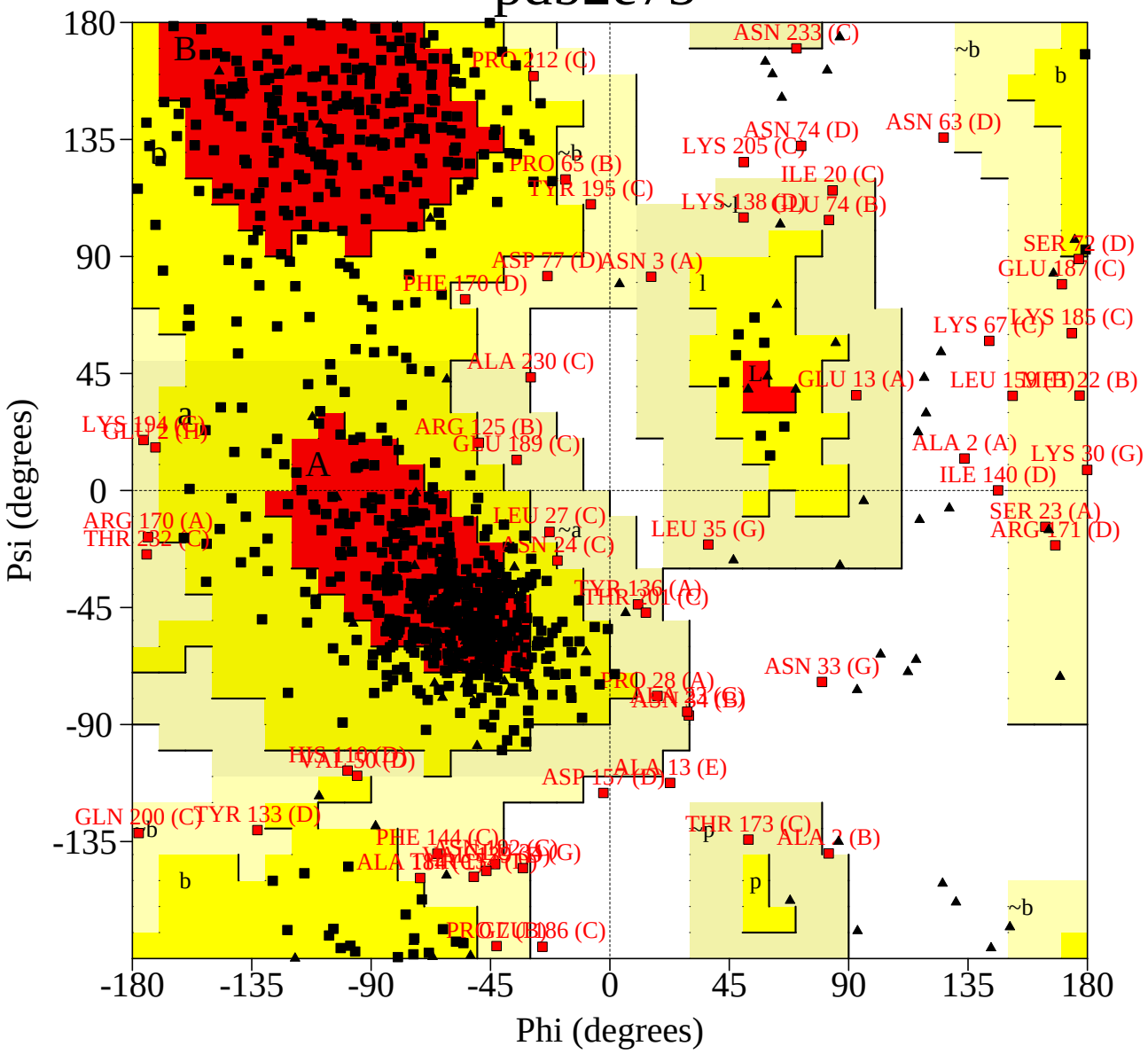
Ramachandran Plot

pdb2e75



Plot statistics

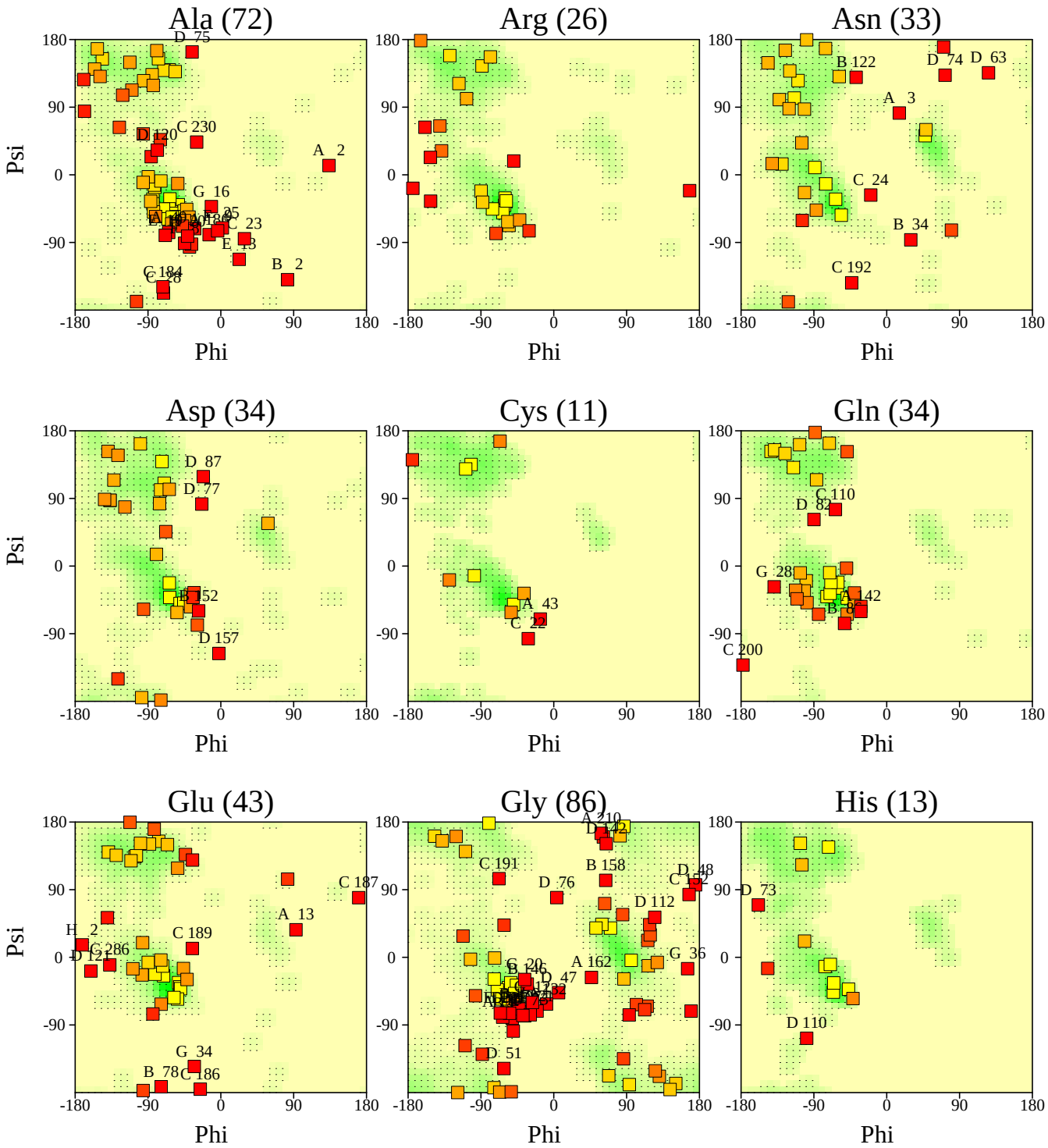
Residues in most favoured regions [A,B,L]	516	65.1%
Residues in additional allowed regions [a,b,l,p]	224	28.2%
Residues in generously allowed regions [~a,~b,~l,~p]	41	5.2%
Residues in disallowed regions	12	1.5%
	----	------
Number of non-glycine and non-proline residues	793	100.0%
Number of end-residues (excl. Gly and Pro)	17	
Number of glycine residues (shown as triangles)	87	
Number of proline residues	62	

