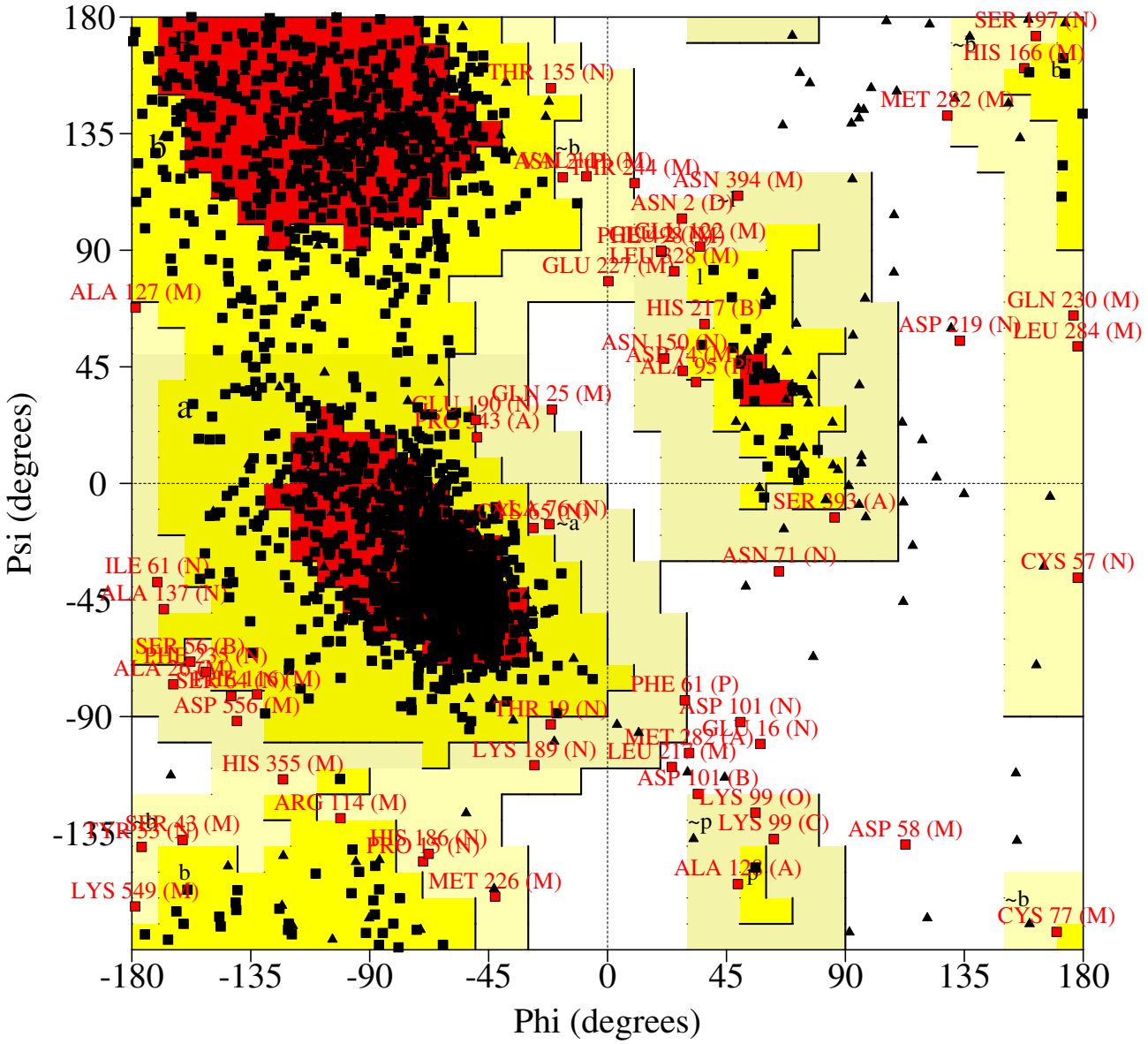
PROCHECK

Ramachandran Plot

2b76



Plot statistics

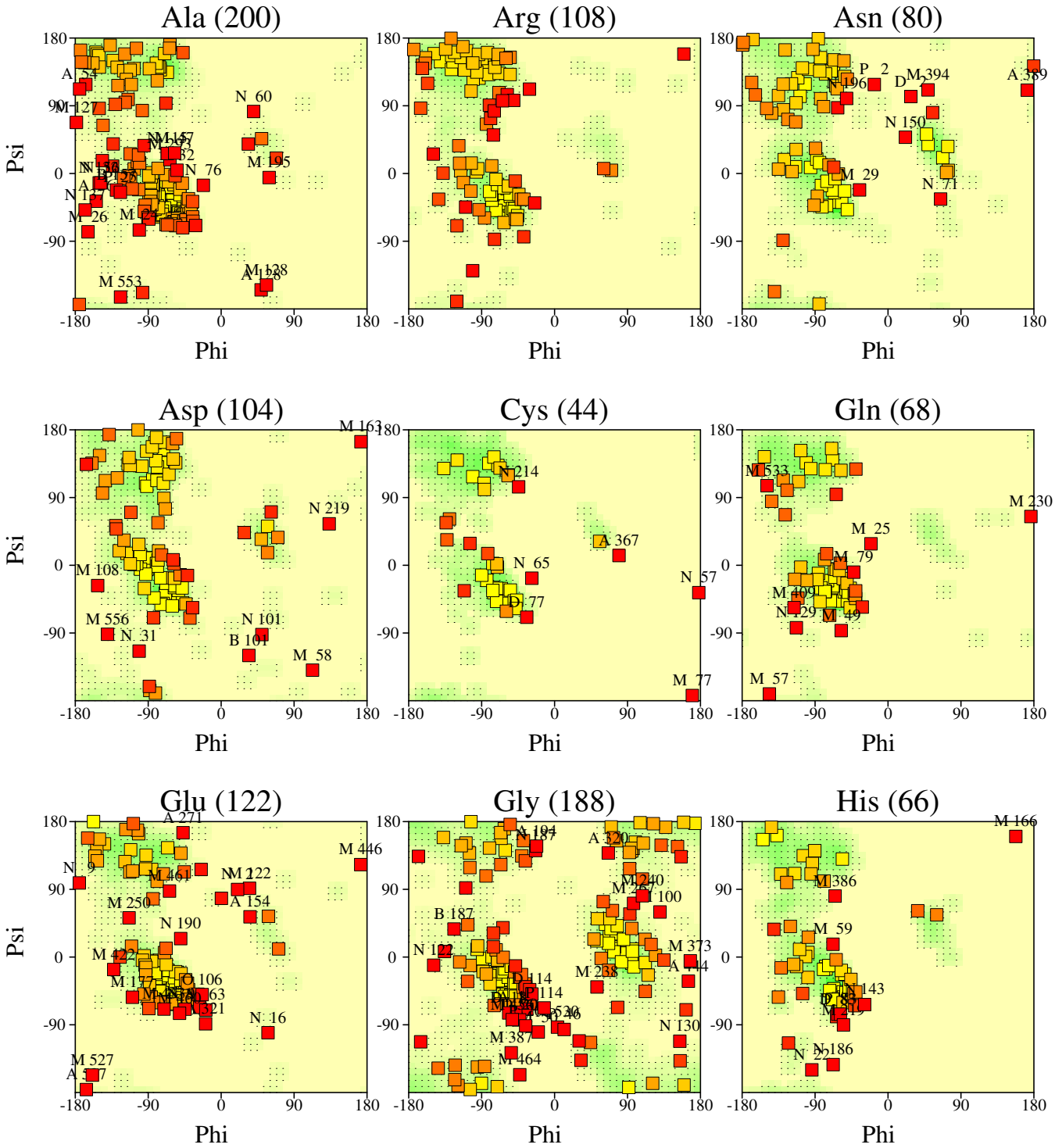
Residues in most favoured regions [A,B,L]	1347	73.8%
Residues in additional allowed regions [a,b,l,p]	421	23.1%
Residues in generously allowed regions [~a,~b,~l,~p]	47	2.6%
Residues in disallowed regions	10	0.5%
	----	------
Number of non-glycine and non-proline residues	1825	100.0%
Number of end-residues (excl. Gly and Pro)	16	
Number of glycine residues (shown as triangles)	188	
Number of proline residues	104	

Total number of residues	2133	

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

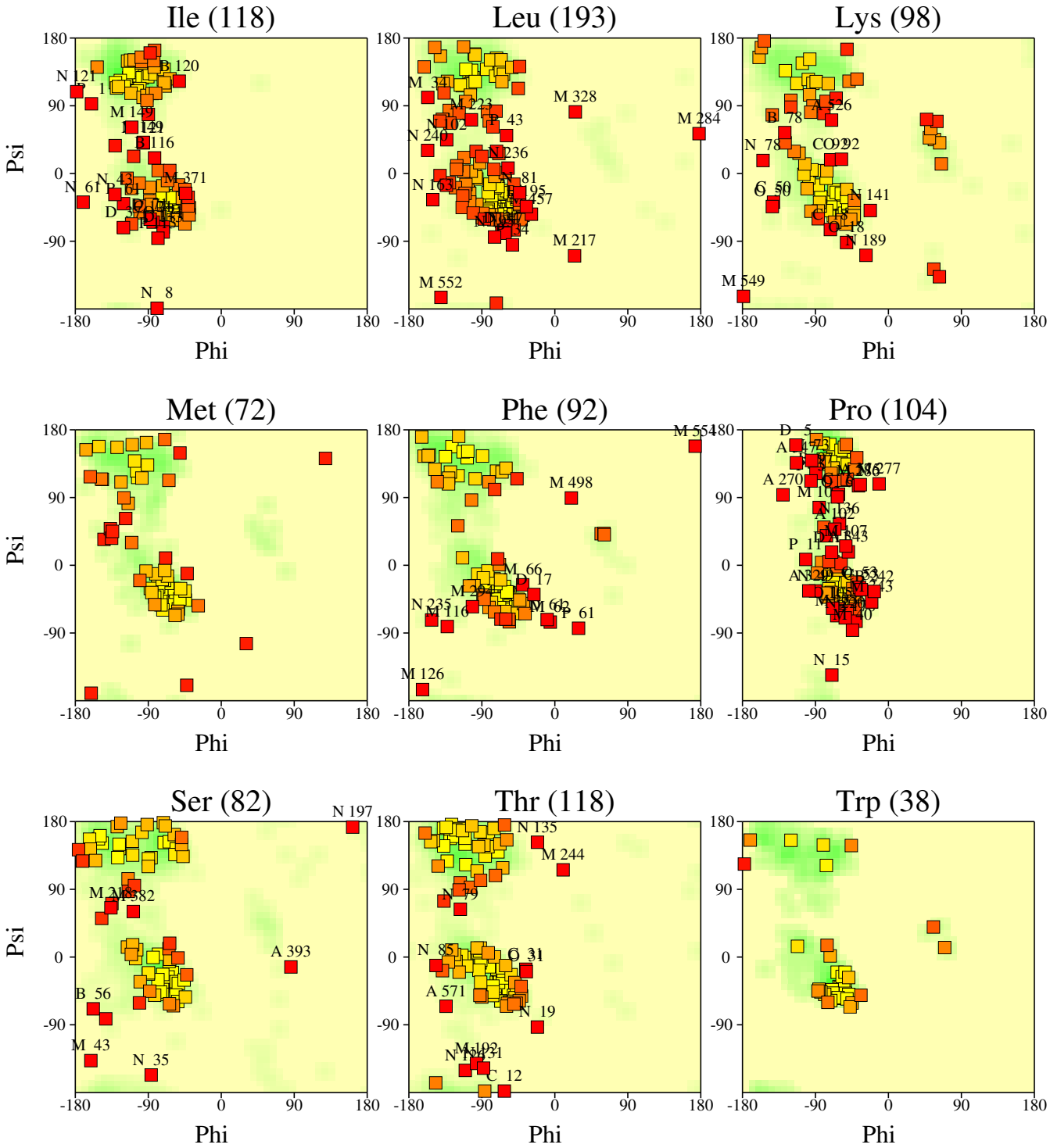
2b76



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

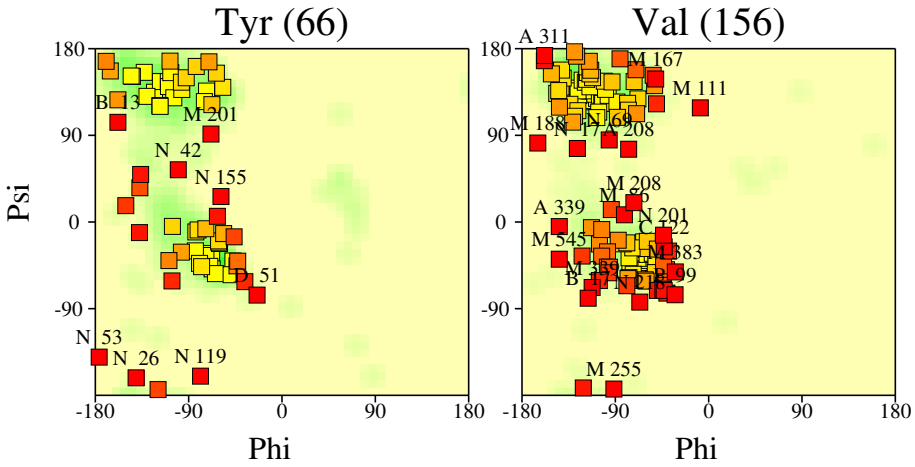
2b76



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

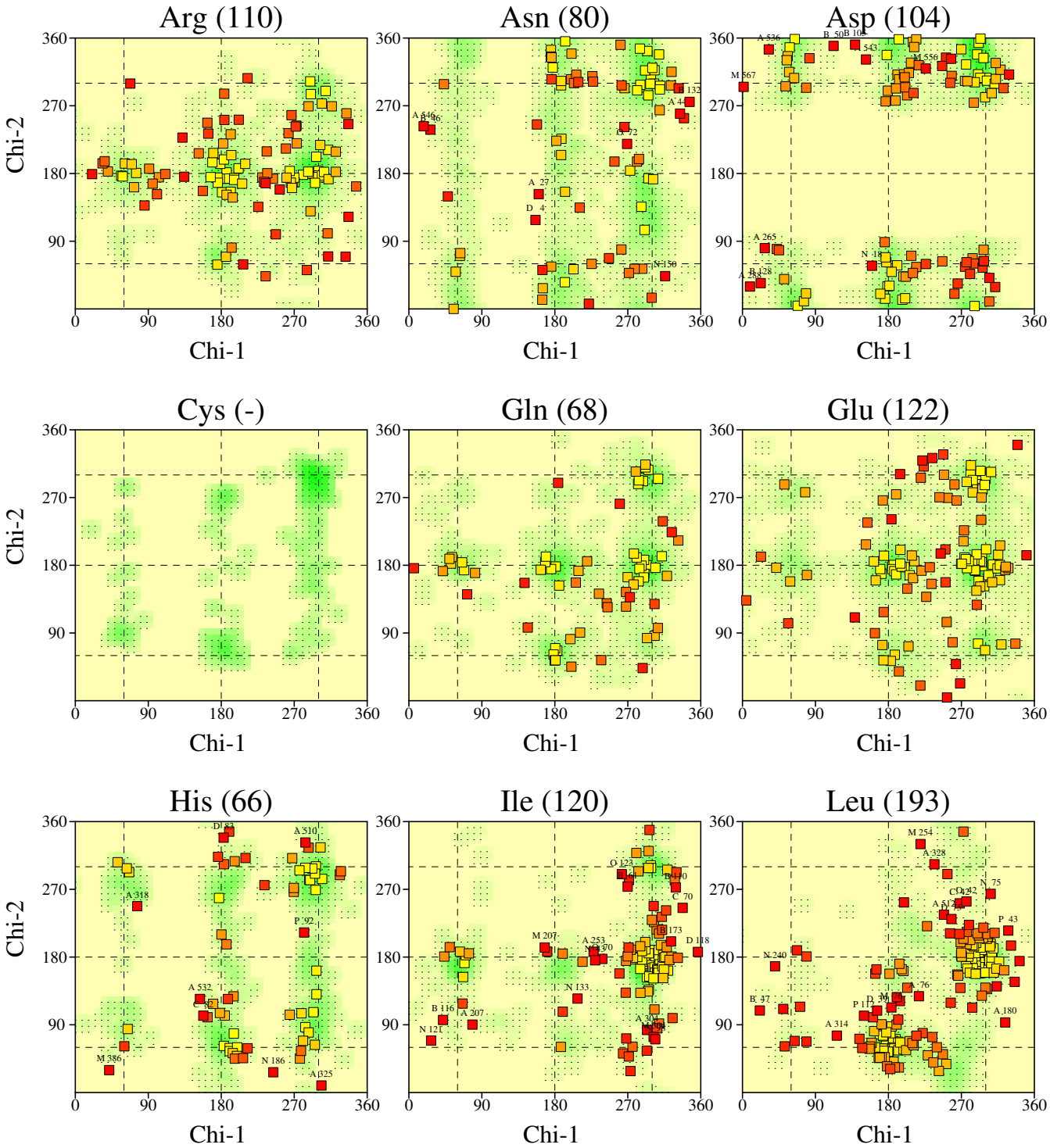
2b76



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

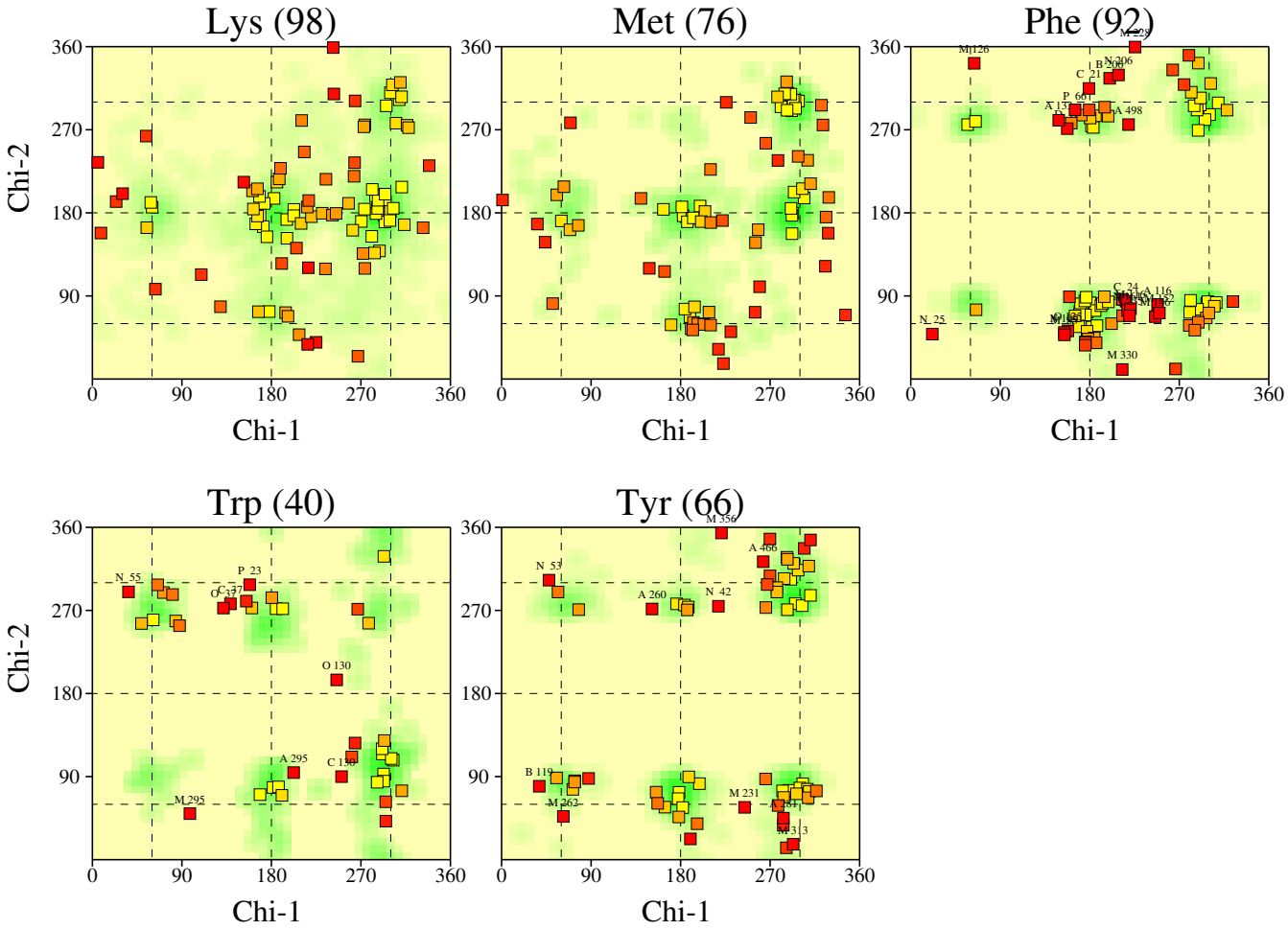
2b76



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

2b76



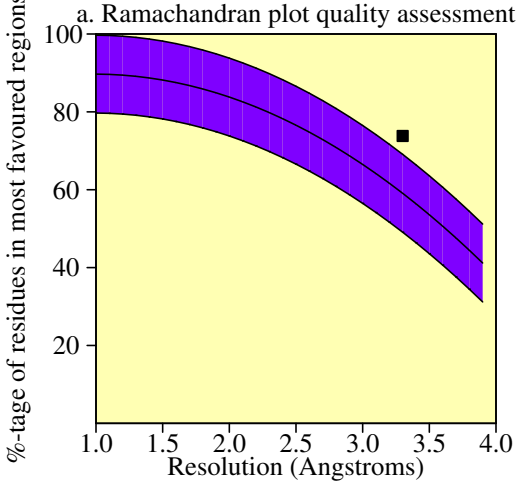
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

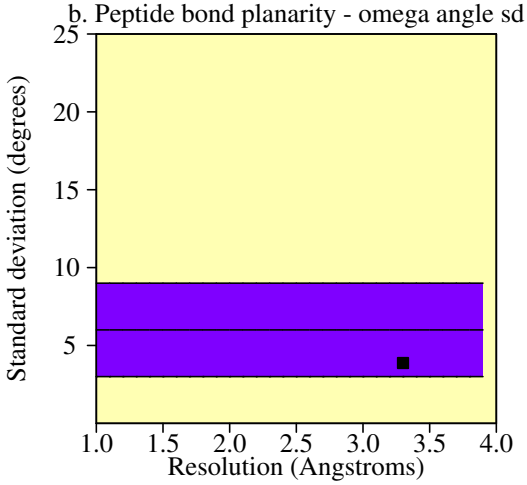
Main-chain parameters

2b76

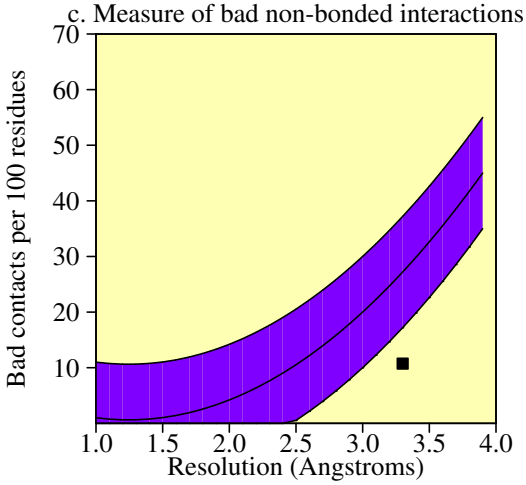
a. Ramachandran plot quality assessment



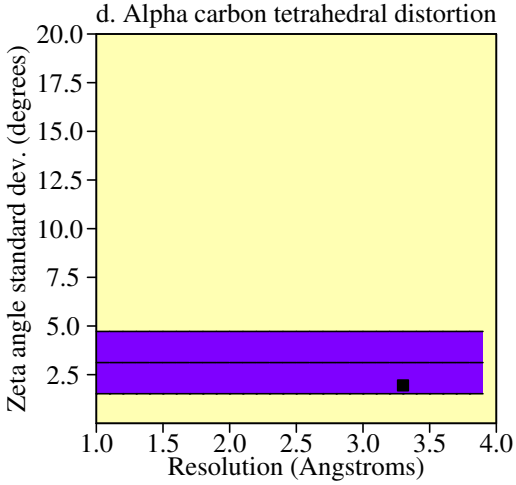
b. Peptide bond planarity - omega angle sd



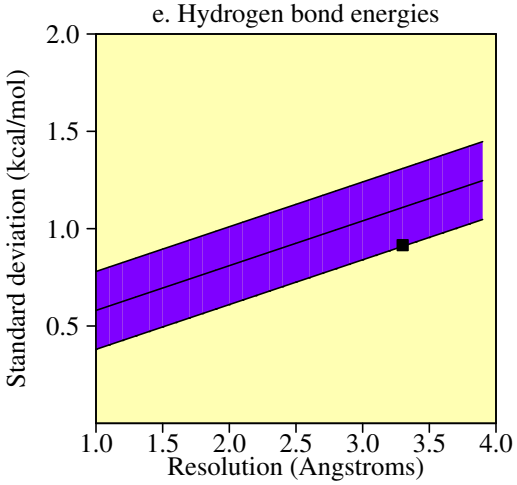
c. Measure of bad non-bonded interactions



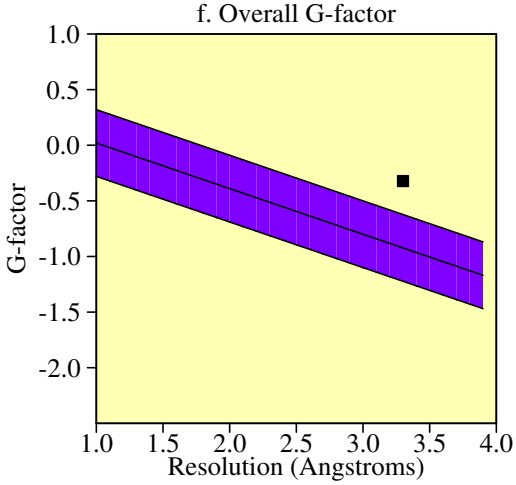
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor



