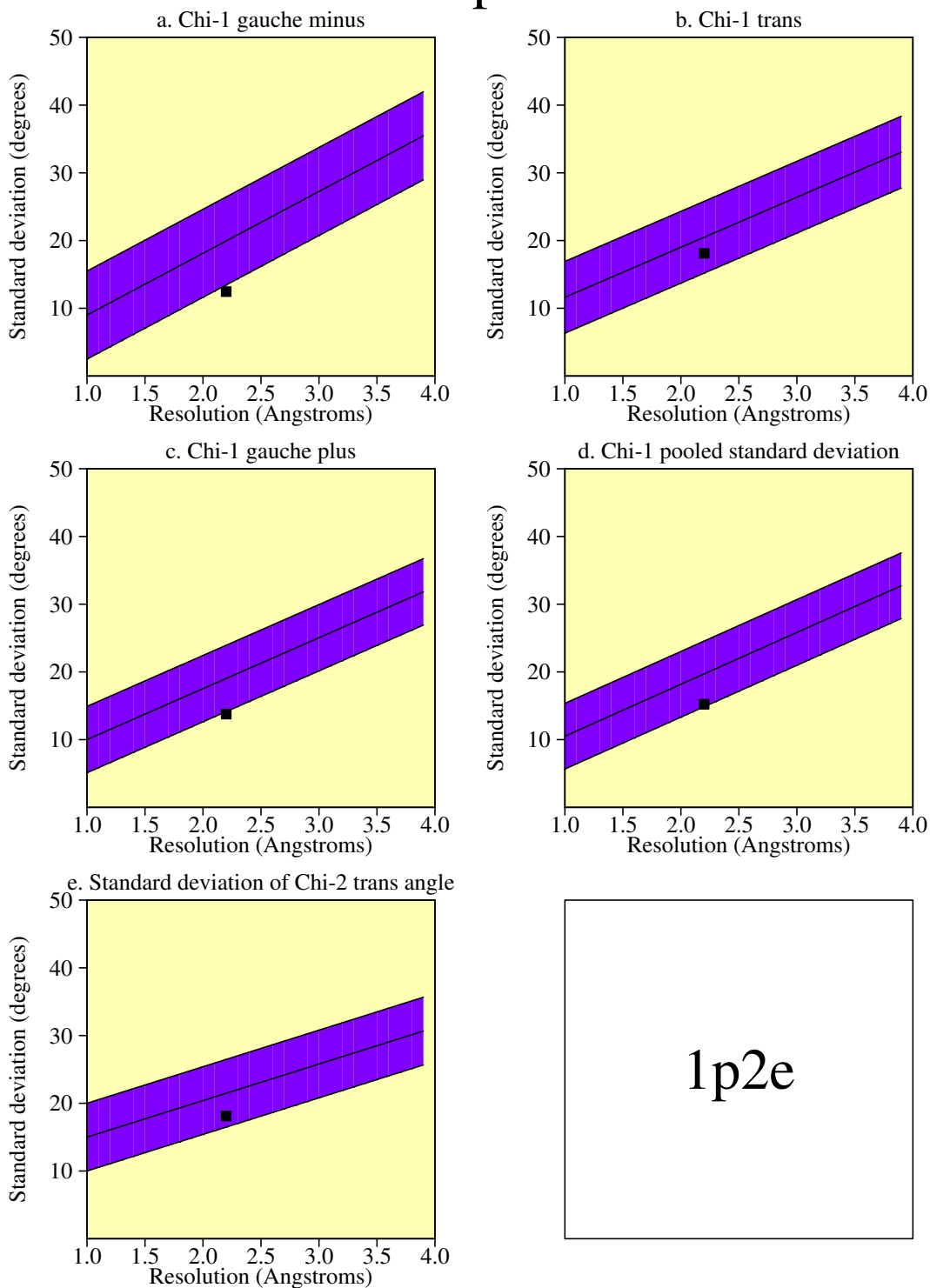


Plot statistics

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	488	87.9	81.3	10.0	0.7	Inside
b. Omega angle st dev	567	5.5	6.0	3.0	-0.2	Inside
c. Bad contacts / 100 residues	96	16.9	6.4	10.0	1.1	WORSE
d. Zeta angle st dev	507	2.9	3.1	1.6	-0.1	Inside
e. H-bond energy st dev	346	0.8	0.9	0.2	-0.5	Inside
f. Overall G-factor	568	-0.4	-0.5	0.3	0.2	Inside

Side-chain parameters

1p2e



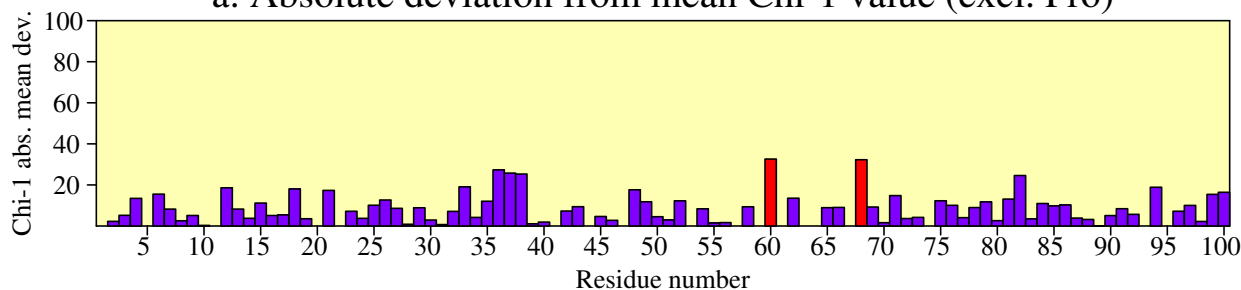
Plot statistics

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	78	12.5	19.9	6.5	-1.2	BETTER
b. Chi-1 trans st dev	136	18.1	20.5	5.3	-0.4	Inside
c. Chi-1 gauche plus st dev	203	13.8	19.0	4.9	-1.1	BETTER
d. Chi-1 pooled st dev	417	15.2	19.7	4.8	-0.9	Inside
e. Chi-2 trans st dev	116	18.1	21.5	5.0	-0.7	Inside

