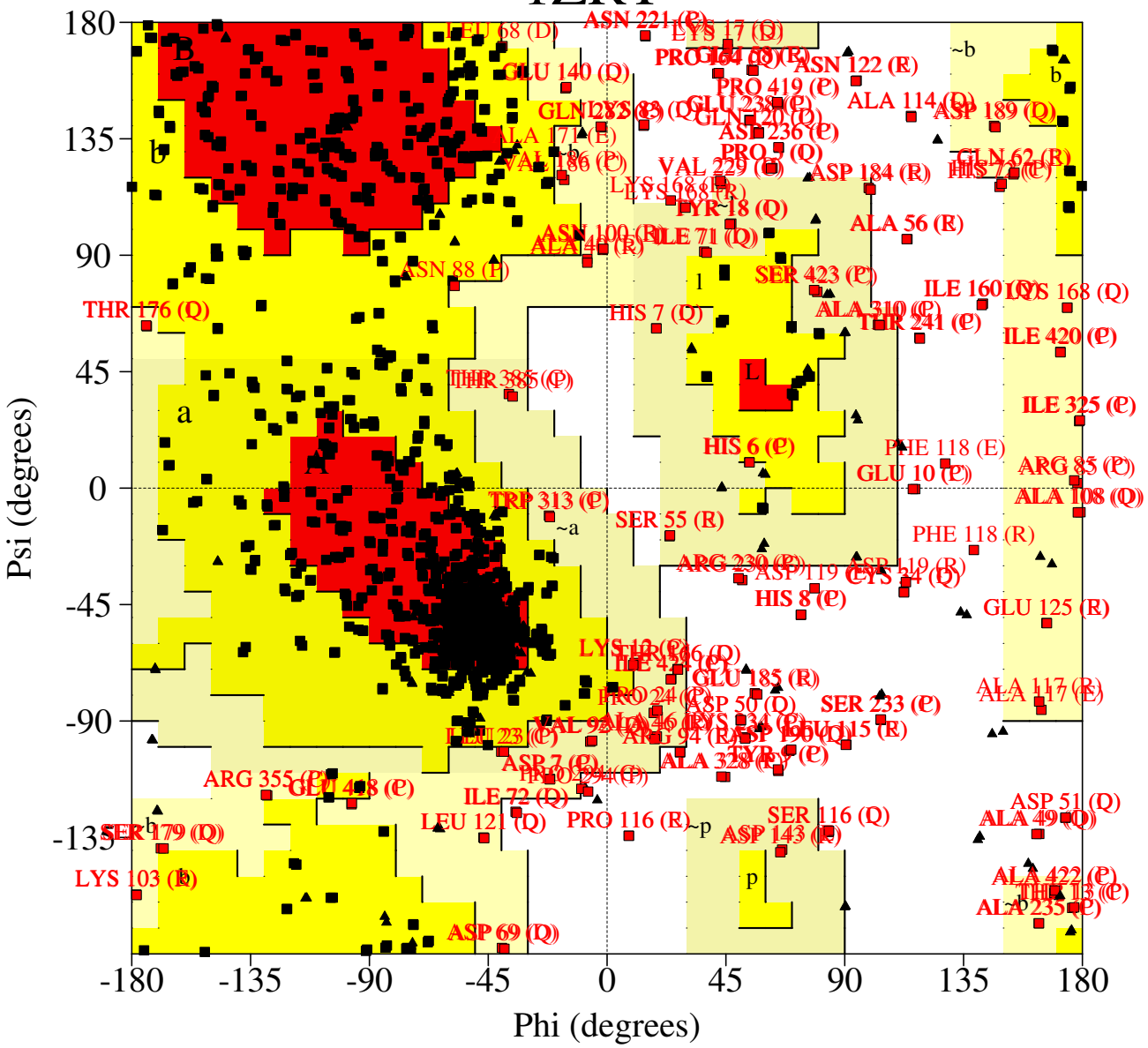
Ramachandran Plot

1ZRT



Plot statistics

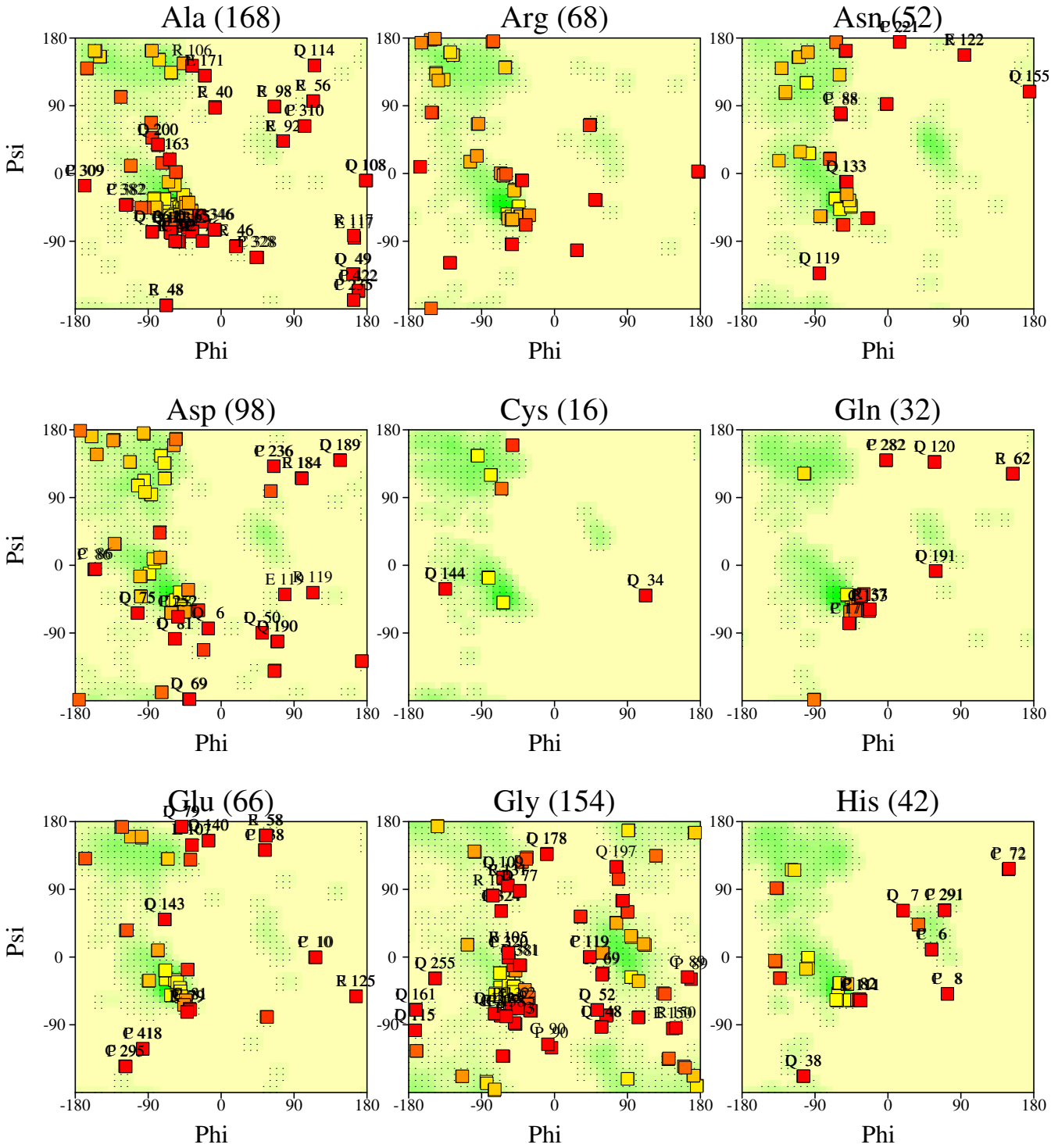
Residues in most favoured regions [A,B,L]	899	62.3%
Residues in additional allowed regions [a,b,l,p]	388	26.9%
Residues in generously allowed regions [~a,~b,~l,~p]	91	6.3%
Residues in disallowed regions	64	4.4%
	----	------
Number of non-glycine and non-proline residues	1442	100.0%
Number of end-residues (excl. Gly and Pro)	10	
Number of glycine residues (shown as triangles)	156	
Number of proline residues	112	

Total number of residues	1720	

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

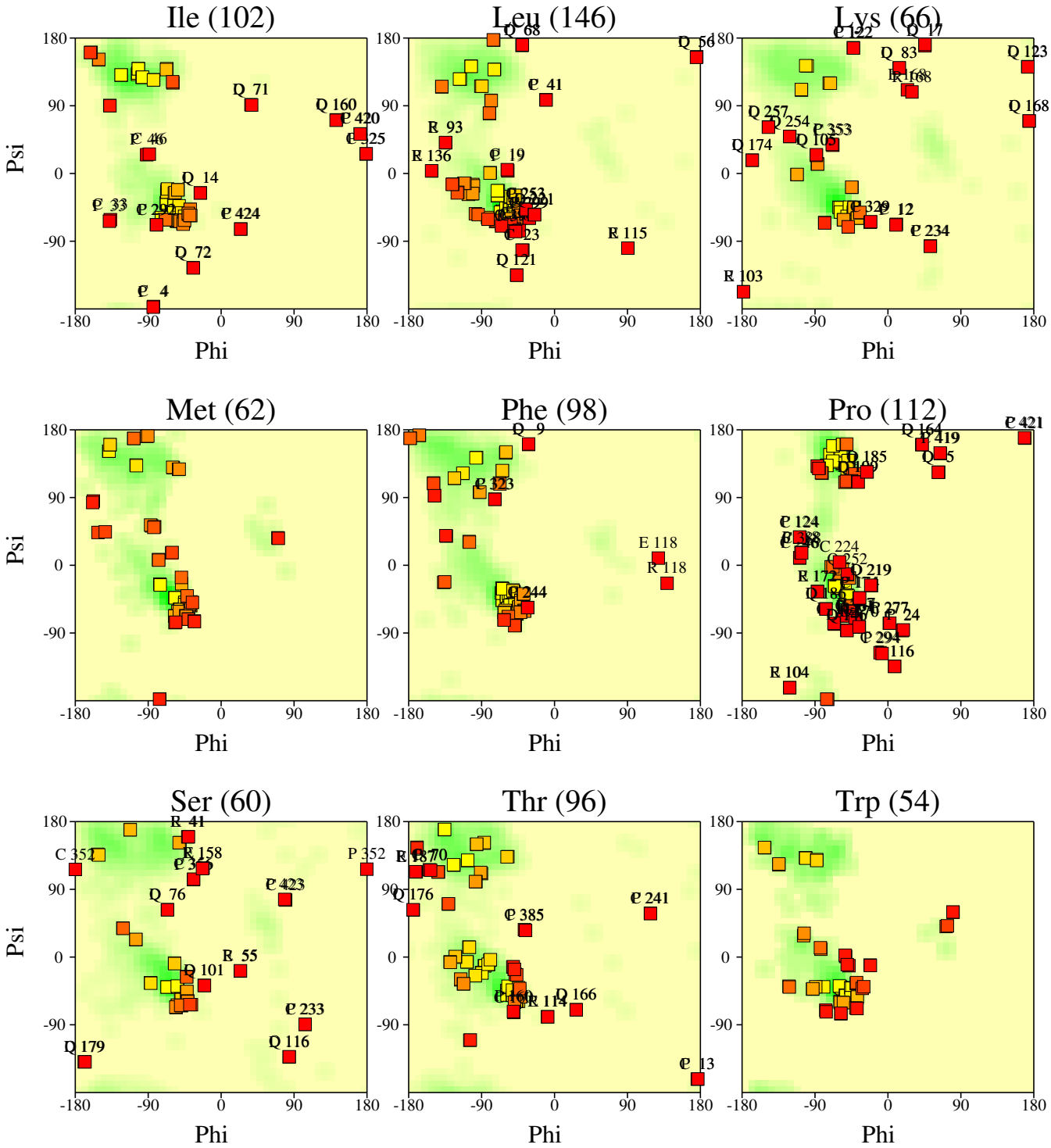
1ZRT



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

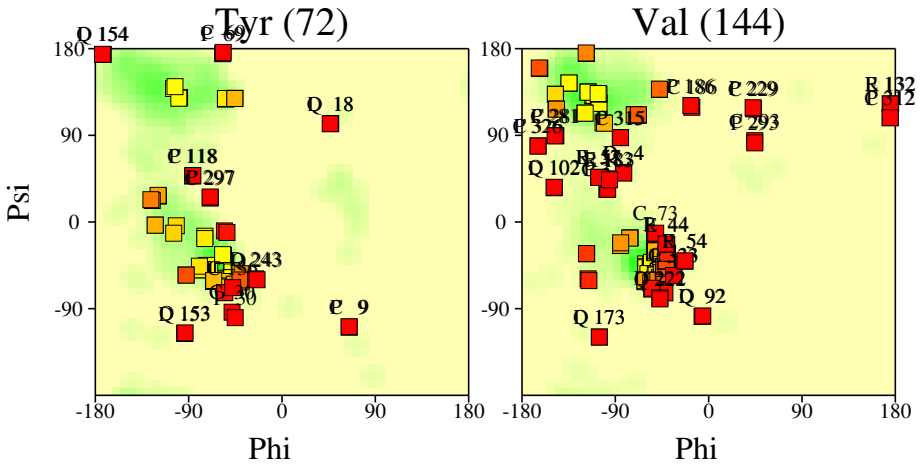
1ZRT



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

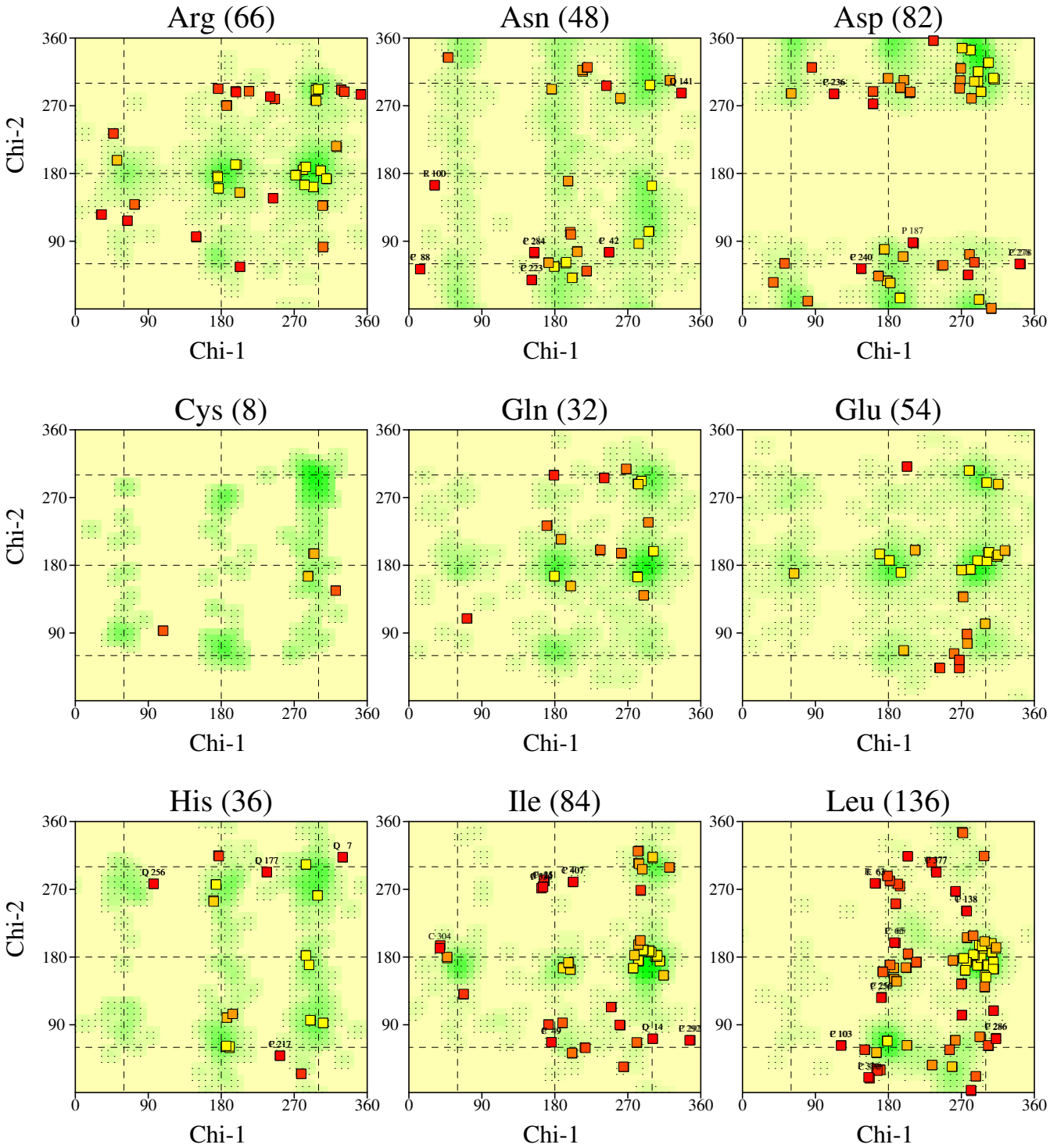
1ZRT



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

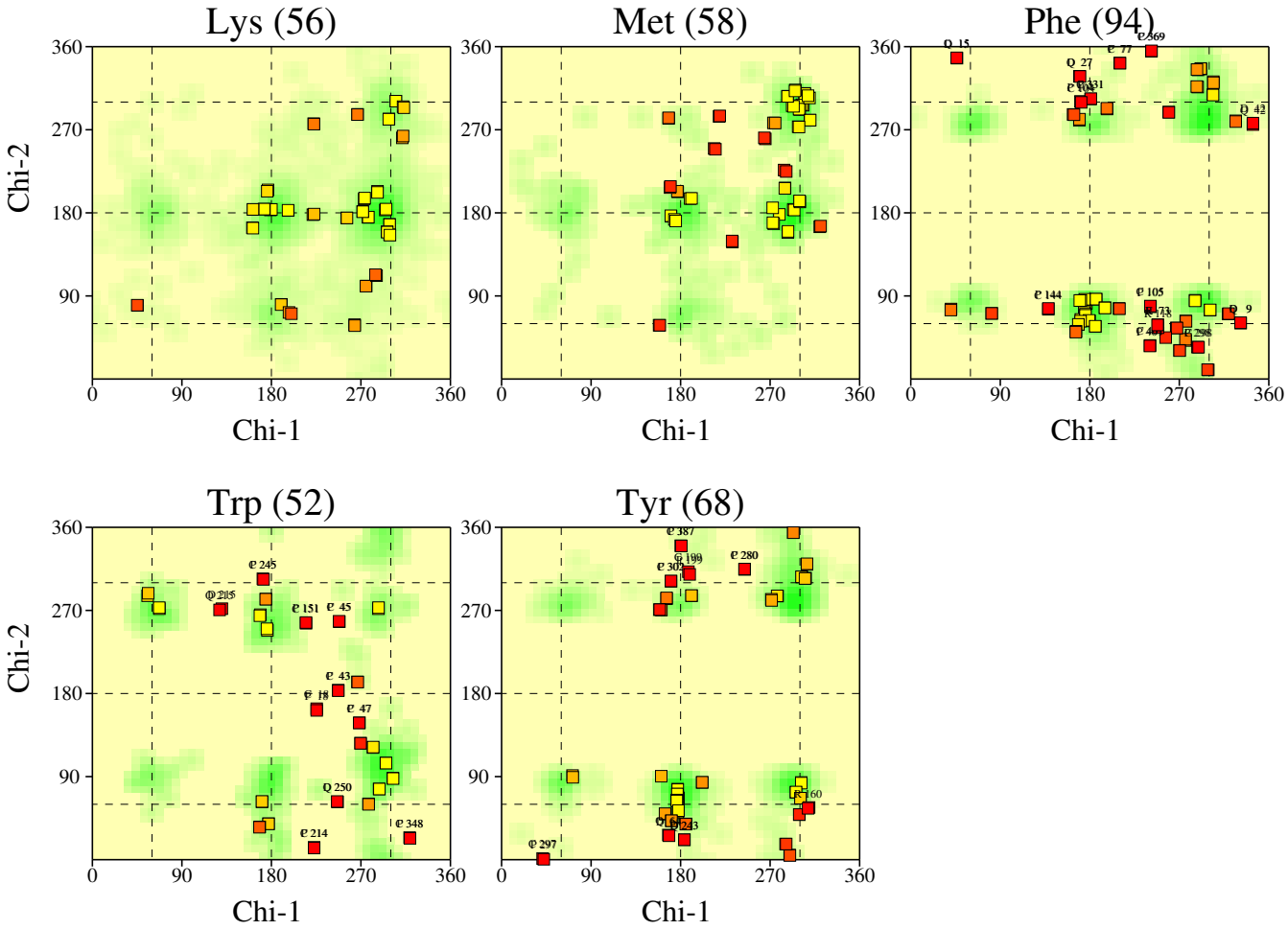
1ZRT



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

1ZRT



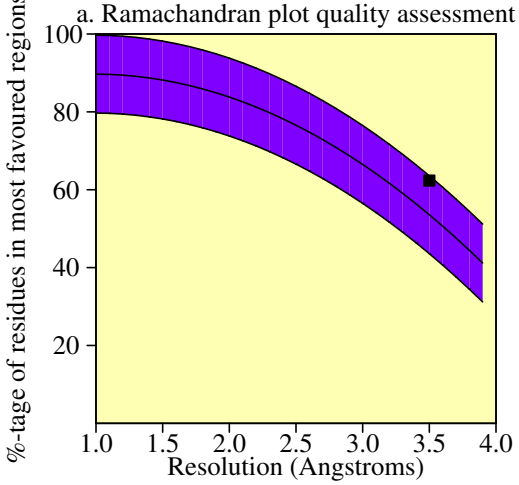
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

