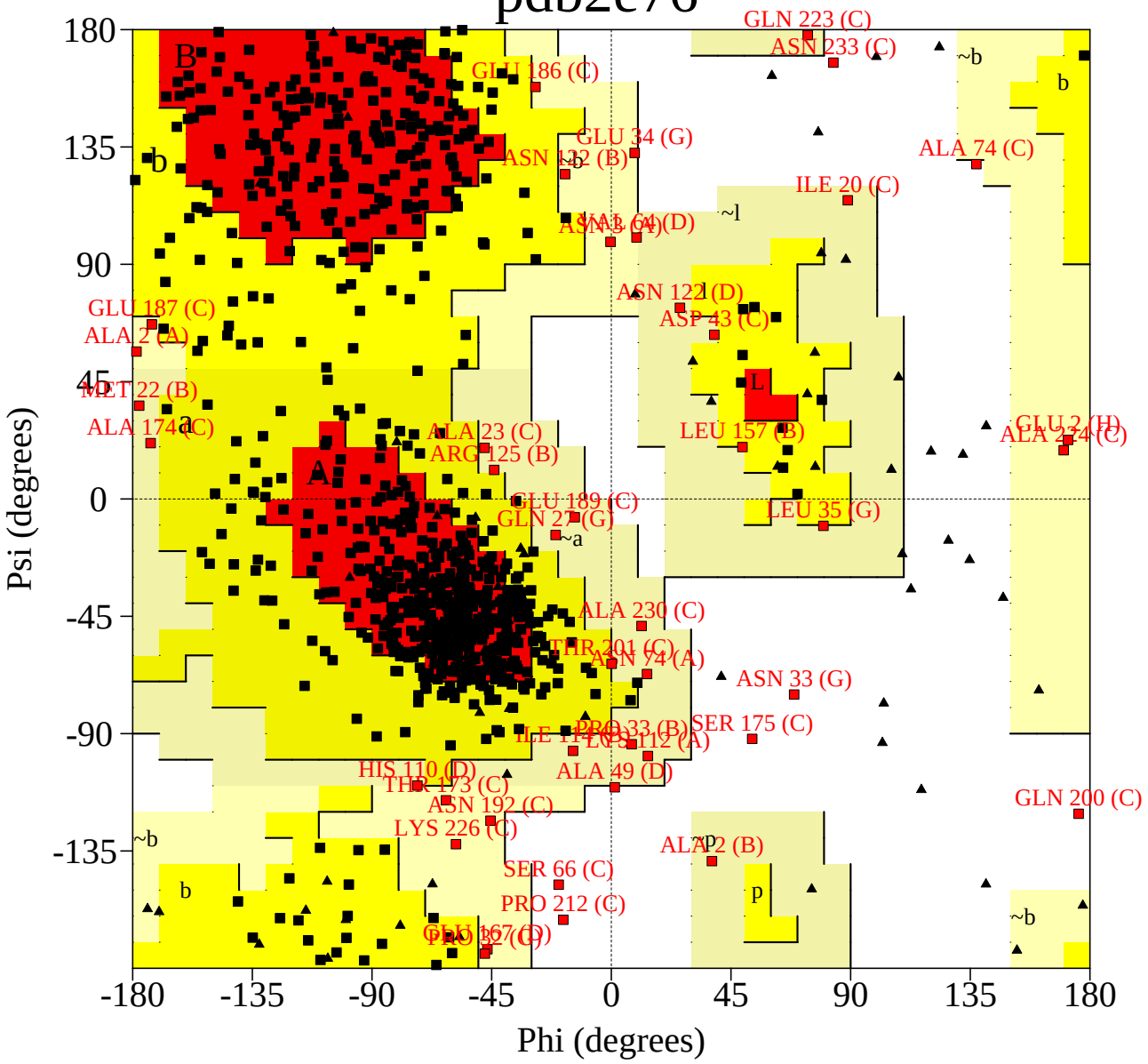
Ramachandran Plot

pdb2e76



Plot statistics

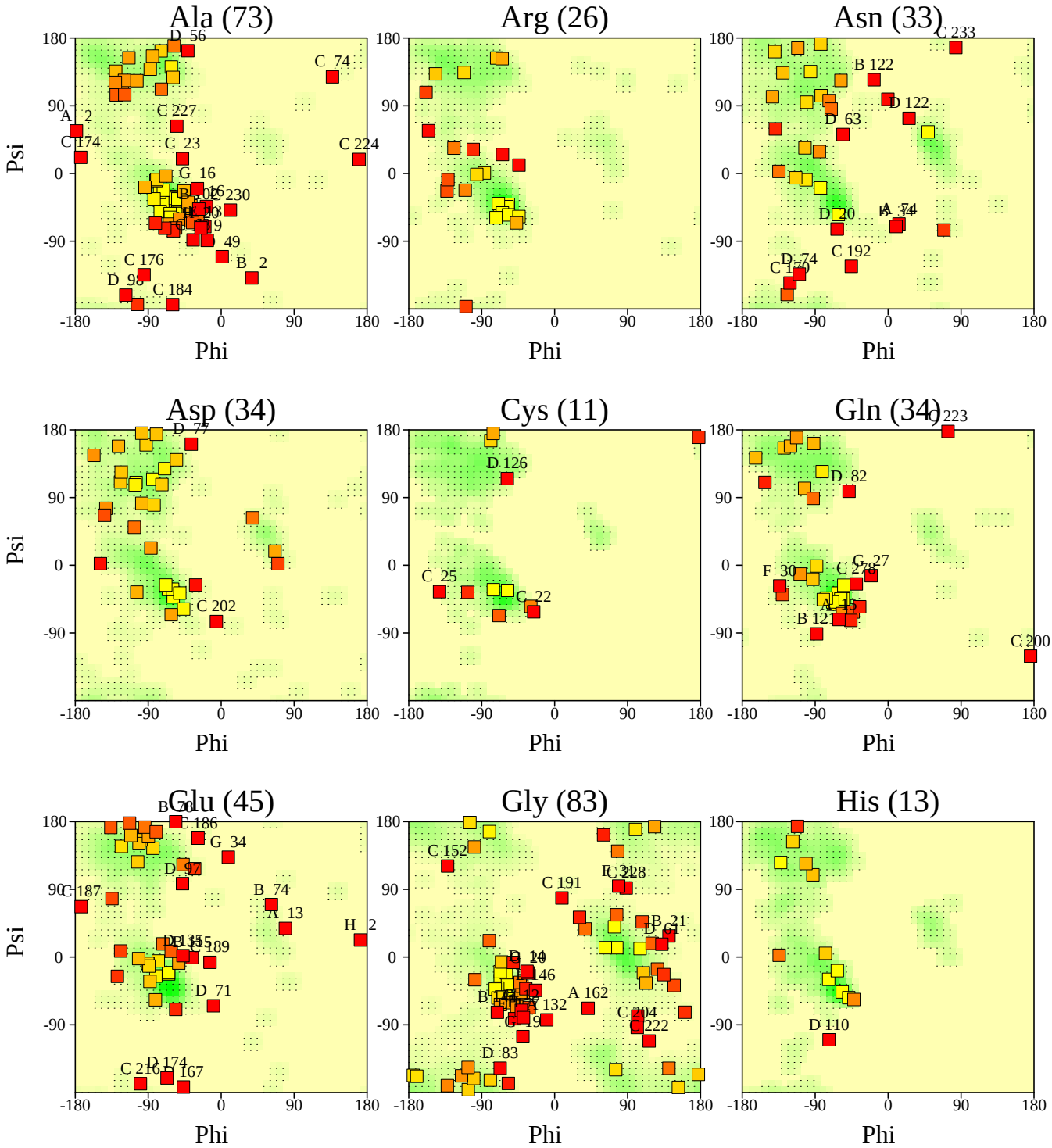
Residues in most favoured regions [A,B,L]	550	68.9%
Residues in additional allowed regions [a,b,l,p]	209	26.2%
Residues in generously allowed regions [~a,~b,~l,~p]	32	4.0%
Residues in disallowed regions	7	0.9%
	----	------
Number of non-glycine and non-proline residues	798	100.0%
Number of end-residues (excl. Gly and Pro)	17	
Number of glycine residues (shown as triangles)	84	
Number of proline residues	62	