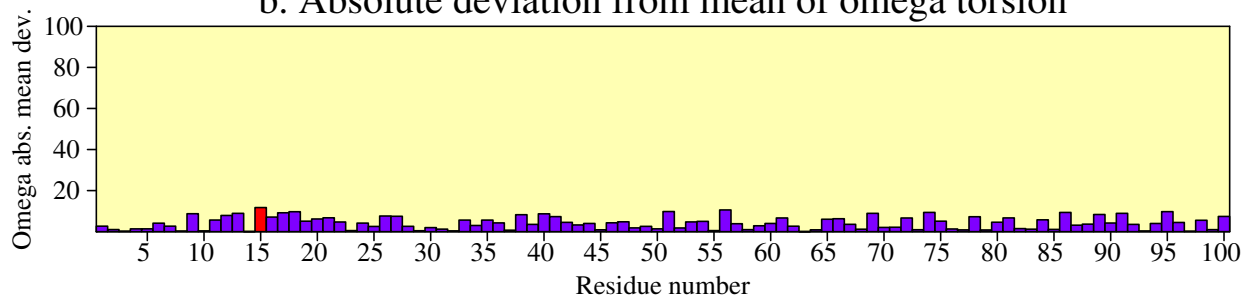
Residue properties

1p2e

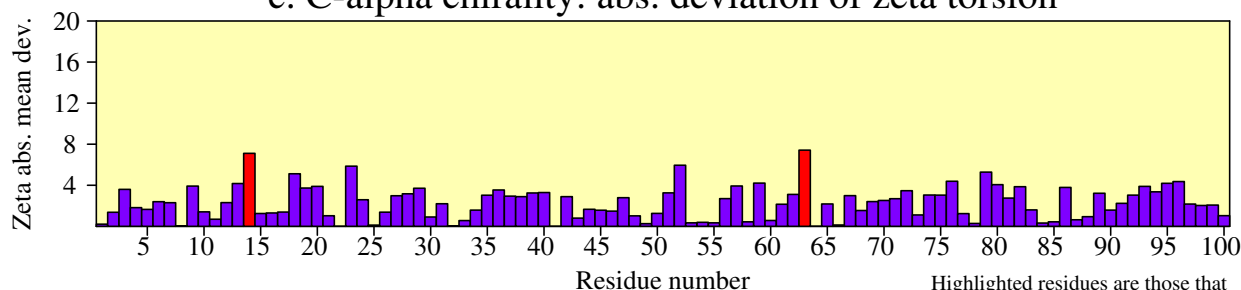
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

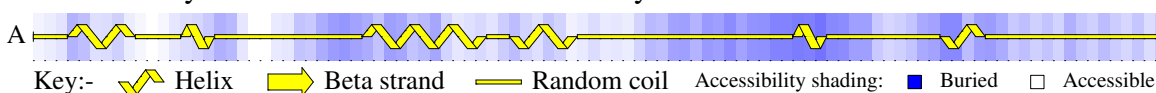


c. C-alpha chirality: abs. deviation of zeta torsion



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

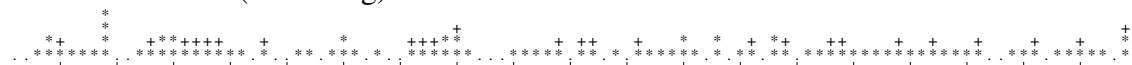
d. Secondary structure & estimated accessibility



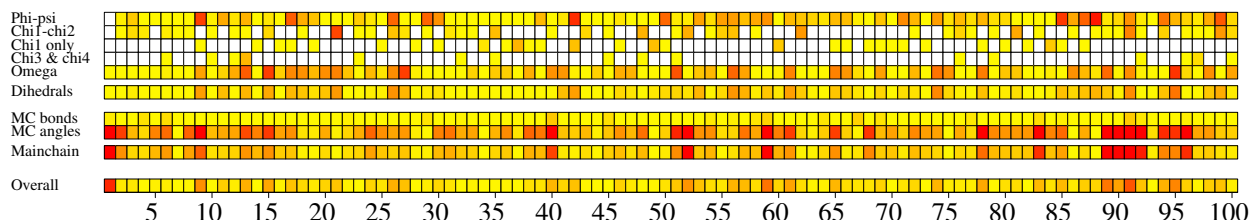
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

ADNLAEFHVQNECDSCHTPDGELSNDLSLTENTQCVSCHGTLAEVAETTKHEHYNAHASAFPGEVACTSCHSAHEKSMVYCDSCHSFDFNMPYAKKWL

f. Max. deviation (see listing)



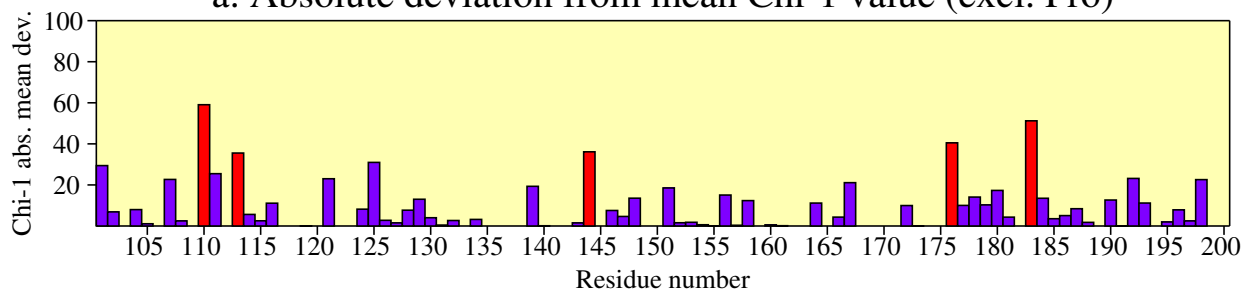
g. G-factors



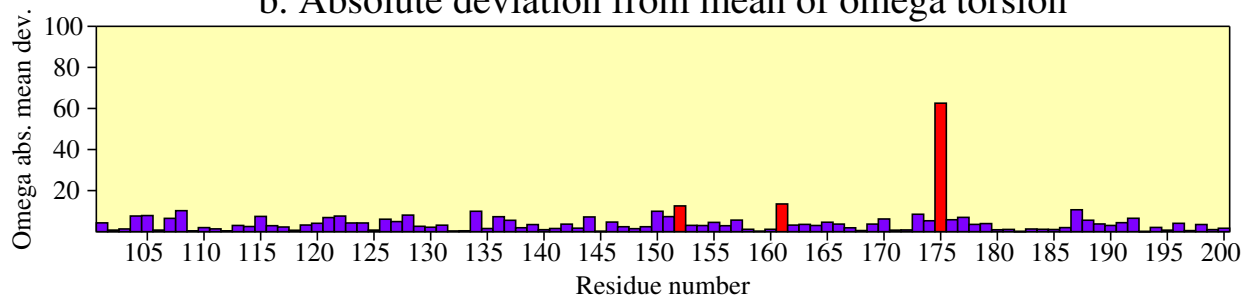
Residue properties

1p2e

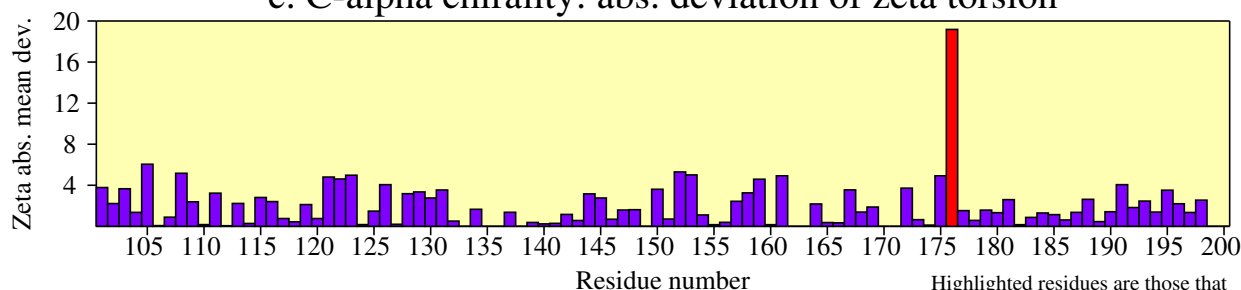
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

