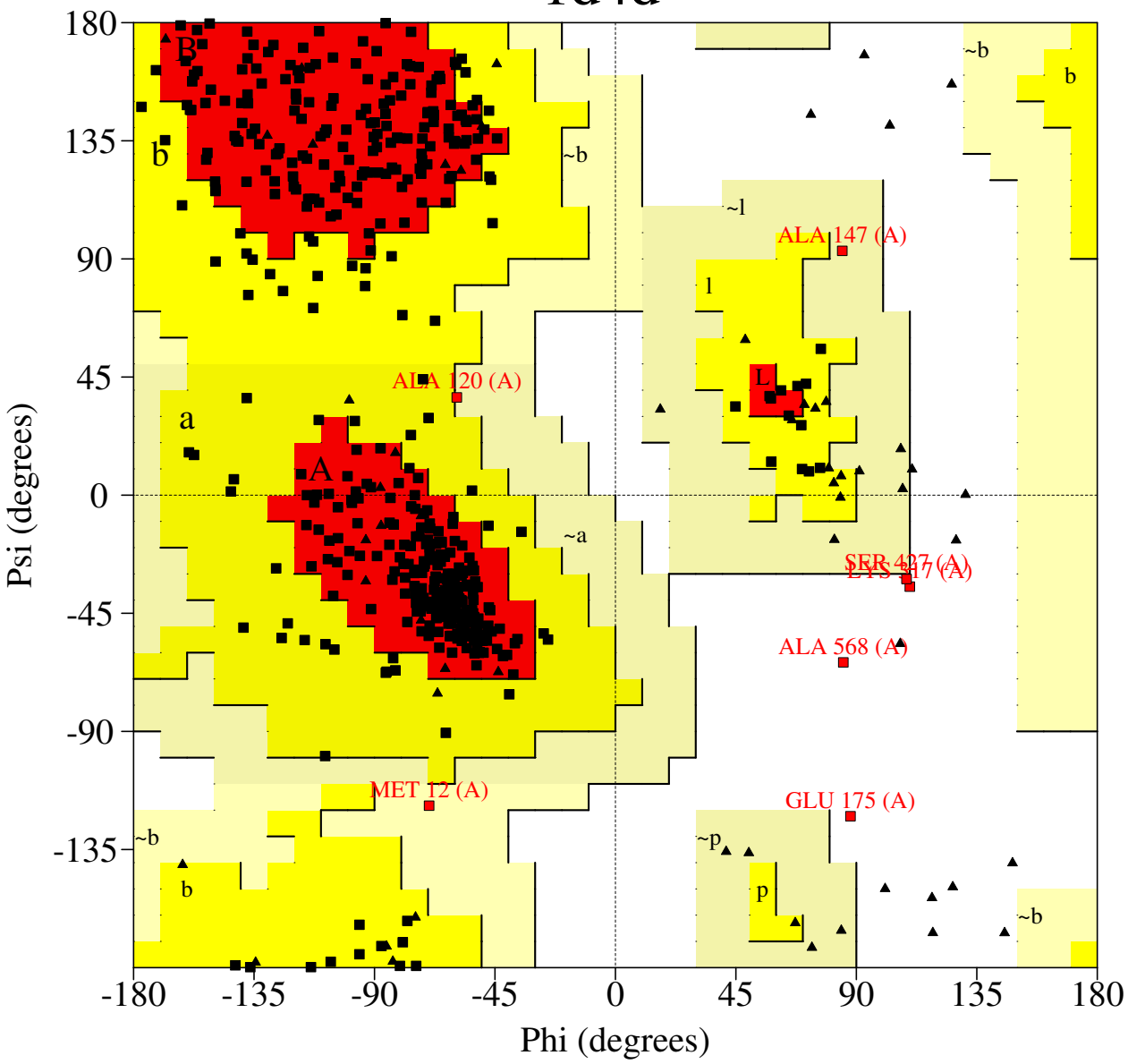
PROCHECK

Ramachandran Plot

1d4d



Plot statistics

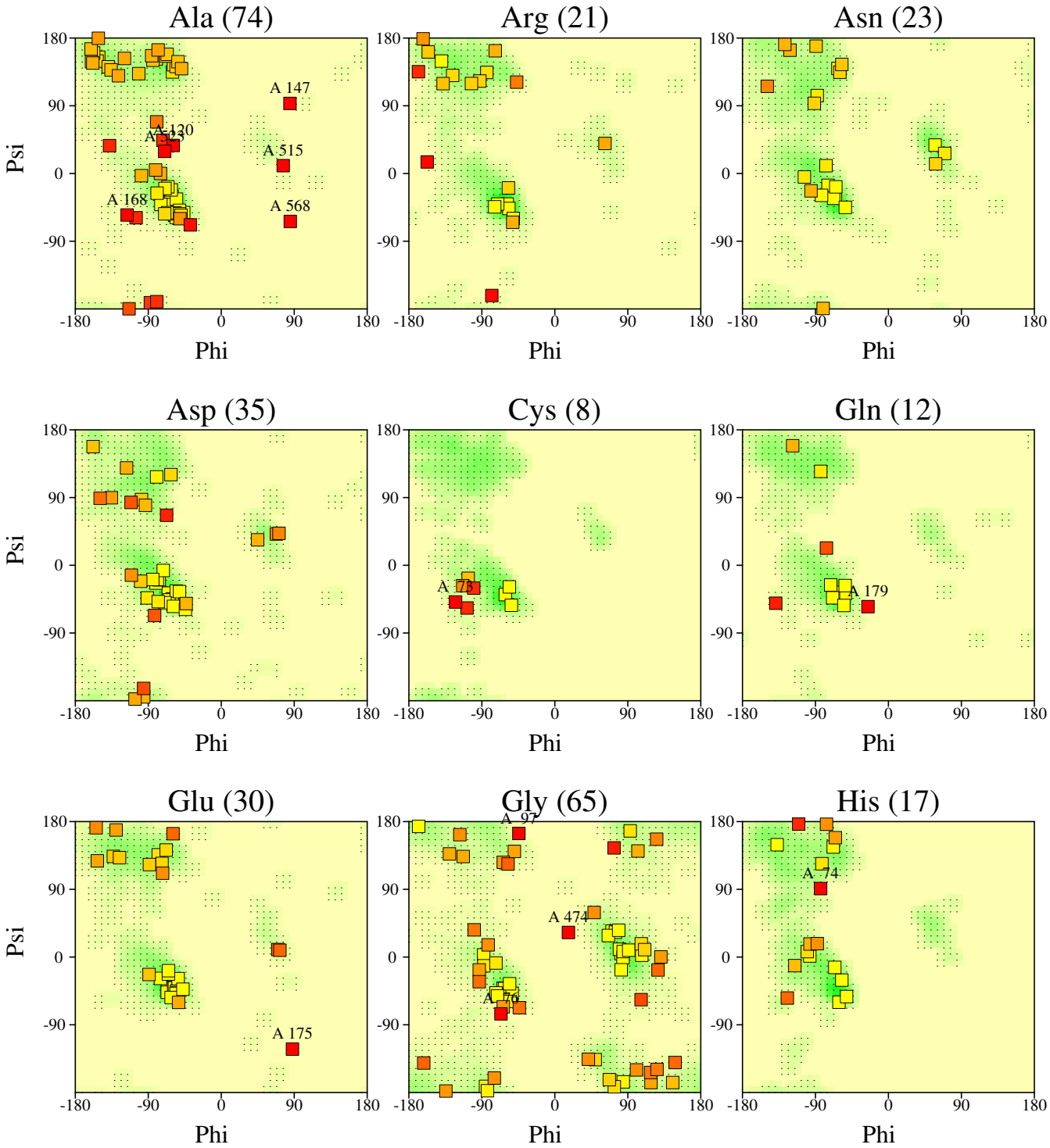
Residues in most favoured regions [A,B,L]	382	81.4%
Residues in additional allowed regions [a,b,l,p]	80	17.1%
Residues in generously allowed regions [~a,~b,~l,~p]	3	0.6%
Residues in disallowed regions	4	0.9%
	----	------
Number of non-glycine and non-proline residues	469	100.0%
Number of end-residues (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