Total number of residues	961	

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

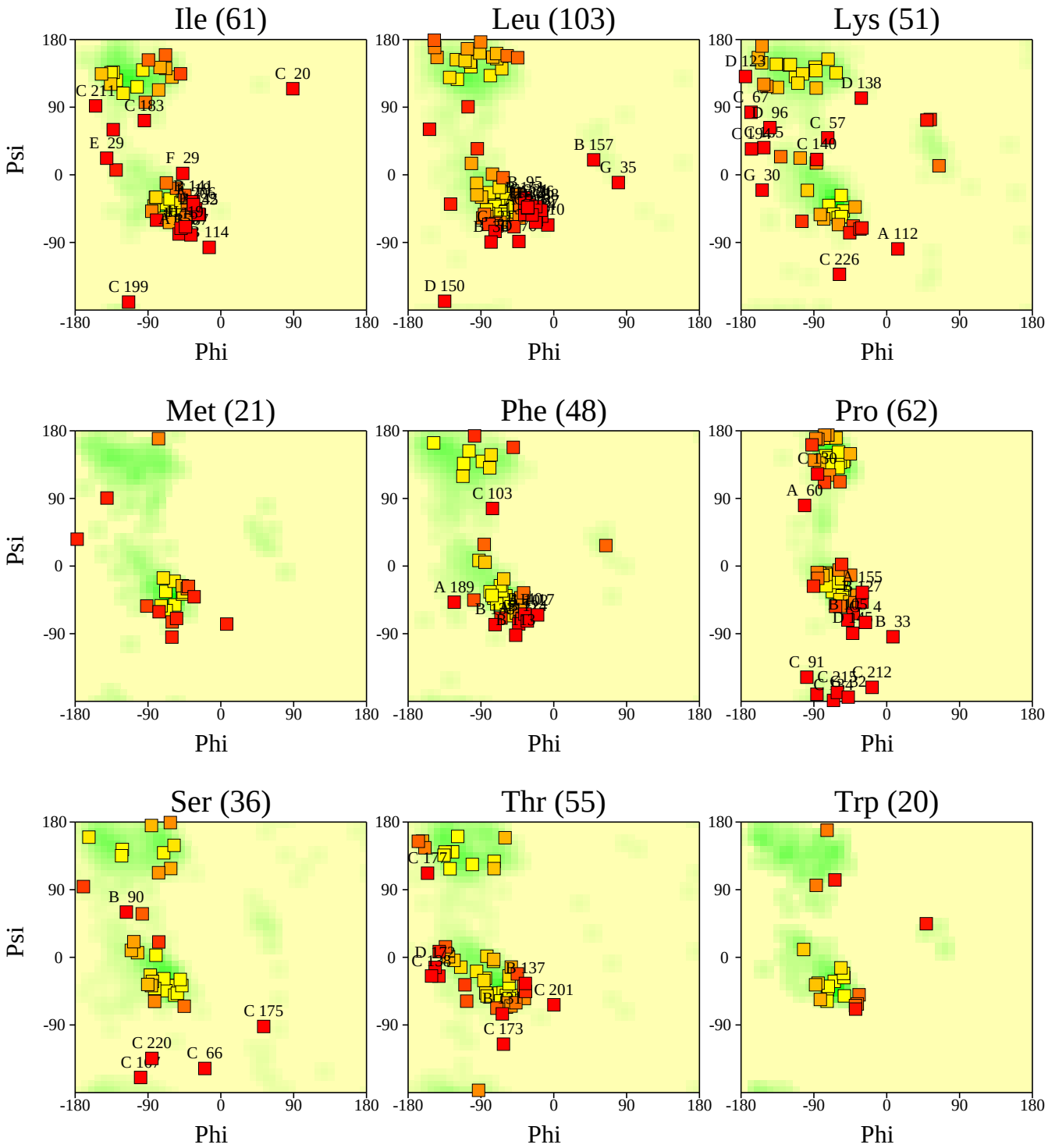
pdb2e76



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

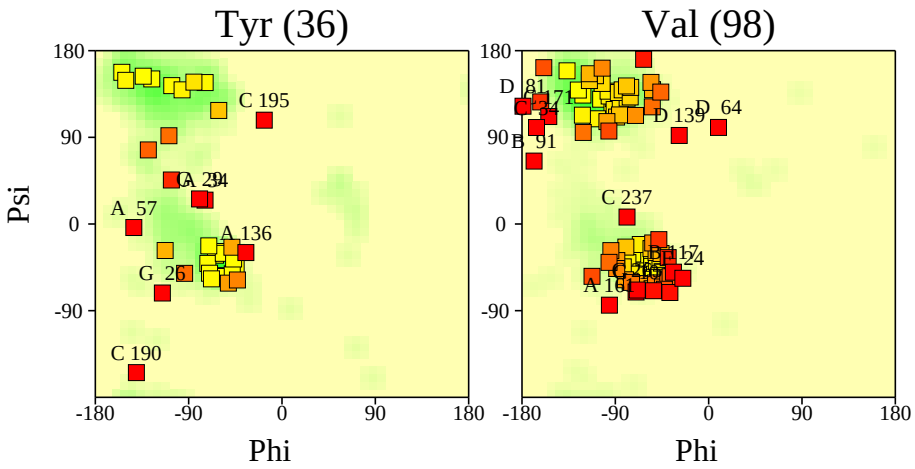
pdb2e76



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

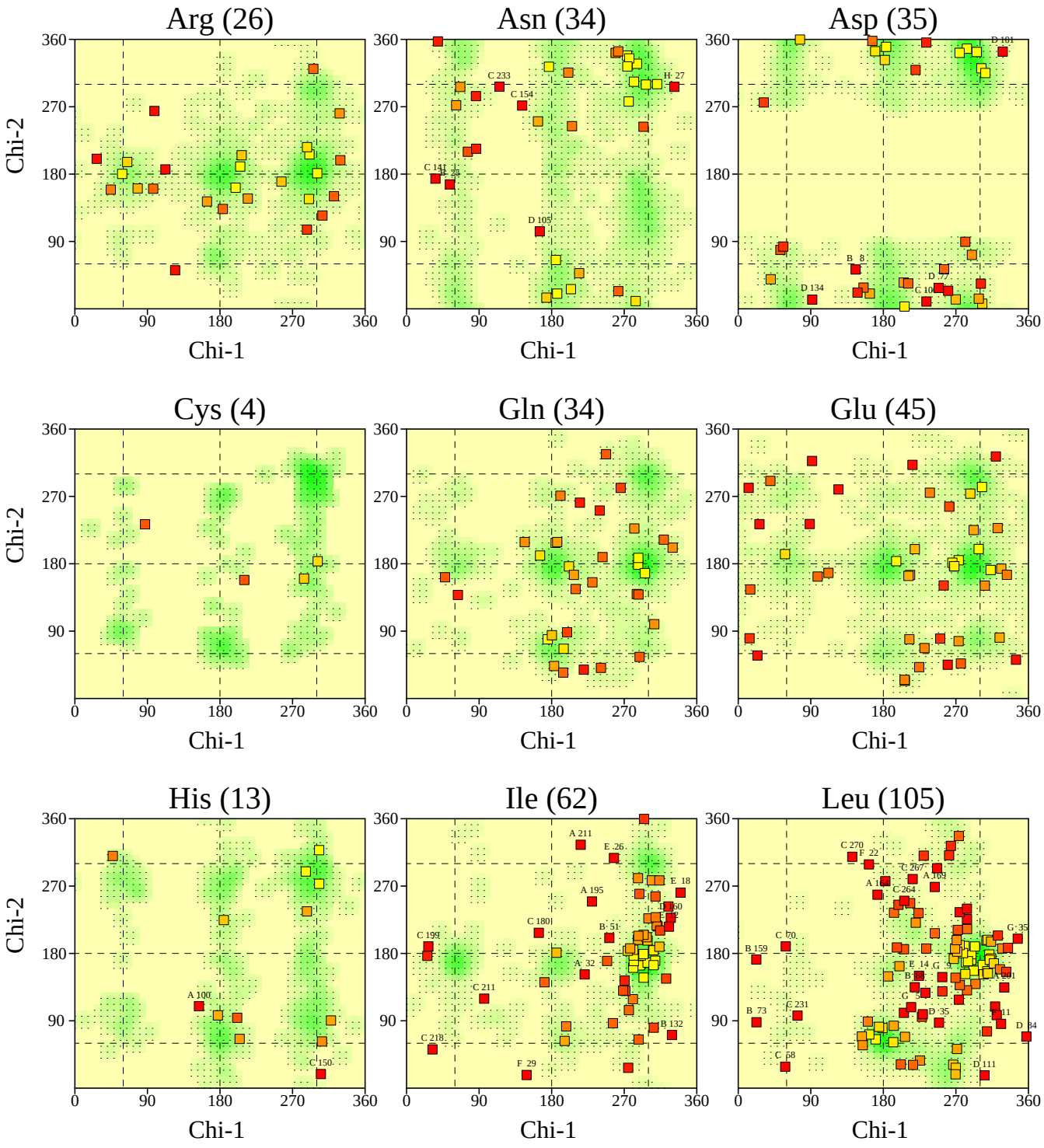
pdb2e76



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

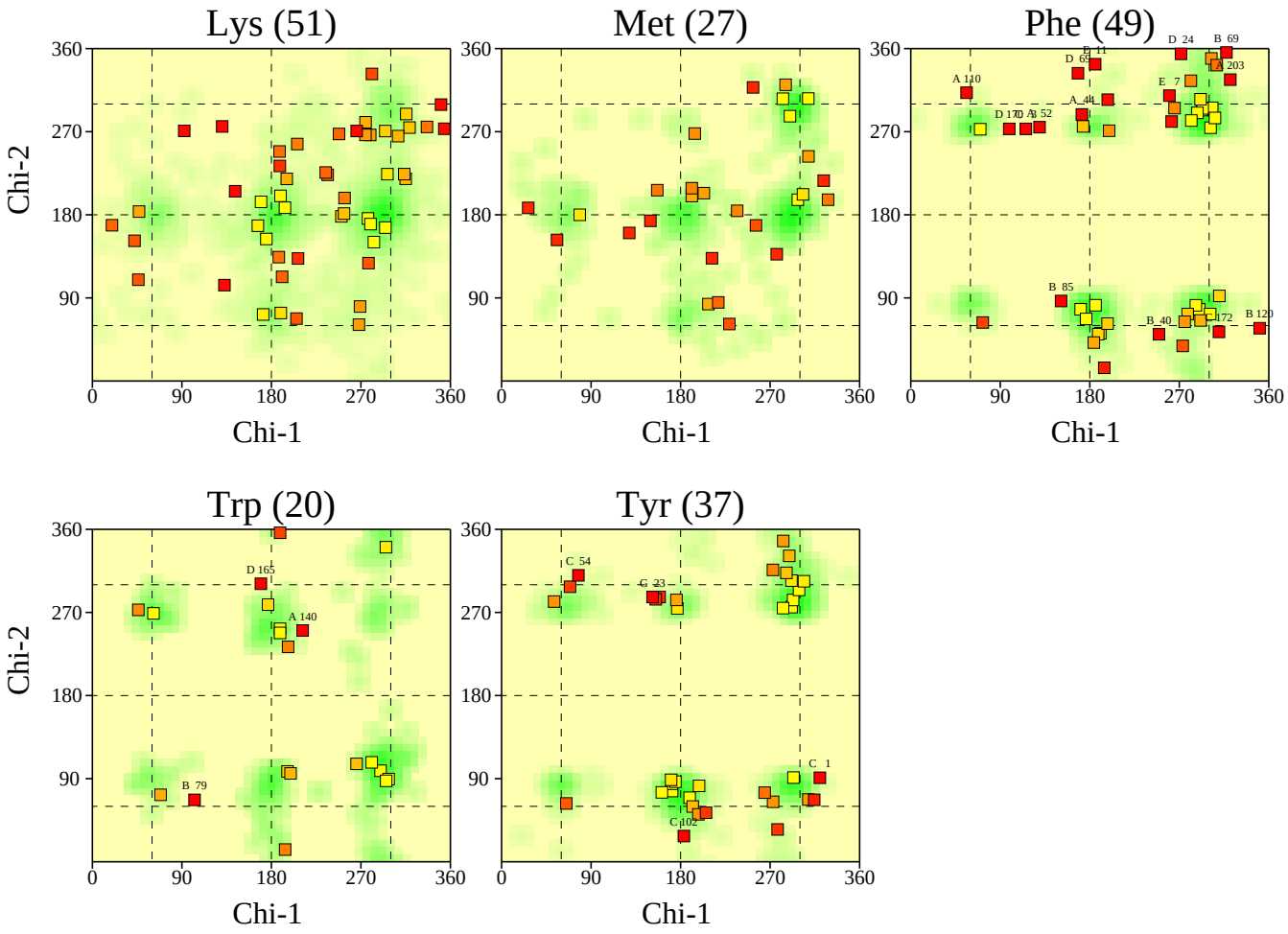
pdb2e76



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

pdb2e76

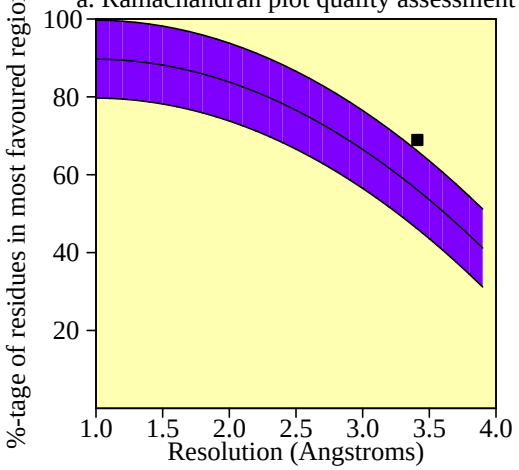


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

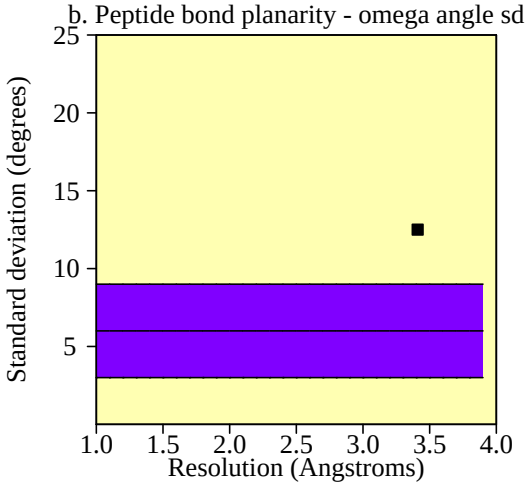
PROCHECK

Main-chain parameters
pdb2e76

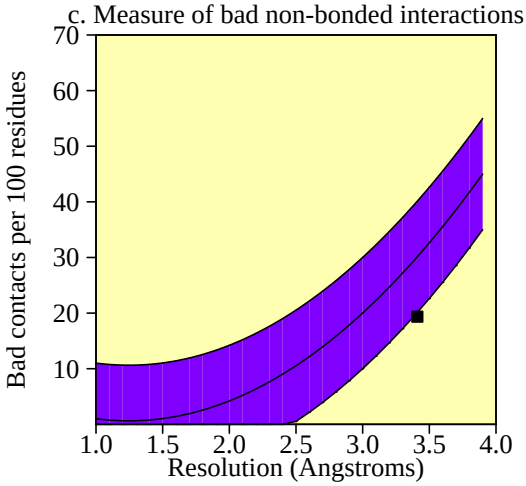
a. Ramachandran plot quality assessment



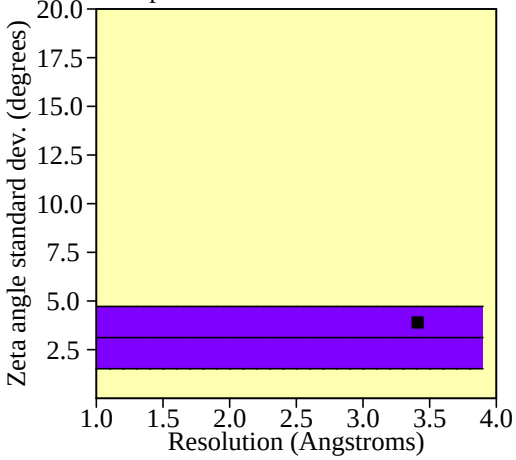
b. Peptide bond planarity - omega angle sd



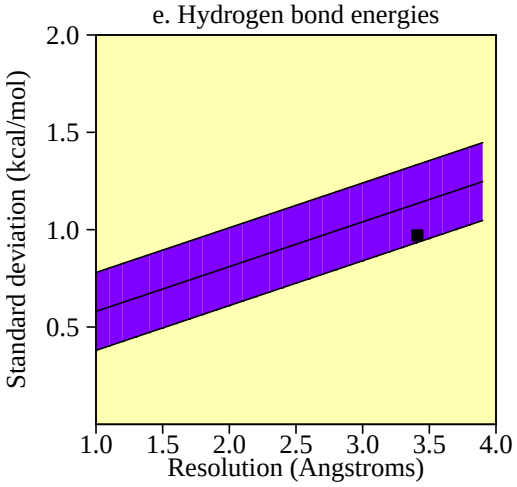
c. Measure of bad non-bonded interactions



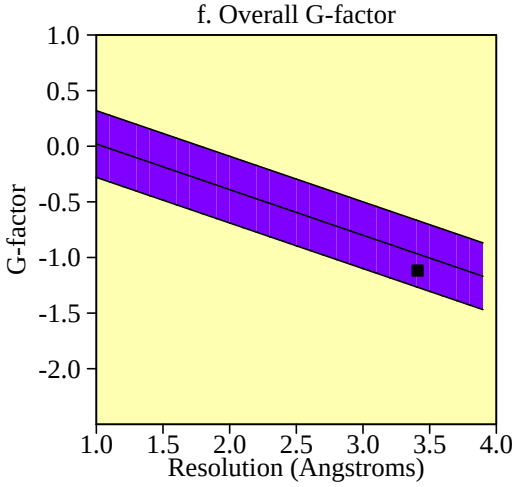
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor

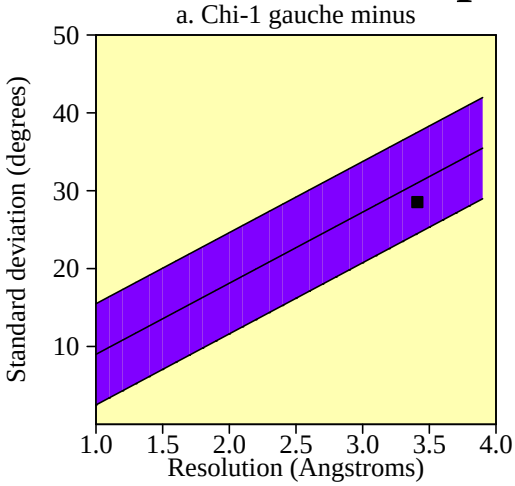


Plot statistics

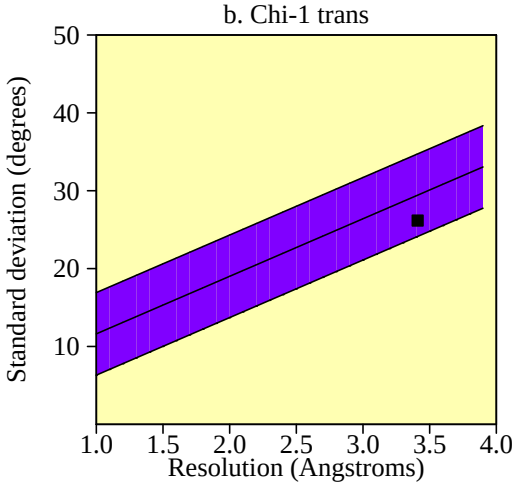
Stereochemical parameter	No. of data pts	Parameter value	Comparison values: Typical value	Comparison values: Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	798	68.9	56.1	10.0	1.3	BETTER
b. Omega angle st dev	950	12.5	6.0	3.0	2.2	WORSE
c. Bad contacts / 100 residues	186	19.4	30.1	10.0	-1.1	BETTER
d. Zeta angle st dev	877	3.9	3.1	1.6	0.5	Inside
e. H-bond energy st dev	584	1.0	1.1	0.2	-0.8	Inside
f. Overall G-factor	961	-1.1	-1.0	0.3	-0.5	Inside

Side-chain parameters
pdb2e76

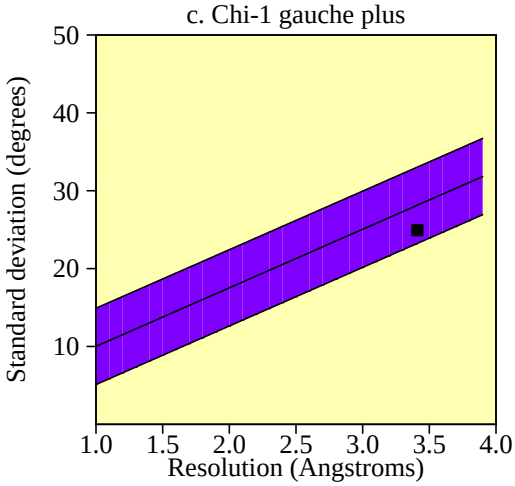
a. Chi-1 gauche minus



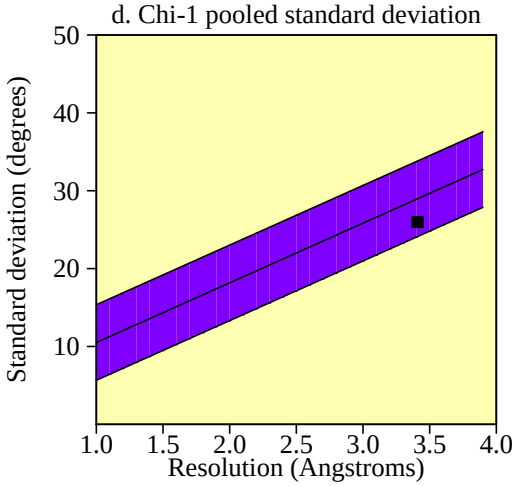
b. Chi-1 trans



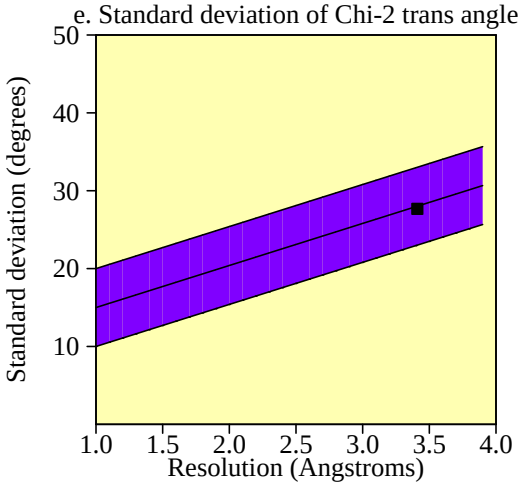
c. Chi-1 gauche plus



d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



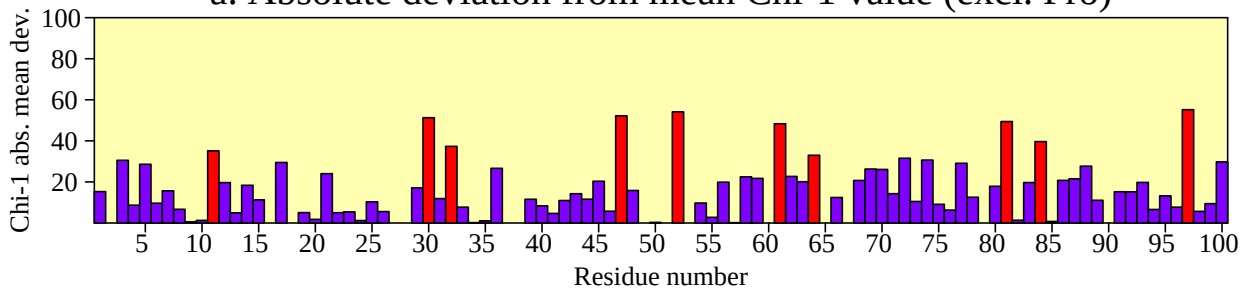
pdb2e76

Plot statistics

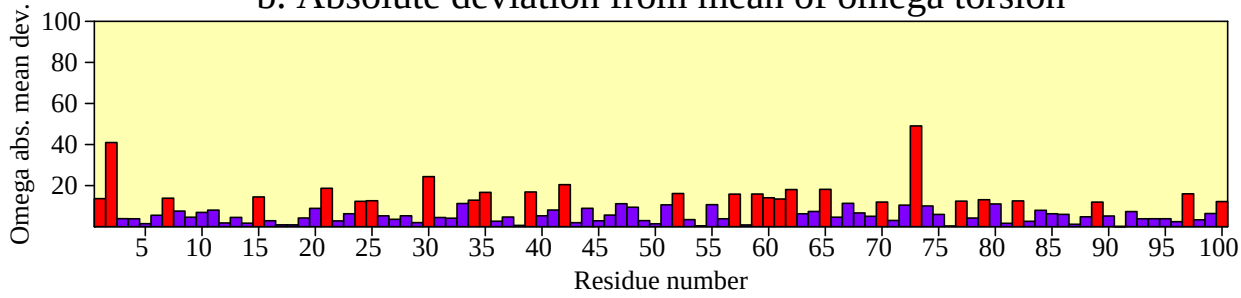
Stereochemical parameter	No. of data pts	Parameter value	Comparison values: Typical value	Comparison values: Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	113	28.5	31.0	6.5	-0.4	Inside
b. Chi-1 trans st dev	277	26.2	29.4	5.3	-0.6	Inside
c. Chi-1 gauche plus st dev	351	24.9	28.1	4.9	-0.7	Inside
d. Chi-1 pooled st dev	741	26.0	29.0	4.8	-0.6	Inside
e. Chi-2 trans st dev	207	27.7	28.0	5.0	-0.1	Inside

Residue properties
pdb2e76

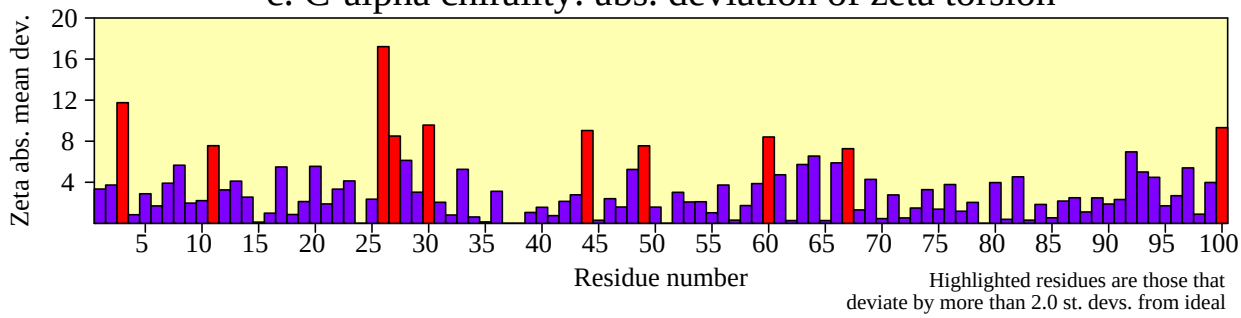
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

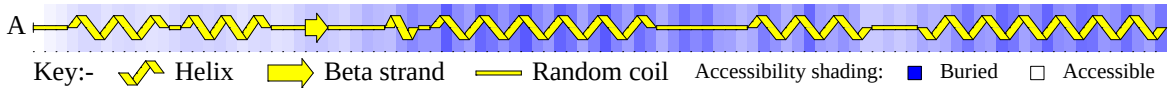


c. C-alpha chirality: abs. deviation of zeta torsion

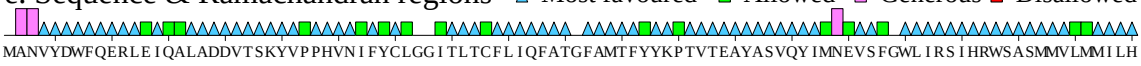


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

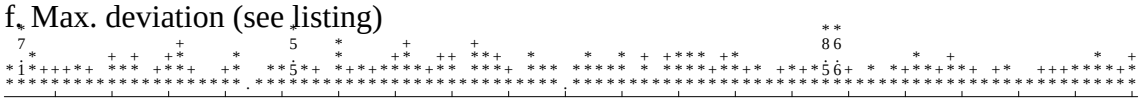
d. Secondary structure & estimated accessibility



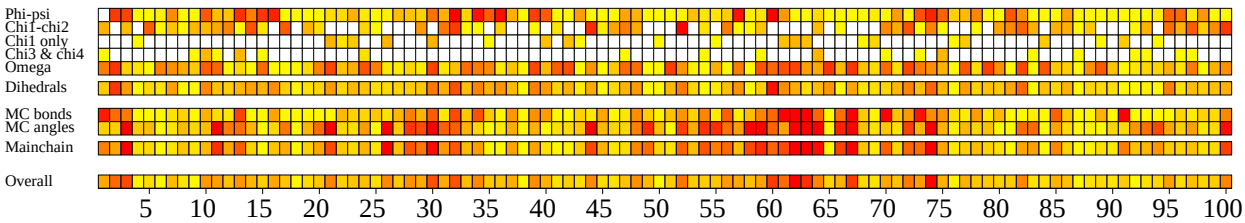
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