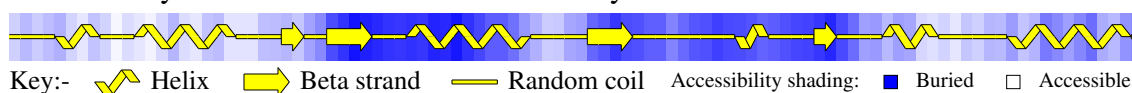


c. C-alpha chirality: abs. deviation of zeta torsion



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

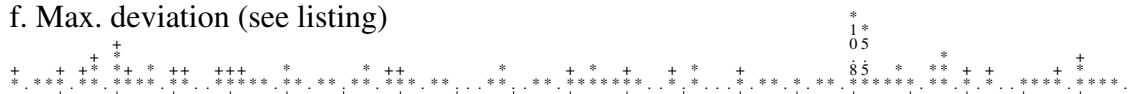
d. Secondary structure & estimated accessibility



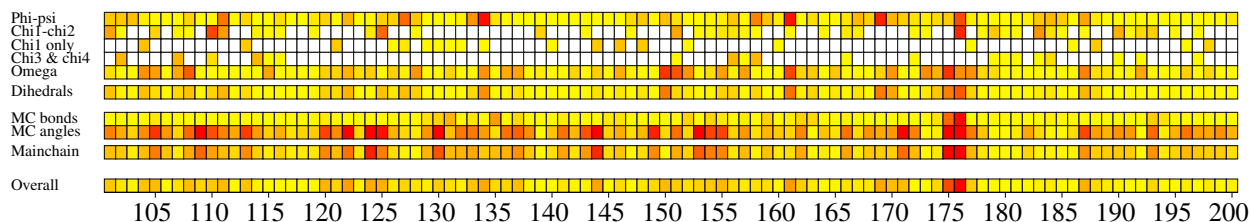
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



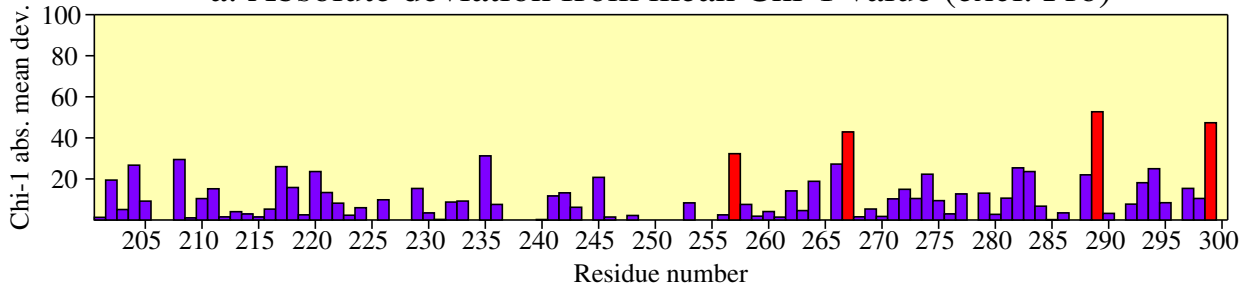
g. G-factors



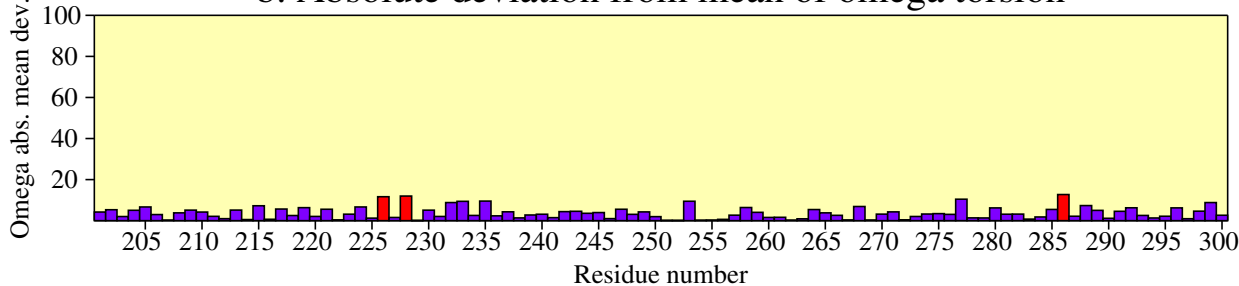
Residue properties

1p2e

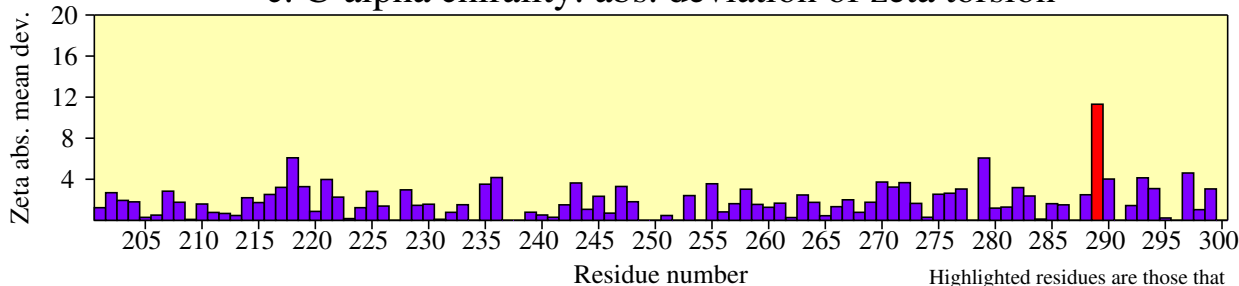
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

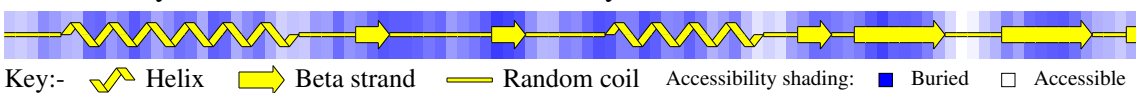


c. C-alpha chirality: abs. deviation of zeta torsion



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

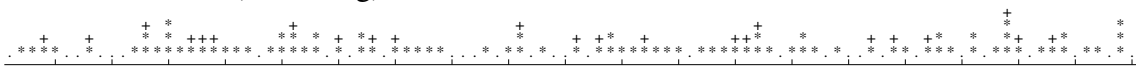
d. Secondary structure & estimated accessibility