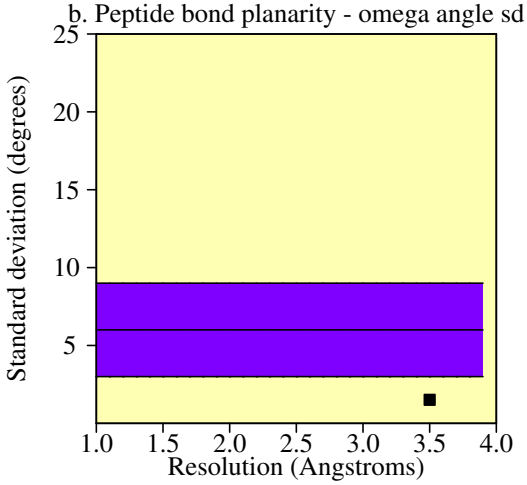
Main-chain parameters

1ZRT

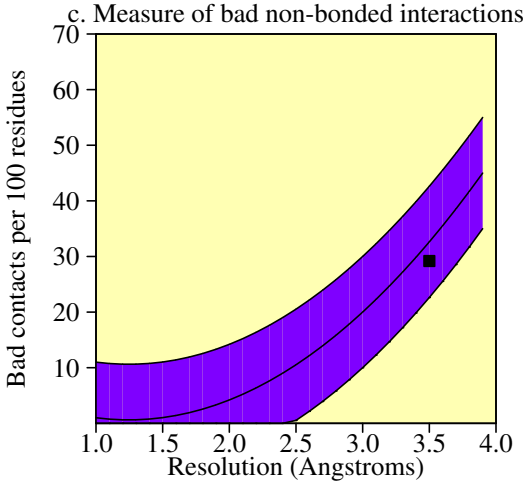
a. Ramachandran plot quality assessment



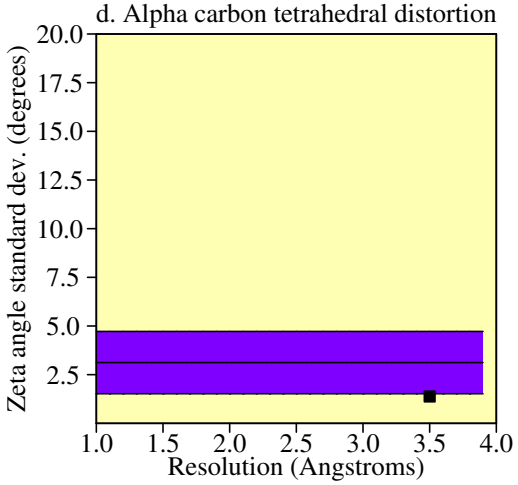
b. Peptide bond planarity - omega angle sd



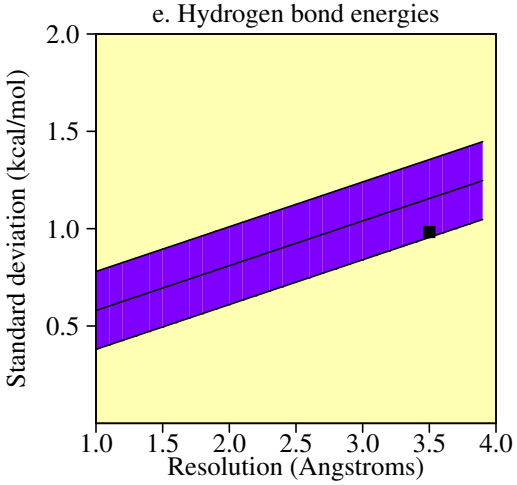
c. Measure of bad non-bonded interactions



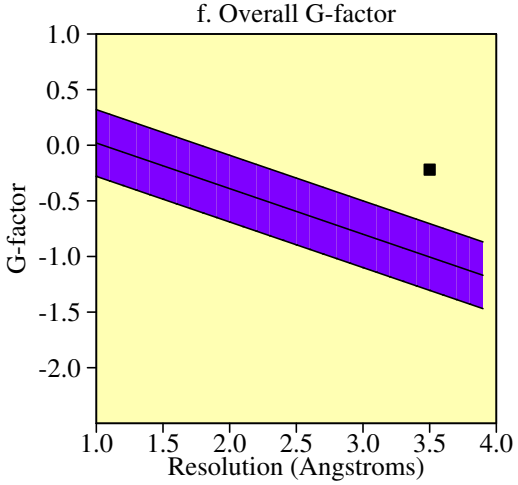
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor



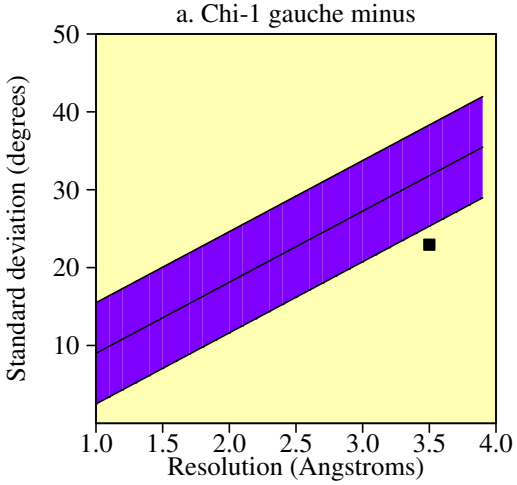
Plot statistics

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	1442	62.3	53.6	10.0	0.9	Inside
b. Omega angle st dev	1708	1.5	6.0	3.0	-1.5	BETTER
c. Bad contacts / 100 residues	502	29.2	32.6	10.0	-0.3	Inside
d. Zeta angle st dev	1560	1.4	3.1	1.6	-1.1	BETTER
e. H-bond energy st dev	977	1.0	1.2	0.2	-0.9	Inside
f. Overall G-factor	1720	-0.2	-1.0	0.3	2.6	BETTER

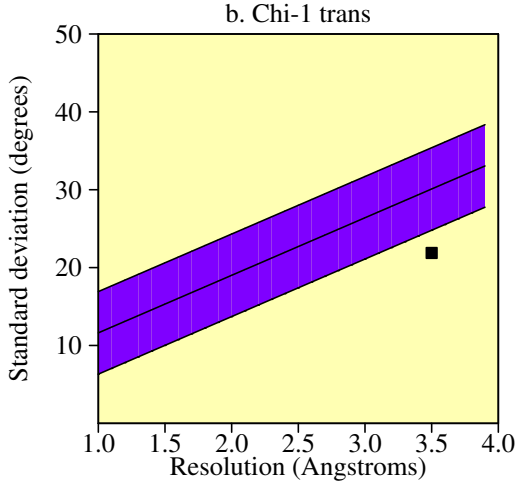
Side-chain parameters

1ZRT

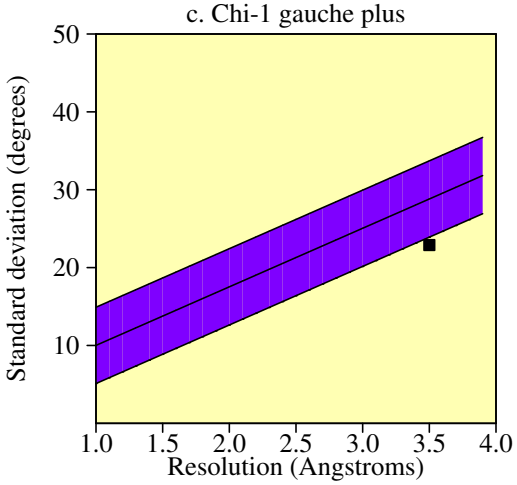
a. Chi-1 gauche minus



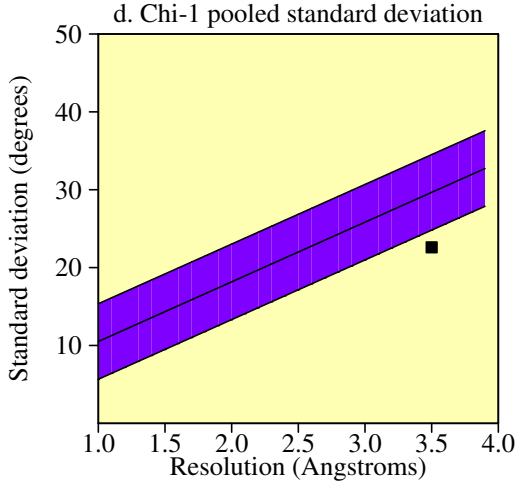
b. Chi-1 trans



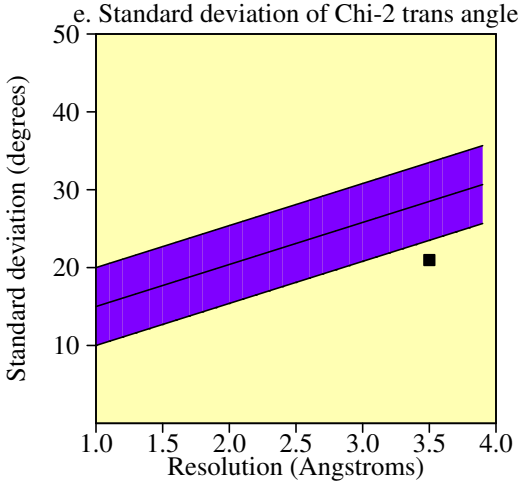
c. Chi-1 gauche plus

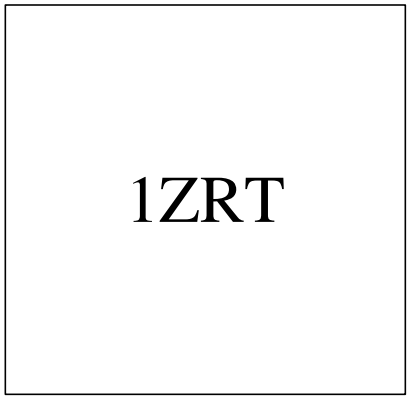


d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



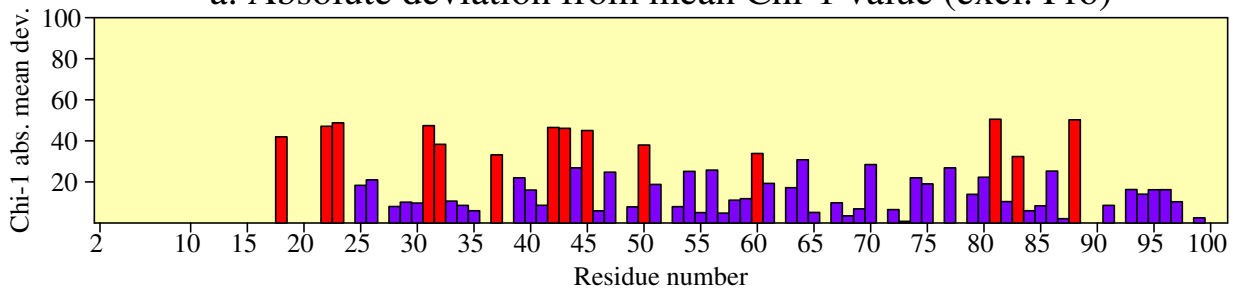


Plot statistics

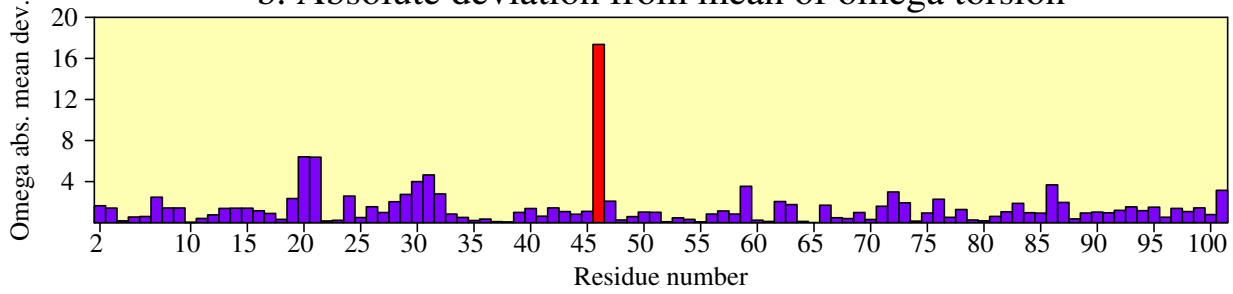
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	138	22.9	31.8	6.5	-1.4	BETTER
b. Chi-1 trans st dev	472	21.9	30.1	5.3	-1.6	BETTER
c. Chi-1 gauche plus st dev	564	22.9	28.8	4.9	-1.2	BETTER
d. Chi-1 pooled st dev	1174	22.6	29.7	4.8	-1.5	BETTER
e. Chi-2 trans st dev	268	21.0	28.5	5.0	-1.5	BETTER

Residue properties
1ZRT

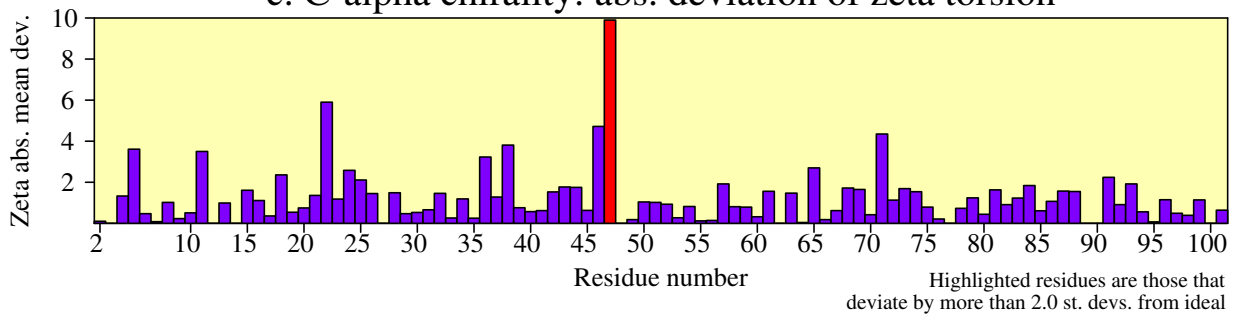
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

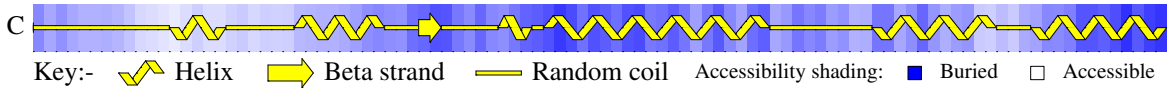


c. C-alpha chirality: abs. deviation of zeta torsion



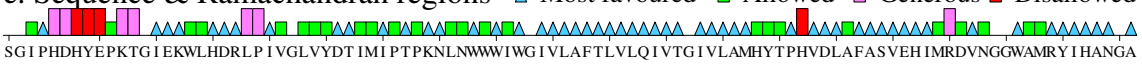
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



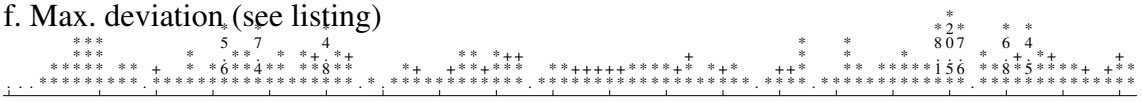
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

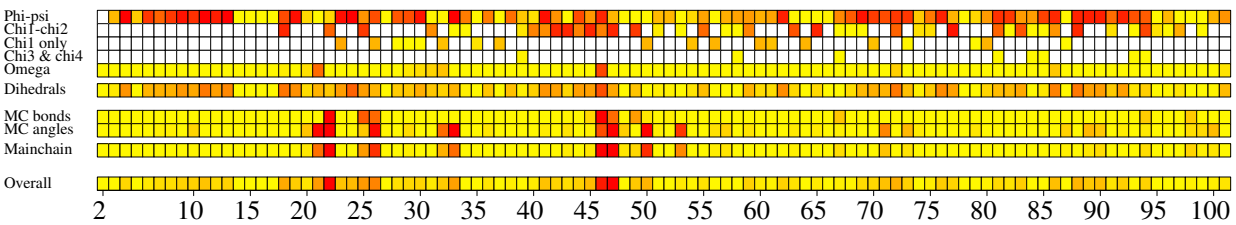


SG I PHDHYEPKTG I EKWLHDRLP I VGLVYDT IM I P T PKNLNWWW I WG I VLAFTLVLQ I VTG I VLAMHYTPHVDLAFASVEH IMRDVNGGWAMRY I HANGA

f. Max. deviation (see listing)

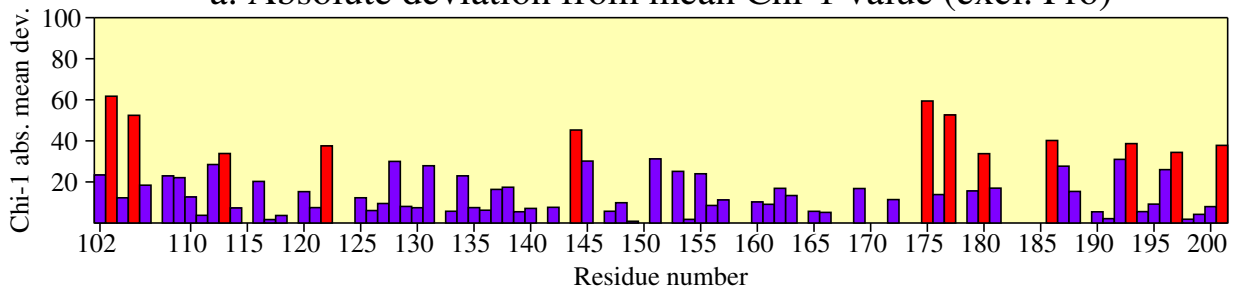


g. G-factors

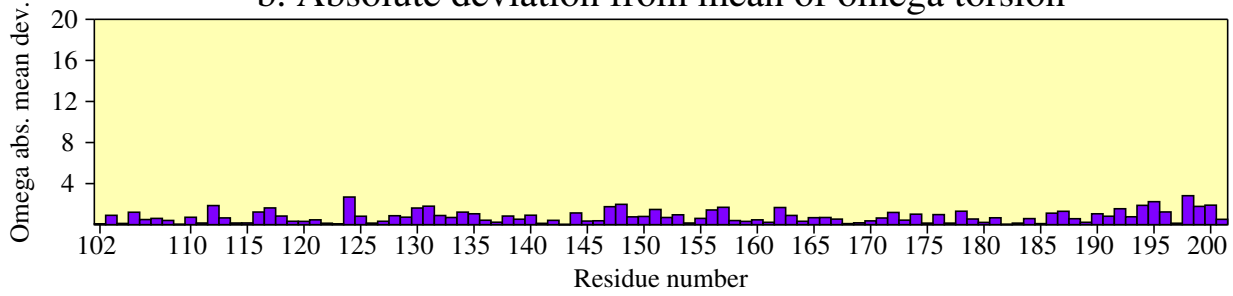


Residue properties
1ZRT

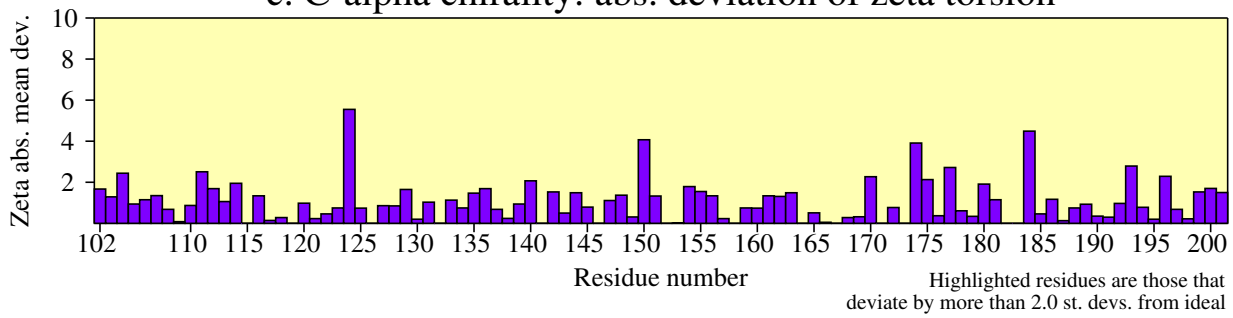
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