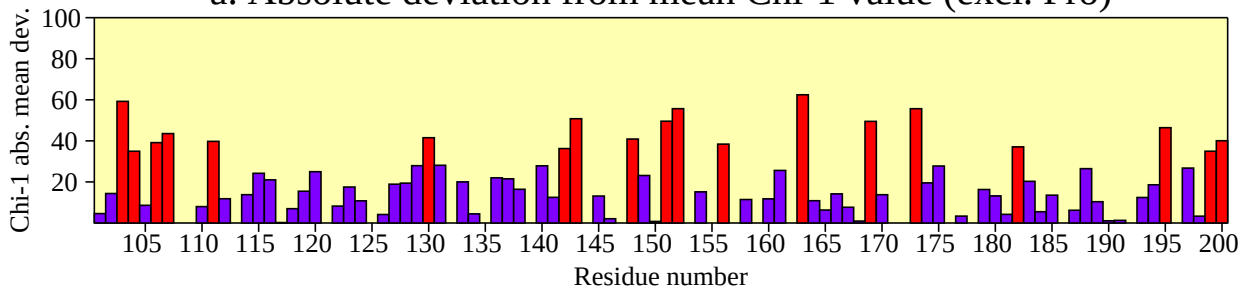


g. G-factors

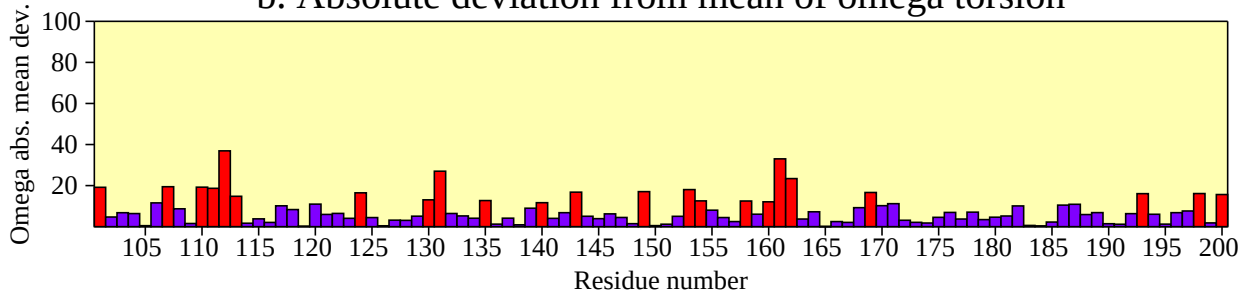


Residue properties
pdb2e76

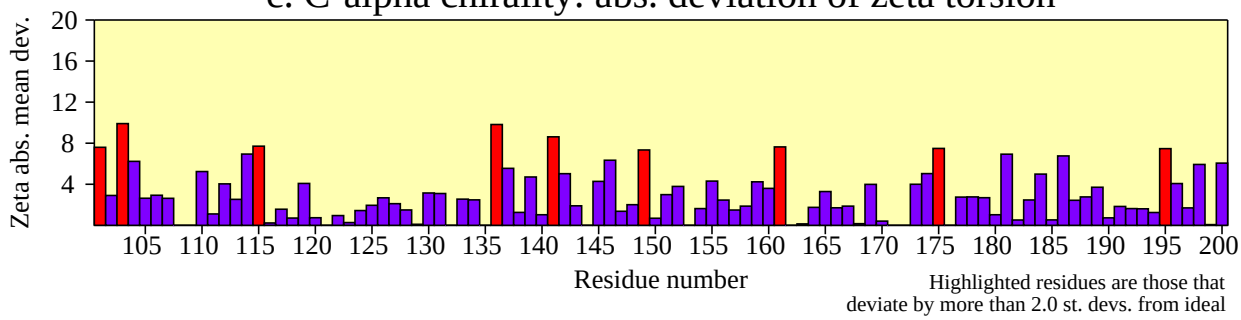
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

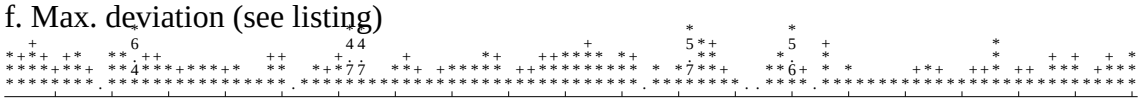
d. Secondary structure & estimated accessibility

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

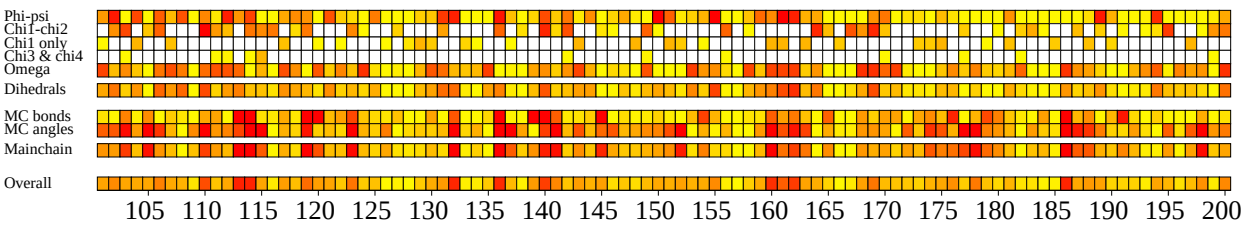
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

VFRVYLTGGFKKPRELTWISGVILAVITVSFGVTGYSLPWDQVGYWAVKIVSGVPEAIPVVGVLISDLLRGGSSVGQATLTRYYSAHTFVLPWLIAVFML

f. Max. deviation (see listing)

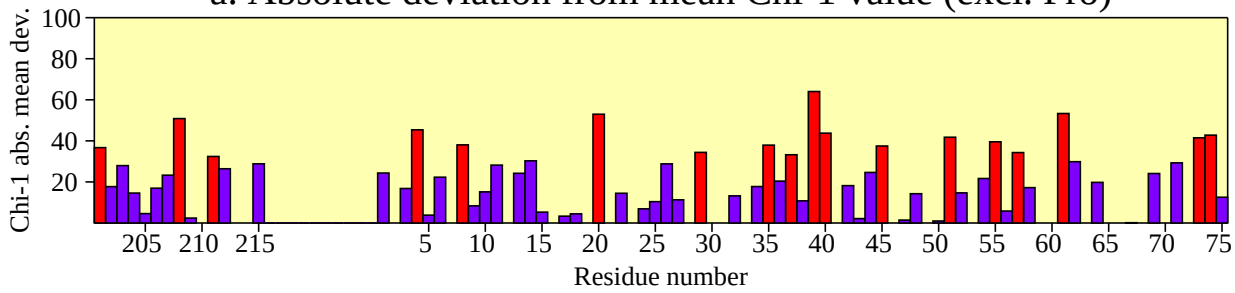


g. G-factors

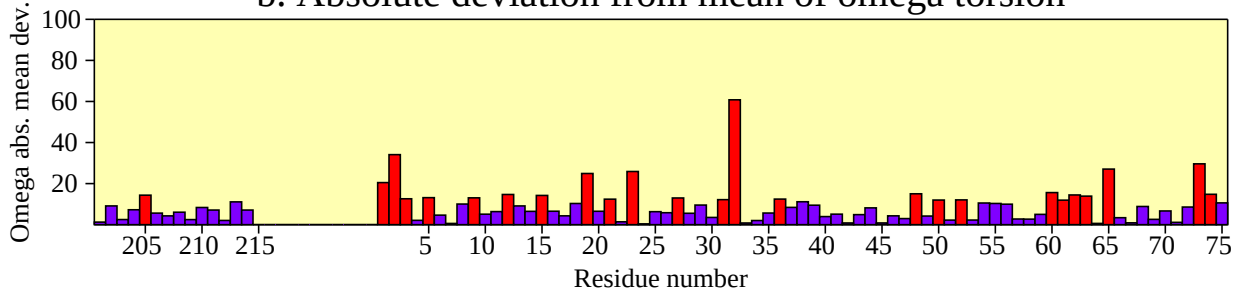


Residue properties
pdb2e76

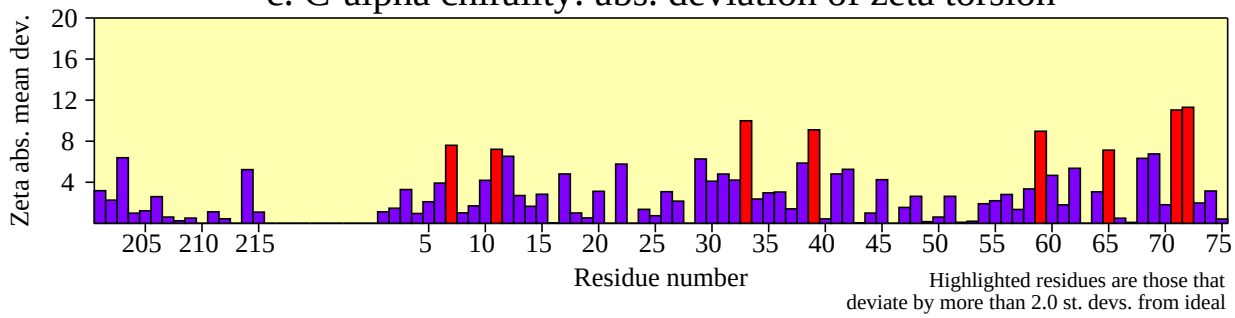
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

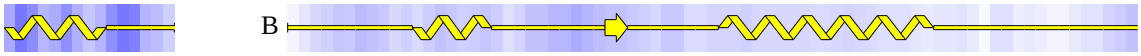


c. C-alpha chirality: abs. deviation of zeta torsion



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

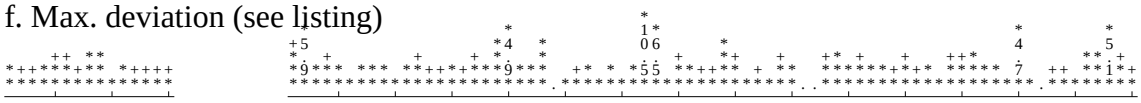
d. Secondary structure & estimated accessibility



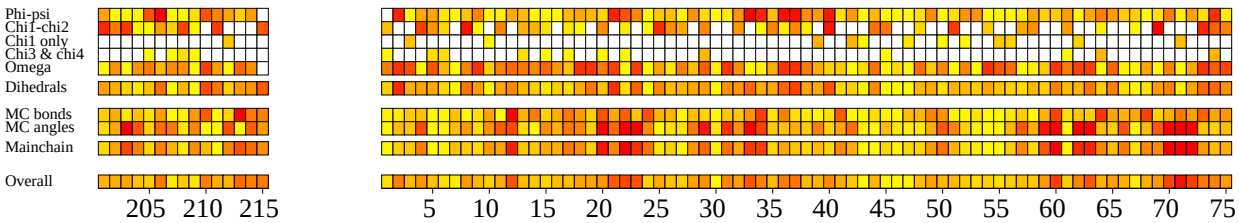
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

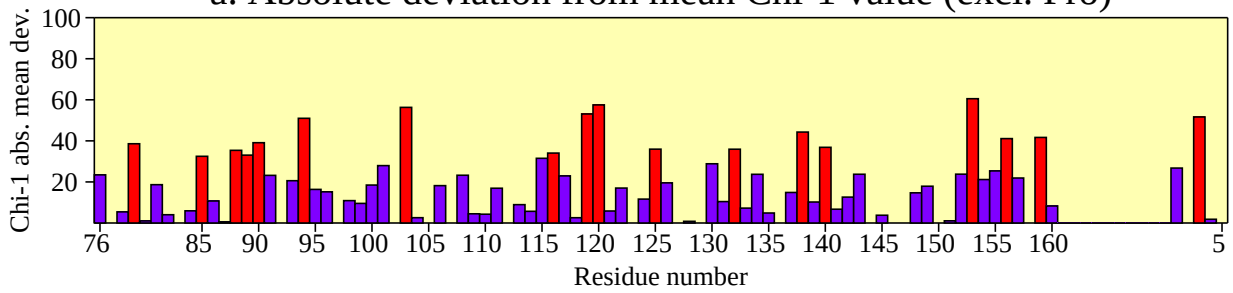


g. G-factors

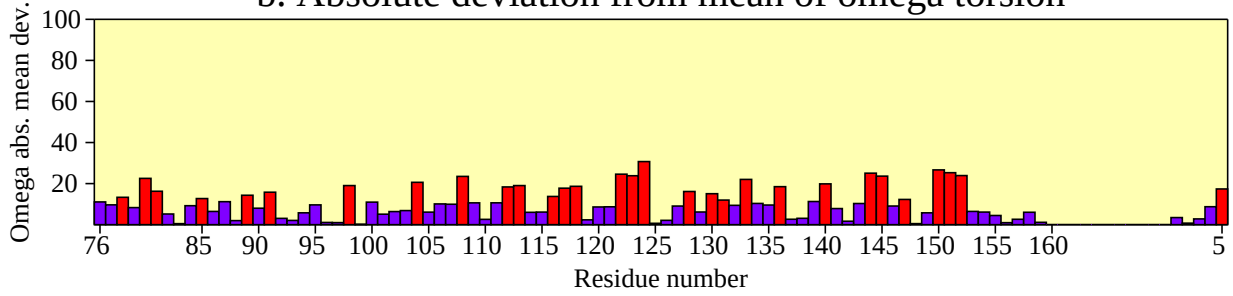


Residue properties
pdb2e76

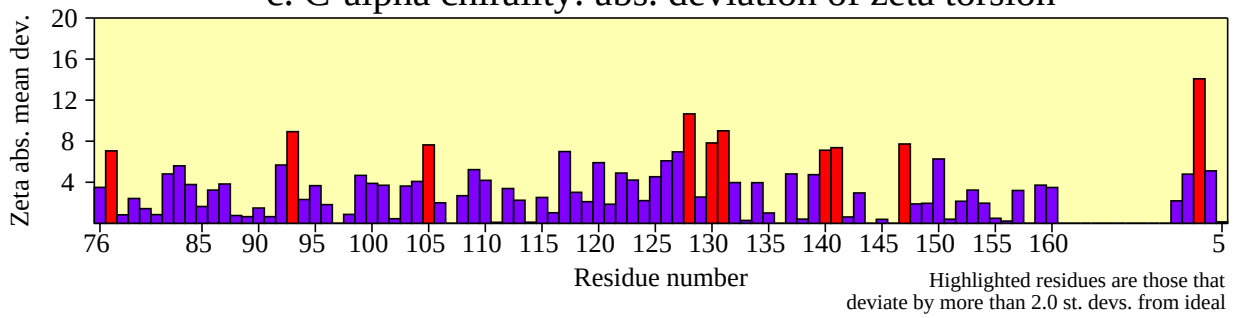
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

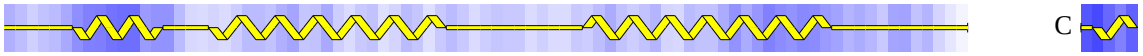


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

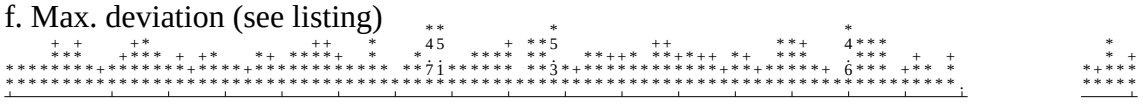


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

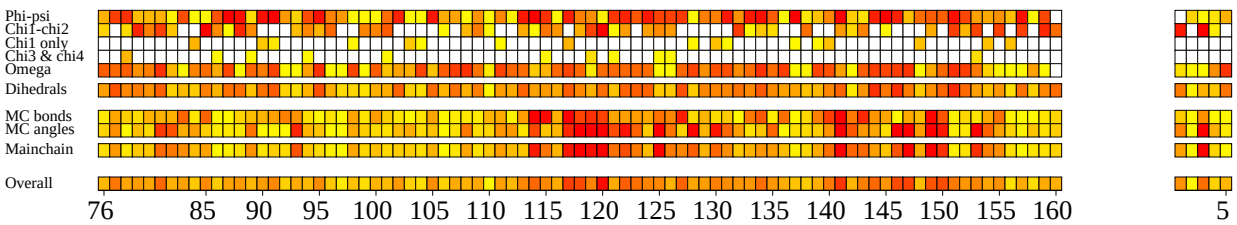
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

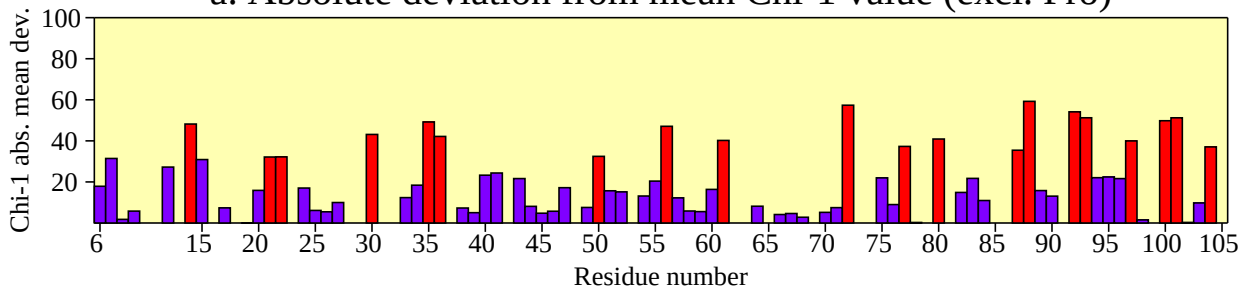


g. G-factors

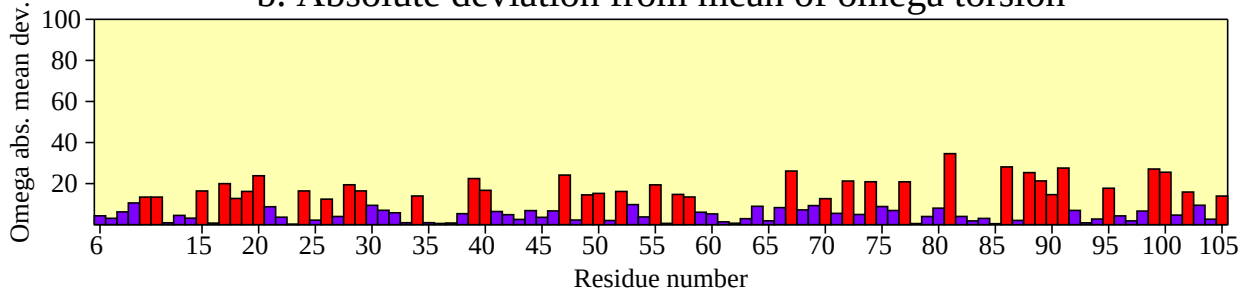


Residue properties
pdb2e76

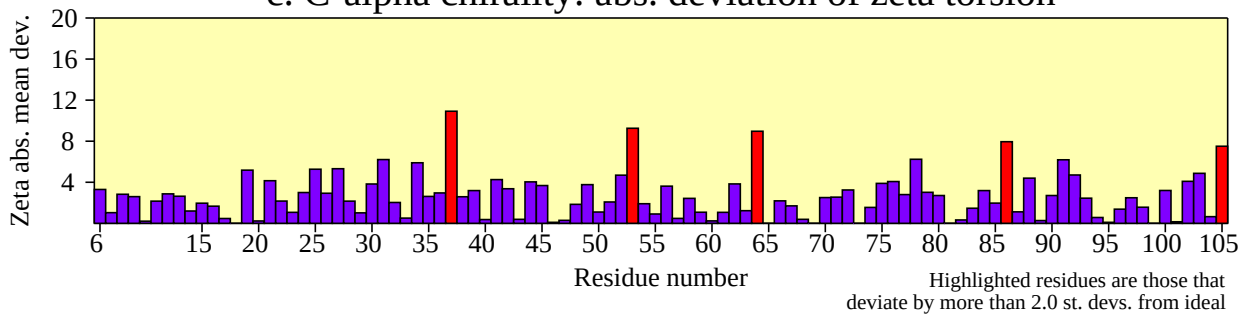
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