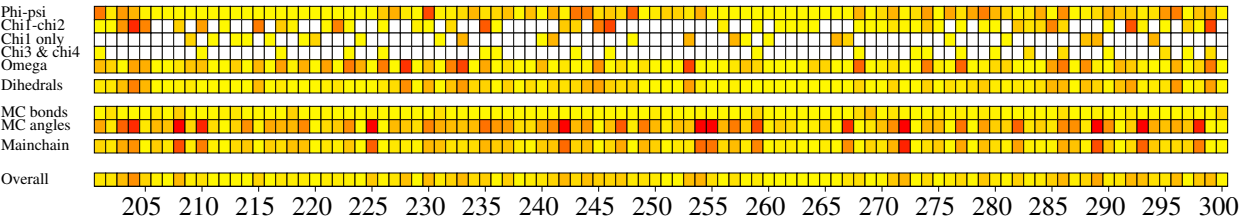
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



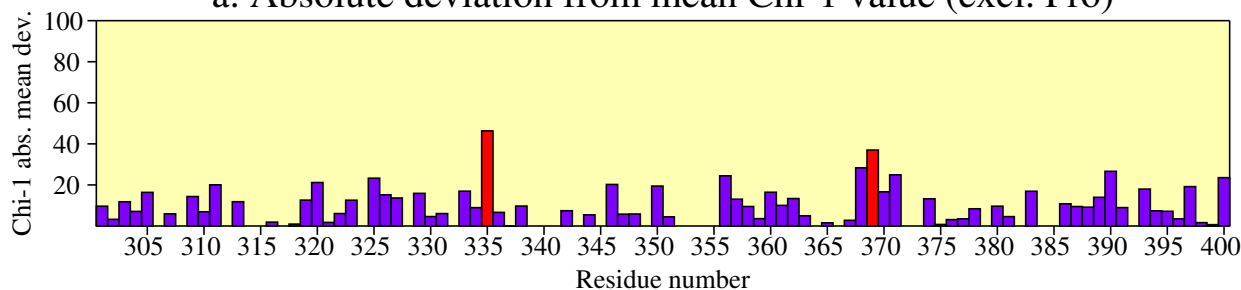
g. G-factors



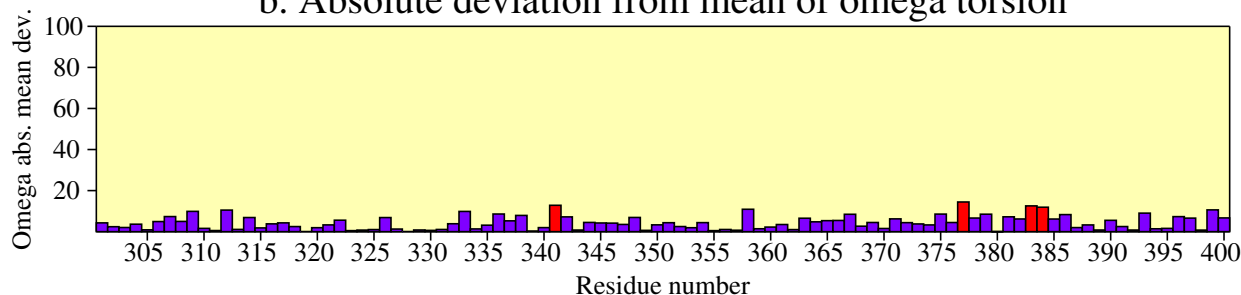
Residue properties

1p2e

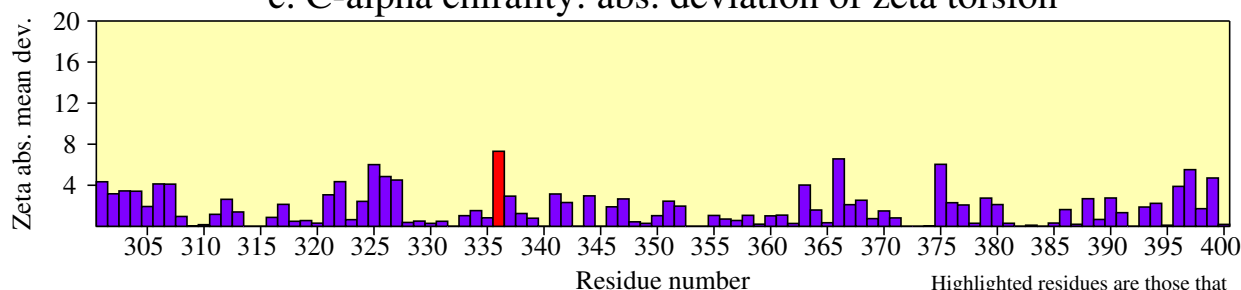
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

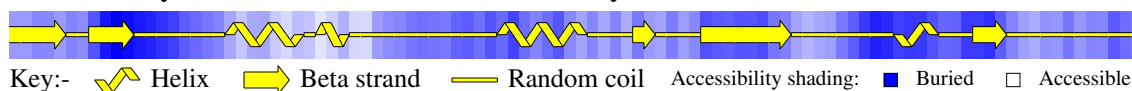


c. C-alpha chirality: abs. deviation of zeta torsion



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

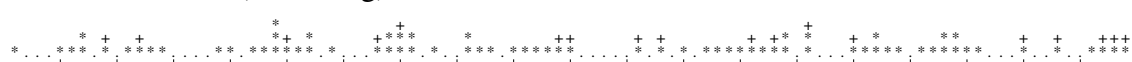
d. Secondary structure & estimated accessibility



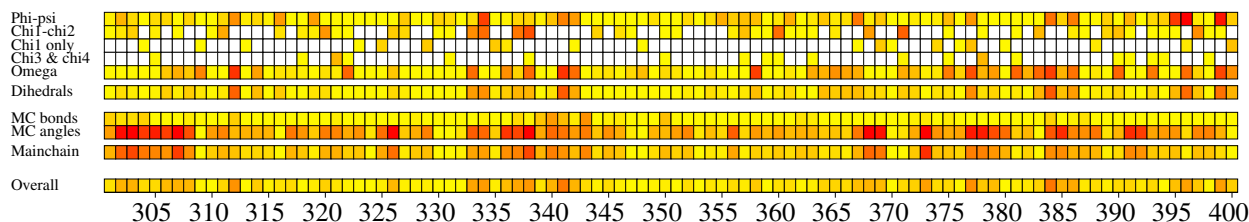
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