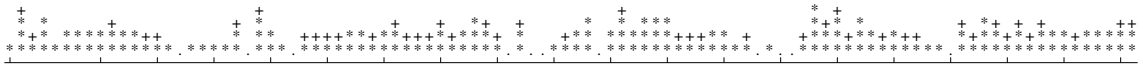
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

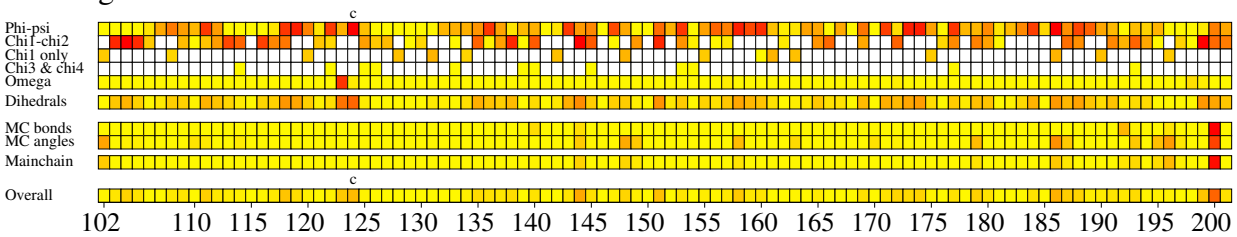
Most favoured Allowed Generous Disallowed

SLFFLAVYIHIFRGLYYGSYKAPREITWIVGMVIYLLMMGTAFMGYVLPWGQMSFWGATVITGLFGAIPGIGPSIQAWLLGGPAVDNATLNRFFSLHYLL

f. Max. deviation (see listing)



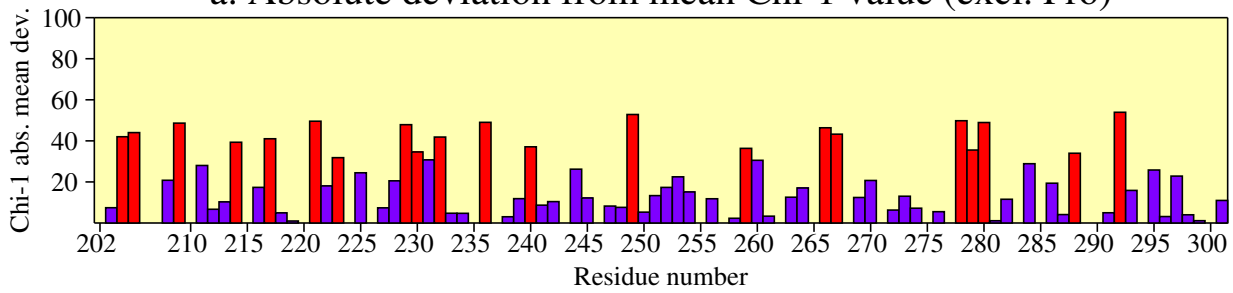
g. G-factors



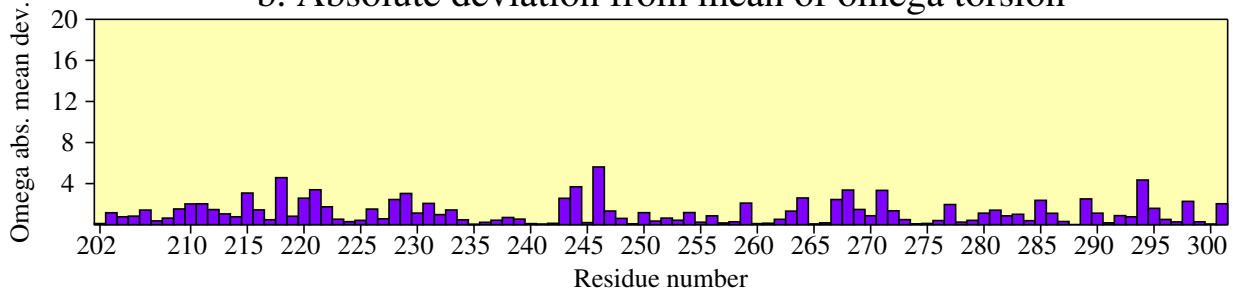
c = cis-peptide

Residue properties
1ZRT

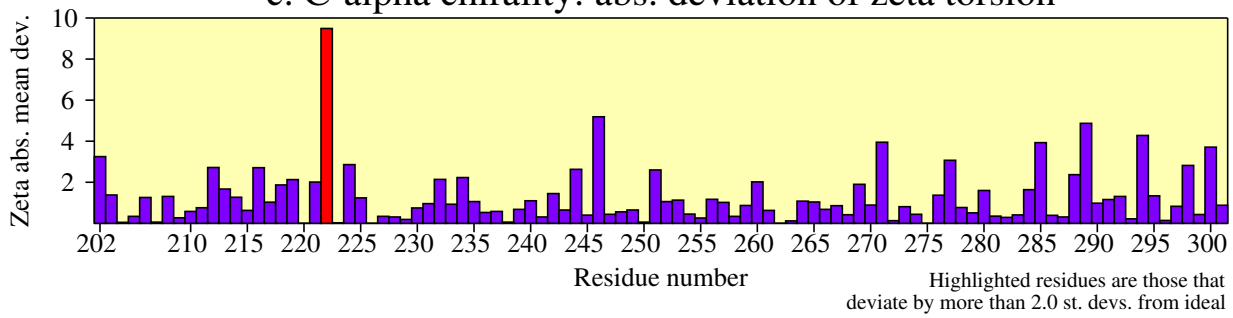
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

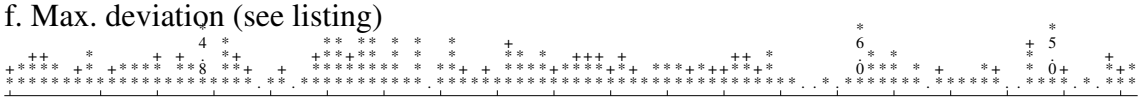
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

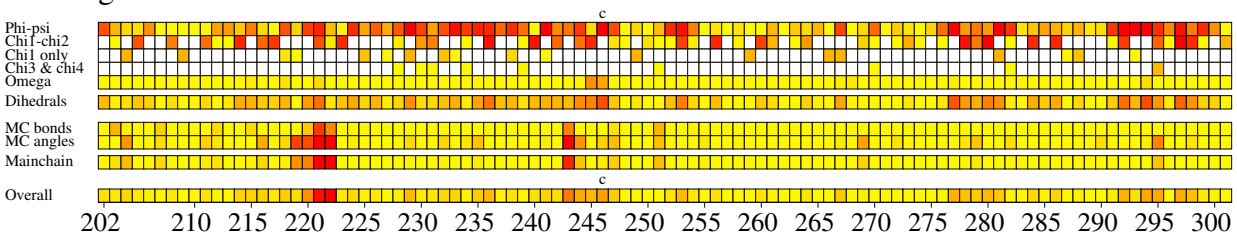
Most favoured Allowed Generous Disallowed

PFVIAALVAIHIWAFHTTGNNNPTGVEVRRTSKADAEKDTLPFWPYFVIKDLFALALVLLGFFAVVAYMPNYLGHPDNYVQANPLSTPAHIVPEWYFLPF

f. Max. deviation (see listing)



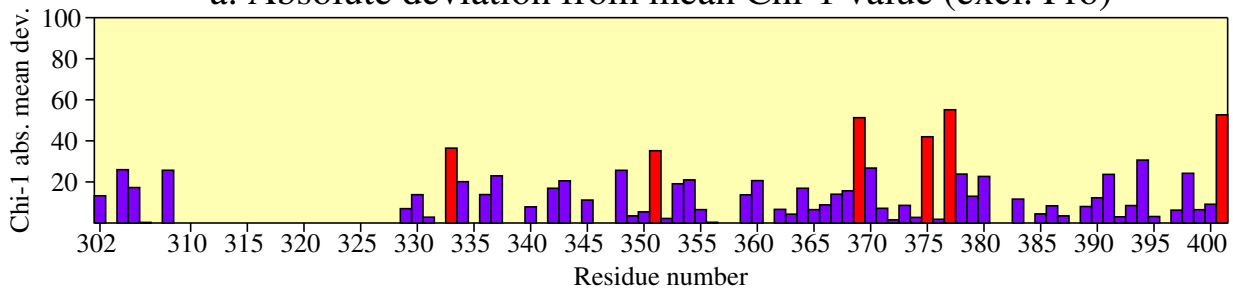
g. G-factors



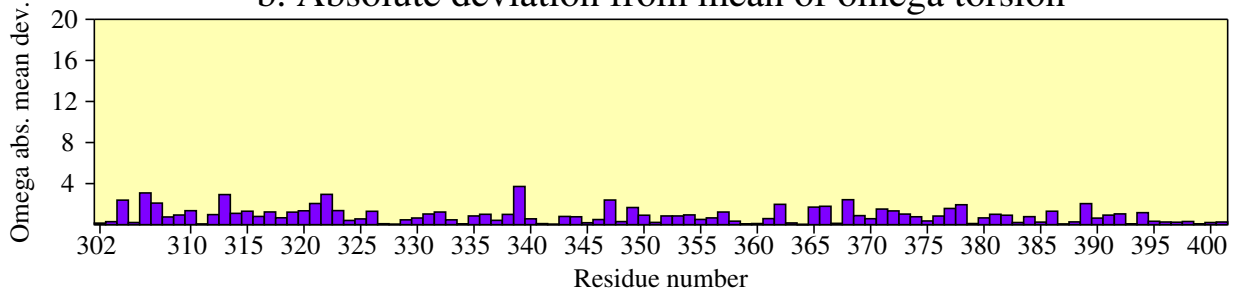
c = cis-peptide

Residue properties
1ZRT

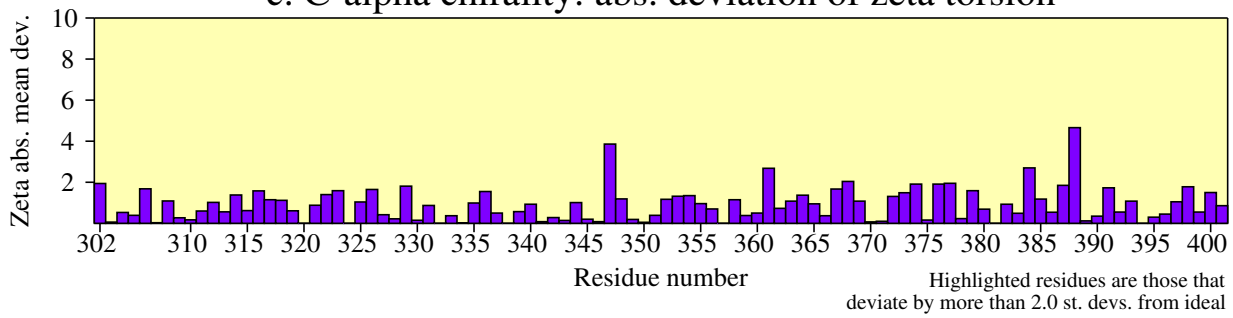
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

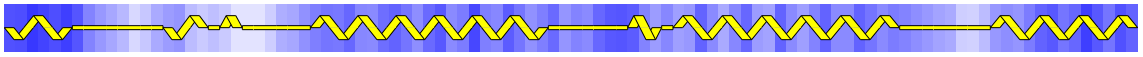


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



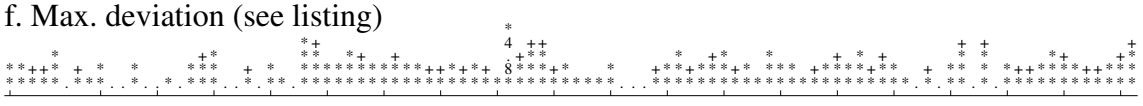
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

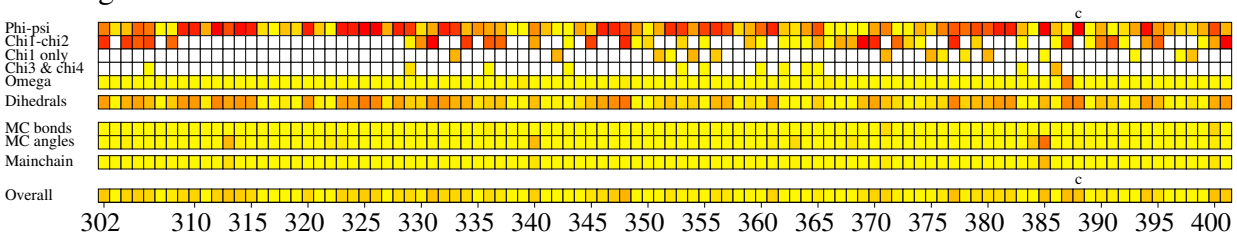
Most favoured Allowed Generous Disallowed

YA I LRAFAADVWVV I LVDGLTFG I VDAKFFGV I AMFGA I AVMALAPWLDTSKVRSGAYRPKFRMWFWFLVLDFVVLTWVGAMPTEYPYDWI SL I AS TYWF

f. Max. deviation (see listing)



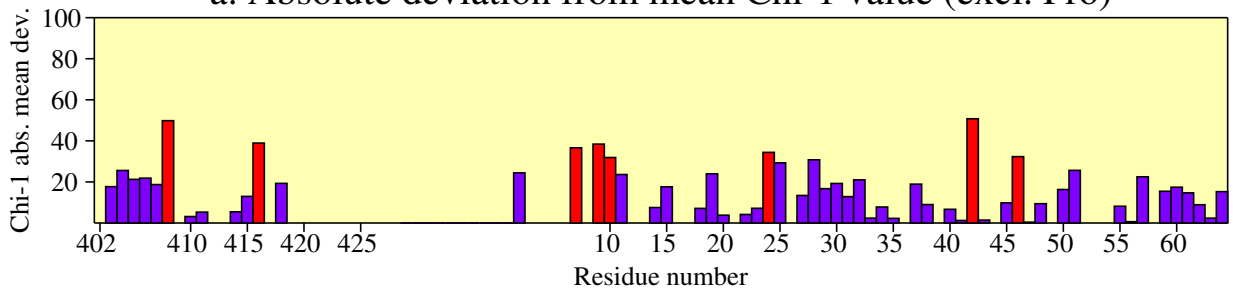
g. G-factors



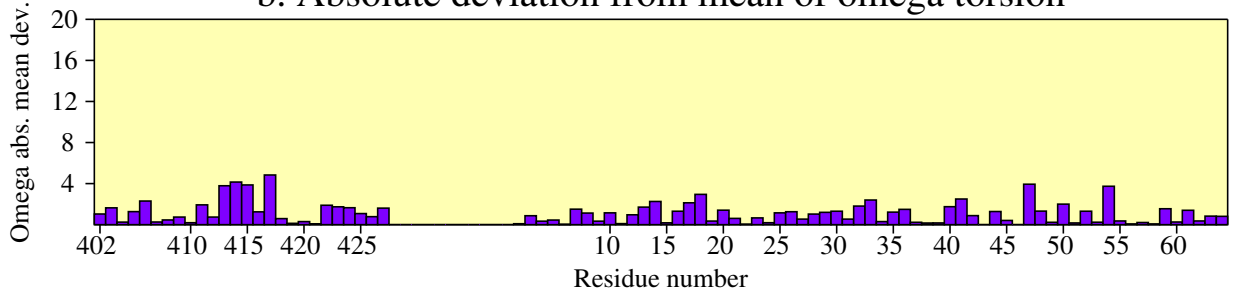
c = cis-peptide

Residue properties
1ZRT

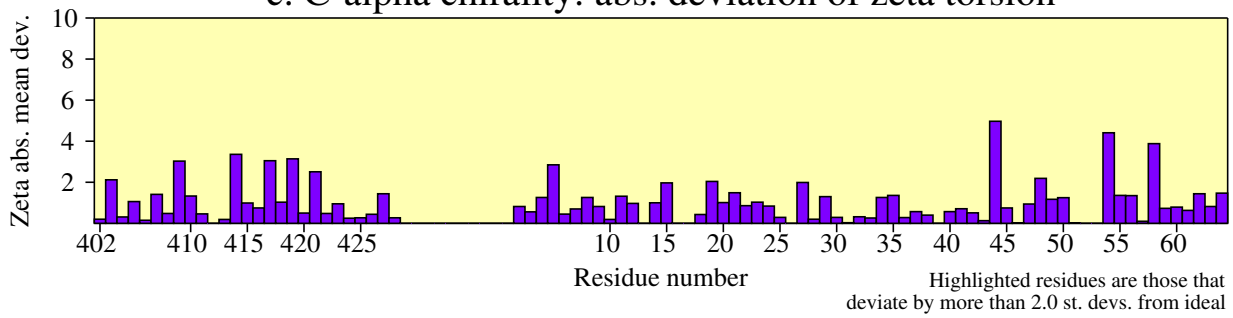
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

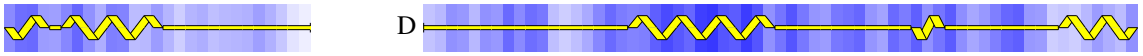


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

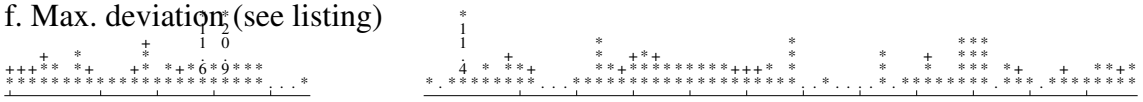


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

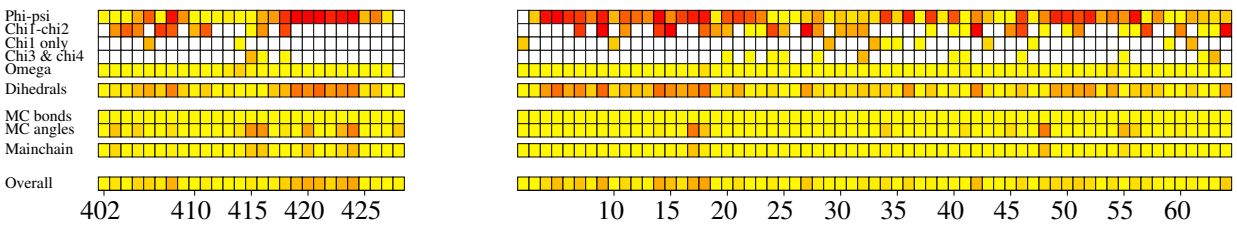
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