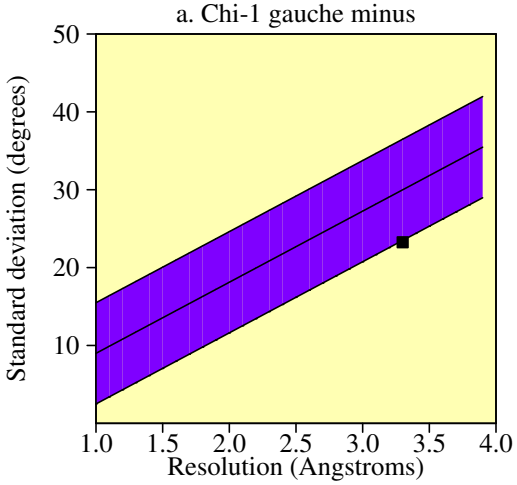
Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	1825	73.8	59.1	10.0	1.5	BETTER
b. Omega angle st dev	2125	3.9	6.0	3.0	-0.7	Inside
c. Bad contacts / 100 residues	229	10.7	27.2	10.0	-1.6	BETTER
d. Zeta angle st dev	1945	1.9	3.1	1.6	-0.7	Inside
e. H-bond energy st dev	1281	0.9	1.1	0.2	-1.0	Inside
f. Overall G-factor	2133	-0.3	-0.9	0.3	2.0	BETTER

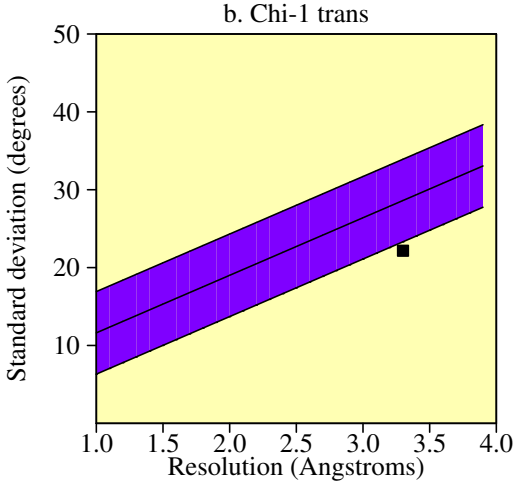
Side-chain parameters

2b76

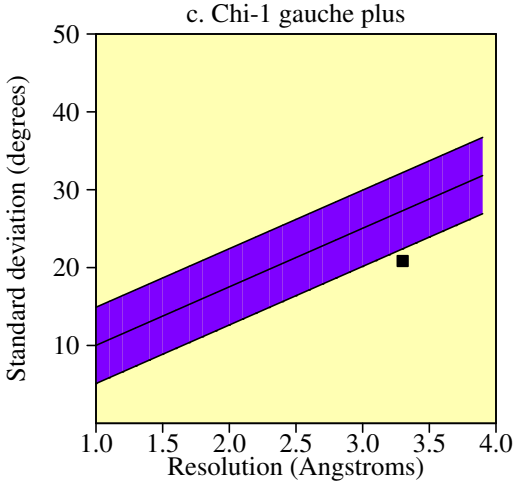
a. Chi-1 gauche minus



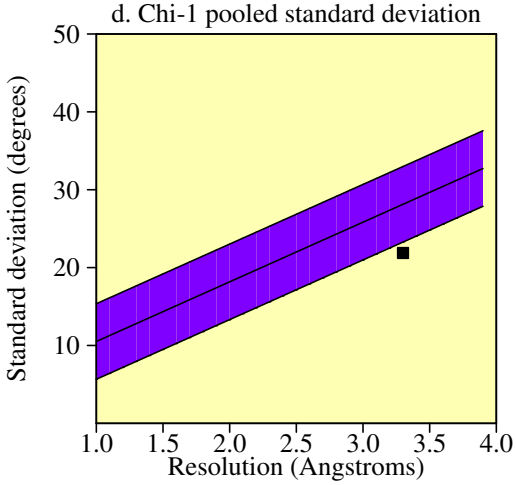
b. Chi-1 trans



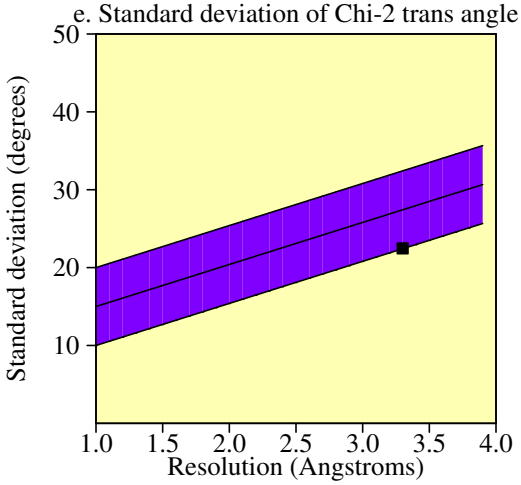
c. Chi-1 gauche plus

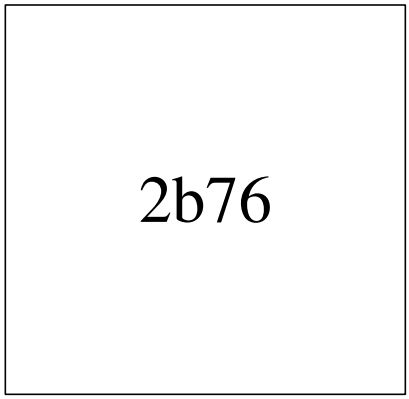


d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



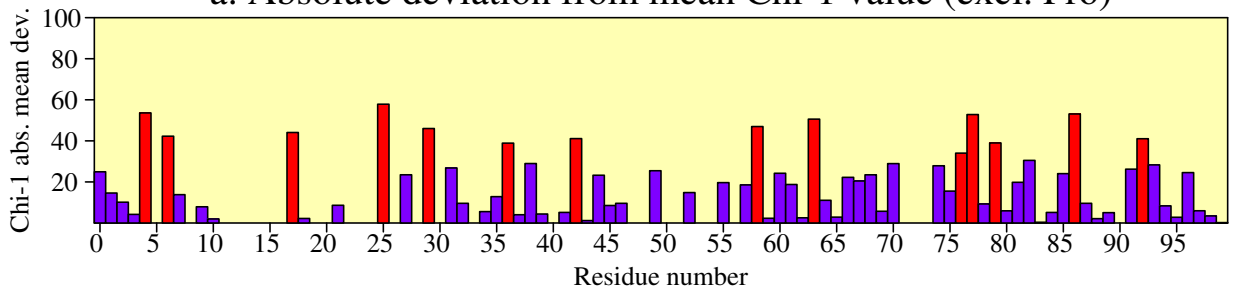


Plot statistics

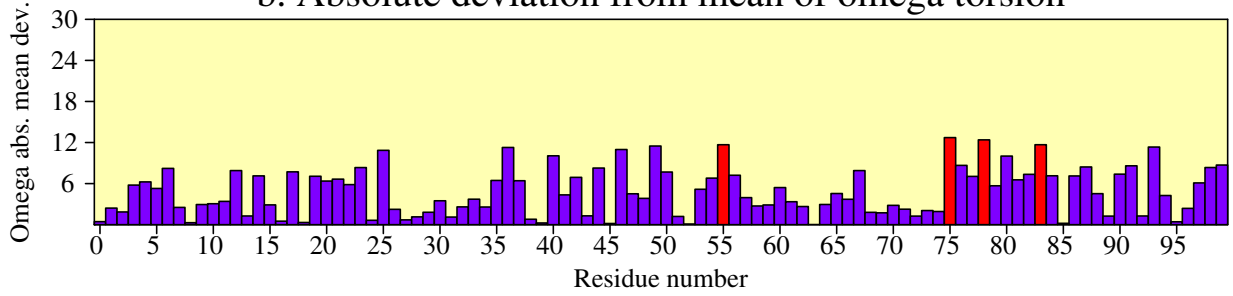
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	251	23.3	30.0	6.5	-1.0	BETTER
b. Chi-1 trans st dev	614	22.2	28.6	5.3	-1.2	BETTER
c. Chi-1 gauche plus st dev	773	20.8	27.3	4.9	-1.3	BETTER
d. Chi-1 pooled st dev	1638	21.9	28.1	4.8	-1.3	BETTER
e. Chi-2 trans st dev	496	22.5	27.4	5.0	-1.0	Inside

Residue properties
2b76

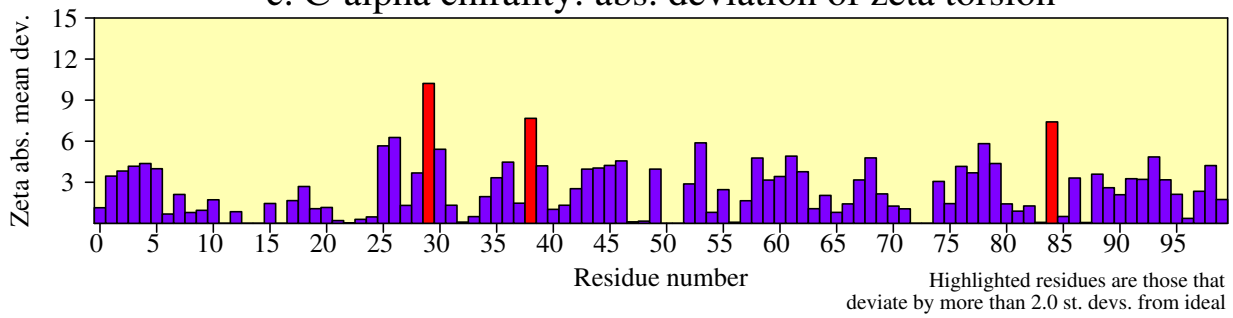
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

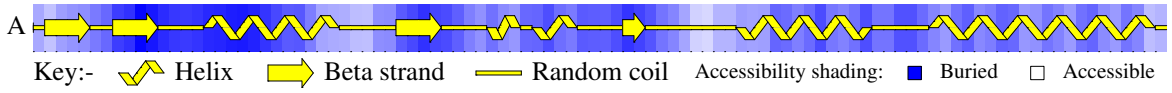


c. C-alpha chirality: abs. deviation of zeta torsion

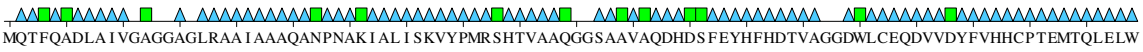


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

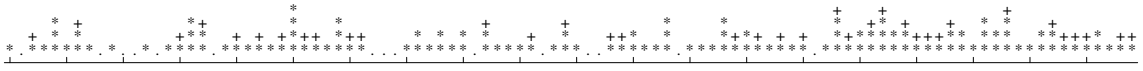
d. Secondary structure & estimated accessibility



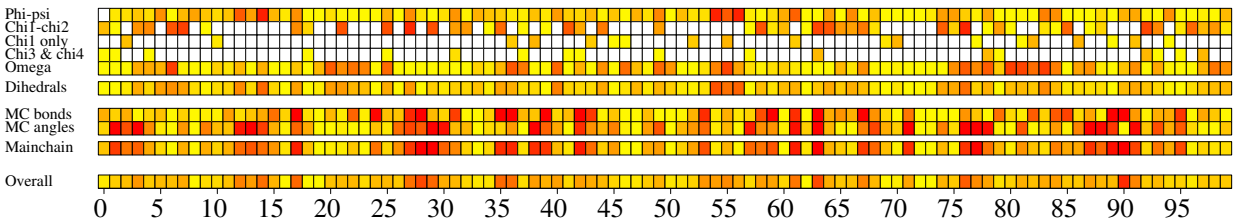
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

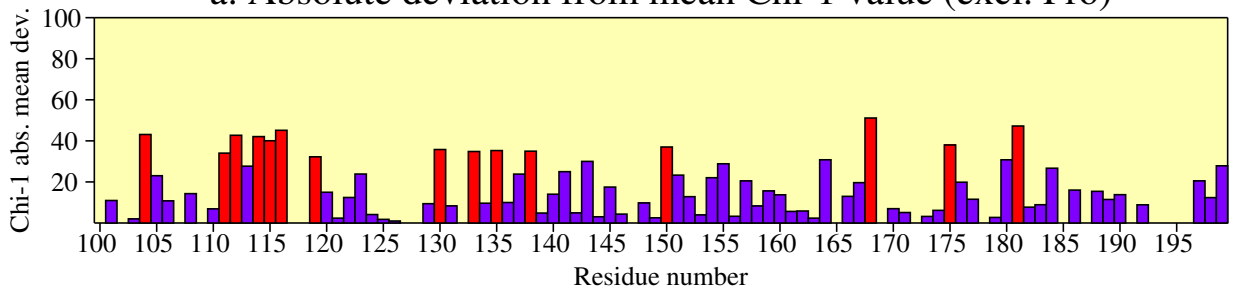


g. G-factors

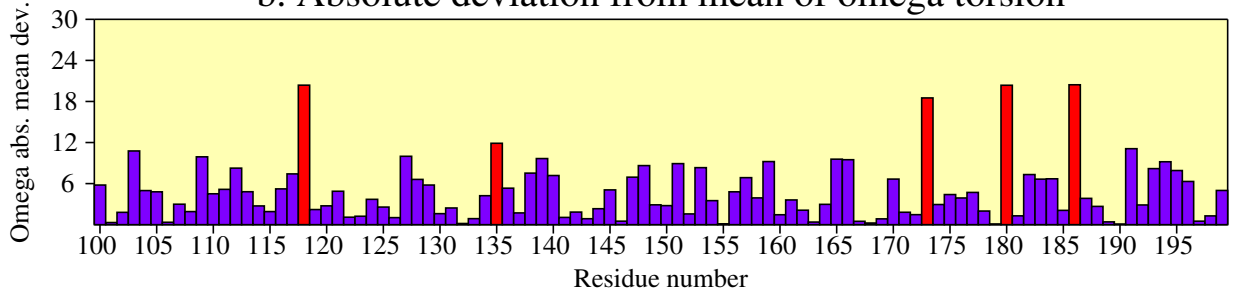


Residue properties
2b76

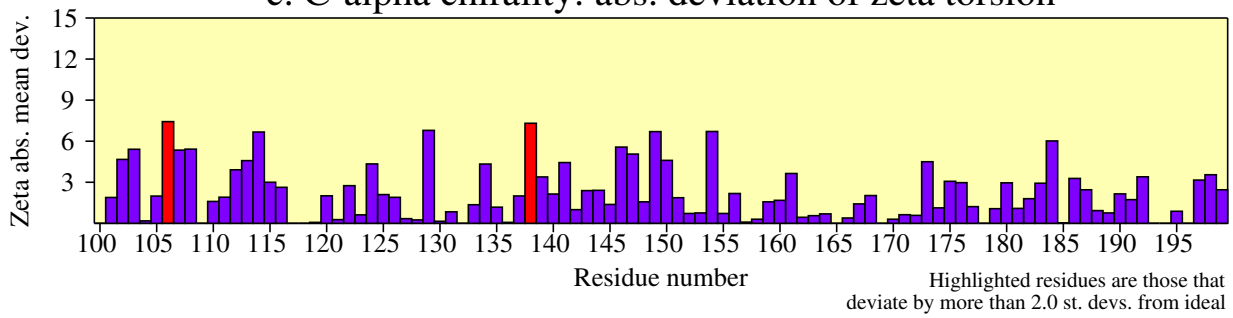
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

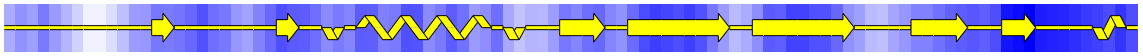


c. C-alpha chirality: abs. deviation of zeta torsion



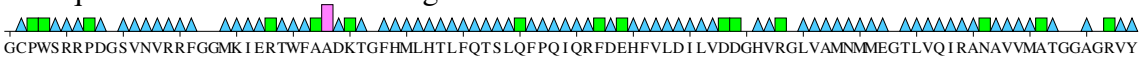
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



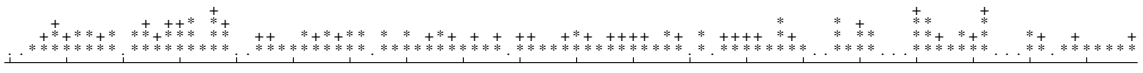
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

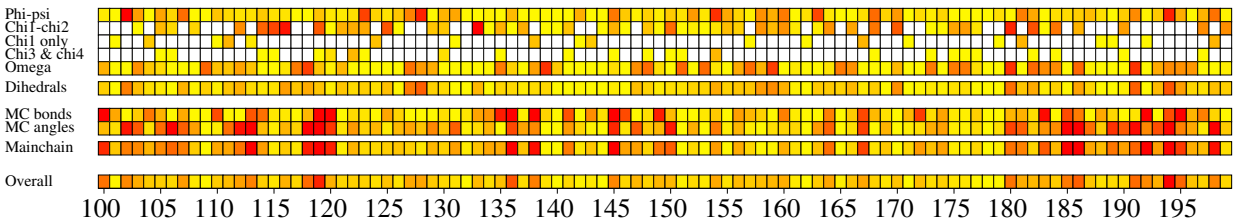


GCPWSRRPDGSVNVRRFGGMKIERTWFAADKTGFHMLHTLFQTSLQFPQIQRFDEHFVLDILVDDGHVRGLVAMNMMEGTLVQIRANAVVMATGGAGRVY

f. Max. deviation (see listing)

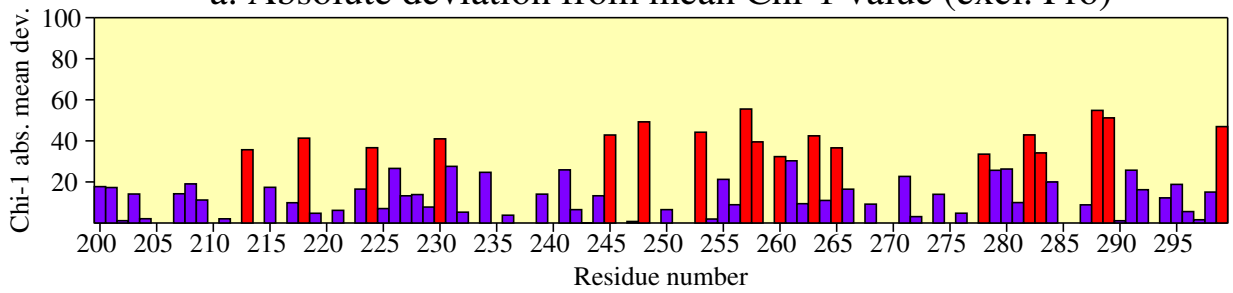


g. G-factors

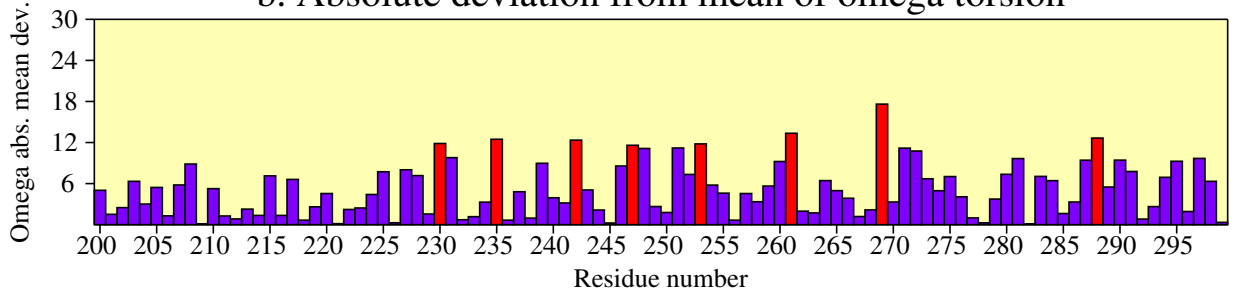


Residue properties
2b76

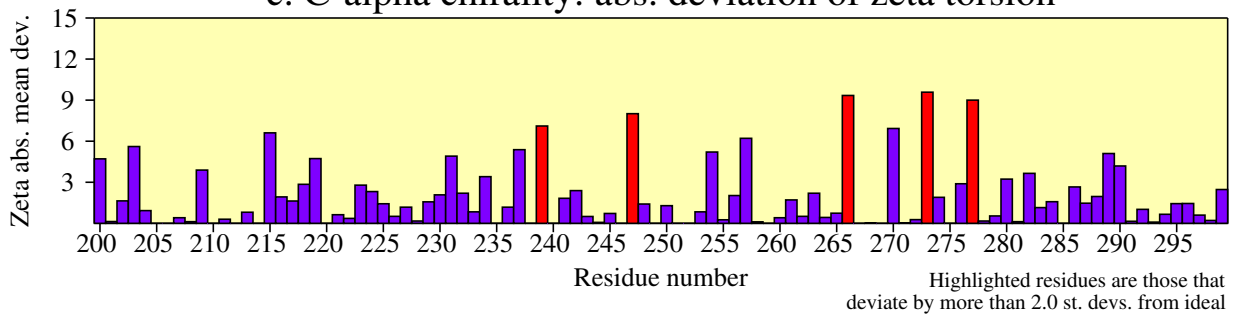
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

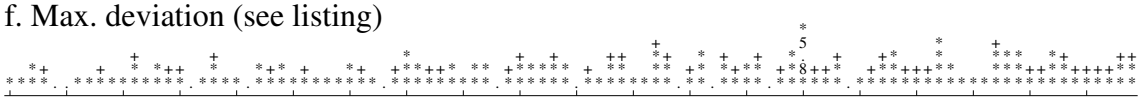
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

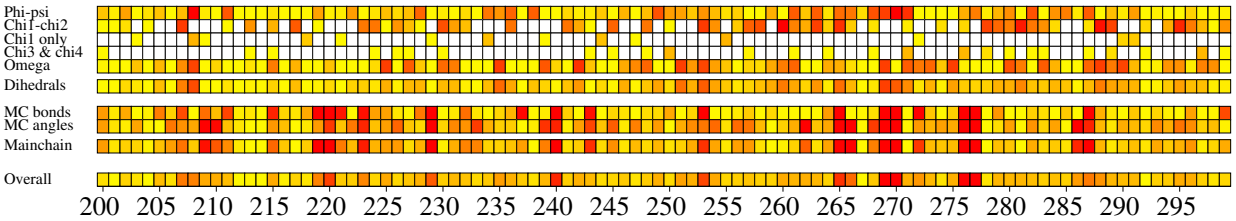
Most favoured Allowed Generous Disallowed

RYNTNGGIVTGDGMGMALSHGVPLRDMEFVQYHPTGLPGSGILMTEGCRGEGGILVNKNGYRYLQDYGMGPETPLGEPKNKYMELGPRDKVSQAFWHEWR

f. Max. deviation (see listing)

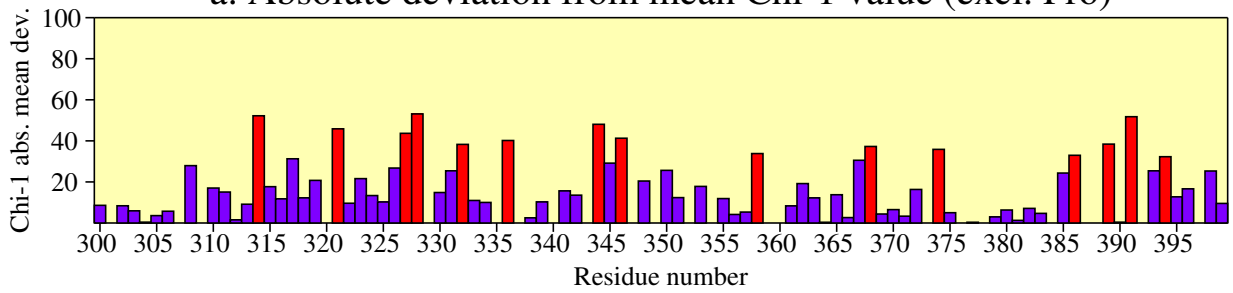


g. G-factors

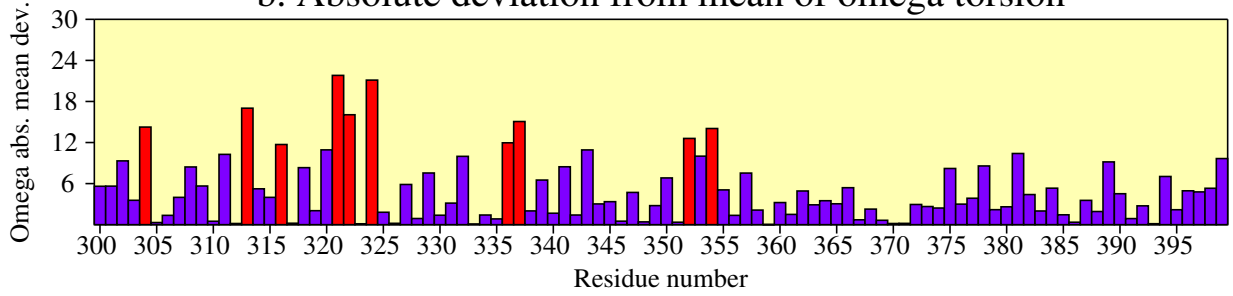


Residue properties
2b76

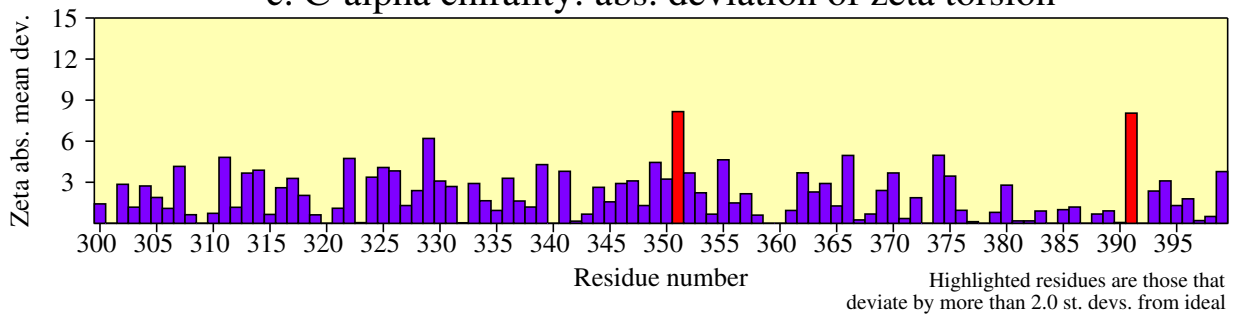
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