Total number of residues	959	

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

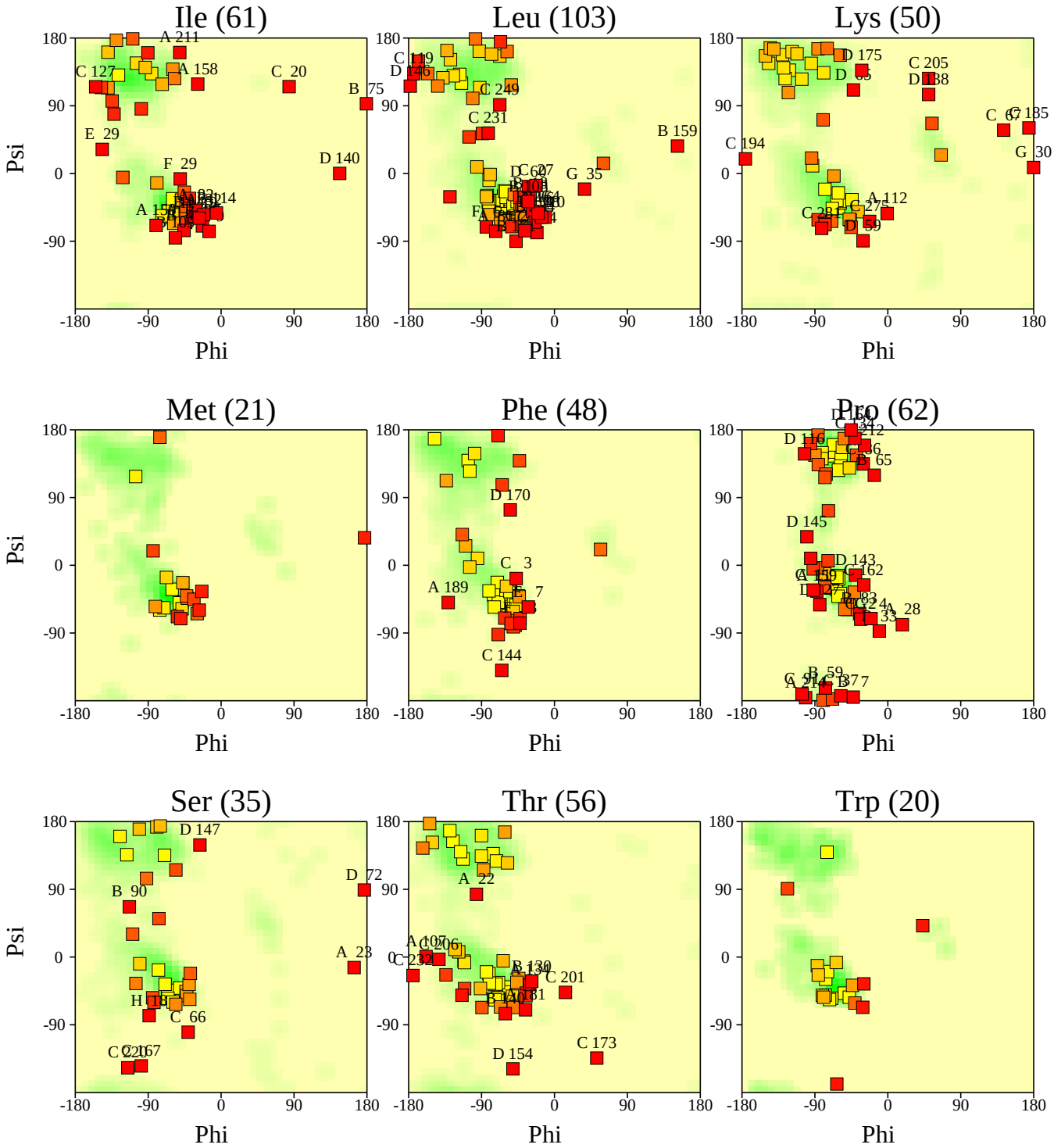
pdb2e75



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

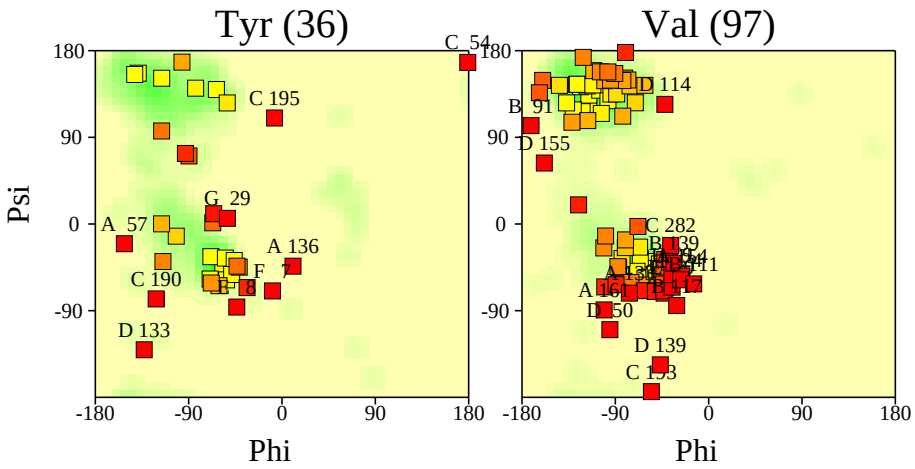
pdb2e75



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

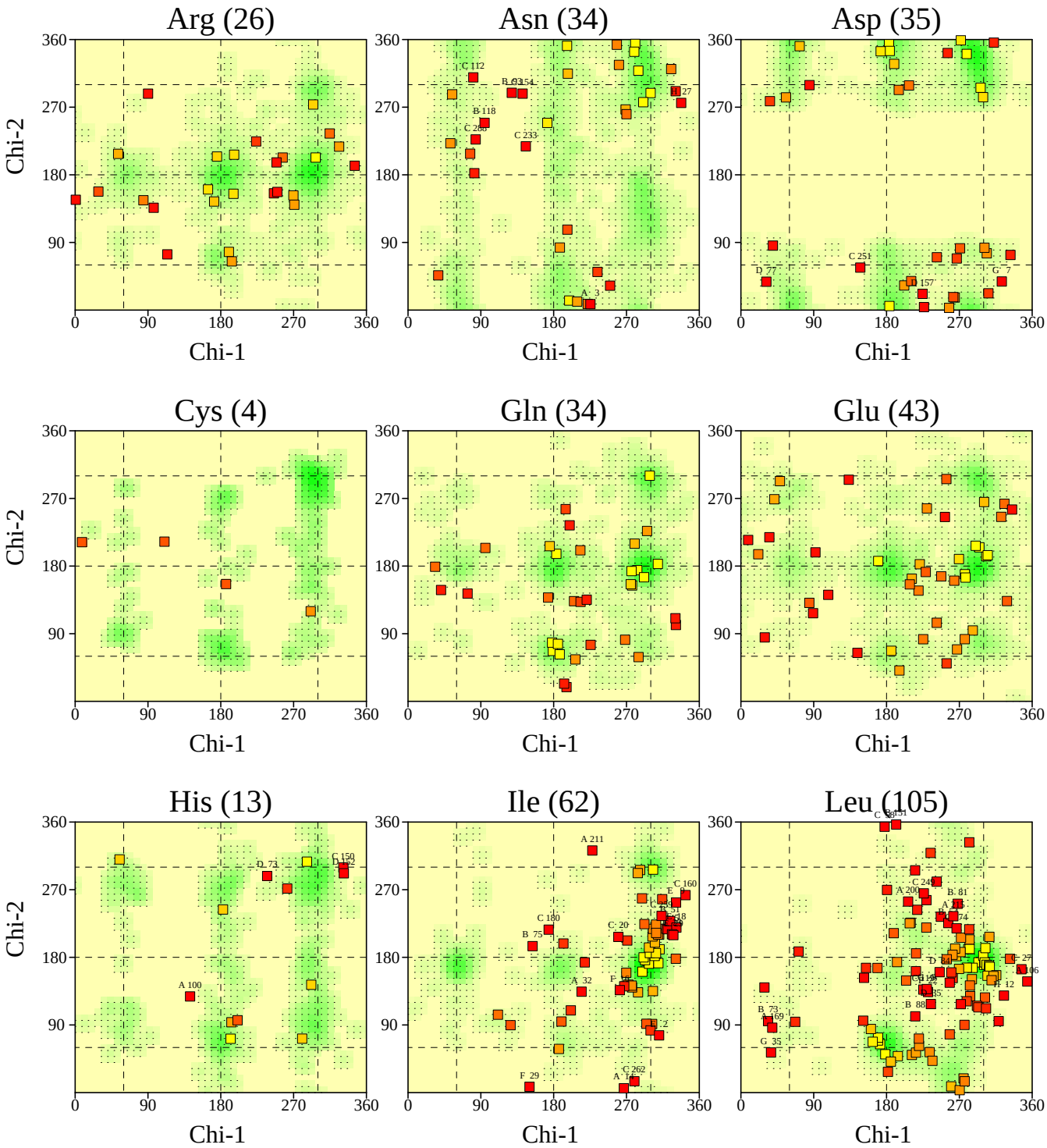
pdb2e75



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

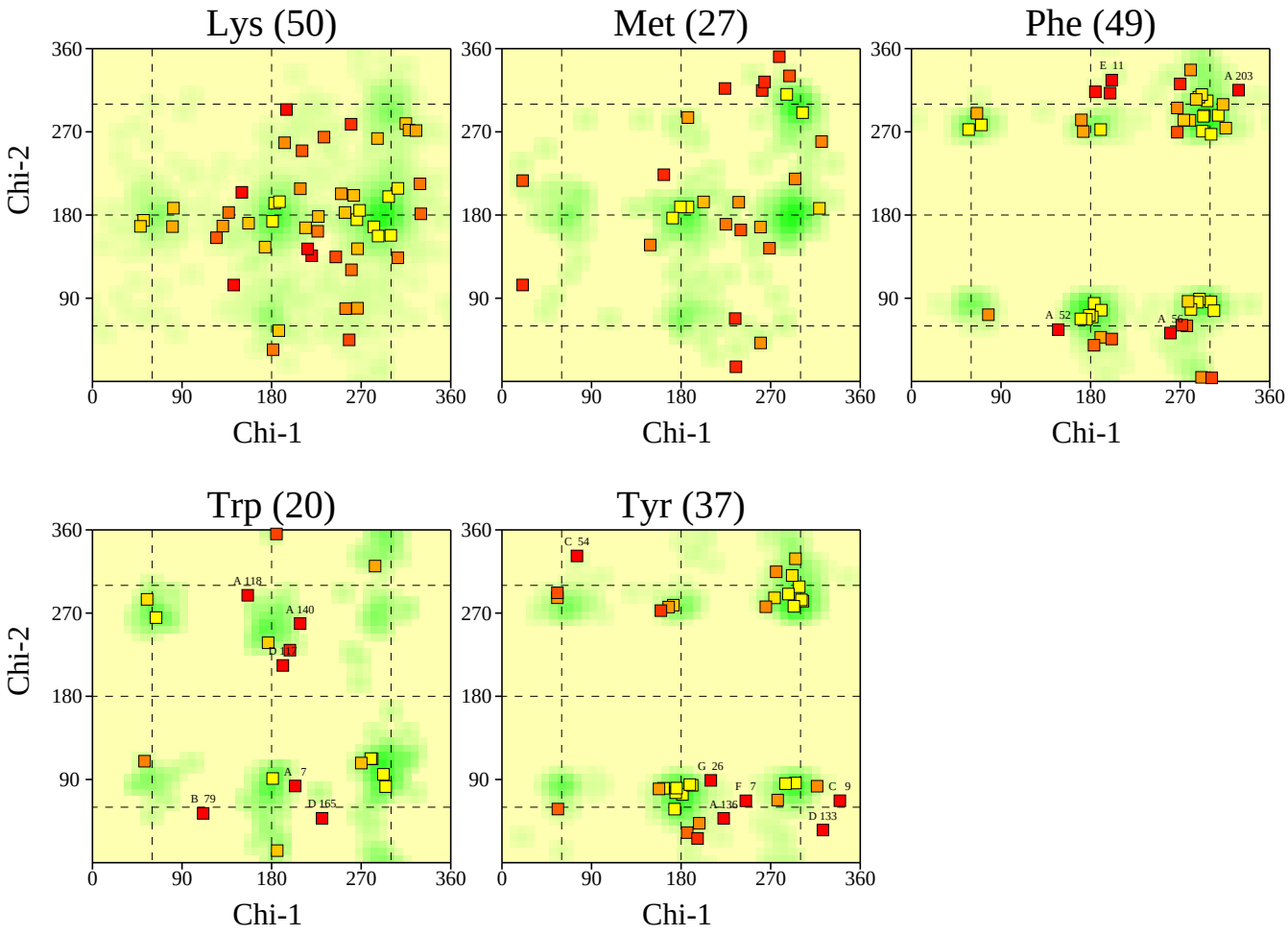
pdb2e75



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

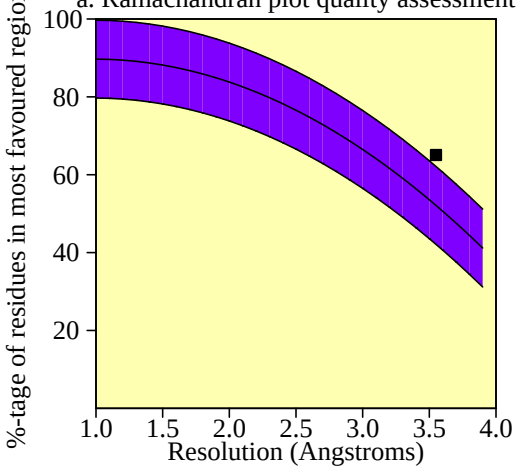
pdb2e75



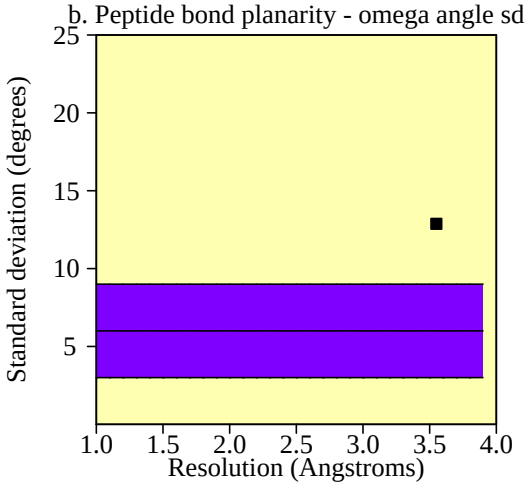
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

Main-chain parameters
pdb2e75

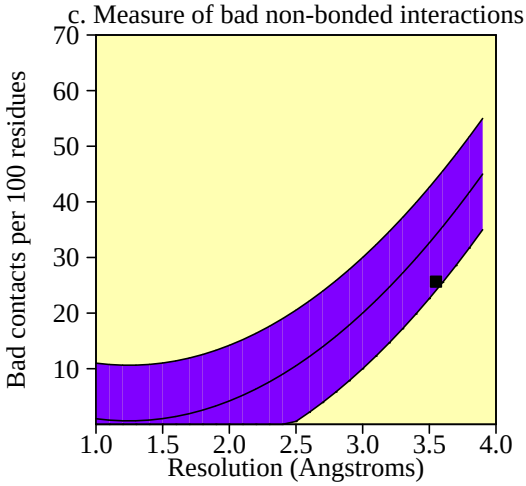
a. Ramachandran plot quality assessment



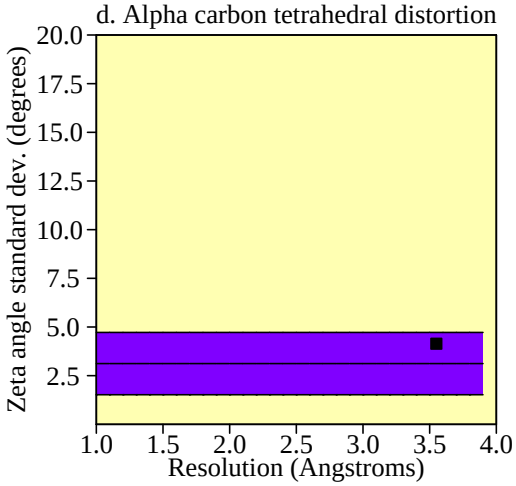
b. Peptide bond planarity - omega angle sd



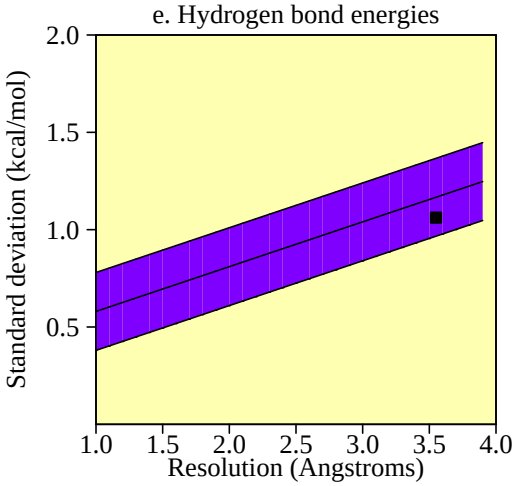
c. Measure of bad non-bonded interactions



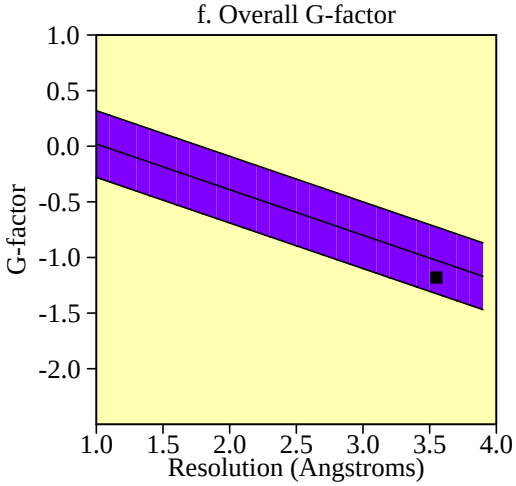
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor

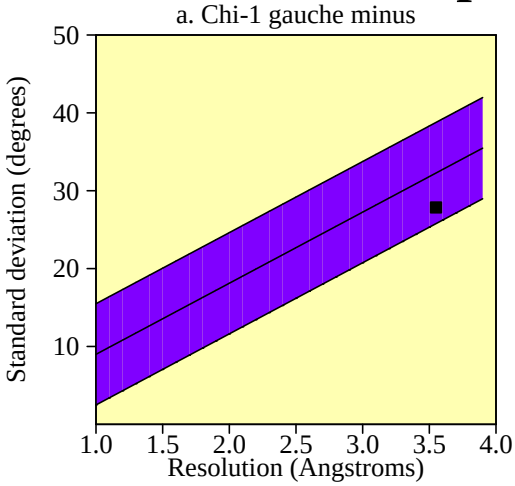


Plot statistics

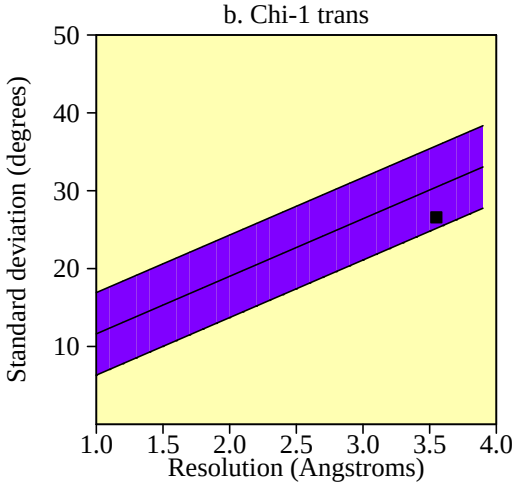
Stereochemical parameter	No. of data pts	Parameter value	Comparison values: Typical value	Comparison values: Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	793	65.1	52.1	10.0	1.3	BETTER
b. Omega angle st dev	949	12.9	6.0	3.0	2.3	WORSE
c. Bad contacts / 100 residues	246	25.7	34.1	10.0	-0.8	Inside
d. Zeta angle st dev	872	4.1	3.1	1.6	0.6	Inside
e. H-bond energy st dev	592	1.1	1.2	0.2	-0.5	Inside
f. Overall G-factor	959	-1.2	-1.0	0.3	-0.5	Inside

Side-chain parameters
pdb2e75

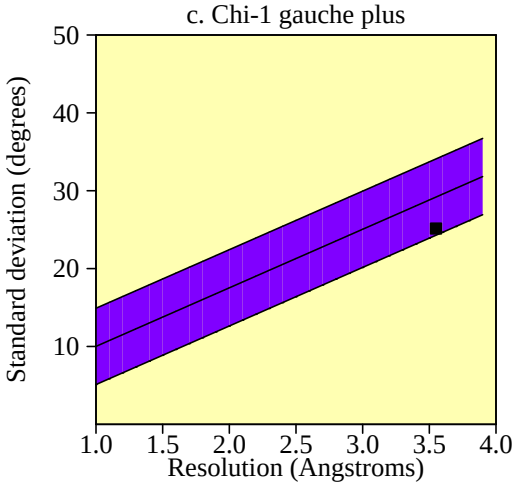
a. Chi-1 gauche minus



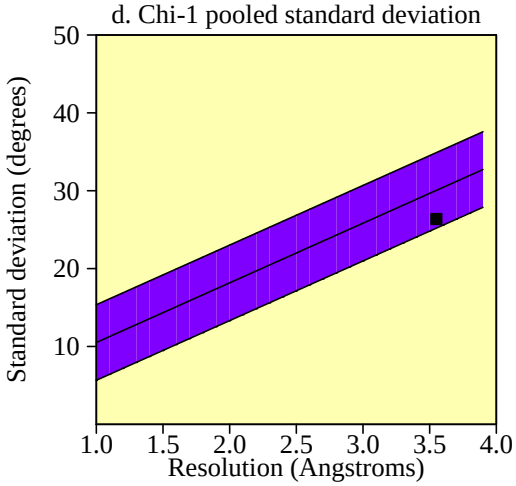
b. Chi-1 trans



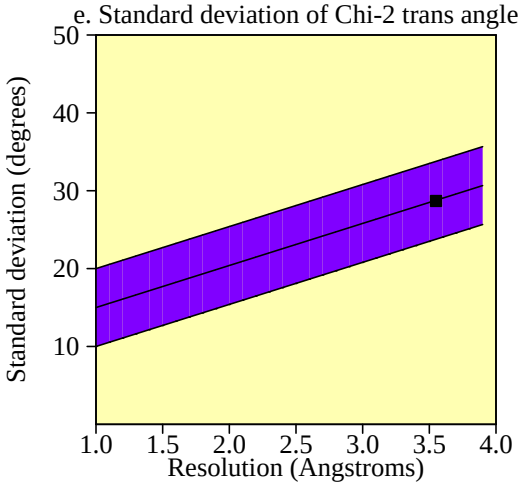
c. Chi-1 gauche plus



d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



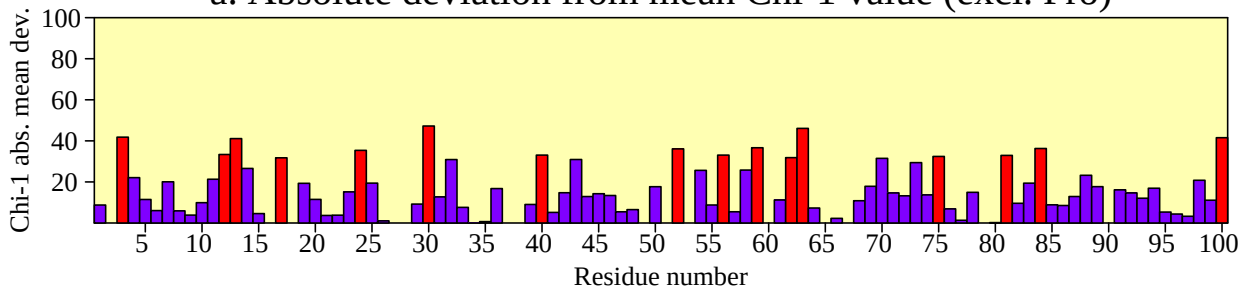
pdb2e75

Plot statistics

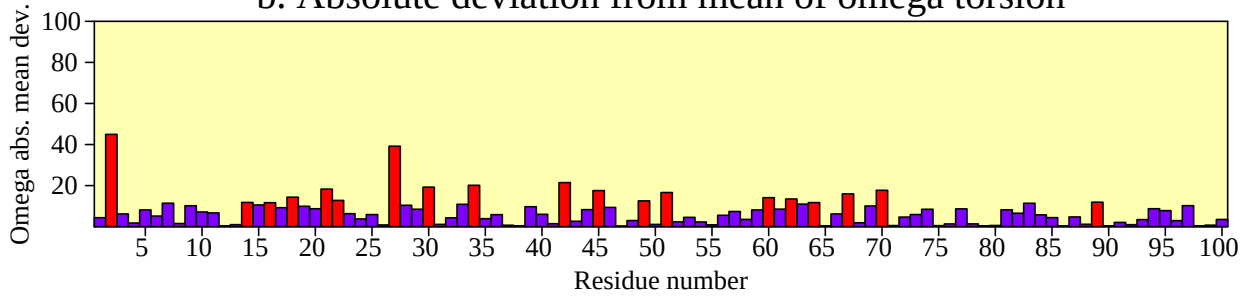
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	109	27.9	32.3	6.5	-0.7	Inside
b. Chi-1 trans st dev	289	26.6	30.5	5.3	-0.7	Inside
c. Chi-1 gauche plus st dev	338	25.1	29.2	4.9	-0.8	Inside
d. Chi-1 pooled st dev	736	26.4	30.0	4.8	-0.8	Inside
e. Chi-2 trans st dev	217	28.7	28.8	5.0	0.0	Inside

Residue properties
pdb2e75

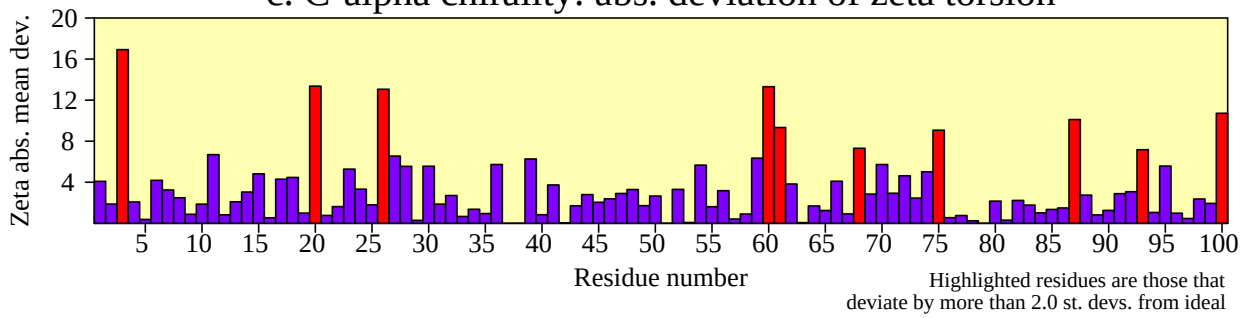
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

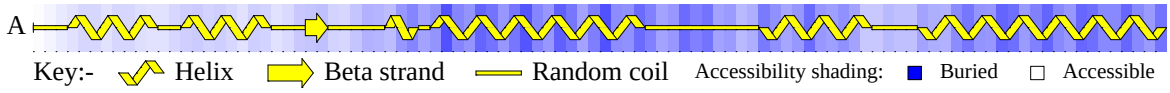


c. C-alpha chirality: abs. deviation of zeta torsion



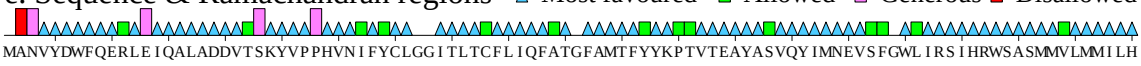
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



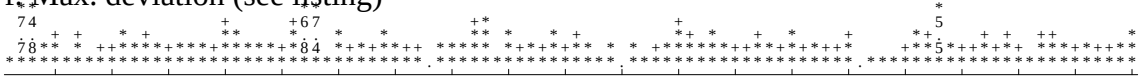
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

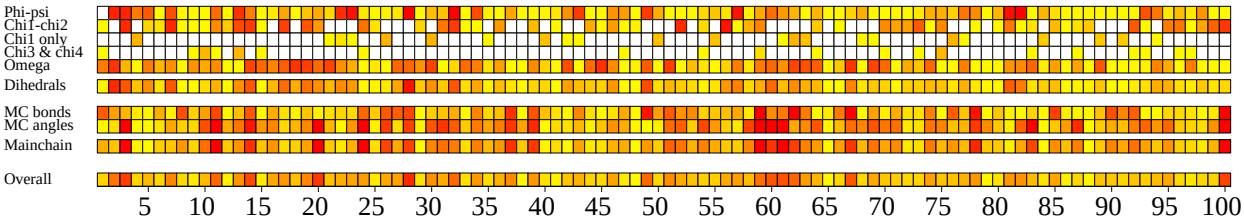


MANVYDWFQERLEIQALADDVTSKYVPPHVNIFYCLGGITLTCFLIQFATGFAMTFYYKPTVTEAYASVQYIMNEVSFGWLIRSIHRWSASMMVLMMILH

f. Max. deviation (see listing)