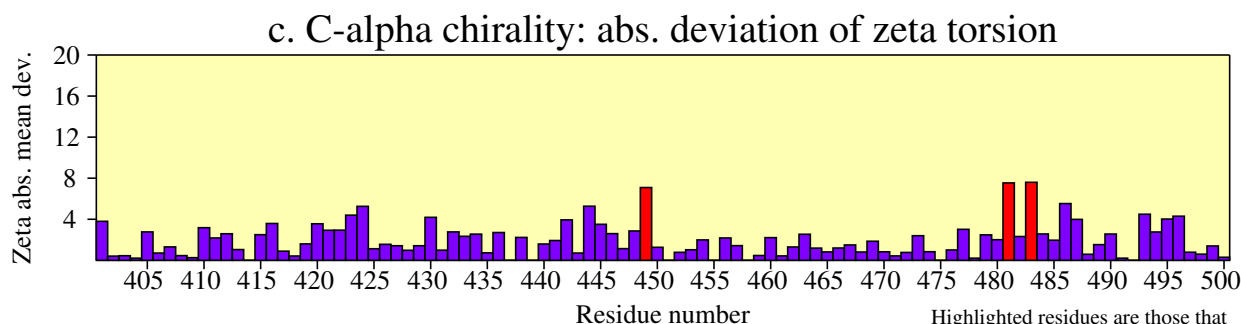
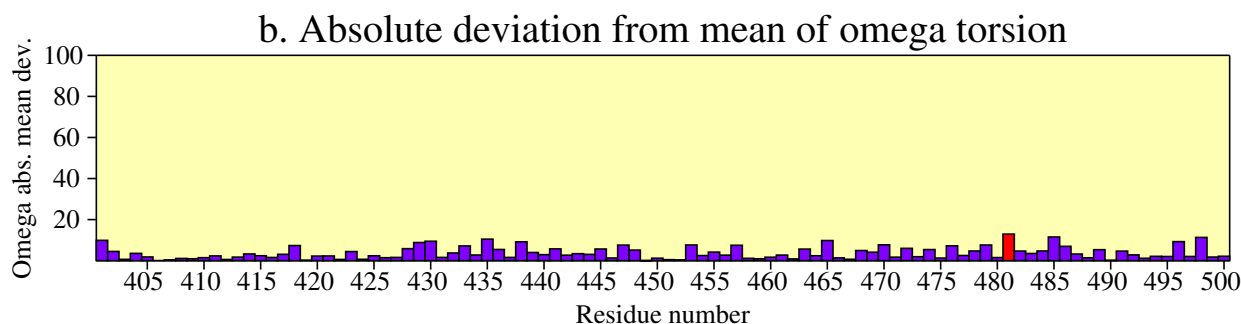
f. Max. deviation (see listing)



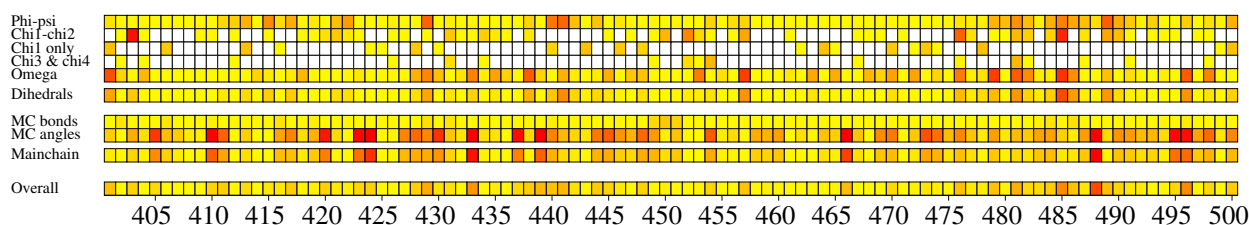
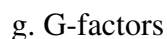
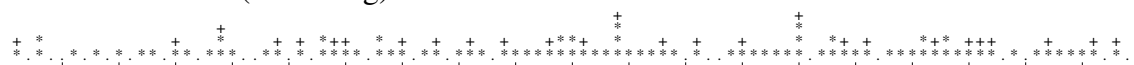
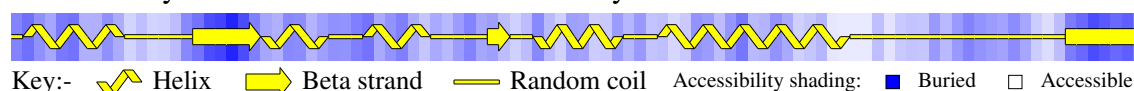
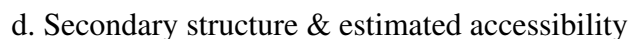
g. G-factors



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



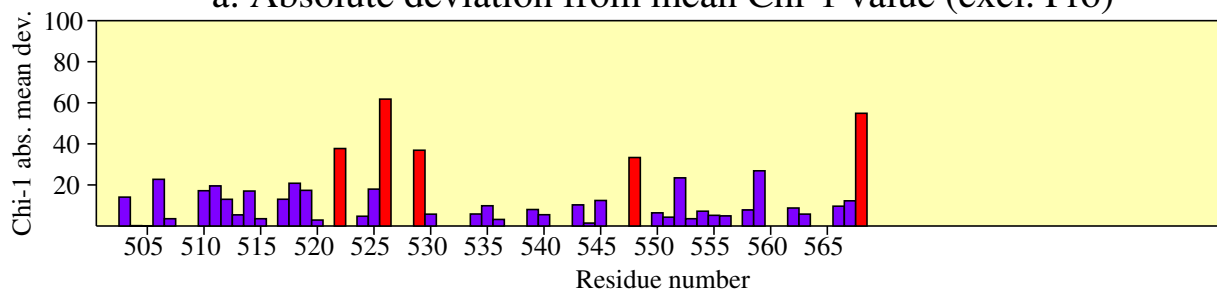
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal