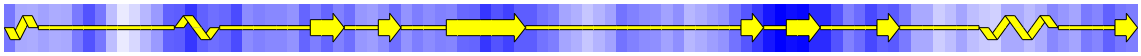


c. C-alpha chirality: abs. deviation of zeta torsion



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

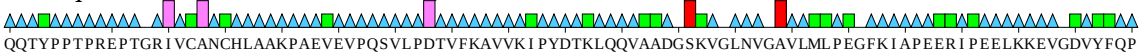
d. Secondary structure & estimated accessibility



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

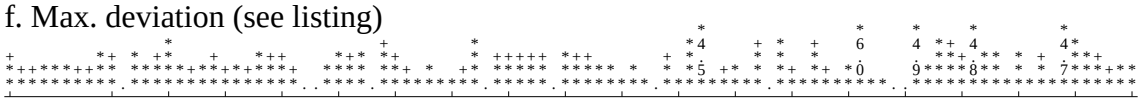
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

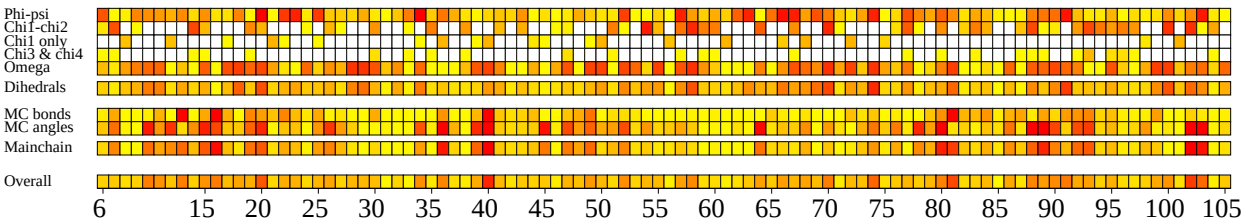


QQTYPPTPREPTGRIVCANCHLAAKPAEVEVPQSVLPDTVFKAVVKIPYDTKLQQVAADGSKVGLNVGAVLMLPEGFKIAPEERIPEELKKEVGDVYFQP

f. Max. deviation (see listing)

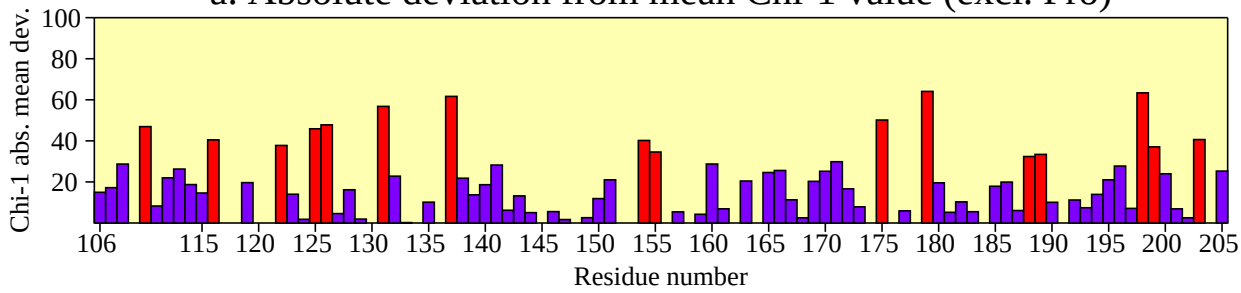


g. G-factors

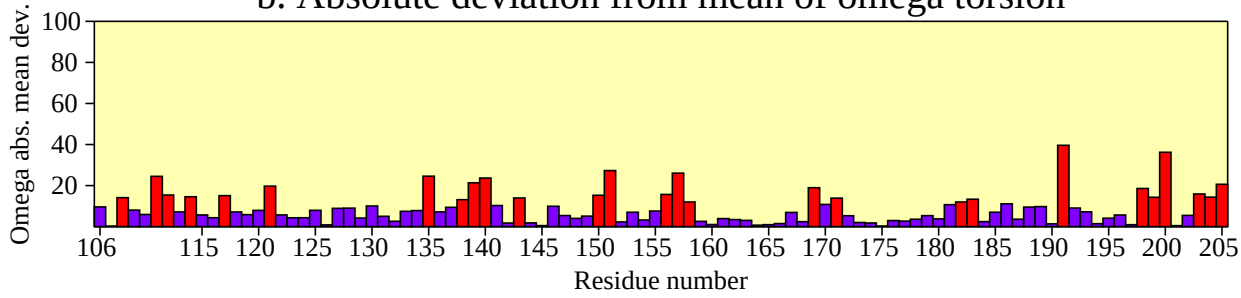


Residue properties
pdb2e76

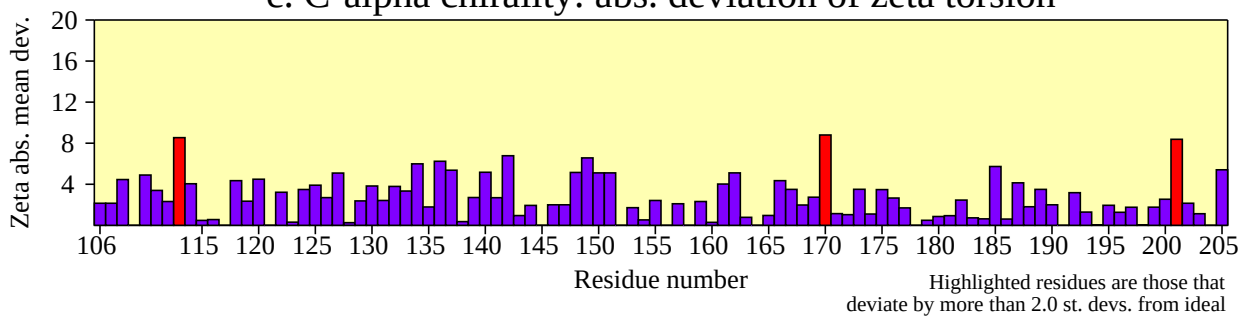
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

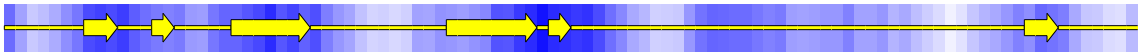


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



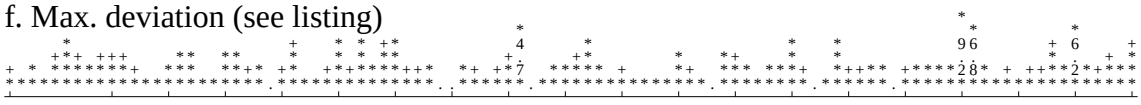
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

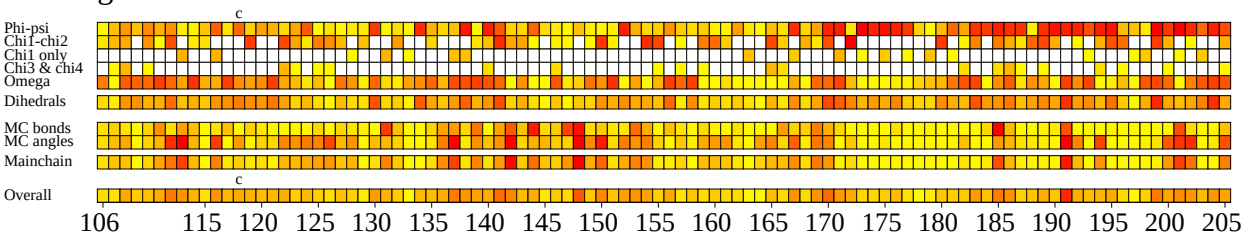
Most favoured Allowed Generous Disallowed

YKEGQDNVLLVGPLPGEQYQE IVFPVLSPNPTTDKN IHFGKYA IHLGANRGRGQ I YPTGEKSNNNVFTASATGT I TK I AKEEDEYGNVKYQVS I QTDSGK

f. Max. deviation (see listing)



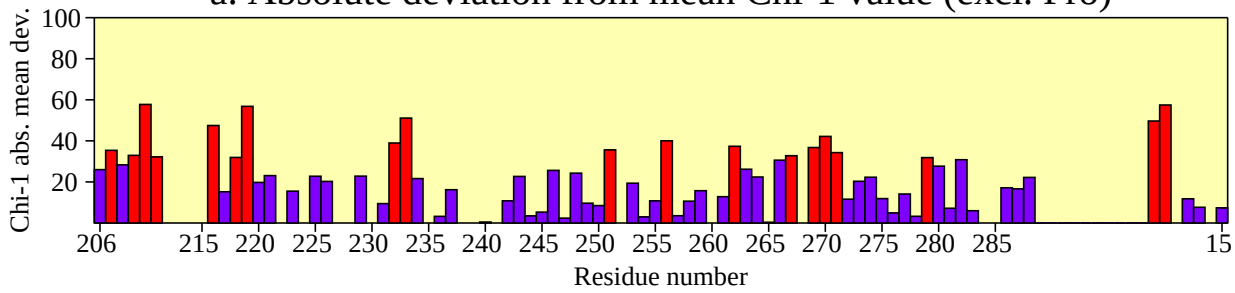
g. G-factors



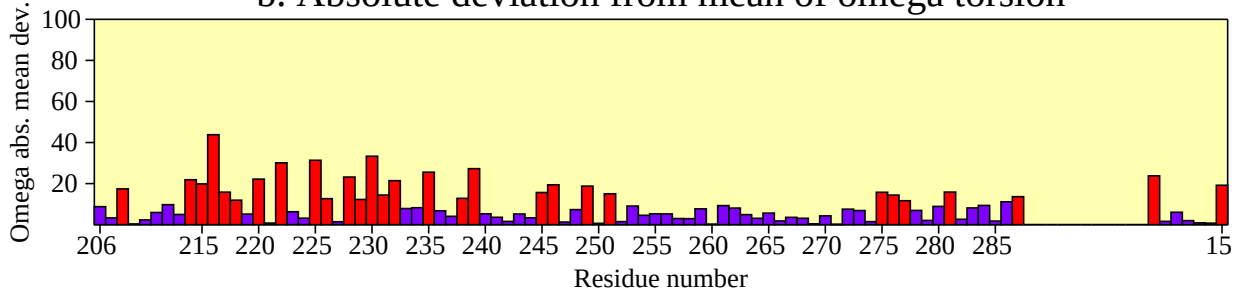
c = cis-peptide

Residue properties
pdb2e76

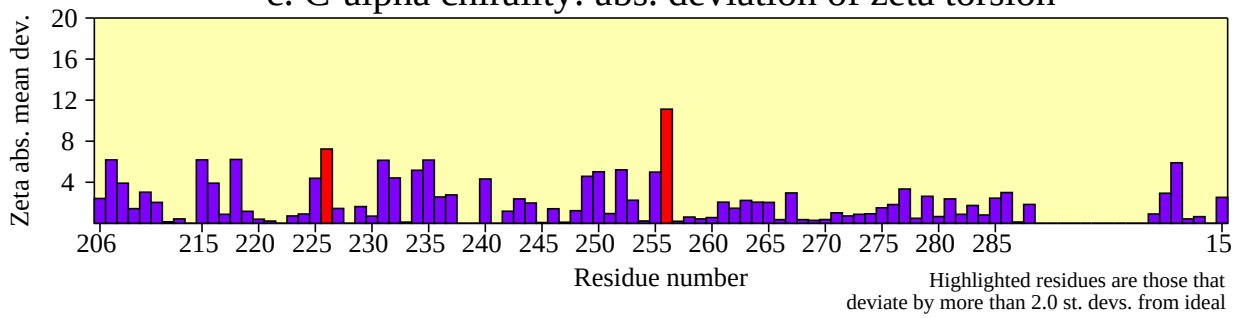
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

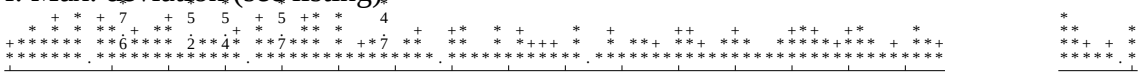
d. Secondary structure & estimated accessibility

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

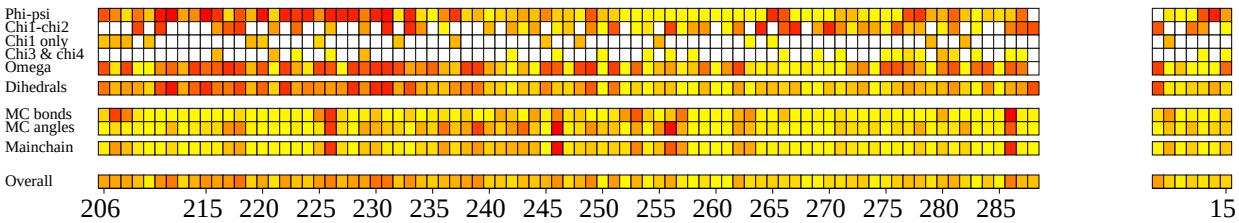
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

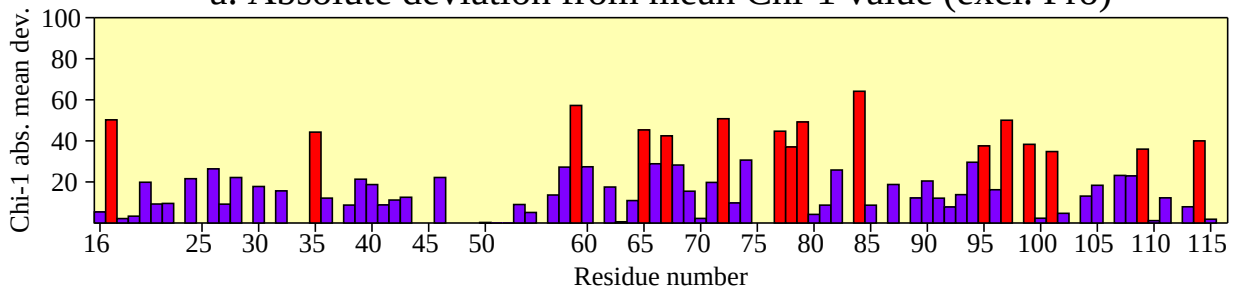


g. G-factors

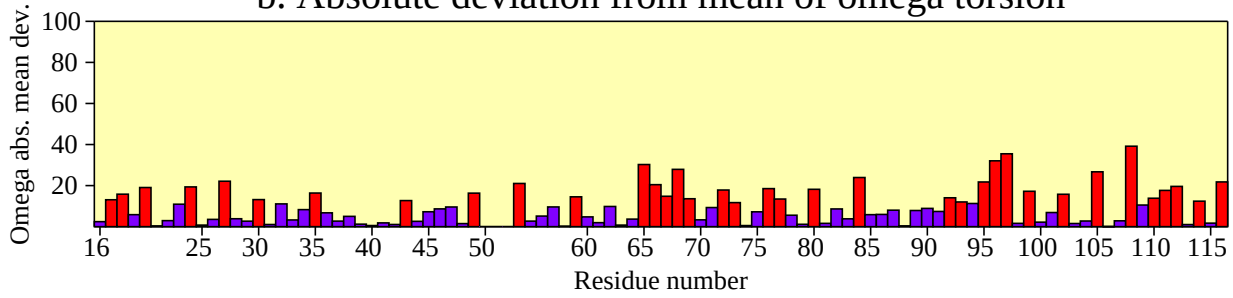


Residue properties
pdb2e76

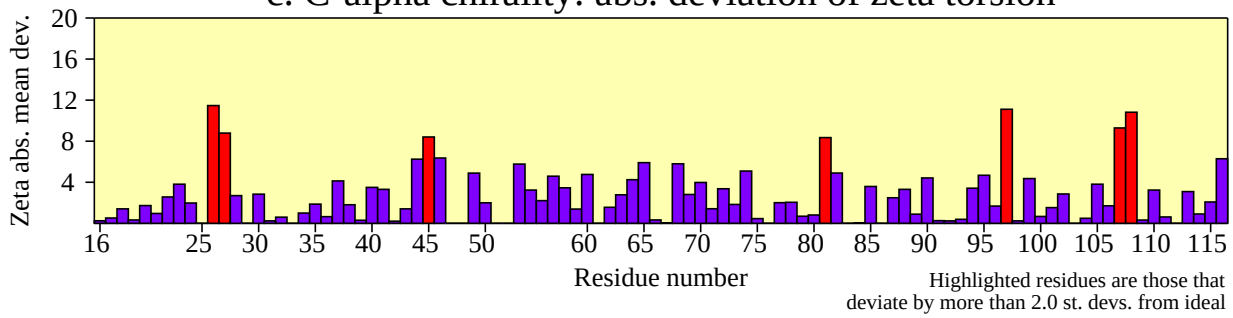
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



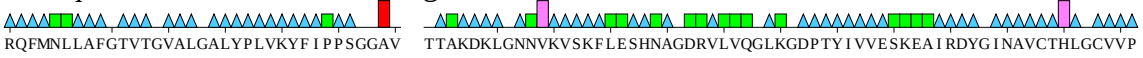
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

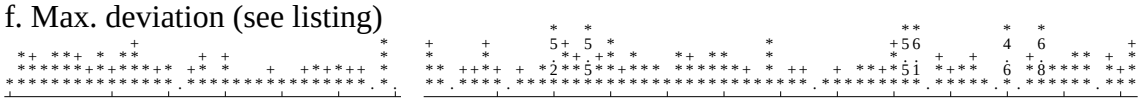
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

