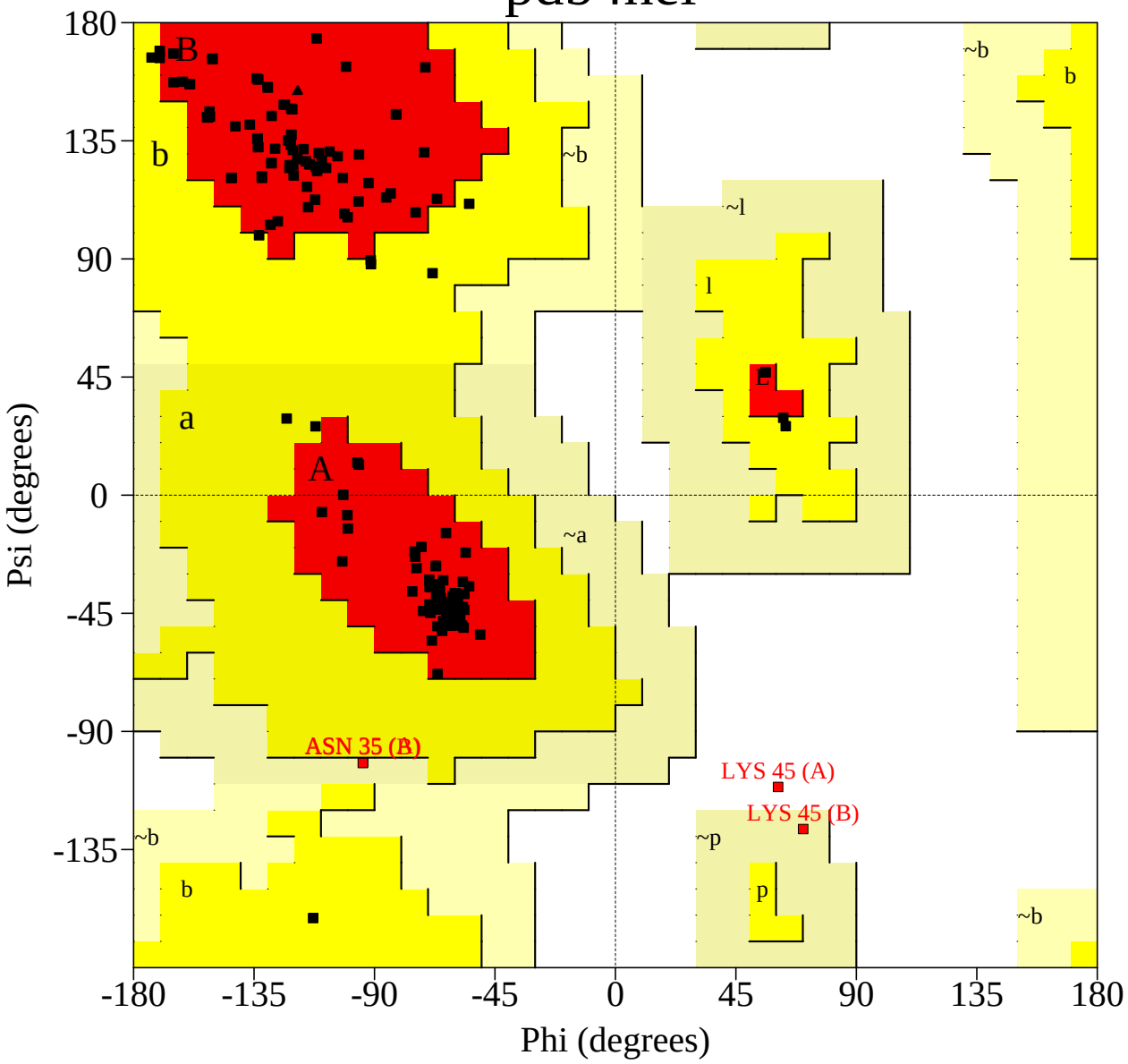
PROCHECK

Ramachandran Plot

pdb4hei



Plot statistics

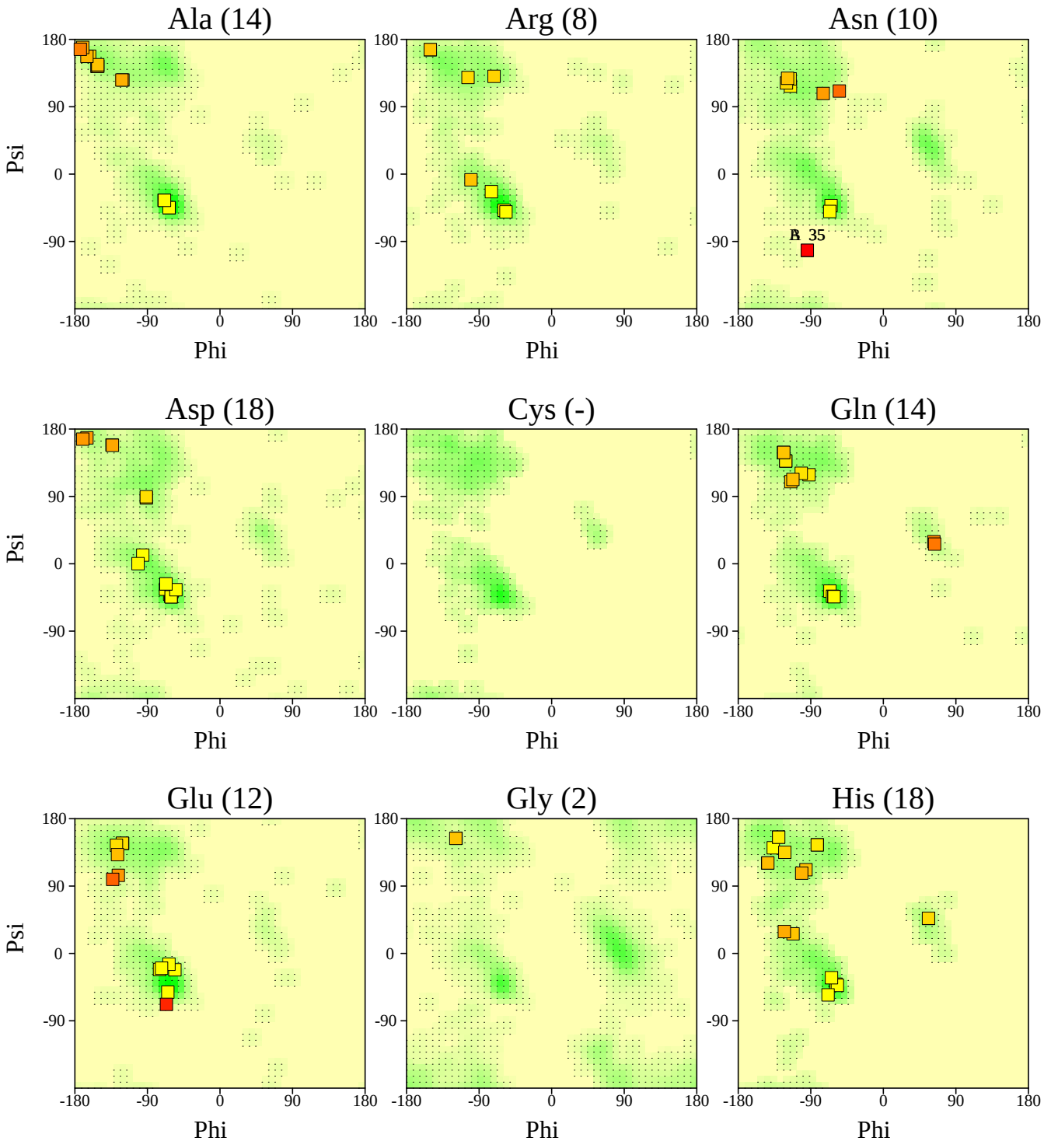
Residues in most favoured regions [A,B,L]	160	90.4%
Residues in additional allowed regions [a,b,l,p]	13	7.3%
Residues in generously allowed regions [~a,~b,~l,~p]	3	1.7%
Residues in disallowed regions	1	0.6%
	----	------
Number of non-glycine and non-proline residues	177	100.0%
Number of end-residues (excl. Gly and Pro)	4	
Number of glycine residues (shown as triangles)	2	
Number of proline residues	0	