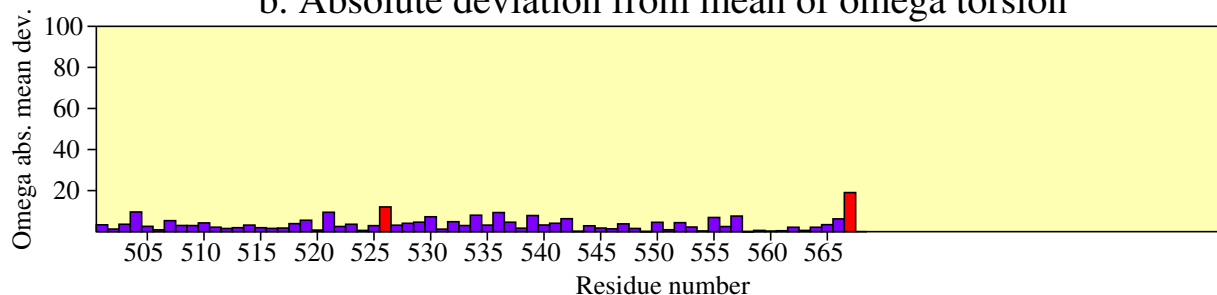
Residue properties

1p2e

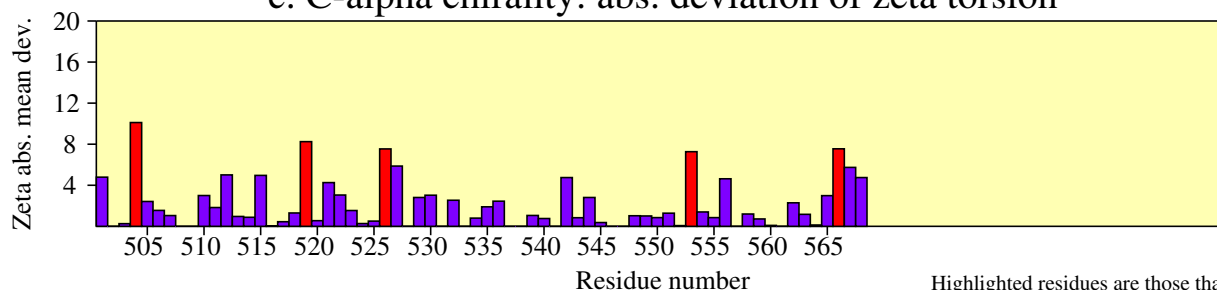
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

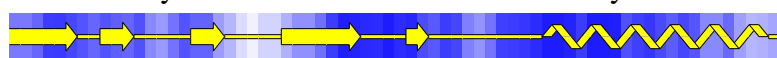


c. C-alpha chirality: abs. deviation of zeta torsion



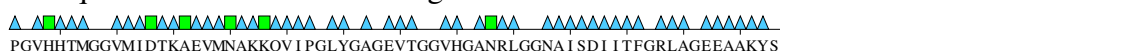
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



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

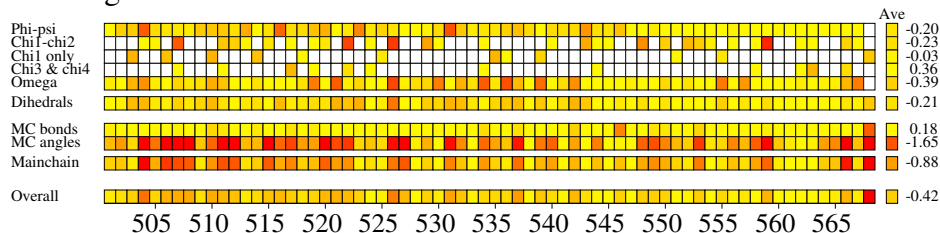
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