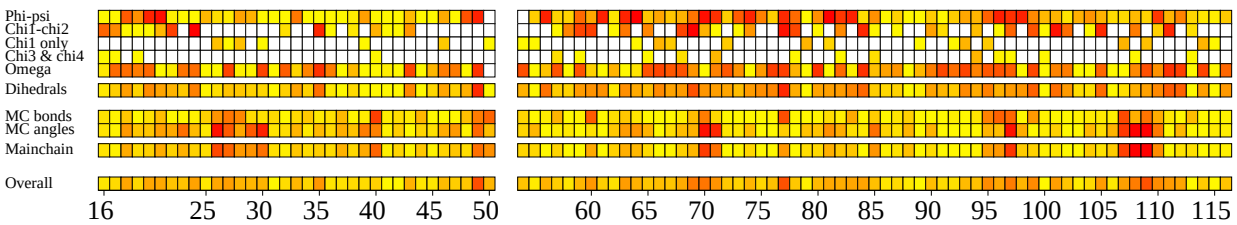
Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

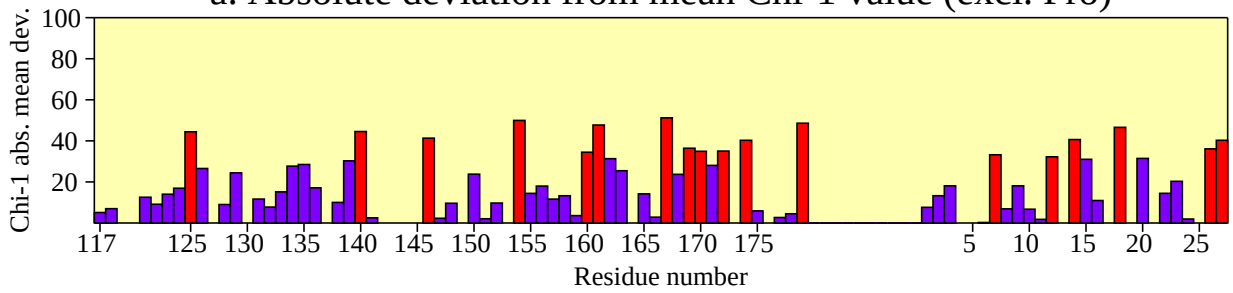


g. G-factors

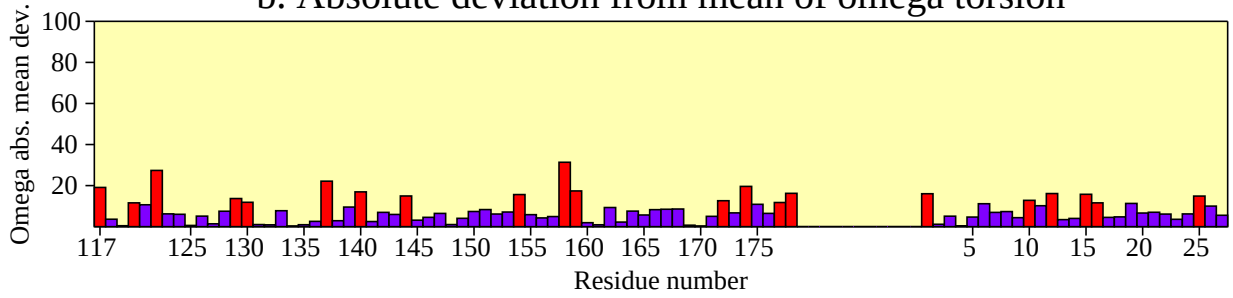


Residue properties
pdb2e76

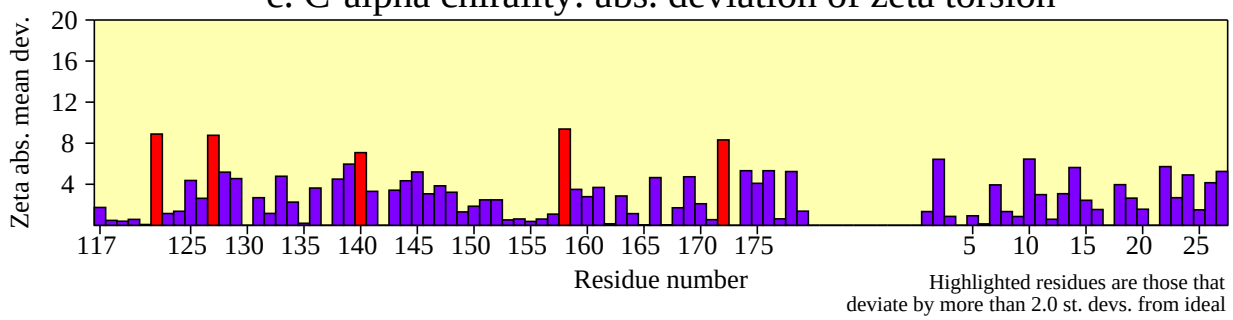
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

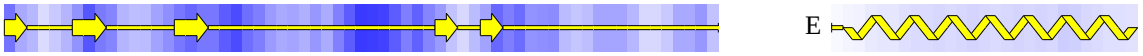


c. C-alpha chirality: abs. deviation of zeta torsion



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

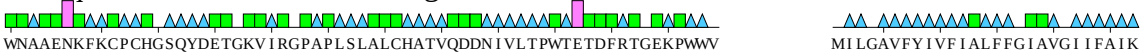
d. Secondary structure & estimated accessibility



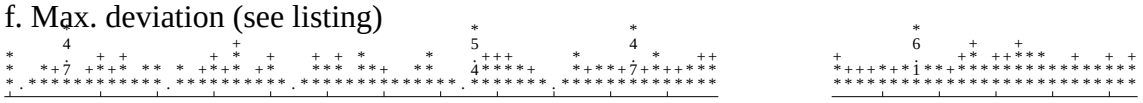
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

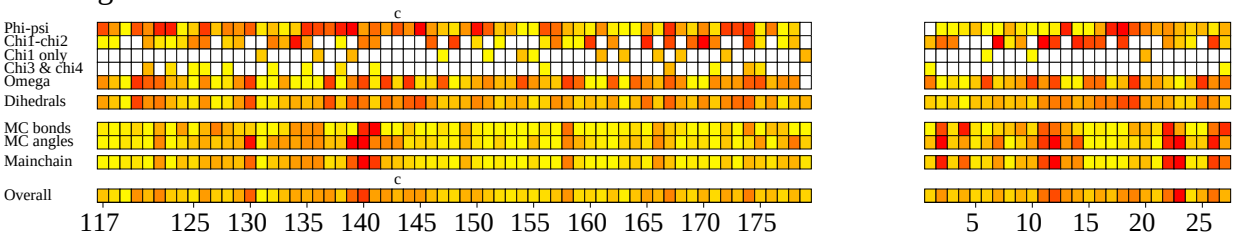
Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



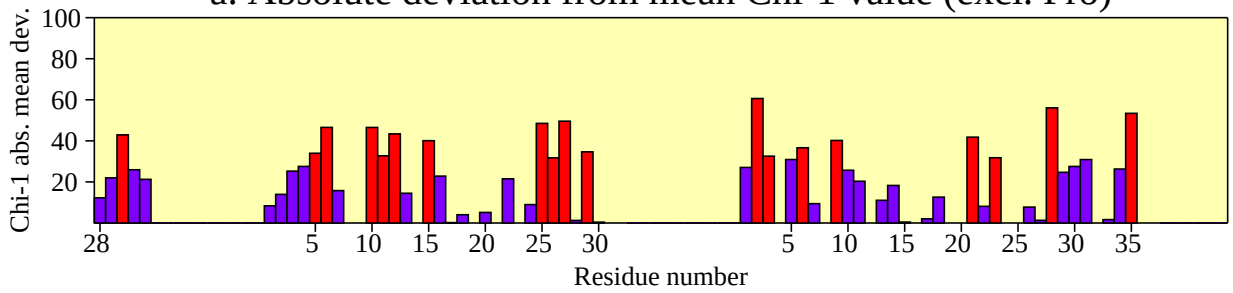
g. G-factors



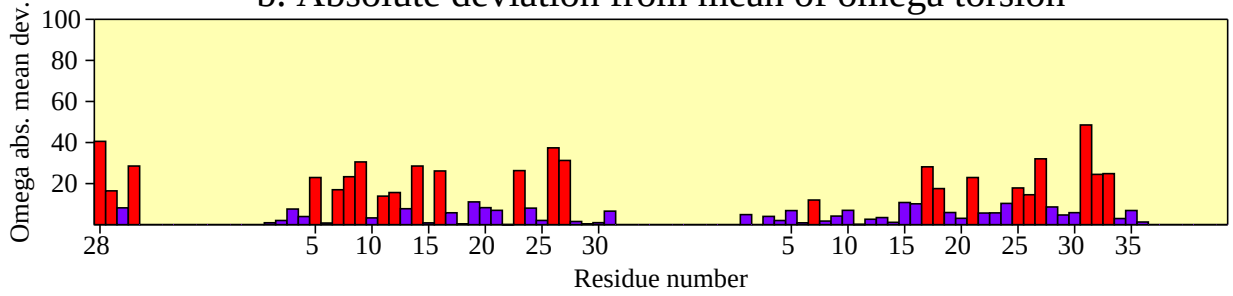
c = cis-peptide

Residue properties
pdb2e76

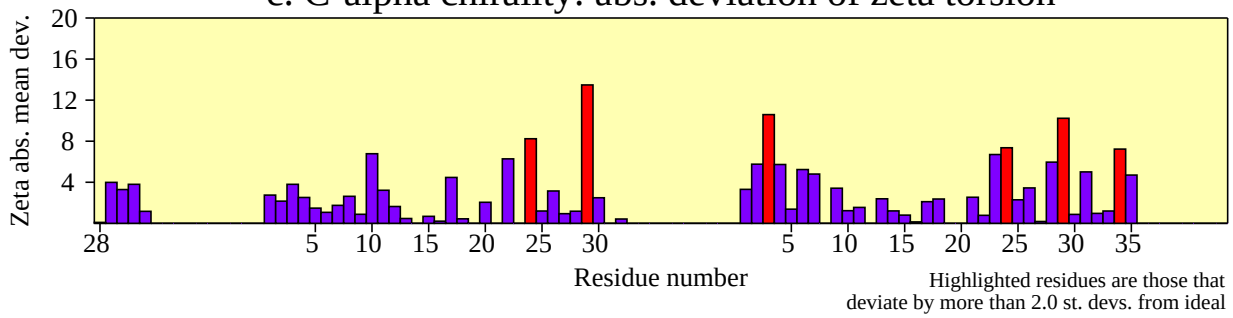
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

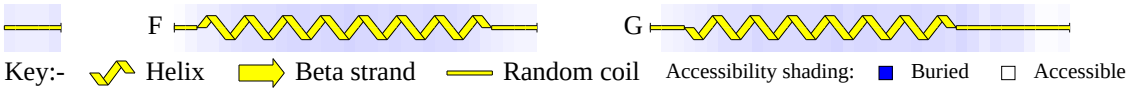


c. C-alpha chirality: abs. deviation of zeta torsion

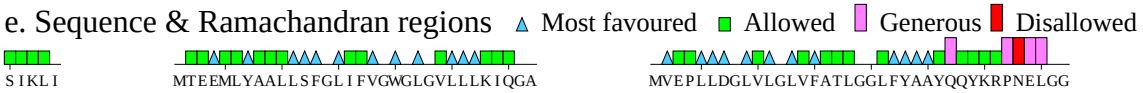


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

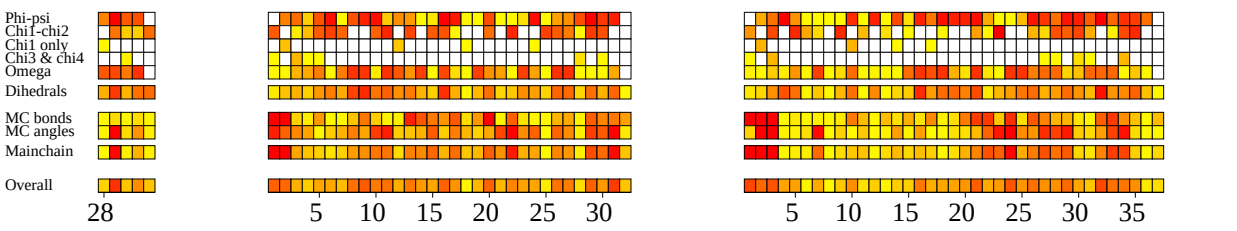


e. Sequence & Ramachandran regions



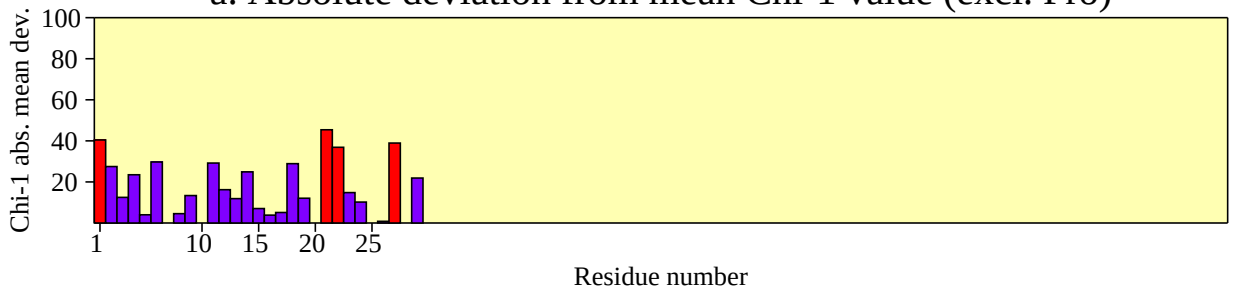
f. Max. deviation (see listing)

g. G-factors

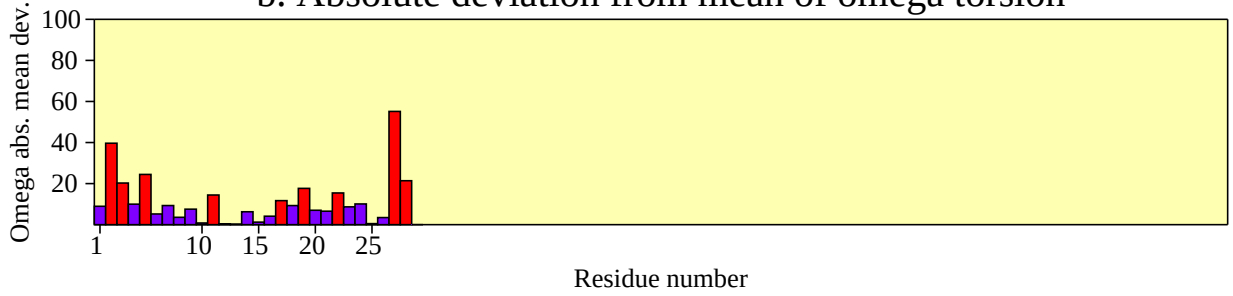


Residue properties
pdb2e76

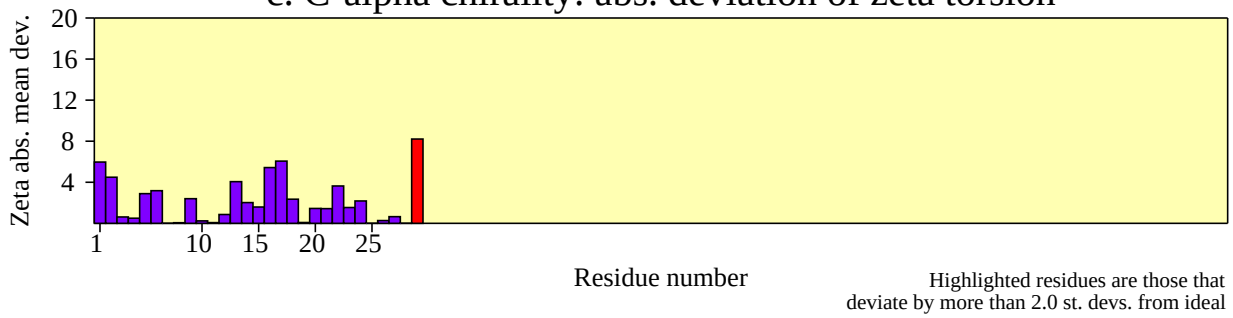
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

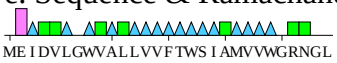


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

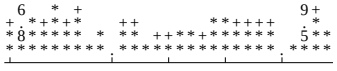
d. Secondary structure & estimated accessibility

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

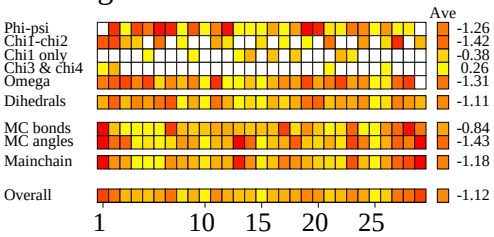
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