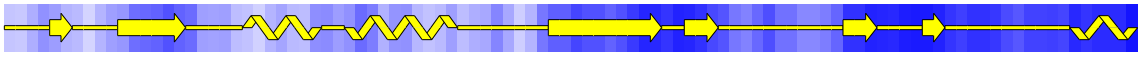


c. C-alpha chirality: abs. deviation of zeta torsion



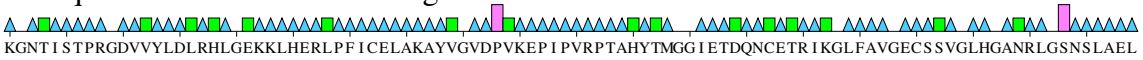
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



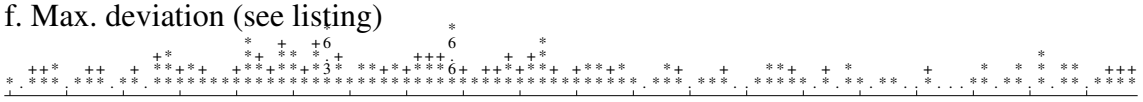
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

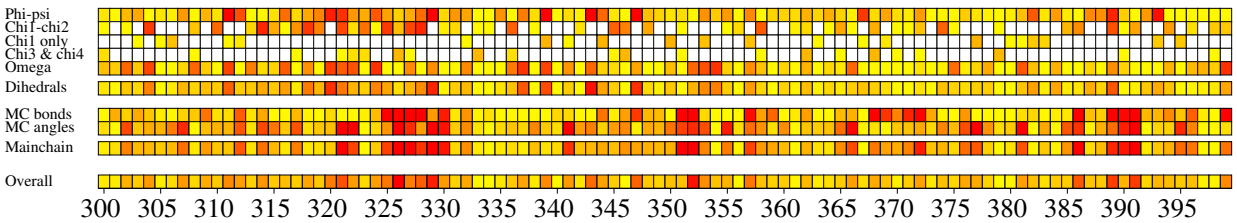


KGNT I S T P R G D V V Y L D L R H L G E K K L H E R L P F I C E L A K A Y V G V D P V K E P I P V R P T A H Y T M G G I E T D Q N C E T R I K G L F A V G E C S S V G L H G A N R L G S N S L A E L

f. Max. deviation (see listing)

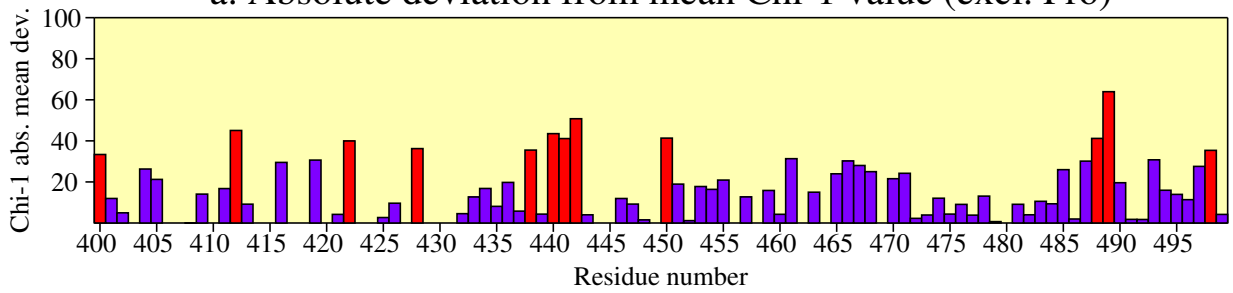


g. G-factors

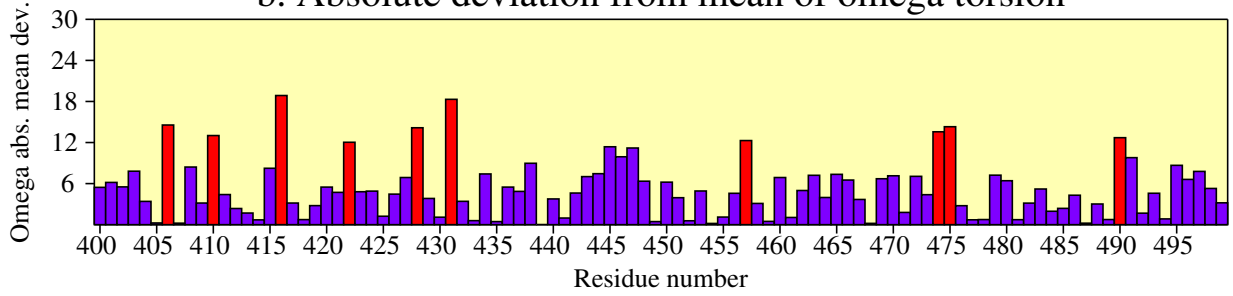


Residue properties
2b76

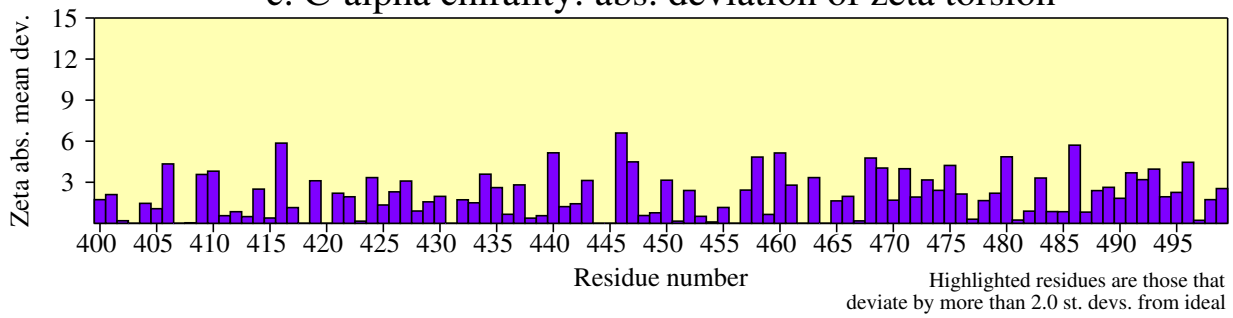
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

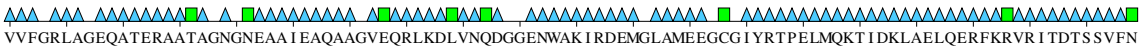


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

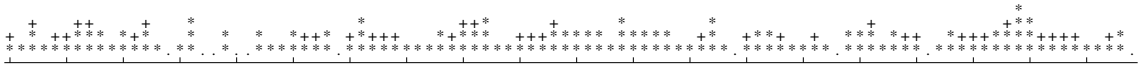
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

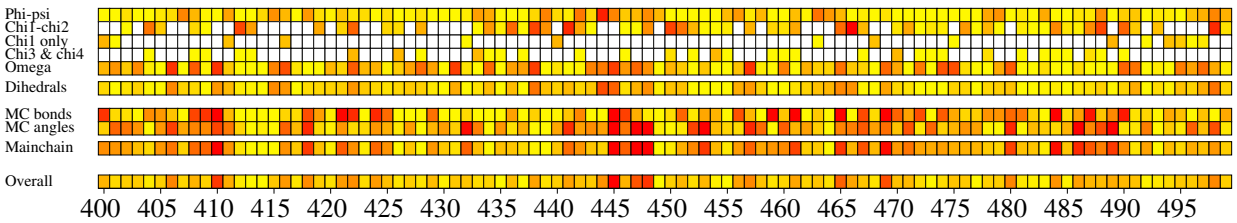


VVFGRLAGEQATERAATAGNGNEAAIEAQAAGVEQRLKDLVNQDGGENWAKIRDEMGLAMEEGCGIYRTPELMQKTIDKLAELQERFKRVRITDTSSVFN

f. Max. deviation (see listing)

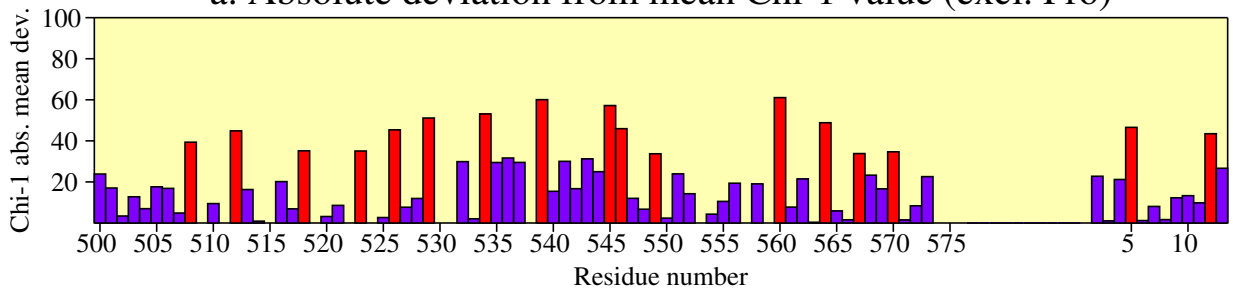


g. G-factors

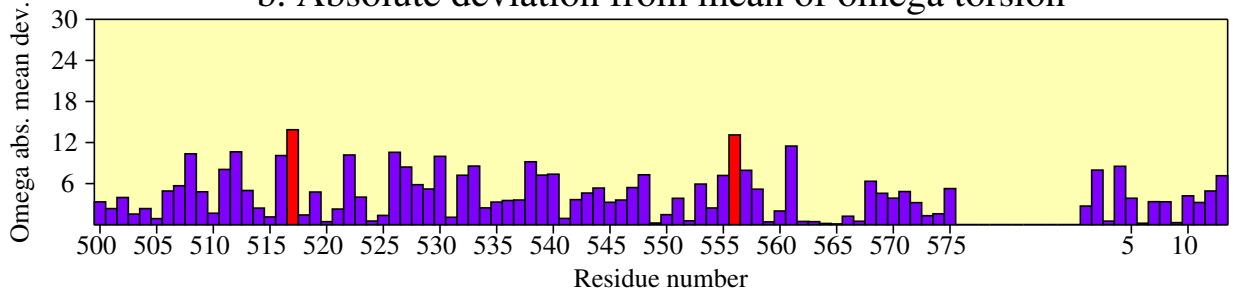


Residue properties
2b76

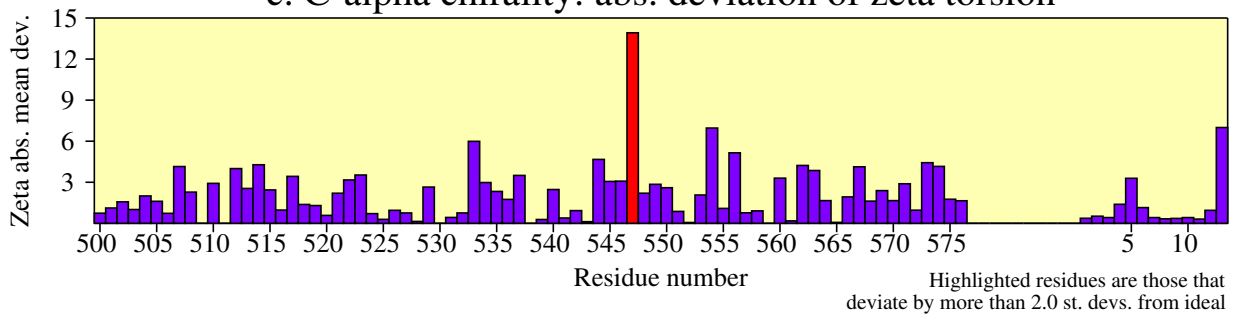
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

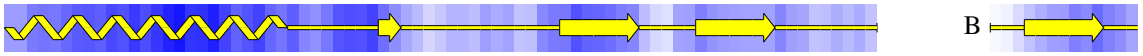


c. C-alpha chirality: abs. deviation of zeta torsion



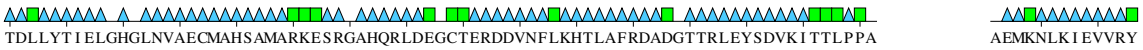
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

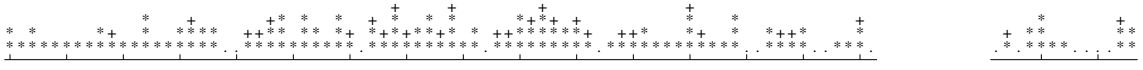


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

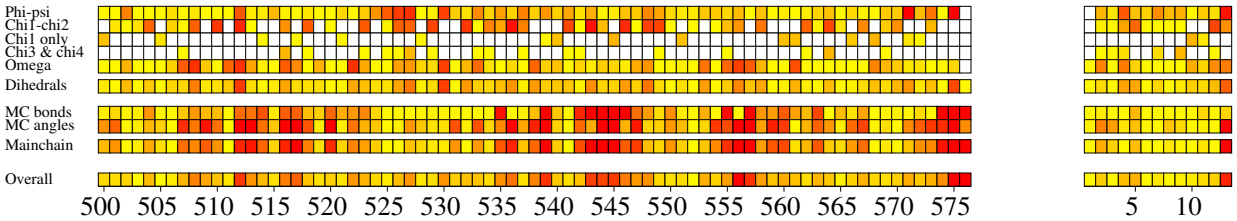
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

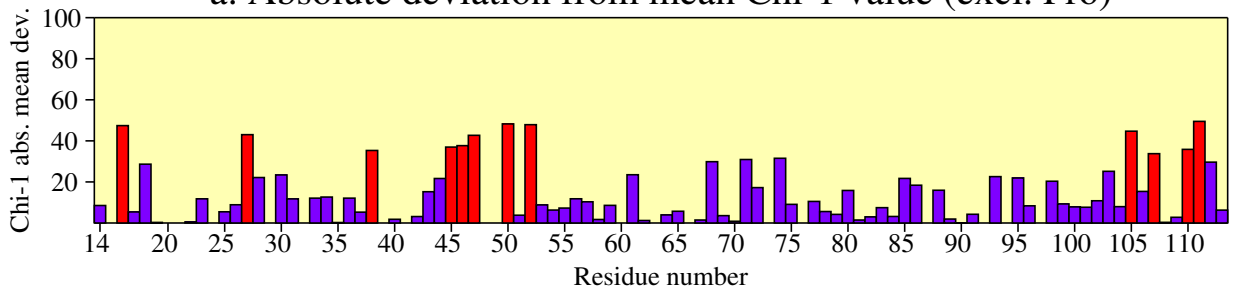


g. G-factors

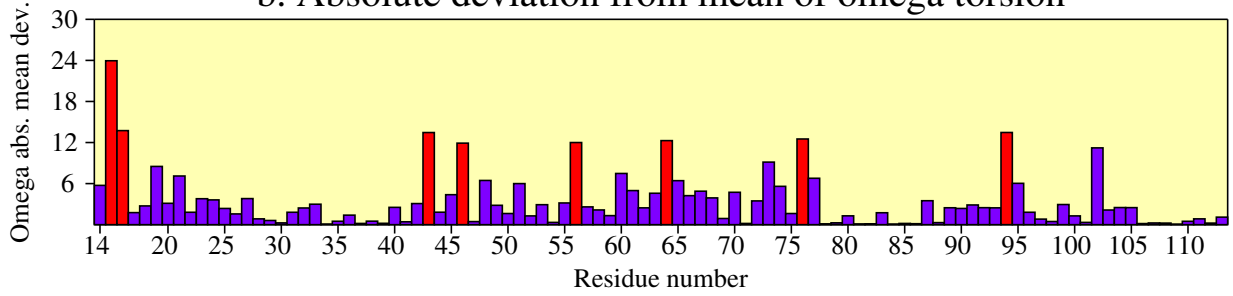


Residue properties
2b76

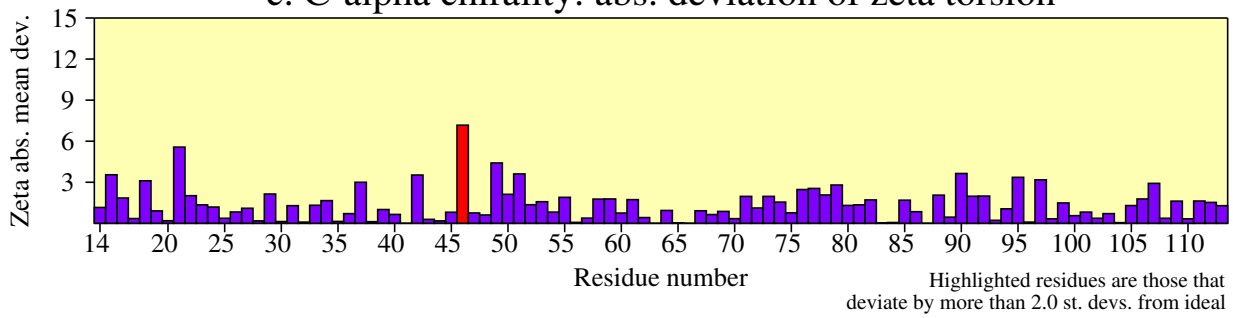
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

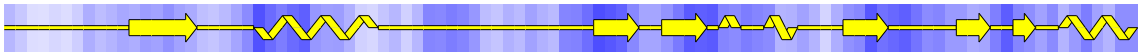


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



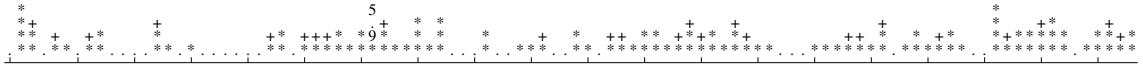
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

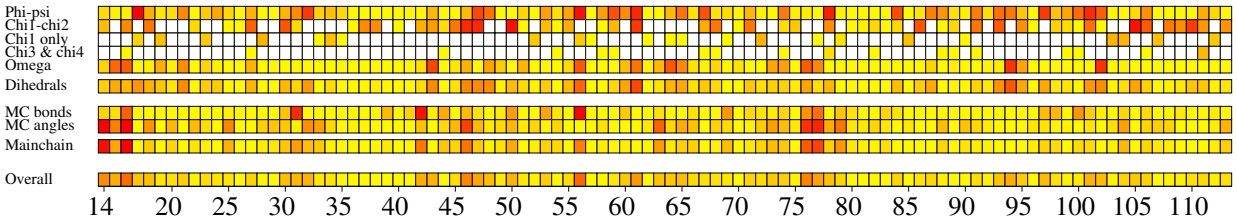
Most favoured Allowed Generous Disallowed

NPEVDTAPHSAFYEVPYDATTSLLDALGYIKDNLAPDLSYRWSCRMAICGSCGMMVNNVPKLACKTFLRDYTDGMKVEALANFPIERDLVVDMTHFIESL

f. Max. deviation (see listing)

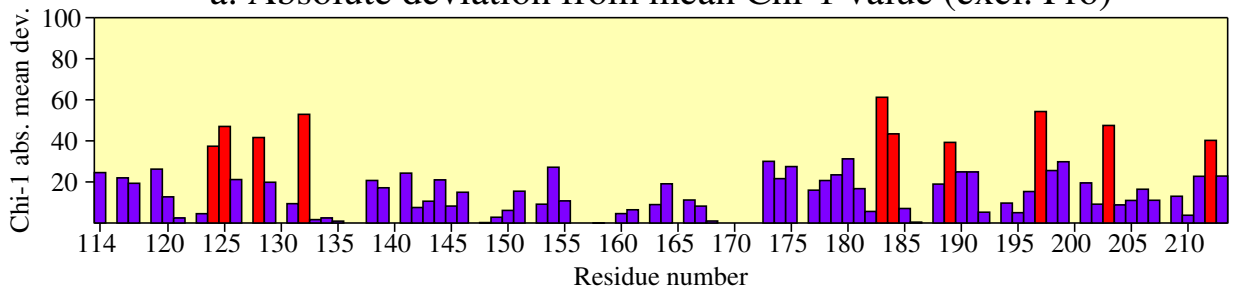


g. G-factors

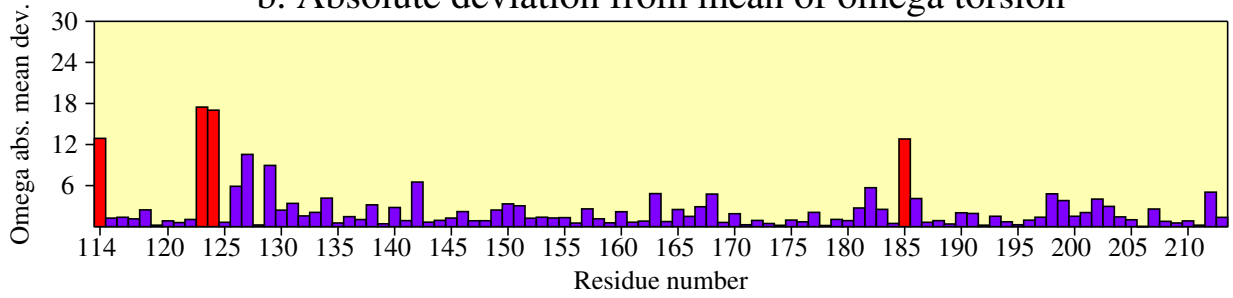


Residue properties
2b76

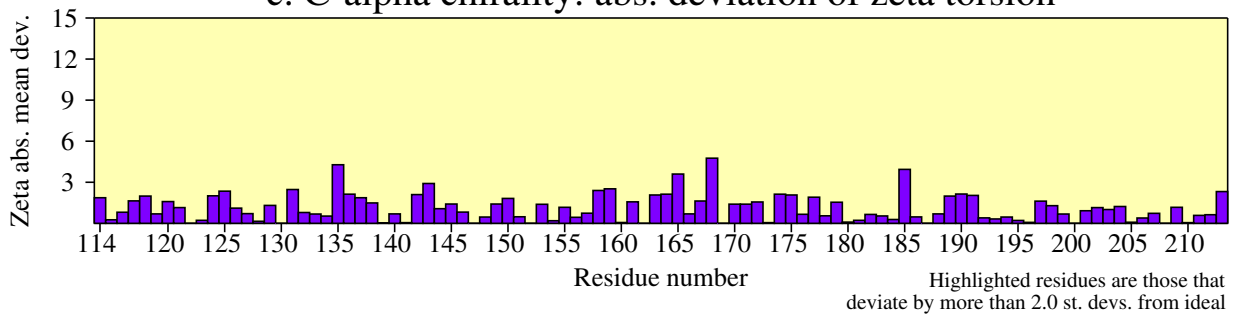
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

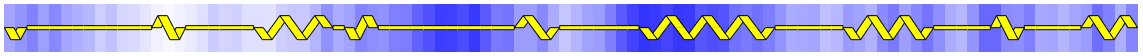


c. C-alpha chirality: abs. deviation of zeta torsion



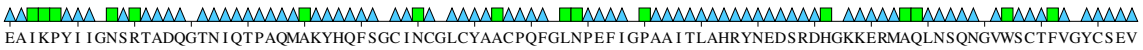
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



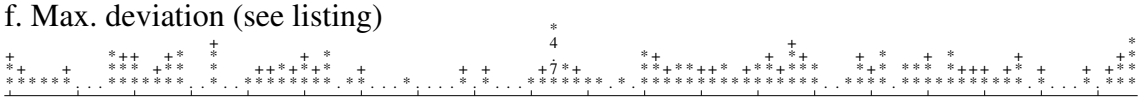
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

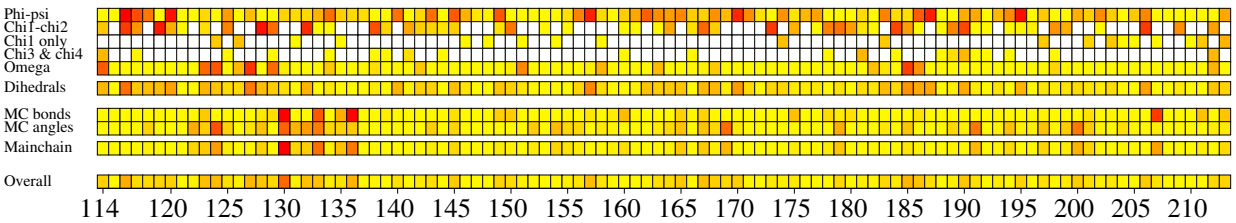


EAIKPYIIGNSRTADQGTNIQTPAQMAKYHQFSGCINCGLCYAACPQFGLNPEFIGPAAITLAHRYNEDSRDHGKKERMAQLNSQNGVWSCTFVGYCSEV

f. Max. deviation (see listing)