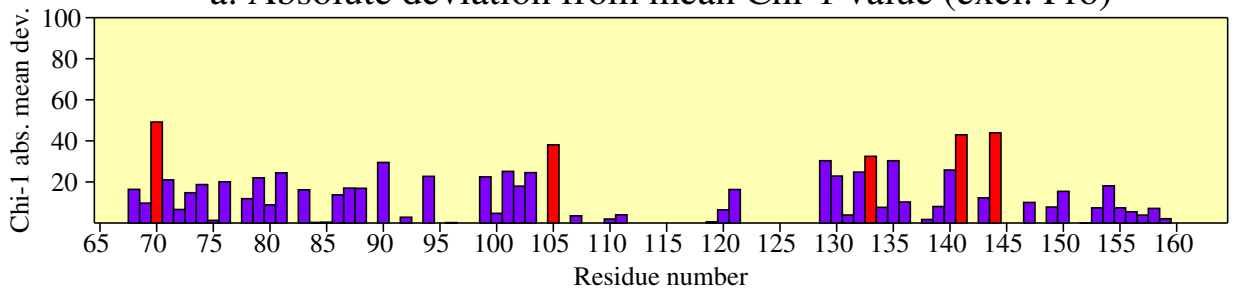


g. G-factors

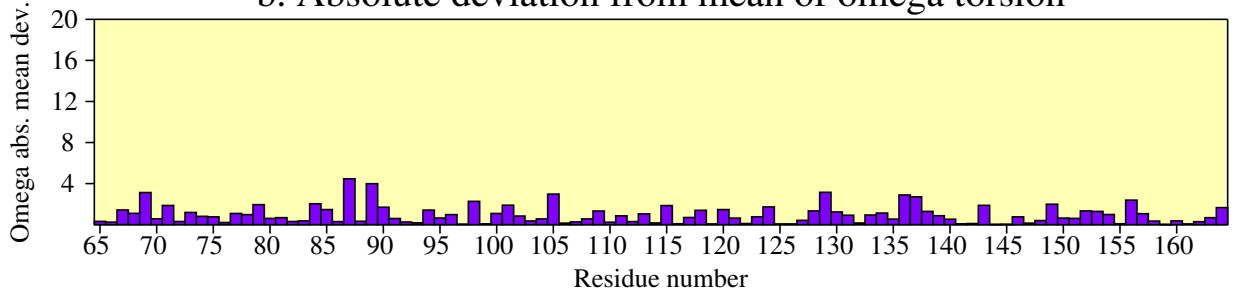


Residue properties
1ZRT

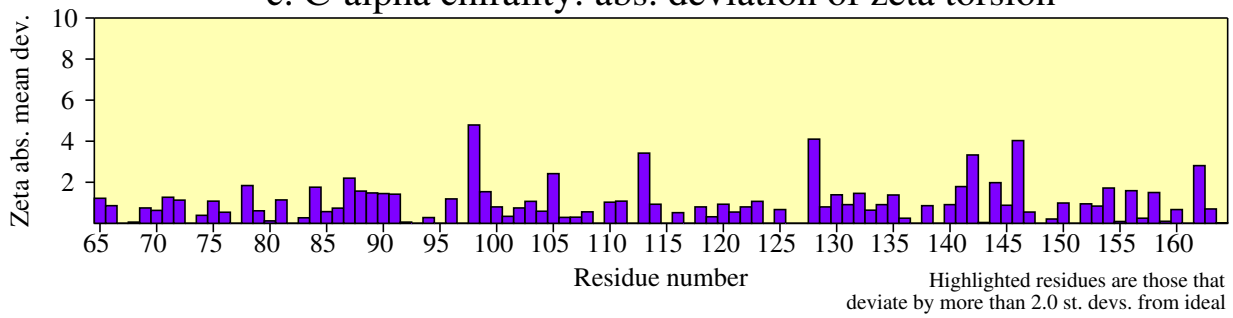
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

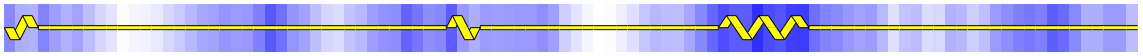


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



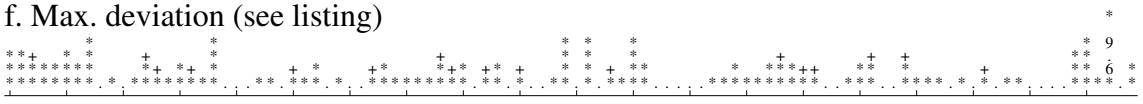
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

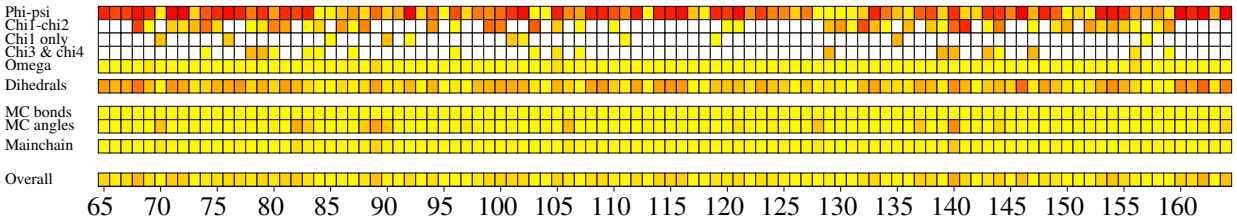
Most favoured Allowed Generous Disallowed

AAGLDTIIDKDSGEERDRKETDMFPTRVGDGMGPDLSVMAKARAGFSGPAGSGMNQLFKGMGGPEYIYNYVIGFEENPECAPEGIDGYYYNKTFQIGPDT

f. Max. deviation (see listing)

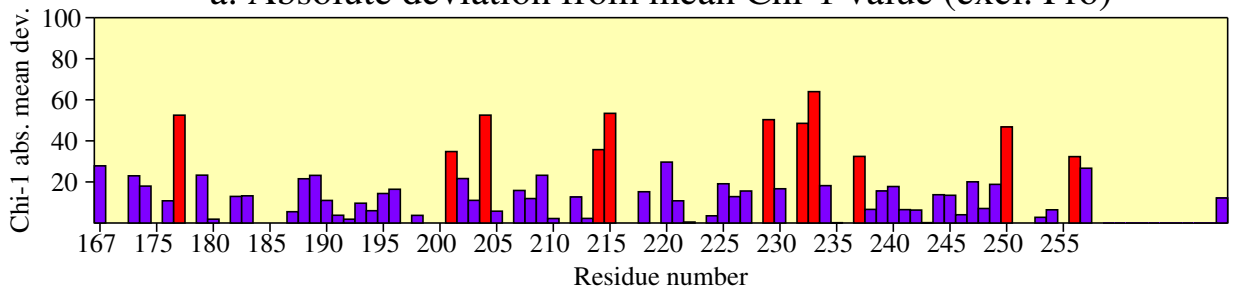


g. G-factors

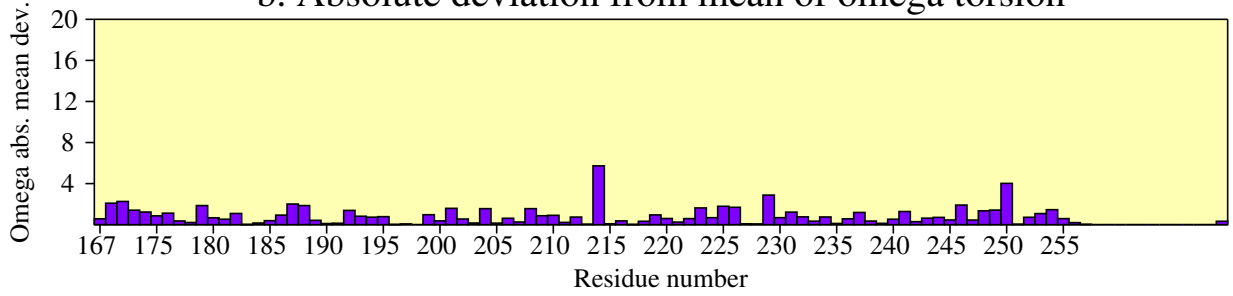


Residue properties
1ZRT

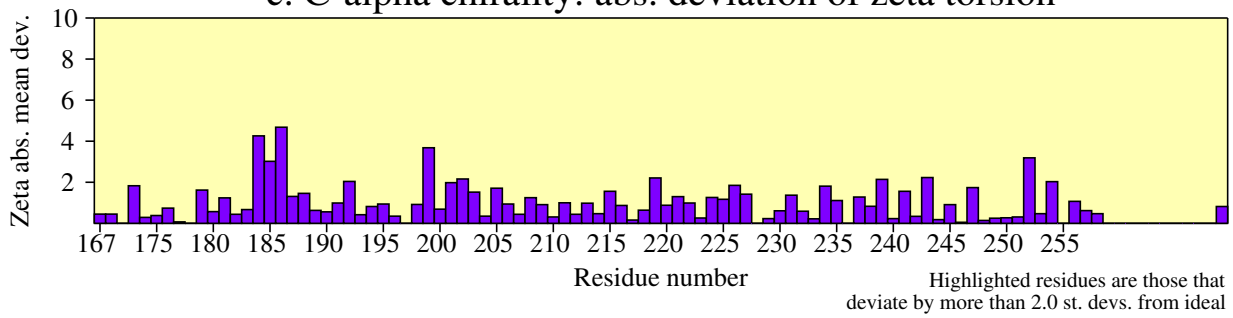
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

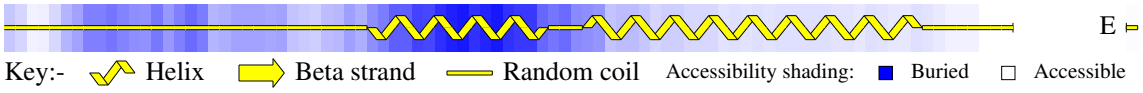


c. C-alpha chirality: abs. deviation of zeta torsion



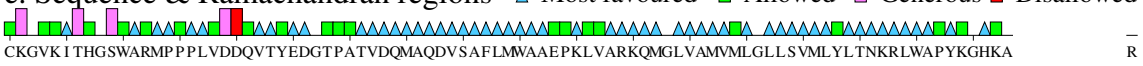
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

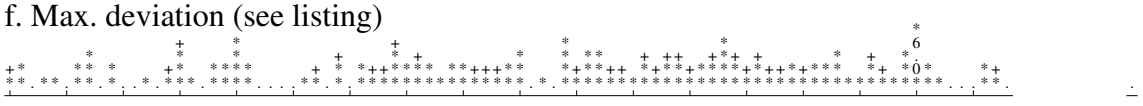


e. Sequence & Ramachandran regions

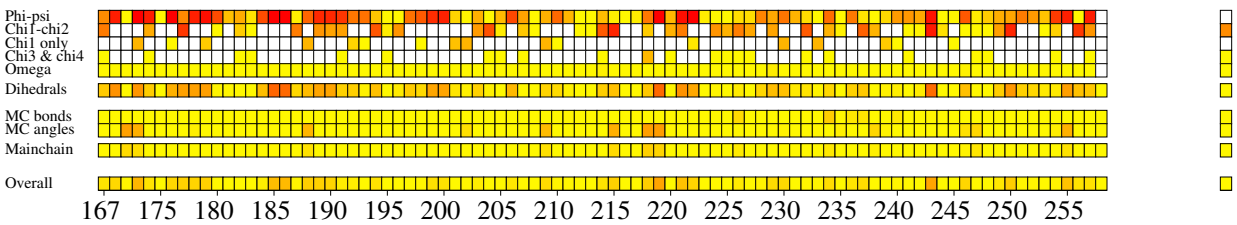
Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

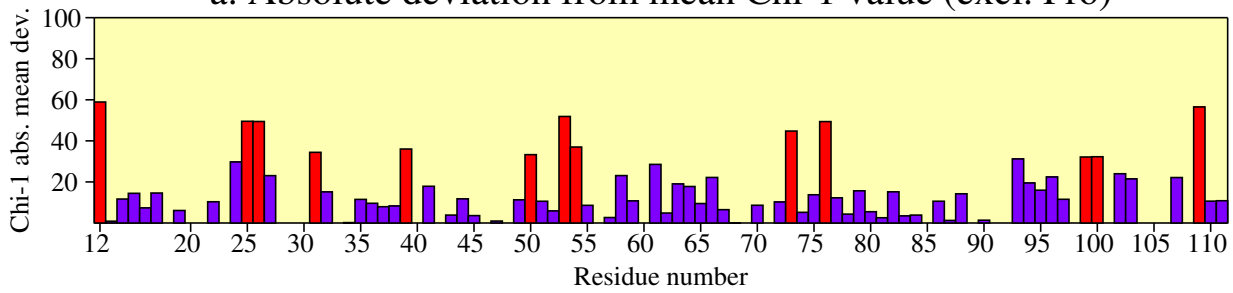


g. G-factors

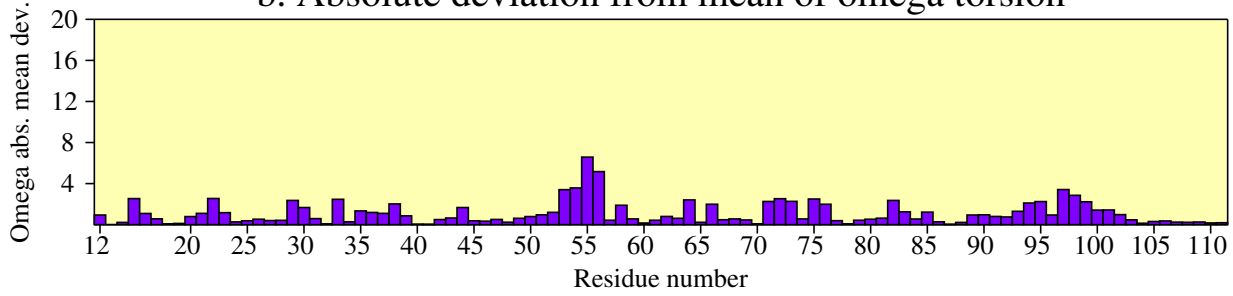


Residue properties
1ZRT

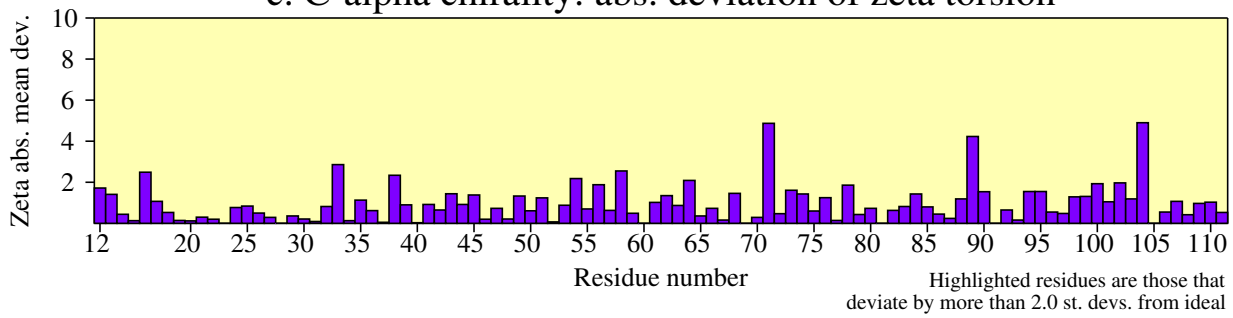
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

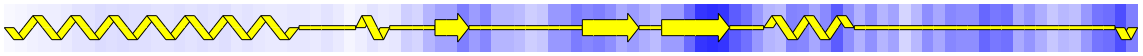


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



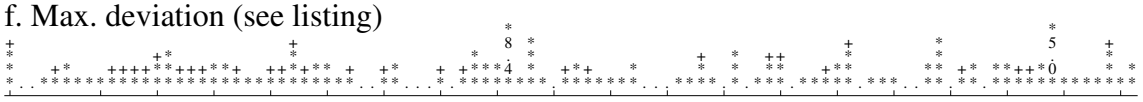
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

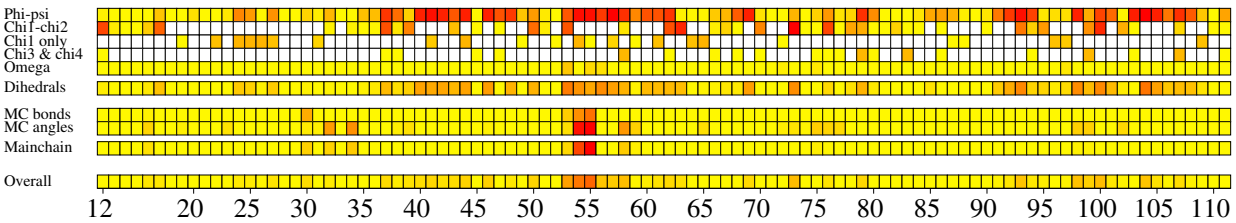
Most favoured Allowed Generous Disallowed

RDFLYHATAATGVVVTGAAVWPLINQMNASADVKAMASIFVDVSAVEVGTQLTVKWRGKPVFIRRRDEKDIELARSVPLGALRDTSAENANKPGAEATDE

f. Max. deviation (see listing)

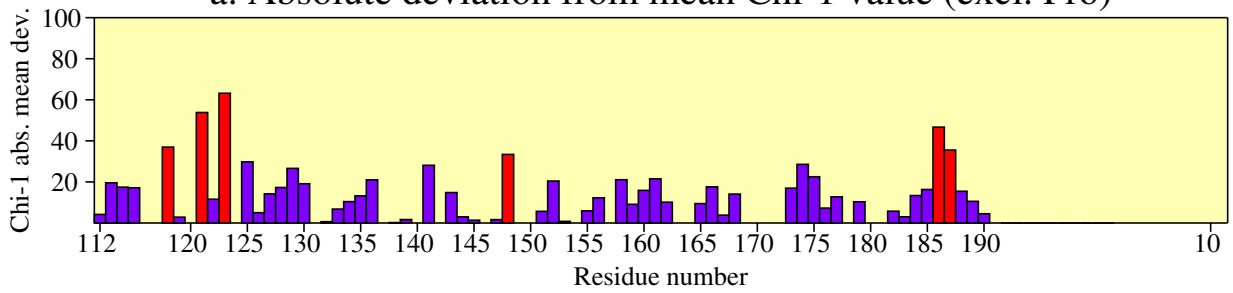


g. G-factors

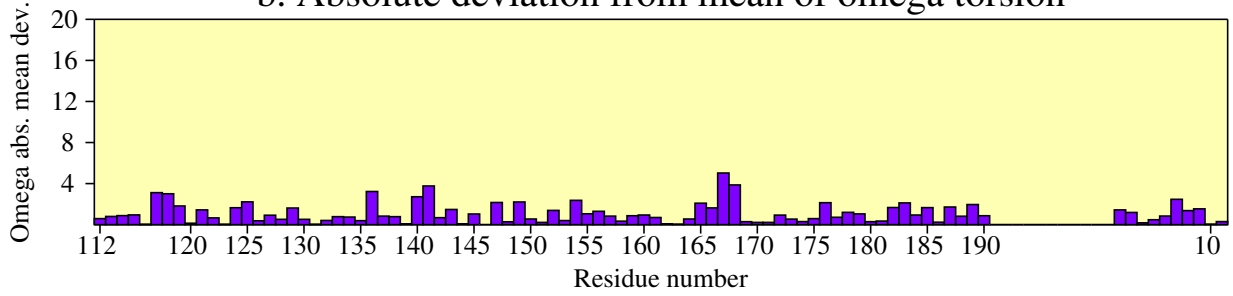


Residue properties
1ZRT

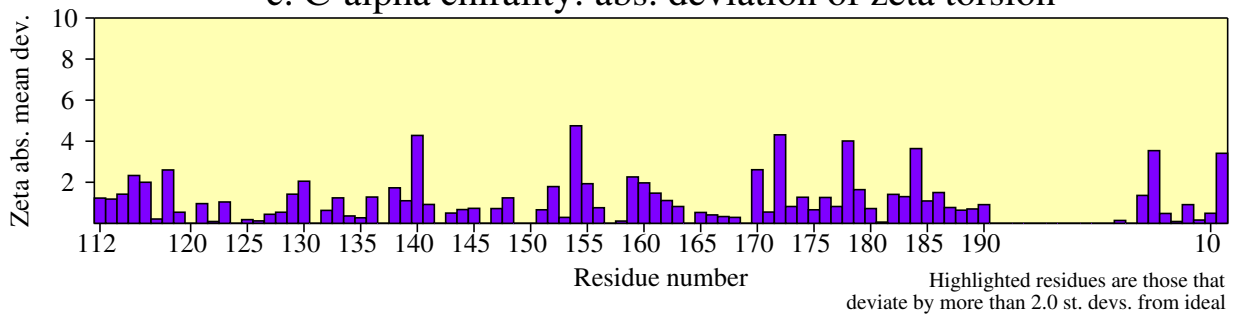
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