Total number of residues	183	

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

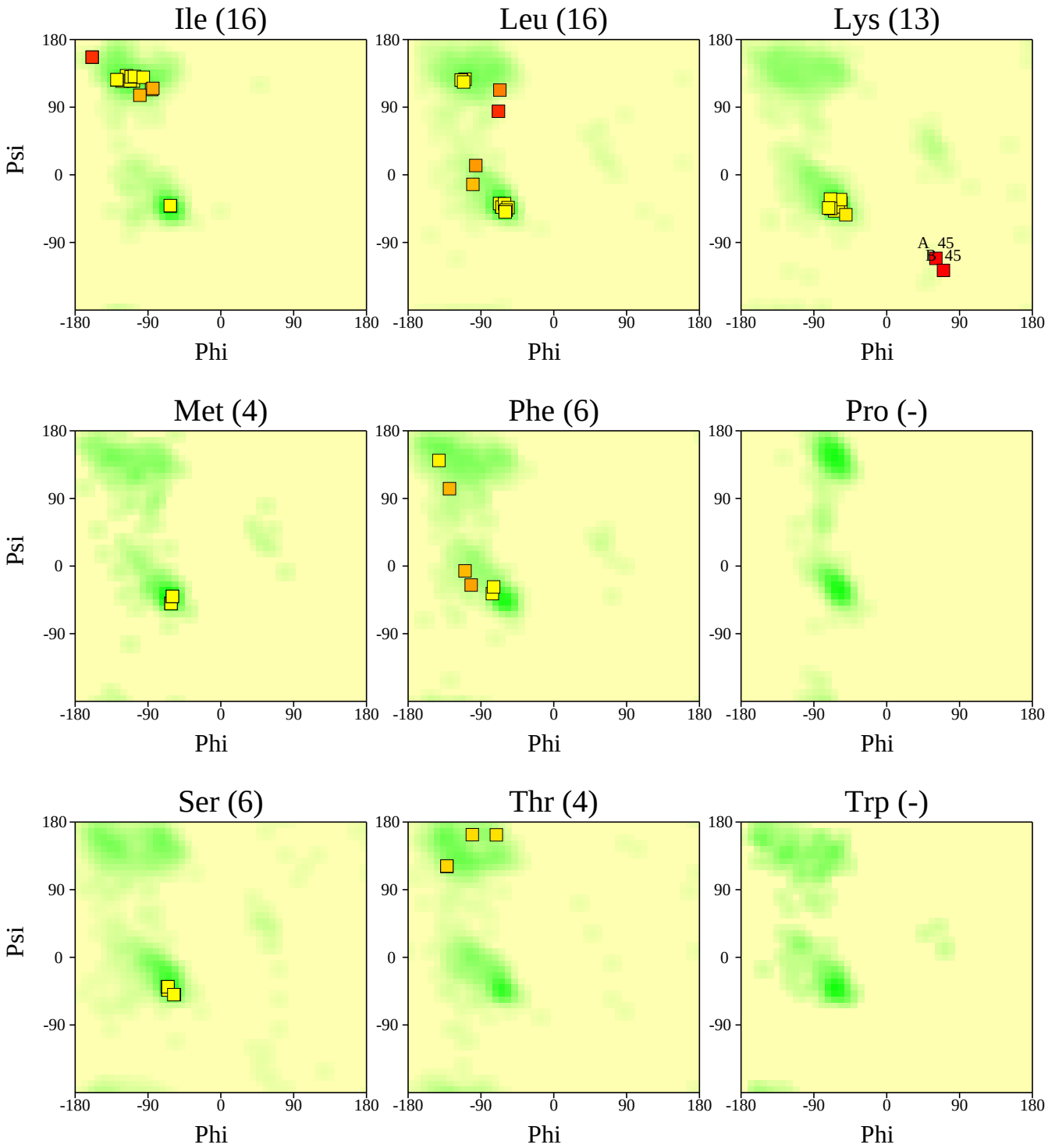
pdb4hei



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

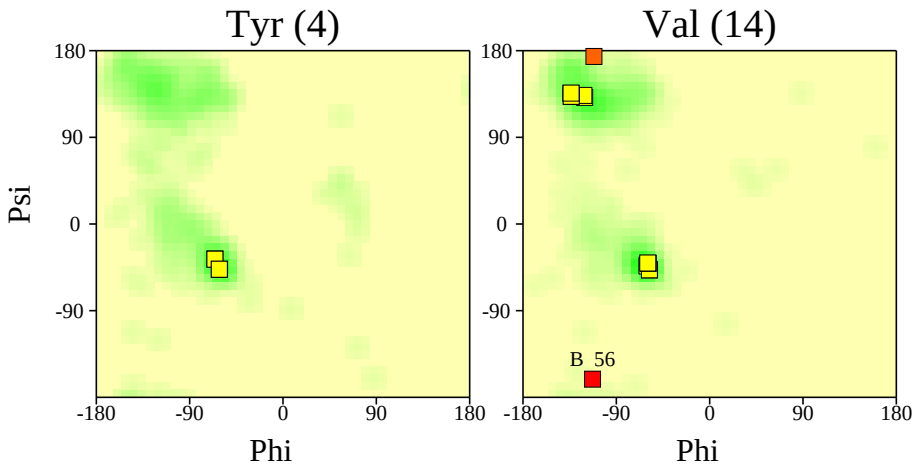
pdb4hei



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

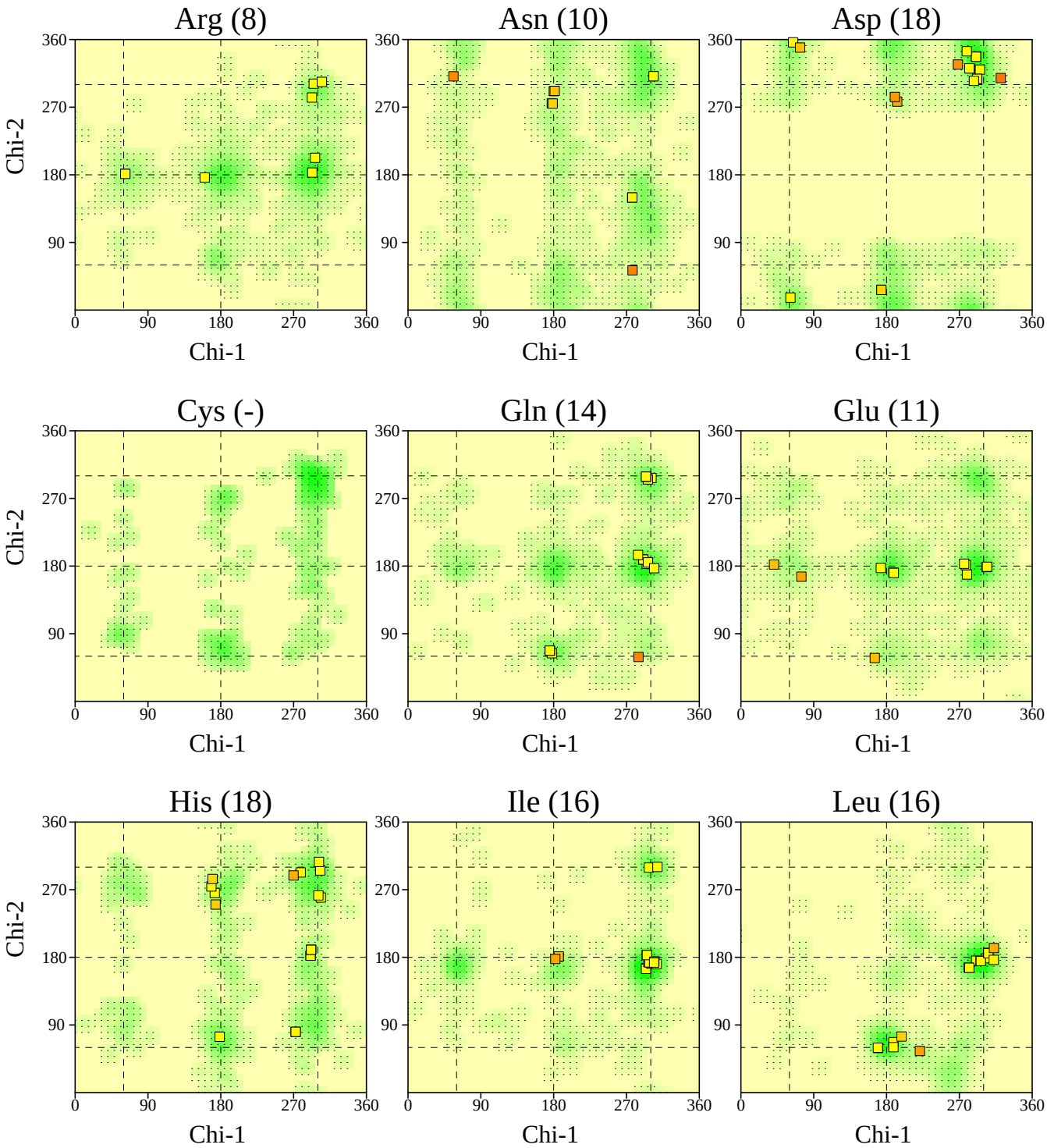
pdb4hei