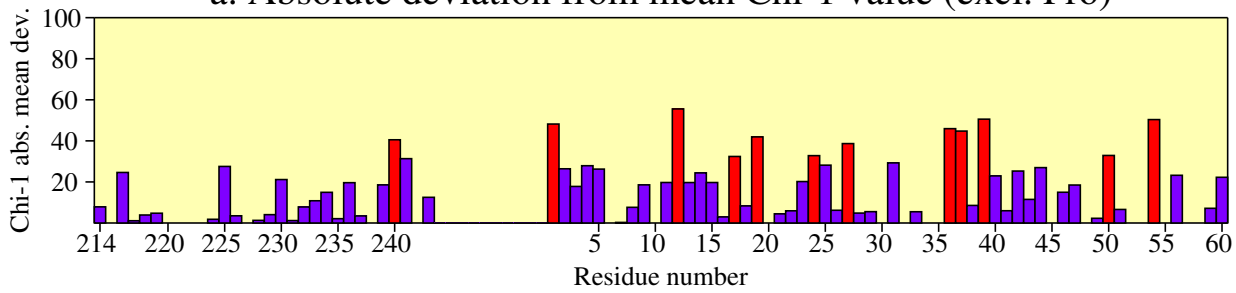


g. G-factors

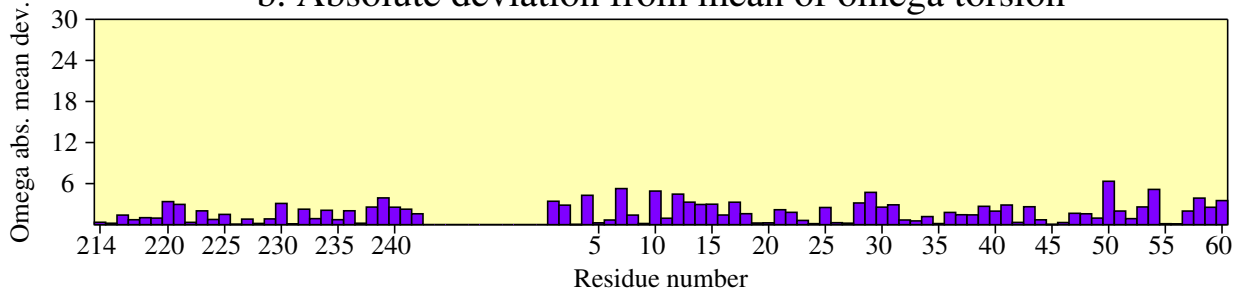


Residue properties
2b76

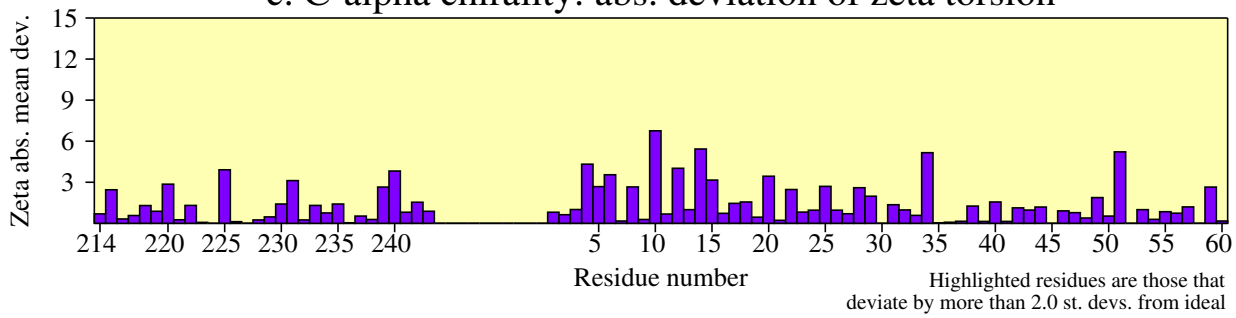
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

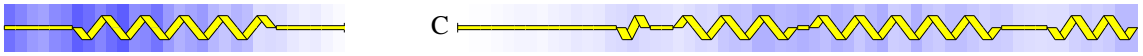


c. C-alpha chirality: abs. deviation of zeta torsion



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

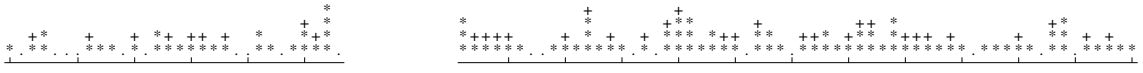
d. Secondary structure & estimated accessibility



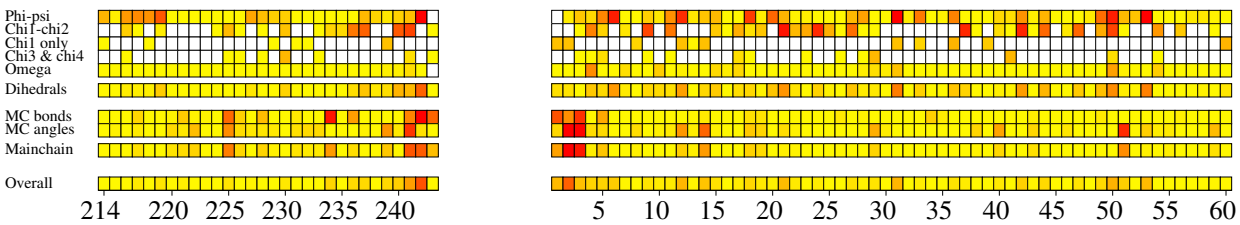
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

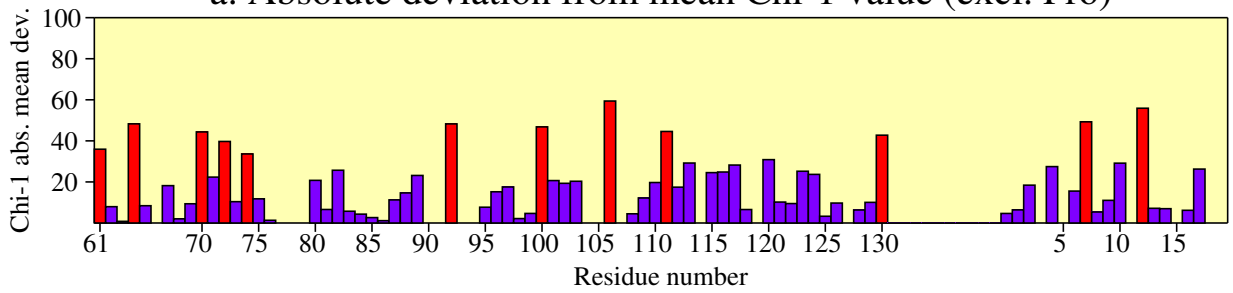


g. G-factors

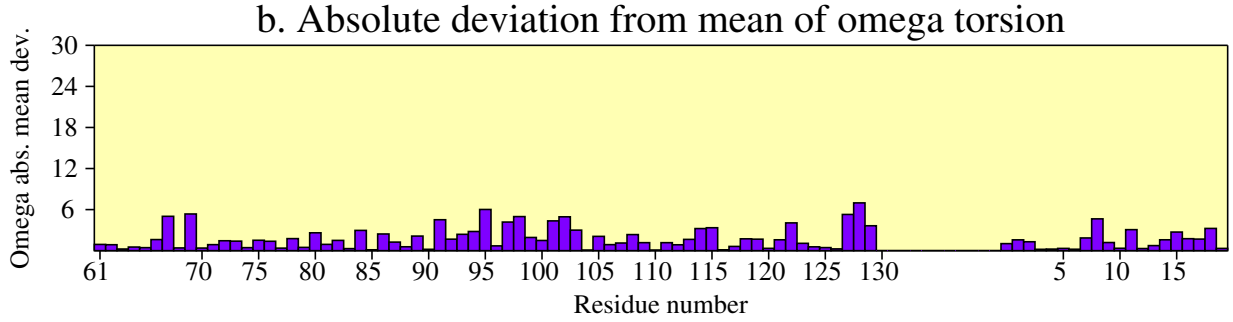


Residue properties
2b76

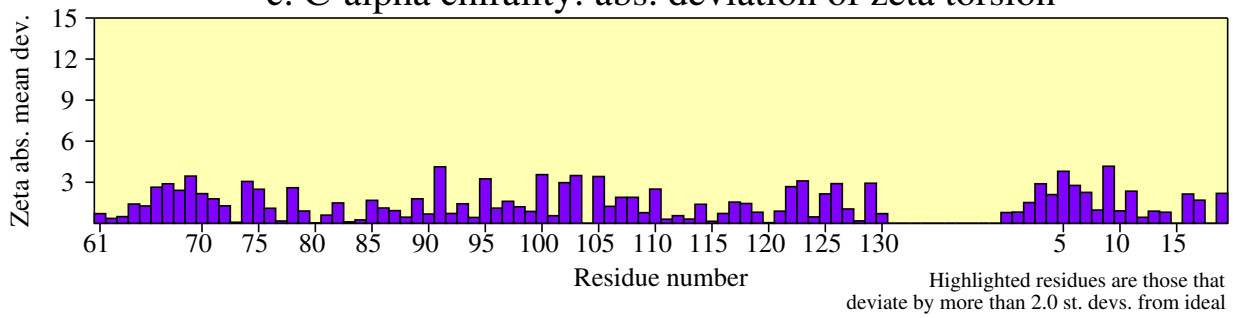
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

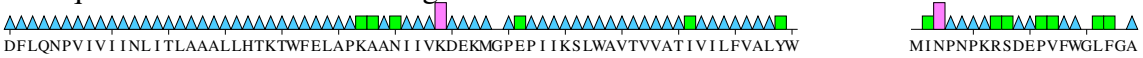


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

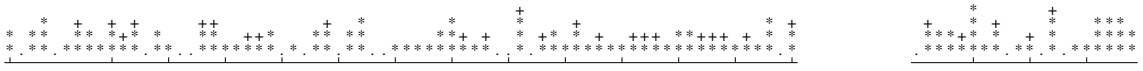
d. Secondary structure & estimated accessibility

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

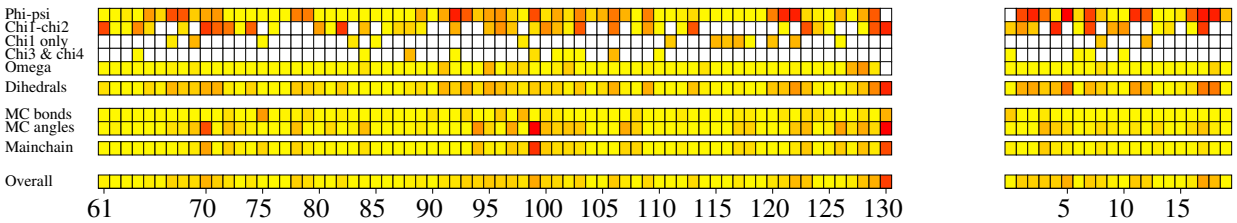
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

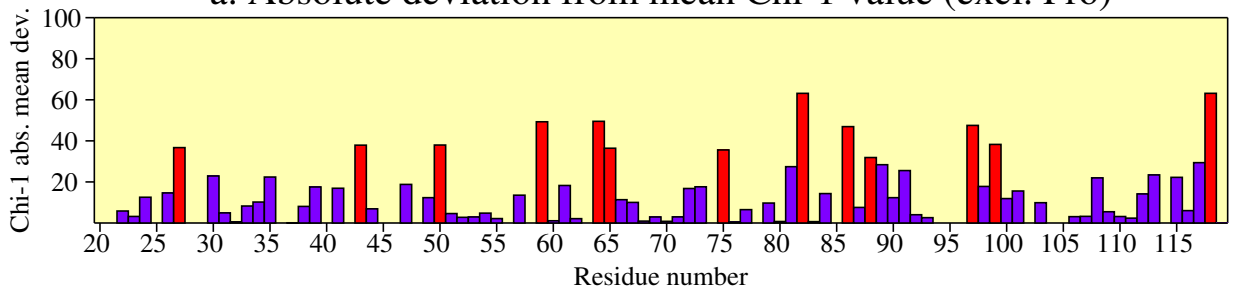


g. G-factors

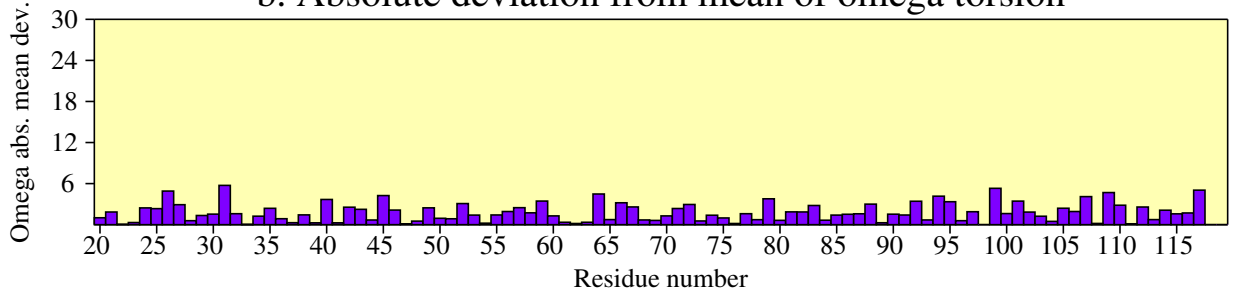


Residue properties
2b76

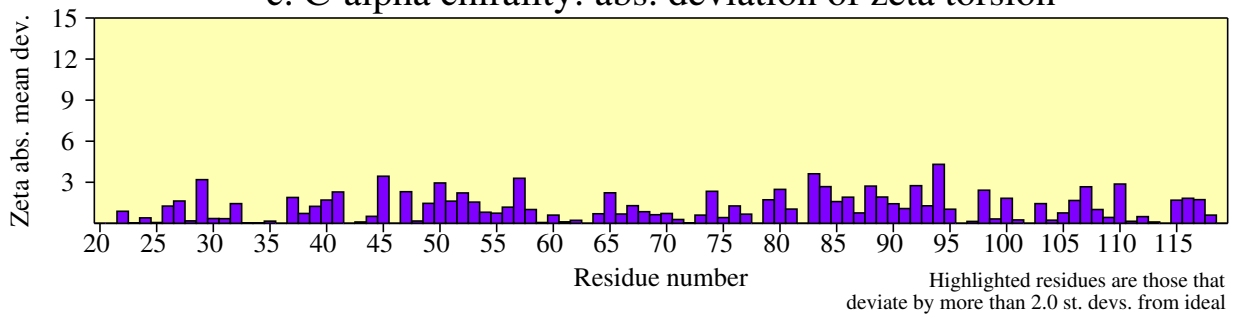
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

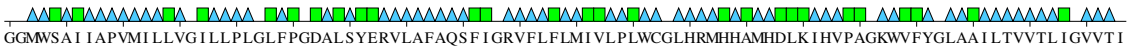


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

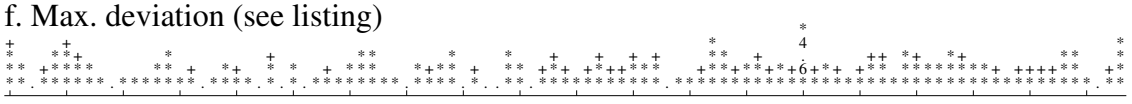
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

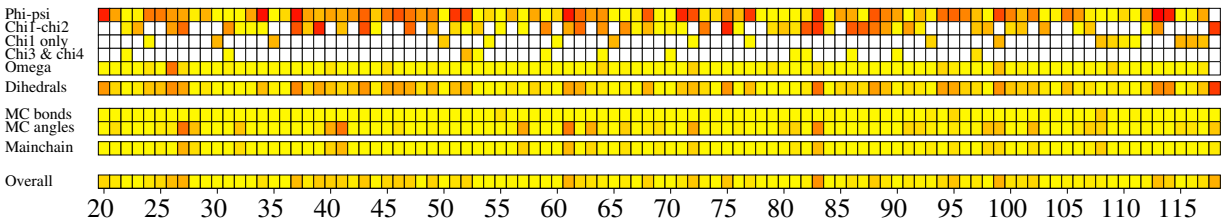


GGMWSAIIAPVMILLVGILLPLGLFPGDALSYERVLAFAQSFIGRVFLFLMIVLPLWCGLHRMHHAMHDLKIHVPAGKWVFYGLAAILTVVTLIGVVTI

f. Max. deviation (see listing)

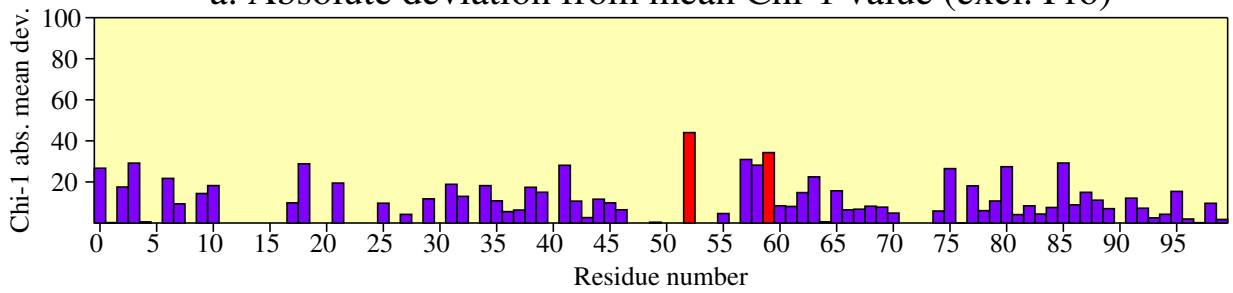


g. G-factors

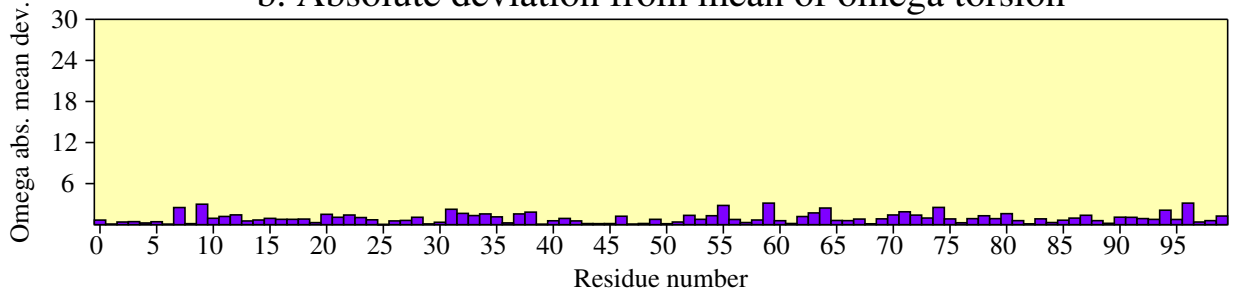


Residue properties
2b76

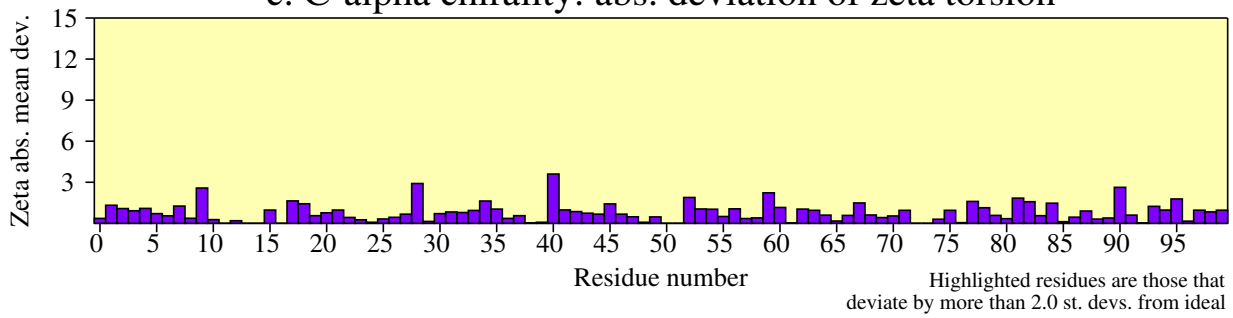
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

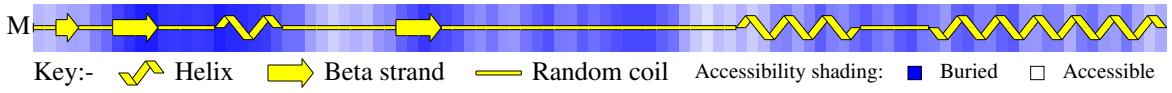


c. C-alpha chirality: abs. deviation of zeta torsion

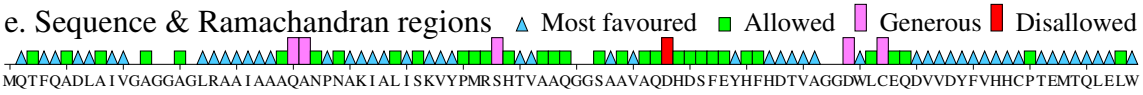


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

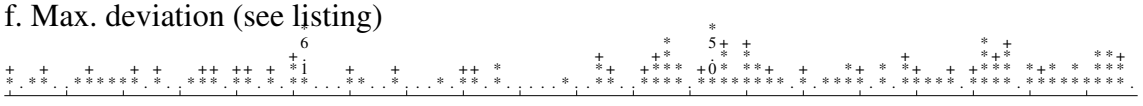
d. Secondary structure & estimated accessibility



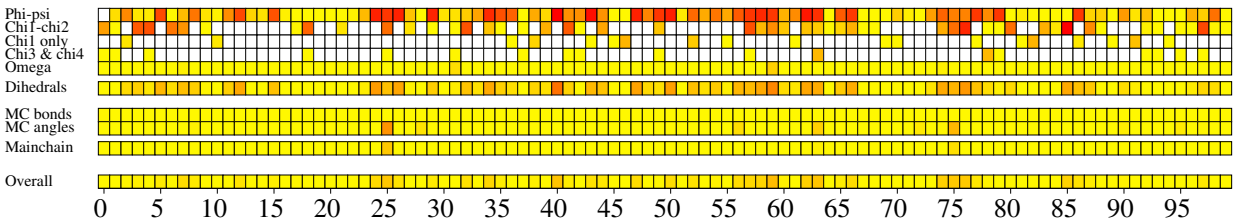
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

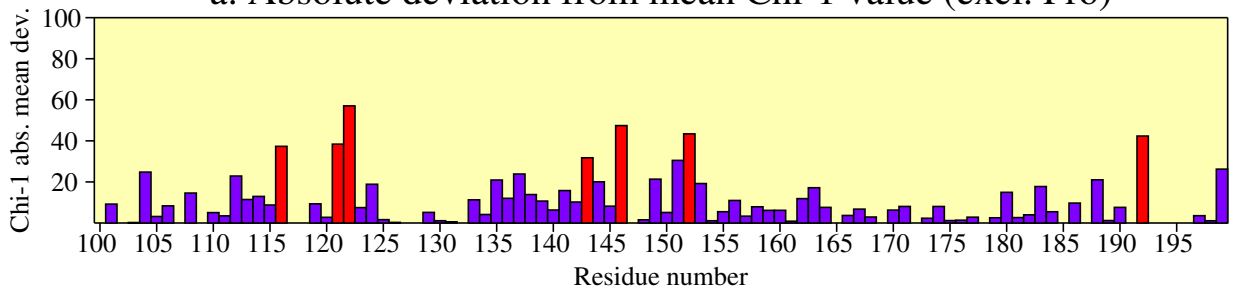


g. G-factors

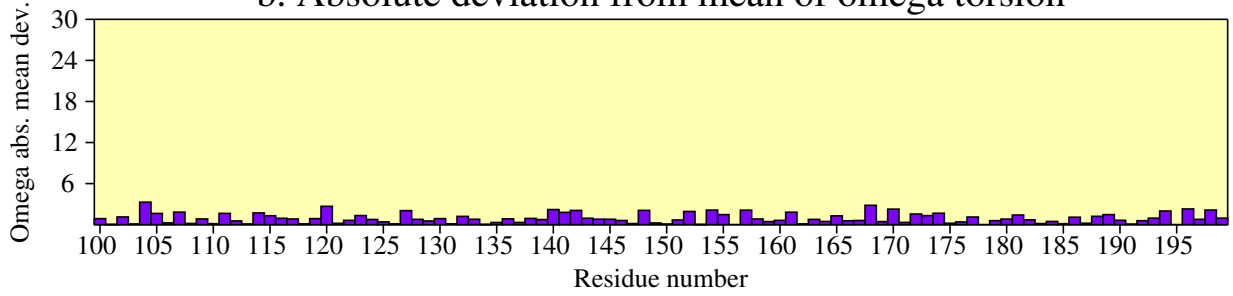


Residue properties
2b76

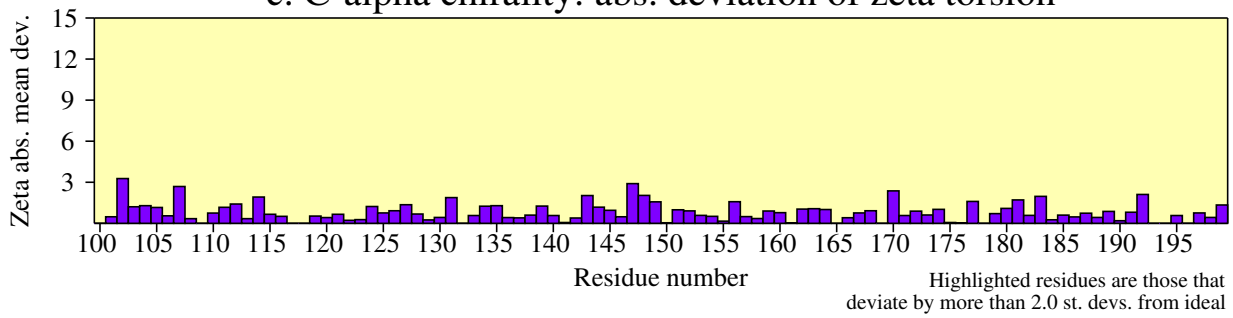
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

