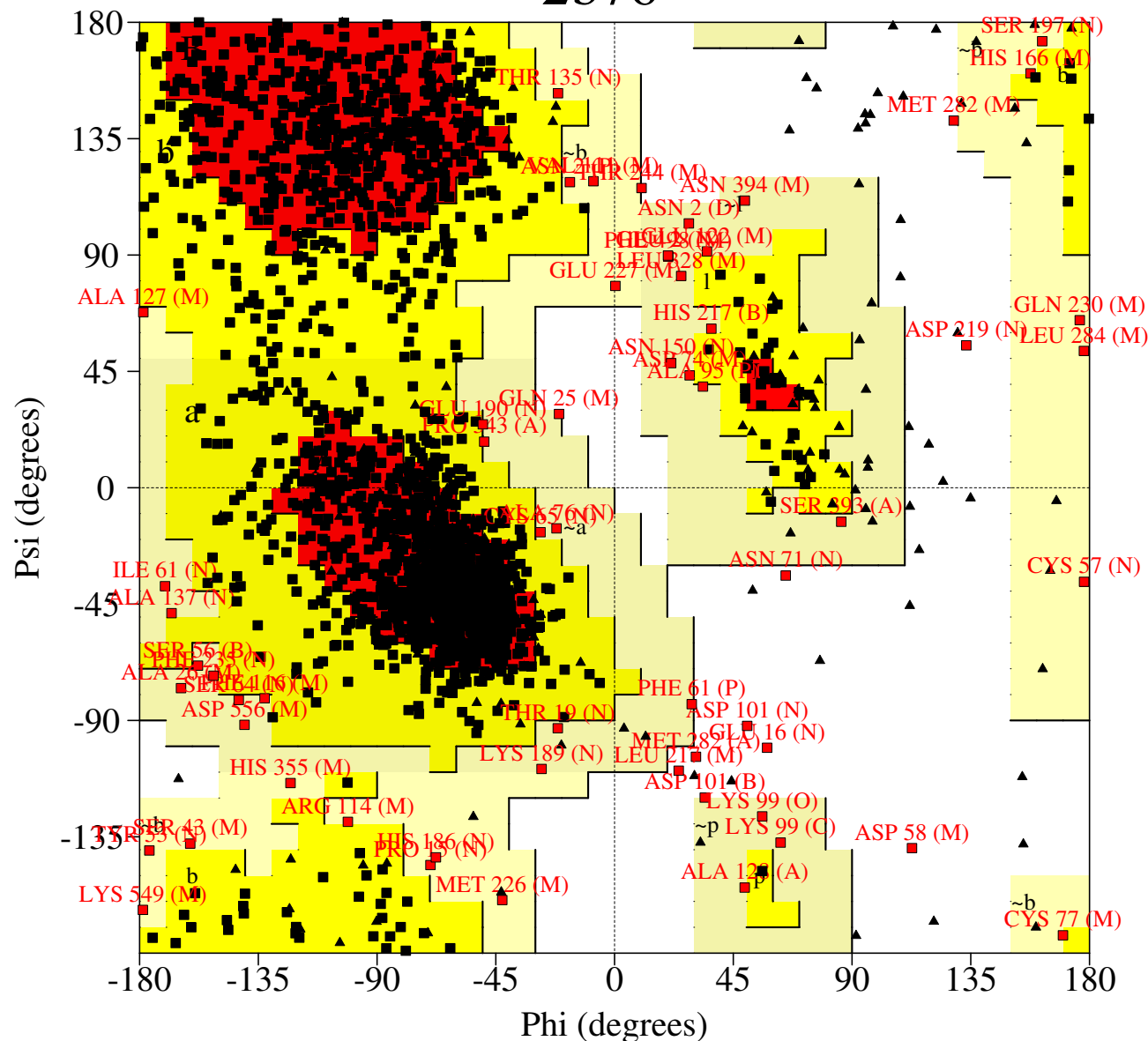


Ramachandran Plot

2b76



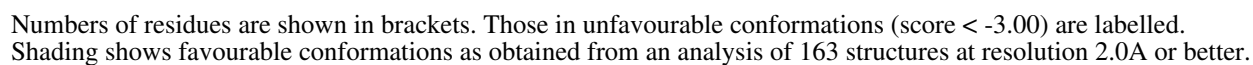
Residues in most favoured regions [A,B,L]	1347	73.8%
Residues in additional allowed regions [a,b,l,p]	421	23.1%
Residues in generously allowed regions [-a,-b,-l,-p]	47	2.6%
Residues in disallowed regions	10	0.5%