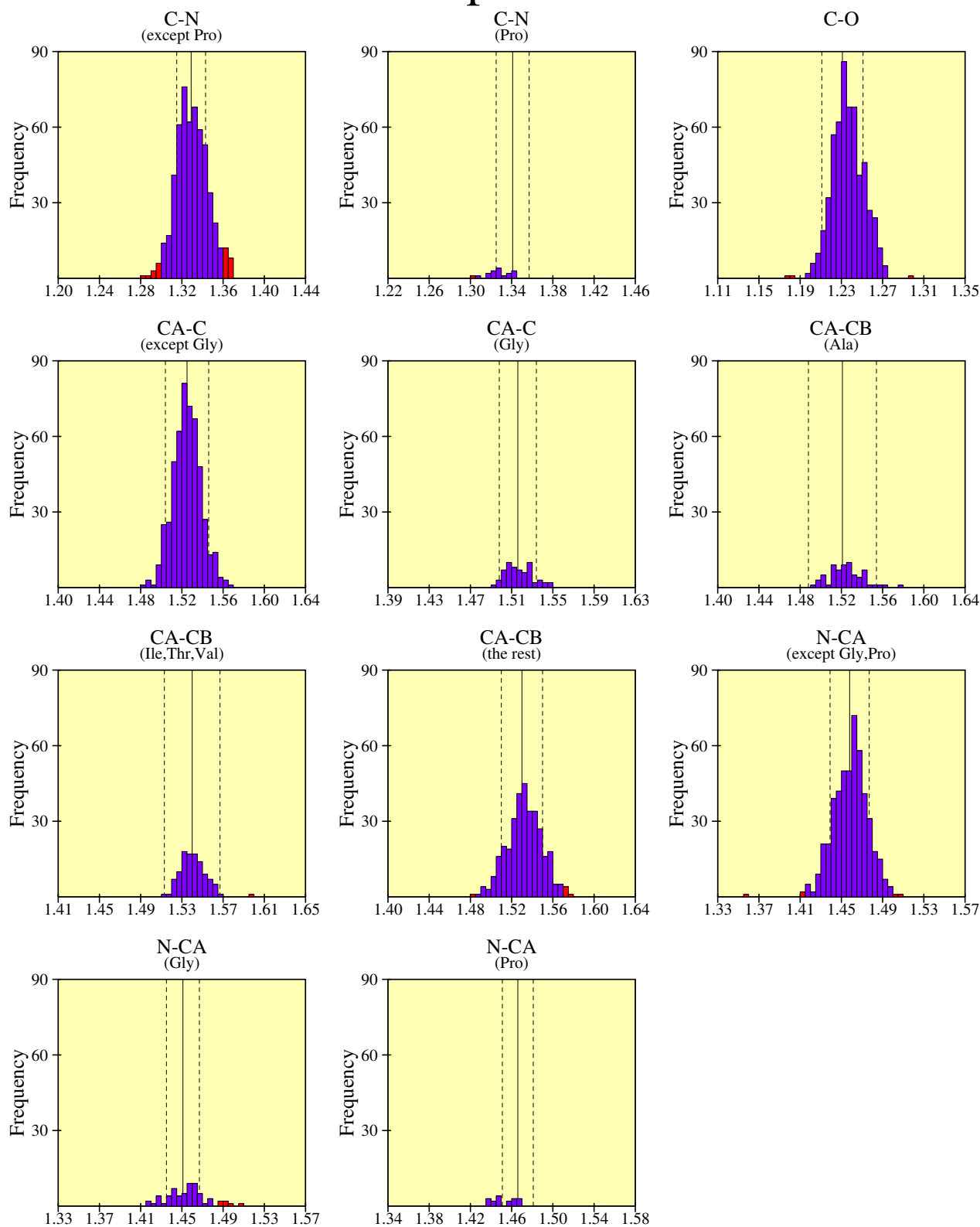


g. G-factors



Main-chain bond lengths

1p2e

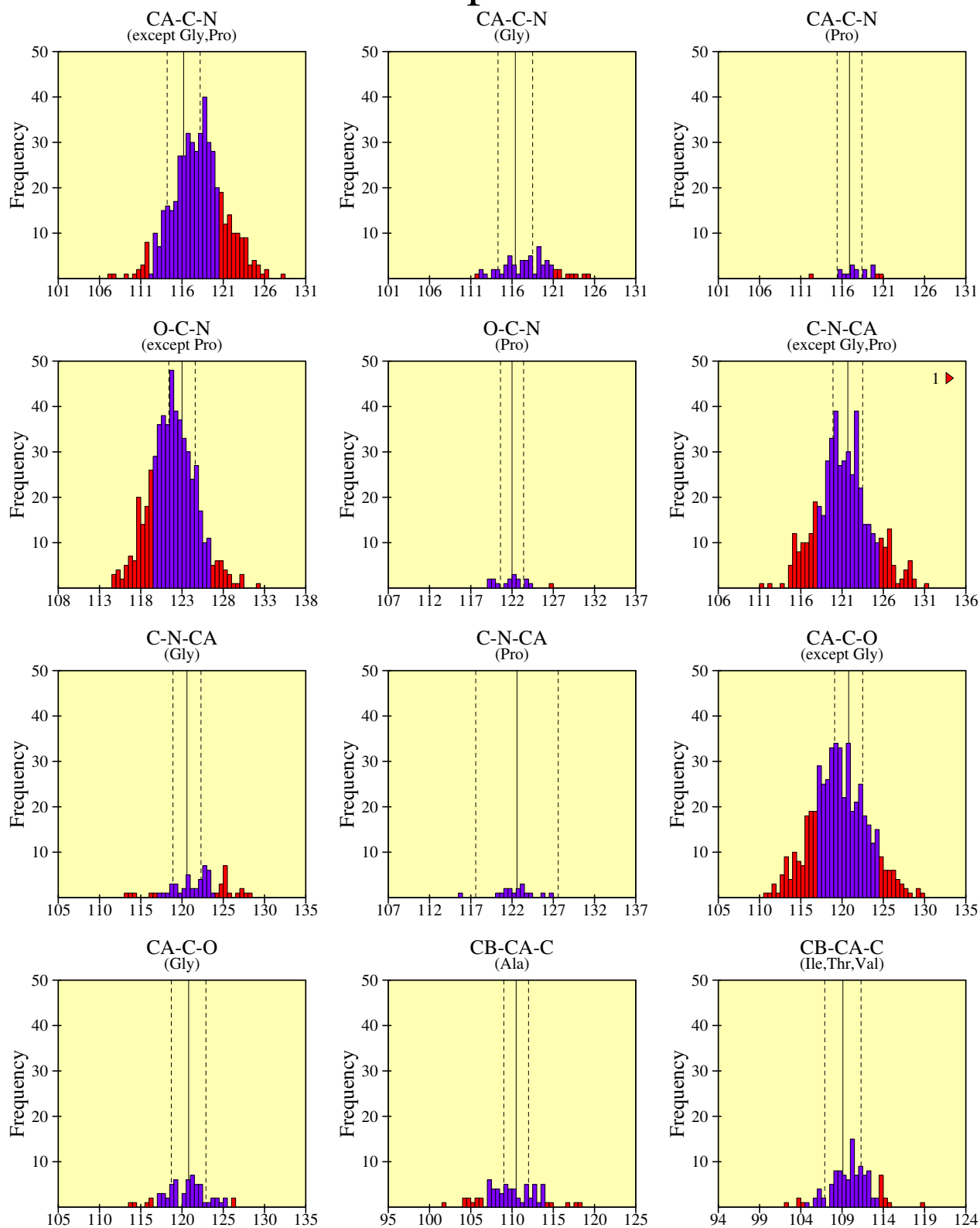


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

1p2e



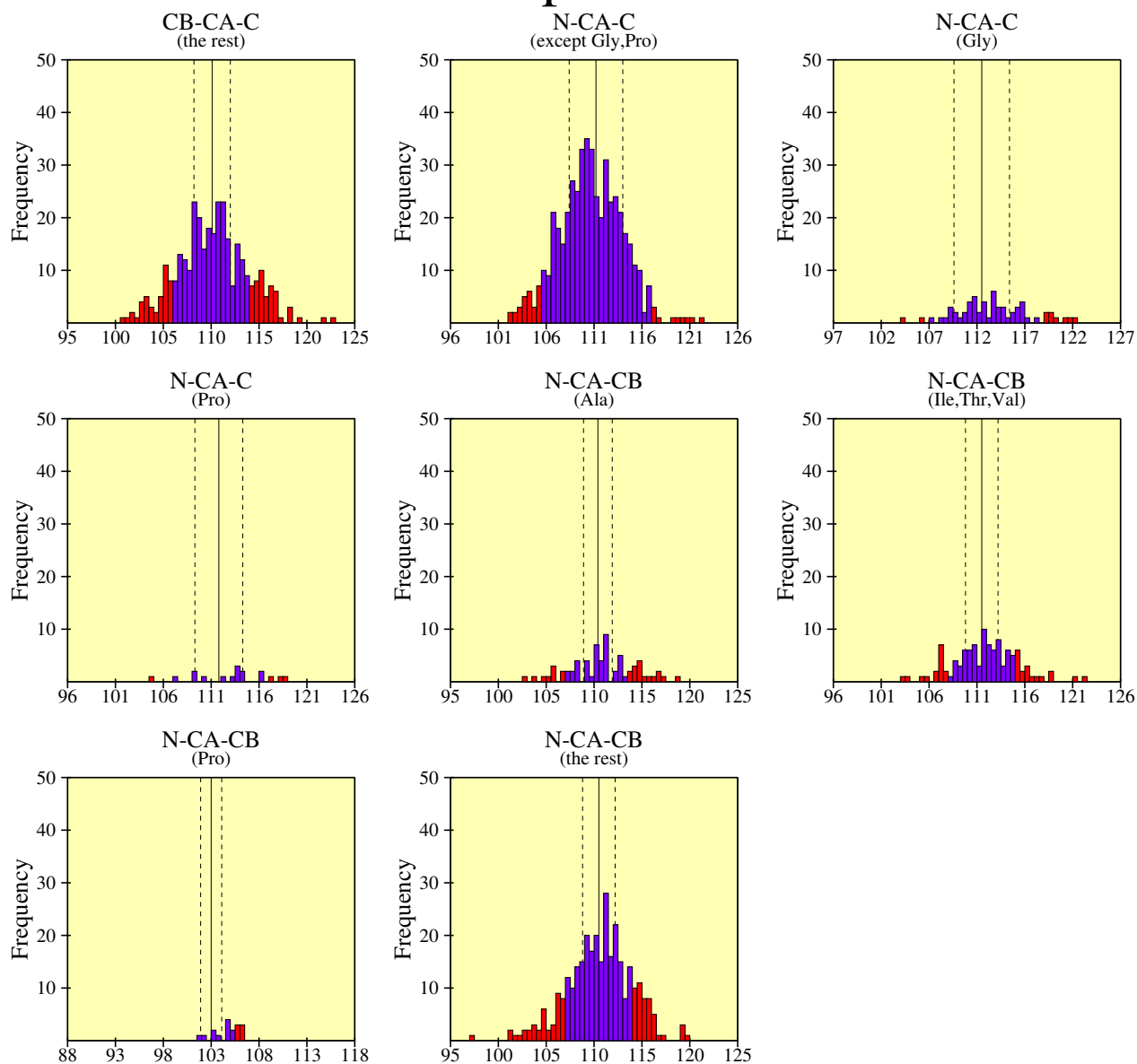
Black bars > 2.0 st. devs. from mean.