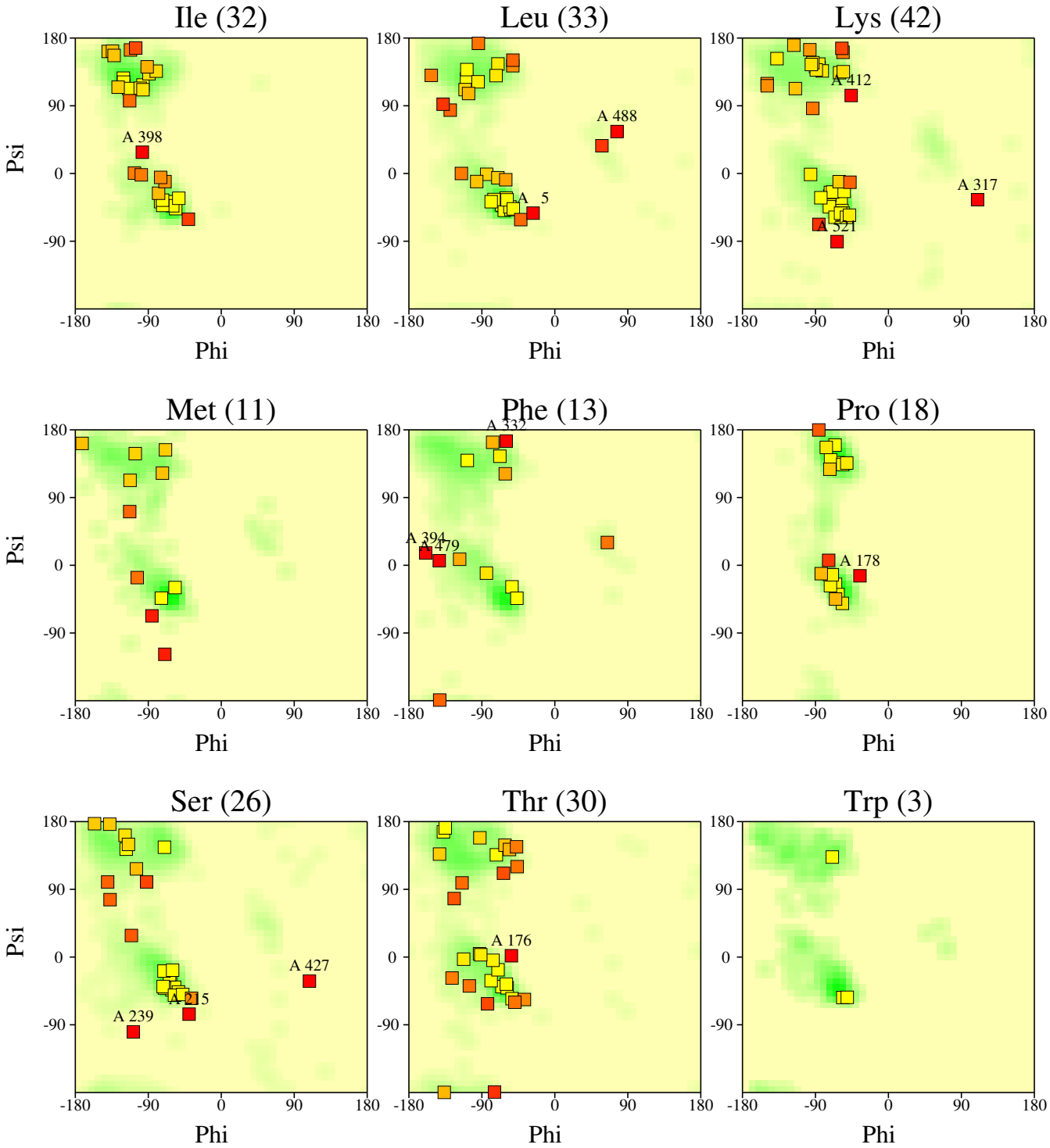
1d4d



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

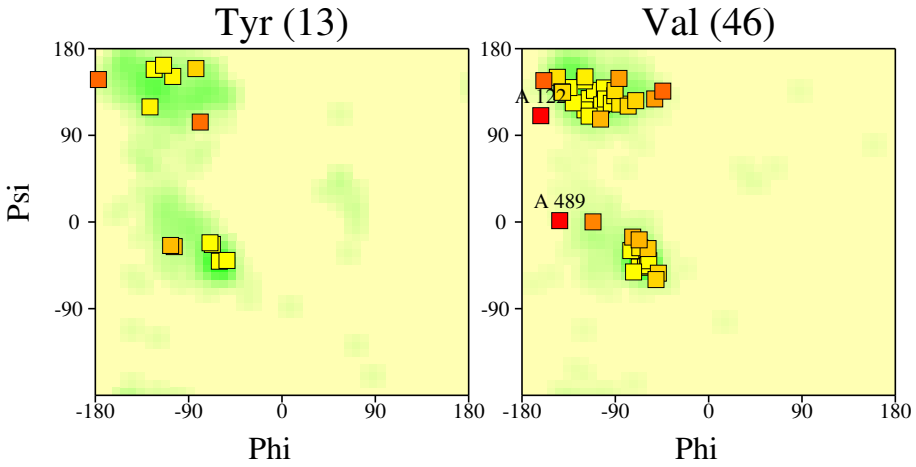
1d4d



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

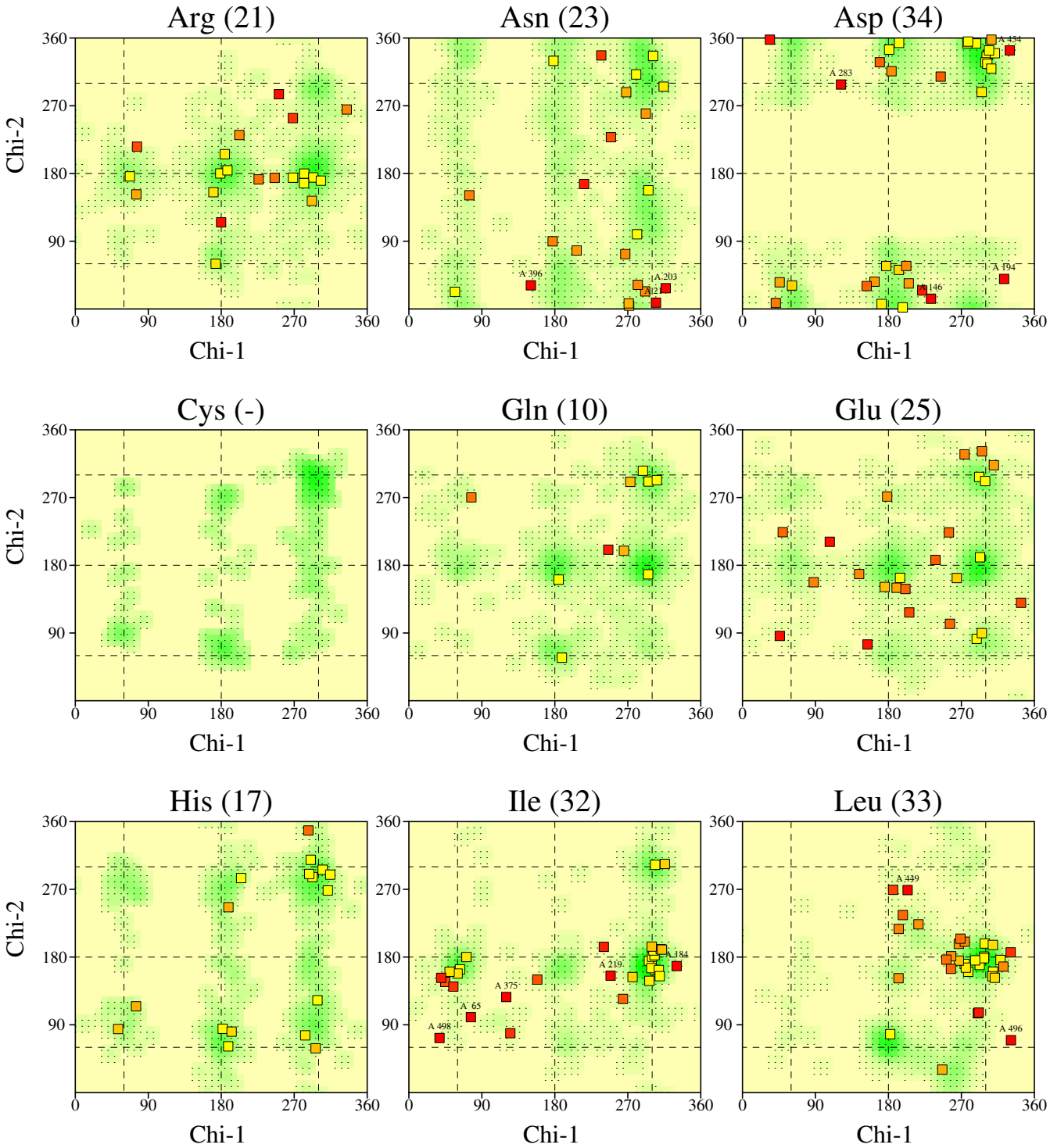
1d4d



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

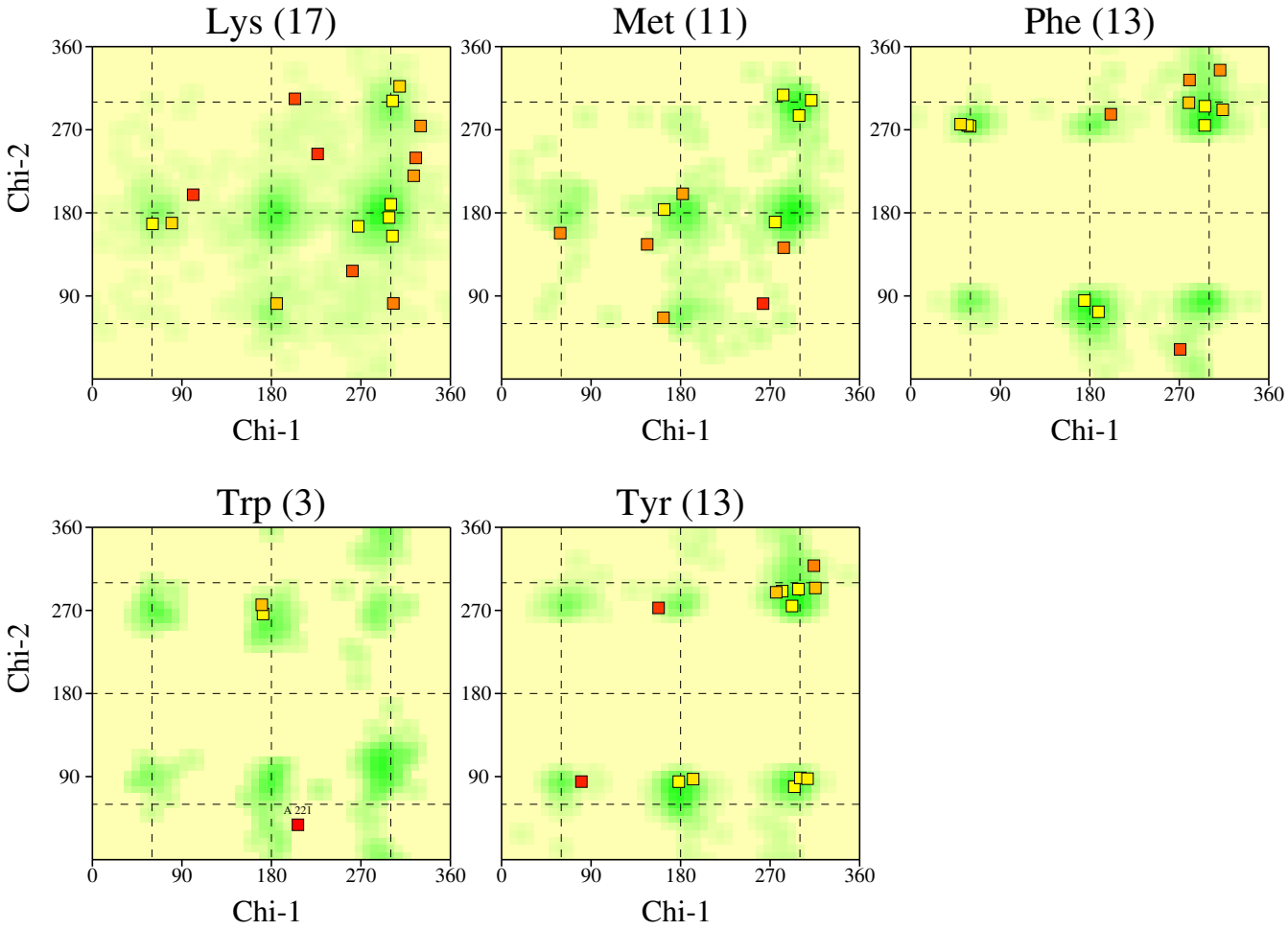
1d4d



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

1d4d



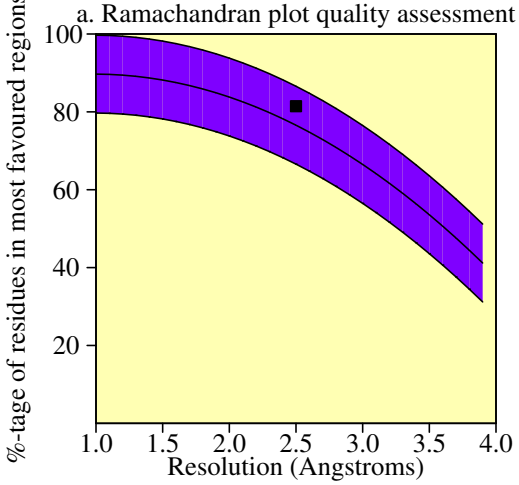
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