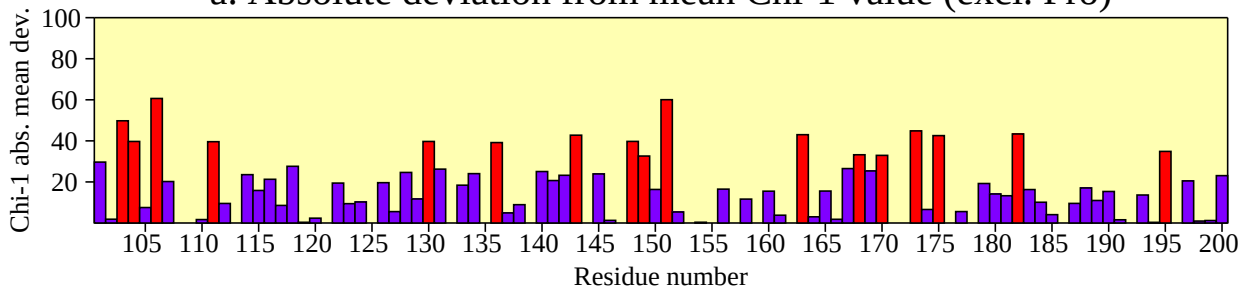


g. G-factors

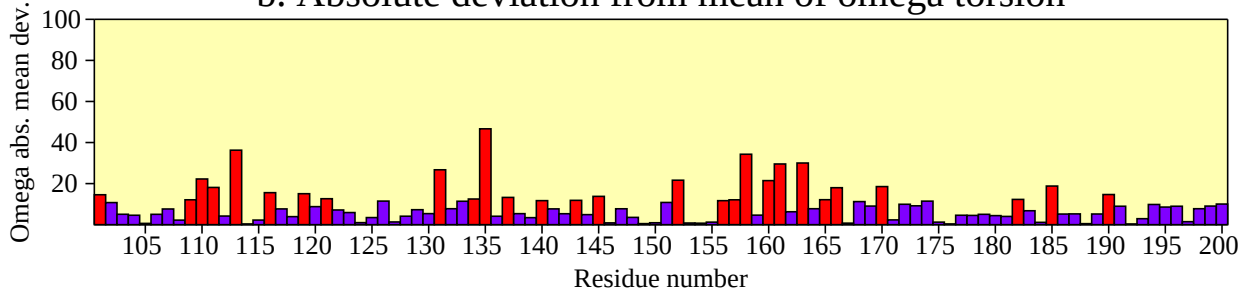


Residue properties
pdb2e75

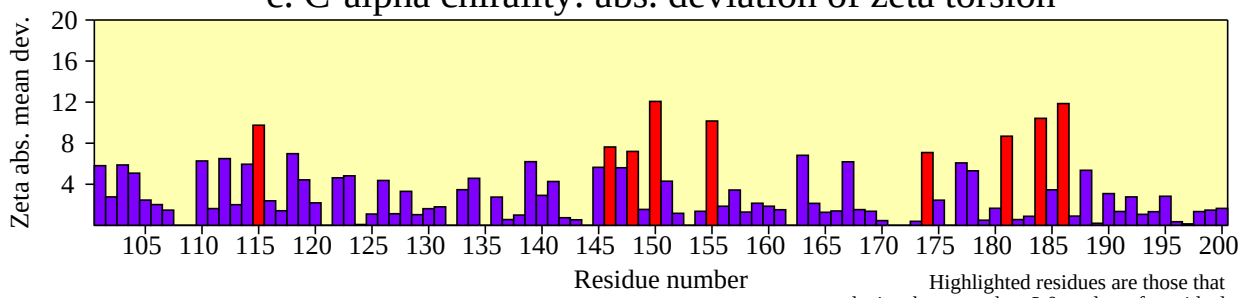
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

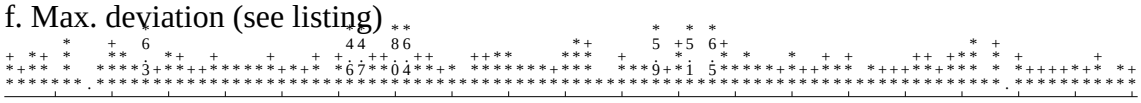
d. Secondary structure & estimated accessibility

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

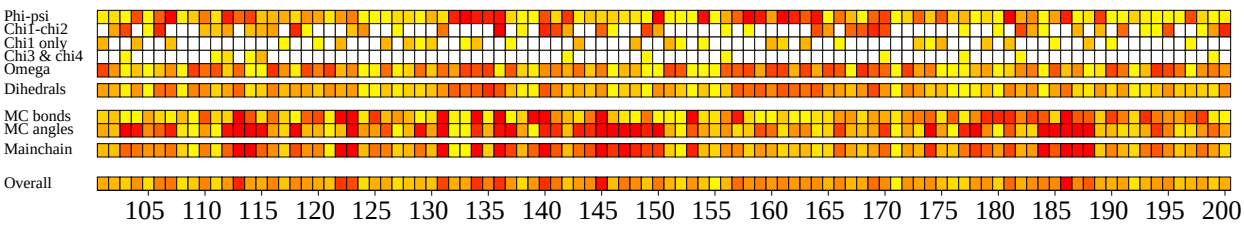
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

VFRVYLTGGFKKPRELTWISGVILAVITVSFGVTGYSLPWDQVGYWAVKIVSGVPEAIPVVGVLISDLLRGGSSVGQATLTRYYSAHTFVLPWLIAVFML

f. Max. deviation (see listing)

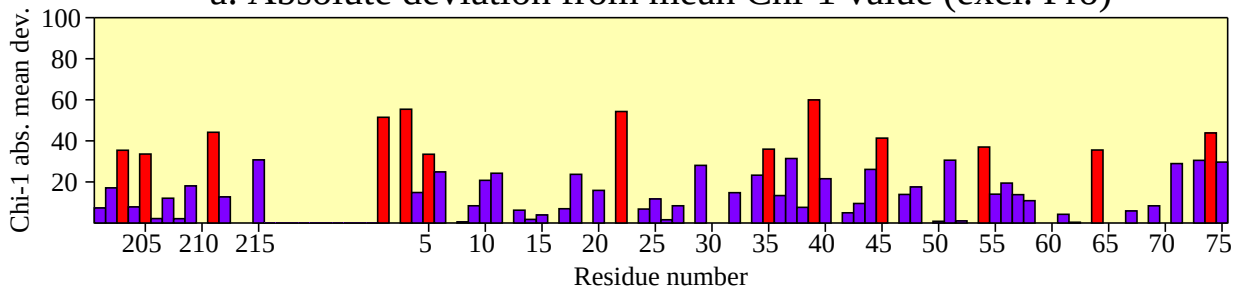


g. G-factors

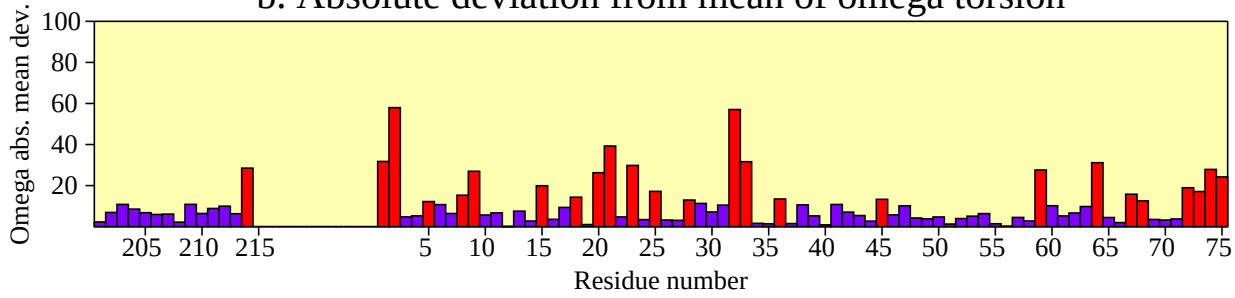


Residue properties
pdb2e75

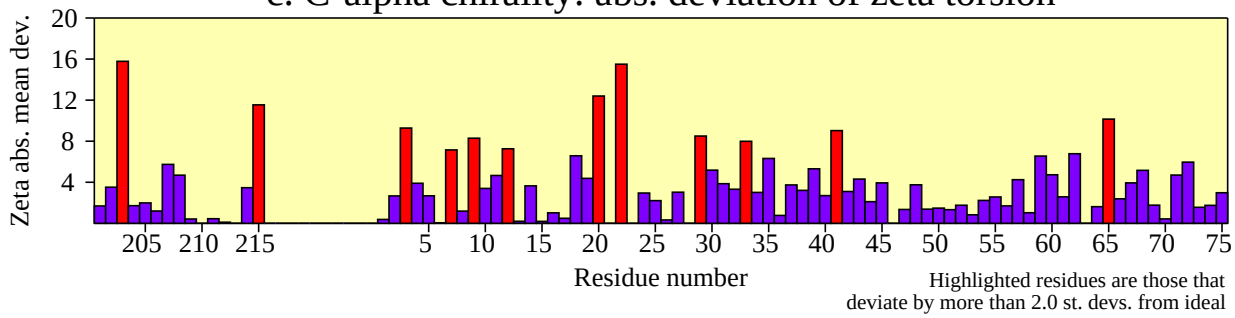
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

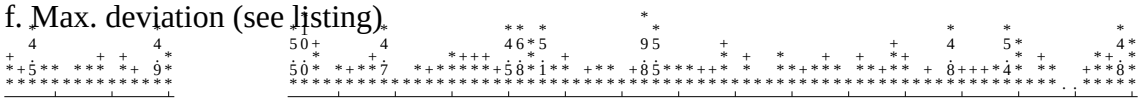


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

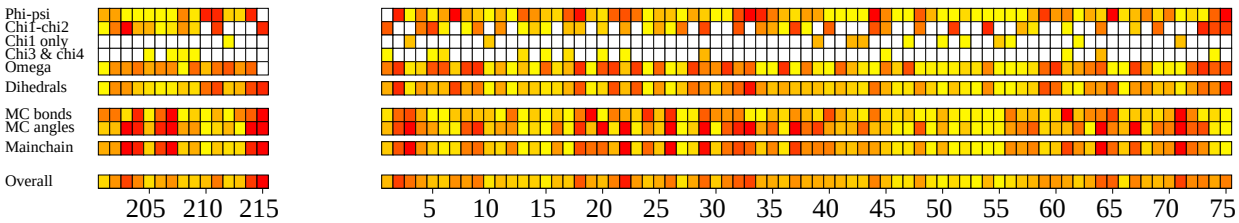
d. Secondary structure & estimated accessibility

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

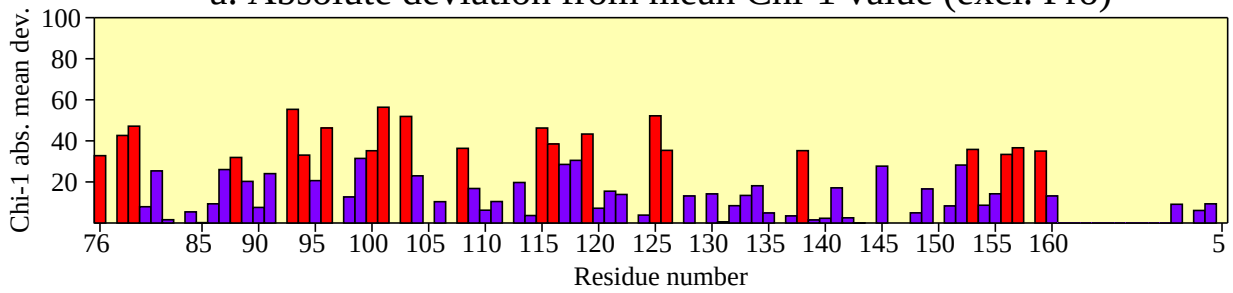


g. G-factors

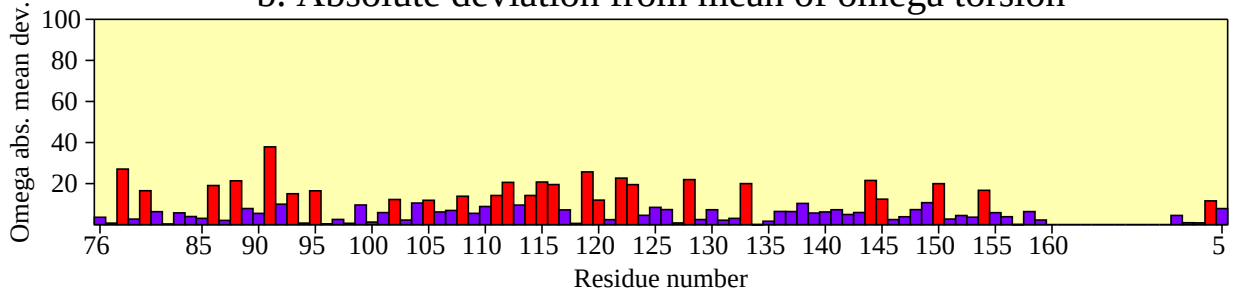


Residue properties
pdb2e75

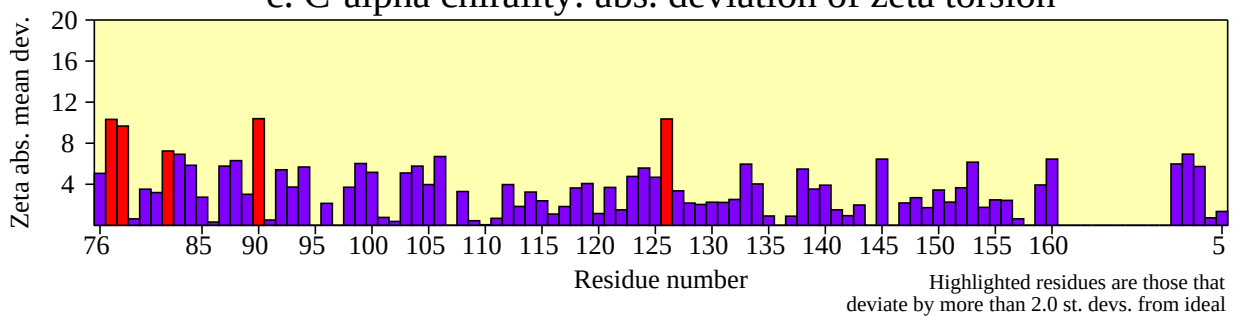
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

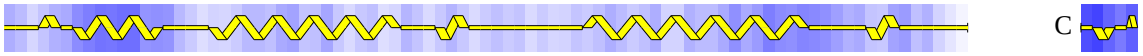


c. C-alpha chirality: abs. deviation of zeta torsion



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

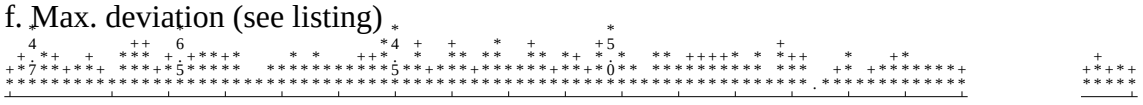
d. Secondary structure & estimated accessibility



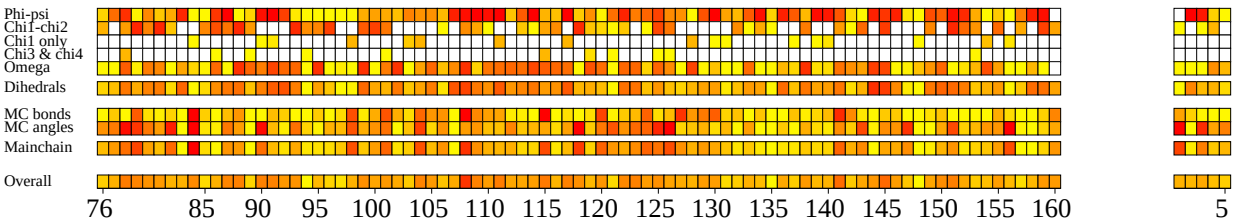
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

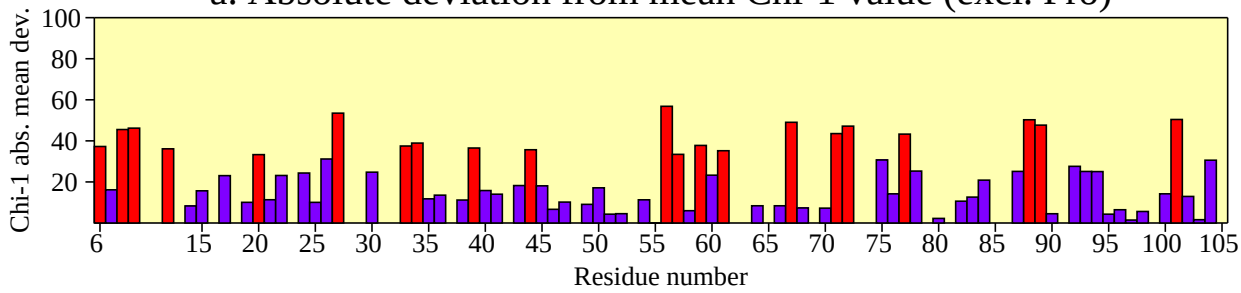


g. G-factors

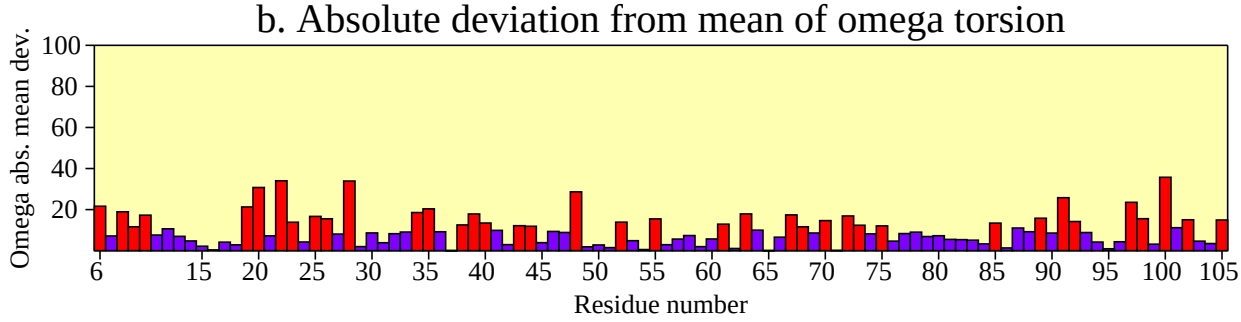


Residue properties
pdb2e75

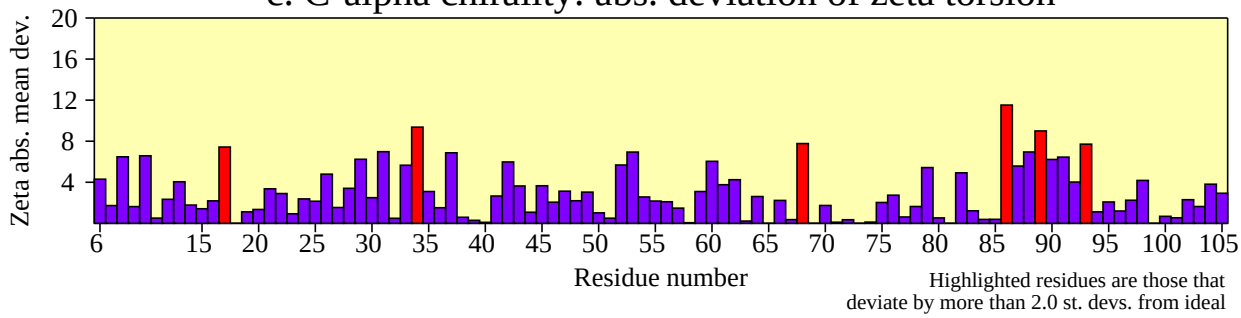
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