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	

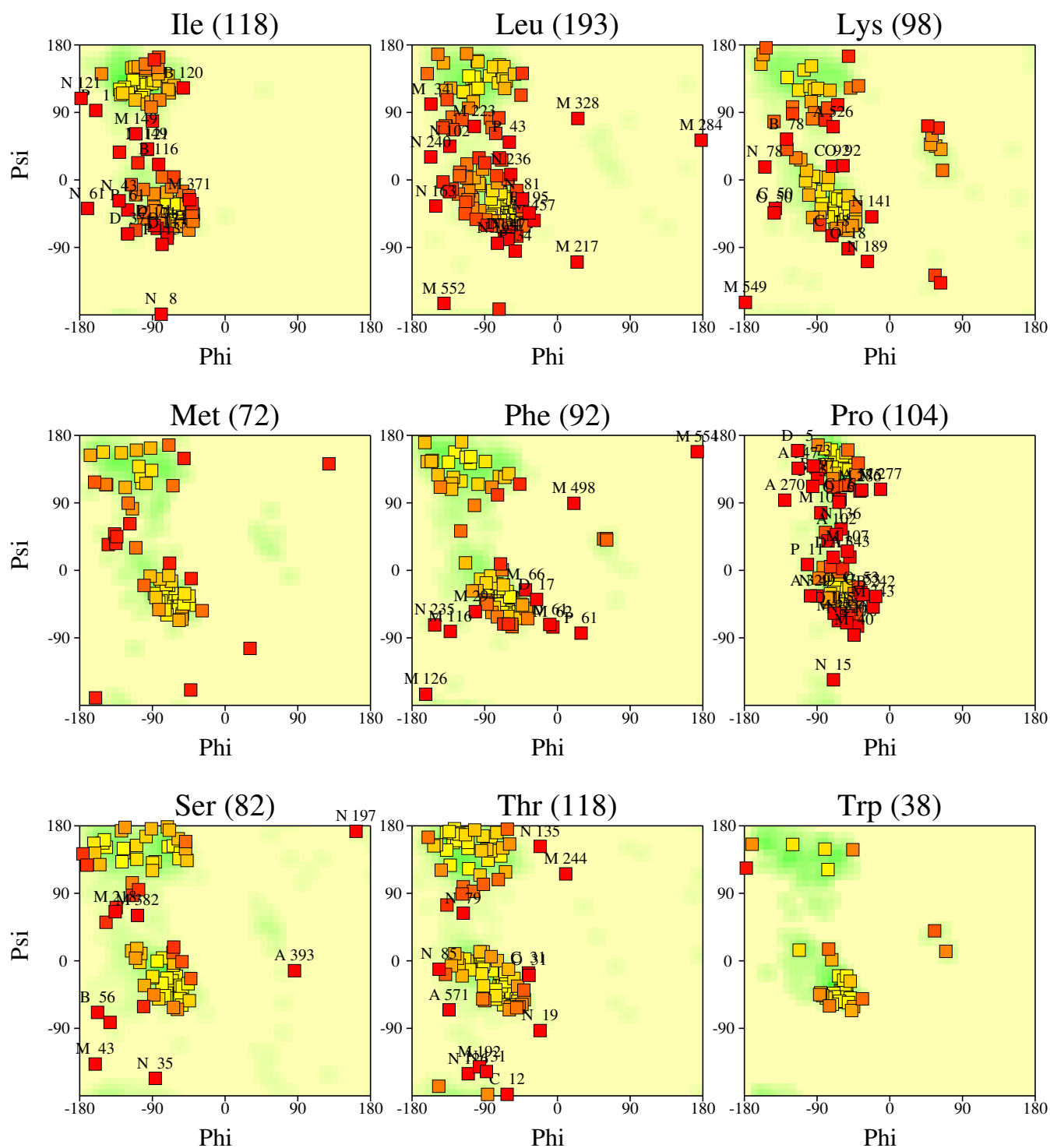
Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