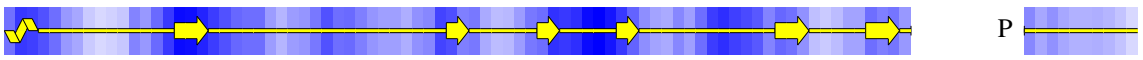


c. C-alpha chirality: abs. deviation of zeta torsion



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

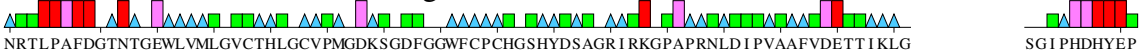
d. Secondary structure & estimated accessibility



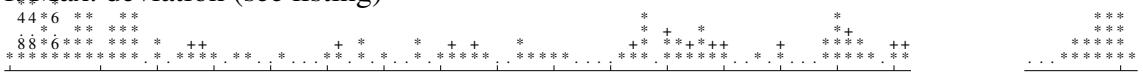
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

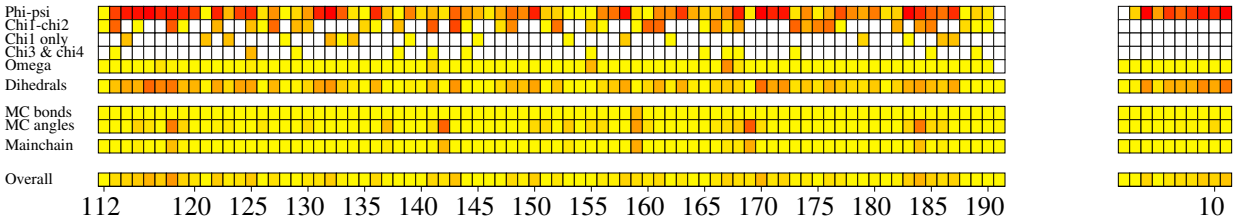
Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

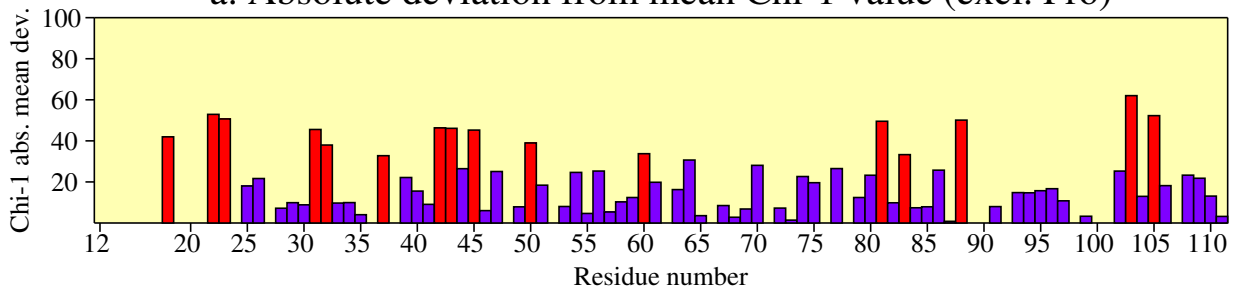


g. G-factors

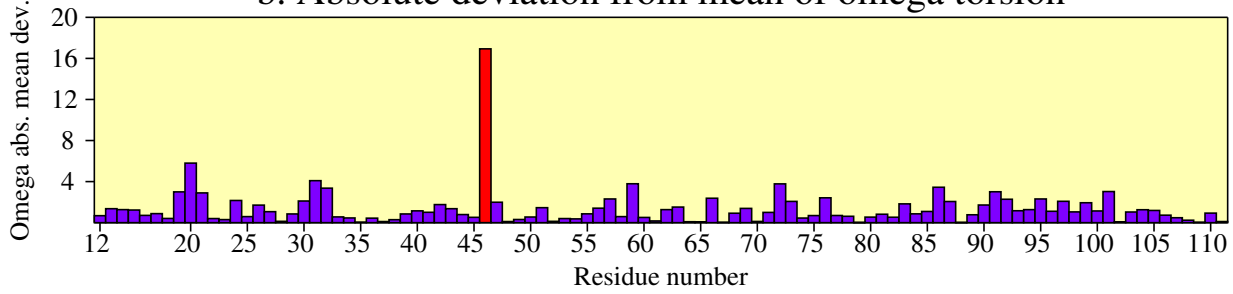


Residue properties
1ZRT

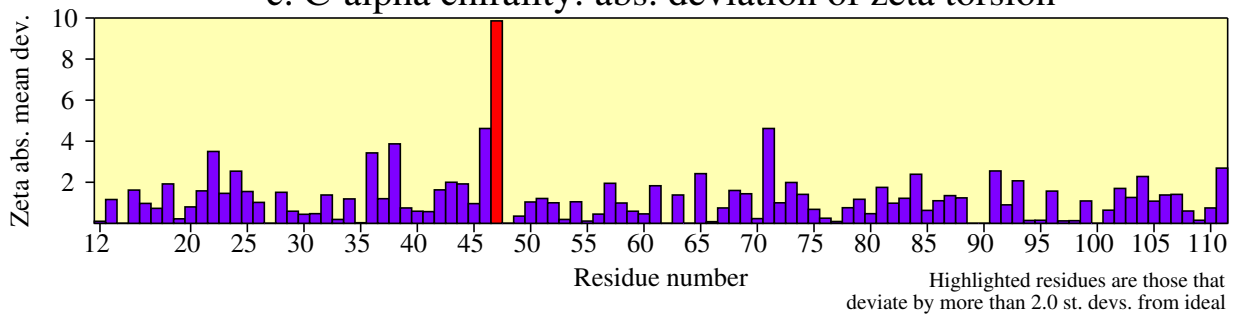
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



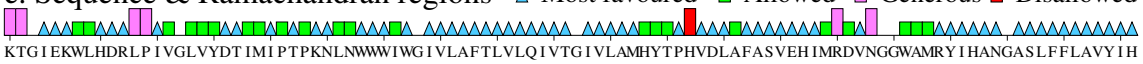
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

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

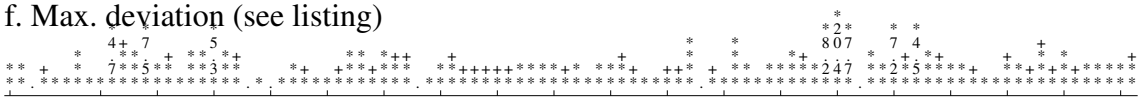
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

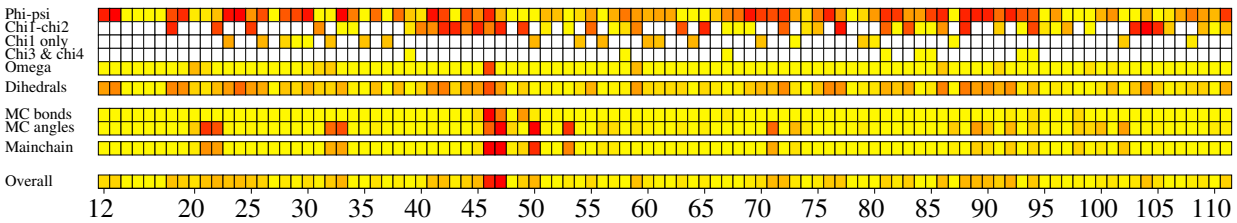


KTG I EKWLHDRLP I VGLVYDT IMI P T PKNLNWWW I WG I VLAFTLVLQ I VTG I VLAMHYTPHVDLAFASVEH IMRDVNGGWAMRY I HANGASLFFLAVY I H

f. Max. deviation (see listing)

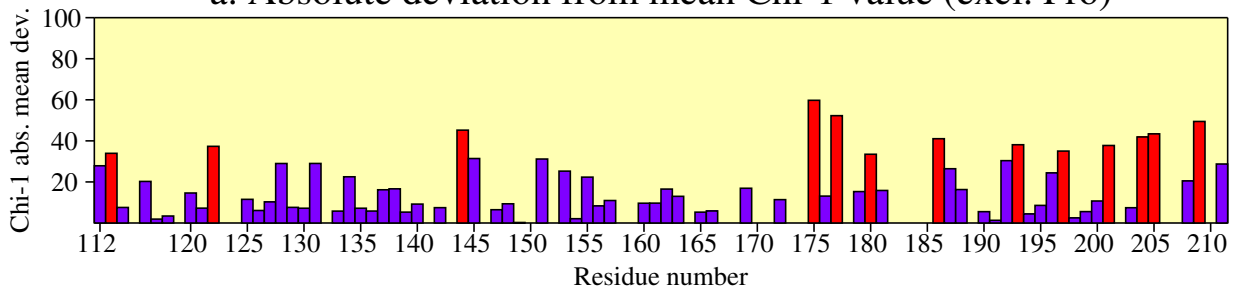


g. G-factors

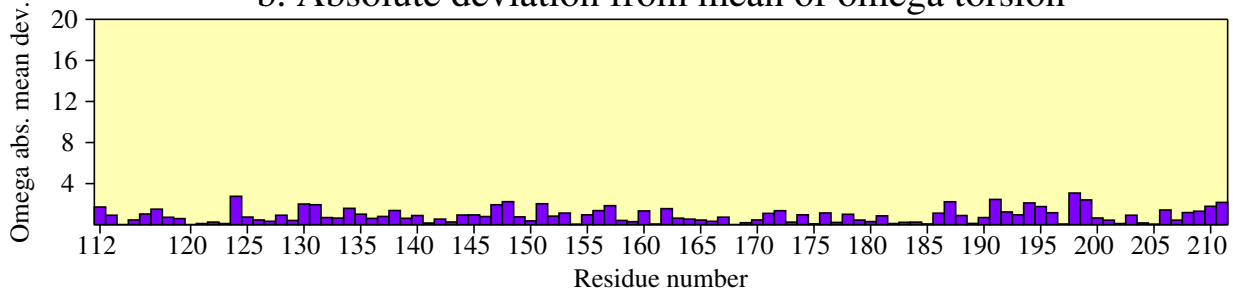


Residue properties
1ZRT

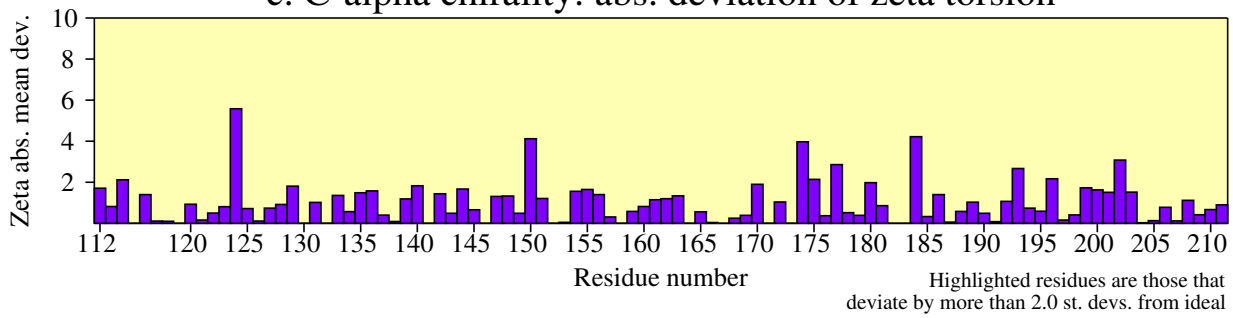
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

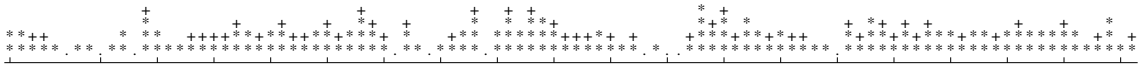
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

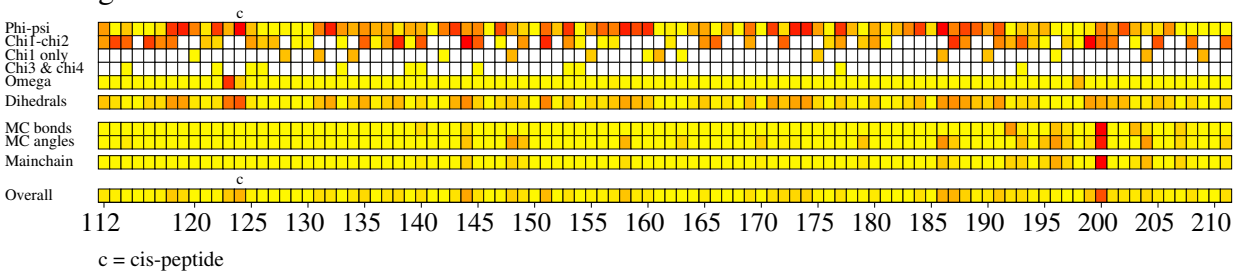
Most favoured Allowed Generous Disallowed

I F R G L Y Y G S Y K A P R E I T W I V G M V I Y L L M M G T A F M G Y V L P W G Q M S F W G A T V I T G L F G A I P G I G P S I Q A W L L G G P A V D N A T L N R F F S L H Y L L P F V I A A L V A I

f. Max. deviation (see listing)



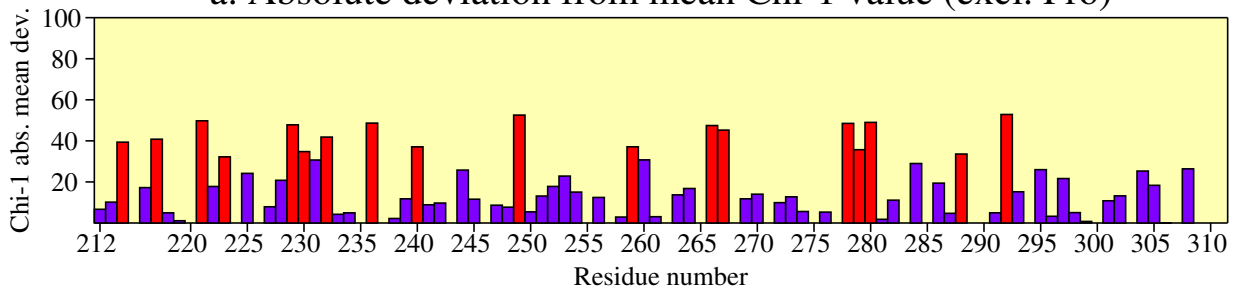
g. G-factors



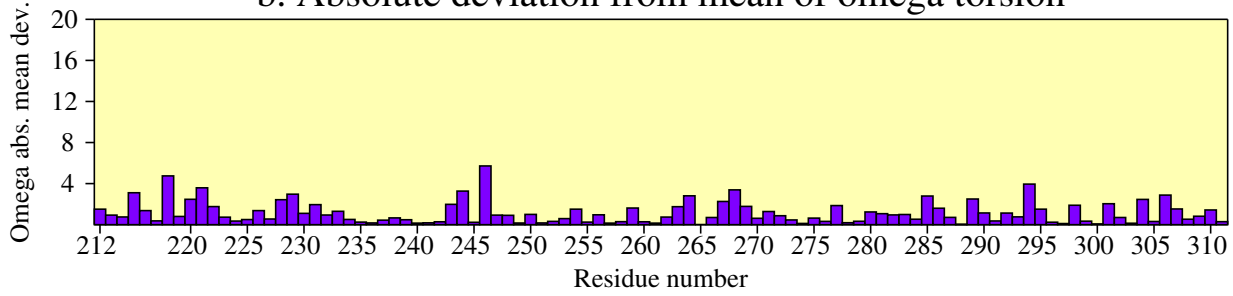
c = cis-peptide

Residue properties
1ZRT

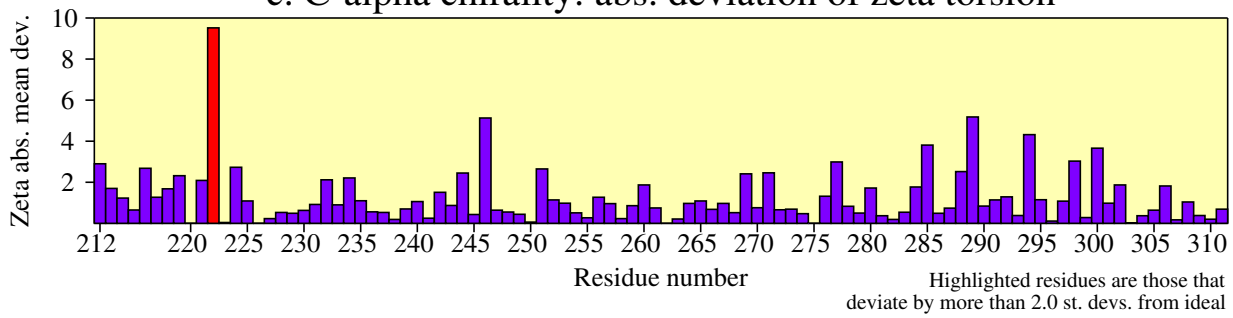
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

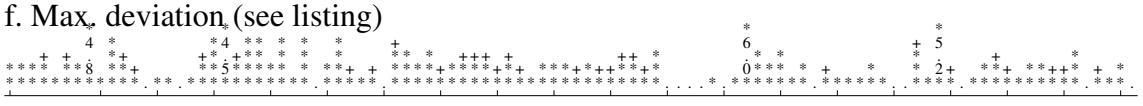
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

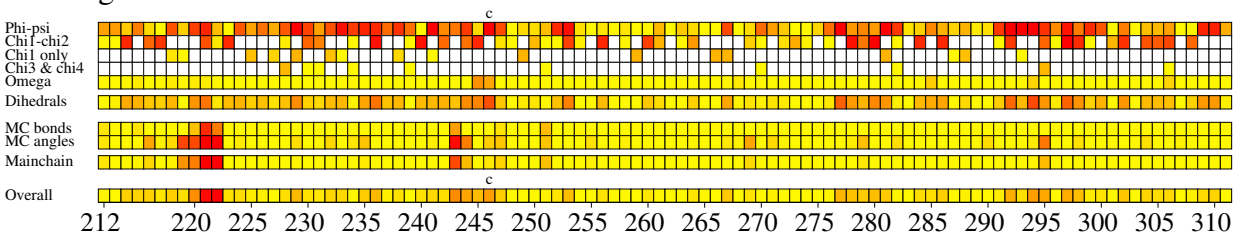
Most favoured Allowed Generous Disallowed

H I W A F H T T G N N N P T G V E V R R T S K A D A E K D T L P F W P Y F V I K D L F A L A L V L L G F F A V V A Y M P N Y L G H P D N Y V Q A N P L S T P A H I V P E W Y F L P F Y A I L R A F A A D

f. Max. deviation (see listing)