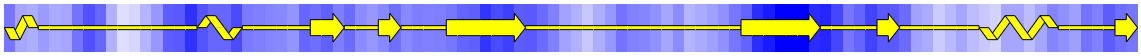


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



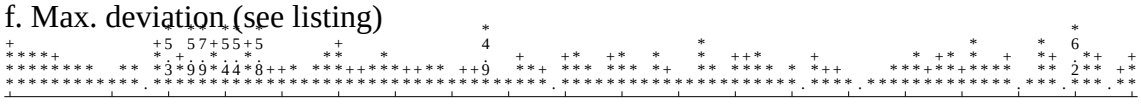
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

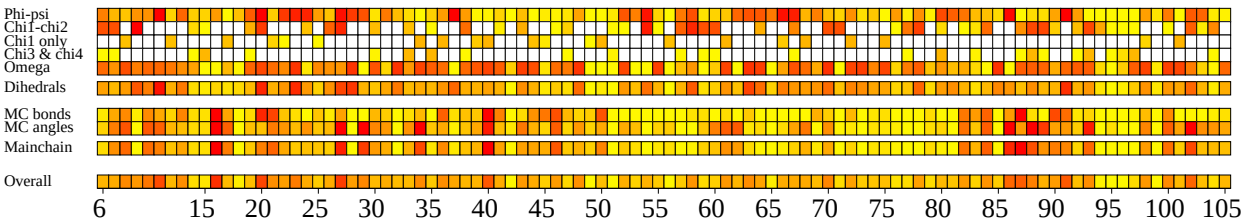
Most favoured Allowed Generous Disallowed

QQTYPPTPREPTGRIVCANCHLAAKPAEVEVPQSVLPDTVFKAVVKIPYDTKLQQVAADGSKVGLNVGAVLMLPEGFKIAPEERIPEELKKEVGDVYFQP

f. Max. deviation (see listing)

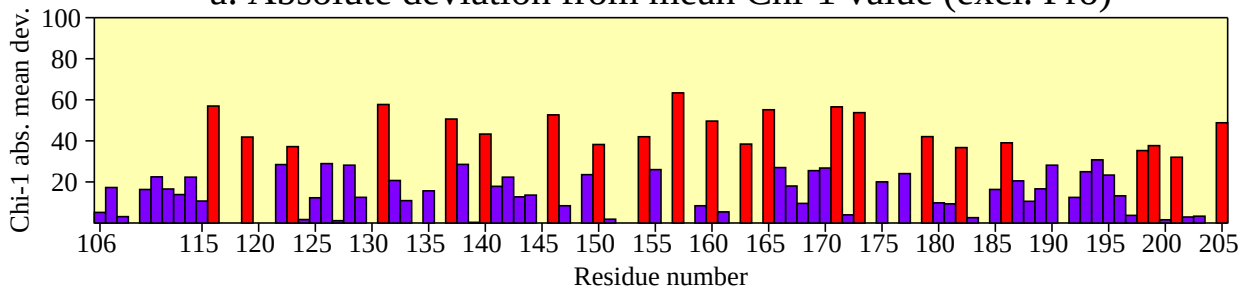


g. G-factors

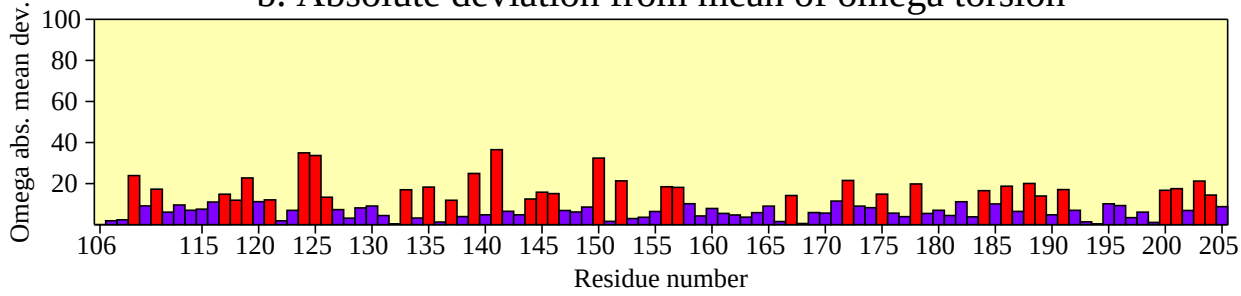


Residue properties
pdb2e75

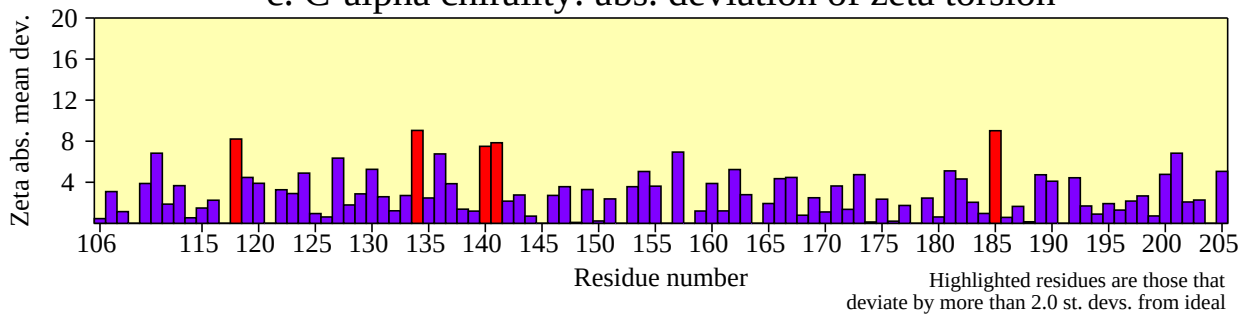
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

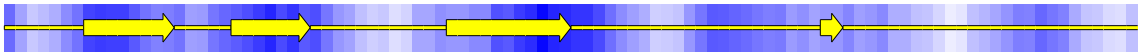


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



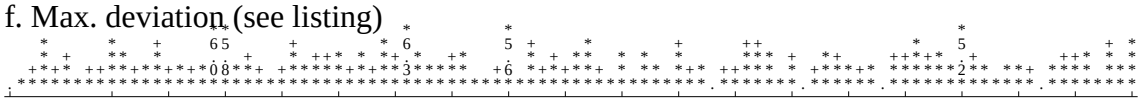
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

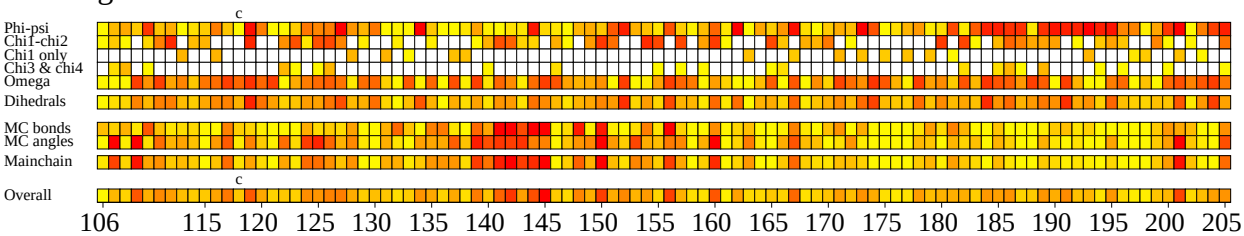
Most favoured Allowed Generous Disallowed

YKEGQDNVLLVGPLPGEQYQE I VF PVLS PNPTTDKN I HFGKYA I HLGANRGRGQ I YPTGEKSNNNVF TASATGT I TK I AKEEDEYGNVKYQVS I QTDSGK

f. Max. deviation (see listing)



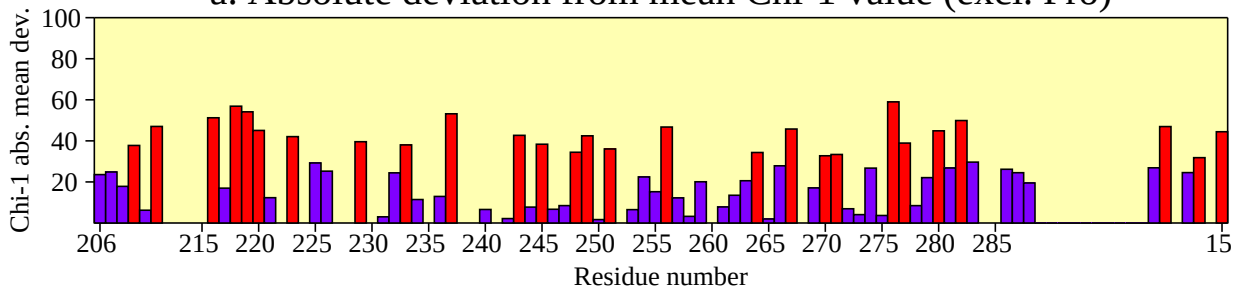
g. G-factors



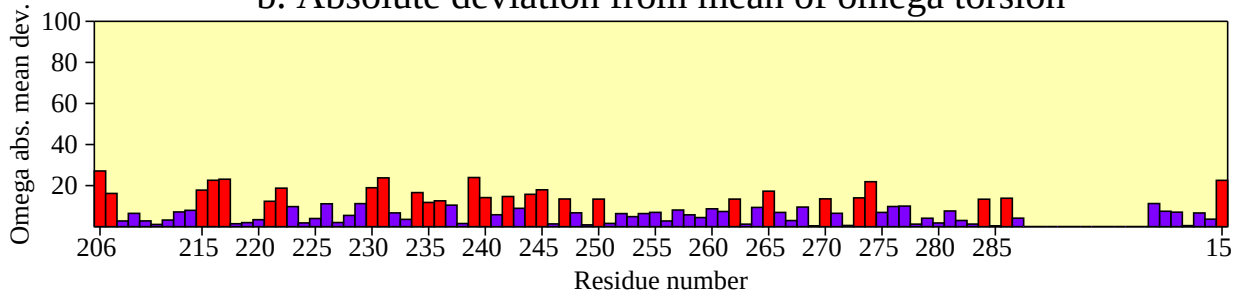
c = cis-peptide

Residue properties
pdb2e75

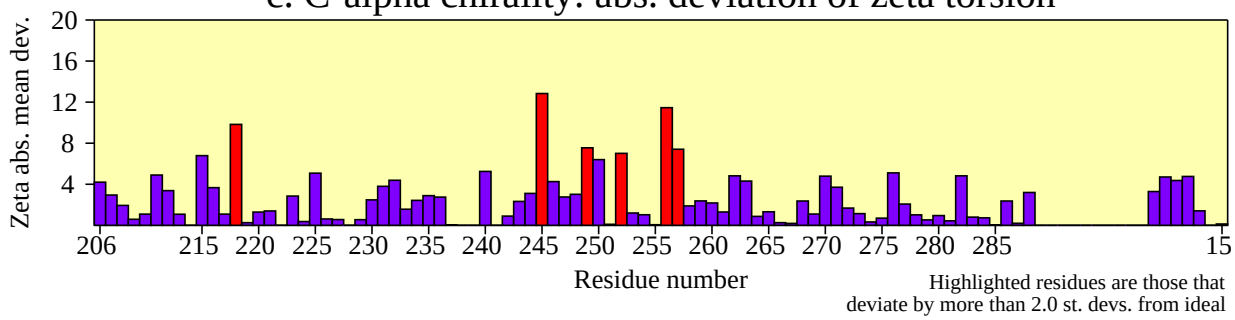
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

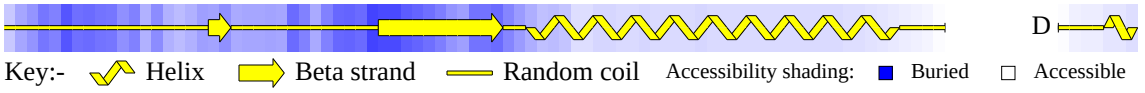


c. C-alpha chirality: abs. deviation of zeta torsion



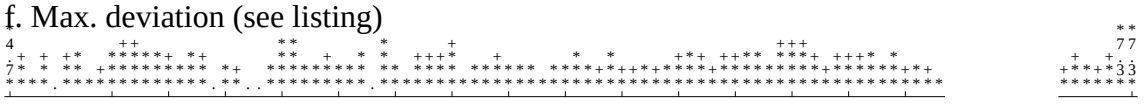
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

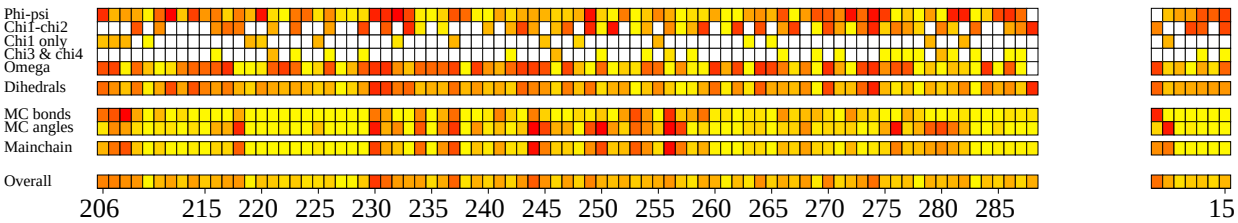


e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

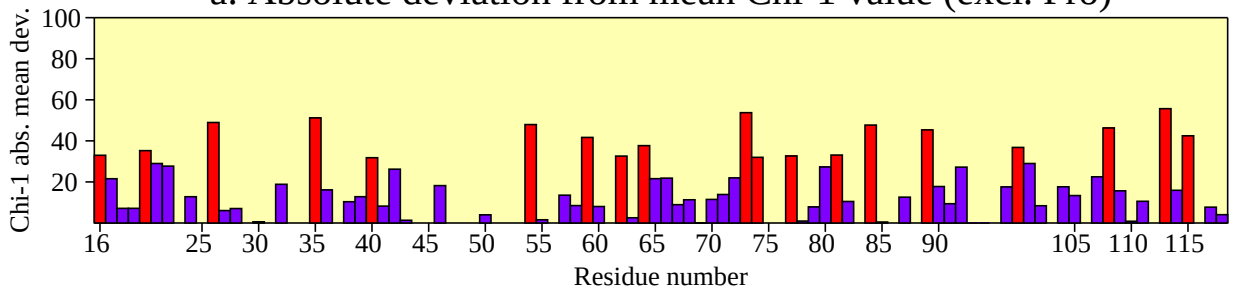


g. G-factors

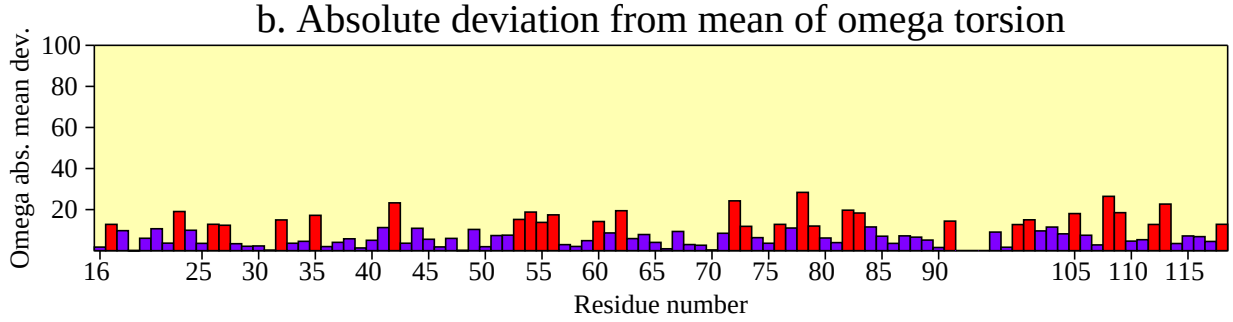


Residue properties
pdb2e75

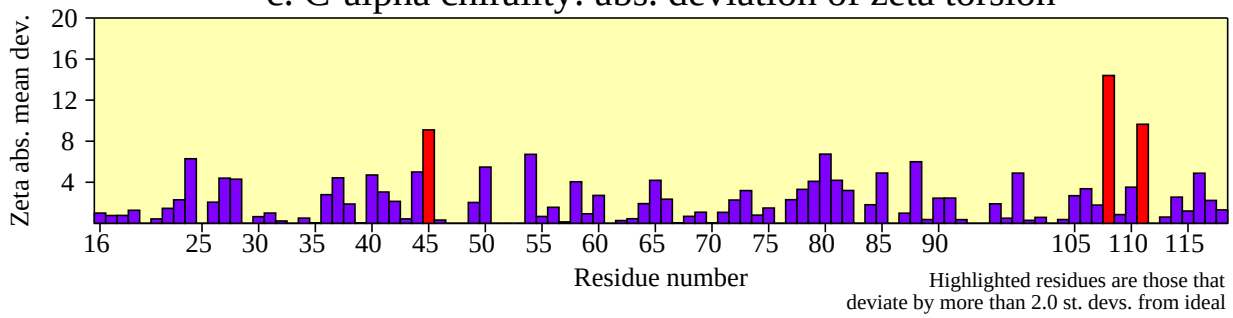
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