◀ 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

1p2e

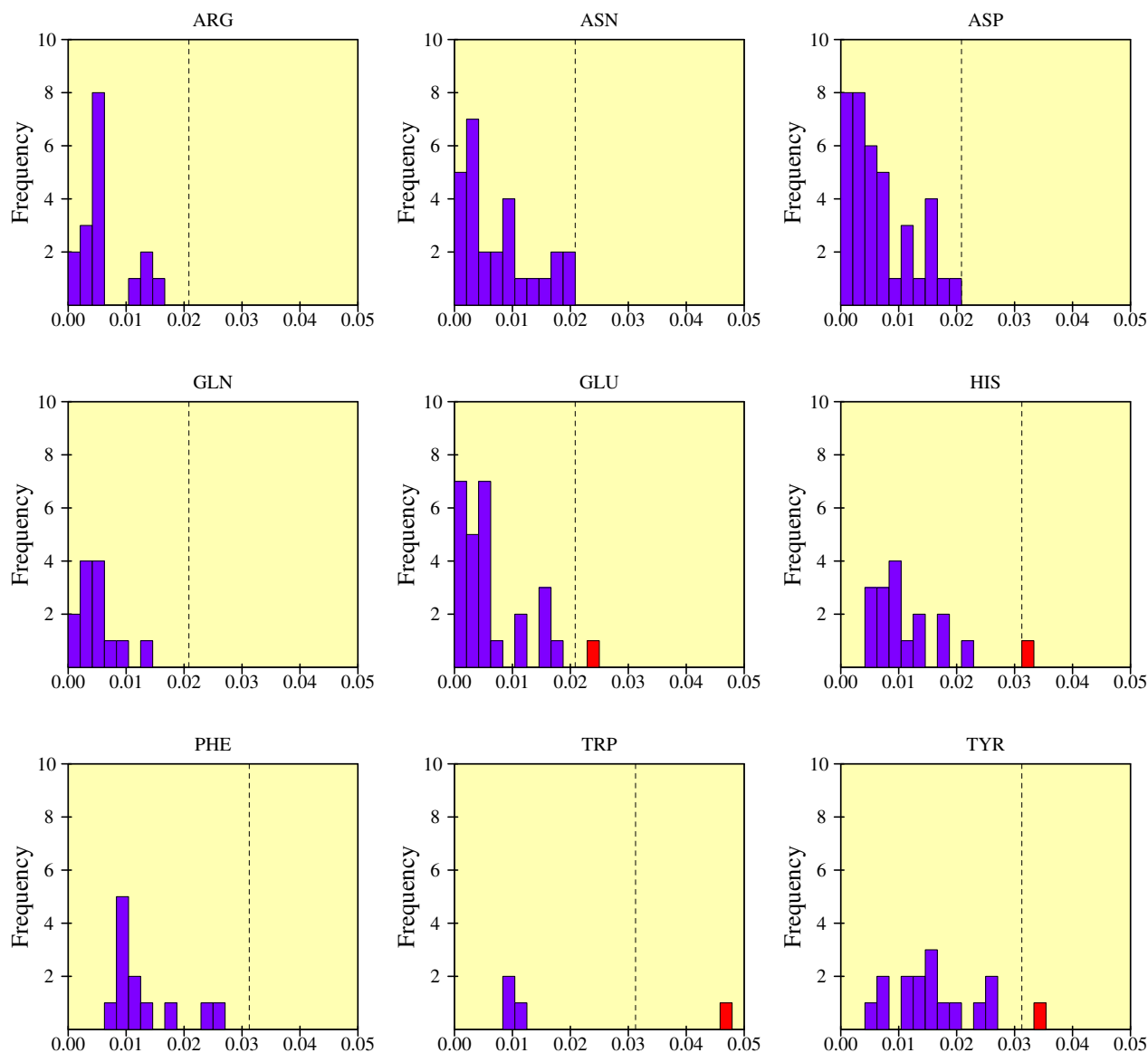


Black bars > 2.0 st. devs. from mean.

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

RMS distances from planarity

1p2e

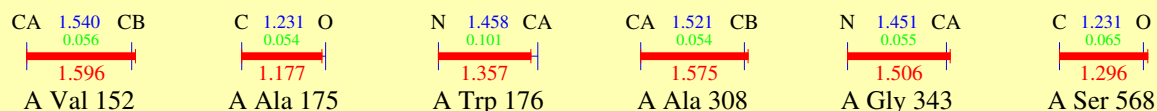


Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

Distorted geometry

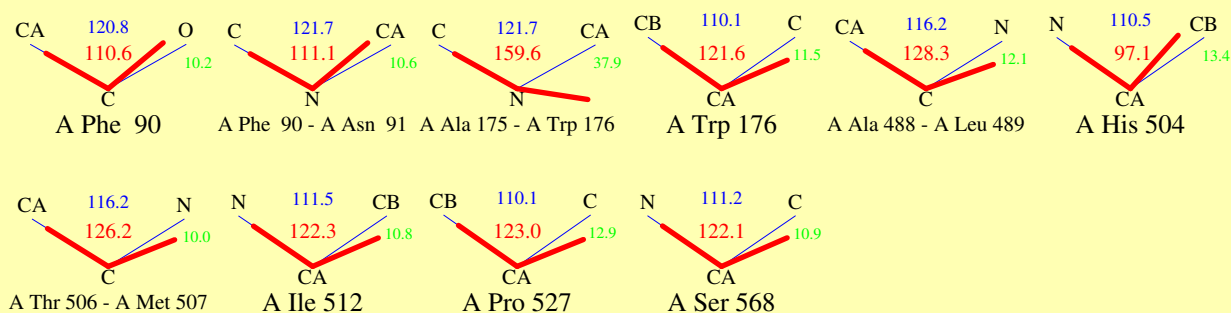
1p2e

Main-chain bond lengths



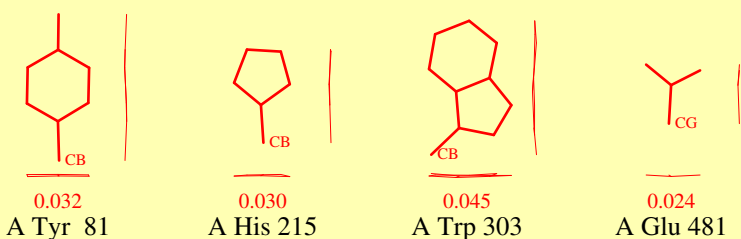
Bonds differing by > 0.05Å from small-molecule values. Values shown: "ideal", difference, actual

Main-chain bond angles



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

Planar groups



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