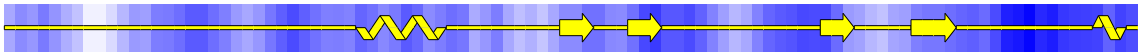


c. C-alpha chirality: abs. deviation of zeta torsion



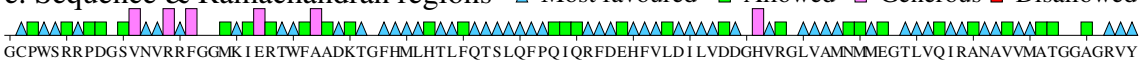
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

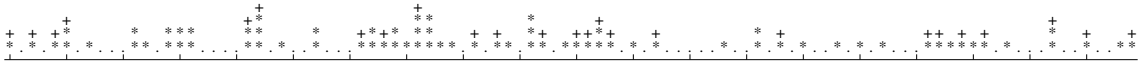


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

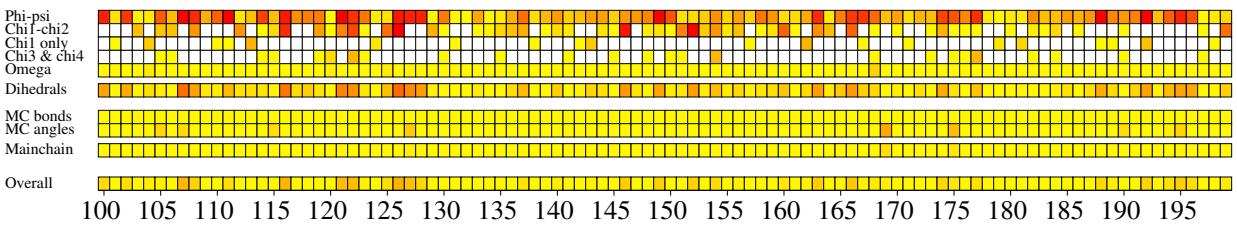
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

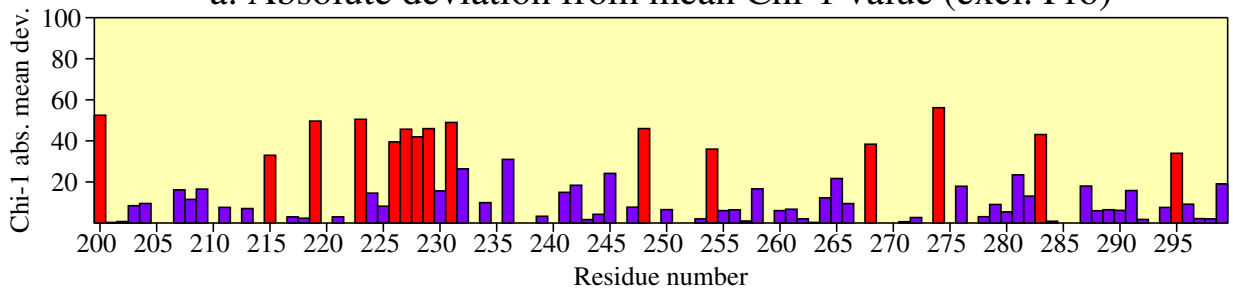


g. G-factors

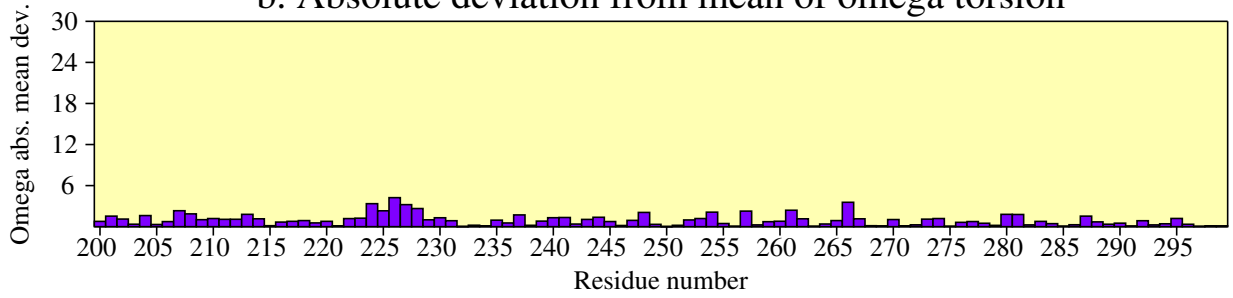


Residue properties
2b76

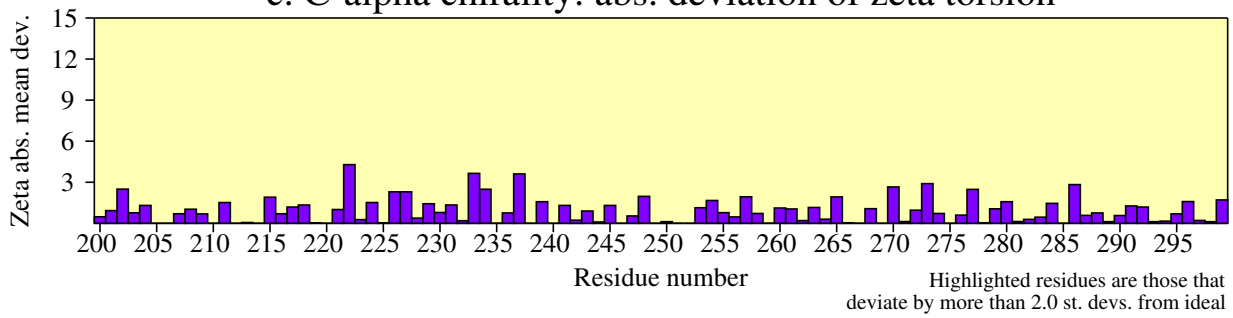
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

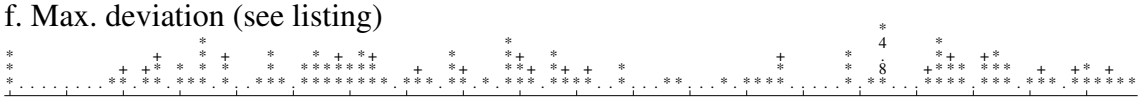
d. Secondary structure & estimated accessibility

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

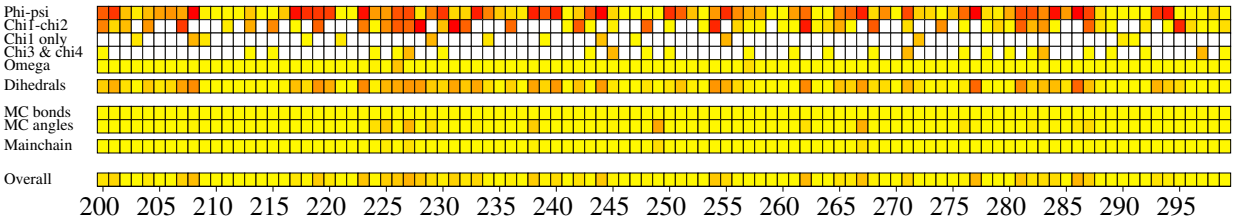
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

RYNTNGGIVTGDGMGMALSHGVPLRDMEFVQYHPTGLPGSGILMTEGCRGEGGILVNKNGYRYLQDYGMGPETPLGEPKNKYMELGPRDKVSQAFWHEWR

f. Max. deviation (see listing)

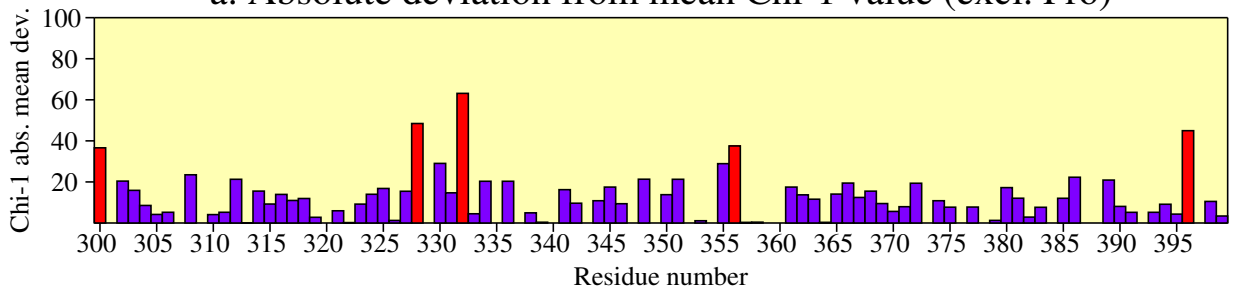


g. G-factors

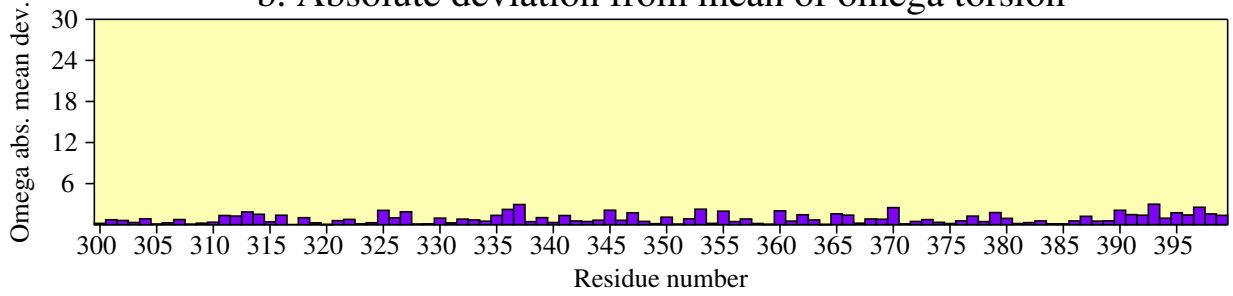


Residue properties
2b76

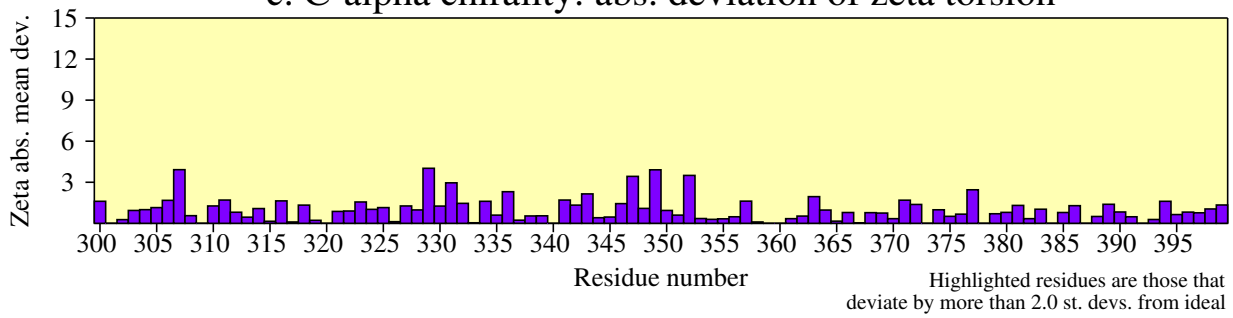
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

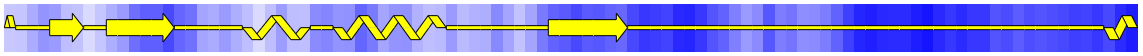


c. C-alpha chirality: abs. deviation of zeta torsion



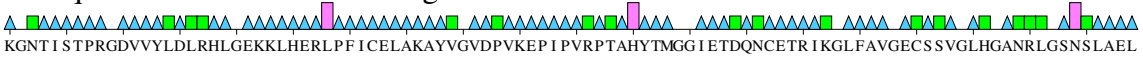
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



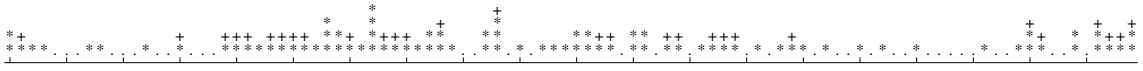
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

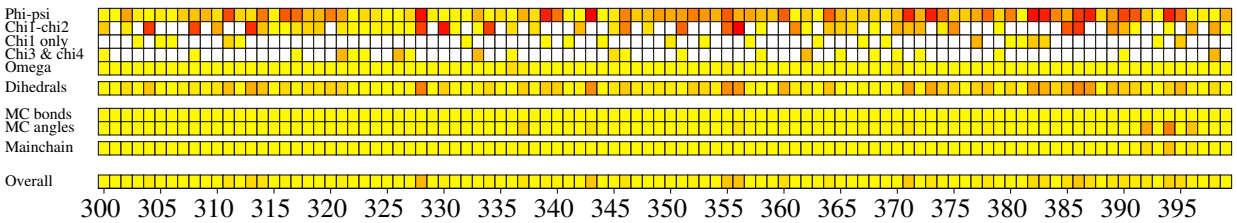


KGNT I S T P R G D V V Y L D L R H L G E K K L H E R L P F I C E L A K A Y V G V D P V K E P I P V R P T A H Y T M G G I E T D Q N C E T R I K G L F A V G E C S S V G L H G A N R L G S N S L A E L

f. Max. deviation (see listing)

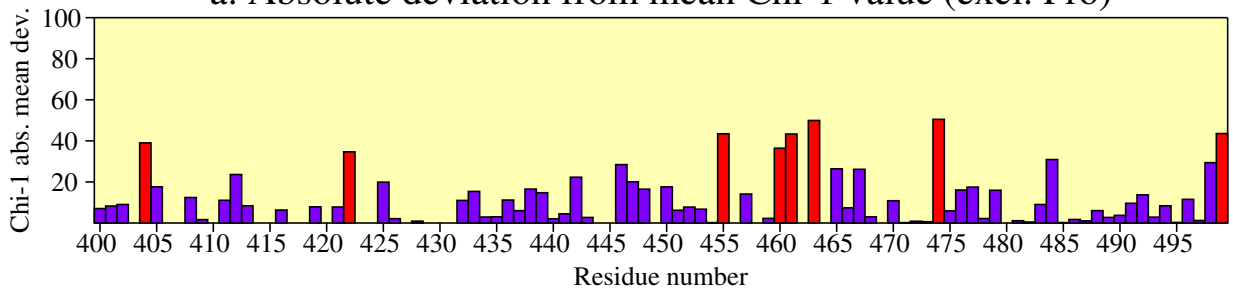


g. G-factors

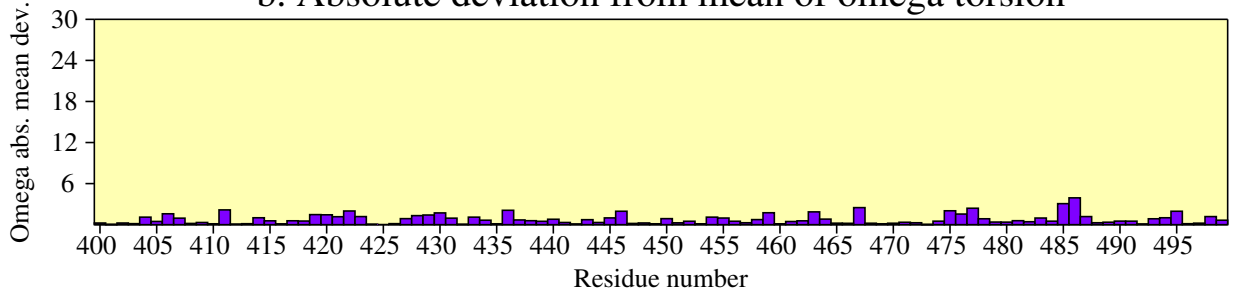


Residue properties
2b76

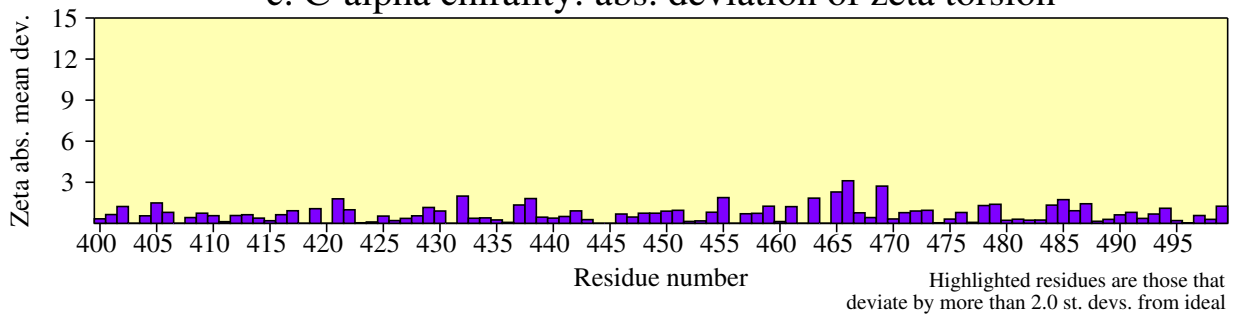
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

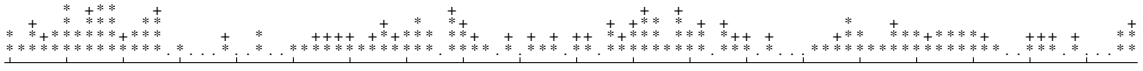
d. Secondary structure & estimated accessibility

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

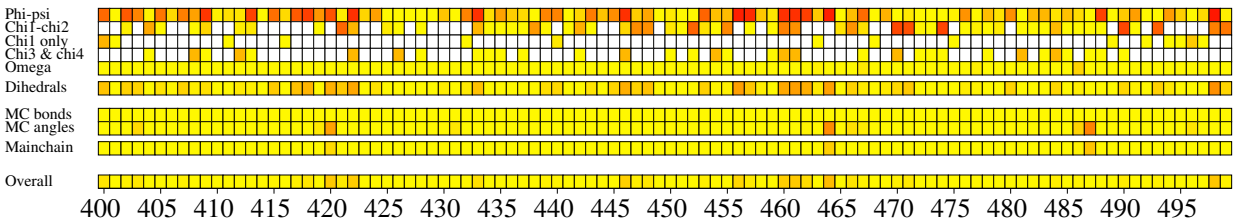
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

VVFGRLAGEQATERAATAGNGNEAAIEAQAAGVEQRLKDLVNQDGGENWAKIRDEMGLAMEEGCGIYRTPELMQKTIDKLAELQERFKRVRITDTSSVFN

f. Max. deviation (see listing)

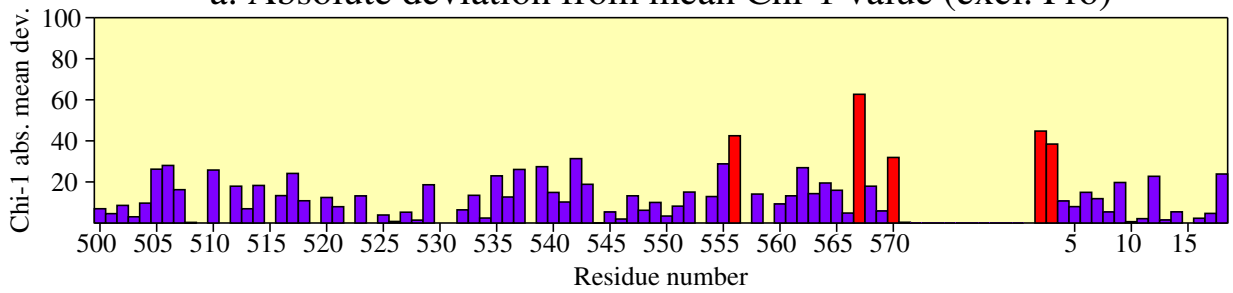


g. G-factors

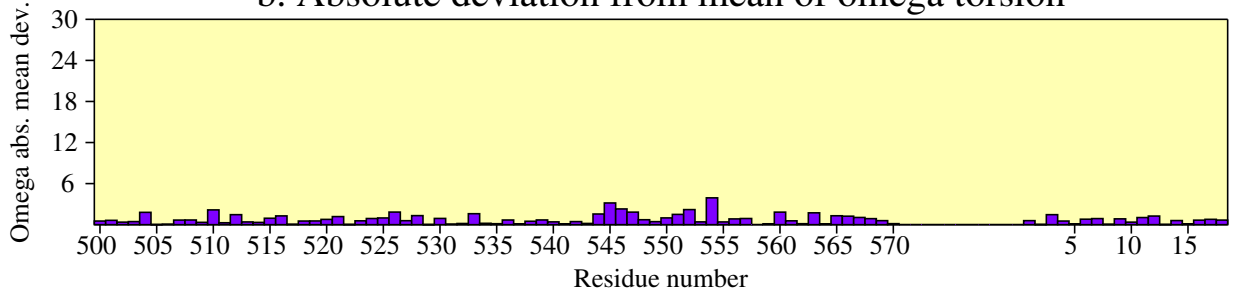


Residue properties
2b76

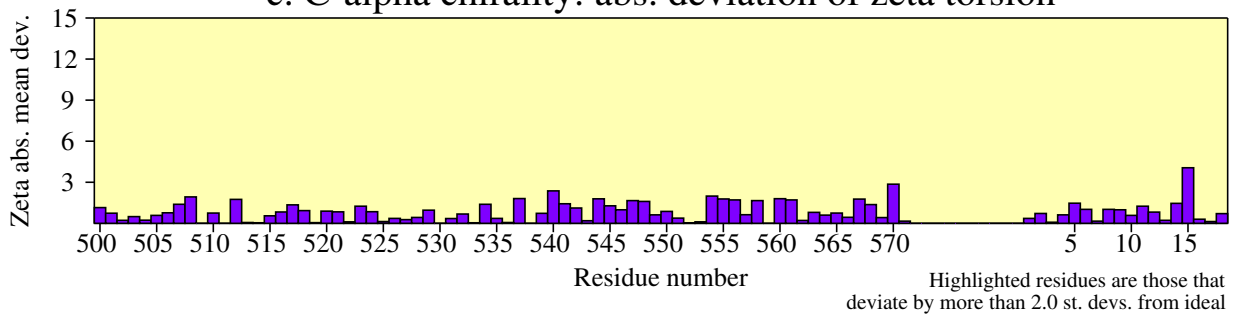
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

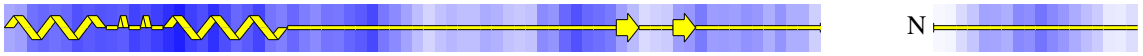


c. C-alpha chirality: abs. deviation of zeta torsion



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

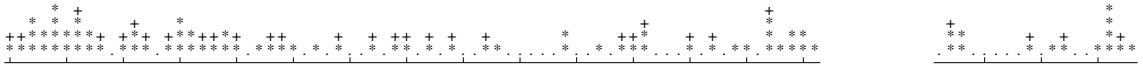
d. Secondary structure & estimated accessibility



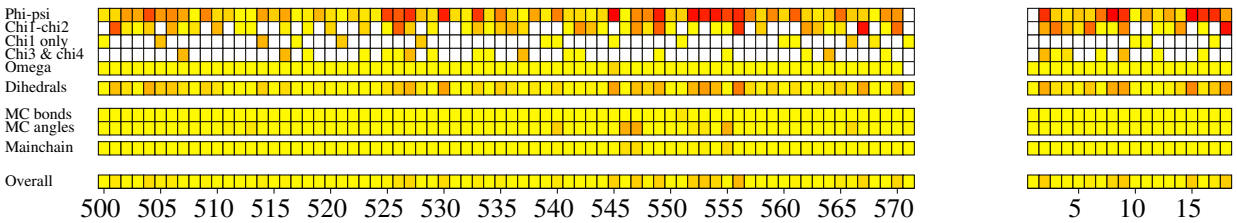
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

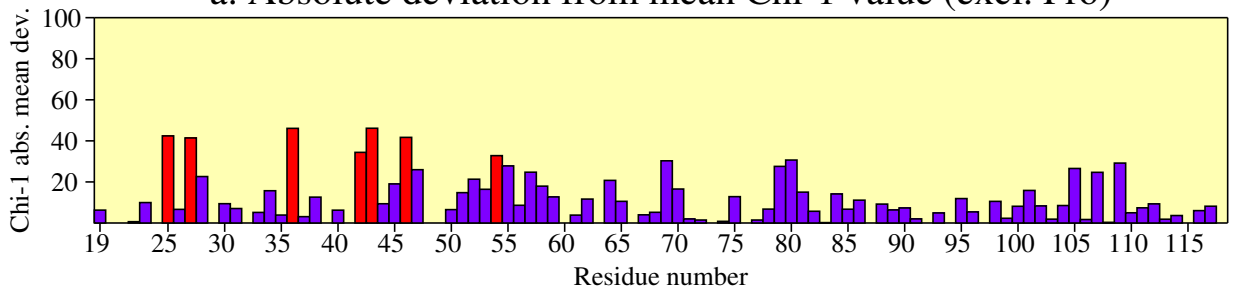


g. G-factors

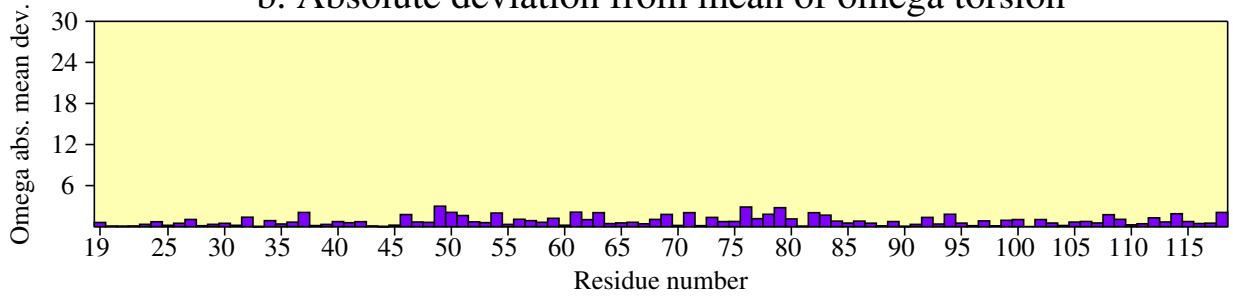


Residue properties
2b76

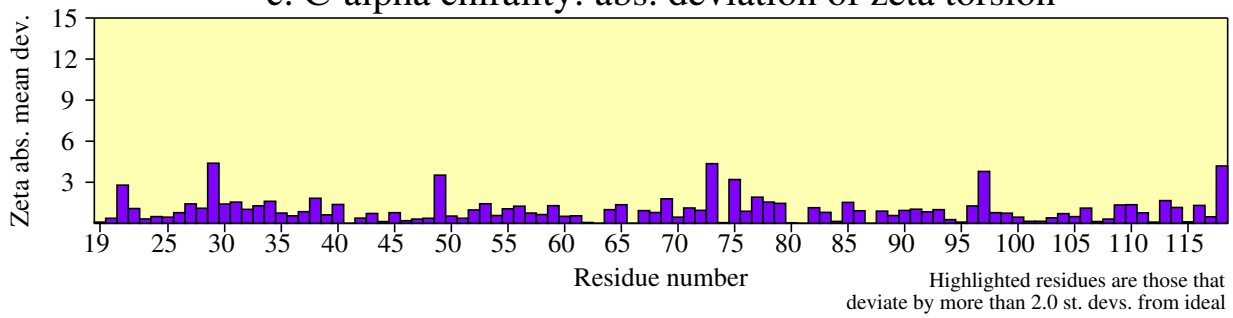
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