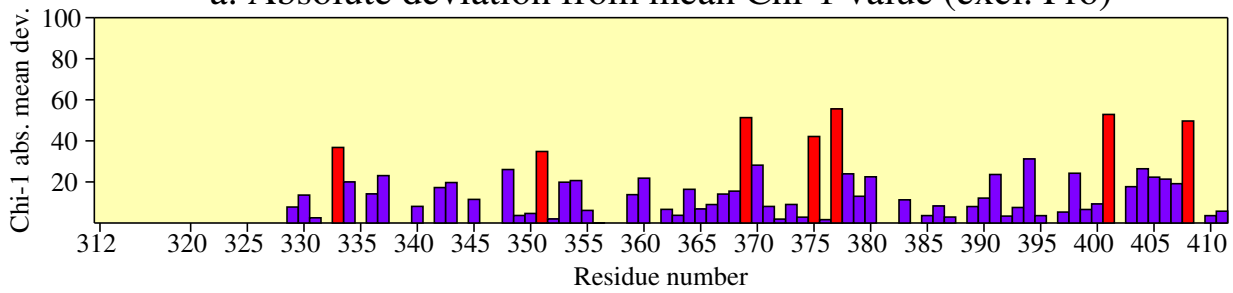
g. G-factors



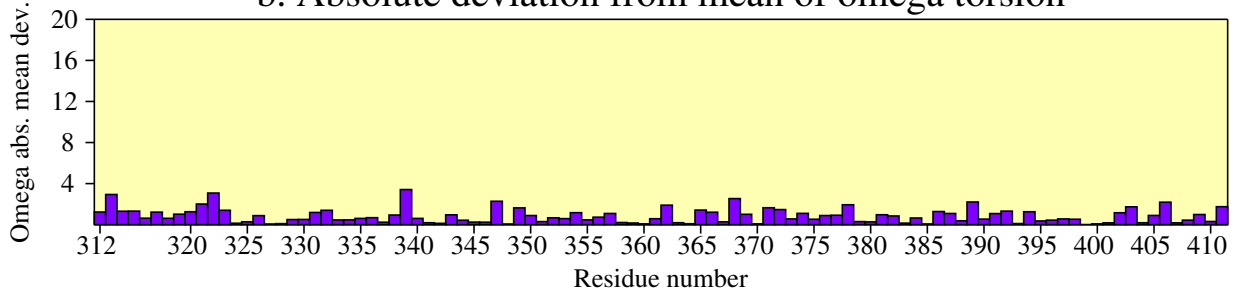
c = cis-peptide

Residue properties
1ZRT

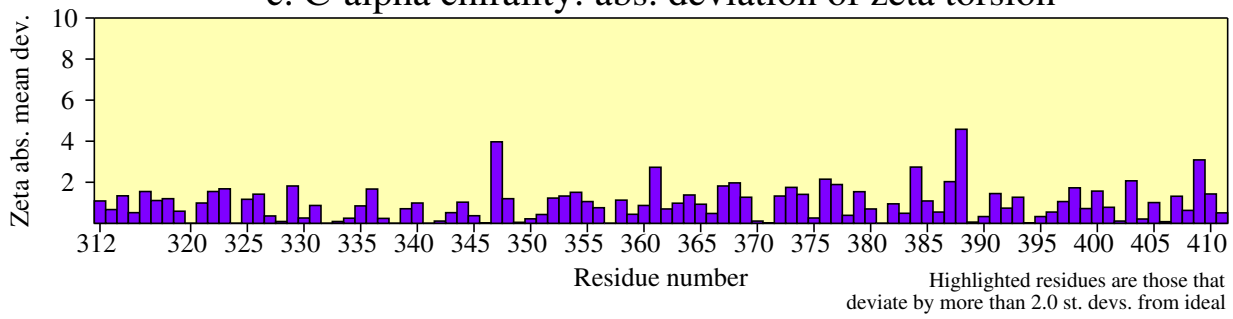
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



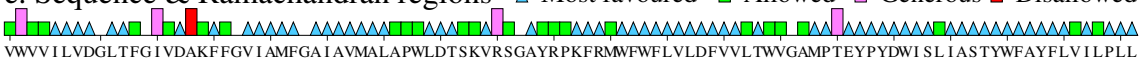
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

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

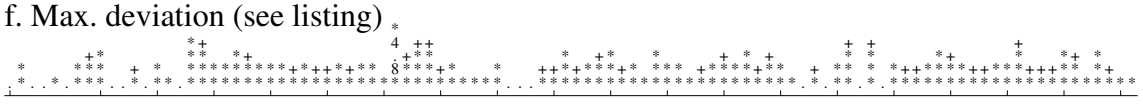
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

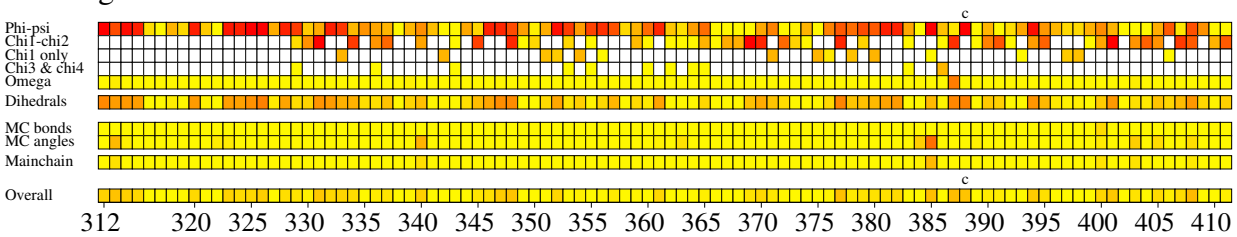


VWVV I L VDGL T FG I VDAK F F GV I AMFGA I AVMAL A PWL D T S KVR S GAYR P K F RMWFWF L VL D F VVL T WVGAMP T EY P YDWI S L I A S T YWF A Y F L V I L P L L

f. Max. deviation (see listing)

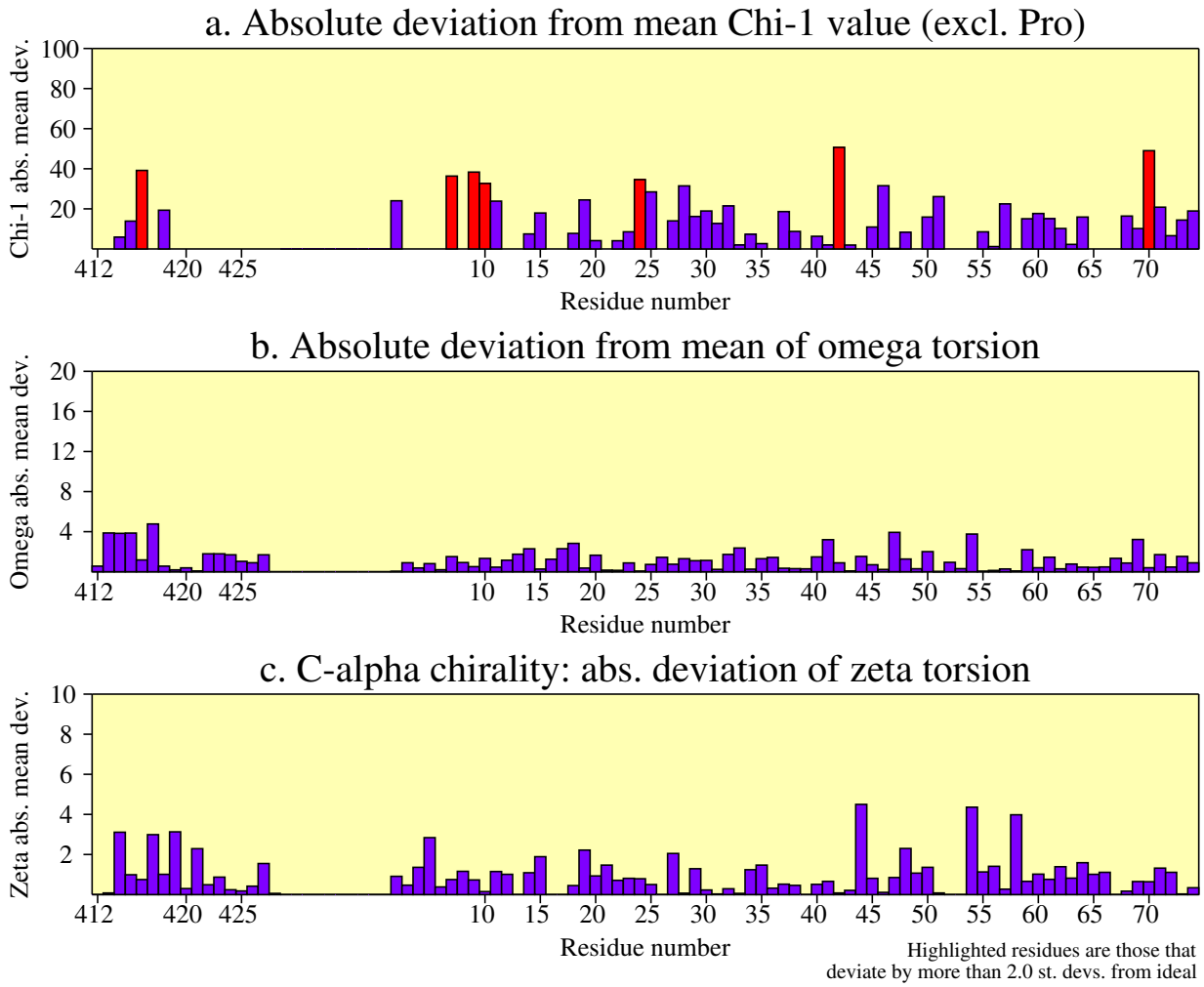


g. G-factors



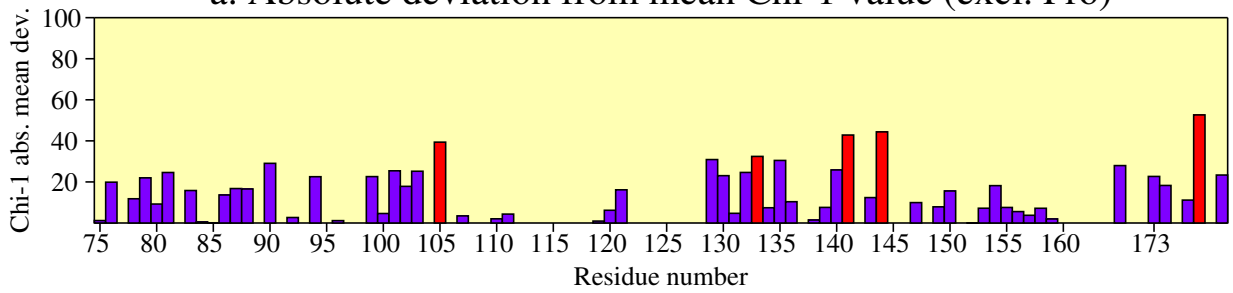
c = cis-peptide

Residue properties
1ZRT

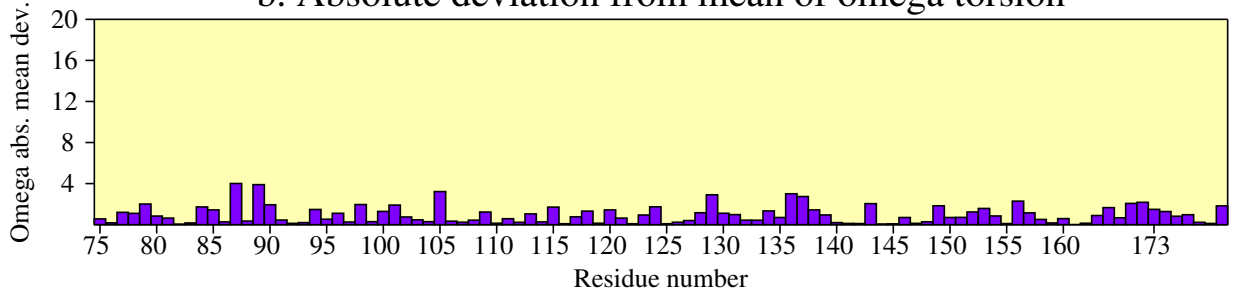


Residue properties
1ZRT

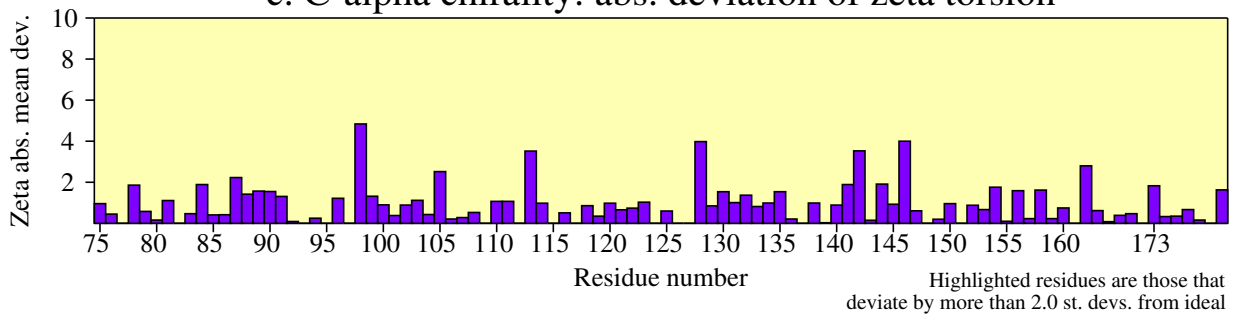
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

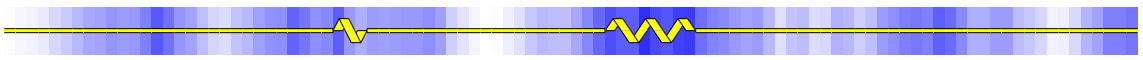


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



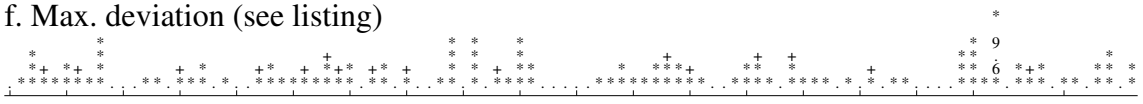
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

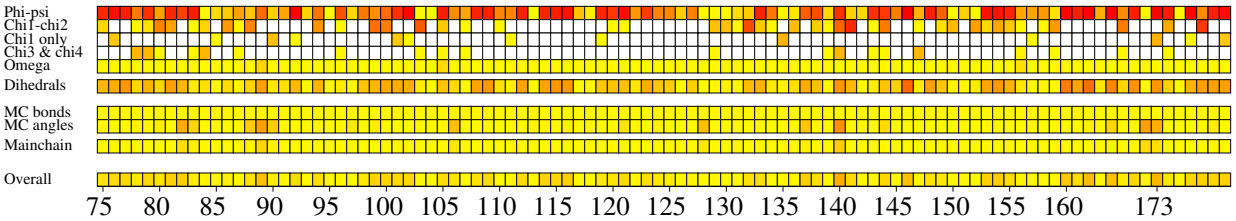
Most favoured Allowed Generous Disallowed

D S G E E R D R K E T D M F P T R V G D G M G P D L S V M A K A R A G F S G P A G S G M N Q L F K G M G G P E Y I Y N Y V I G F E E N P E C A P E G I D G Y Y Y N K T F Q I G P D T C K G V K I T H G S

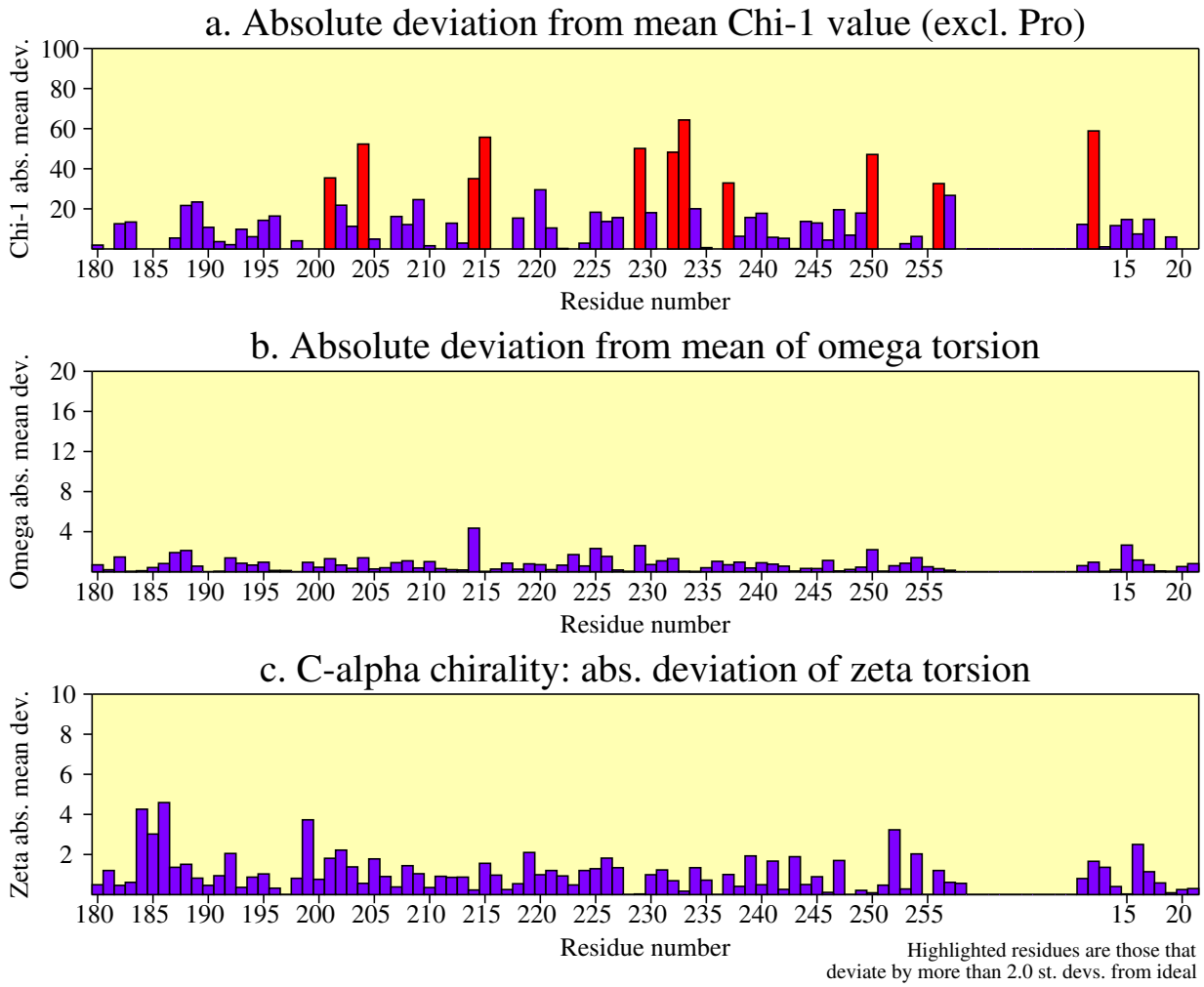
f. Max. deviation (see listing)



g. G-factors

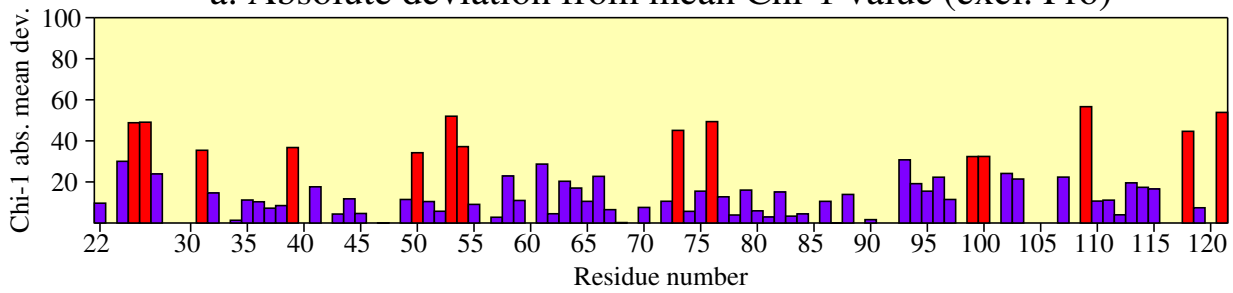


Residue properties
1ZRT

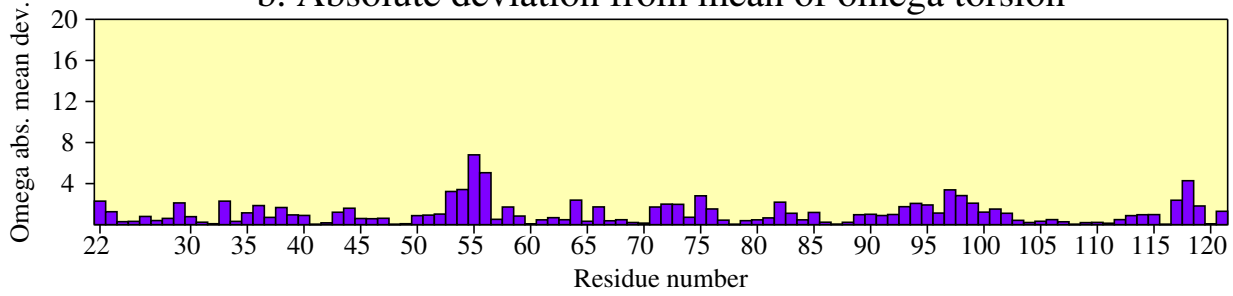


Residue properties
1ZRT

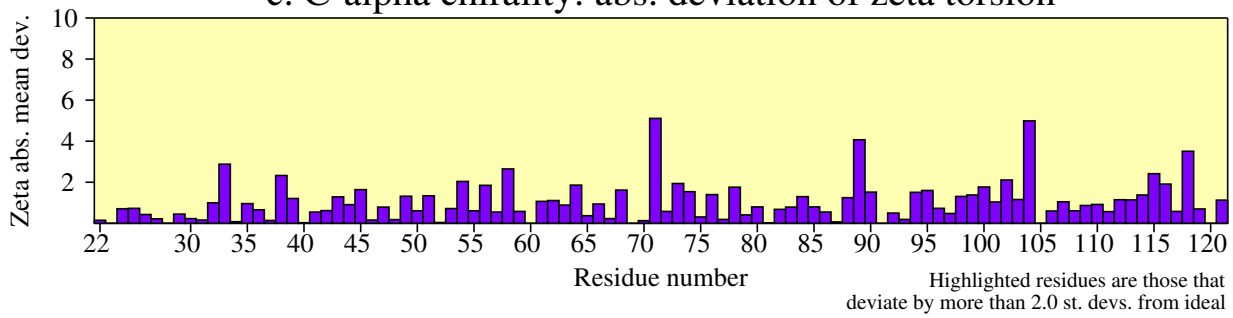
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