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

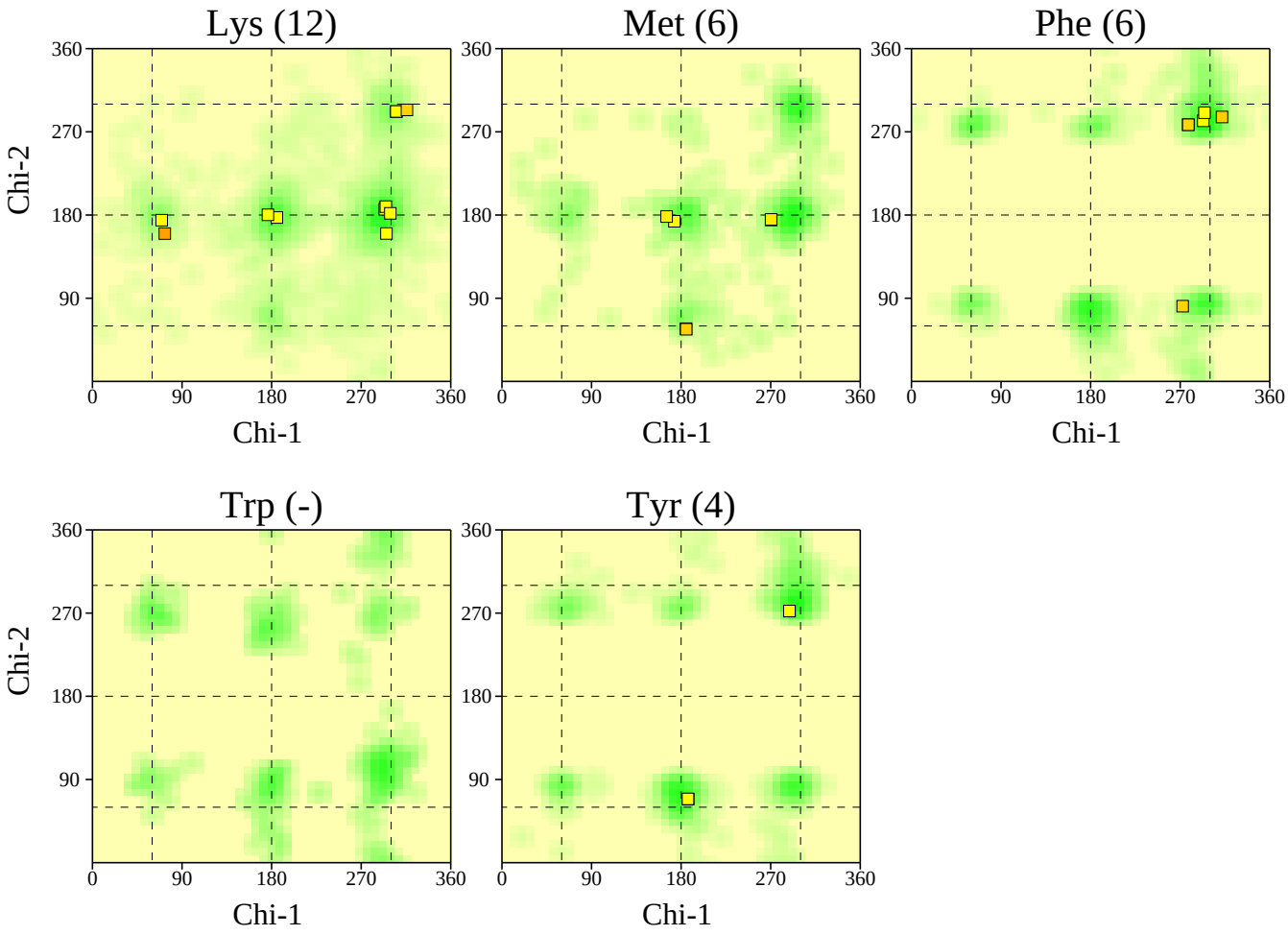
pdb4hei



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

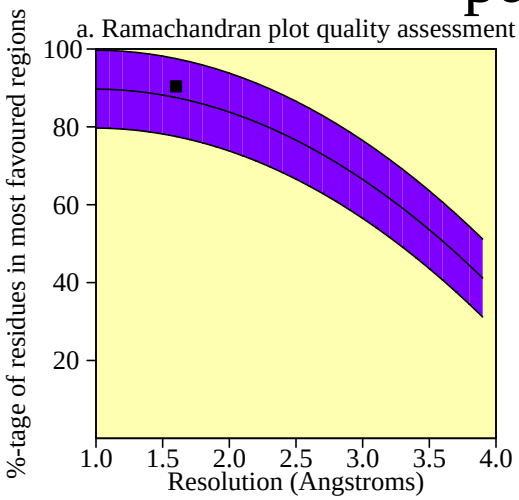
pdb4hei



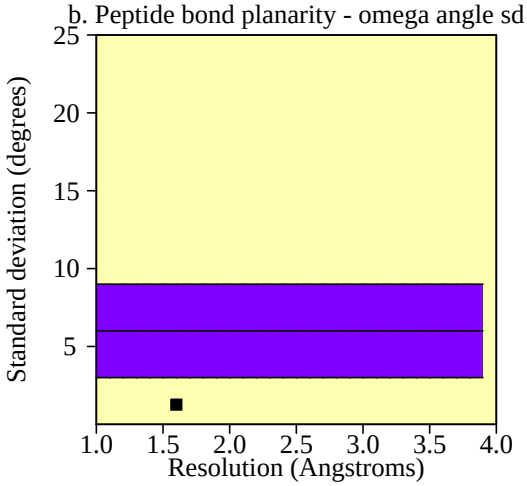
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

Main-chain parameters
pdb4hei