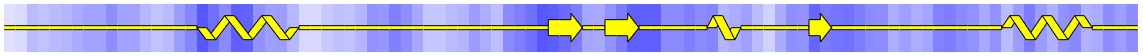


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



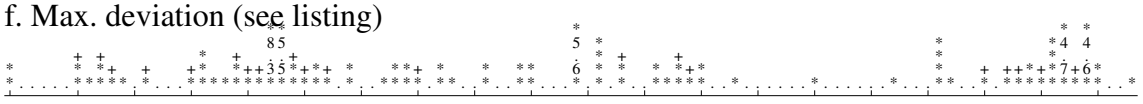
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

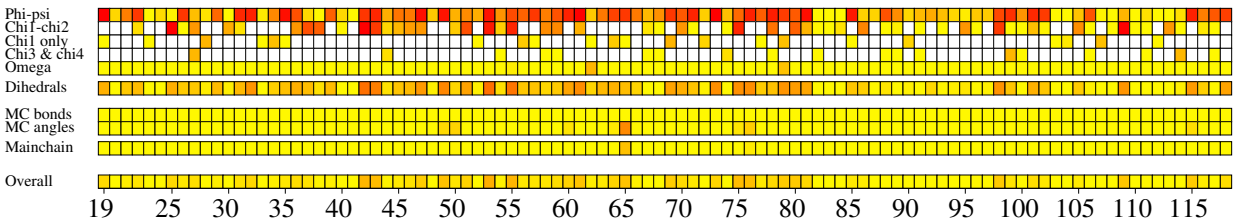
Most favoured Allowed Generous Disallowed

TAPHSAFYEVPYDATTSLLDALGYIKDNLAPDLSYRWSCRMAICGSCGMMVNNVPKLACKTFLRDYTDGMKVEALANFPIERDLVVDMTHFIESLEAIKP

f. Max. deviation (see listing)

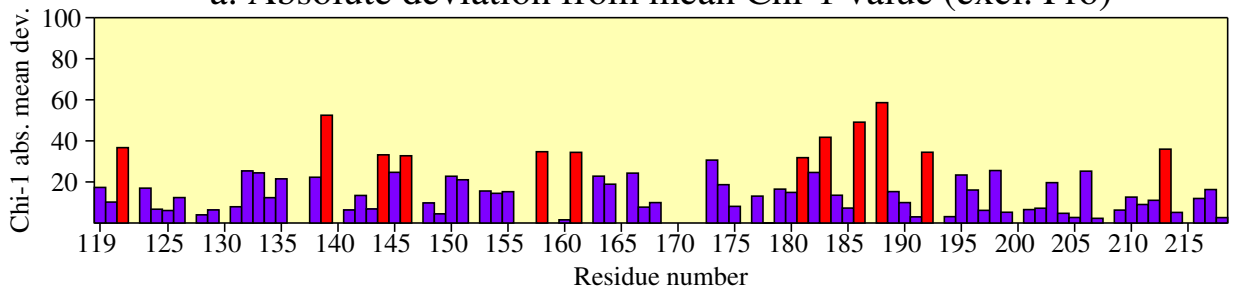


g. G-factors

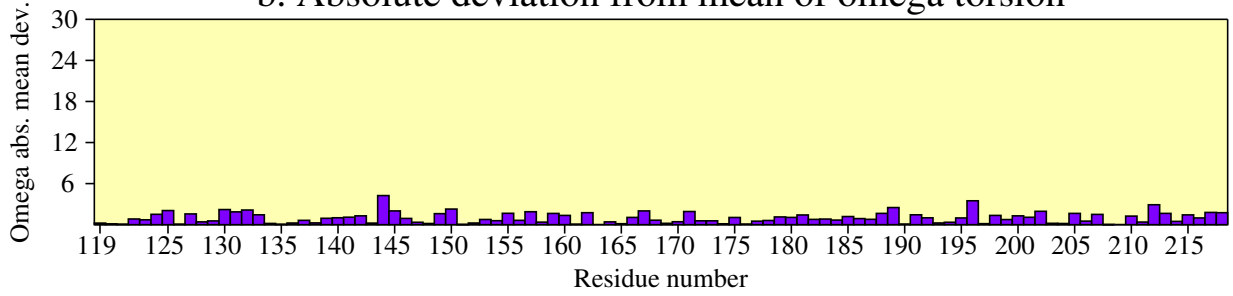


Residue properties
2b76

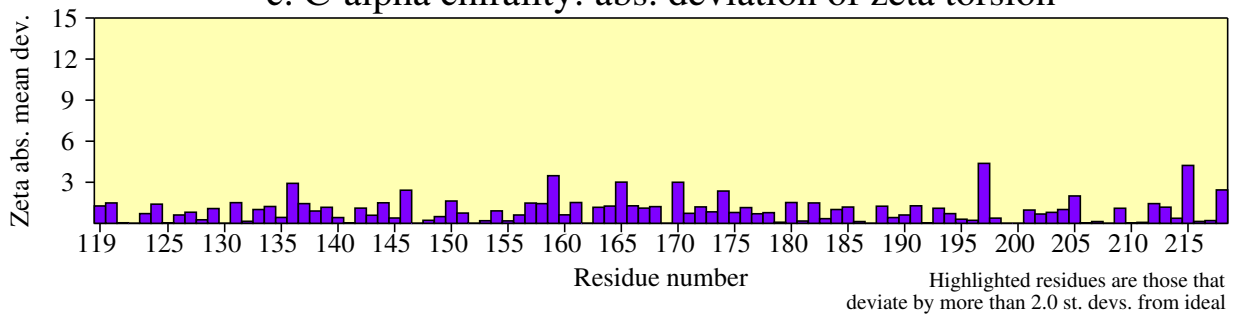
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

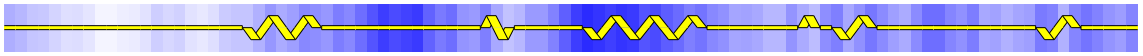


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

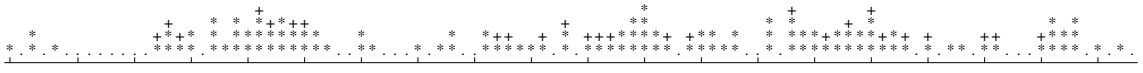


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

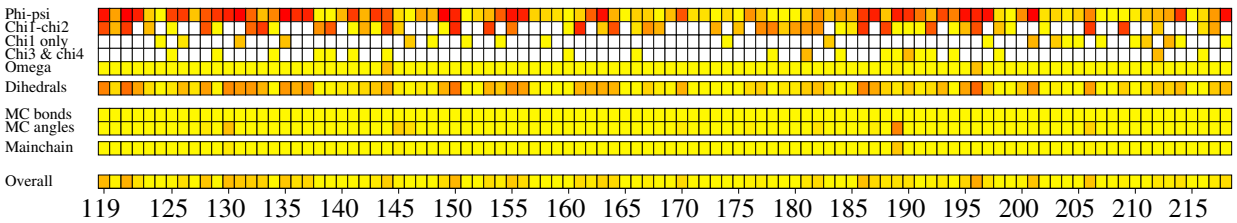
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

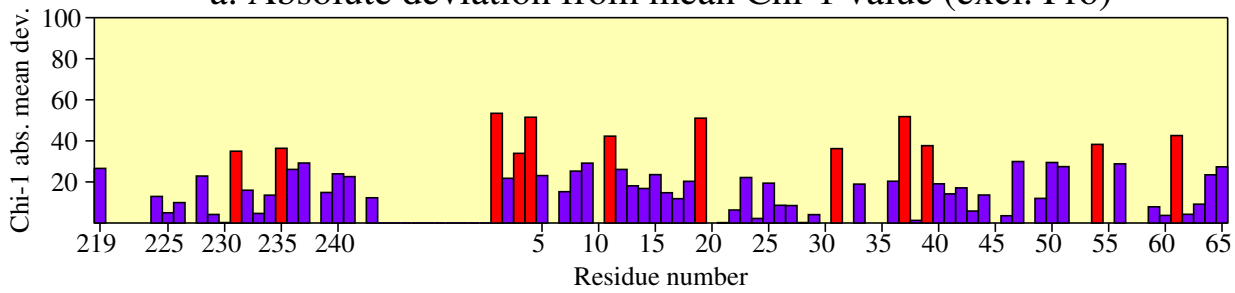


g. G-factors

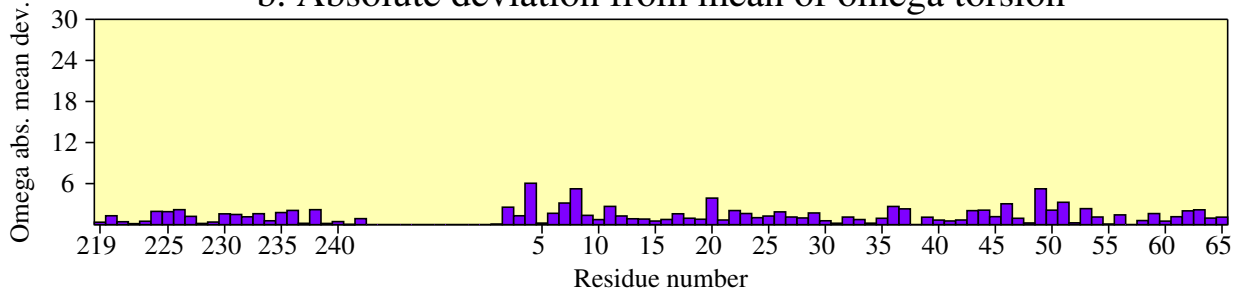


Residue properties
2b76

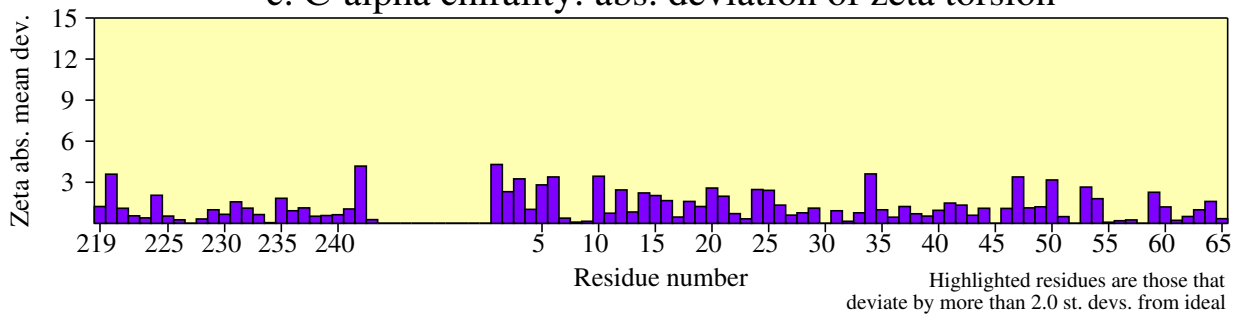
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

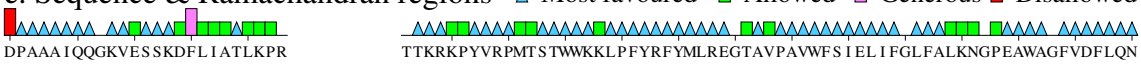


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

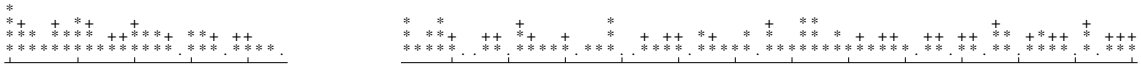
d. Secondary structure & estimated accessibility

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

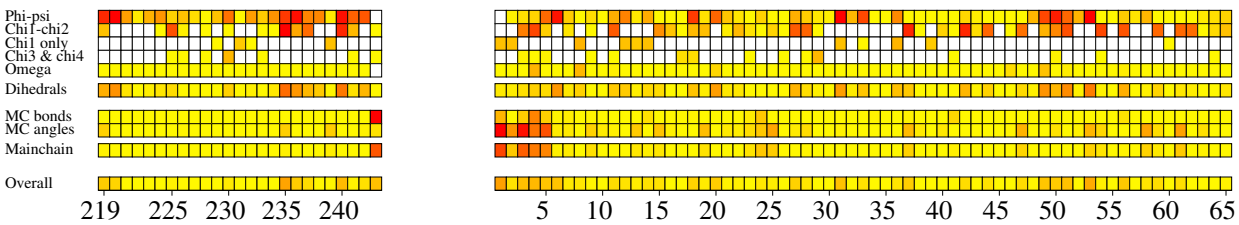
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

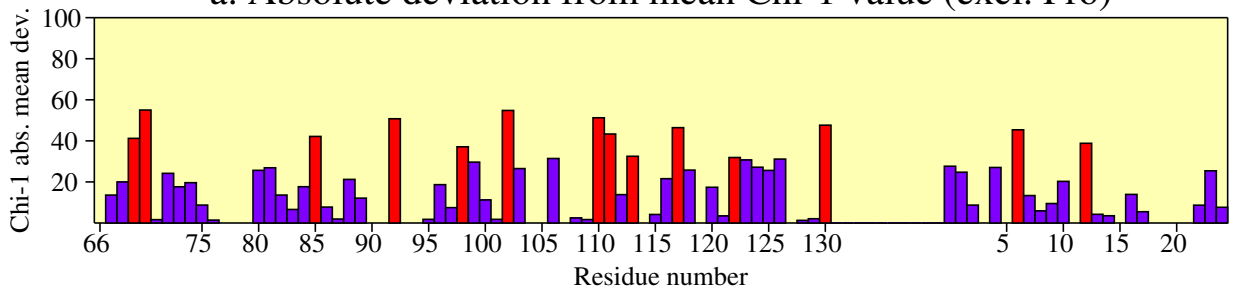


g. G-factors

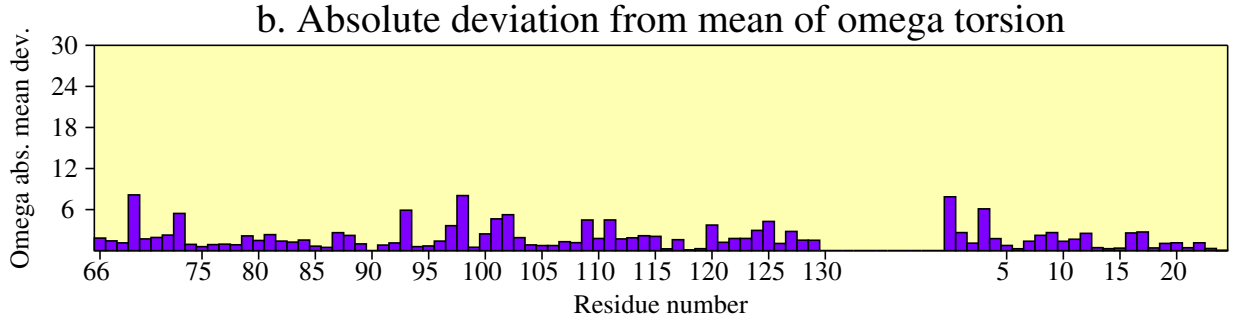


Residue properties
2b76

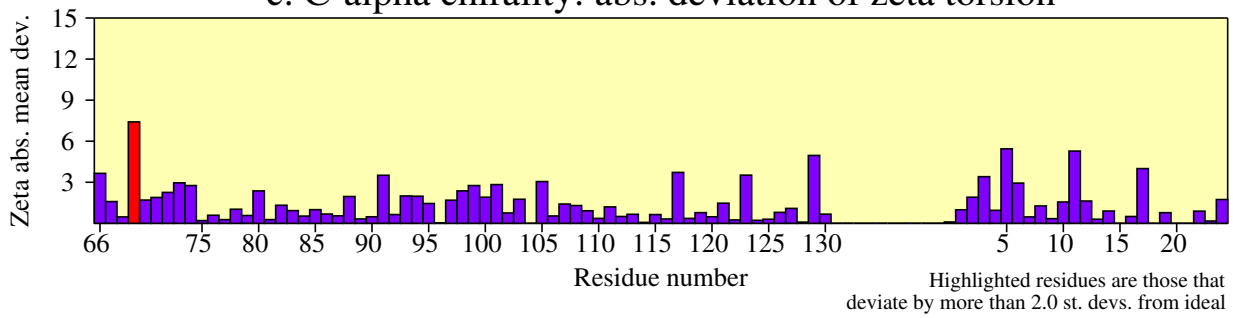
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



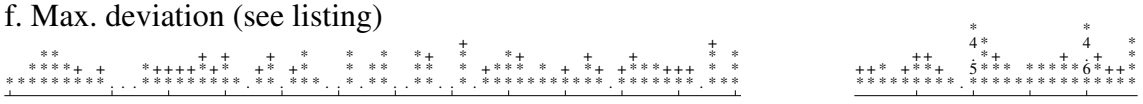
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

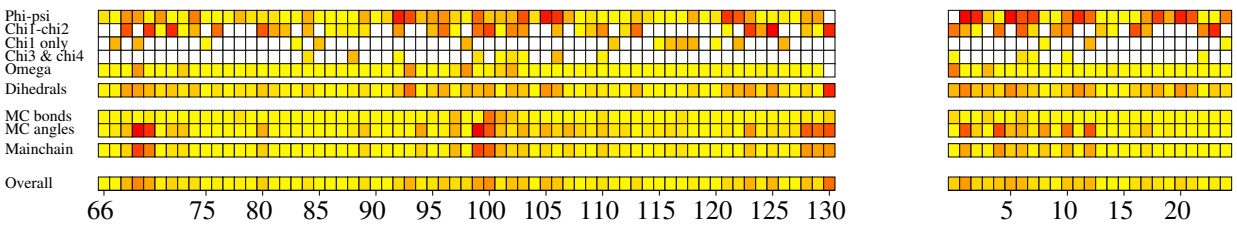
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

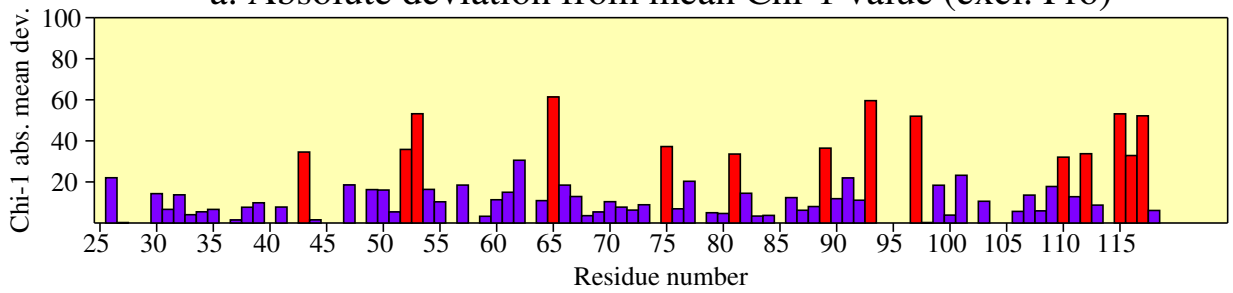


g. G-factors

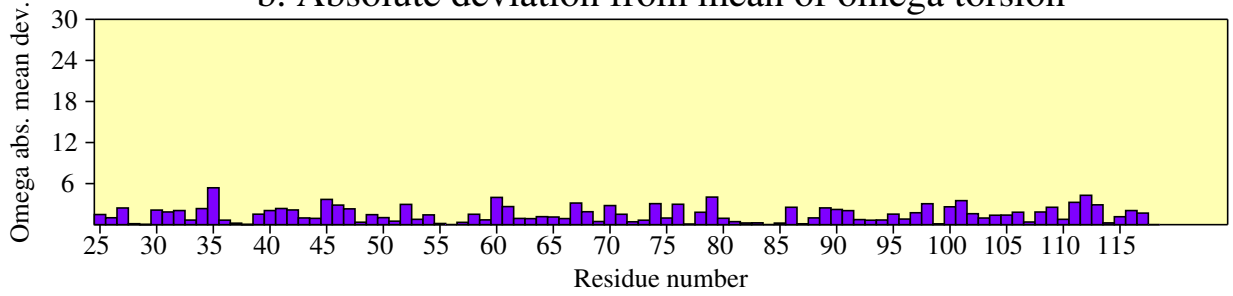


Residue properties
2b76

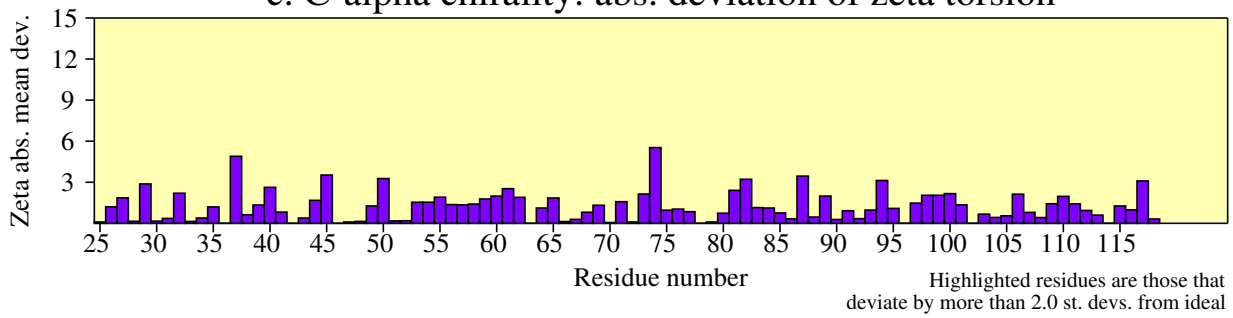
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



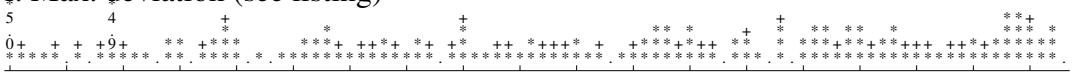
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

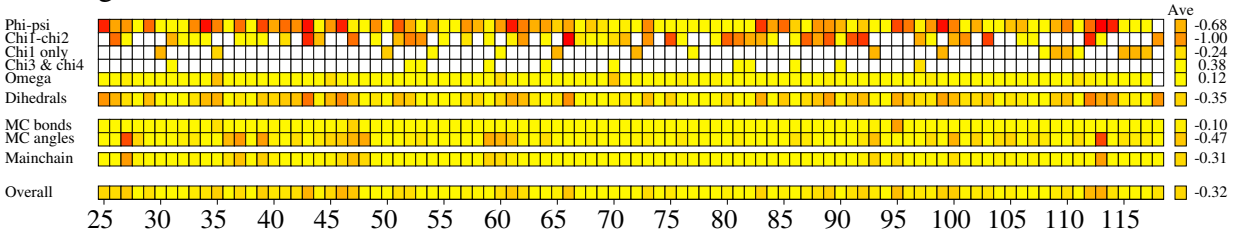
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