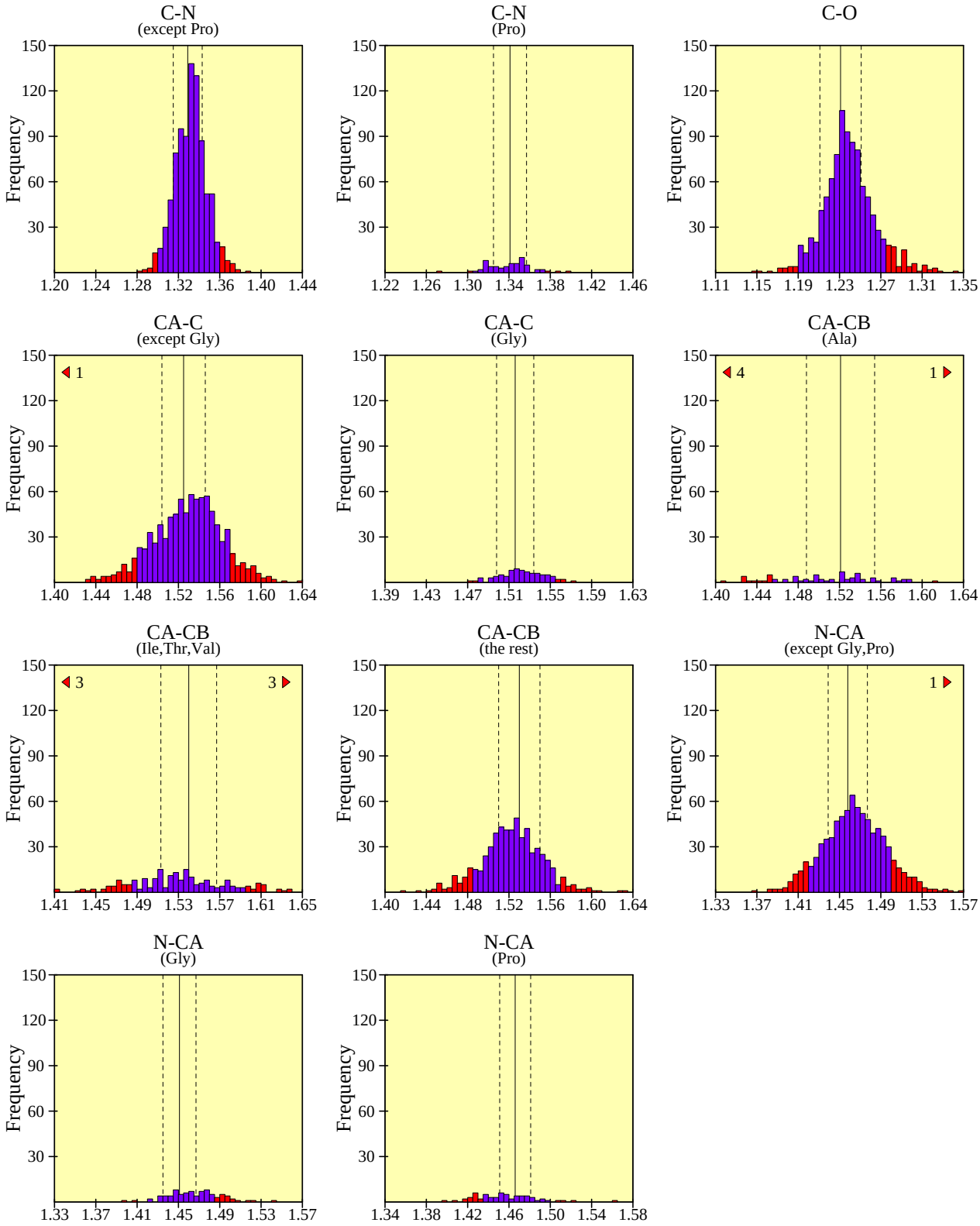


g. G-factors



Main-chain bond lengths

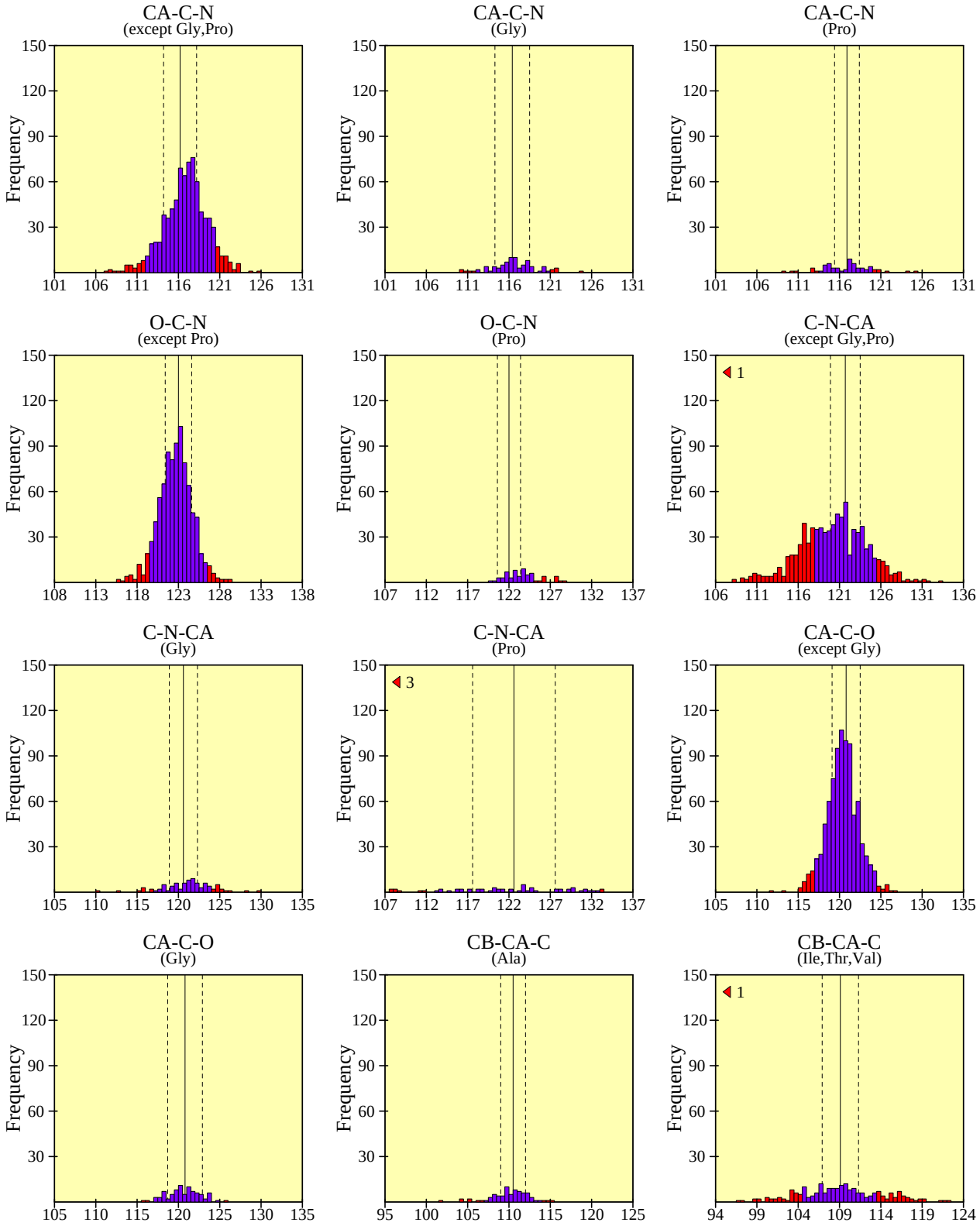
pdb2e76



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

pdb2e76



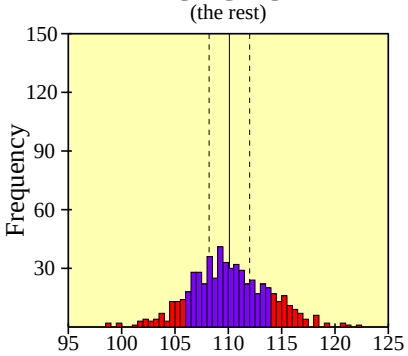
Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

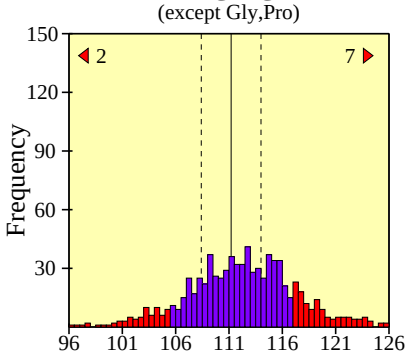
Main-chain bond angles

pdb2e76

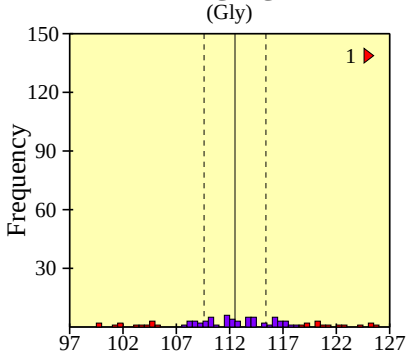
CB-CA-C
(the rest)



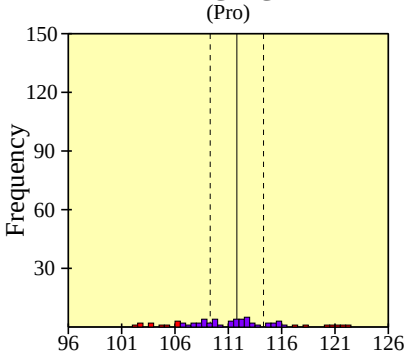
N-CA-C
(except Gly,Pro)



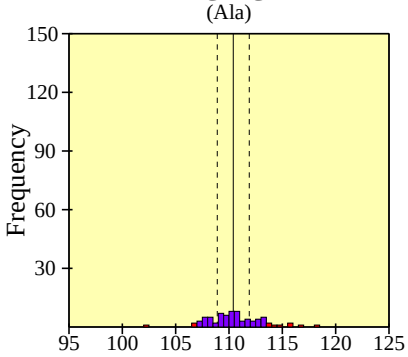
N-CA-C
(Gly)



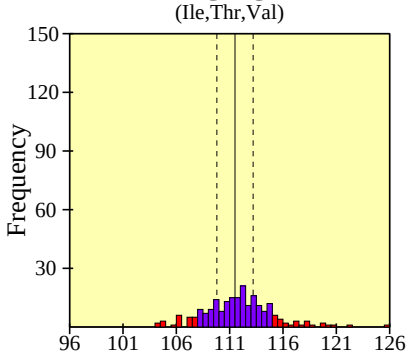
N-CA-C
(Pro)



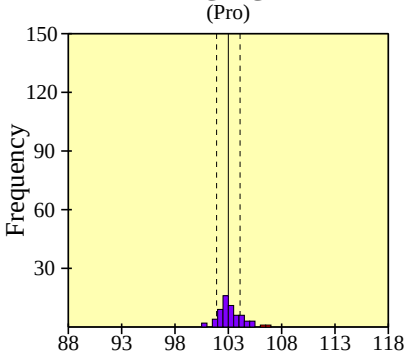
N-CA-CB
(Ala)



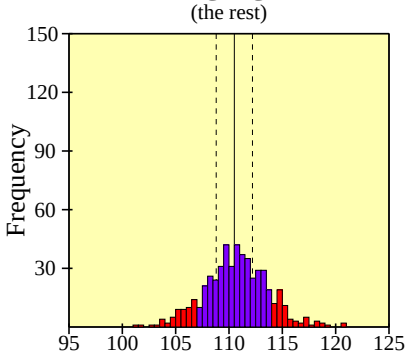
N-CA-CB
(Ile,Thr,Val)



N-CA-CB
(Pro)



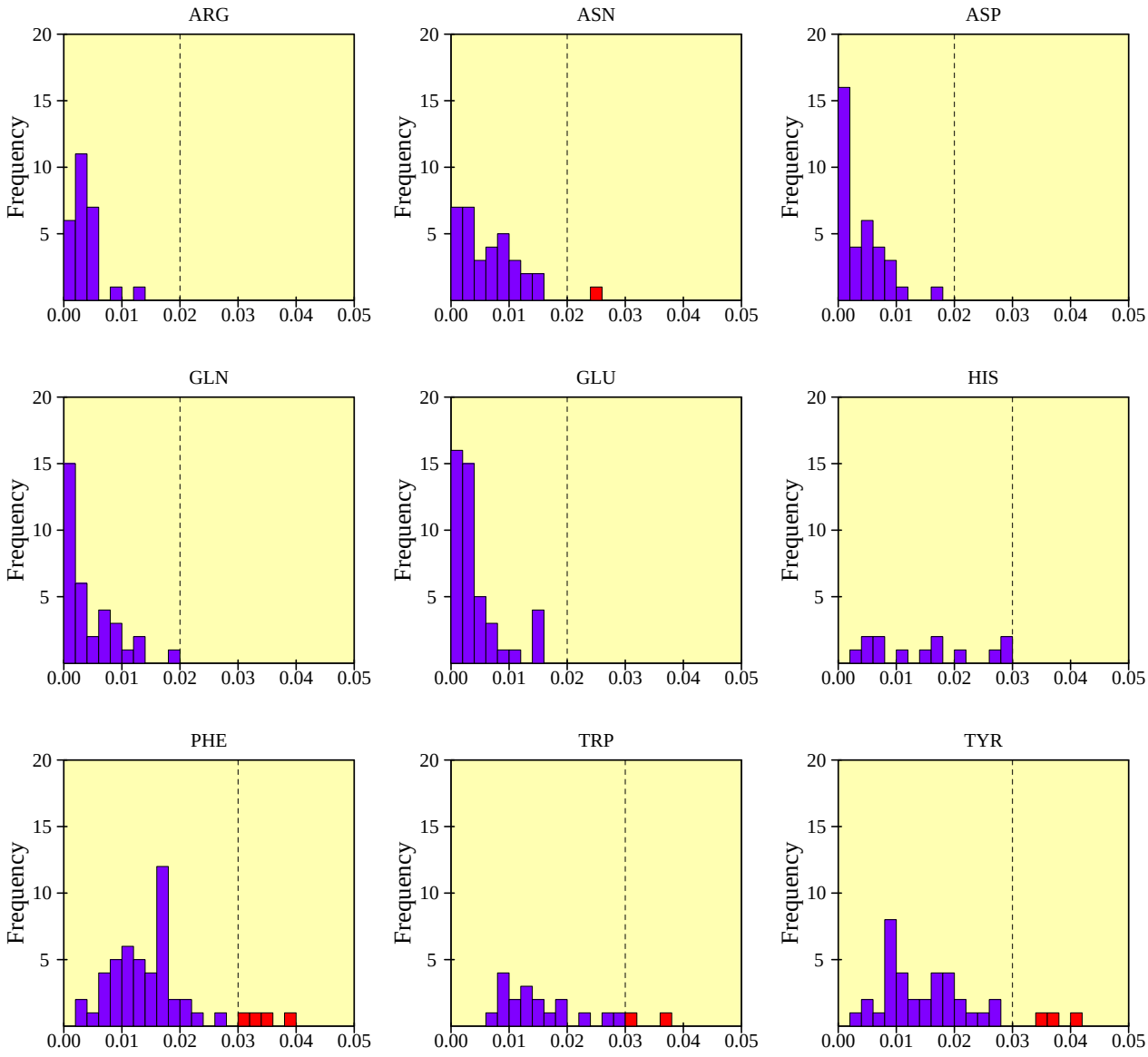
N-CA-CB
(the rest)



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

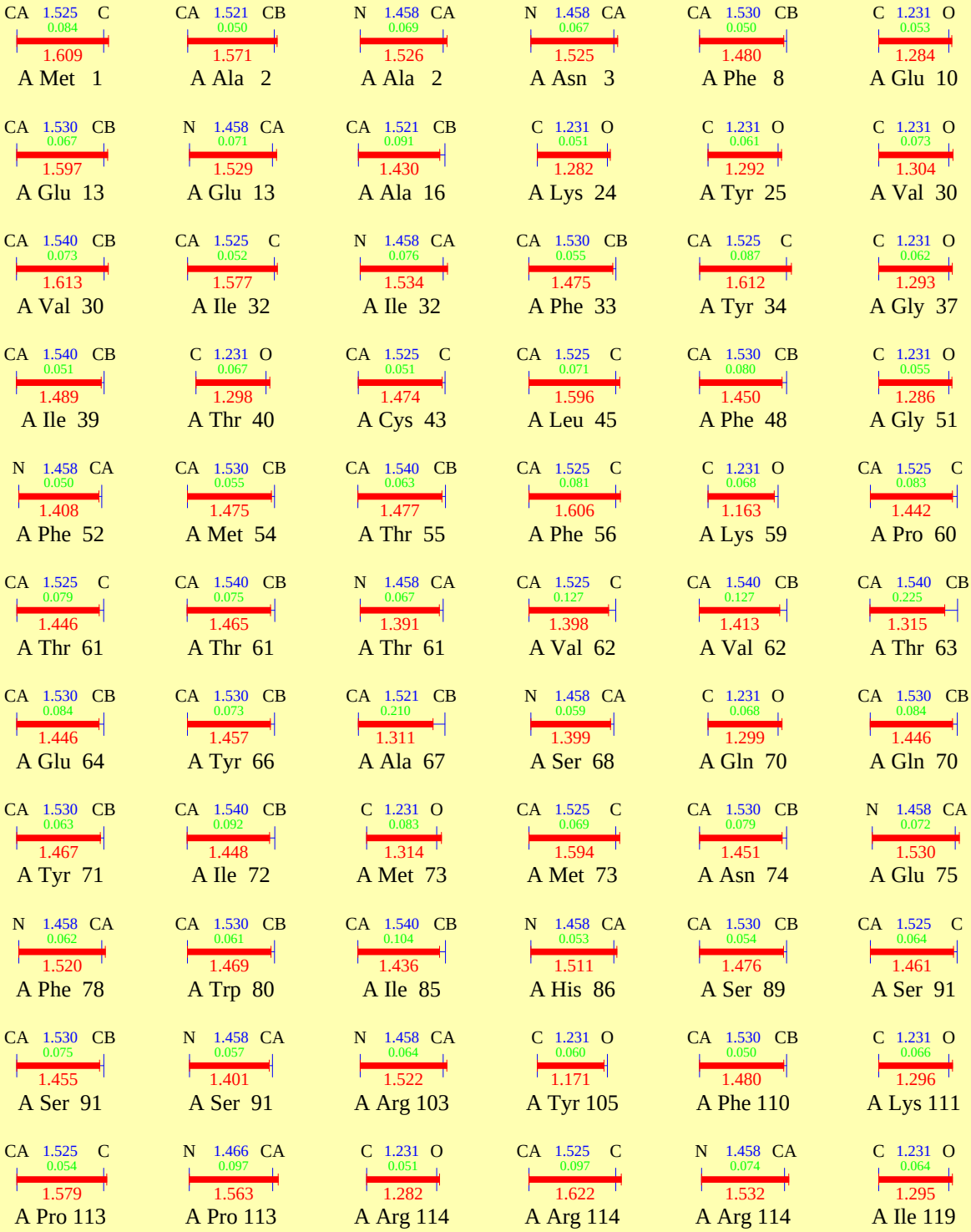
pdb2e76



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
pdb2e76

Main-chain bond lengths



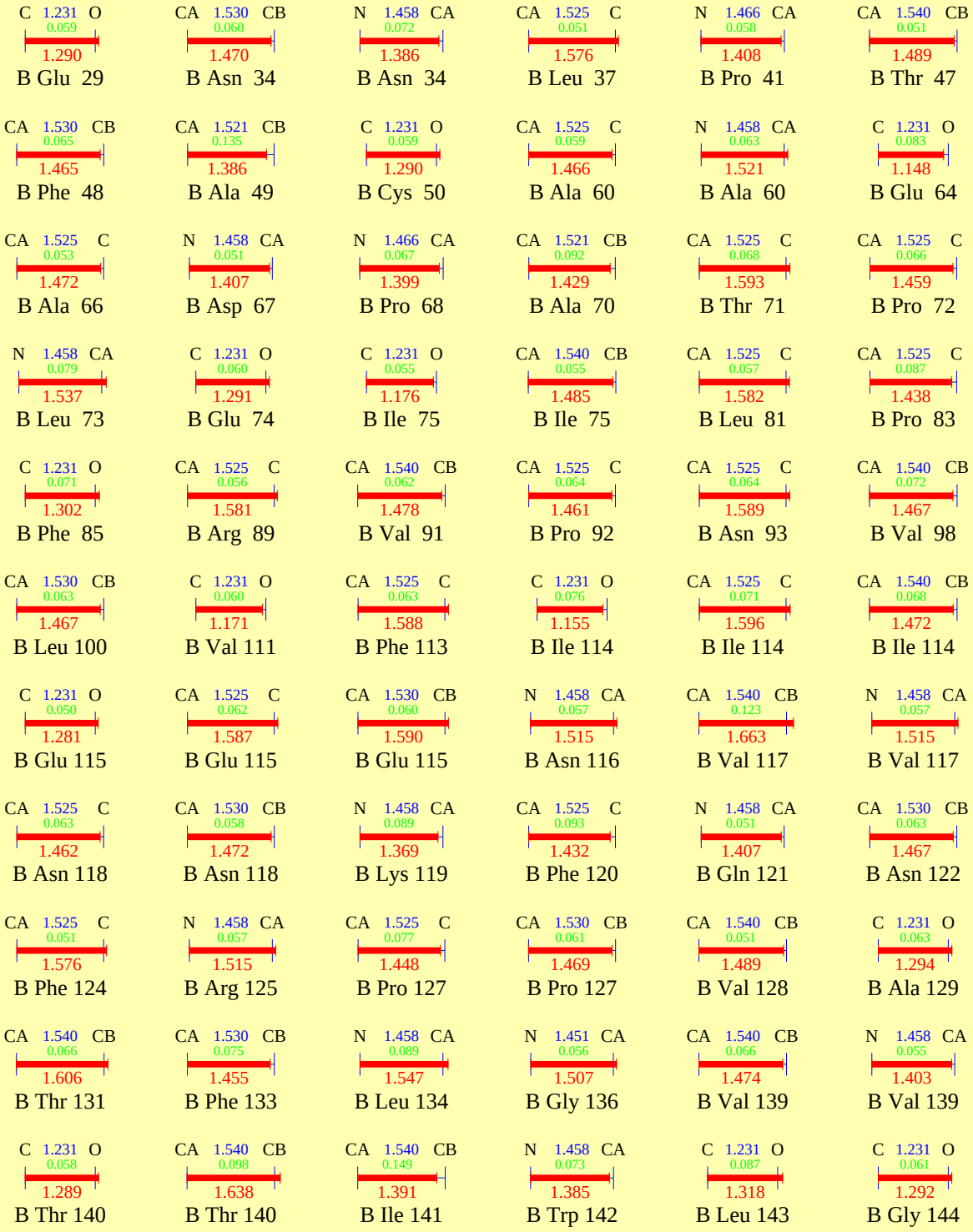
Distorted geometry
pdb2e76

Main-chain bond lengths (contd)