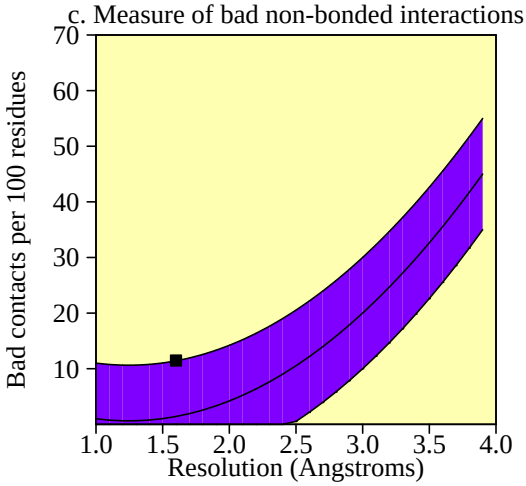
a. Ramachandran plot quality assessment



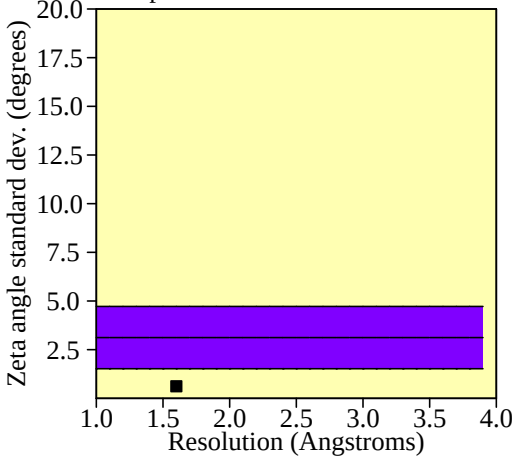
b. Peptide bond planarity - omega angle sd



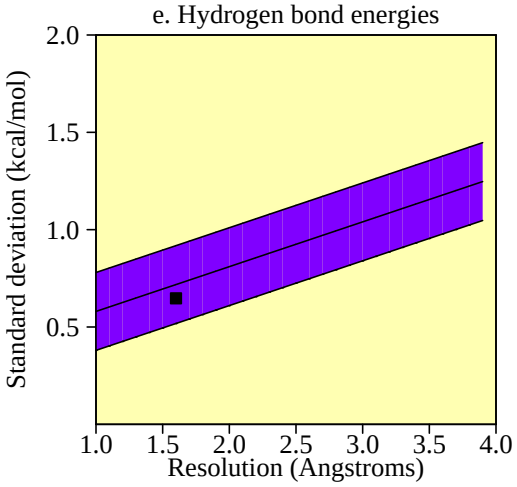
c. Measure of bad non-bonded interactions



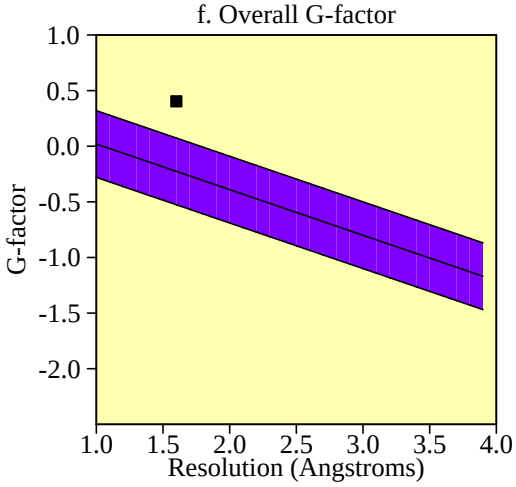
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor