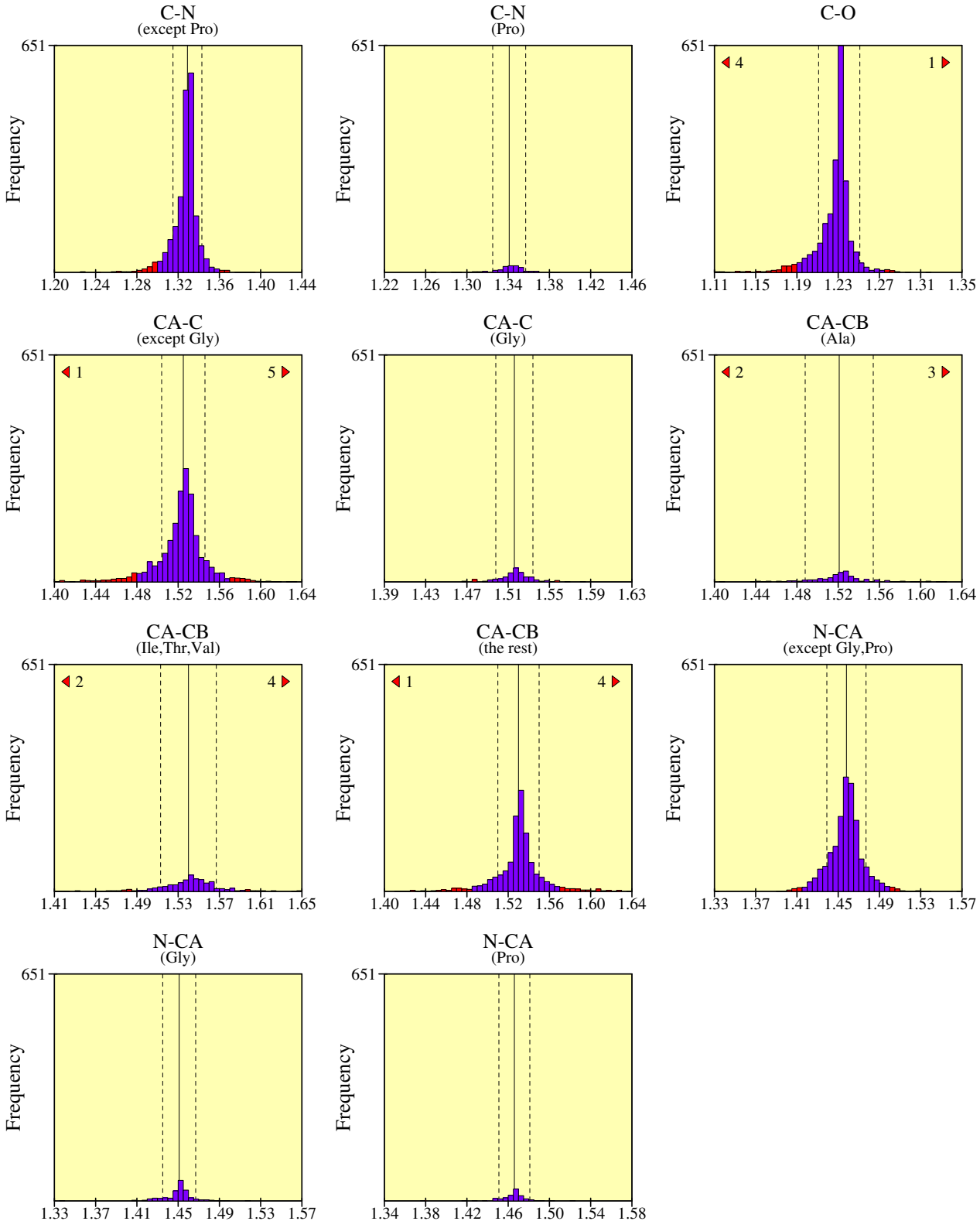


g. G-factors



Main-chain bond lengths

2b76

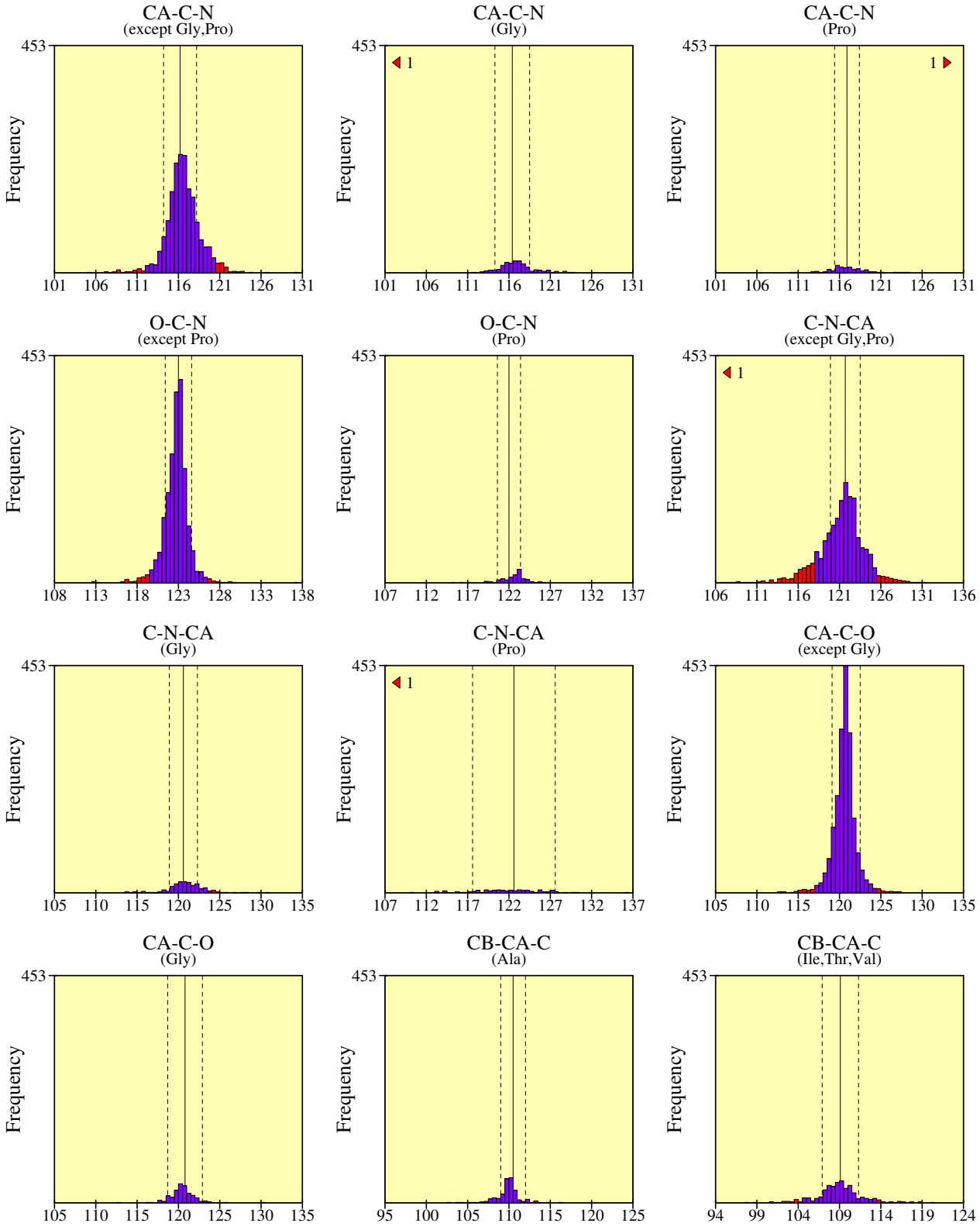


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

2b76

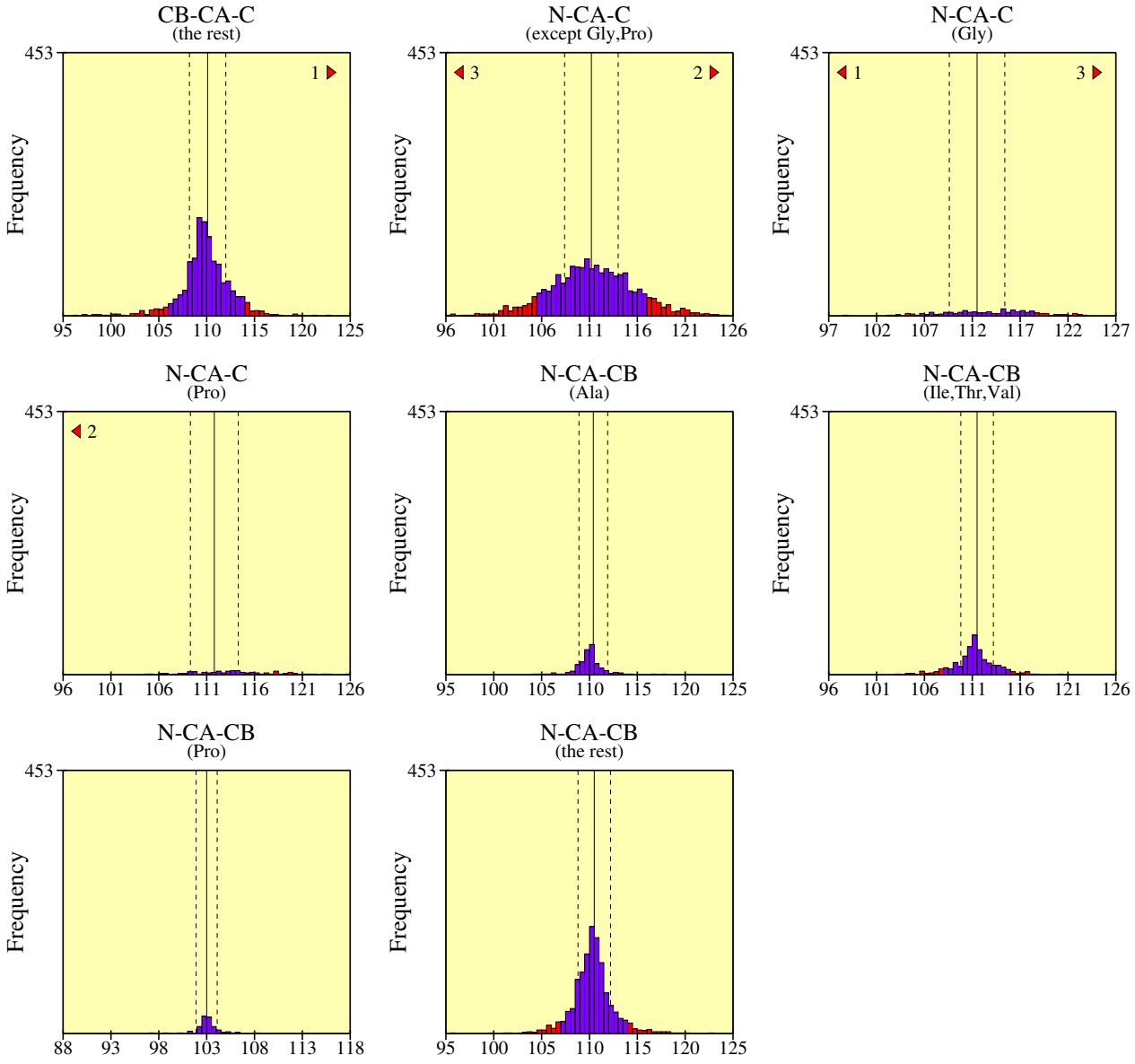


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

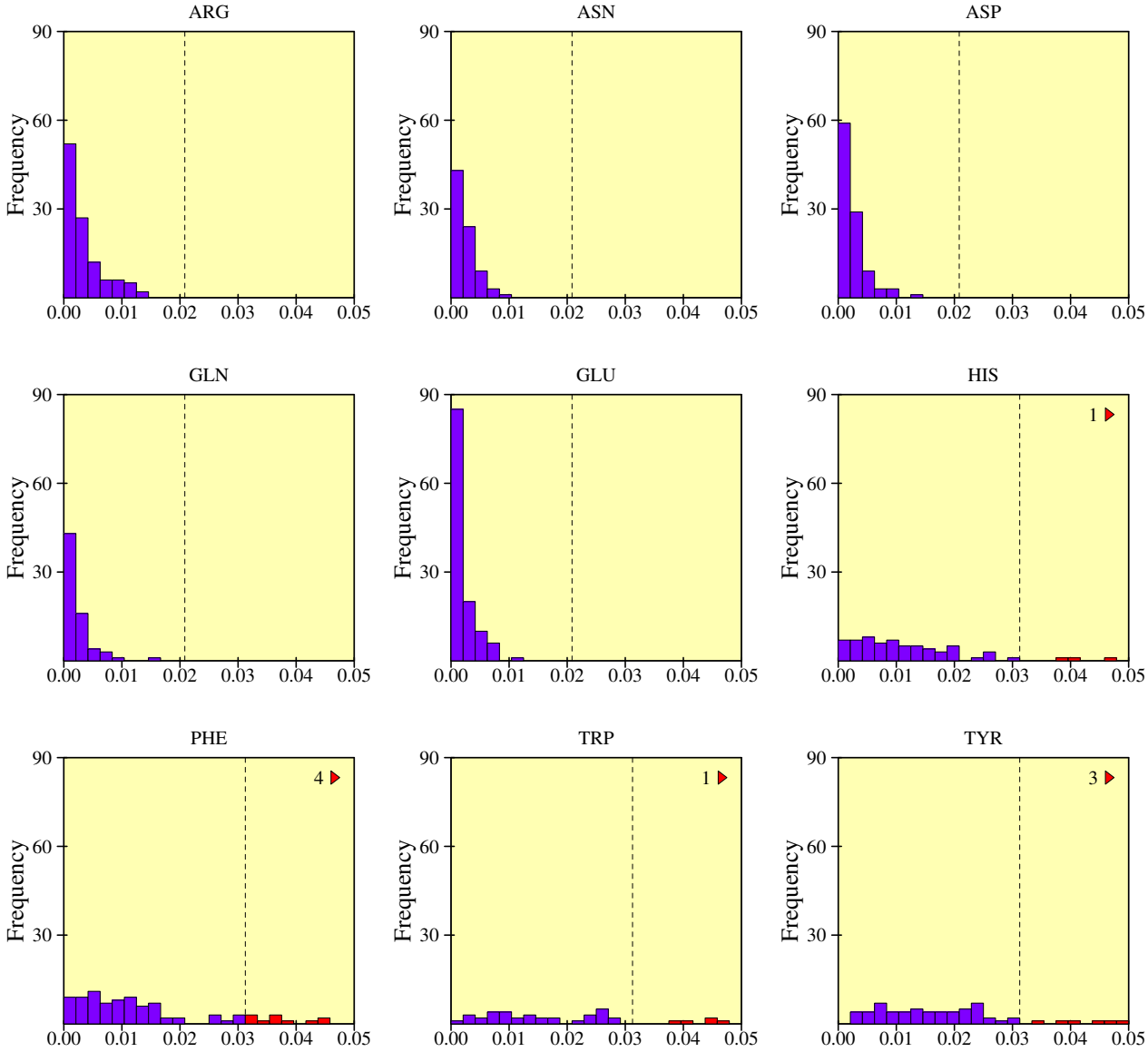
2b76



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

2b76

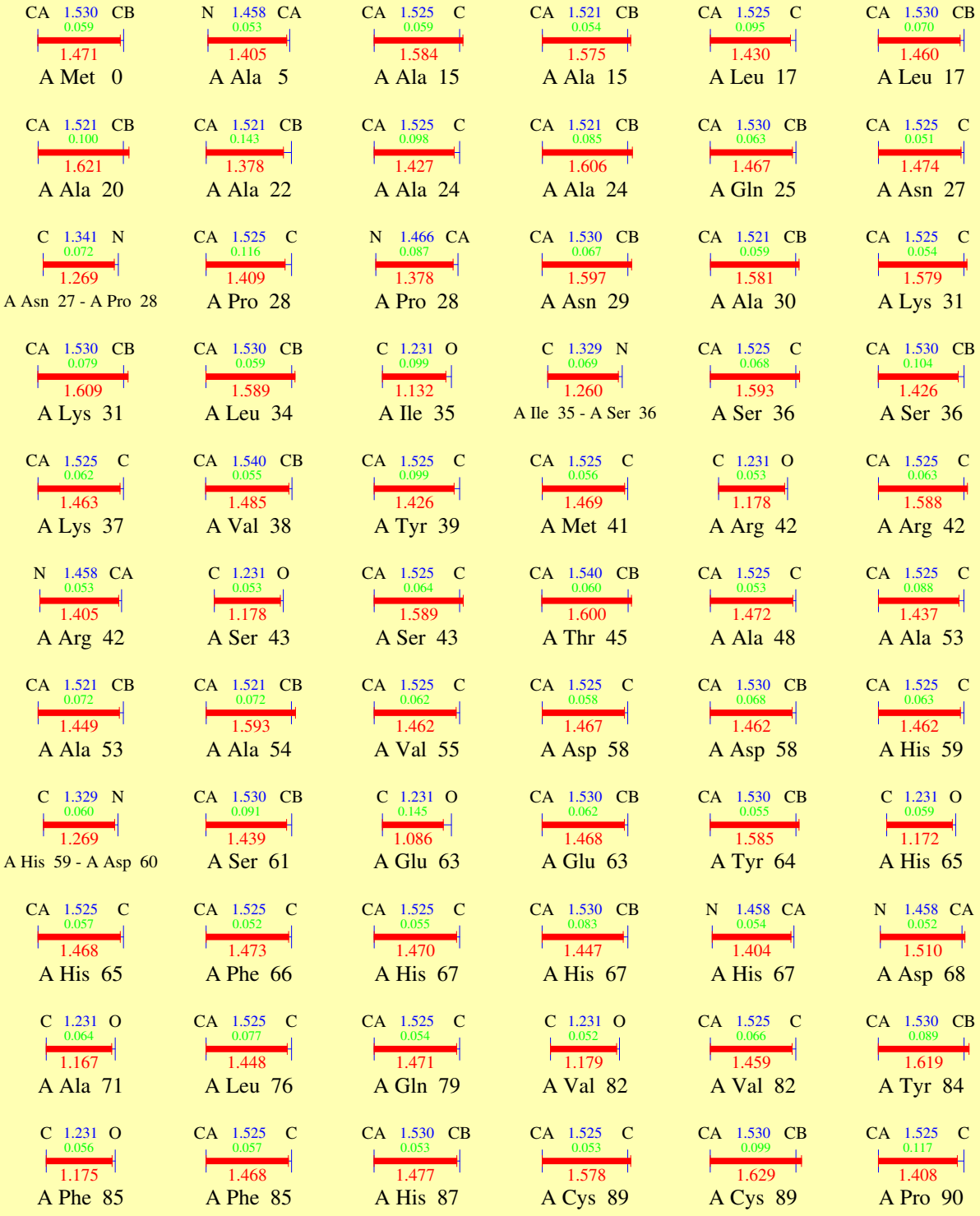


Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

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

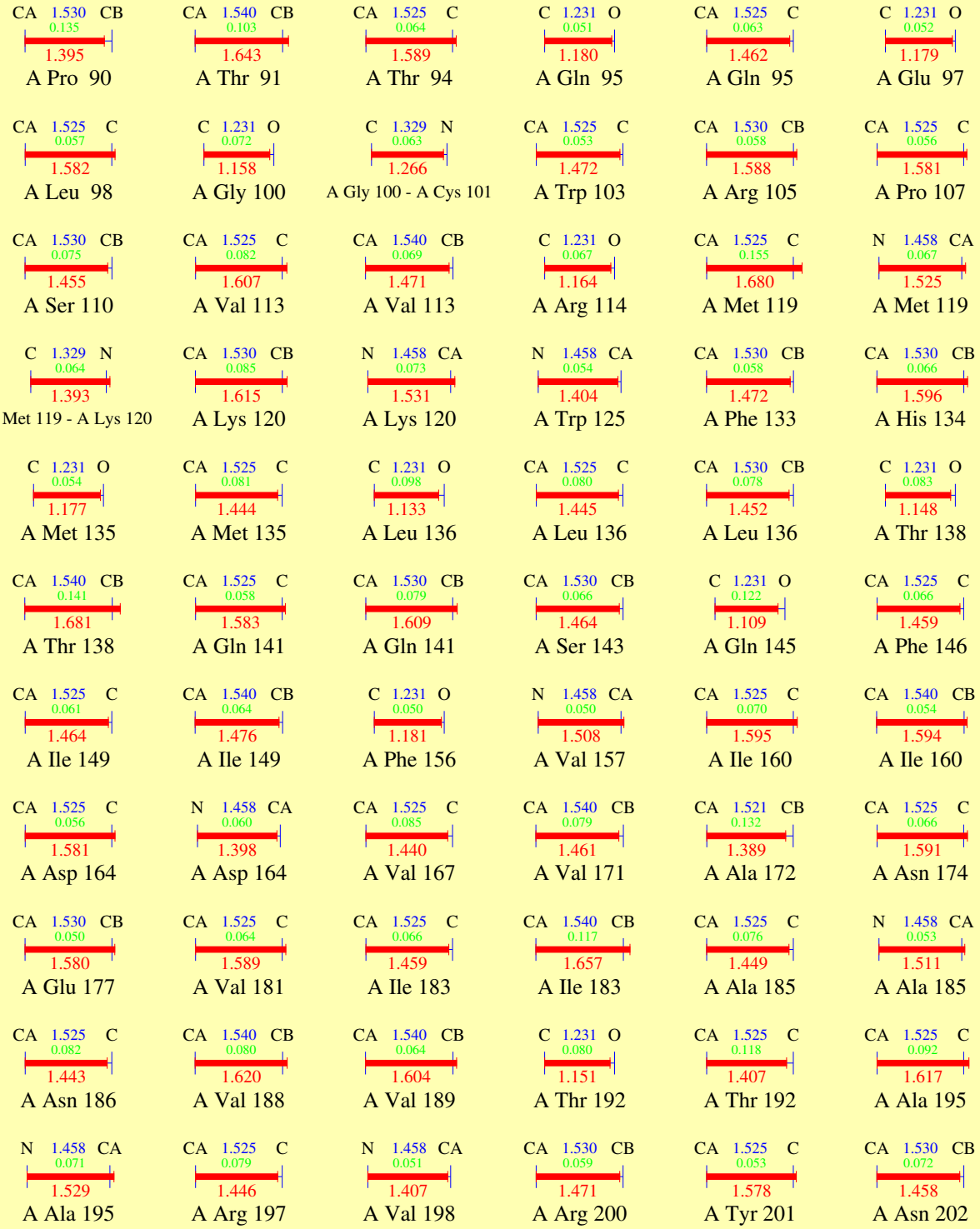
Distorted geometry
2b76

Main-chain bond lengths



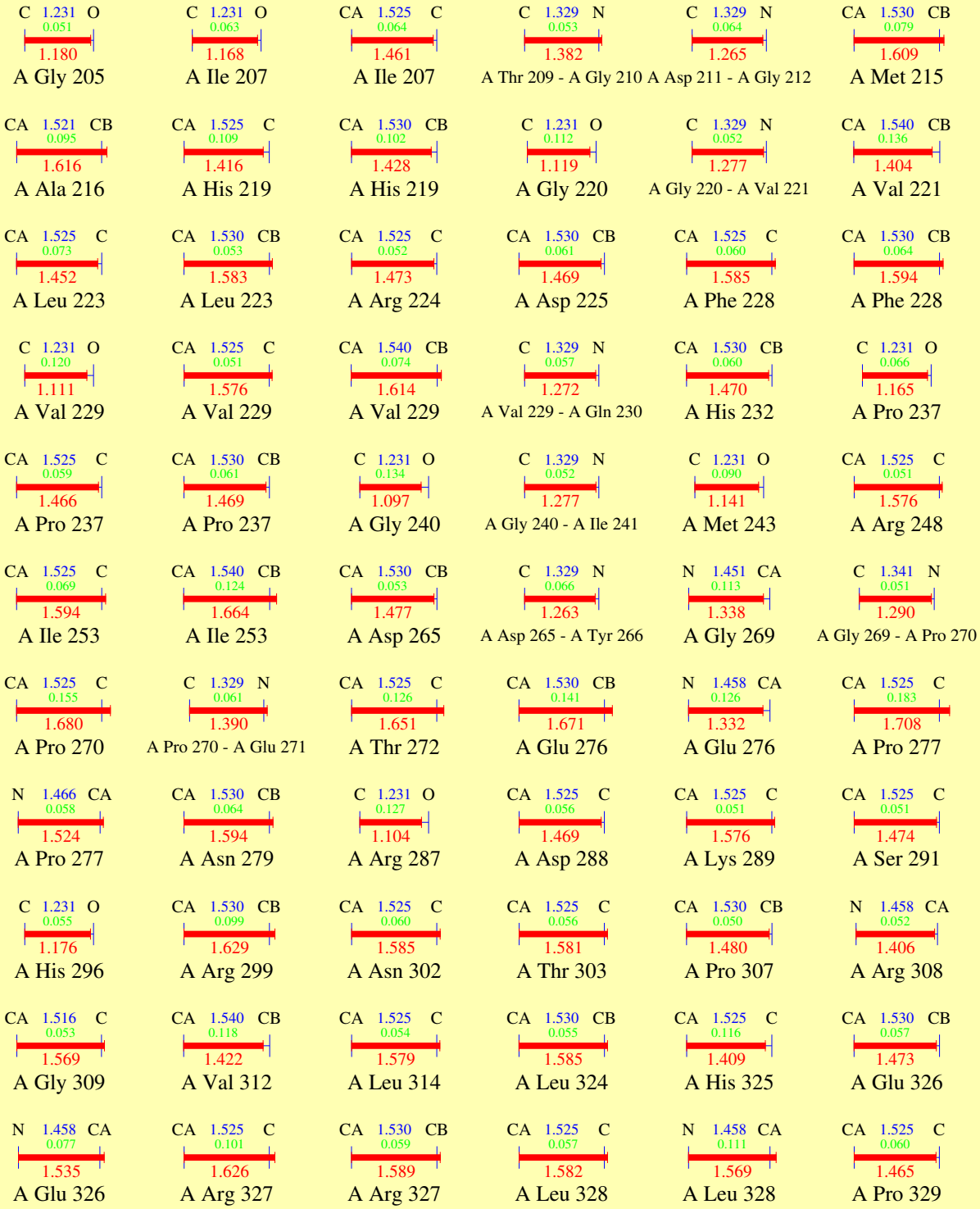
Distorted geometry
2b76

Main-chain bond lengths (contd)