CA 1.525 C 0.076 1.601 A Ile 119
CA 1.540 CB 0.079 1.461 A Ile 119
C 1.231 O 0.087 1.318 A Ser 120
CA 1.525 C 0.081 1.606 A Ser 120
N 1.458 CA 0.051 1.407 A Val 122
C 1.231 O 0.081 1.312 A Ile 123
CA 1.530 CB 0.051 1.479 A Leu 124
CA 1.521 CB 0.072 1.449 A Ala 125
CA 1.540 CB 0.068 1.472 A Ile 127
CA 1.516 C 0.059 1.575 A Gly 132
C 1.231 O 0.053 1.178 A Tyr 136
CA 1.525 C 0.084 1.441 A Tyr 136
CA 1.530 CB 0.060 1.470 A Tyr 136
C 1.231 O 0.054 1.177 A Pro 139
CA 1.525 C 0.058 1.467 A Pro 139
CA 1.530 CB 0.079 1.451 A Pro 139
CA 1.530 CB 0.112 1.418 A Trp 140
N 1.458 CA 0.076 1.382 A Asp 141
C 1.231 O 0.050 1.181 A Tyr 145
CA 1.530 CB 0.089 1.441 A Tyr 145
N 1.458 CA 0.058 1.400 A Tyr 145
CA 1.521 CB 0.051 1.470 A Ala 147
CA 1.540 CB 0.051 1.489 A Val 154
N 1.458 CA 0.074 1.384 A Val 154
CA 1.540 CB 0.052 1.488 A Ile 158
CA 1.540 CB 0.098 1.638 A Val 160
CA 1.525 C 0.052 1.577 A Val 163
CA 1.540 CB 0.061 1.479 A Val 163
CA 1.540 CB 0.109 1.431 A Ile 165
C 1.231 O 0.064 1.295 A Leu 168
CA 1.530 CB 0.055 1.585 A Arg 170
CA 1.530 CB 0.062 1.468 A Ser 173
CA 1.525 C 0.067 1.592 A Ser 174
CA 1.540 CB 0.080 1.460 A Val 175
N 1.451 CA 0.052 1.503 A Gly 176
CA 1.521 CB 0.111 1.410 A Ala 178
C 1.231 O 0.070 1.301 A Thr 179
CA 1.540 CB 0.078 1.462 A Thr 179
C 1.231 O 0.061 1.292 A Tyr 184
CA 1.525 C 0.074 1.451 A Ala 186
CA 1.521 CB 0.163 1.358 A Ala 186
CA 1.530 CB 0.051 1.581 A His 187
CA 1.525 C 0.059 1.465 A Thr 188
N 1.458 CA 0.056 1.513 A Thr 188
CA 1.540 CB 0.073 1.467 A Val 190
C 1.341 N 0.066 1.275 A Leu 191 - A Pro 192
CA 1.530 CB 0.068 1.462 A Phe 198
CA 1.540 CB 0.073 1.467 A Ile 206
N 1.458 CA 0.051 1.407 A Ile 206
CA 1.530 CB 0.068 1.462 A Gln 209
C 1.231 O 0.082 1.313 A Gly 213
C 1.341 N 0.057 1.398 A Gly 213 - A Pro 214
CA 1.525 C 0.068 1.593 A Leu 215
CA 1.521 CB 0.064 1.585 B Ala 2
N 1.458 CA 0.060 1.518 B Leu 4
CA 1.525 C 0.057 1.582 B Ser 10
CA 1.525 C 0.090 1.435 B Pro 12
CA 1.530 CB 0.058 1.472 B Pro 12
C 1.231 O 0.063 1.294 B Lys 13
C 1.231 O 0.063 1.294 B Leu 14
CA 1.521 CB 0.092 1.429 B Ala 16
CA 1.521 CB 0.069 1.452 B Ala 19
C 1.231 O 0.091 1.322 B Lys 20
N 1.458 CA 0.056 1.402 B Met 22
CA 1.530 CB 0.079 1.451 B His 24
CA 1.530 CB 0.052 1.478 B Tyr 26

Distorted geometry
pdb2e76

Main-chain bond lengths (contd)



Distorted geometry
pdb2e76

Main-chain bond lengths (contd)

CA 1.540 CB 0.069 1.470 B Ile 145
C 1.231 O 0.050 1.281 B Ala 147
N 1.458 CA 0.083 1.541 B Phe 149
CA 1.525 C 0.086 1.439 B Pro 150
CA 1.525 C 0.061 1.464 B Leu 155
N 1.458 CA 0.057 1.515 B Leu 155

CA 1.525 C 0.059 1.584 C Phe 3
CA 1.530 CB 0.055 1.585 C Phe 3
CA 1.530 CB 0.052 1.582 C Pro 11
C 1.231 O 0.053 1.284 C Pro 13
CA 1.525 C 0.077 1.602 C Pro 13
N 1.458 CA 0.062 1.520 C Glu 15

C 1.231 O 0.113 1.344 C Pro 16
CA 1.540 CB 0.081 1.459 C Thr 17
CA 1.525 C 0.058 1.467 C Val 21
CA 1.525 C 0.085 1.610 C Cys 22
CA 1.525 C 0.065 1.590 C Ala 23
CA 1.525 C 0.071 1.454 C Cys 25

CA 1.521 CB 0.054 1.467 C Ala 29
C 1.231 O 0.059 1.172 C Val 36
CA 1.525 C 0.053 1.578 C Ser 39
CA 1.525 C 0.088 1.437 C Val 40
CA 1.540 CB 0.137 1.403 C Val 40
N 1.458 CA 0.063 1.395 C Val 40

CA 1.521 CB 0.086 1.435 C Ala 48
CA 1.540 CB 0.102 1.438 C Val 49
CA 1.540 CB 0.054 1.486 C Ile 52
CA 1.540 CB 0.057 1.483 C Val 72
CA 1.525 C 0.066 1.591 C Glu 80
N 1.451 CA 0.092 1.543 C Gly 81

C 1.231 O 0.054 1.285 C Lys 83
CA 1.540 CB 0.091 1.449 C Ile 84
CA 1.521 CB 0.051 1.572 C Ala 85
CA 1.525 C 0.058 1.467 C Pro 86
CA 1.525 C 0.056 1.469 C Glu 87
N 1.466 CA 0.050 1.416 C Pro 91

N 1.458 CA 0.056 1.402 C Glu 92
CA 1.525 C 0.054 1.471 C Glu 93
N 1.451 CA 0.052 1.399 C Gly 99
CA 1.530 CB 0.058 1.472 C Tyr 102
CA 1.525 C 0.056 1.469 C Asp 111
CA 1.540 CB 0.065 1.475 C Val 113

CA 1.525 C 0.051 1.474 C Leu 114
C 1.231 O 0.052 1.283 C Gly 117
CA 1.530 CB 0.052 1.478 C Leu 119
CA 1.525 C 0.086 1.439 C Val 131
CA 1.540 CB 0.071 1.610 C Val 131
CA 1.540 CB 0.072 1.612 C Thr 137

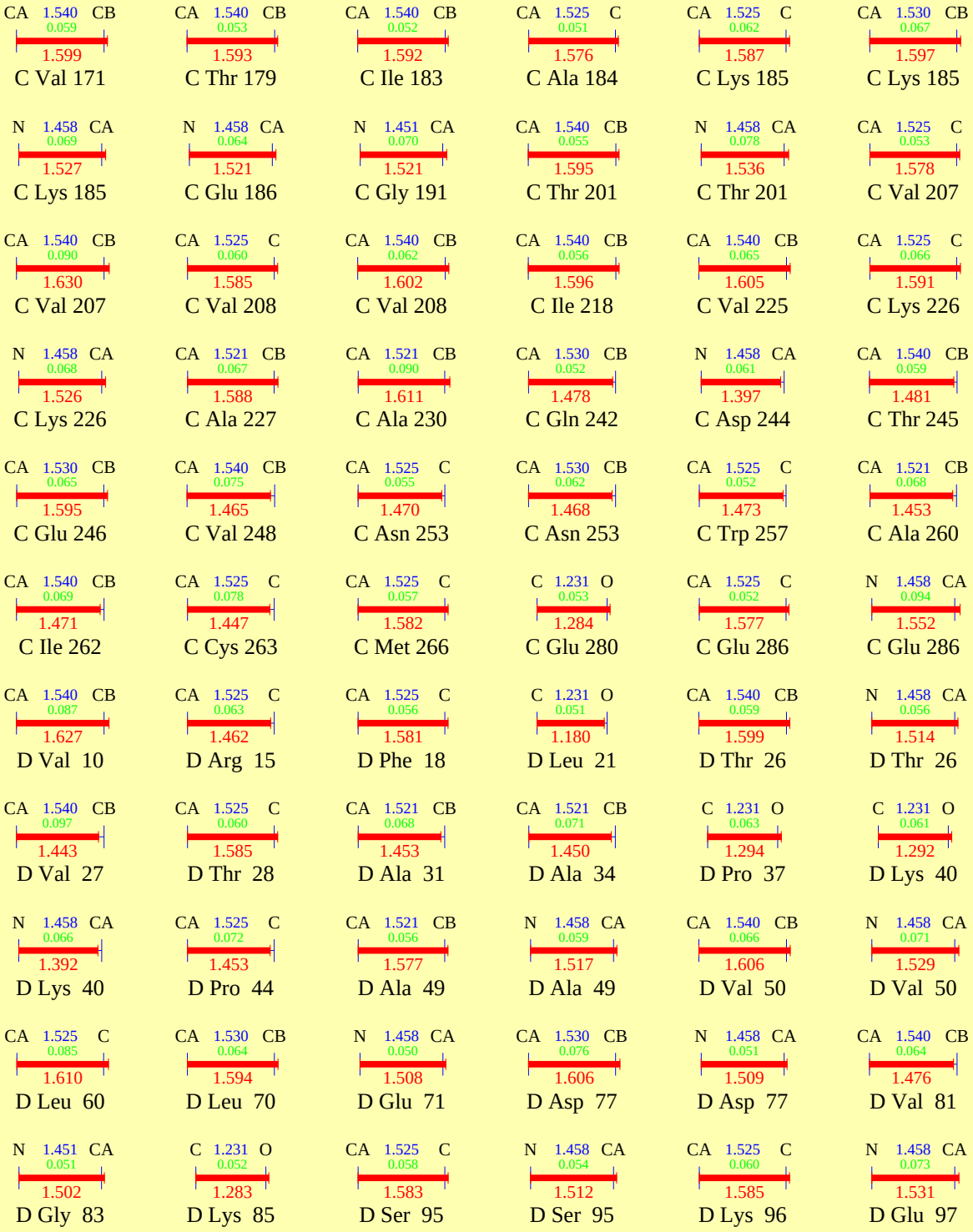
CA 1.530 CB 0.052 1.478 C Asp 139
N 1.458 CA 0.057 1.515 C Asn 141
C 1.231 O 0.070 1.301 C Ile 142
CA 1.540 CB 0.066 1.474 C Ile 142
CA 1.525 C 0.068 1.457 C His 143
CA 1.530 CB 0.097 1.433 C Phe 144

C 1.231 O 0.092 1.323 C Tyr 147
CA 1.521 CB 0.141 1.380 C Ala 148
N 1.458 CA 0.063 1.521 C Ala 148
CA 1.540 CB 0.058 1.482 C Ile 149
CA 1.525 C 0.059 1.466 C His 150
CA 1.525 C 0.062 1.463 C Ala 153

N 1.458 CA 0.059 1.517 C Ala 153
CA 1.525 C 0.070 1.455 C Asn 154
N 1.458 CA 0.061 1.519 C Lys 166
CA 1.525 C 0.053 1.472 C Ser 167
CA 1.525 C 0.064 1.461 C Asn 169
N 1.458 CA 0.054 1.512 C Asn 170

Distorted geometry
pdb2e76

Main-chain bond lengths (contd)



Distorted geometry
pdb2e76

Main-chain bond lengths (contd)

CA 1.540 CB 0.072 1.612 D Ile 99
CA 1.540 CB 0.128 1.412 D Val 107
CA 1.525 C 0.069 1.456 D Thr 109
N 1.458 CA 0.052 1.406 D Thr 109
CA 1.525 C 0.056 1.469 D Cys 113
CA 1.525 C 0.057 1.468 D Ala 120

N 1.458 CA 0.056 1.514 D Asn 122
CA 1.525 C 0.059 1.584 D Cys 126
CA 1.525 C 0.076 1.449 D Pro 127
CA 1.525 C 0.063 1.588 D Cys 128
CA 1.525 C 0.059 1.466 D His 129
N 1.458 CA 0.067 1.525 D Asp 134

CA 1.525 C 0.067 1.592 D Glu 135
CA 1.525 C 0.059 1.584 D Thr 136
N 1.458 CA 0.054 1.512 D Thr 136
CA 1.525 C 0.074 1.599 D Ile 140
N 1.458 CA 0.108 1.566 D Arg 141
CA 1.521 CB 0.050 1.571 D Ala 144

CA 1.521 CB 0.062 1.459 D Ala 149
N 1.458 CA 0.052 1.510 D Ala 149
CA 1.525 C 0.073 1.598 D Asp 158
CA 1.540 CB 0.072 1.612 D Thr 166
N 1.458 CA 0.053 1.511 D Glu 167
CA 1.540 CB 0.068 1.608 D Thr 172

CA 1.525 C 0.073 1.598 D Glu 174
N 1.458 CA 0.059 1.517 D Trp 177
C 1.231 O 0.080 1.311 E Ile 2
CA 1.540 CB 0.065 1.605 E Ile 2
C 1.231 O 0.091 1.322 E Gly 4
CA 1.521 CB 0.066 1.455 E Ala 5

C 1.231 O 0.053 1.284 E Phe 7
C 1.231 O 0.051 1.282 E Ile 9
CA 1.540 CB 0.068 1.472 E Ile 9
C 1.231 O 0.054 1.285 E Phe 11
C 1.231 O 0.072 1.303 E Ile 12
CA 1.521 CB 0.096 1.425 E Ala 13

CA 1.521 CB 0.088 1.433 E Ala 19
CA 1.540 CB 0.056 1.596 E Ile 22
C 1.329 N 0.058 1.387 E Ile 22 - E Ile 23
N 1.458 CA 0.063 1.521 E Ile 23
CA 1.540 CB 0.088 1.628 E Ile 26
CA 1.530 CB 0.074 1.604 E Lys 27

N 1.458 CA 0.060 1.518 E Lys 27
CA 1.540 CB 0.066 1.606 E Ile 29
CA 1.525 C 0.056 1.469 E Leu 31
CA 1.525 C 0.111 1.636 F Met 1
N 1.458 CA 0.064 1.522 F Met 1
CA 1.540 CB 0.141 1.681 F Thr 2