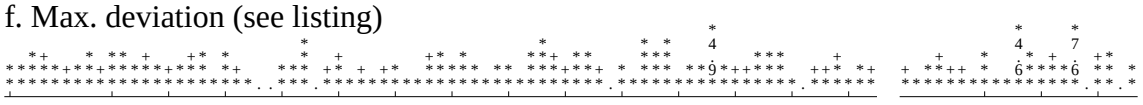
d. Secondary structure & estimated accessibility

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

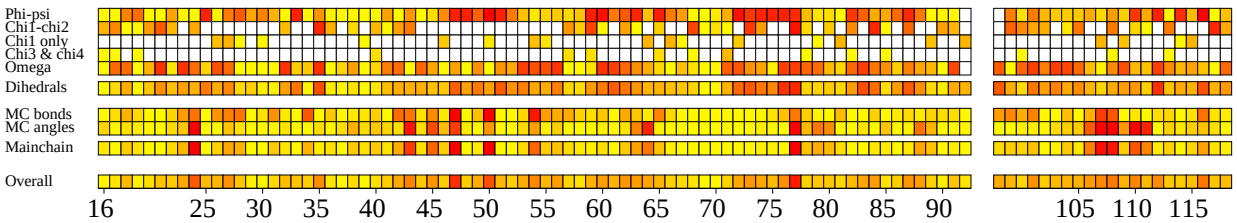
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

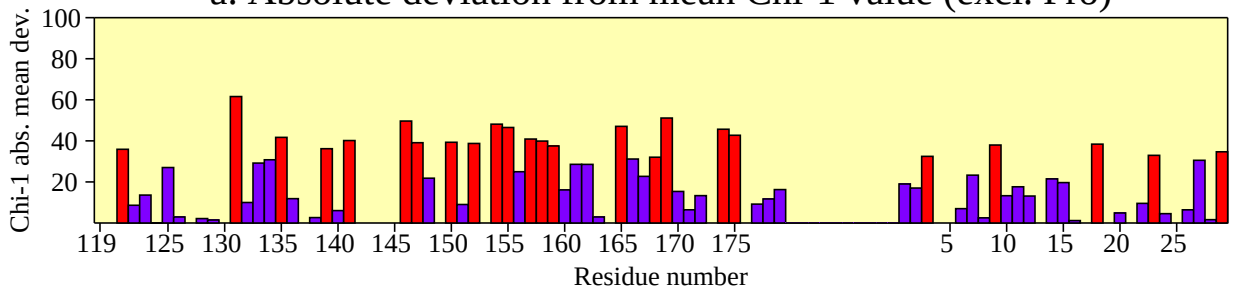


g. G-factors

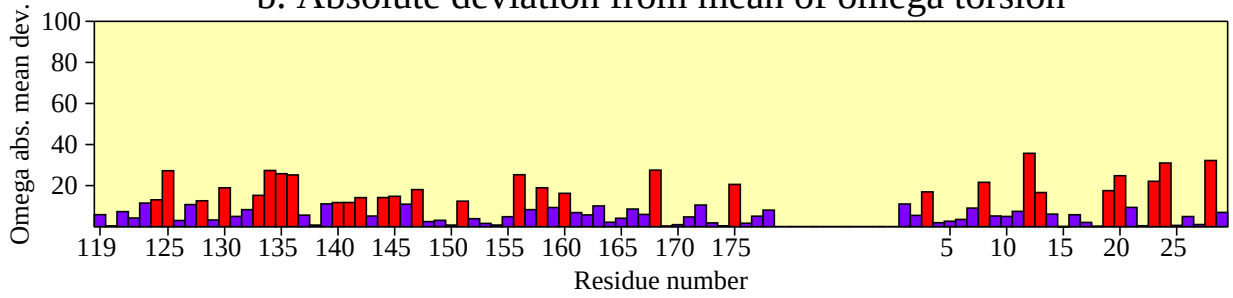


Residue properties
pdb2e75

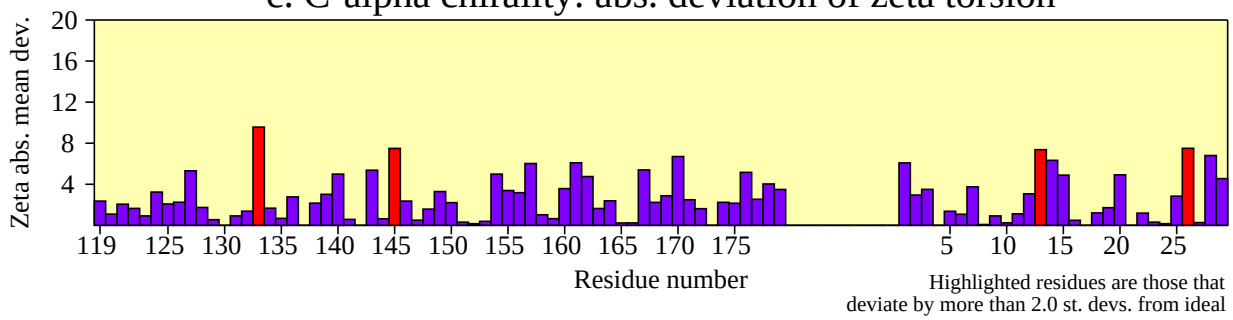
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

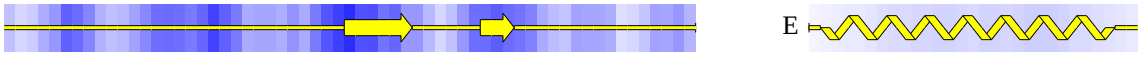


c. C-alpha chirality: abs. deviation of zeta torsion



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

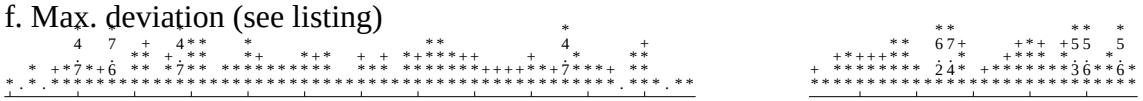
d. Secondary structure & estimated accessibility



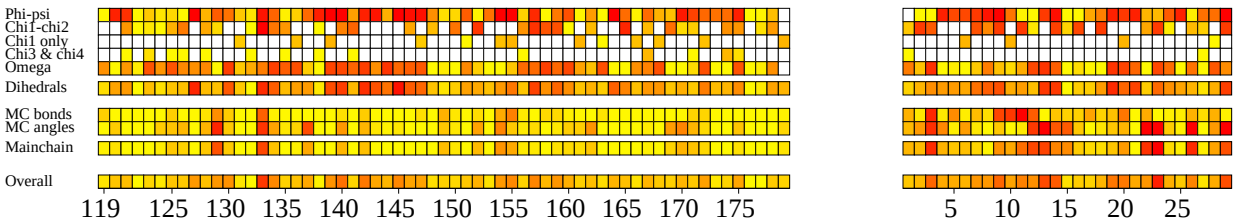
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

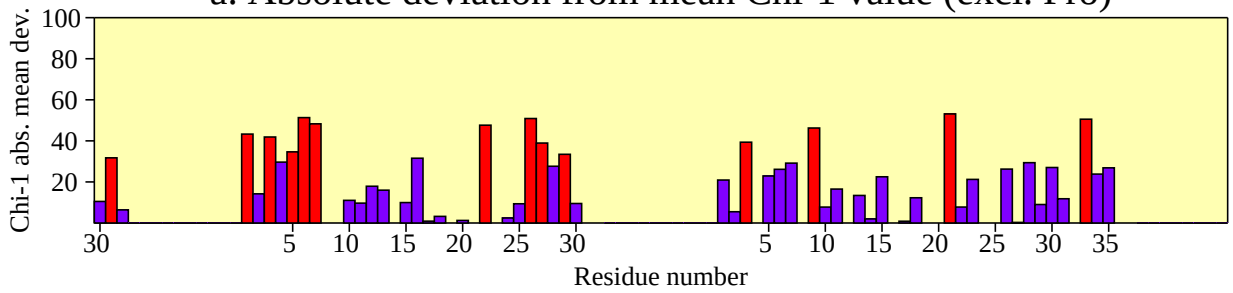


g. G-factors

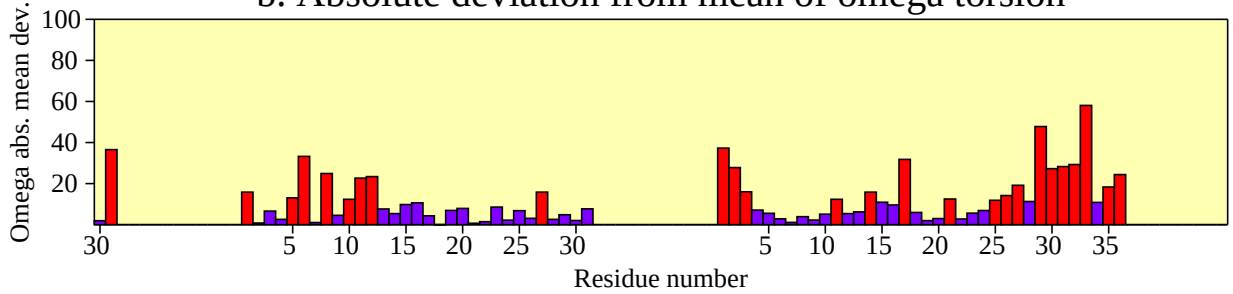


Residue properties
pdb2e75

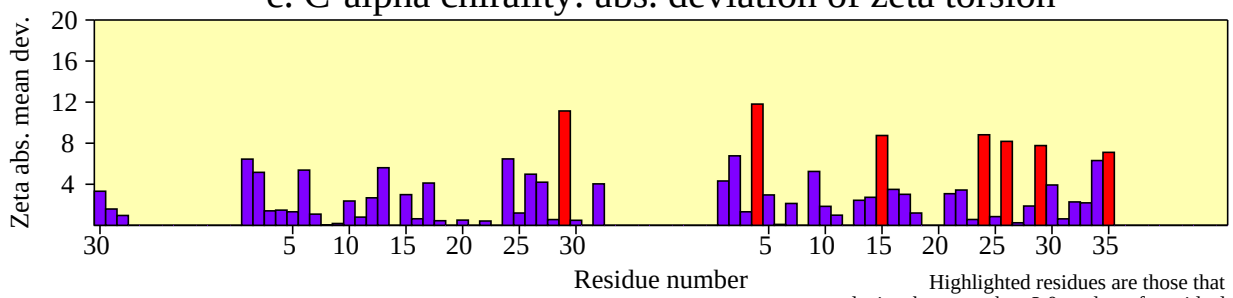
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



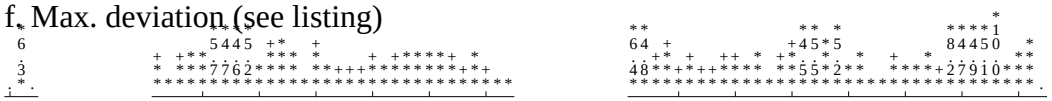
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

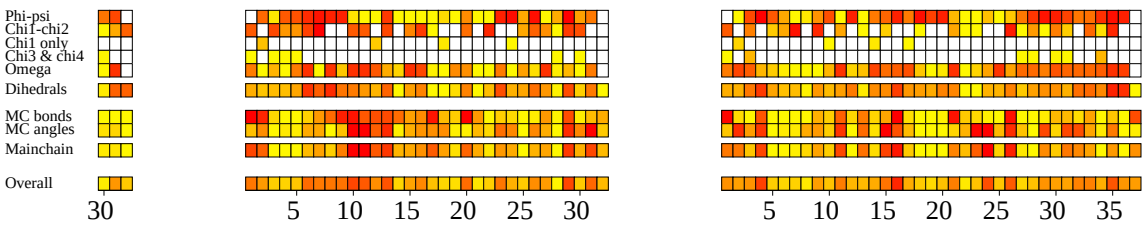
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

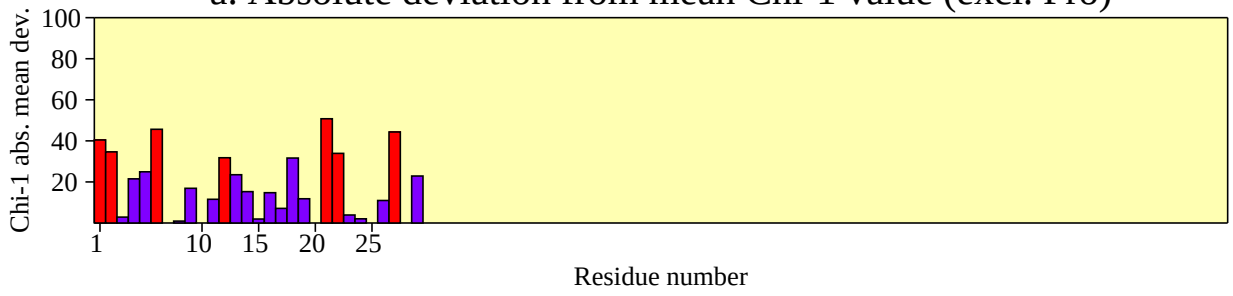


g. G-factors

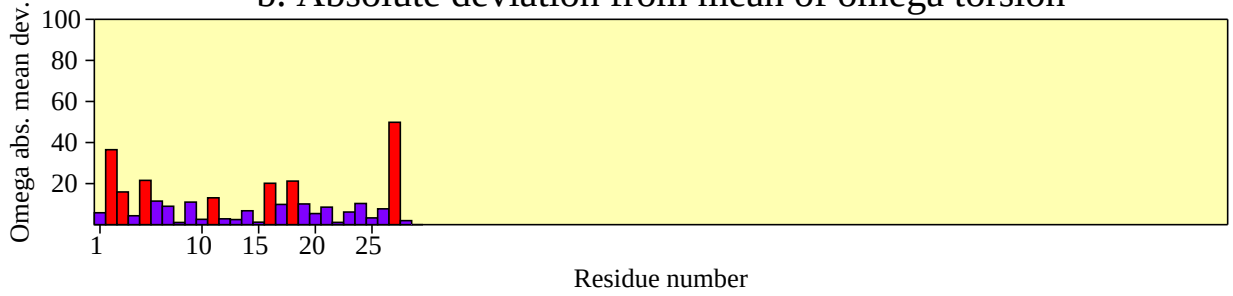


Residue properties
pdb2e75

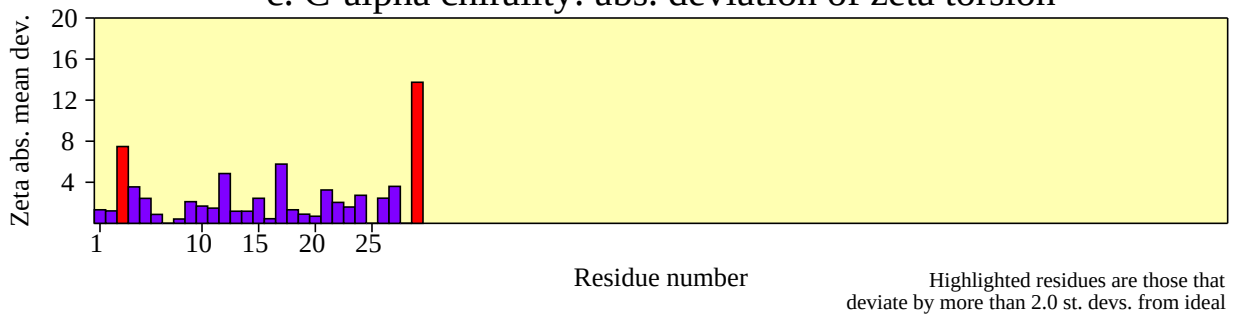
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



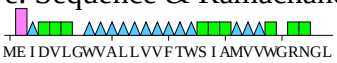
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

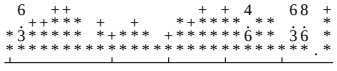
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

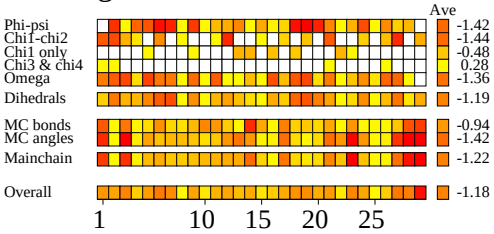
Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