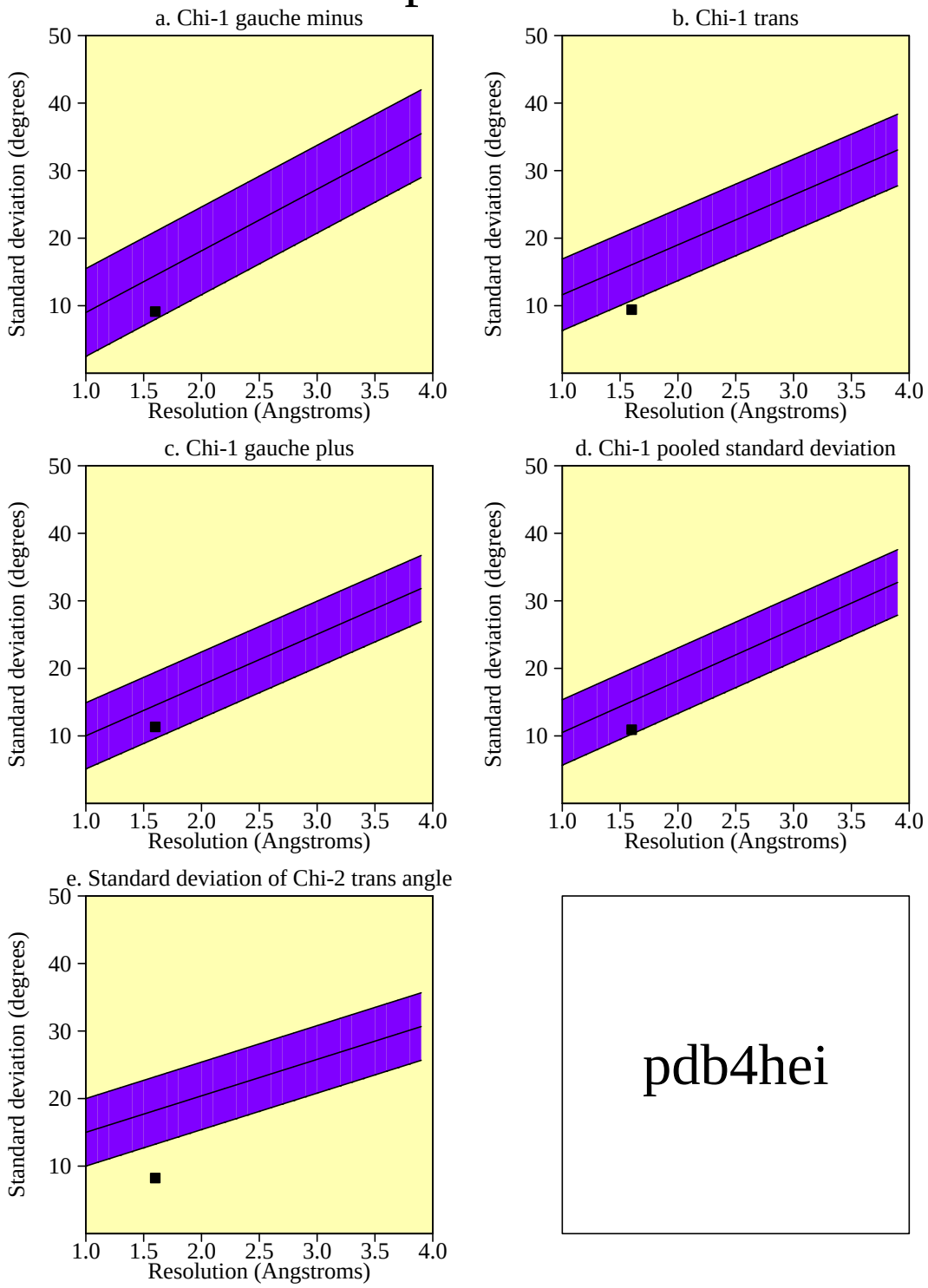


Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values: Typical value	Comparison values: Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	177	90.4	87.5	10.0	0.3	Inside
b. Omega angle st dev	181	1.3	6.0	3.0	-1.6	BETTER
c. Bad contacts / 100 residues	21	11.5	1.4	10.0	1.0	WORSE
d. Zeta angle st dev	179	0.6	3.1	1.6	-1.6	BETTER
e. H-bond energy st dev	136	0.6	0.7	0.2	-0.4	Inside
f. Overall G-factor	183	0.4	-0.2	0.3	2.1	BETTER

Side-chain parameters

pdb4hei

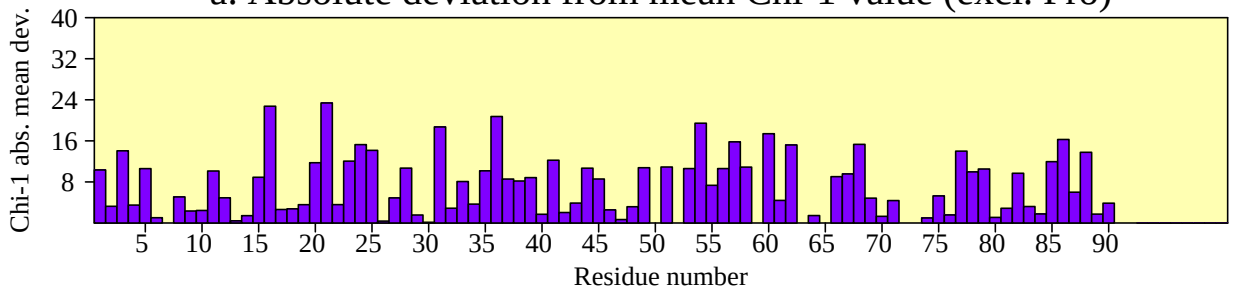


Plot statistics

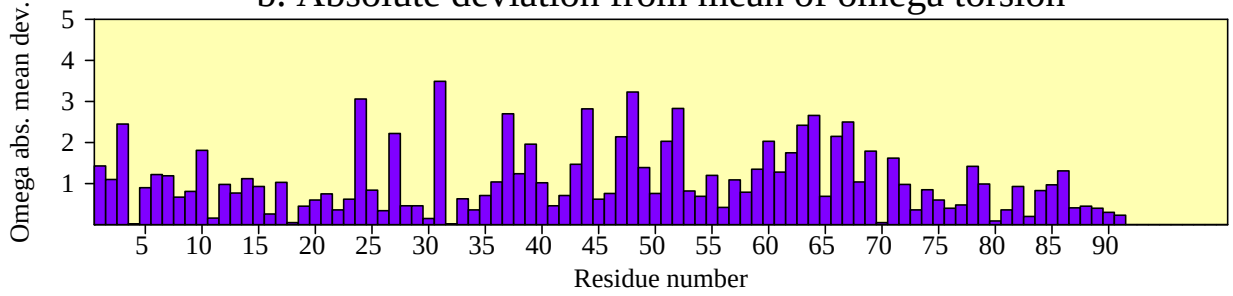
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	12	9.1	14.5	6.5	-0.8	Inside
b. Chi-1 trans st dev	56	9.4	16.1	5.3	-1.3	BETTER
c. Chi-1 gauche plus st dev	96	11.3	14.5	4.9	-0.7	Inside
d. Chi-1 pooled st dev	164	10.9	15.1	4.8	-0.9	Inside
e. Chi-2 trans st dev	58	8.2	18.2	5.0	-2.0	BETTER

Residue properties
pdb4hei

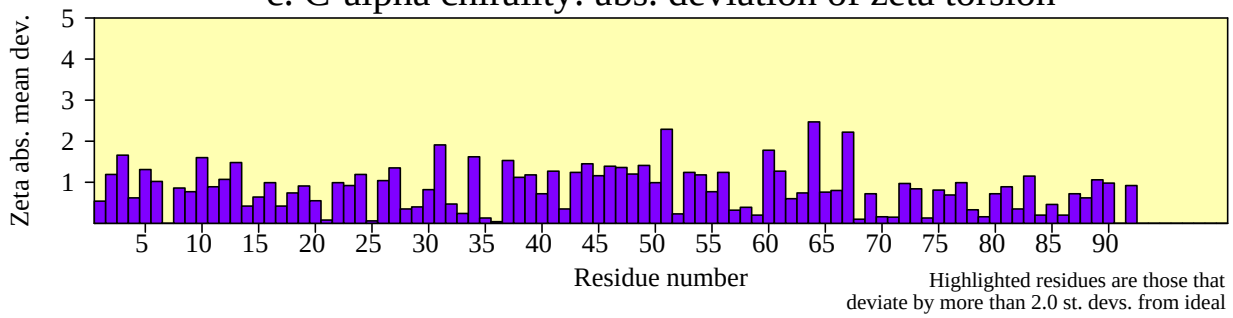
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

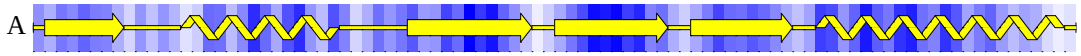


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

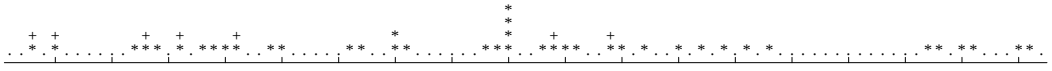


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

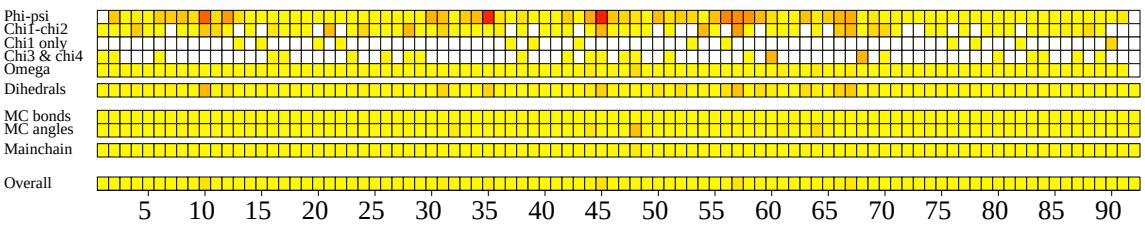
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