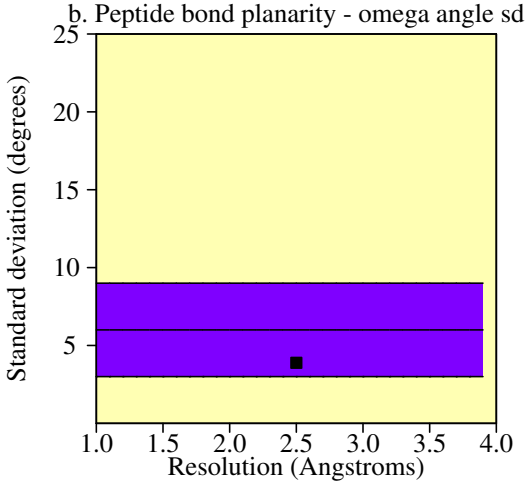
Main-chain parameters

1d4d

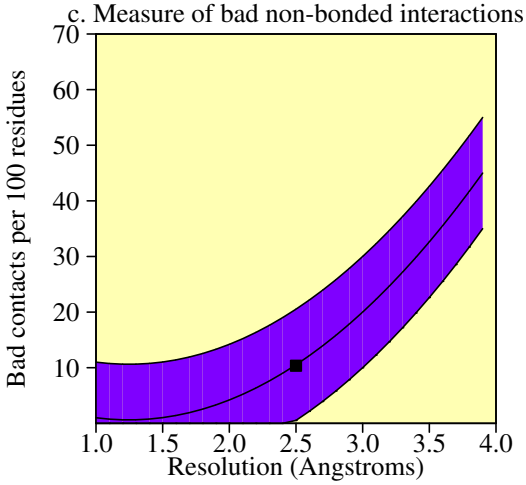
a. Ramachandran plot quality assessment



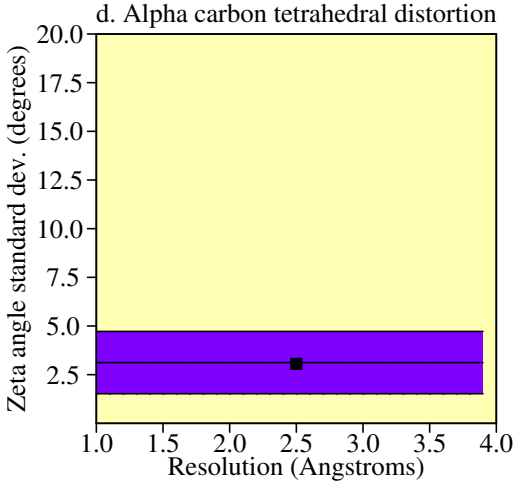
b. Peptide bond planarity - omega angle sd



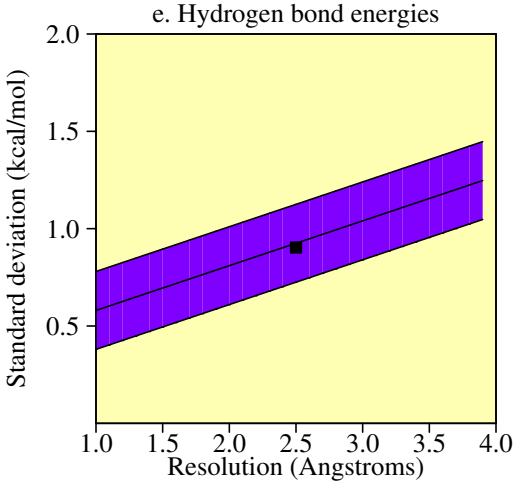
c. Measure of bad non-bonded interactions



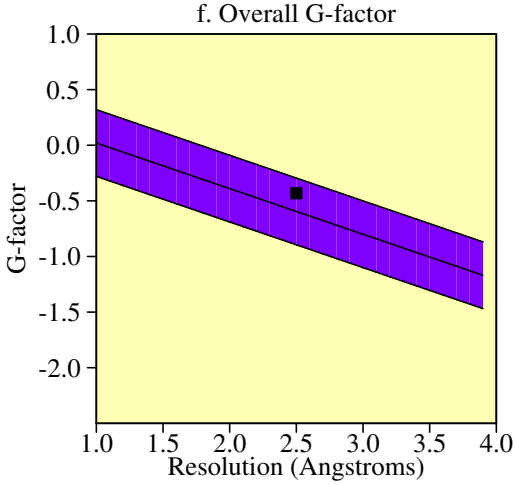
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor



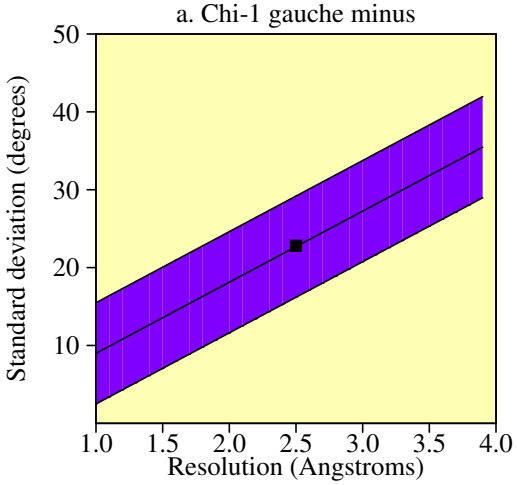
Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	469	81.4	76.6	10.0	0.5	Inside
b. Omega angle st dev	555	3.9	6.0	3.0	-0.7	Inside
c. Bad contacts / 100 residues	58	10.4	10.5	10.0	0.0	Inside
d. Zeta angle st dev	490	3.1	3.1	1.6	0.0	Inside
e. H-bond energy st dev	338	0.9	0.9	0.2	-0.1	Inside
f. Overall G-factor	560	-0.4	-0.6	0.3	0.5	Inside