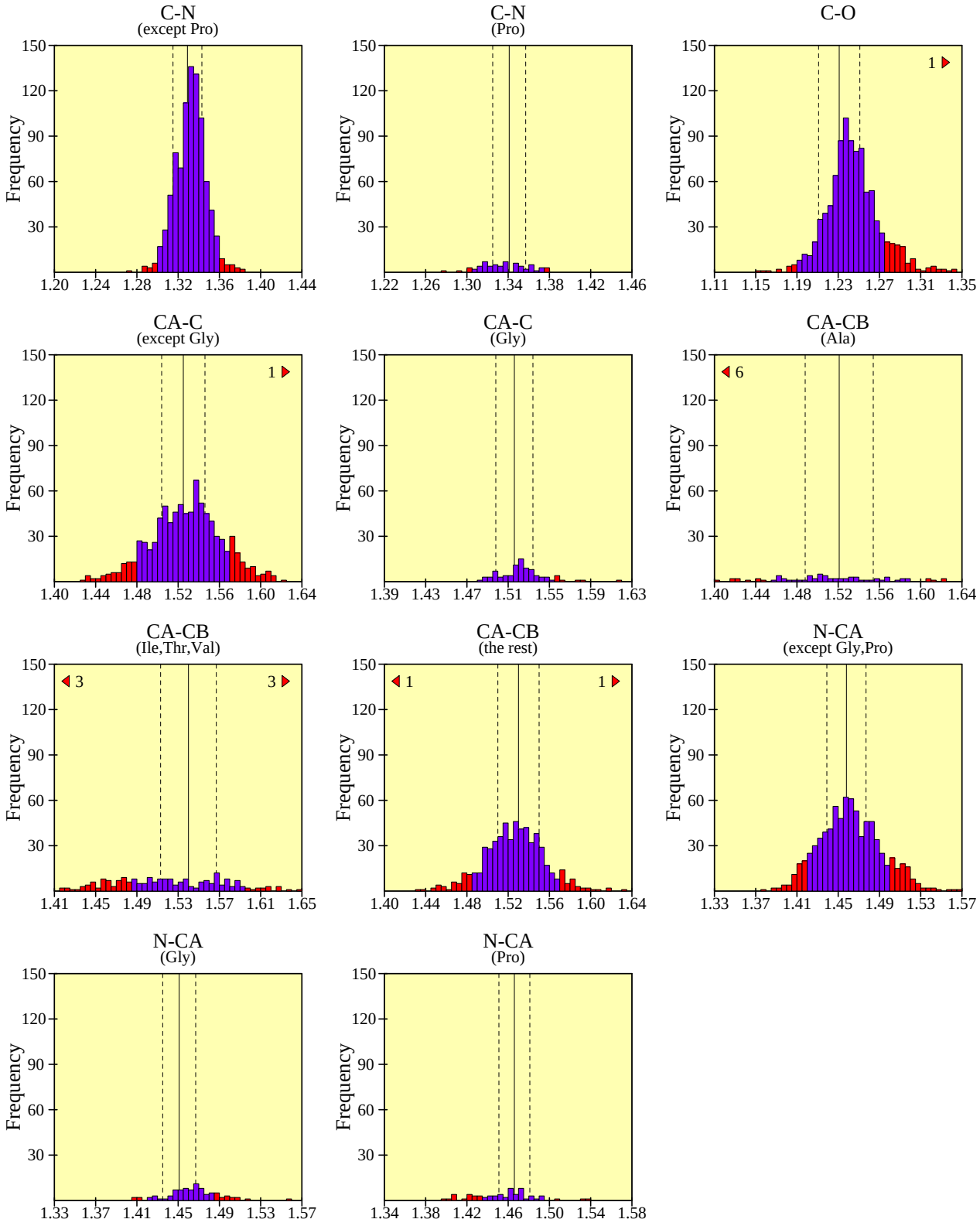


g. G-factors



Main-chain bond lengths

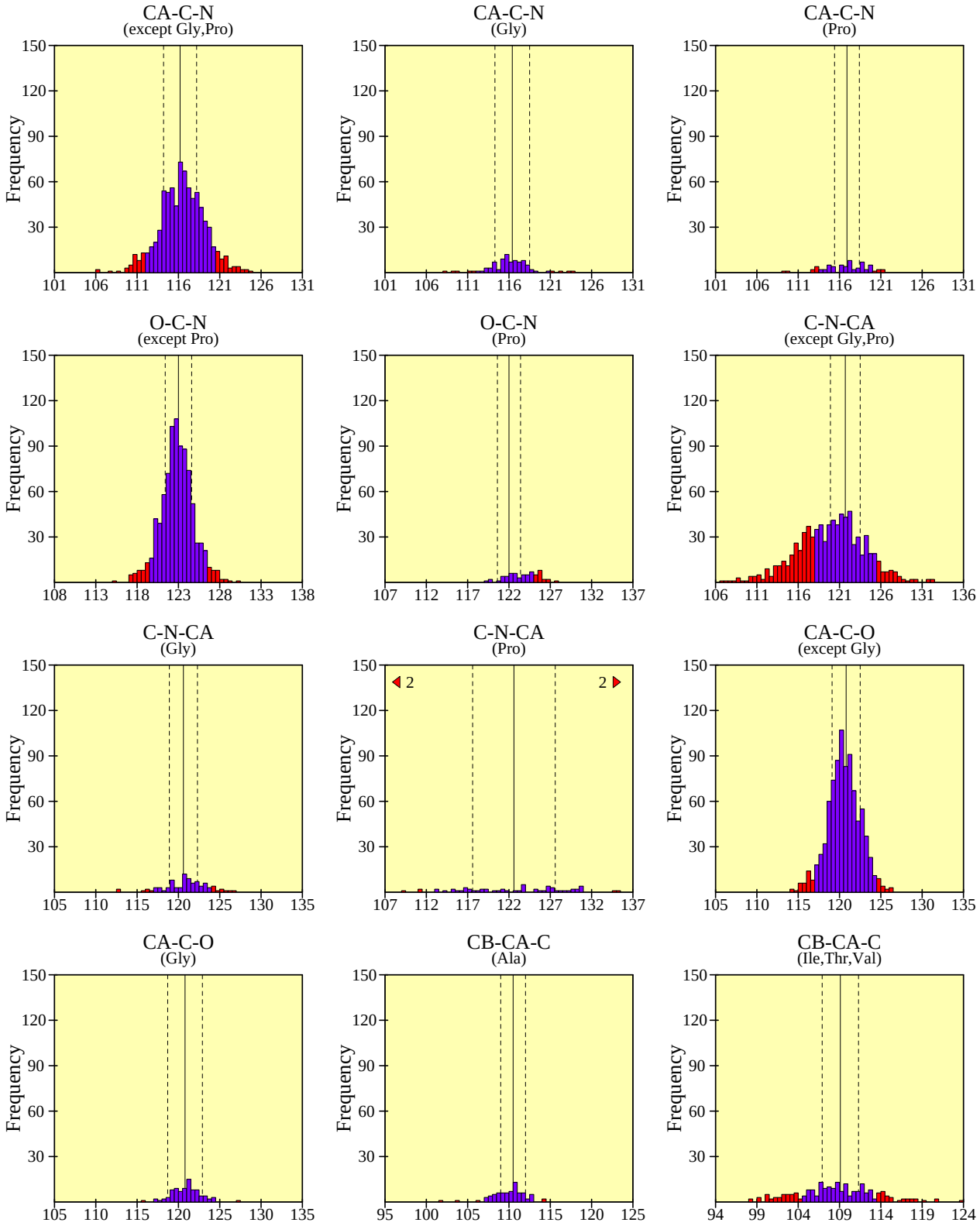
pdb2e75



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

pdb2e75



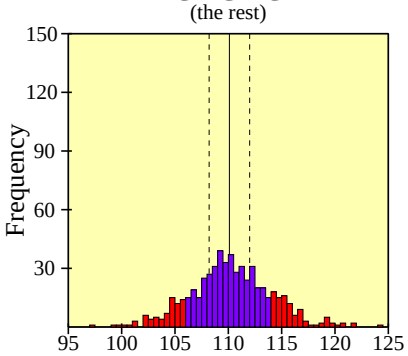
Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

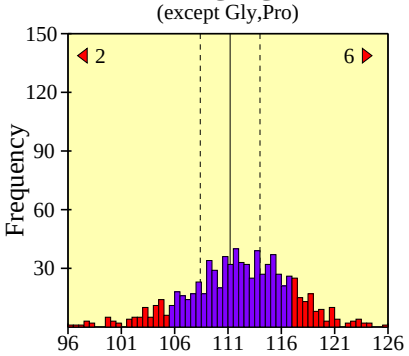
Main-chain bond angles

pdb2e75

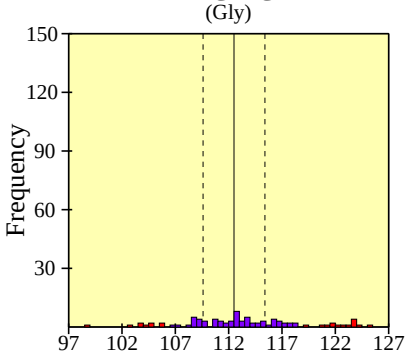
CB-CA-C
(the rest)



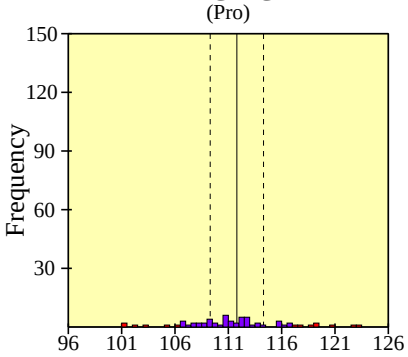
N-CA-C
(except Gly,Pro)



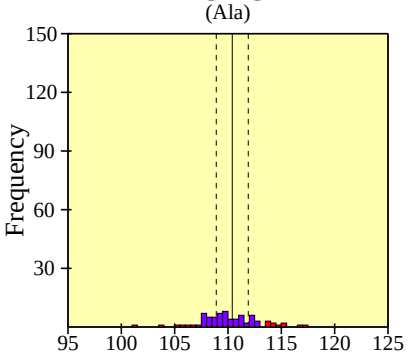
N-CA-C
(Gly)



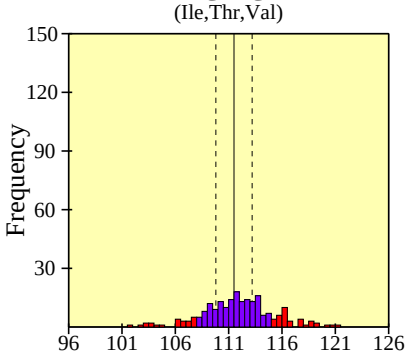
N-CA-C
(Pro)



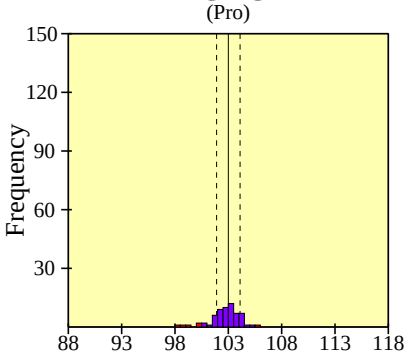
N-CA-CB
(Ala)



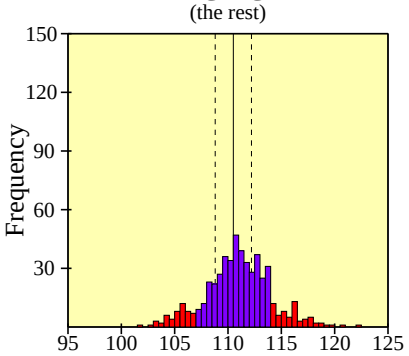
N-CA-CB
(Ile,Thr,Val)



N-CA-CB
(Pro)



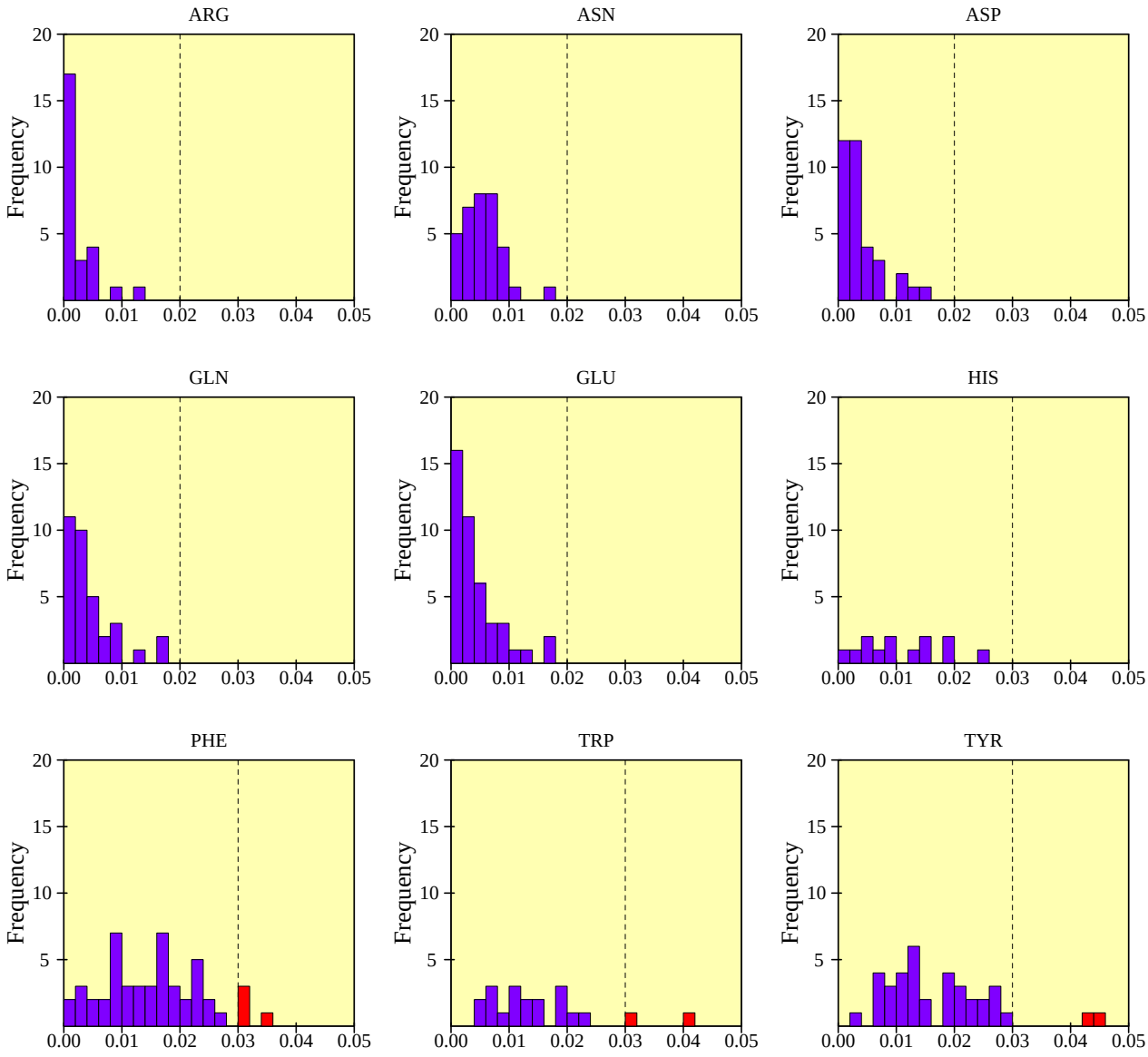
N-CA-CB
(the rest)



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

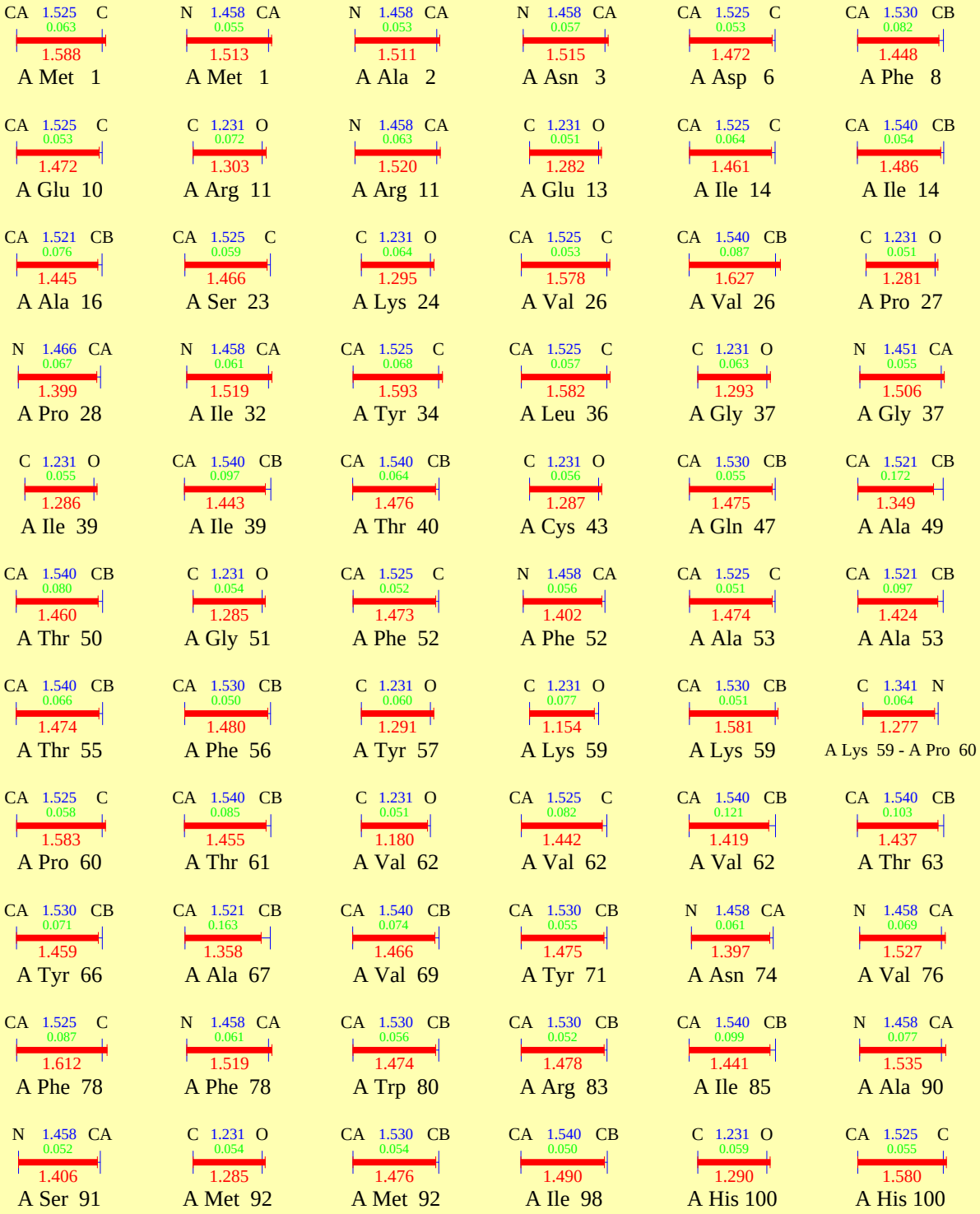
pdb2e75



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.