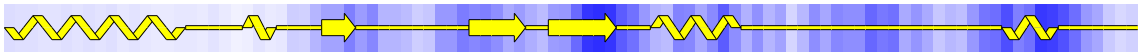


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



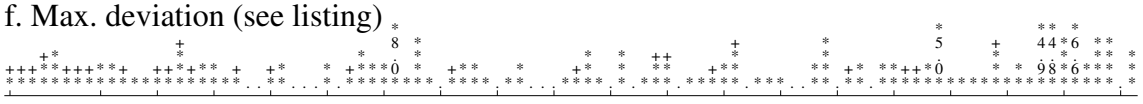
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

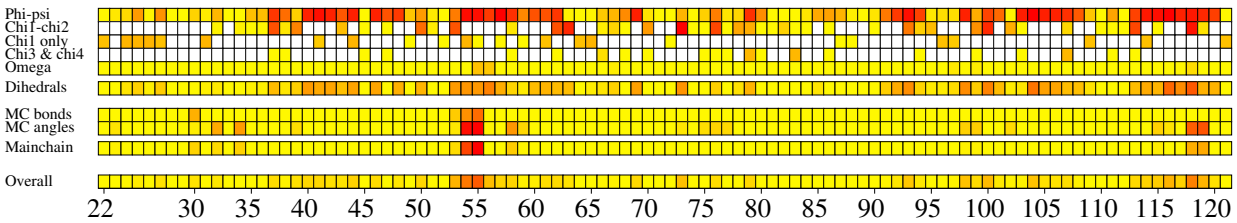
Most favoured Allowed Generous Disallowed

TGVVVTGAAVWPLINQMNASADVKAMASIFVDVSAVEVGTQLTVKWRGKPVFIRRRDEKDIELARSVPLGALRDTSAENANKPGAEATDENRTLPAFDGT

f. Max. deviation (see listing)

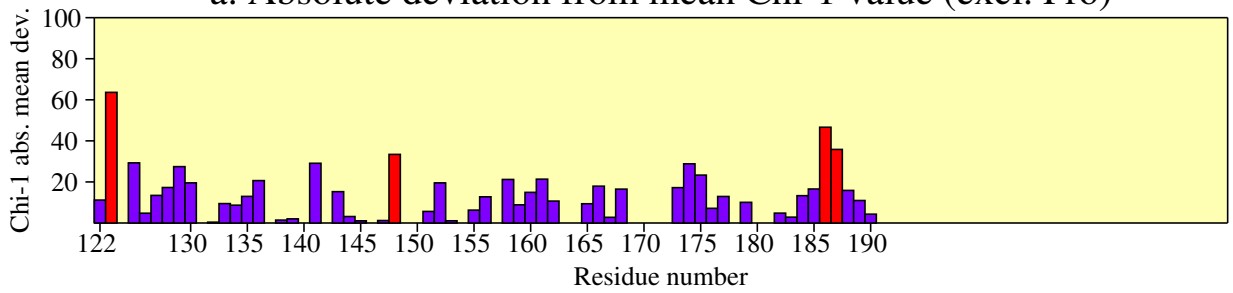


g. G-factors

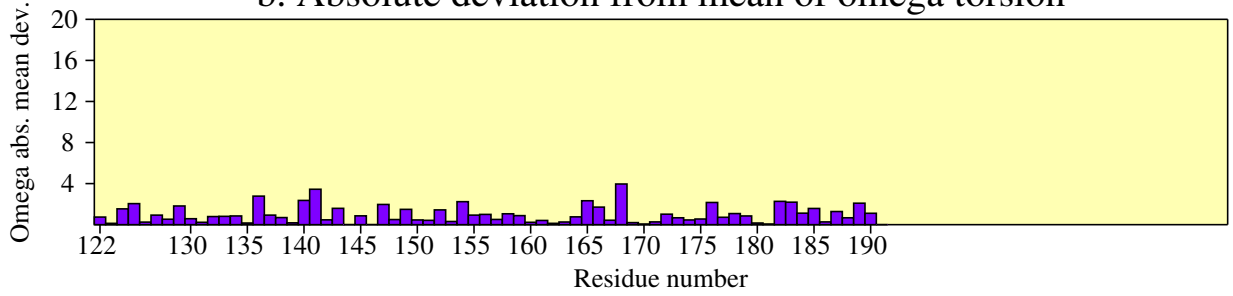


Residue properties
1ZRT

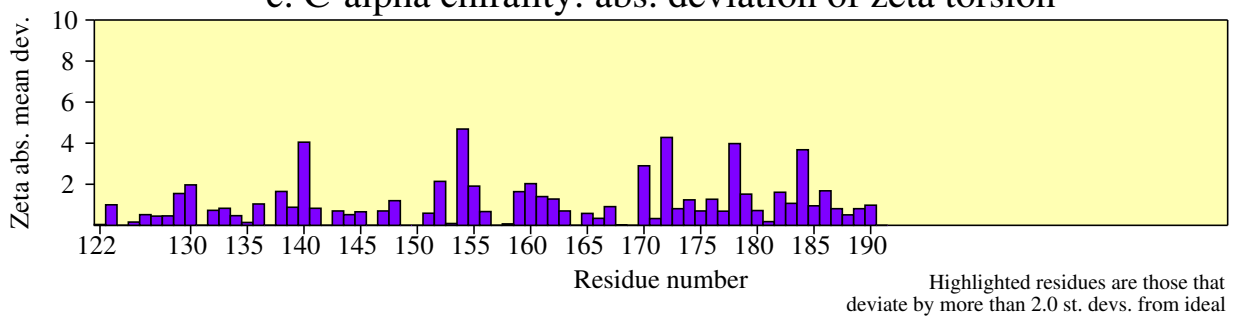
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

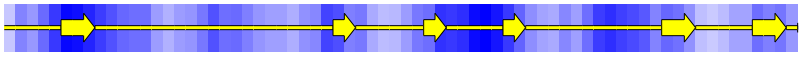


c. C-alpha chirality: abs. deviation of zeta torsion



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

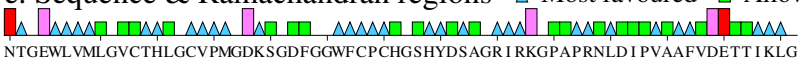
d. Secondary structure & estimated accessibility



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

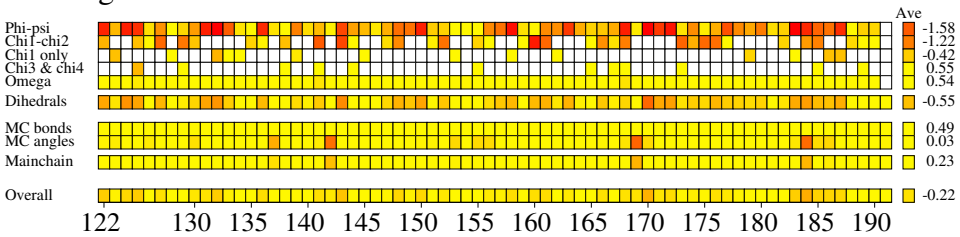
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed



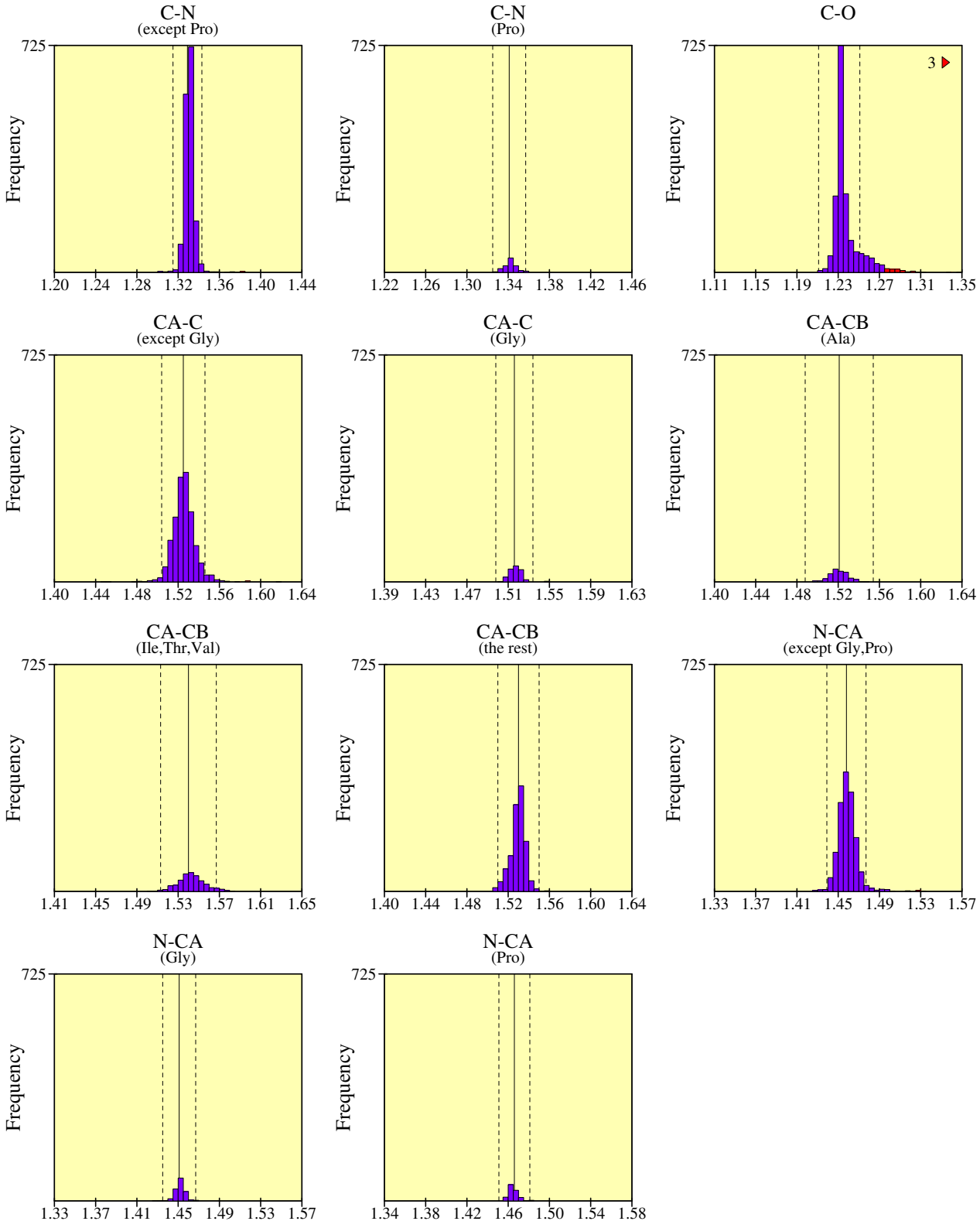
f. Max. deviation (see listing)