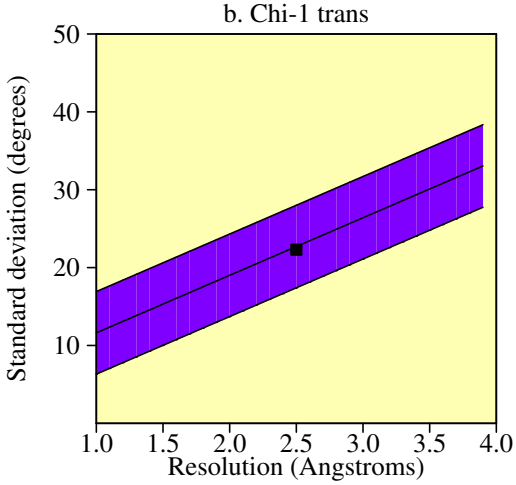
Side-chain parameters

1d4d

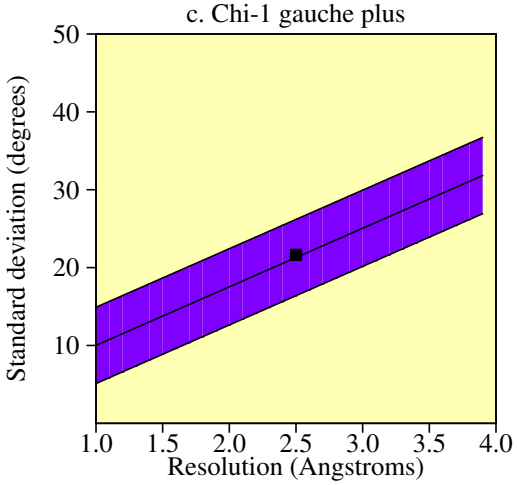
a. Chi-1 gauche minus



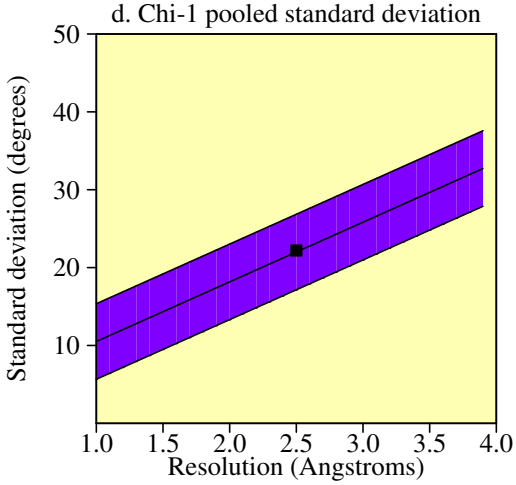
b. Chi-1 trans



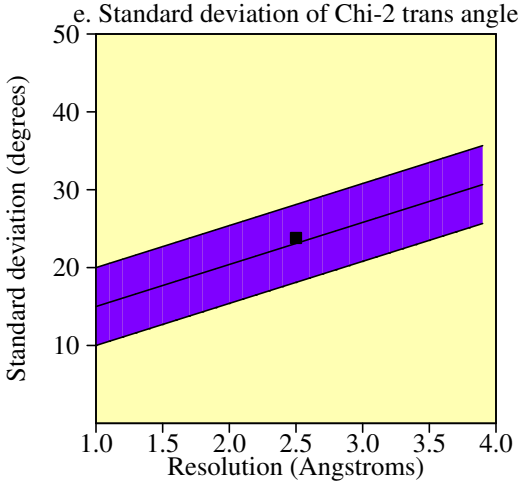
c. Chi-1 gauche plus

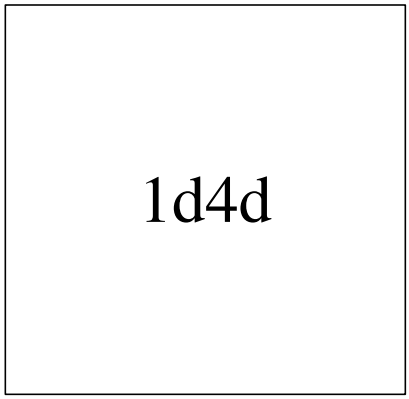


d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



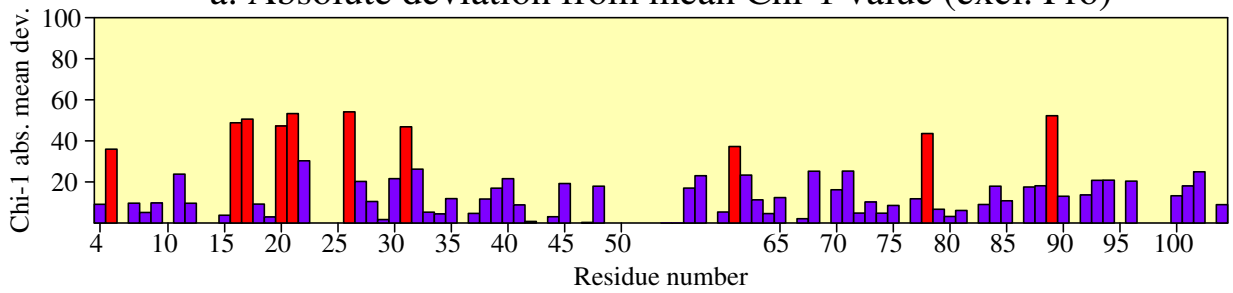


Plot statistics

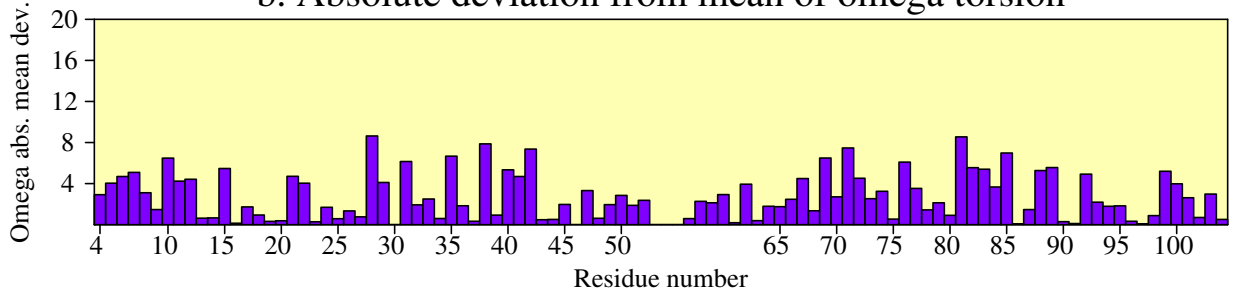
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	63	22.8	22.7	6.5	0.0	Inside
b. Chi-1 trans st dev	119	22.3	22.7	5.3	-0.1	Inside
c. Chi-1 gauche plus st dev	176	21.6	21.3	4.9	0.1	Inside
d. Chi-1 pooled st dev	358	22.2	22.0	4.8	0.0	Inside
e. Chi-2 trans st dev	101	23.8	23.1	5.0	0.1	Inside

Residue properties
1d4d

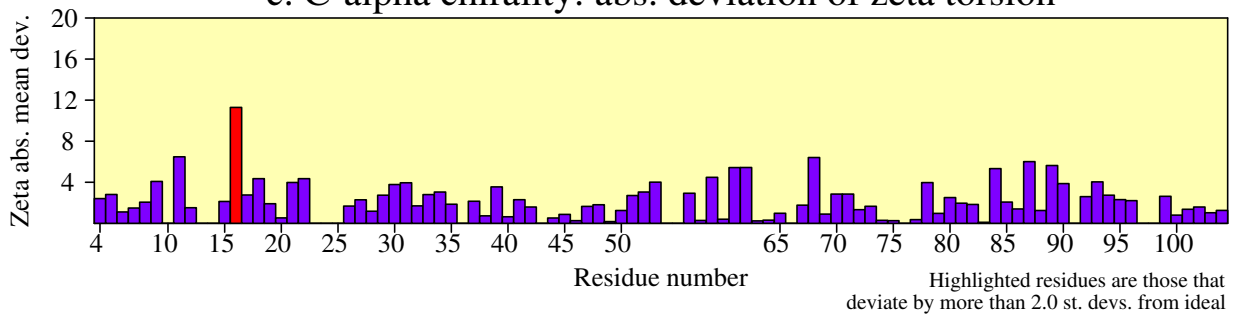
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

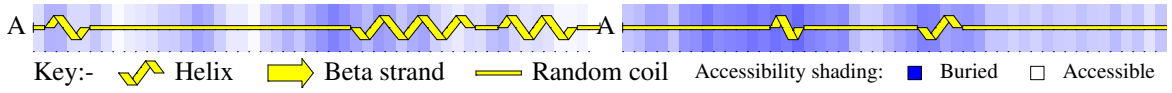


c. C-alpha chirality: abs. deviation of zeta torsion



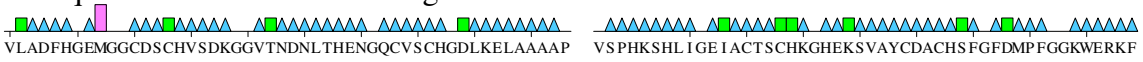
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

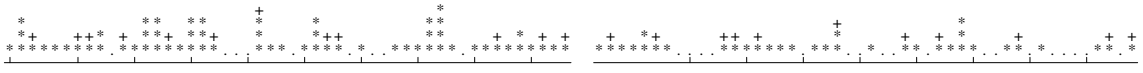


e. Sequence & Ramachandran regions

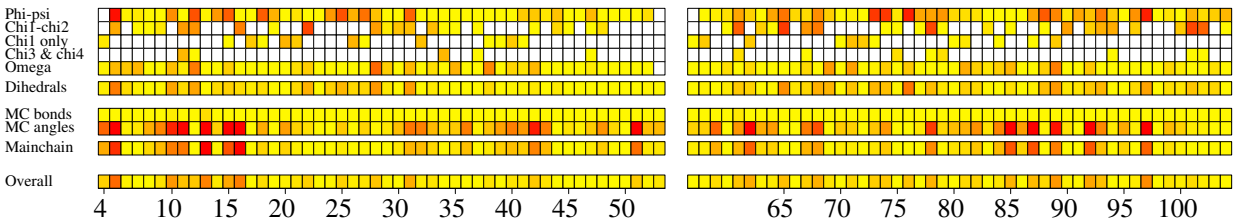
Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

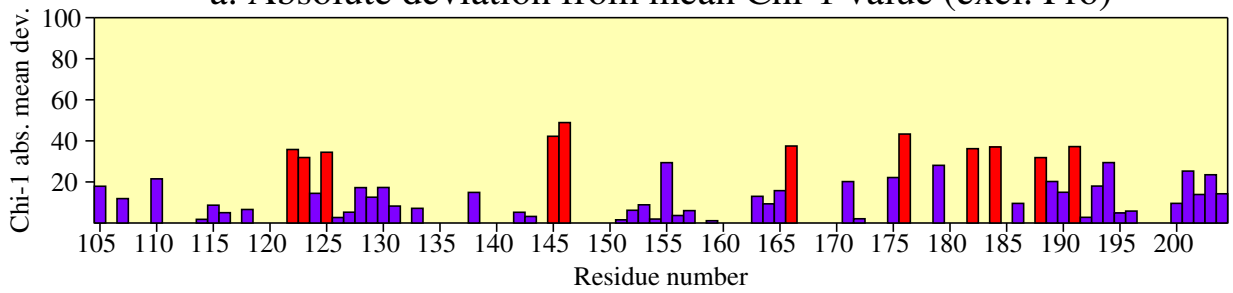


g. G-factors

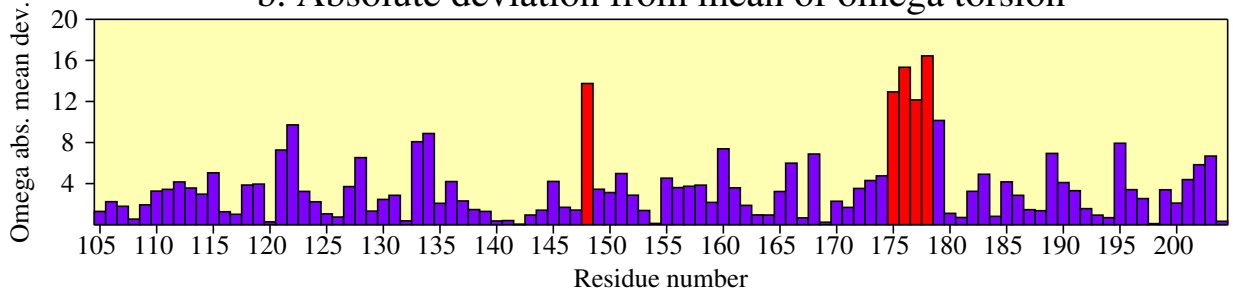


Residue properties
1d4d

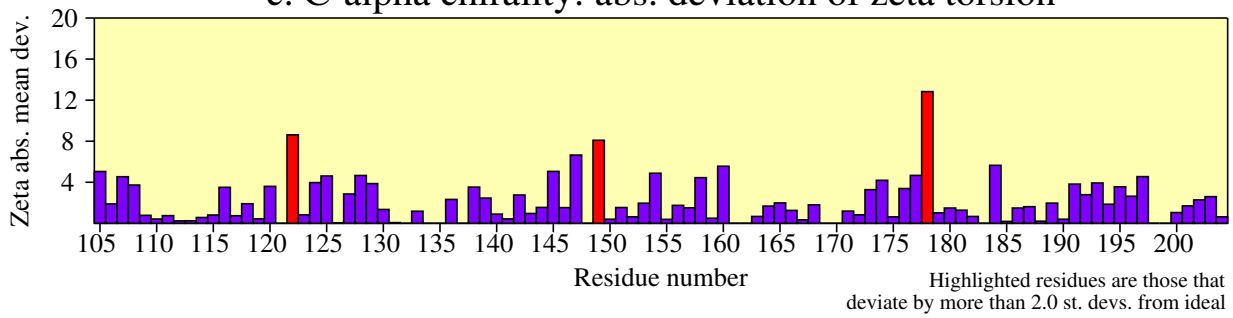
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

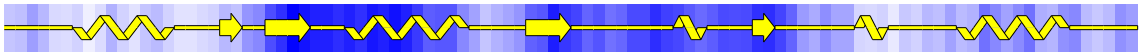


c. C-alpha chirality: abs. deviation of zeta torsion



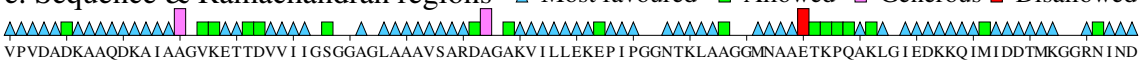
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



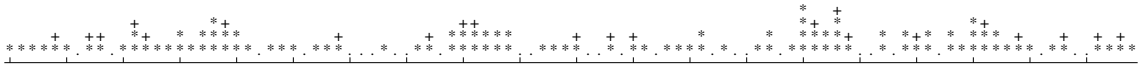
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