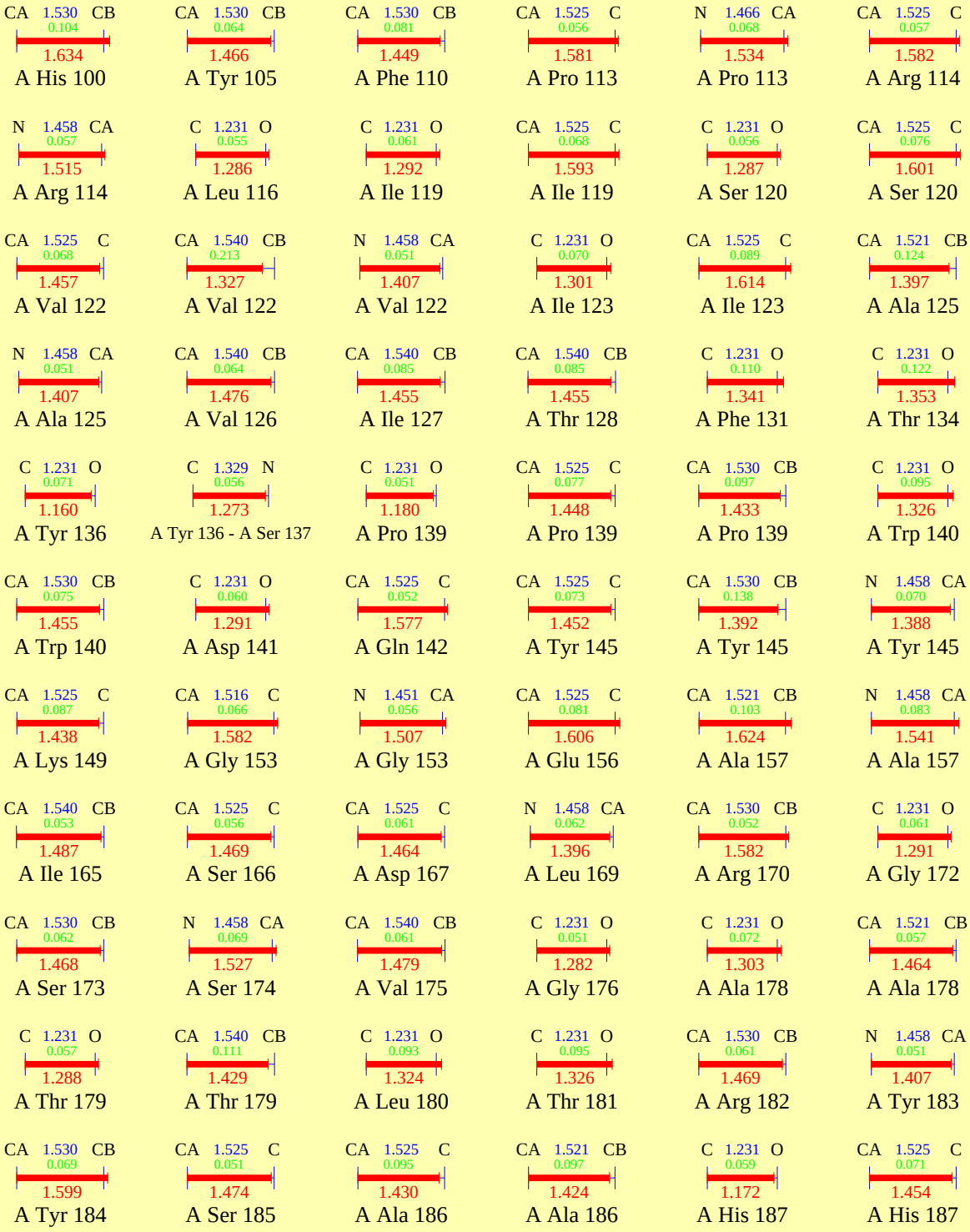
Distorted geometry
pdb2e75

Main-chain bond lengths



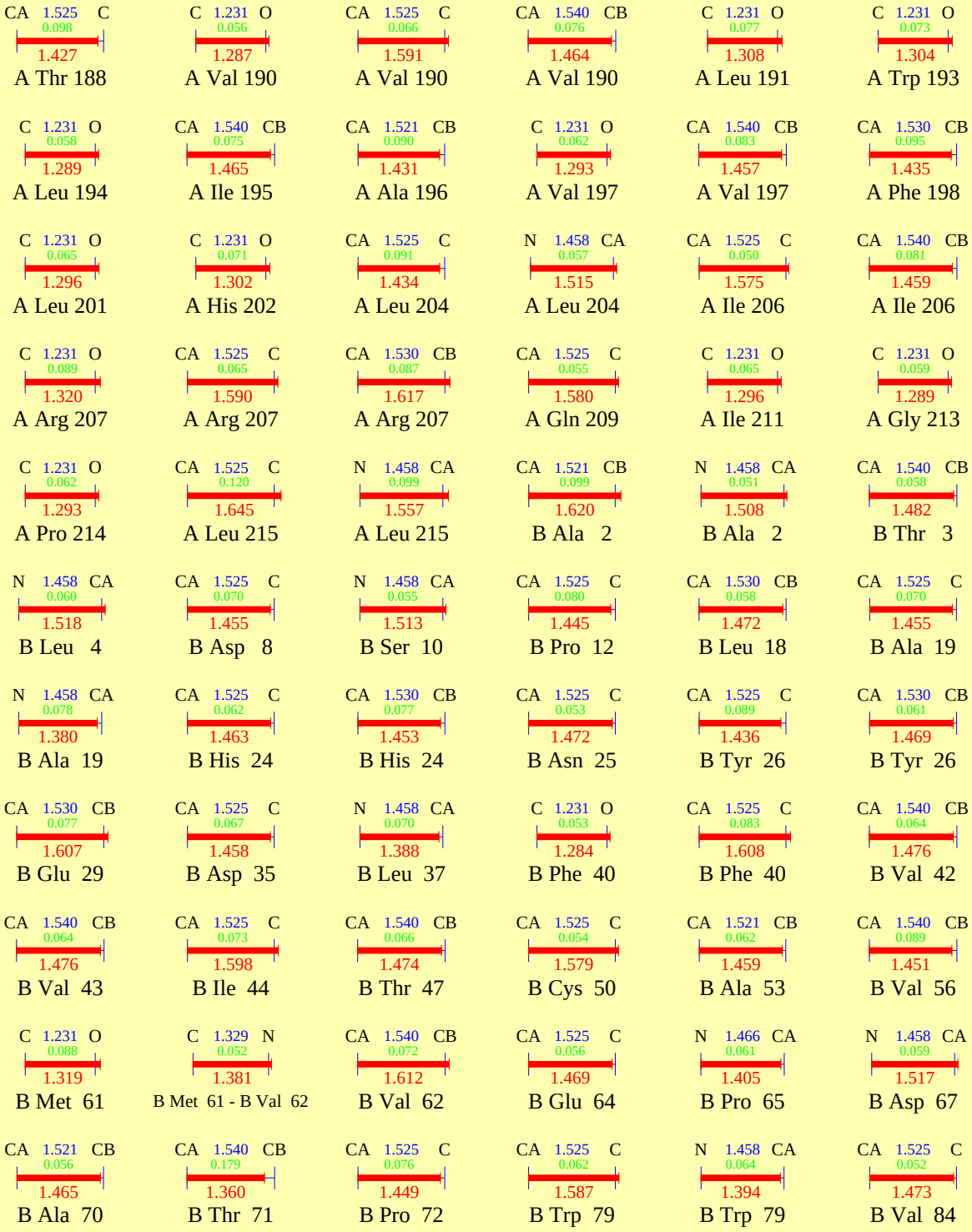
Distorted geometry
pdb2e75

Main-chain bond lengths (contd)



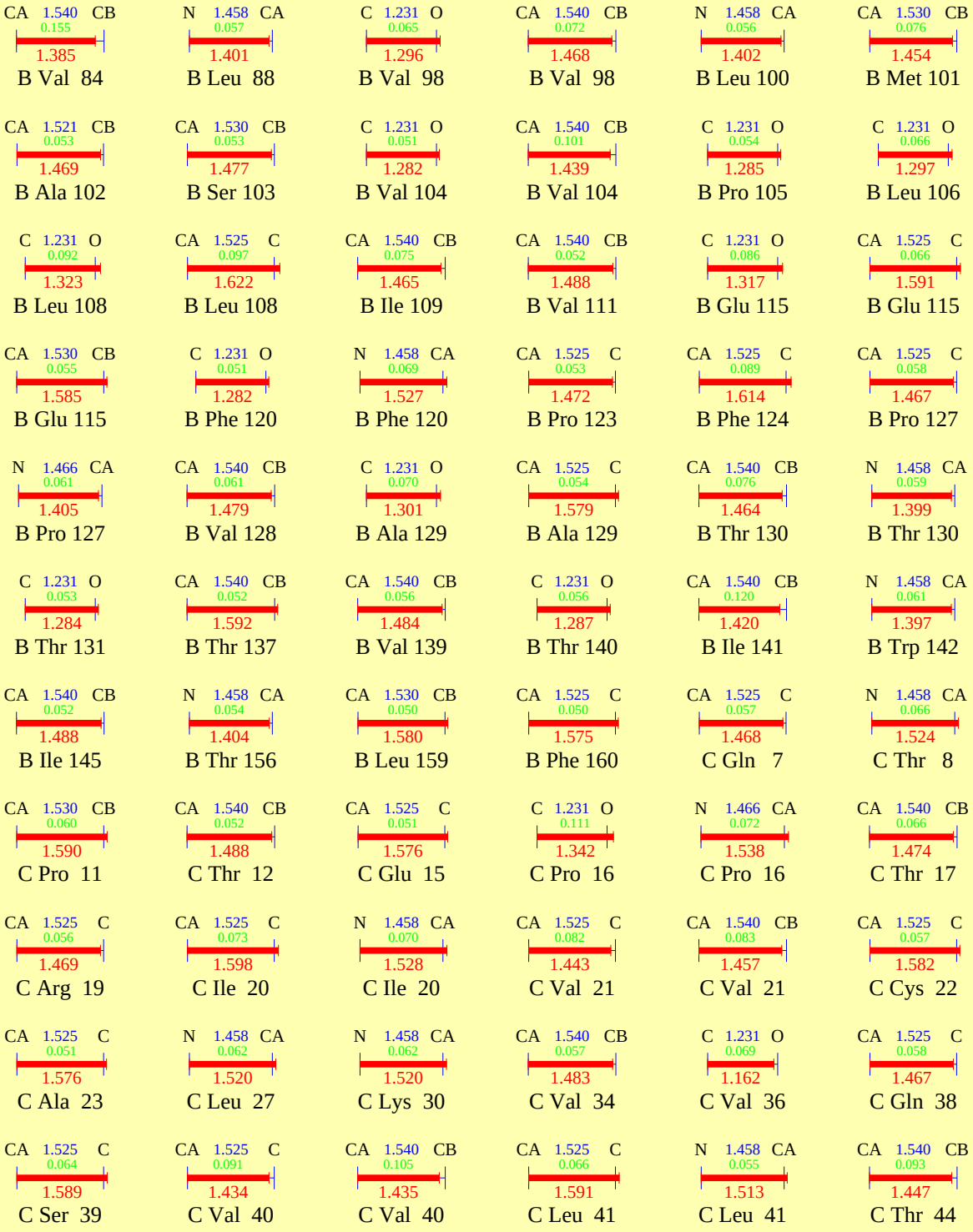
Distorted geometry
pdb2e75

Main-chain bond lengths (contd)



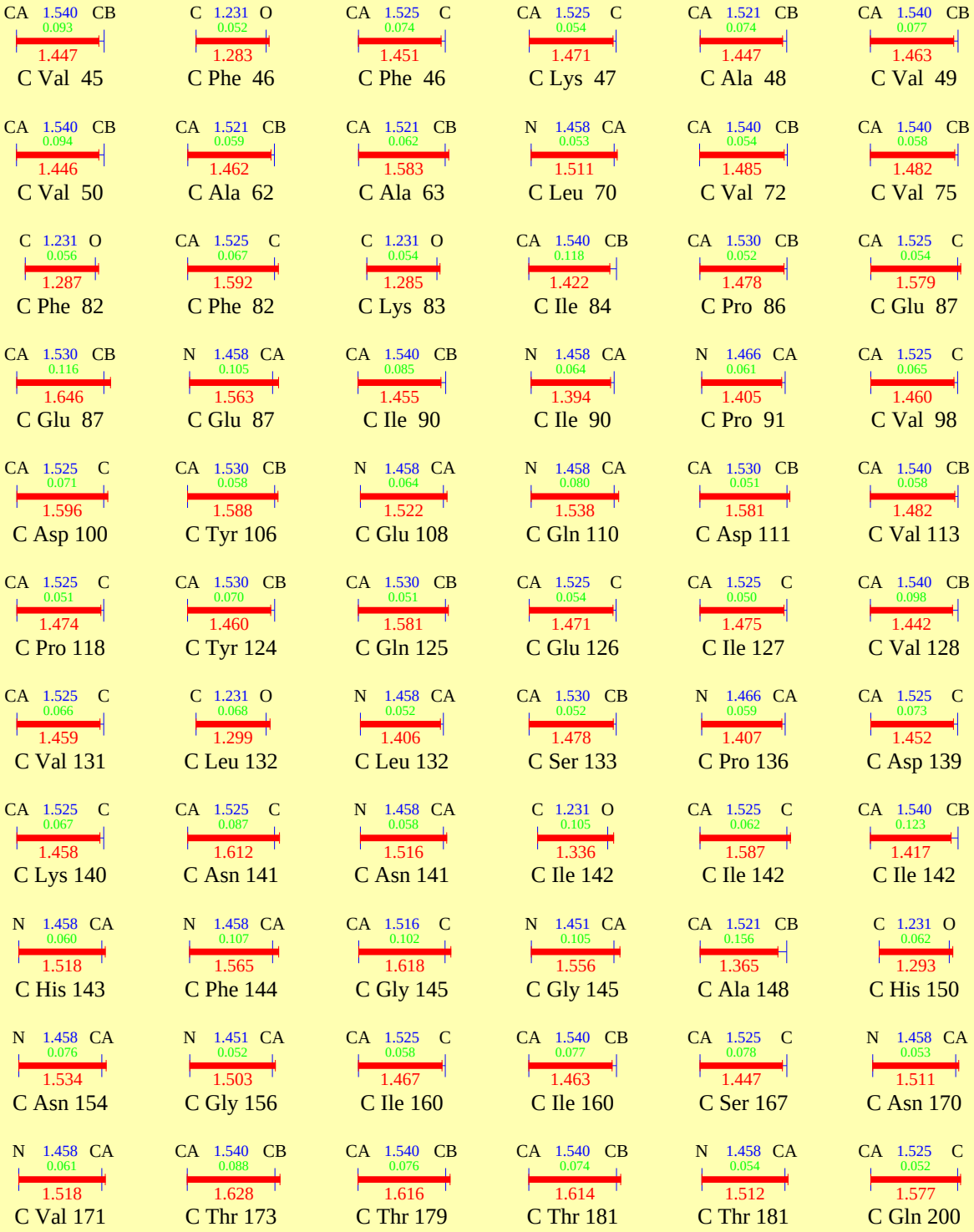
Distorted geometry
pdb2e75

Main-chain bond lengths (contd)



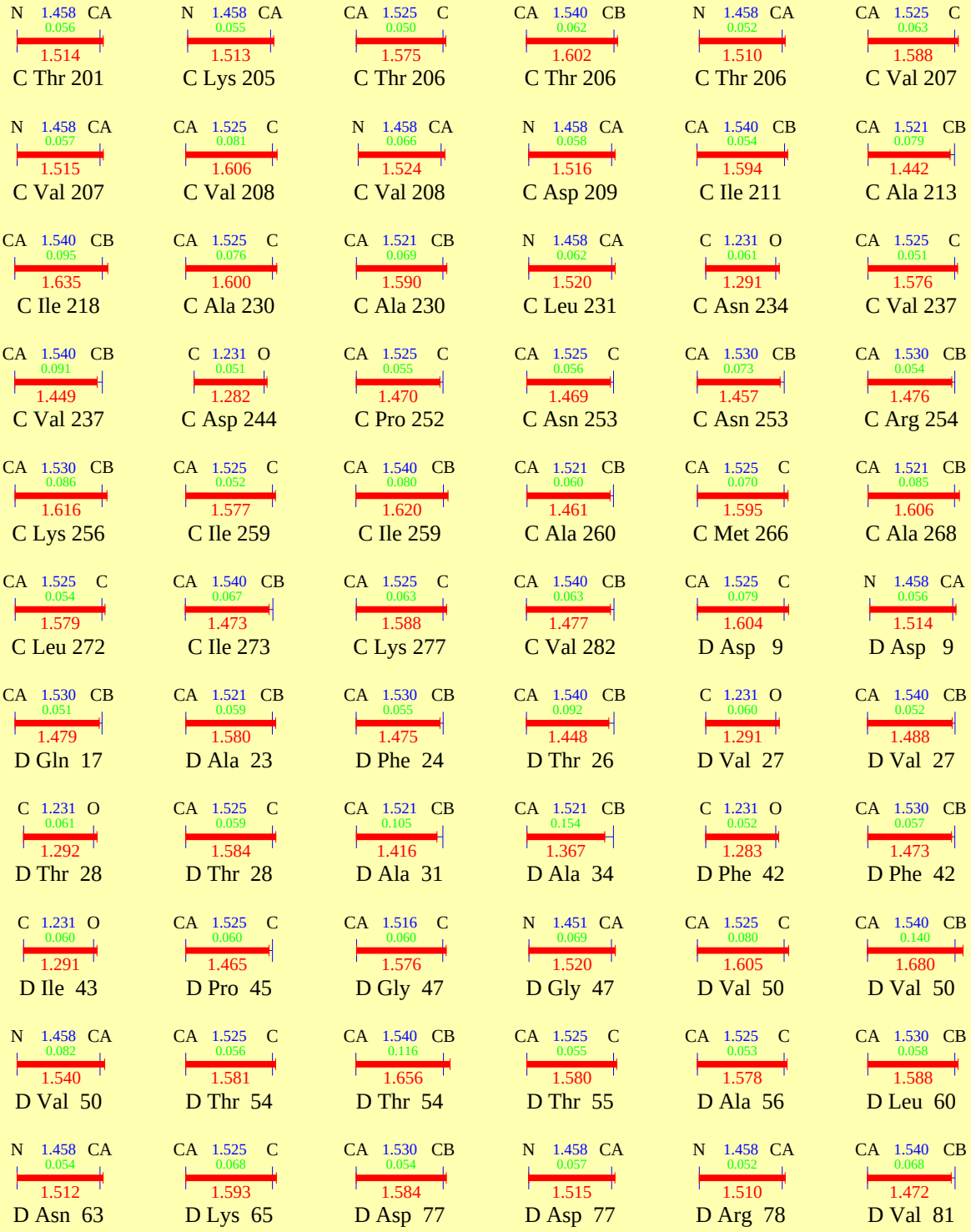
Distorted geometry
pdb2e75

Main-chain bond lengths (contd)



Distorted geometry
pdb2e75

Main-chain bond lengths (contd)



Distorted geometry
pdb2e75

Main-chain bond lengths (contd)