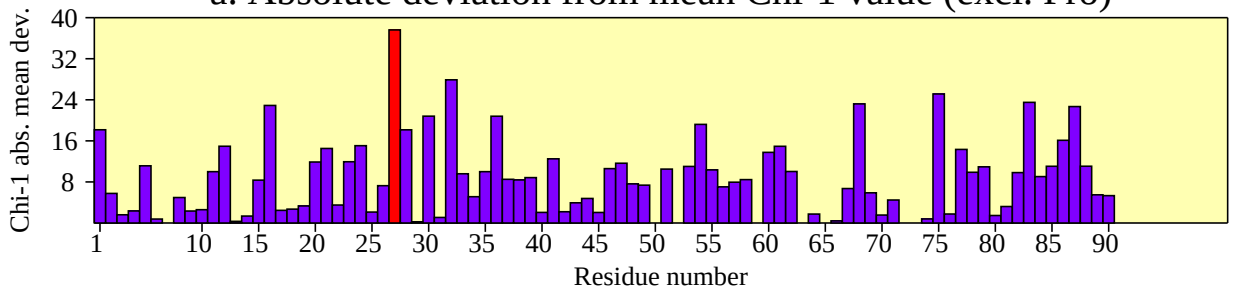


g. G-factors

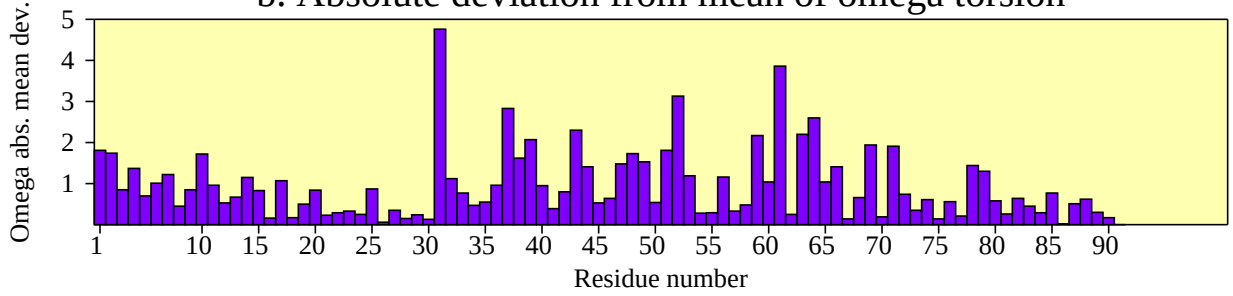


Residue properties
pdb4hei

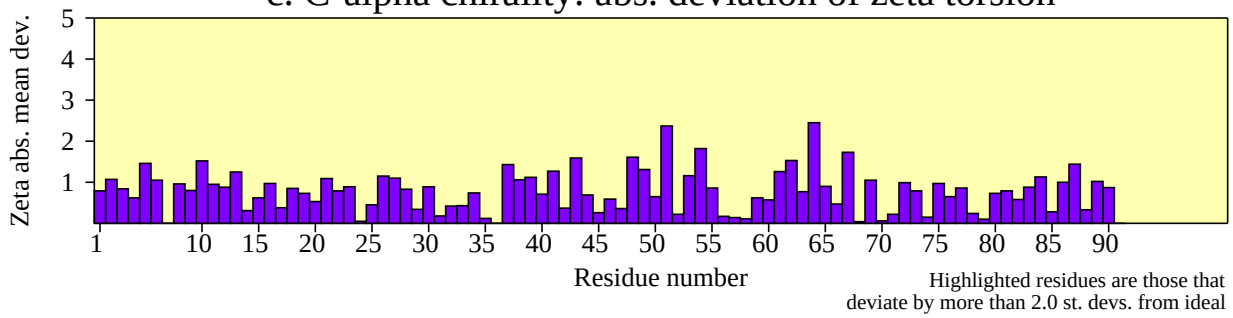
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

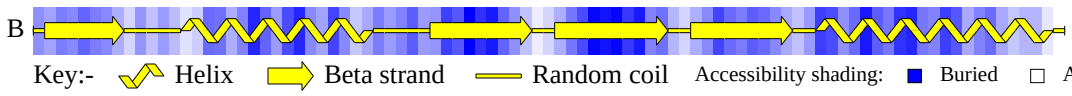


c. C-alpha chirality: abs. deviation of zeta torsion



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

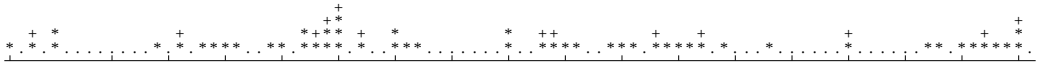
d. Secondary structure & estimated accessibility



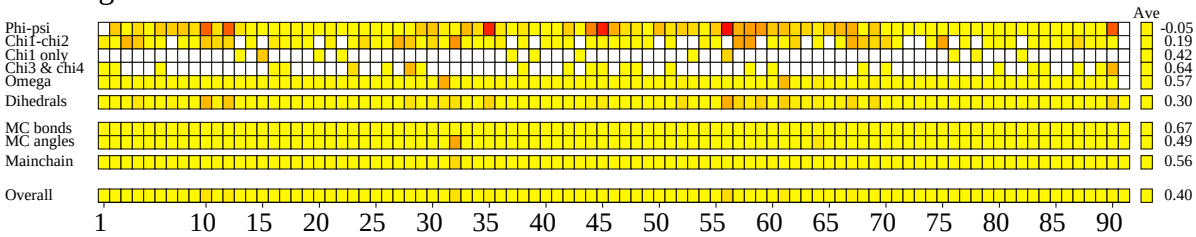
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