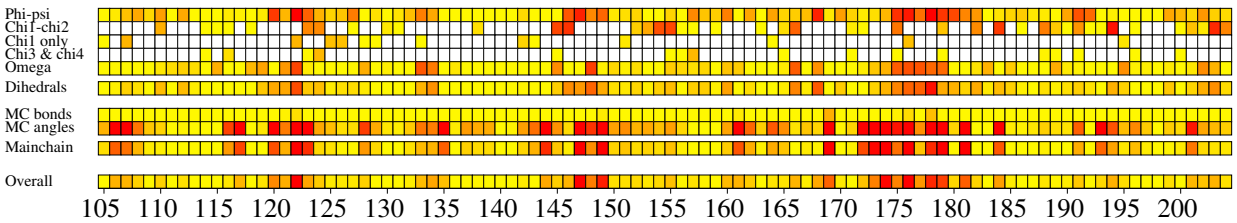


V P V D A D K A A Q D K A I A A G V K E T T D V V I I G S G G A G L A A A V S A R D A G A K V I L L E K E P I P G G N T K L A A G G M N A A E T K P Q A K L G I E D K K Q I M I D D T M K G G R N I N D

f. Max. deviation (see listing)

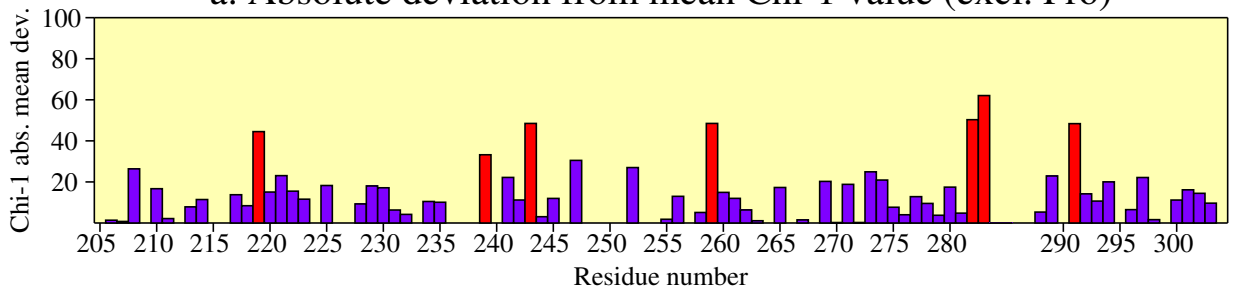


g. G-factors

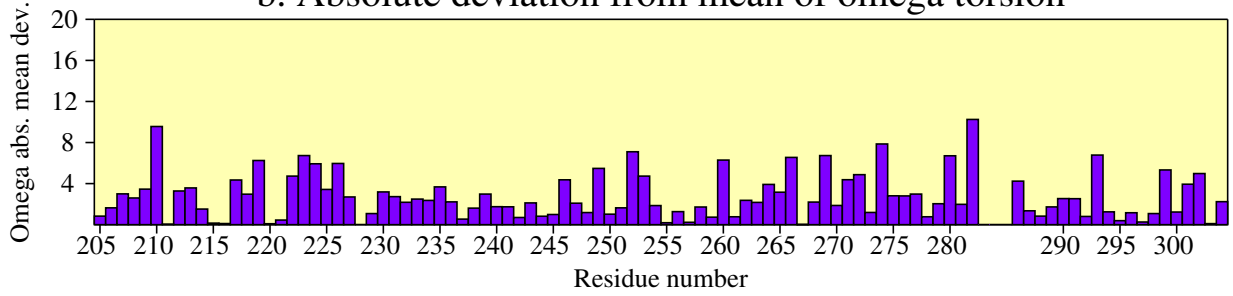


Residue properties
1d4d

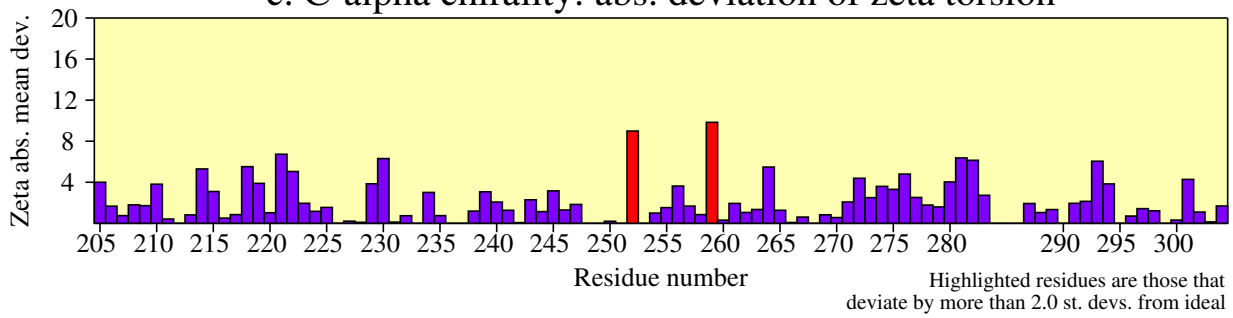
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



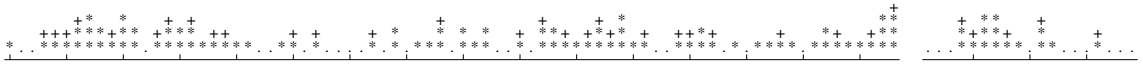
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

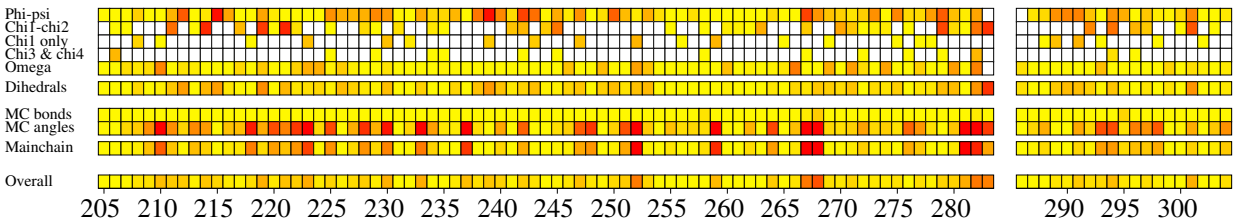
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

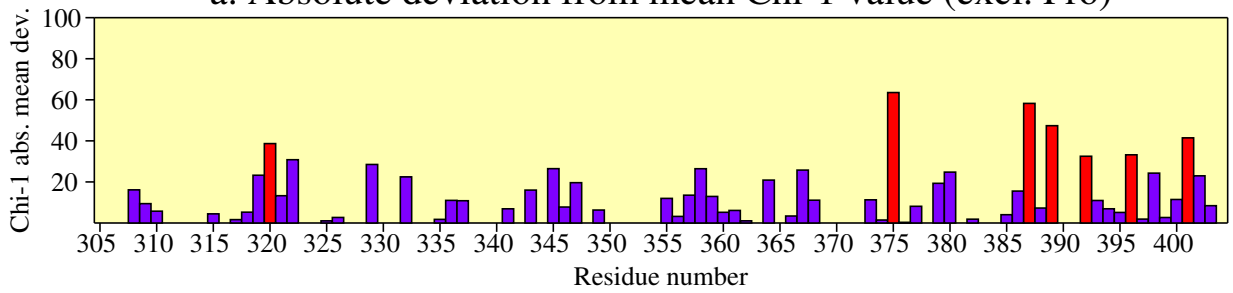


g. G-factors

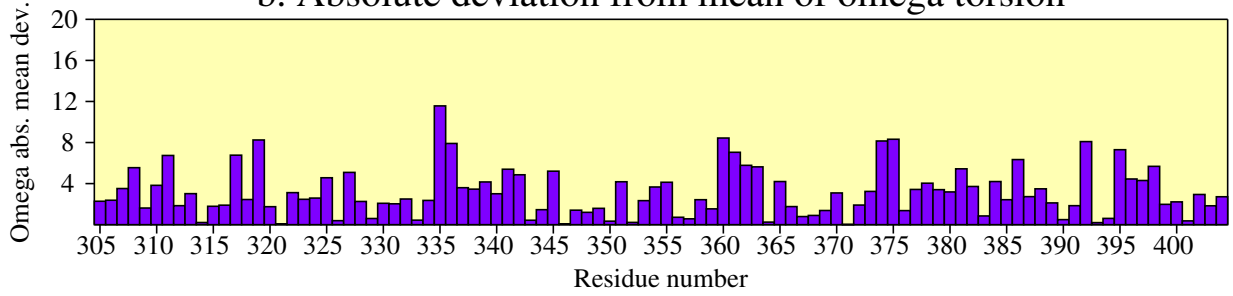


Residue properties
1d4d

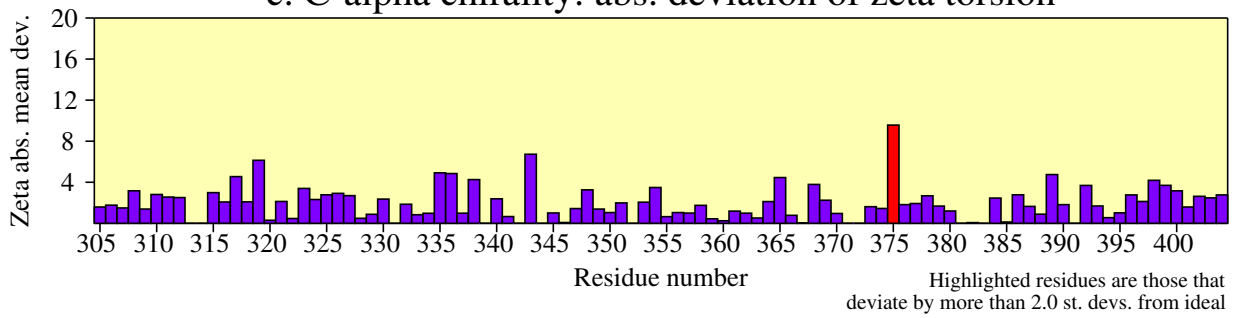
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

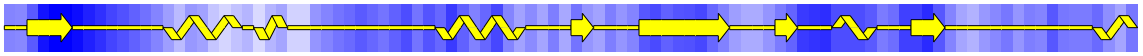


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

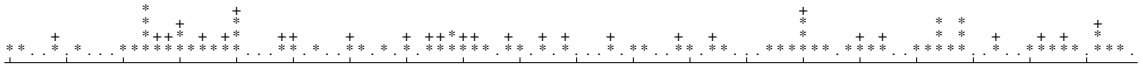


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

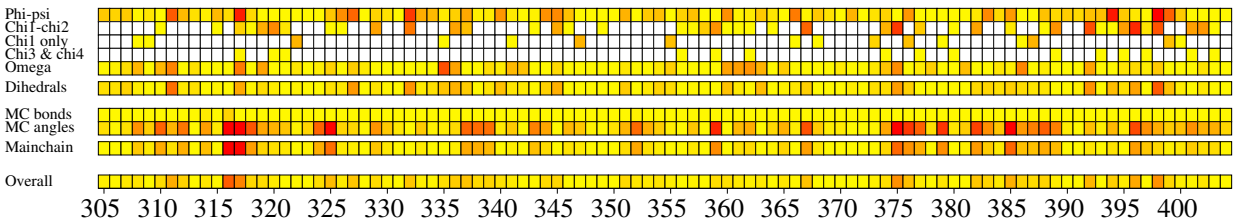
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