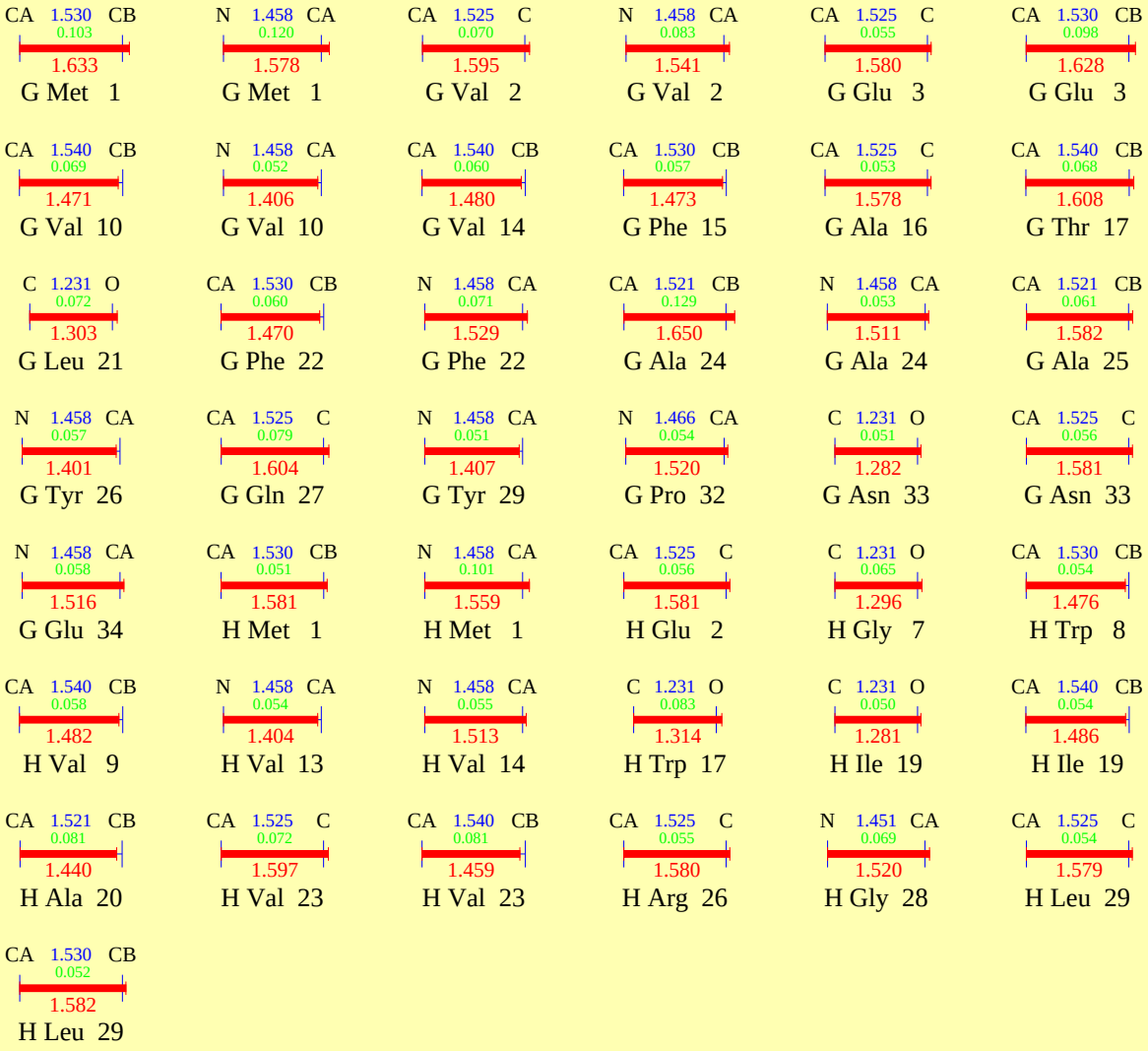
N 1.458 CA 0.093 1.551 F Thr 2
CA 1.530 CB 0.057 1.587 F Glu 3
CA 1.530 CB 0.073 1.457 F Met 5
CA 1.521 CB 0.067 1.454 F Ala 8
CA 1.525 C 0.065 1.590 F Ala 9
CA 1.525 C 0.066 1.591 F Phe 13

CA 1.530 CB 0.064 1.466 F Phe 13
C 1.231 O 0.078 1.309 F Gly 14
C 1.231 O 0.063 1.294 F Ile 16
CA 1.530 CB 0.066 1.464 F Phe 17
C 1.231 O 0.061 1.292 F Gly 19
C 1.231 O 0.096 1.327 F Trp 20

CA 1.525 C 0.068 1.593 F Leu 22
CA 1.525 C 0.066 1.459 F Leu 27
CA 1.540 CB 0.123 1.663 F Ile 29
CA 1.525 C 0.071 1.454 F Gln 30
CA 1.521 CB 0.062 1.583 F Ala 32
N 1.458 CA 0.051 1.509 F Ala 32

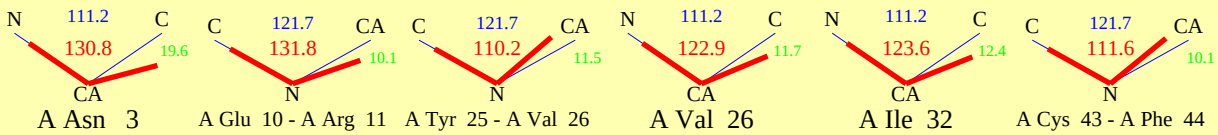
Distorted geometry
pdb2e76

Main-chain bond lengths (contd)



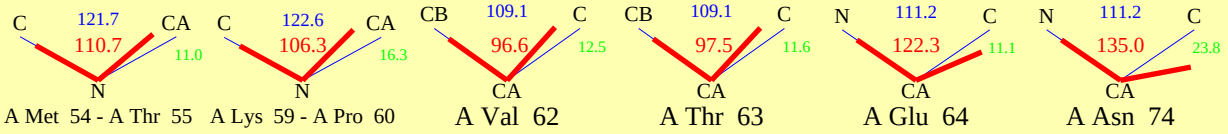
Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

Main-chain bond angles

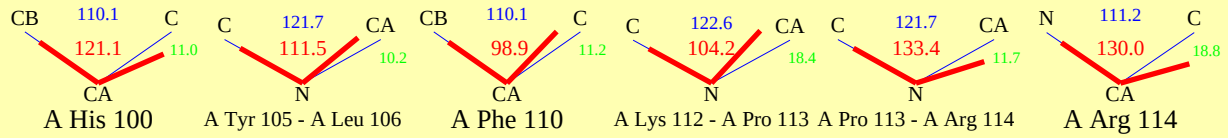


Distorted geometry
pdb2e76

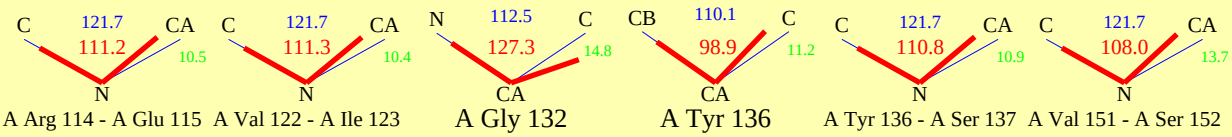
Main-chain bond angles (contd)



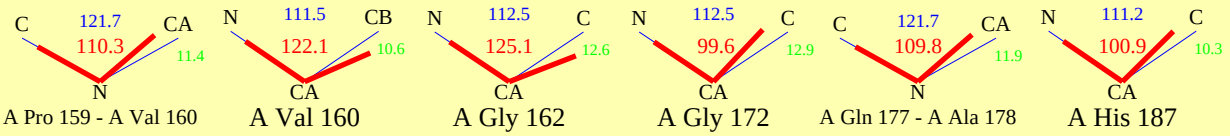
A Met 54 - A Thr 55 | A Lys 59 - A Pro 60 | A Val 62 | A Thr 63 | A Glu 64 | A Asn 74



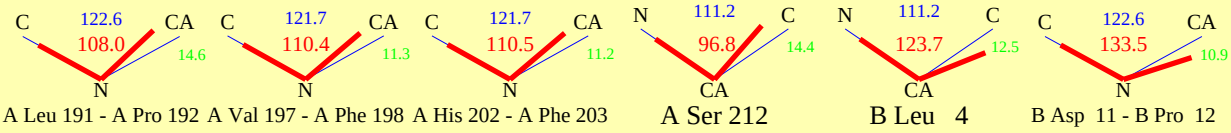
A His 100 | A Tyr 105 - A Leu 106 | A Phe 110 | A Lys 112 - A Pro 113 | A Pro 113 - A Arg 114 | A Arg 114



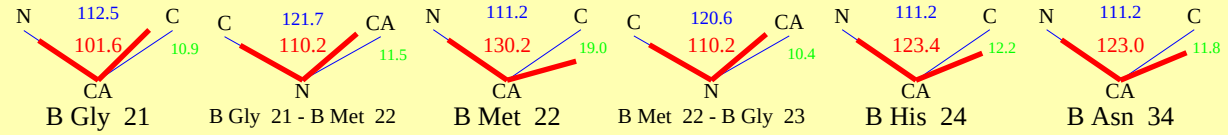
A Arg 114 - A Glu 115 | A Val 122 - A Ile 123 | A Gly 132 | A Tyr 136 | A Tyr 136 - A Ser 137 | A Val 151 - A Ser 152



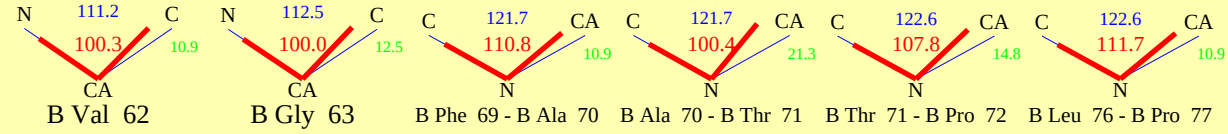
A Pro 159 - A Val 160 | A Val 160 | A Gly 162 | A Gly 172 | A Gln 177 - A Ala 178 | A His 187



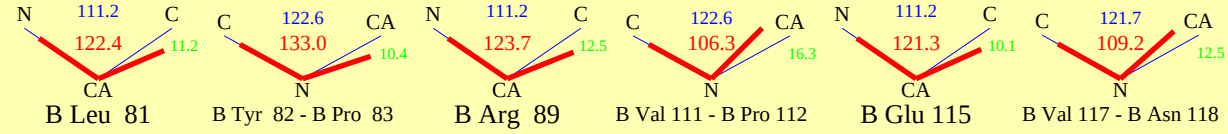
A Leu 191 - A Pro 192 | A Val 197 - A Phe 198 | A His 202 - A Phe 203 | A Ser 212 | B Leu 4 | B Asp 11 - B Pro 12



B Gly 21 | B Gly 21 - B Met 22 | B Met 22 | B Met 22 - B Gly 23 | B His 24 | B Asn 34



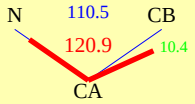
B Val 62 | B Gly 63 | B Phe 69 - B Ala 70 | B Ala 70 - B Thr 71 | B Thr 71 - B Pro 72 | B Leu 76 - B Pro 77



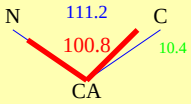
B Leu 81 | B Tyr 82 - B Pro 83 | B Arg 89 | B Val 111 - B Pro 112 | B Glu 115 | B Val 117 - B Asn 118

Distorted geometry
pdb2e76

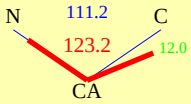
Main-chain bond angles (contd)



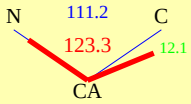
B Phe 120



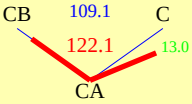
B Gln 121



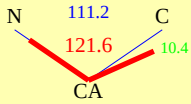
B Asn 122



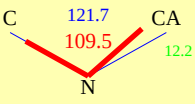
B Arg 125



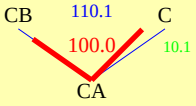
B Thr 130



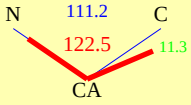
B Ile 141



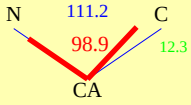
B Gly 146 - B Ala 147



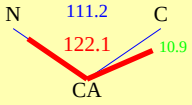
B Phe 149



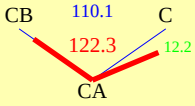
B Phe 149



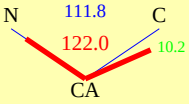
B Lys 153



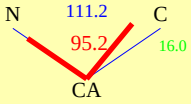
B Thr 154



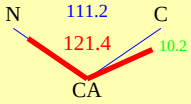
C Phe 3



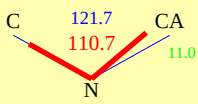
C Pro 10



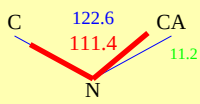
C Val 36



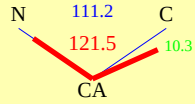
C Ser 39



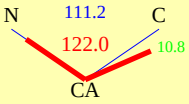
C Ser 39 - C Val 40



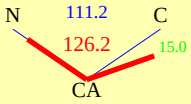
C Leu 41 - C Pro 42



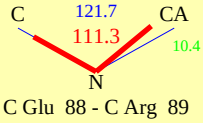
C Lys 51



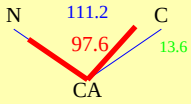
C Leu 70



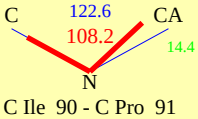
C Glu 80



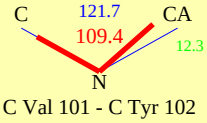
C Glu 88 - C Arg 89



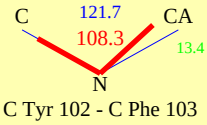
C Ile 90



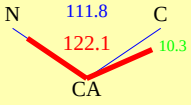
C Ile 90 - C Pro 91



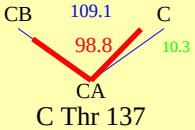
C Val 101 - C Tyr 102



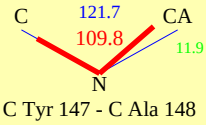
C Tyr 102 - C Phe 103



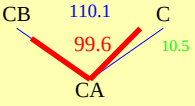
C Pro 118



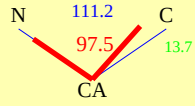
C Thr 137



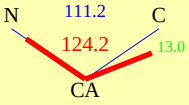
C Tyr 147 - C Ala 148



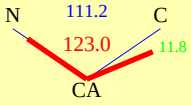
C His 150



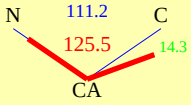
C Ser 167



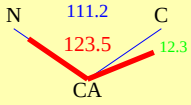
C Asn 192



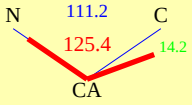
C Lys 194



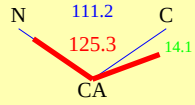
C Gln 200



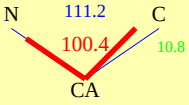
C Thr 201



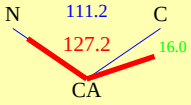
C Asp 202



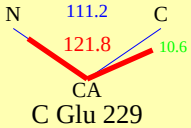
C Lys 205



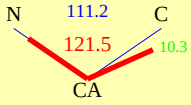
C Leu 217



C Lys 226



C Glu 229



C Asn 234

C Gly 239

C Glu 246

C Leu 249

C Glu 286

D Val 27

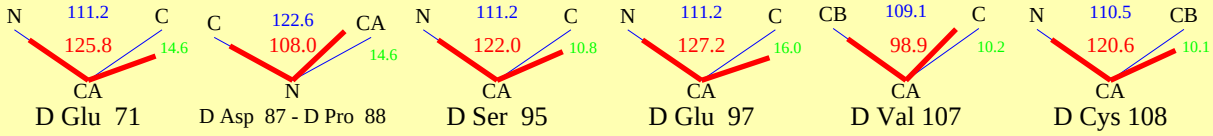
D Gly 29 - D Val 30

D Asn 63

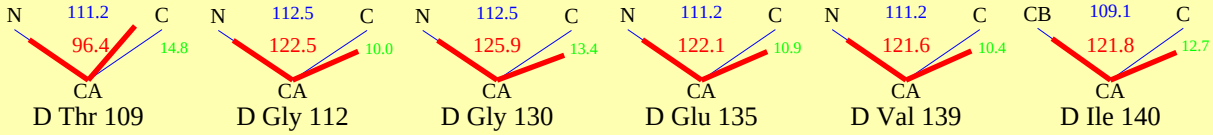
D Leu 70

Distorted geometry
pdb2e76

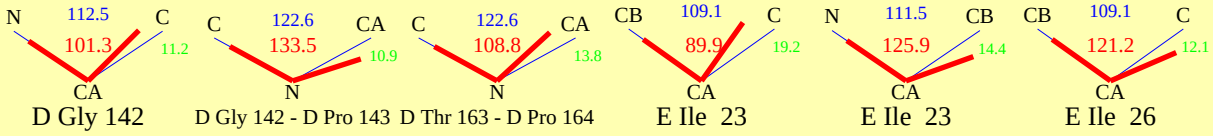
Main-chain bond angles (contd)



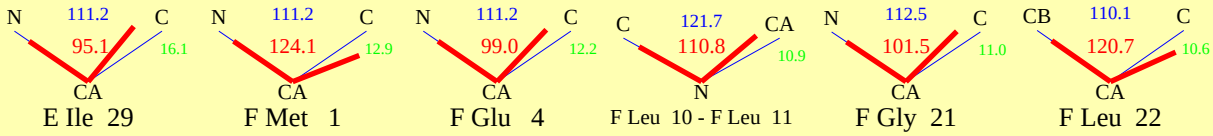
D Glu 71 | D Asp 87 - D Pro 88 | D Ser 95 | D Glu 97 | D Val 107 | D Cys 108



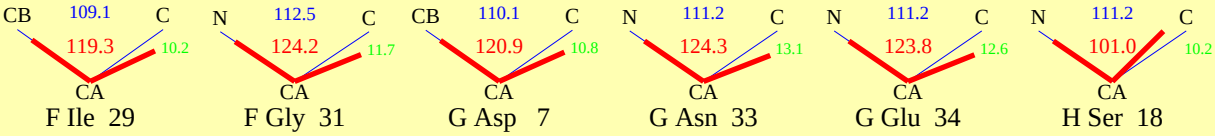
D Thr 109 | D Gly 112 | D Gly 130 | D Glu 135 | D Val 139 | D Ile 140



D Gly 142 | D Gly 142 - D Pro 143 | D Thr 163 - D Pro 164 | E Ile 23 | E Ile 23 | E Ile 26



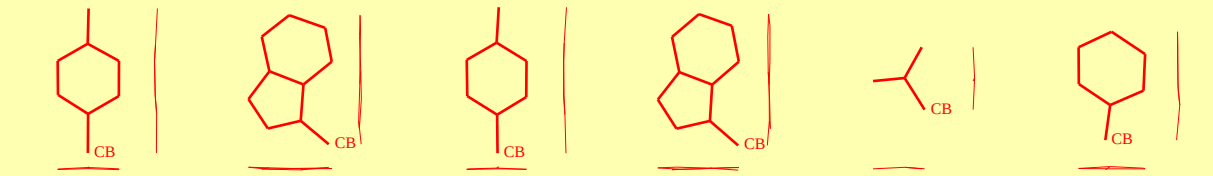
E Ile 29 | F Met 1 | F Glu 4 | F Leu 10 - F Leu 11 | F Gly 21 | F Leu 22



F Ile 29 | F Gly 31 | G Asp 7 | G Asn 33 | G Glu 34 | H Ser 18

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

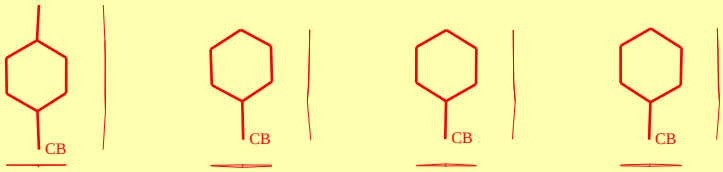
Planar groups



0.038 A Tyr 57 | 0.031 A Trp 140 | 0.041 A Tyr 184 | 0.038 A Trp 193 | 0.026 B Asn 34 | 0.035 B Phe 40

Distorted geometry
pdb2e76

Planar groups (contd)



0.035 B Tyr 80 | 0.038 B Phe 149 | 0.031 D Phe 124 | 0.033 G Phe 22

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