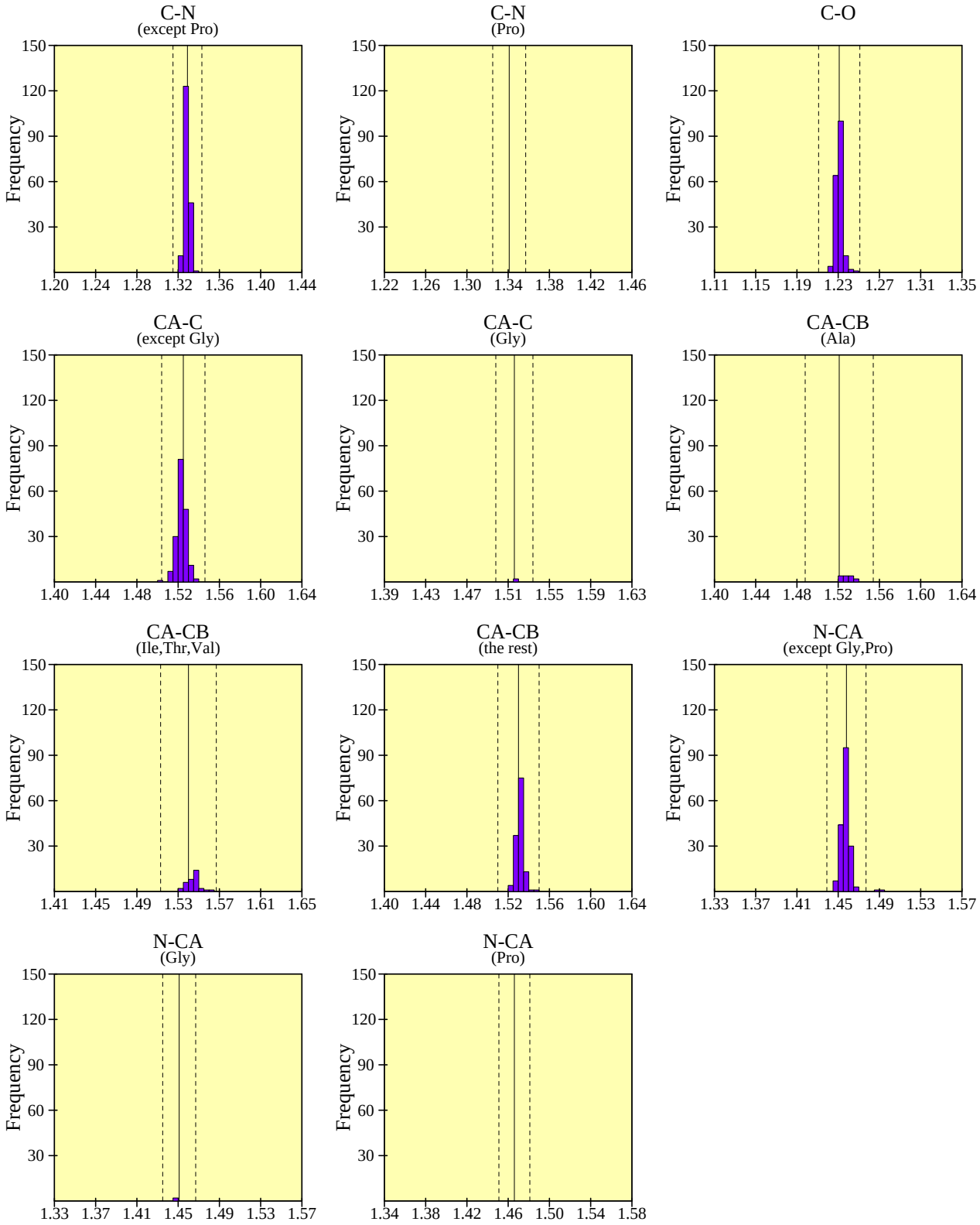


g. G-factors



Main-chain bond lengths

pdb4hei

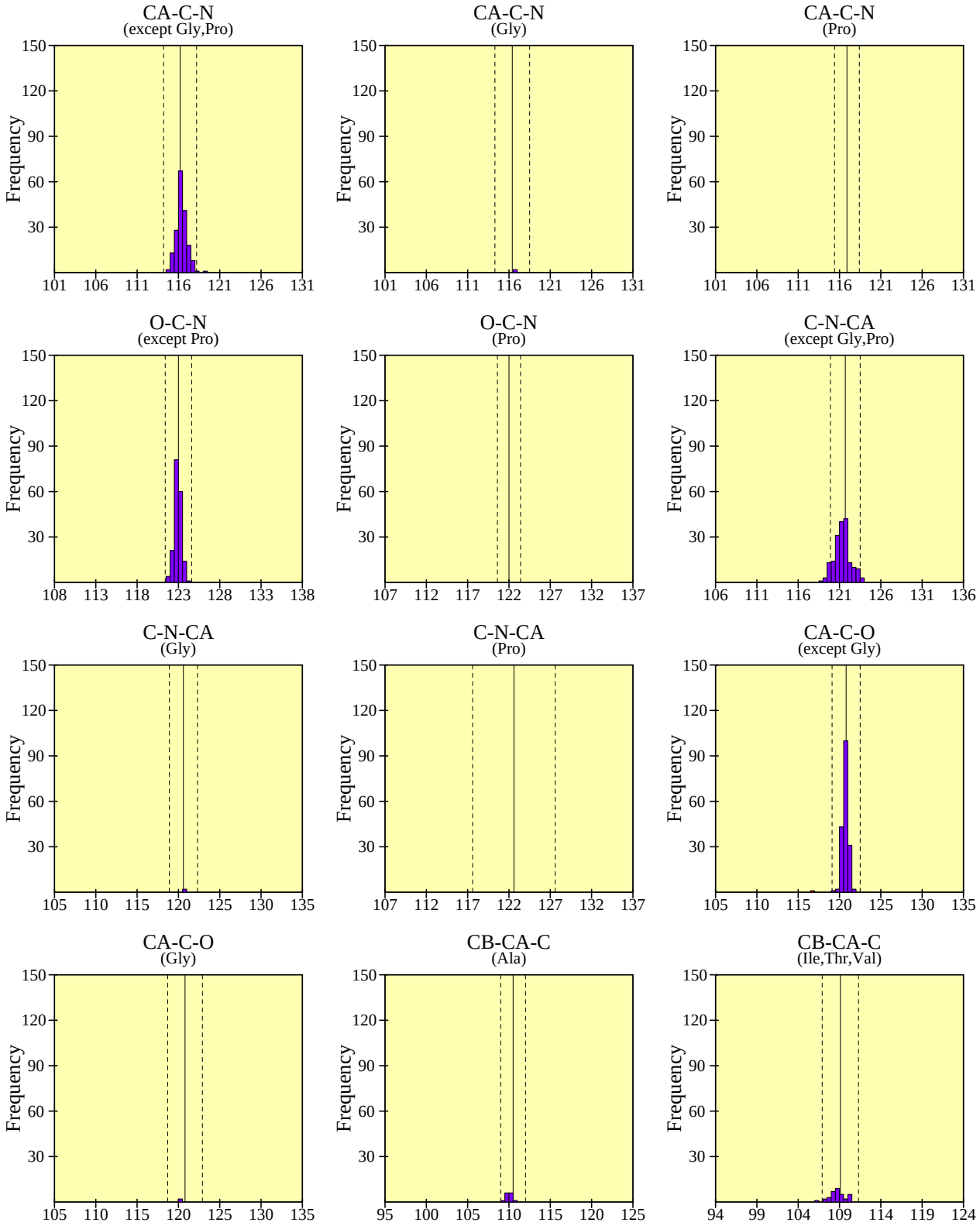


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

pdb4hei

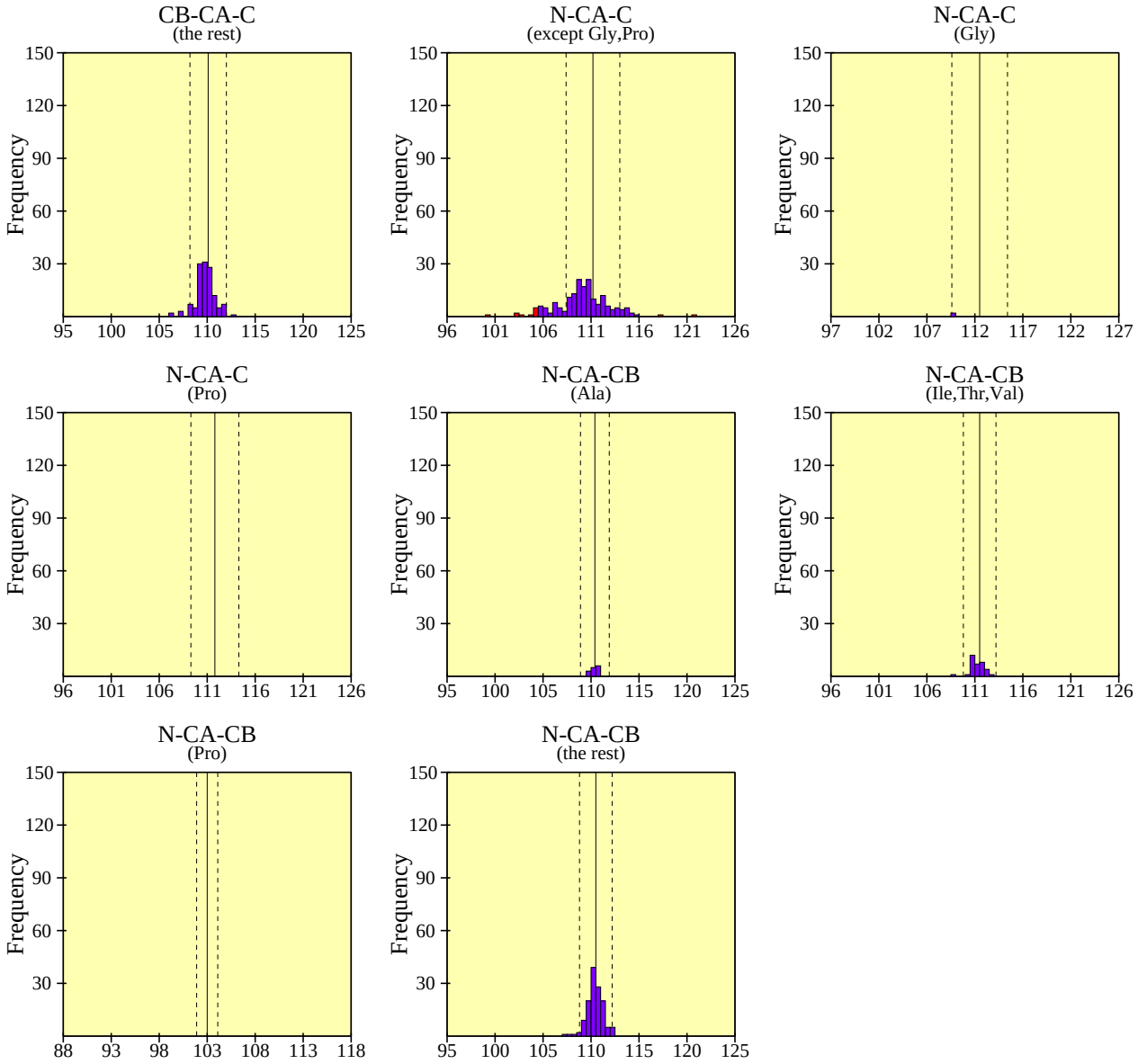


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

pdb4hei

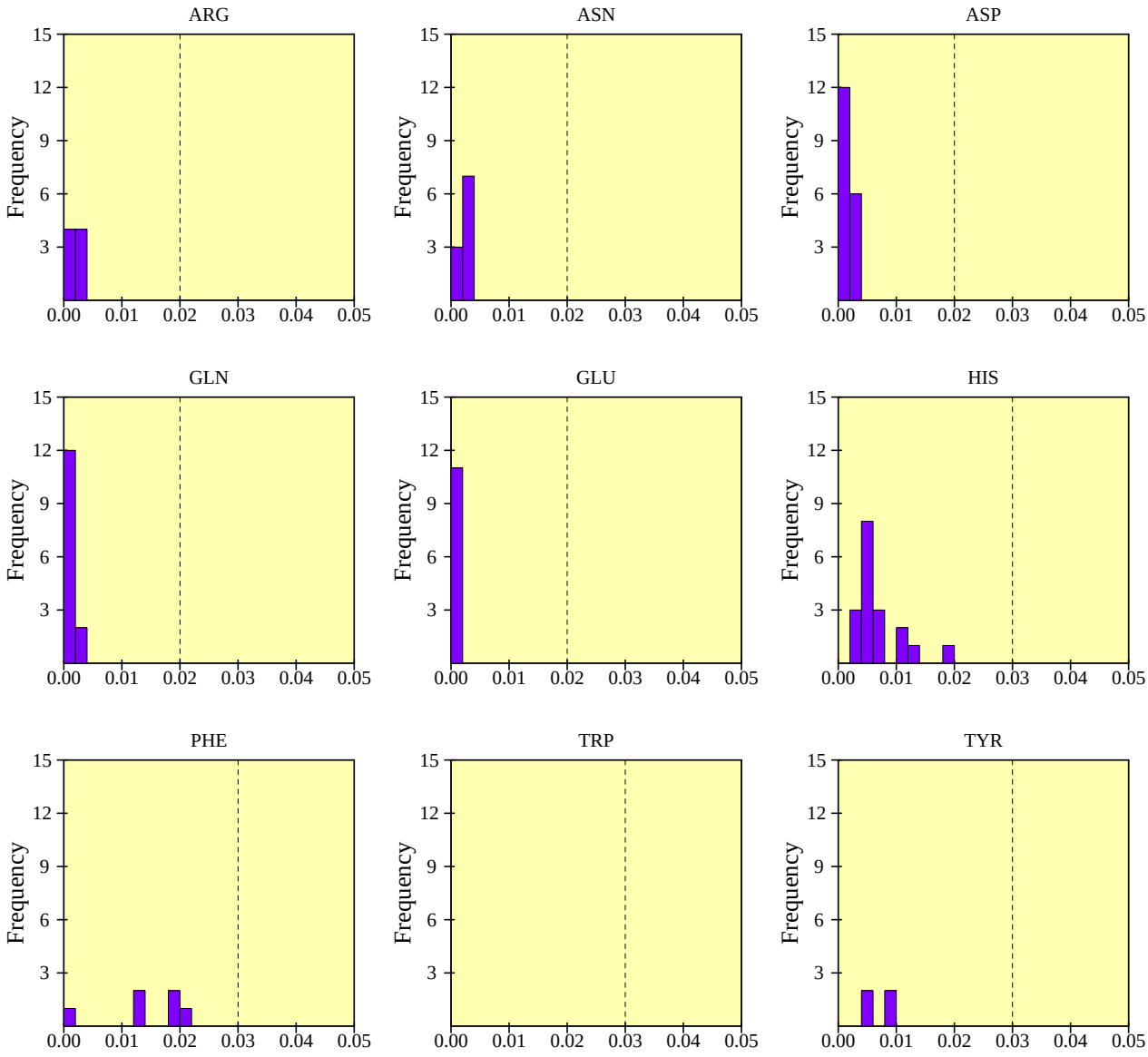


Black bars > 2.0 st. devs. from mean.

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

RMS distances from planarity

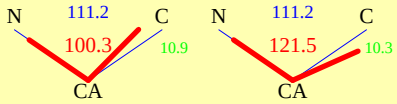
pdb4hei



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
pdb4hei

Main-chain bond angles



A Gln 48 B Asp 32

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