ADAVV I AAGGF AKNNERV SKYDPKLKGF KATNHPGATGDGLDVALQAGAATRDLQY I QAHPTYS PAGGVMI TEAVRGNGA I VVNREGNRFMNE I TTRDKA

f. Max. deviation (see listing)

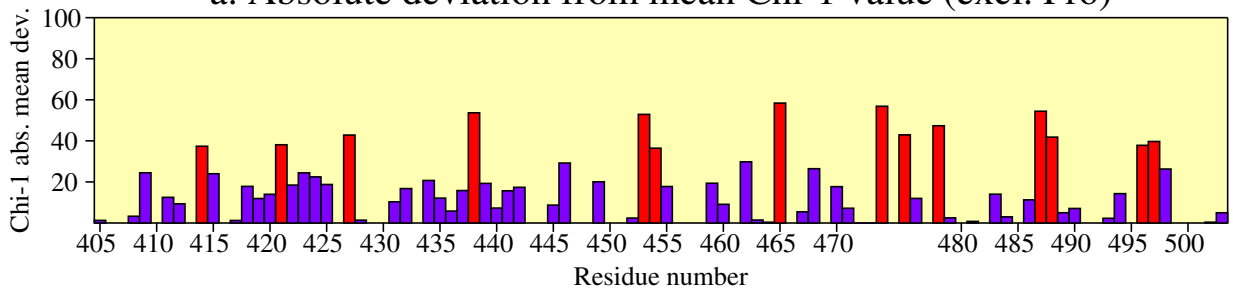


g. G-factors

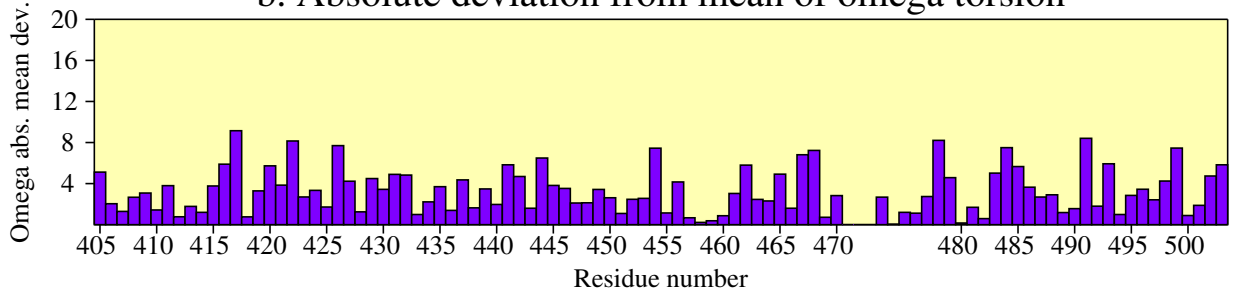


Residue properties
1d4d

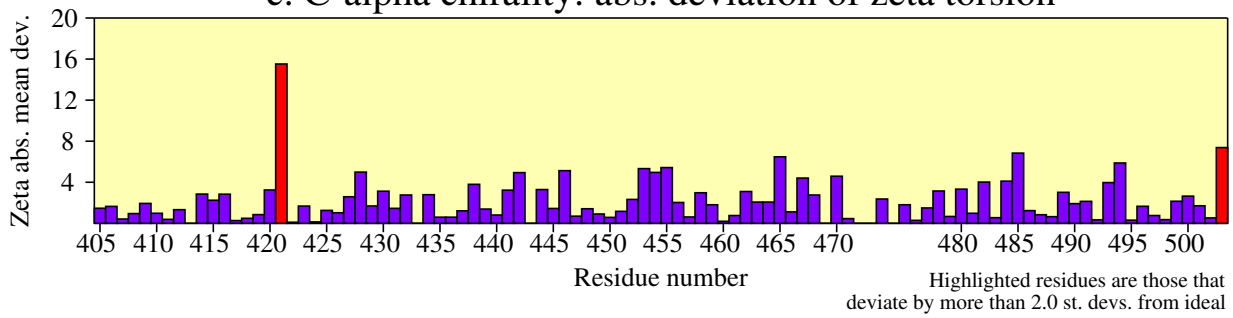
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



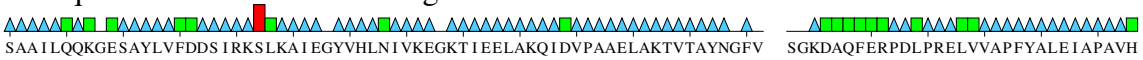
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

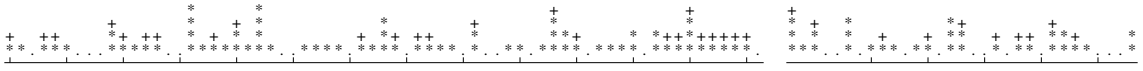
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

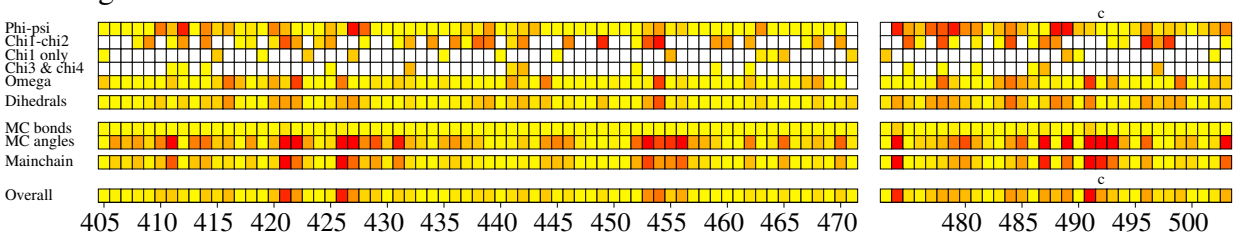
Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



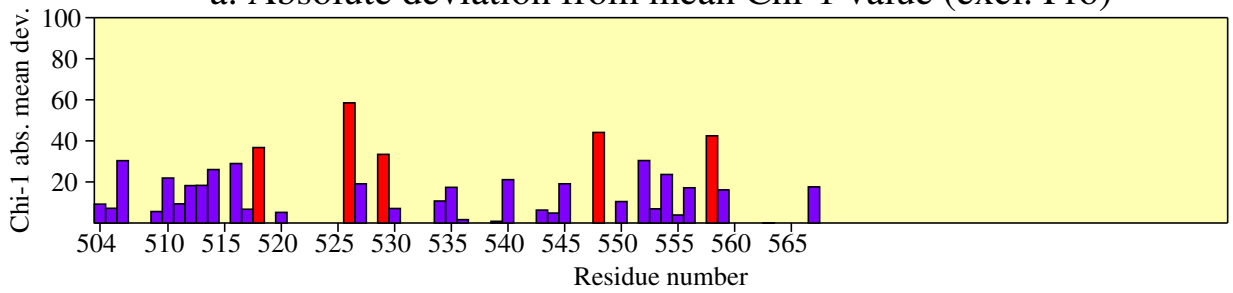
g. G-factors



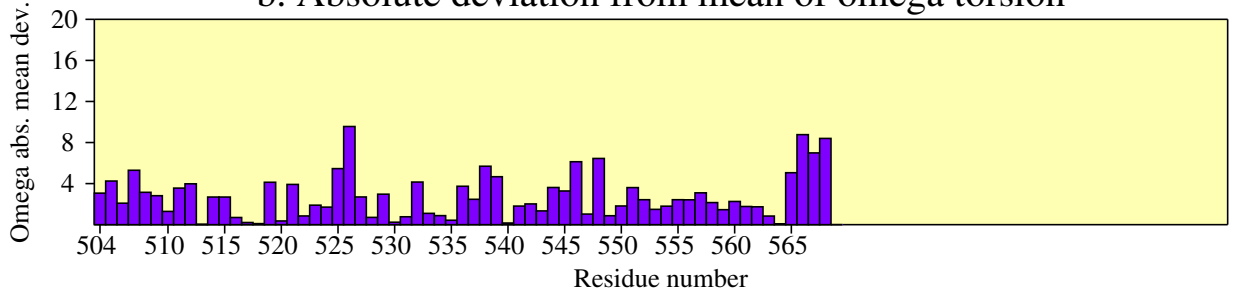
c = cis-peptide

Residue properties
1d4d

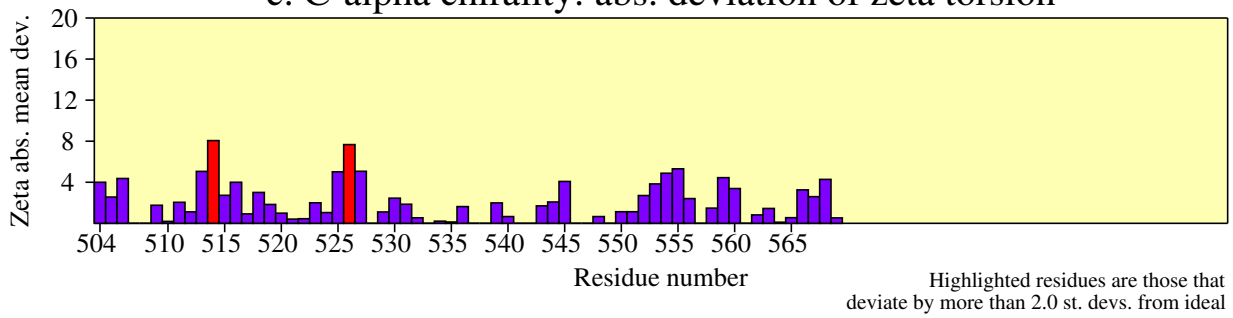
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

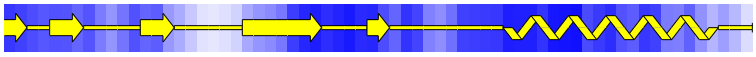


c. C-alpha chirality: abs. deviation of zeta torsion



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

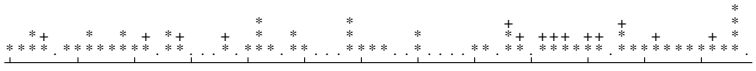
d. Secondary structure & estimated accessibility