g. G-factors



Main-chain bond lengths

1ZRT

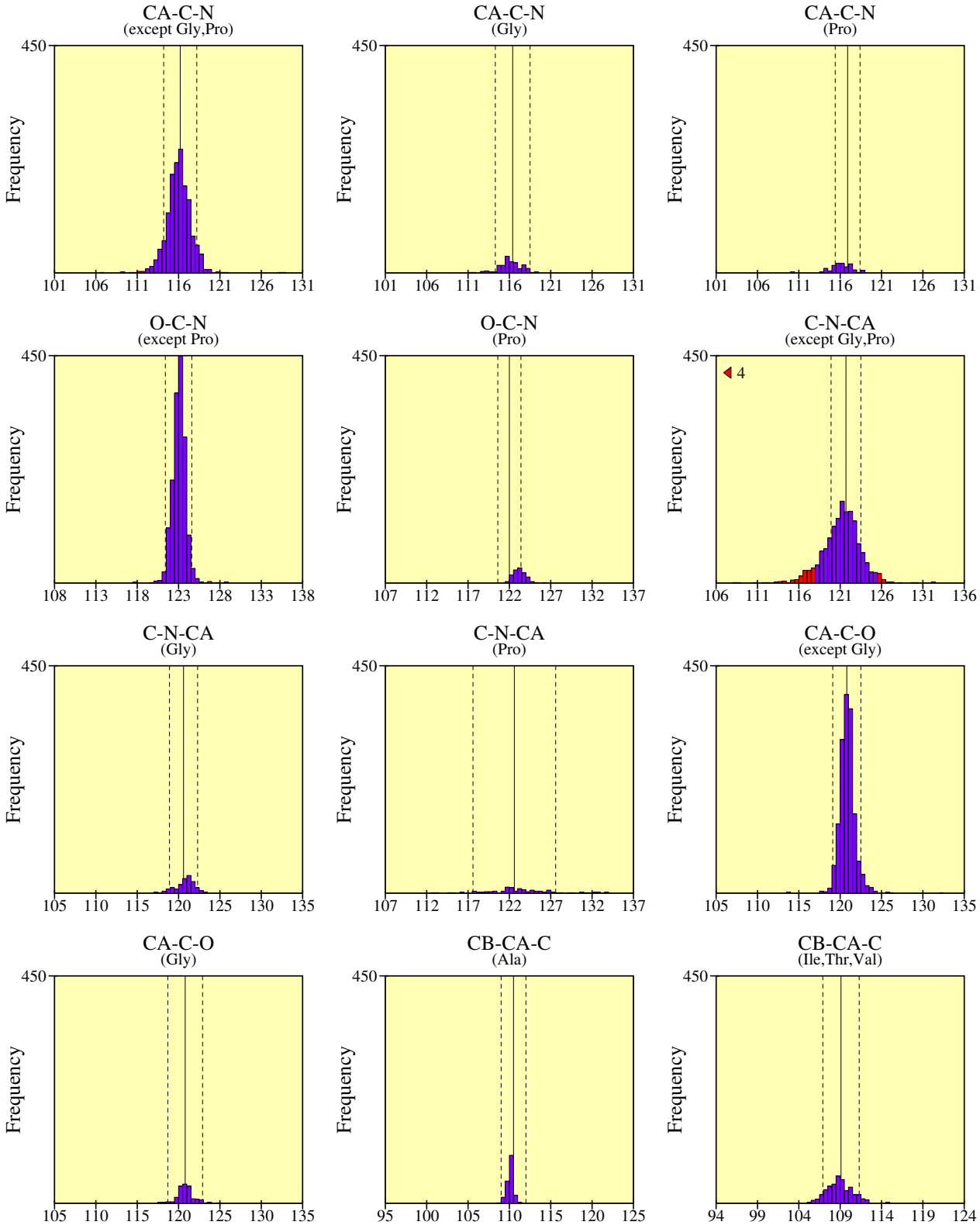


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

1ZRT

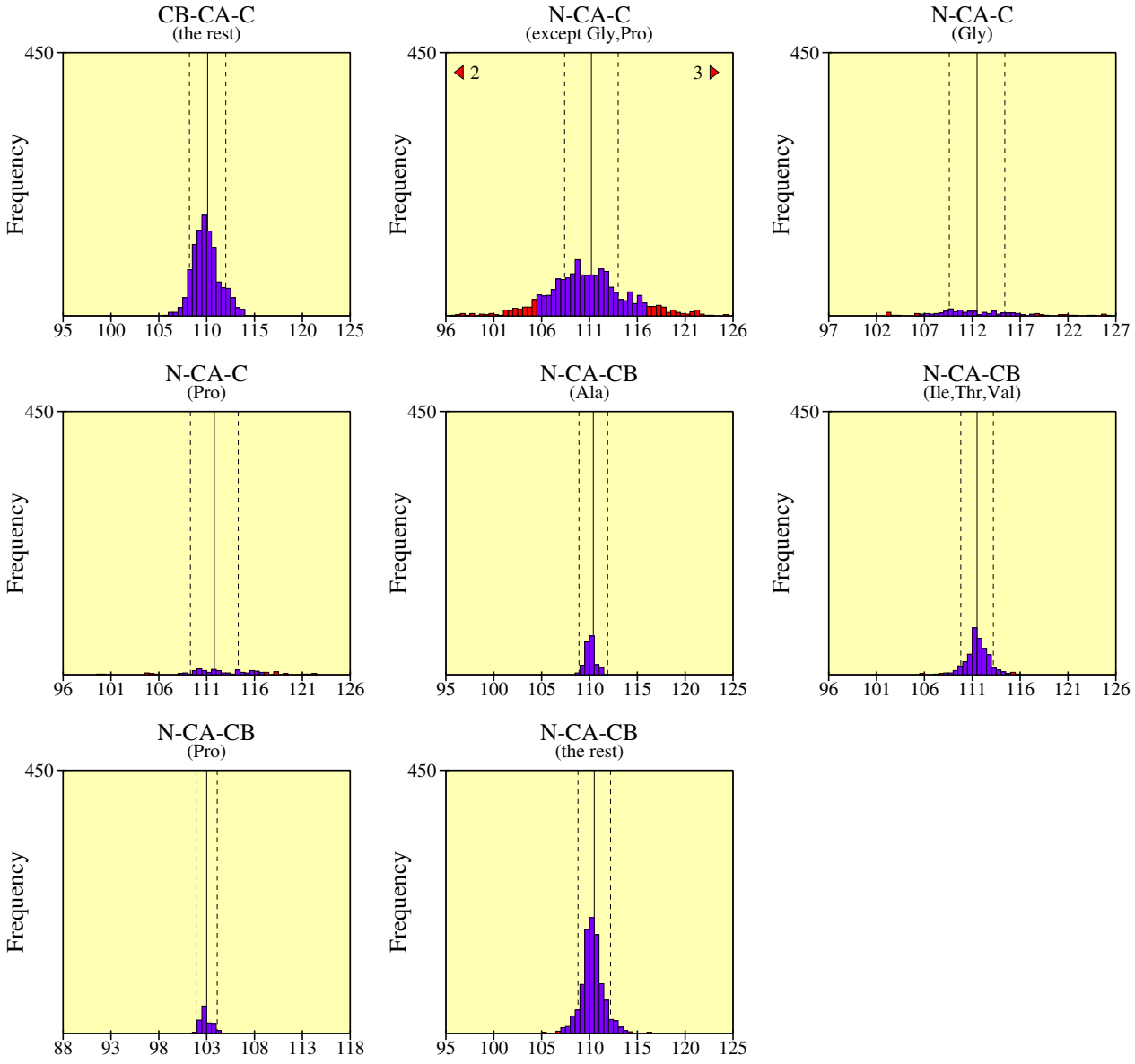


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

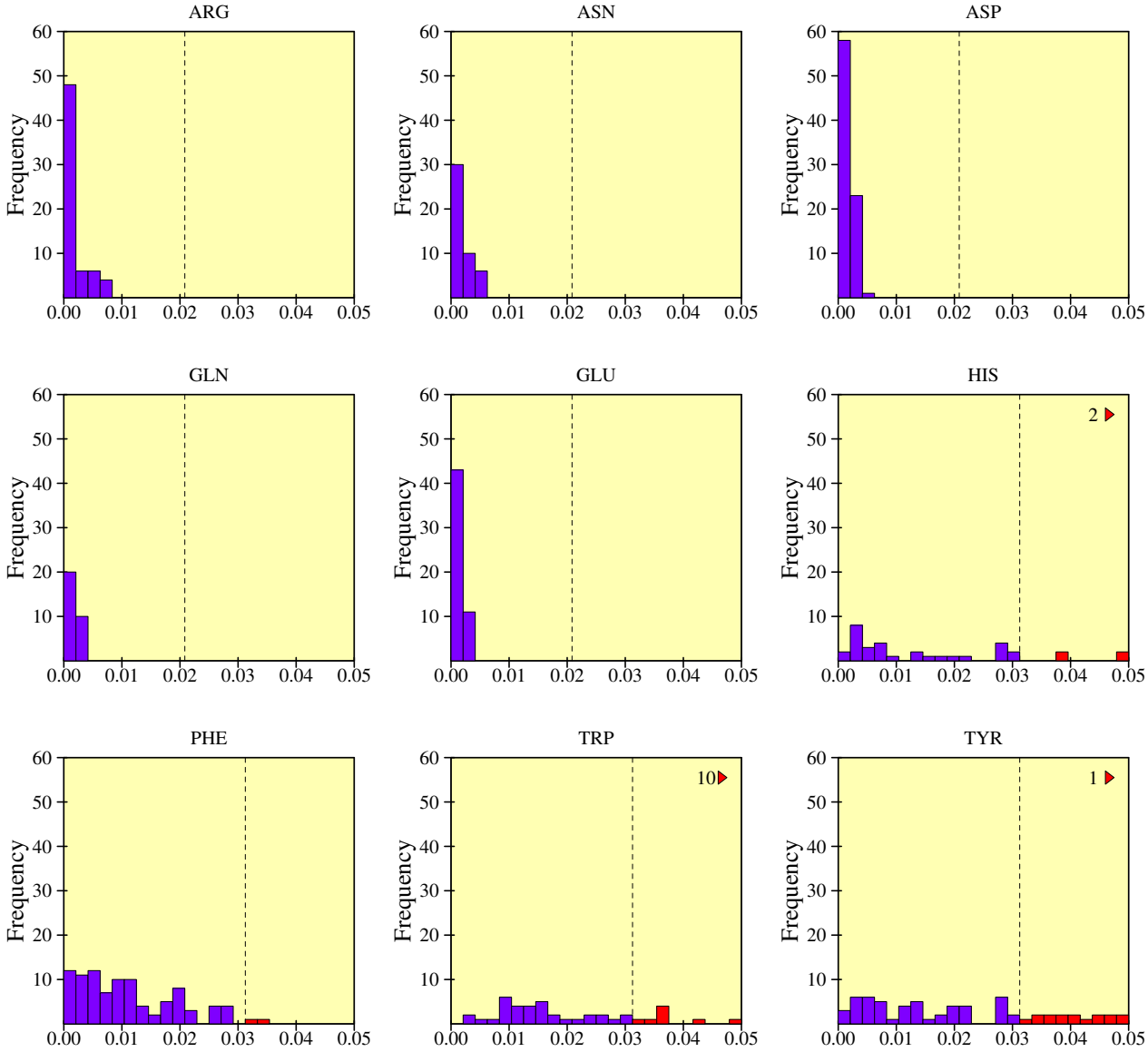
1ZRT



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

1ZRT

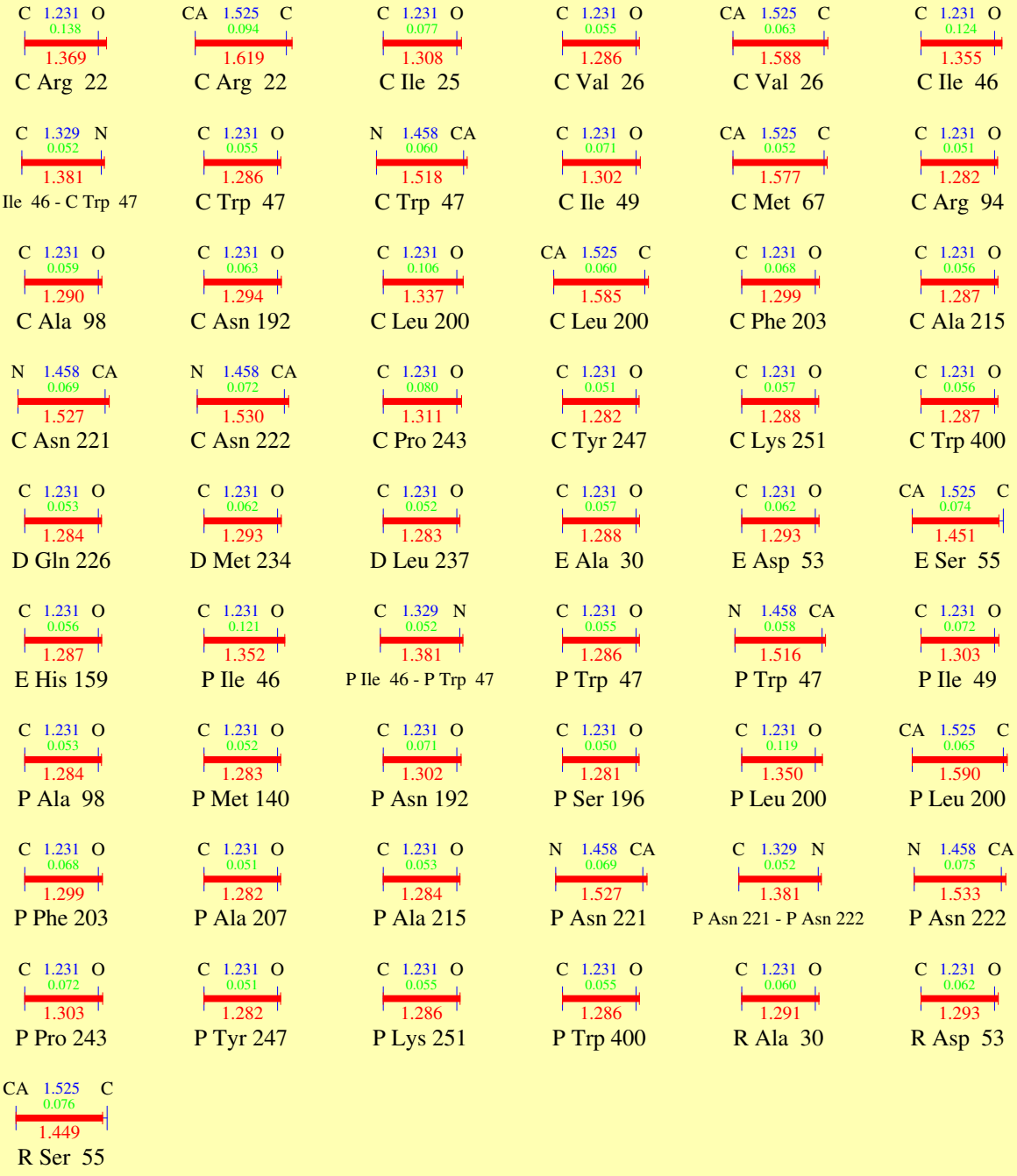


Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

▸ signifies data points off the graph in the direction shown.

Distorted geometry
1ZRT

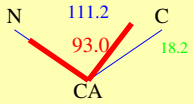
Main-chain bond lengths



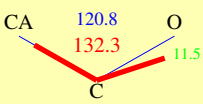
Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

Distorted geometry
1ZRT

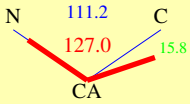
Main-chain bond angles



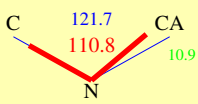
C Asp 21



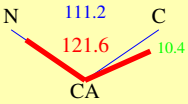
C Arg 22



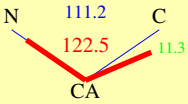
C Arg 22



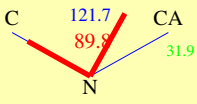
C Ile 25 - C Val 26



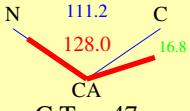
C Thr 32



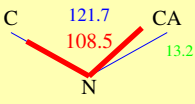
C Ile 33



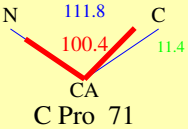
C Ile 46 - C Trp 47



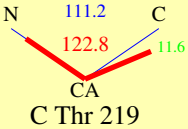
C Trp 47



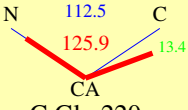
C Ile 49 - C Val 50



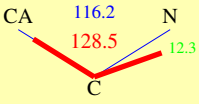
C Pro 71



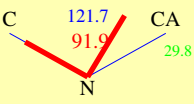
C Thr 219



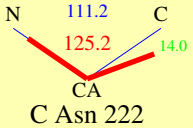
C Gly 220



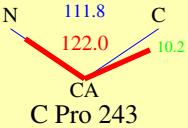
C Asn 221 - C Asn 222



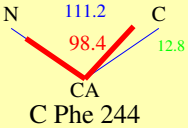
C Asn 221 - C Asn 222



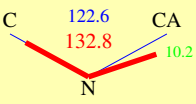
C Asn 222



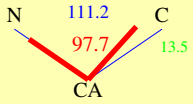
C Pro 243



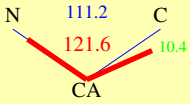
C Phe 244



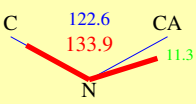
C Val 293 - C Pro 294



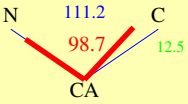
C Glu 295



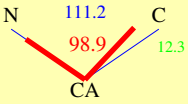
C Thr 385



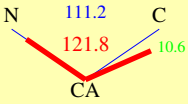
C Tyr 387 - C Pro 388



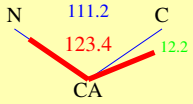
C Glu 415



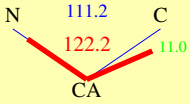
C Lys 416



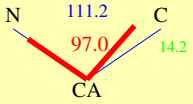
C Ile 420



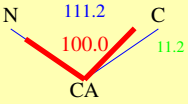
C Ile 424



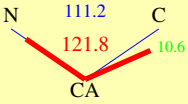
D Lys 17



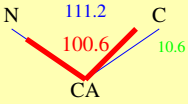
D Leu 48



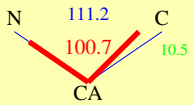
D Gln 55



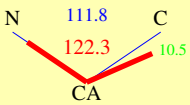
D Glu 140



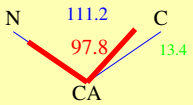
D Val 173



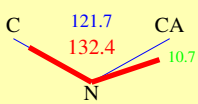
D Val 188



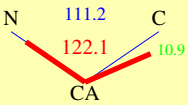
D Pro 219



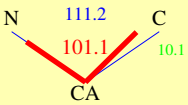
E Val 54



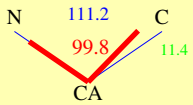
E Val 54 - E Ser 55



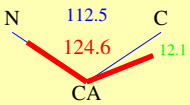
E Glu 58



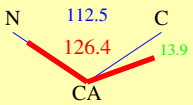
E Ala 98



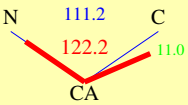
E Phe 118



E Gly 142



E Gly 169



E Asp 184

P Asp 21

P Arg 22

P Thr 32

P Ile 33

P Ile 46 - P Trp 47

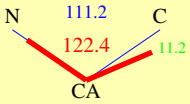
P Trp 47

P Ile 49 - P Val 50

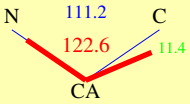
P Pro 71

Distorted geometry
1ZRT

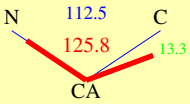
Main-chain bond angles (contd)



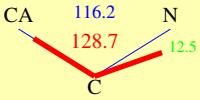
P Leu 200



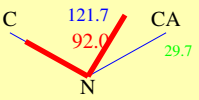
P Thr 219



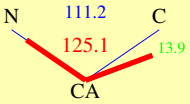
P Gly 220



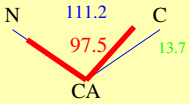
P Asn 221 - P Asn 222



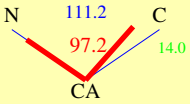
P Asn 221 - P Asn 222



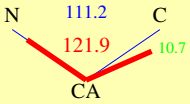
P Asn 222



P Phe 244

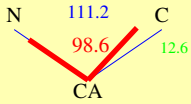


P Glu 295

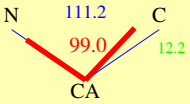


P Thr 385

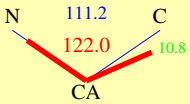
P Tyr 387 - P Pro 388



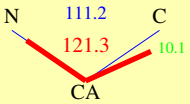
P Glu 415



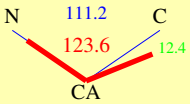
P Lys 416



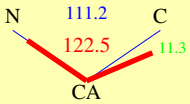
P Ile 420



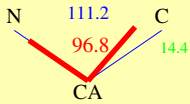
P Ser 423



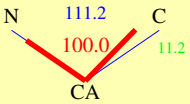
P Ile 424



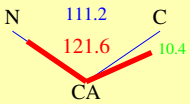
Q Lys 17



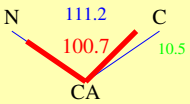
Q Leu 48



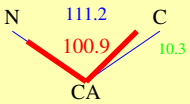
Q Gln 55



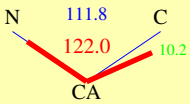
Q Glu 140



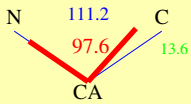
Q Val 173



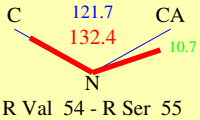
Q Val 188



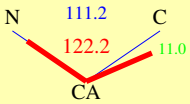
Q Pro 219



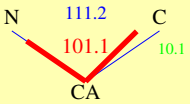
R Val 54



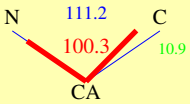
R Val 54 - R Ser 55



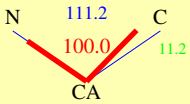
R Glu 58



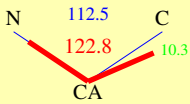
R Ala 98



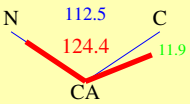
R Phe 118



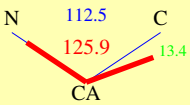
R Asp 119



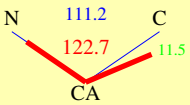
R Gly 137



R Gly 142



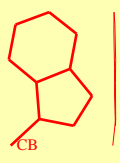
R Gly 169



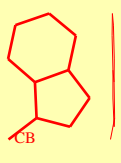
R Asp 184

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

Planar groups

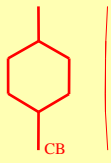


0.035
C Trp 43

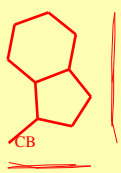


0.047
C Trp 45

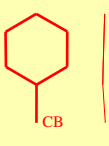
0.034
C Trp 47



0.036
C Tyr 69



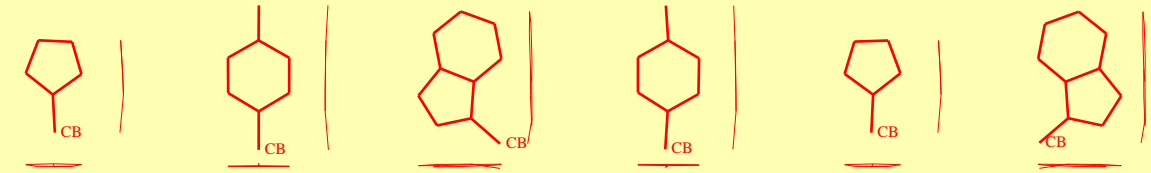
0.066
C Trp 91



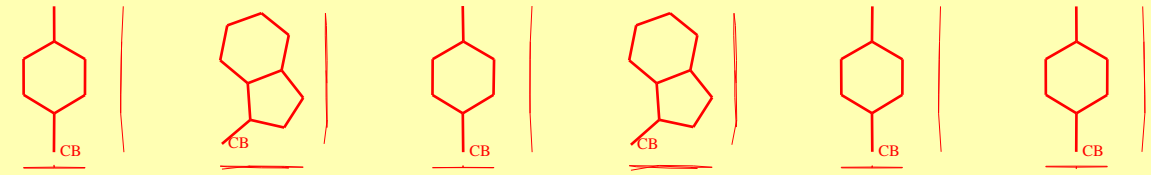
0.034
C Phe 105

Distorted geometry
1ZRT

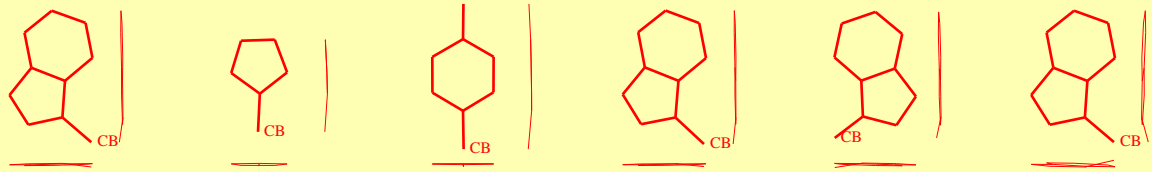
Planar groups (contd)



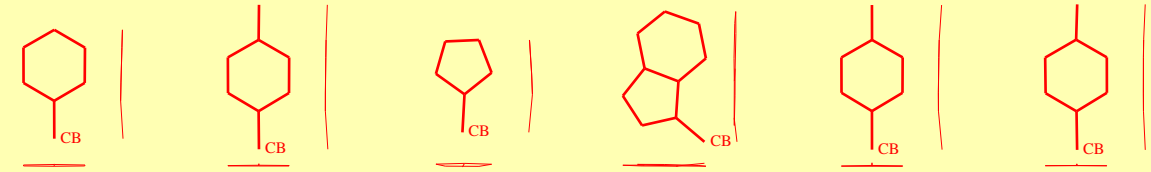
0.051 C His 111 | 0.048 C Tyr 136 | 0.051 C Trp 151 | 0.042 C Tyr 199 | 0.046 C His 212 | 0.050 C Trp 214



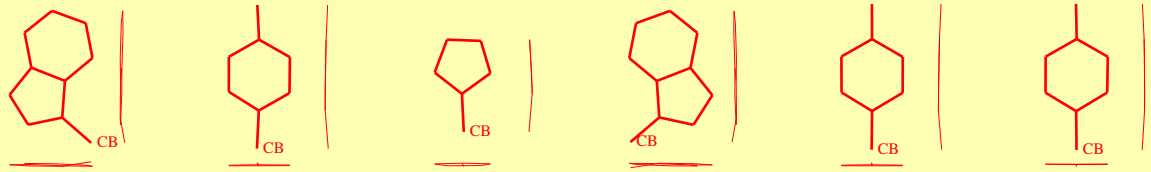
0.045 C Tyr 269 | 0.036 C Trp 296 | 0.034 C Tyr 297 | 0.056 C Trp 368 | 0.034 C Tyr 389 | 0.039 C Tyr 399



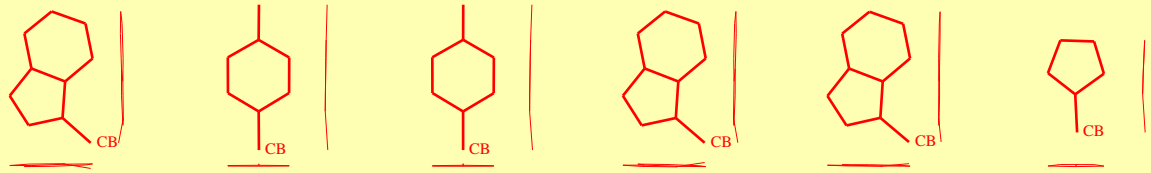
0.041 E Trp 32 | 0.038 E His 135 | 0.047 E Tyr 160 | 0.034 P Trp 43 | 0.051 P Trp 45 | 0.078 P Trp 91



0.032 P Phe 105 | 0.035 P Tyr 109 | 0.053 P His 111 | 0.035 P Trp 129 | 0.055 P Tyr 136 | 0.031 P Tyr 147



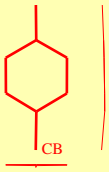
0.054 P Trp 151 | 0.043 P Tyr 199 | 0.047 P His 212 | 0.053 P Trp 214 | 0.045 P Tyr 269 | 0.036 P Tyr 297



0.055 P Trp 368 | 0.033 P Tyr 389 | 0.039 P Tyr 399 | 0.050 R Trp 32 | 0.030 R Trp 126 | 0.037 R His 135

Distorted geometry
1ZRT

Planar groups (contd)



0.043
R Tyr 160

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