CA 1.525 C
0.056
1.469
D Leu 84

CA 1.540 CB
0.067
1.607
D Thr 89

CA 1.540 CB
0.054
1.594
D Ile 91

CA 1.525 C
0.053
1.578
D Ala 98

CA 1.540 CB
0.056
1.596
D Ile 99

N 1.458 CA
0.059
1.517
D Ile 99

CA 1.530 CB
0.060
1.590
D Asp 101

CA 1.540 CB
0.064
1.476
D Ile 104

N 1.458 CA
0.073
1.531
D Val 107

CA 1.530 CB
0.072
1.602
D Cys 108

N 1.458 CA
0.051
1.509
D Cys 108

CA 1.525 C
0.068
1.593
D Pro 116

CA 1.525 C
0.051
1.474
D Trp 117

N 1.458 CA
0.055
1.513
D Ala 119

CA 1.525 C
0.062
1.463
D Lys 125

N 1.458 CA
0.064
1.522
D His 129

CA 1.525 C
0.085
1.610
D Tyr 133

CA 1.525 C
0.062
1.587
D Ala 149

CA 1.540 CB
0.069
1.609
D Thr 154

CA 1.540 CB
0.088
1.628
D Val 155

N 1.458 CA
0.050
1.508
D Thr 172

N 1.458 CA
0.053
1.511
E Met 1

C 1.231 O
0.072
1.303
E Leu 3

CA 1.525 C
0.072
1.597
E Leu 3

CA 1.521 CB
0.104
1.417
E Ala 5

C 1.231 O
0.056
1.287
E Ile 9

CA 1.525 C
0.077
1.602
E Ile 9

C 1.231 O
0.085
1.316
E Val 10

CA 1.525 C
0.056
1.581
E Val 10

C 1.231 O
0.102
1.333
E Phe 11

C 1.329 N
0.052
1.381
E Phe 11 - E Ile 12

C 1.231 O
0.063
1.294
E Ile 12

CA 1.540 CB
0.076
1.464
E Ile 12

CA 1.530 CB
0.061
1.469
E Leu 14

CA 1.525 C
0.053
1.578
E Ile 18

C 1.231 O
0.055
1.286
E Ala 19

CA 1.521 CB
0.060
1.461
E Ala 19

CA 1.540 CB
0.109
1.431
E Val 20

C 1.231 O
0.060
1.291
E Ile 22

CA 1.540 CB
0.075
1.615
E Ile 26

CA 1.530 CB
0.052
1.582
E Ser 28

CA 1.525 C
0.084
1.609
F Met 1

N 1.458 CA
0.064
1.522
F Met 1

CA 1.540 CB
0.117
1.657
F Thr 2

N 1.458 CA
0.056
1.514
F Thr 2

CA 1.521 CB
0.120
1.401
F Ala 8

CA 1.521 CB
0.135
1.386
F Ala 9

CA 1.525 C
0.093
1.432
F Leu 10

N 1.458 CA
0.057
1.515
F Leu 10

C 1.231 O
0.071
1.302
F Leu 11

C 1.231 O
0.080
1.311
F Ser 12

CA 1.525 C
0.067
1.592
F Phe 13

CA 1.530 CB
0.052
1.478
F Phe 13

C 1.231 O
0.074
1.305
F Gly 14

C 1.231 O
0.061
1.292
F Leu 15

CA 1.540 CB
0.096
1.444
F Ile 16

C 1.231 O
0.077
1.308
F Phe 17

CA 1.530 CB
0.076
1.454
F Phe 17

C 1.231 O
0.053
1.283
F Gly 19

C 1.231 O
0.103
1.334
F Trp 20

CA 1.525 C
0.053
1.578
F Trp 20

C 1.231 O
0.062
1.293
F Gly 21

C 1.231 O
0.052
1.283
F Gly 23

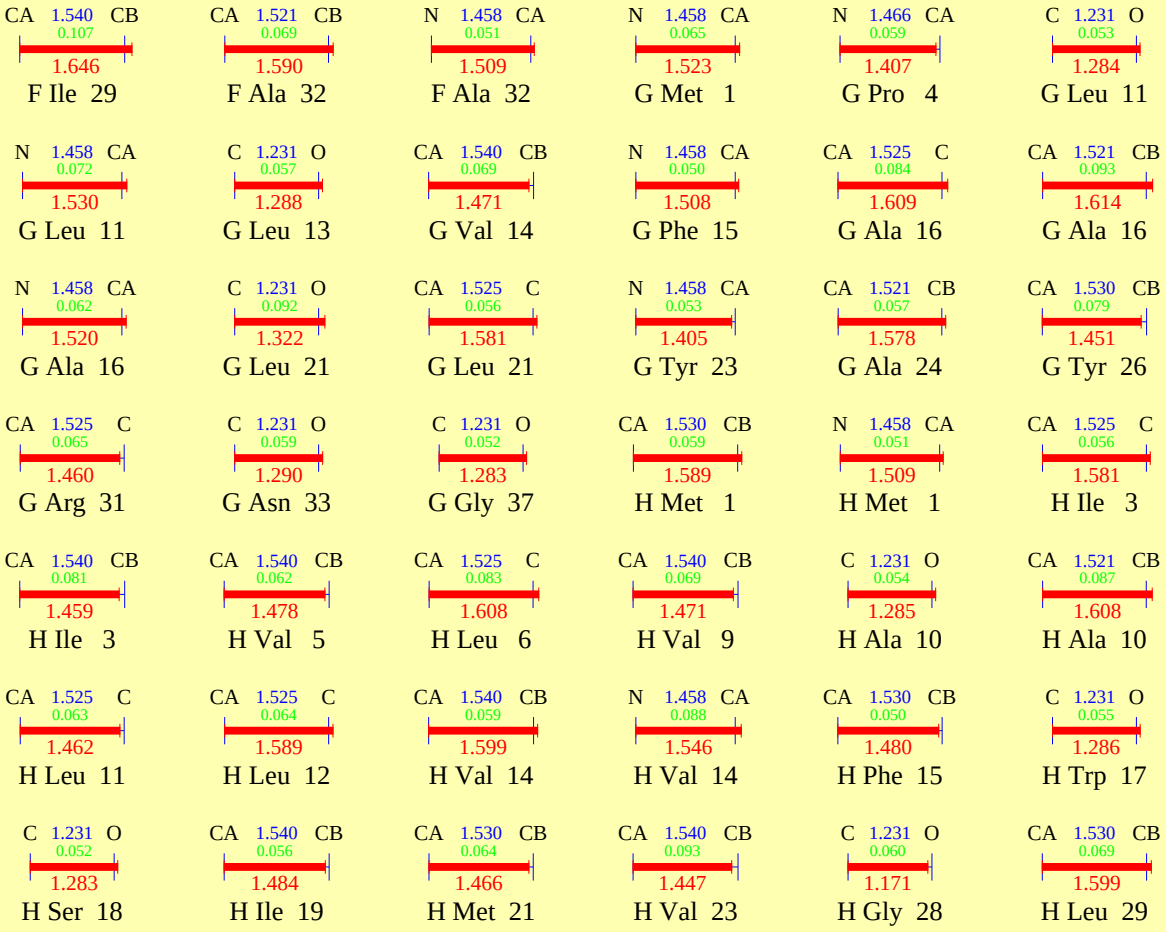
CA 1.540 CB
0.074
1.466
F Val 24

CA 1.530 CB
0.053
1.477
F Leu 27

CA 1.525 C
0.057
1.582
F Ile 29

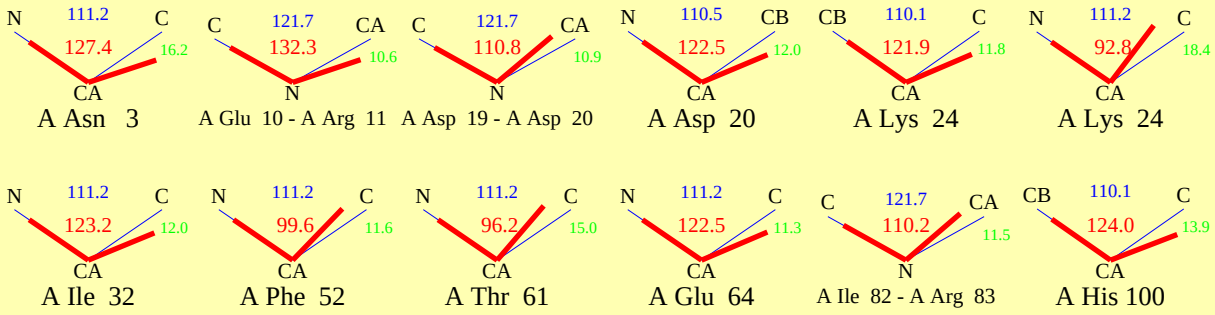
Distorted geometry
pdb2e75

Main-chain bond lengths (contd)



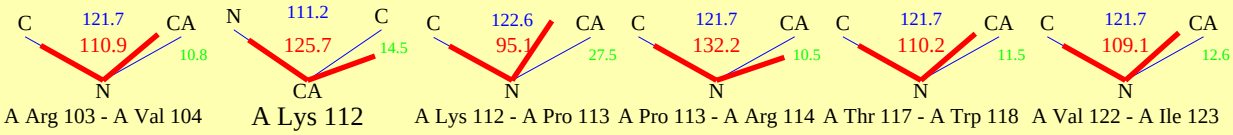
Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

Main-chain bond angles

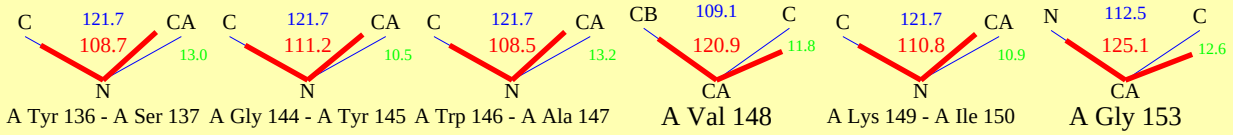


Distorted geometry
pdb2e75

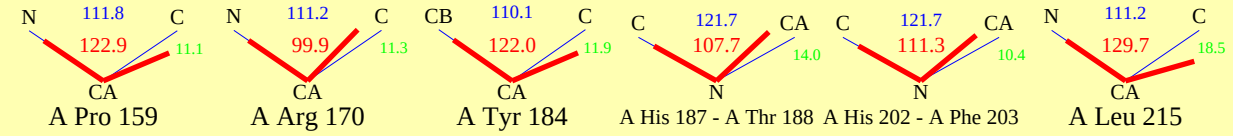
Main-chain bond angles (contd)



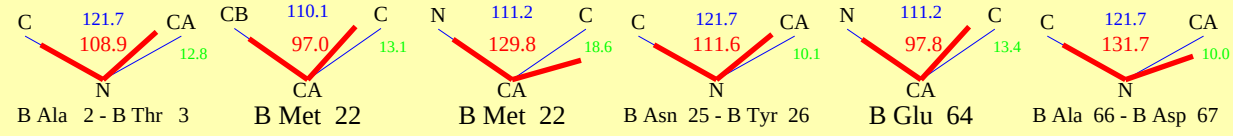
A Arg 103 - A Val 104 | A Lys 112 | A Lys 112 - A Pro 113 | A Pro 113 - A Arg 114 | A Thr 117 - A Trp 118 | A Val 122 - A Ile 123



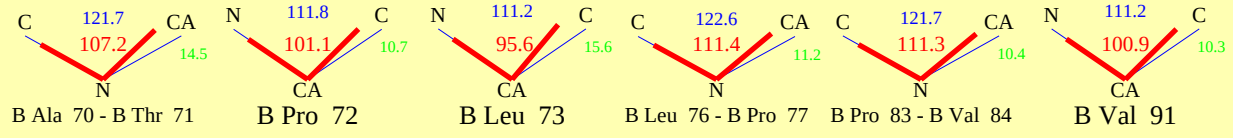
A Tyr 136 - A Ser 137 | A Gly 144 - A Tyr 145 | A Trp 146 - A Ala 147 | A Val 148 | A Lys 149 - A Ile 150 | A Gly 153



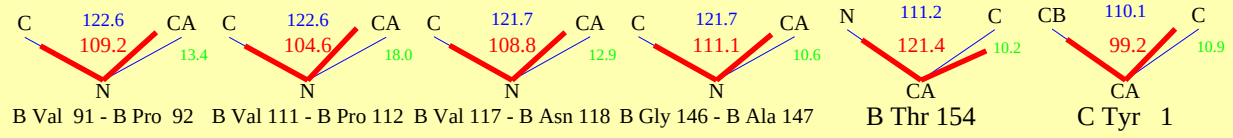
A Pro 159 | A Arg 170 | A Tyr 184 | A His 187 - A Thr 188 | A His 202 - A Phe 203 | A Leu 215



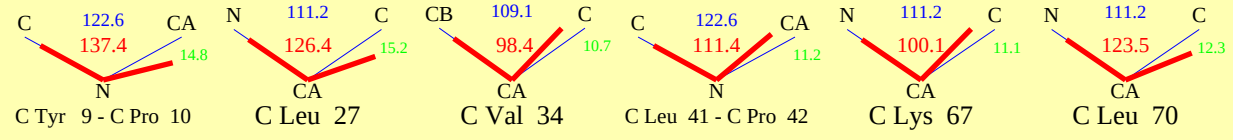
B Ala 2 - B Thr 3 | B Met 22 | B Met 22 | B Asn 25 - B Tyr 26 | B Glu 64 | B Ala 66 - B Asp 67



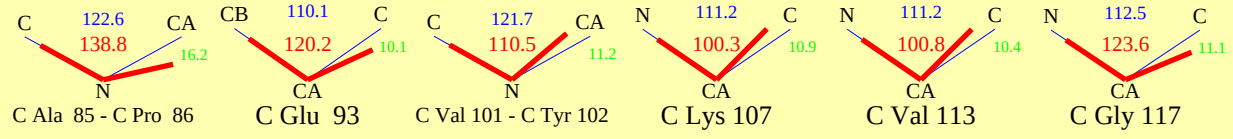
B Ala 70 - B Thr 71 | B Pro 72 | B Leu 73 | B Leu 76 - B Pro 77 | B Pro 83 - B Val 84 | B Val 91



B Val 91 - B Pro 92 | B Val 111 - B Pro 112 | B Val 117 - B Asn 118 | B Gly 146 - B Ala 147 | B Thr 154 | C Tyr 1



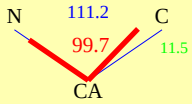
C Tyr 9 - C Pro 10 | C Leu 27 | C Val 34 | C Leu 41 - C Pro 42 | C Lys 67 | C Leu 70



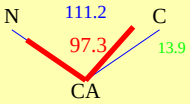
C Ala 85 - C Pro 86 | C Glu 93 | C Val 101 - C Tyr 102 | C Lys 107 | C Val 113 | C Gly 117

Distorted geometry
pdb2e75

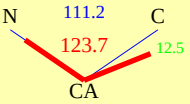
Main-chain bond angles (contd)



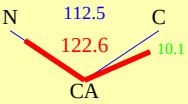
C Leu 119



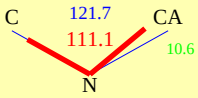
C Gln 125



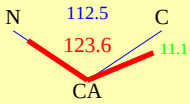
C Asn 141



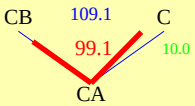
C Gly 145



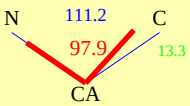
C Ile 149 - C His 150



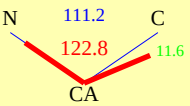
C Gly 156



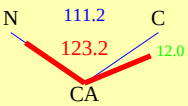
C Ile 160



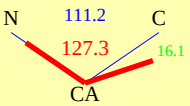
C Ser 167



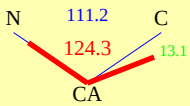
C Phe 172



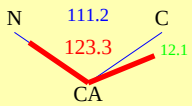
C Gln 200



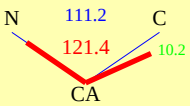
C Thr 201



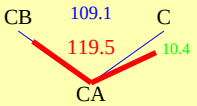
C Lys 205



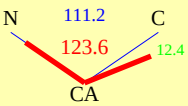
C Val 207



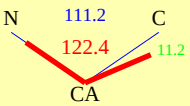
C Val 208



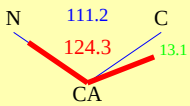
C Ile 218



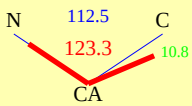
C Ala 230



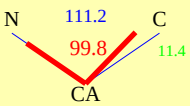
C Leu 231



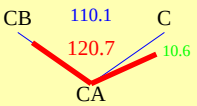
C Asn 234



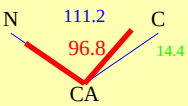
C Gly 239



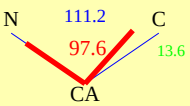
C Asp 244



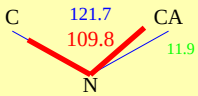
C Lys 256



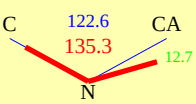
C Glu 280



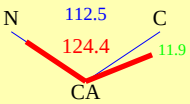
D Val 10



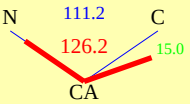
D Ala 23 - D Phe 24



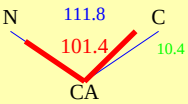
D Pro 44 - D Pro 45



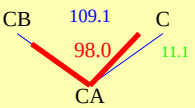
D Gly 47



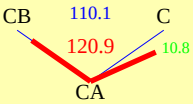
D Asp 77



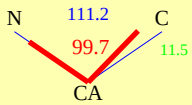
D Pro 88



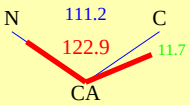
D Val 107



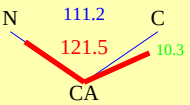
D Cys 108



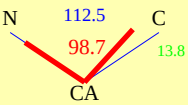
D His 110



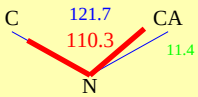
D His 129



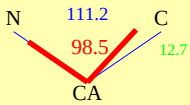
D Asp 134



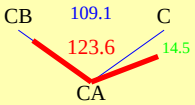
D Gly 137



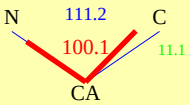
E Ile 22 - E Ile 23



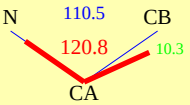
E Ile 23



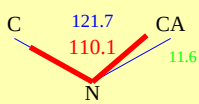
E Ile 26



E Ile 29



F Leu 10



F Leu 10 - F Leu 11

F Ile 29

F Gly 31

G Glu 3 - G Pro 4

G Tyr 23 - G Ala 24

G Tyr 29

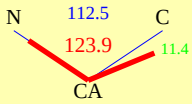
G Pro 32

G Leu 35

H Met 1

Distorted geometry
pdb2e75

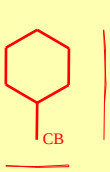
Main-chain bond angles (contd)



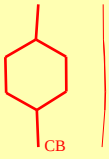
H Gly 28

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

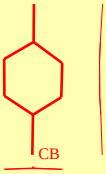
Planar groups



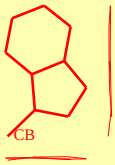
0.030
A Phe 8



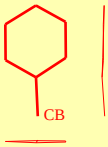
0.043
A Tyr 145



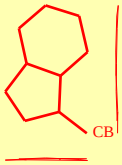
0.045
A Tyr 184



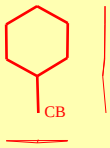
0.040
A Trp 193



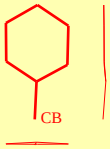
0.032
C Phe 129



0.030
C Trp 257



0.036
E Phe 15



0.031
G Phe 22

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