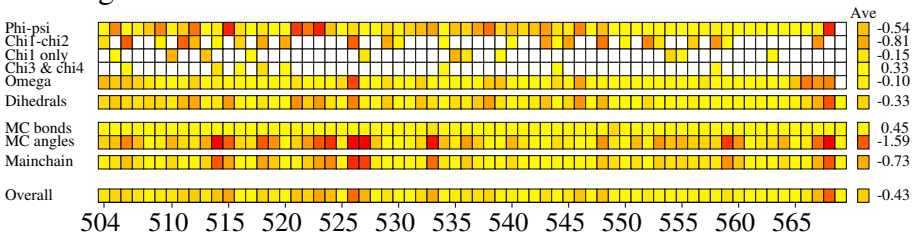
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

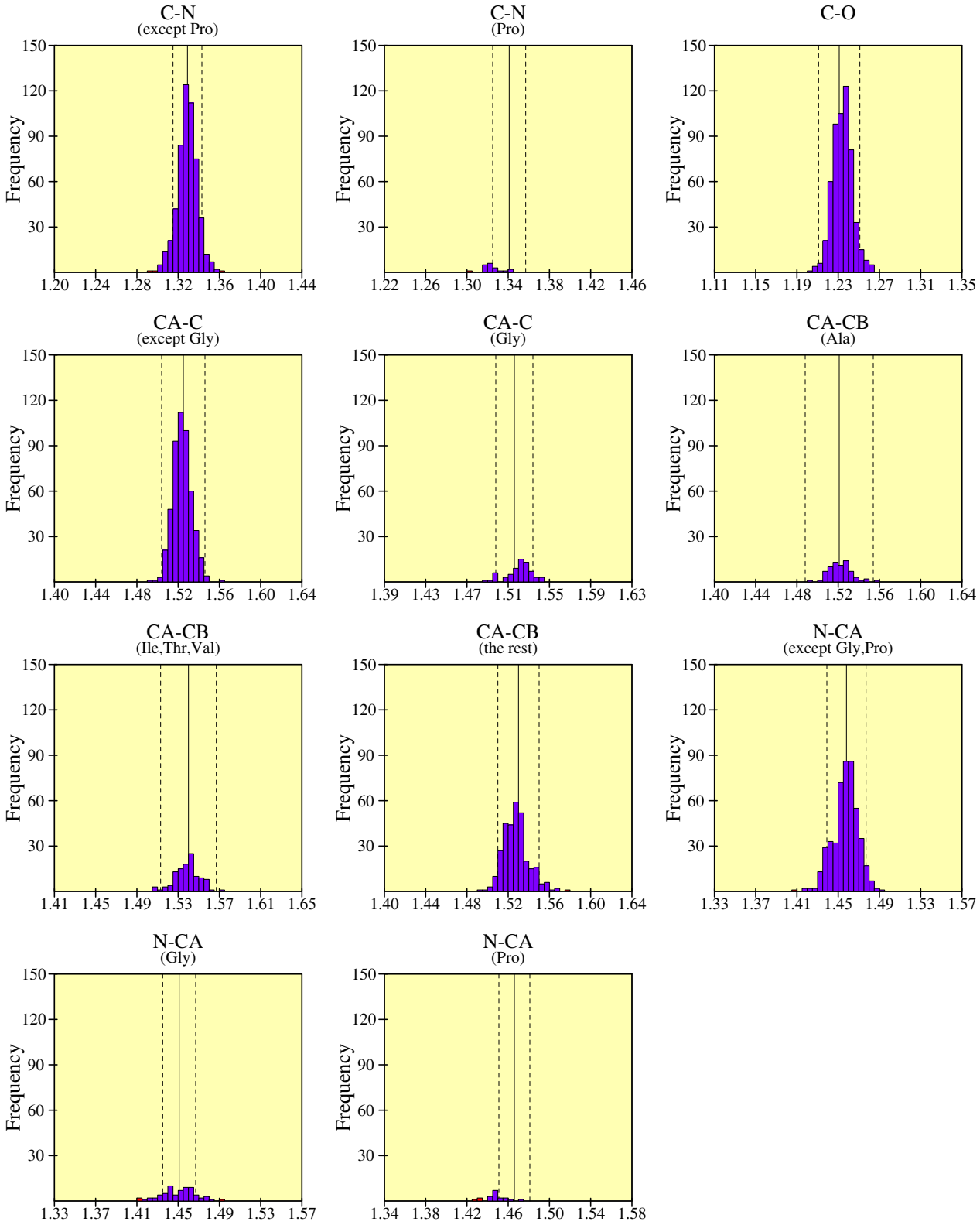


g. G-factors



Main-chain bond lengths

1d4d

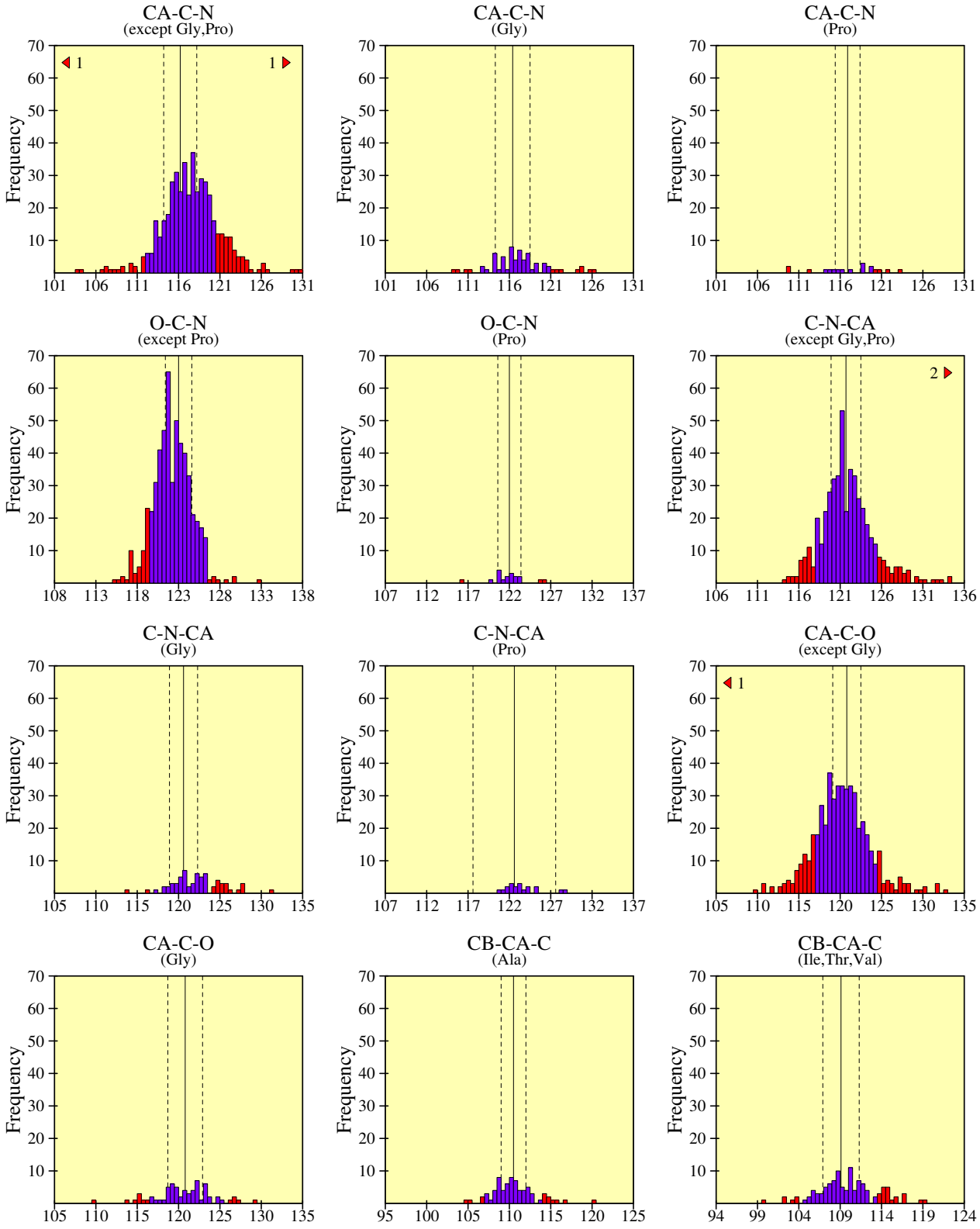


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

1d4d

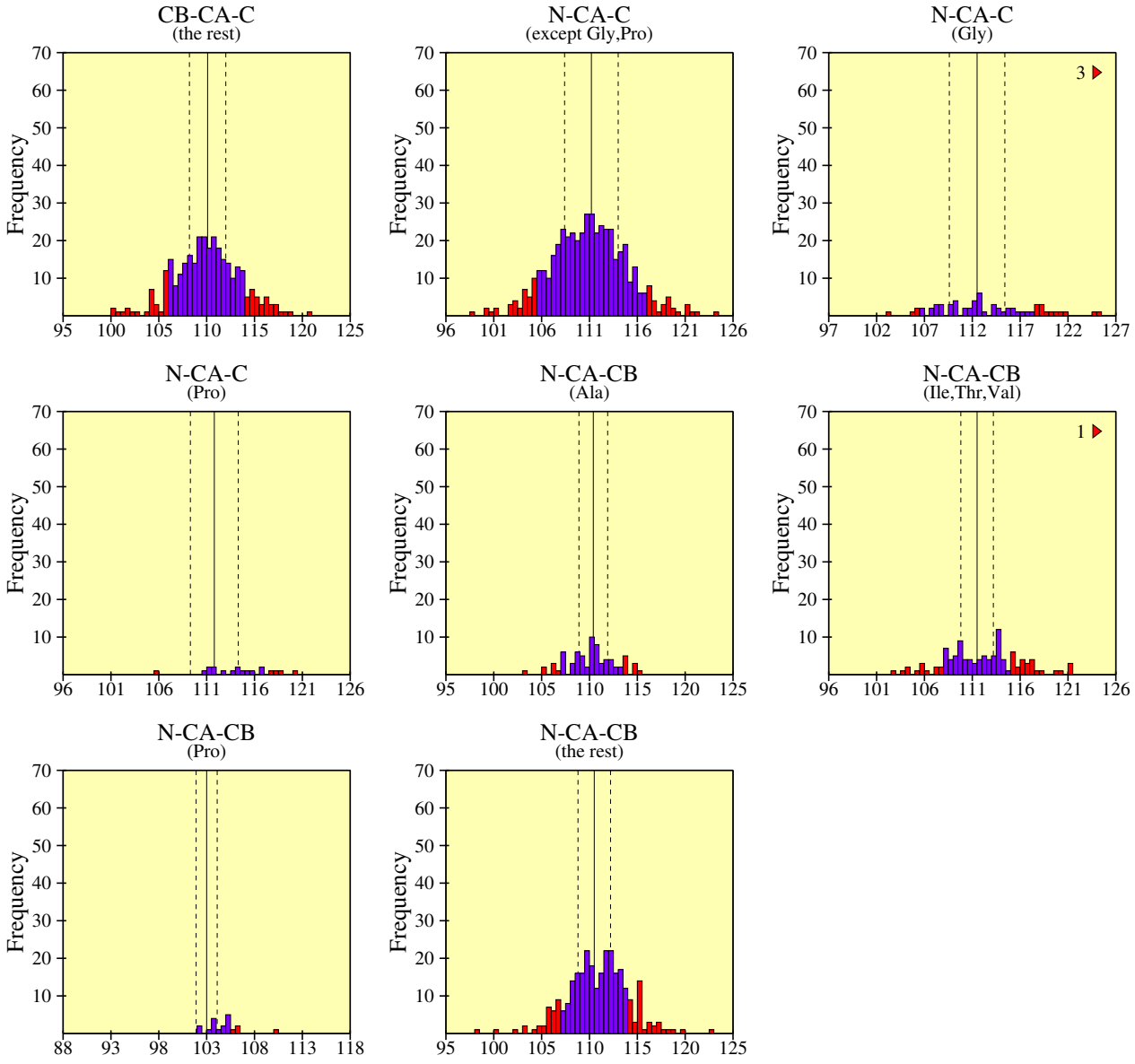


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

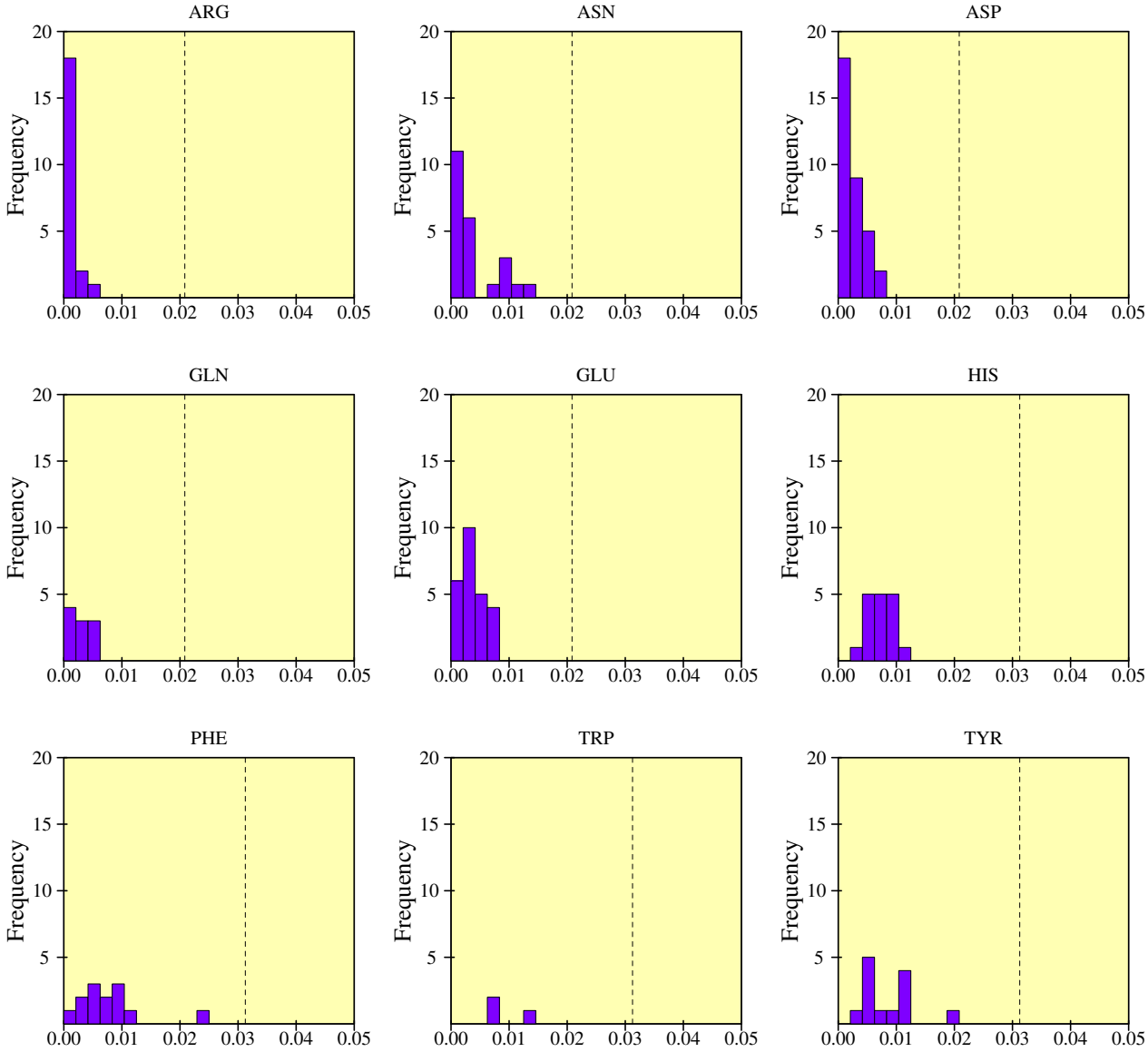
1d4d



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

1d4d



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.

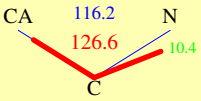
Distorted geometry
1d4d

Main-chain bond lengths

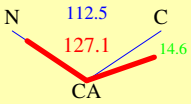
A Thr 176

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

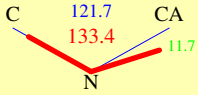
Main-chain bond angles



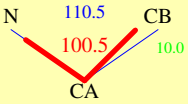
A Leu 5 - A Ala 6



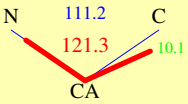
A Gly 13



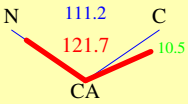
A Cys 15 - A Asp 16



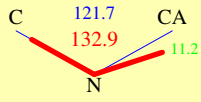
A Asp 16



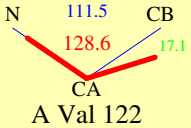
A Cys 87



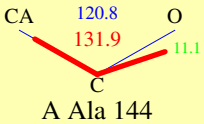
A Ala 120



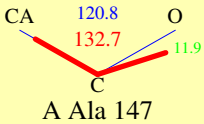
A Gly 121 - A Val 122



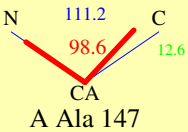
A Val 122



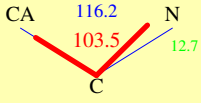
A Ala 144



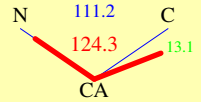
A Ala 147



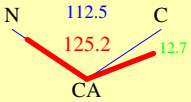
A Ala 147



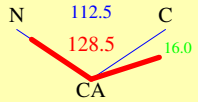
A Ala 147 - A Gly 148



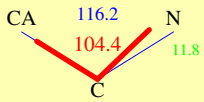
A Ala 149



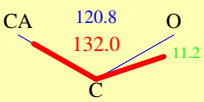
A Gly 161



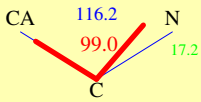
A Gly 169



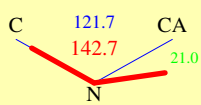
A Ala 173 - A Ala 174



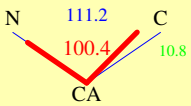
A Ala 174



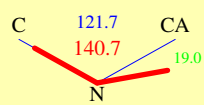