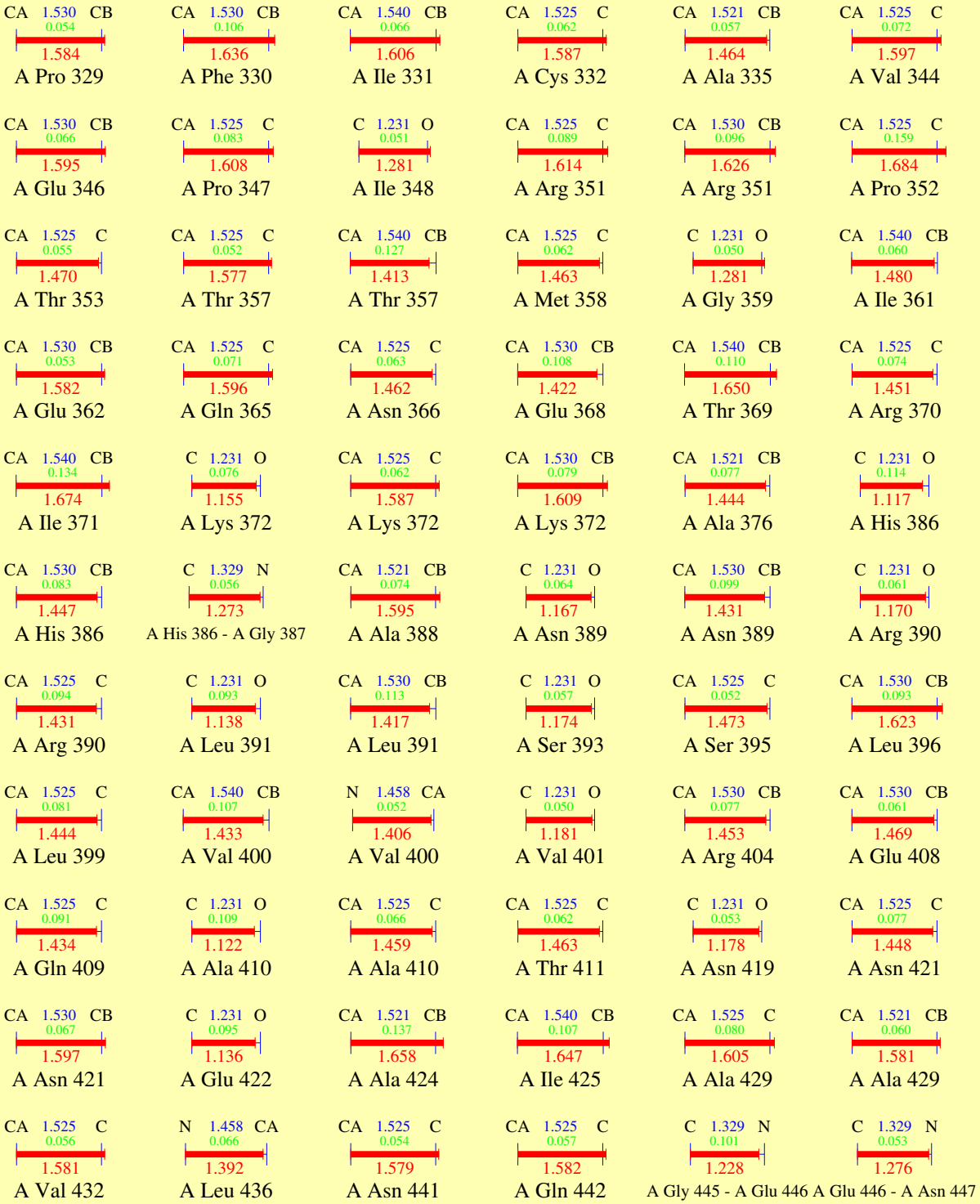
Distorted geometry
2b76

Main-chain bond lengths (contd)



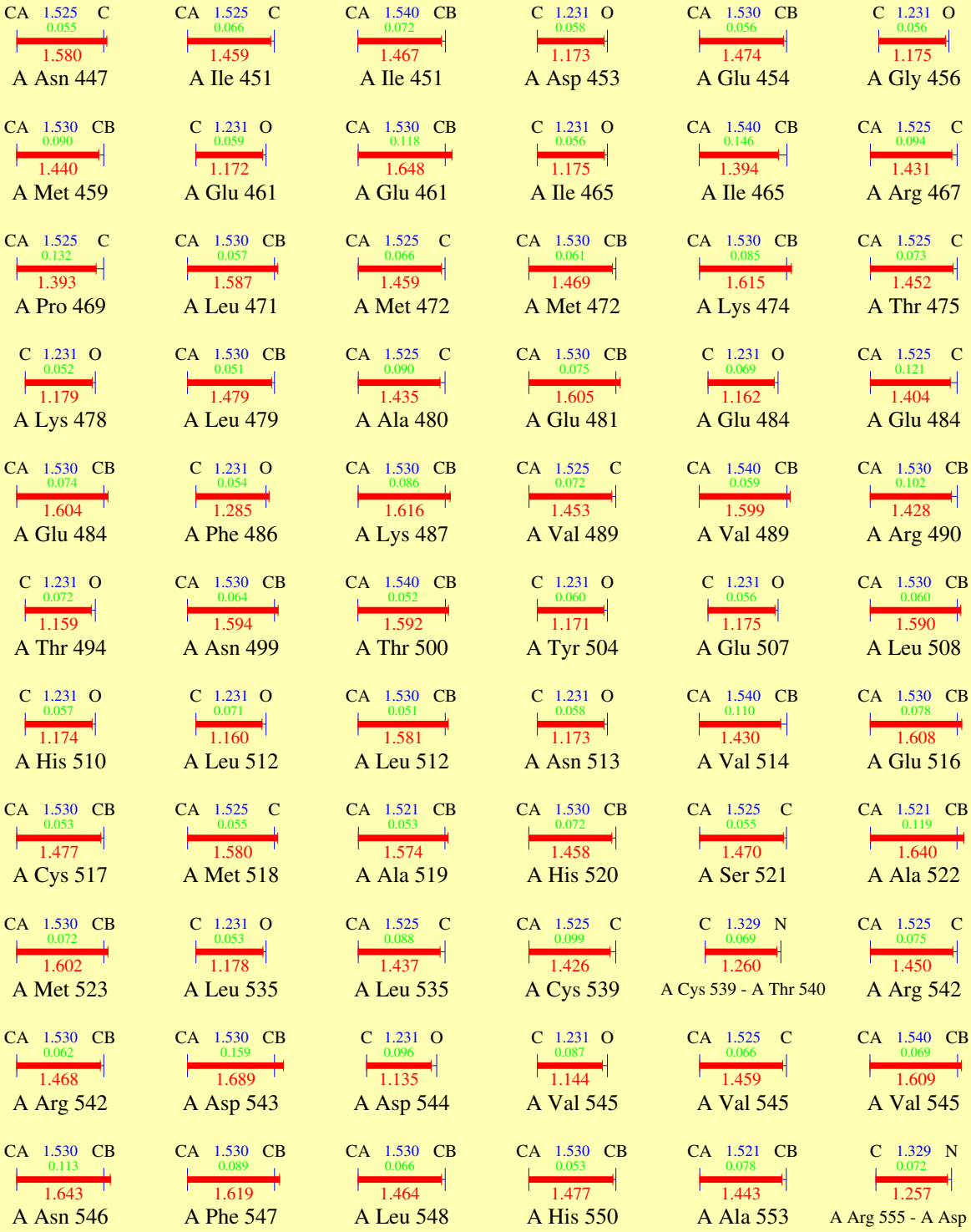
Distorted geometry
2b76

Main-chain bond lengths (contd)



Distorted geometry
2b76

Main-chain bond lengths (contd)



Distorted geometry
2b76

Main-chain bond lengths (contd)

CA 1.525 C 0.109 1.633 A Ala 557
N 1.458 CA 0.063 1.521 A Ala 557
N 1.458 CA 0.053 1.511 A Asp 558
CA 1.540 CB 0.082 1.457 A Thr 560
CA 1.540 CB 0.059 1.481 A Thr 561
CA 1.530 CB 0.055 1.585 A Arg 562
CA 1.530 CB 0.093 1.437 A Leu 563
C 1.231 O 0.051 1.180 A Tyr 565
CA 1.530 CB 0.074 1.456 A Asp 567
CA 1.530 CB 0.117 1.413 A Pro 574
CA 1.525 C 0.100 1.425 A Pro 575
C 1.329 N 0.100 1.229 A Pro 575 - A Ala 576
C 1.231 O 0.063 1.168 A Ala 576
CA 1.521 CB 0.174 1.695 A Ala 576
N 1.458 CA 0.054 1.404 A Ala 576
CA 1.525 C 0.059 1.584 B Asn 5
CA 1.540 CB 0.054 1.486 B Val 11
CA 1.525 C 0.070 1.455 B Glu 16
N 1.458 CA 0.051 1.509 B Glu 16
CA 1.530 CB 0.061 1.469 B Tyr 30
C 1.231 O 0.080 1.151 B Asp 31
CA 1.521 CB 0.085 1.436 B Ala 39
C 1.231 O 0.055 1.176 B Tyr 42
CA 1.530 CB 0.079 1.451 B Tyr 42
CA 1.530 CB 0.057 1.473 B Asn 46
CA 1.530 CB 0.057 1.473 B Asp 50
CA 1.530 CB 0.056 1.474 B Tyr 53
C 1.231 O 0.119 1.112 B Ser 56
CA 1.540 CB 0.090 1.450 B Val 69
CA 1.525 C 0.051 1.474 B Asn 71
CA 1.525 C 0.058 1.467 B Cys 77
C 1.231 O 0.051 1.180 B Thr 79
CA 1.521 CB 0.057 1.464 B Ala 92
CA 1.540 CB 0.080 1.460 B Ile 98
CA 1.540 CB 0.066 1.474 B Val 104
CA 1.516 C 0.069 1.585 B Gly 130
N 1.451 CA 0.064 1.515 B Gly 130
CA 1.525 C 0.063 1.462 B Ile 133
CA 1.540 CB 0.061 1.479 B Ile 133
CA 1.525 C 0.052 1.473 B Thr 135
CA 1.540 CB 0.071 1.469 B Thr 135
C 1.231 O 0.063 1.168 B Pro 136
CA 1.530 CB 0.059 1.471 B Pro 136
CA 1.525 C 0.060 1.465 B Leu 175
CA 1.540 CB 0.121 1.419 B Val 207
CA 1.540 CB 0.060 1.480 B Val 213
CA 1.521 CB 0.068 1.453 B Ala 221
C 1.231 O 0.089 1.142 B Asp 234
C 1.231 O 0.056 1.175 B Leu 236
CA 1.540 CB 0.051 1.591 B Ile 237
CA 1.530 CB 0.080 1.610 B Lys 241
C 1.329 N 0.085 1.244 B Pro 242 - B Arg 243
C 1.231 O 0.087 1.318 C Thr 1
CA 1.540 CB 0.081 1.621 C Thr 1
N 1.458 CA 0.058 1.516 C Thr 1
C 1.231 O 0.055 1.286 C Thr 2
C 1.231 O 0.057 1.288 C Lys 3
CA 1.525 C 0.058 1.467 C Thr 75
CA 1.540 CB 0.065 1.475 C Thr 75
CA 1.521 CB 0.068 1.453 C Ala 93
CA 1.540 CB 0.055 1.595 C Ile 96
CA 1.540 CB 0.057 1.597 C Val 98
CA 1.521 CB 0.054 1.467 C Ala 114
CA 1.540 CB 0.053 1.487 C Val 118
CA 1.530 CB 0.053 1.477 C Trp 130
CA 1.525 C 0.052 1.473 D Pro 3

Distorted geometry
2b76

Main-chain bond lengths (contd)

D Val 93

D Ala 95

D Thr 108

O Thr 1

O Arg 4

O Lys 5

O Val 8

O Thr 14

O Ile 97

O Asp 100

O Asp 100

O Lys 102

O Trp 130

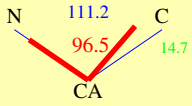
P Lys 6

P Ile 37

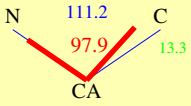
P Ala 95

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

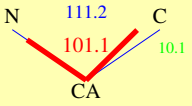
Main-chain bond angles



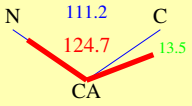
A Gln 1



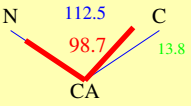
A Phe 3



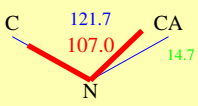
A Gln 4



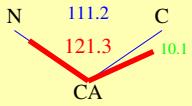
A Ala 12



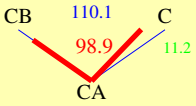
A Gly 13



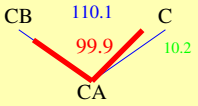
A Pro 28 - A Asn 29



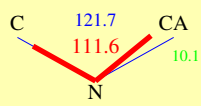
A Ala 30



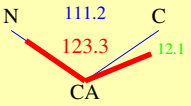
A Ser 61



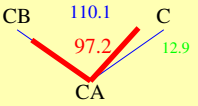
A Asp 68



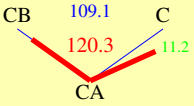
A Leu 76 - A Cys 77



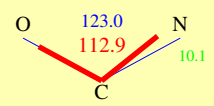
A Arg 105



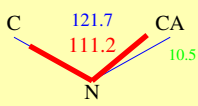
A Arg 106



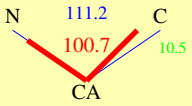
A Val 113



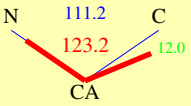
A Gly 118 - A Met 119



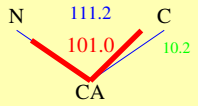
A Gly 118 - A Met 119



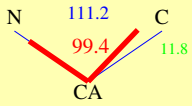
A Ala 127



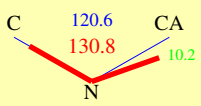
A Thr 131



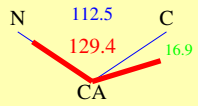
A Val 167



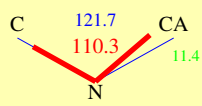
A Val 189



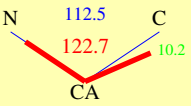
A Gly 193 - A Gly 194



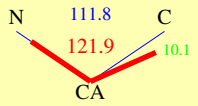
A Gly 194



A Arg 197 - A Val 198



A Gly 206



A Pro 222

A Leu 223

A Val 229 - A Gln 230

A Pro 233

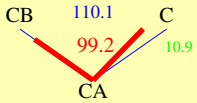
A Met 243

A Gly 249

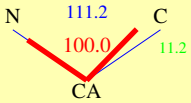
A Tyr 262

Distorted geometry
2b76

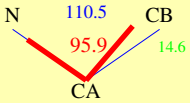
Main-chain bond angles (contd)



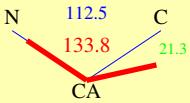
A Asp 265



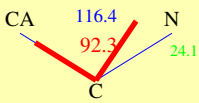
A Tyr 266



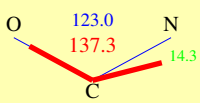
A Tyr 266



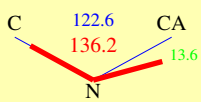
A Gly 269



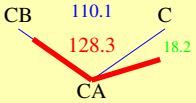
A Gly 269 - A Pro 270



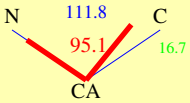
A Gly 269 - A Pro 270



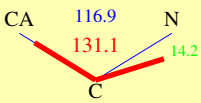
A Gly 269 - A Pro 270



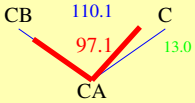
A Pro 270



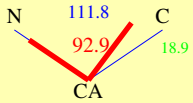
A Pro 270



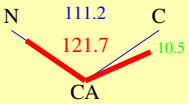
A Pro 270 - A Glu 271



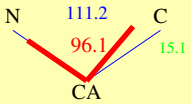
A Glu 276



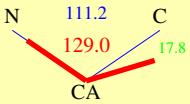
A Pro 277



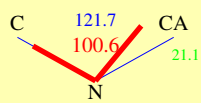
A Asn 302



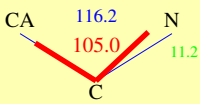
A Val 312



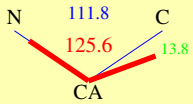
A Glu 321



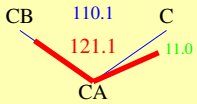
A His 325 - A Glu 326



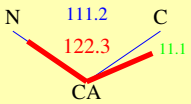
A Glu 326 - A Arg 327



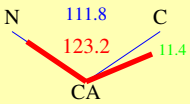
A Pro 329



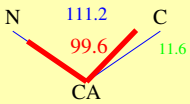
A Phe 330



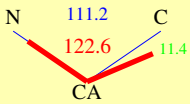
A Val 341



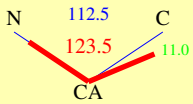
A Pro 343



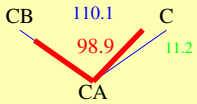
A Glu 346



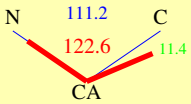
A His 355



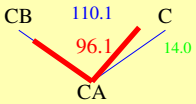
A Gly 360



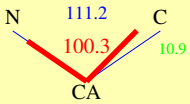
A Asn 366



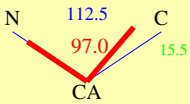
A His 386



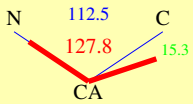
A Leu 391



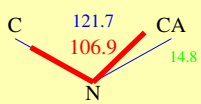
A Ala 410



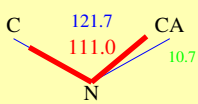
A Gly 418



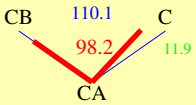
A Gly 445



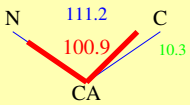
A Glu 446 - A Asn 447



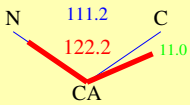
A Asn 447 - A Trp 448



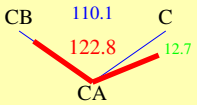
A Trp 448



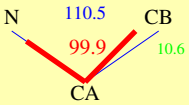
A Val 489



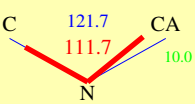
A Thr 492



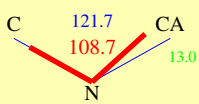
A Cys 517



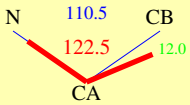
A Cys 517



A Ala 519 - A His 520



A Gly 538 - A Cys 539



A Asp 544

A Val 545

A Phe 547

A Arg 555 - A Asp 556

A Asp 556 - A Ala 557

A Asp 556 - A Ala 557

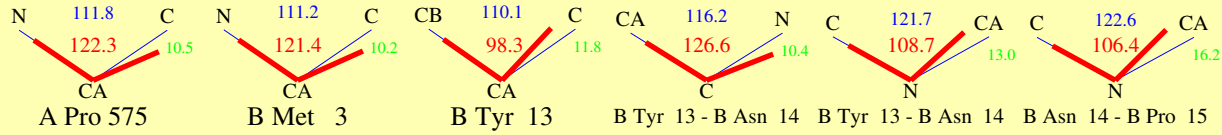
A Thr 560

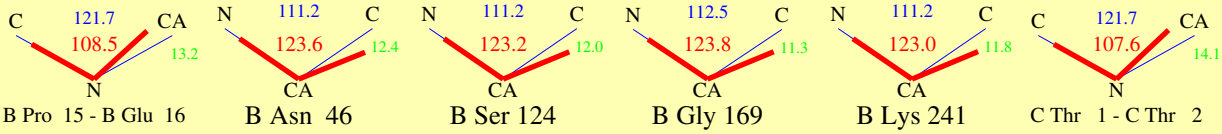
A Ser 566

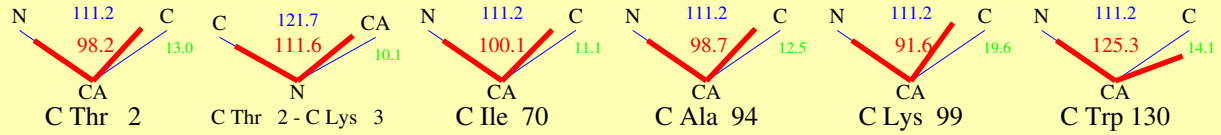
A Leu 573

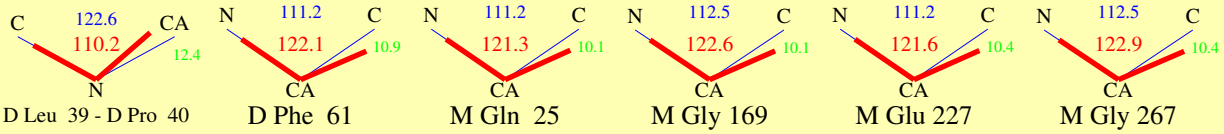
Distorted geometry
2b76

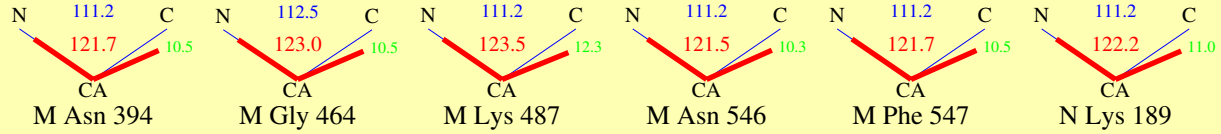
Main-chain bond angles (contd)

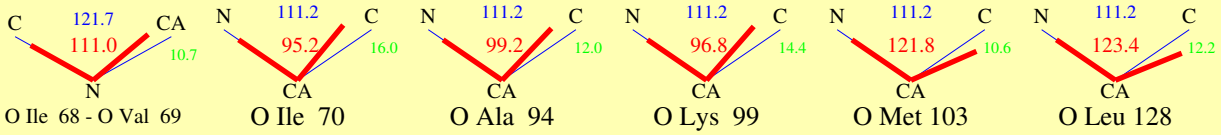


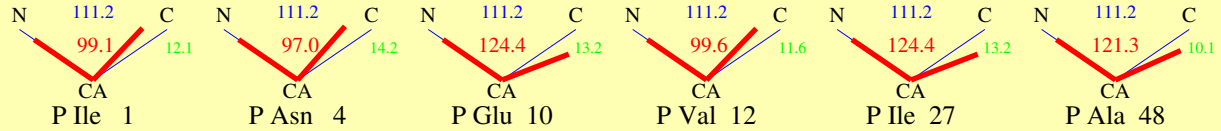








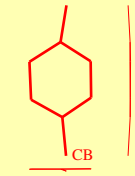




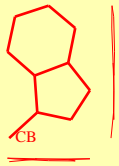
Bond angles differing by > 10.0 degrees from small-molec values. Values shown: "ideal", actual, diff.

Distorted geometry
2b76

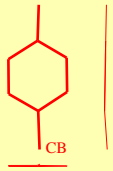
Planar groups



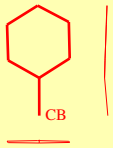
0.037
A Tyr 64



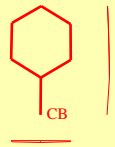
0.043
A Trp 75



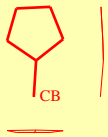
0.033
A Tyr 84



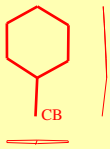
0.043
A Phe 133



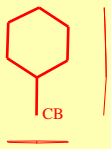
0.034
A Phe 152



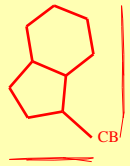
0.045
A His 219



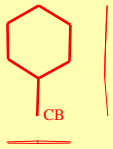
0.060
A Phe 228



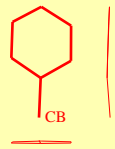
0.034
A Phe 402



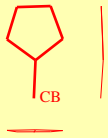
0.046
A Trp 448



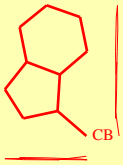
0.043
A Phe 498



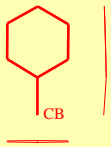
0.040
A Phe 547



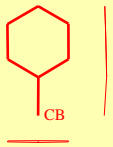
0.036
A His 550



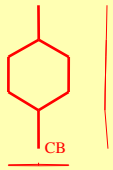
0.044
B Trp 55



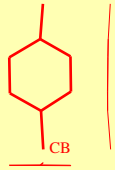
0.033
B Phe 80



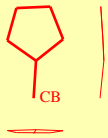
0.032
B Phe 109



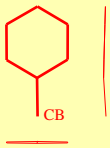
0.038
B Tyr 142



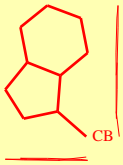
0.045
B Tyr 179



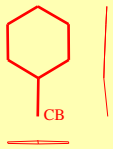
0.055
B His 217



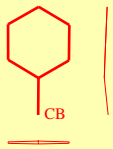
0.031
C Phe 21



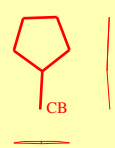
0.039
C Trp 113



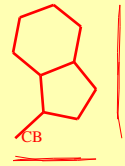
0.052
C Phe 125



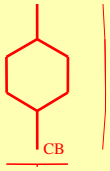
0.050
D Phe 13



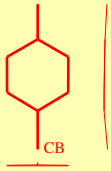
0.040
D His 80



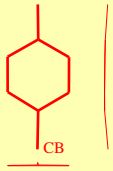
0.053
D Trp 98



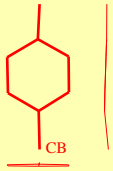
0.043
M Tyr 356



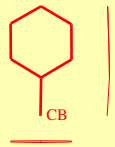
0.050
N Tyr 30



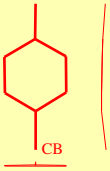
0.053
N Tyr 209



0.047
O Tyr 7



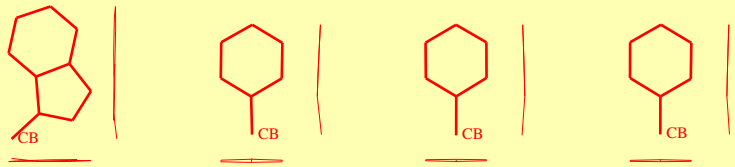
0.031
O Phe 87



0.065
O Tyr 129

Distorted geometry
2b76

Planar groups (contd)



0.038	0.055	0.036	0.034
O Trp 130	P Phe 17	P Phe 66	P Phe 100

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