A Ala 174 - A Glu 175



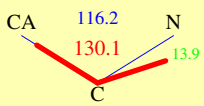
A Glu 175 - A Thr 176



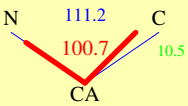
A Lys 177



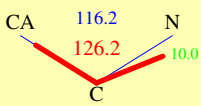
A Pro 178 - A Gln 179



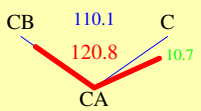
A Lys 181 - A Leu 182



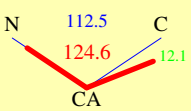
A Met 191



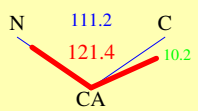
A Asp 193 - A Asp 194



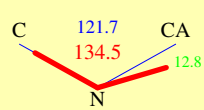
A Leu 222



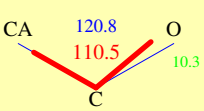
A Gly 237



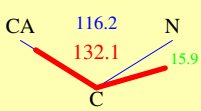
A Arg 242



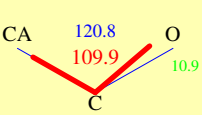
A Gly 251 - A Val 252



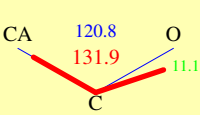
A Arg 267



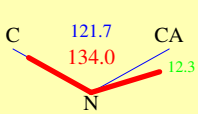
A Arg 267 - A Gly 268



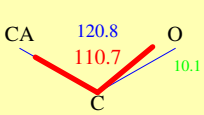
A Gly 268



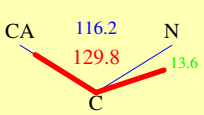
A Leu 281



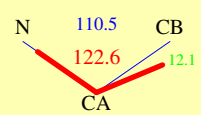
A Leu 281 - A Glu 282



A Ala 316



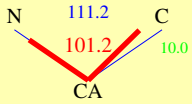
A Ala 316 - A Lys 317



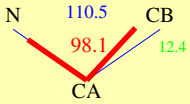
A Lys 317

Distorted geometry
1d4d

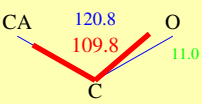
Main-chain bond angles (contd)



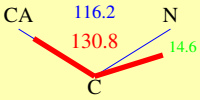
A Asn 396



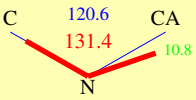
A Asp 421



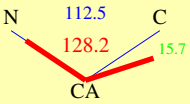
A Lys 426



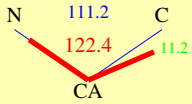
A Lys 426 - A Ser 427



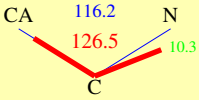
A Ser 473 - A Gly 474



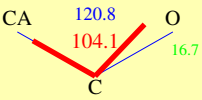
A Gly 474



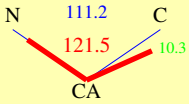
A Glu 487



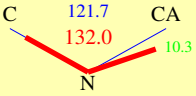
A Glu 487 - A Leu 488



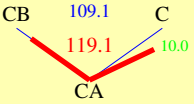
A Ala 491



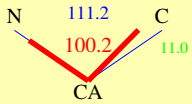
A His 503



A Ala 523 - A Lys 524



A Ile 526



A Ile 526

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