2b76



Ramachandran plots for all residue types

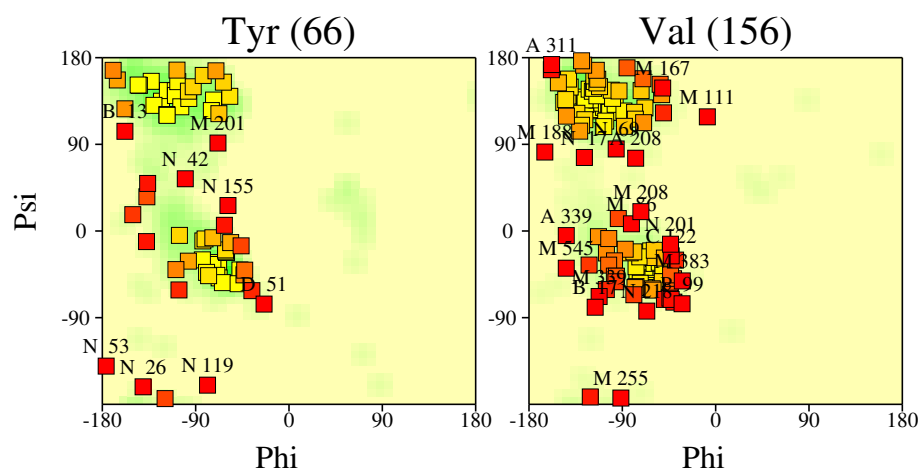
2b76



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

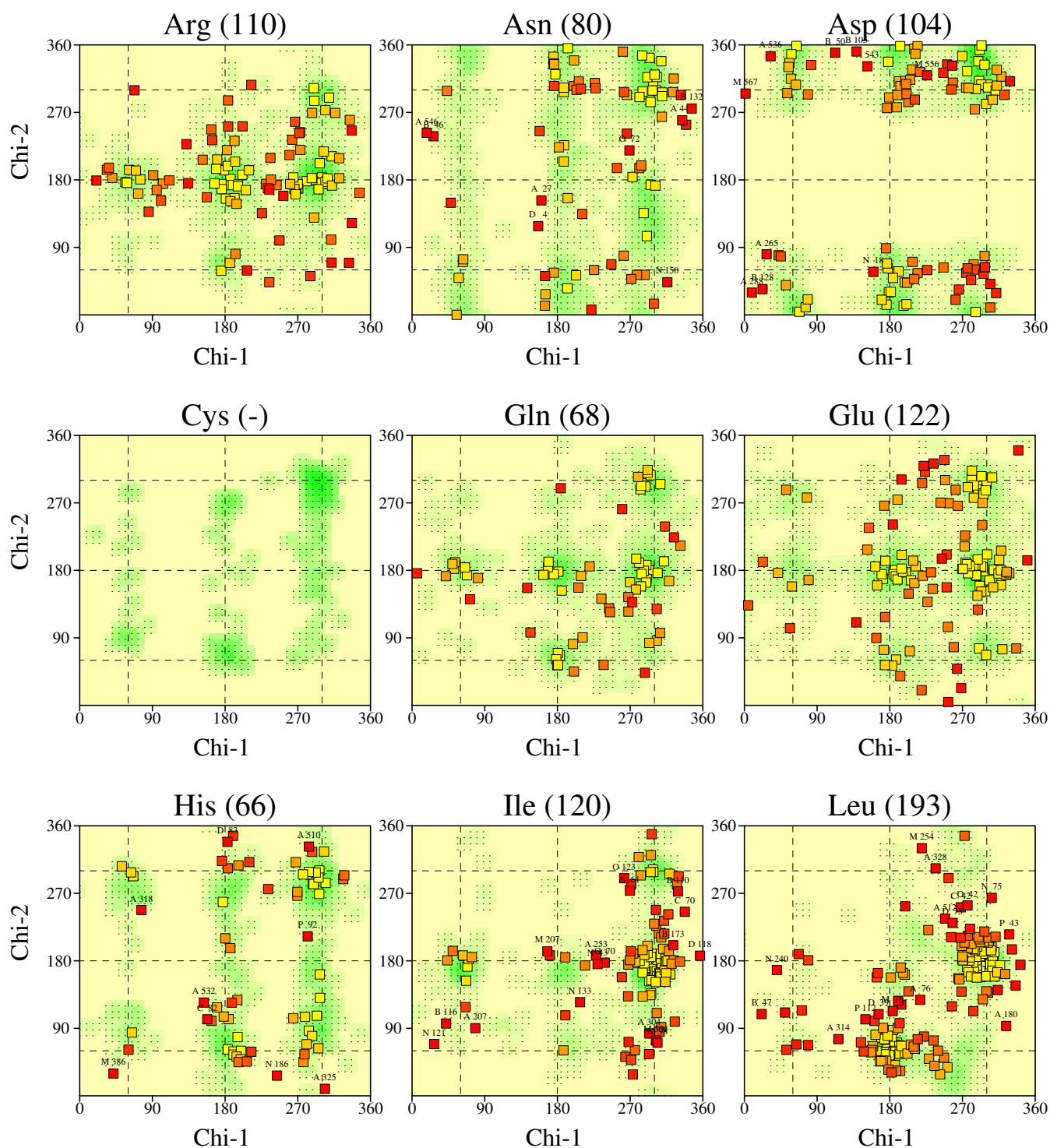
2b76



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 2.0Å or better.

Chi1-Chi2 plots

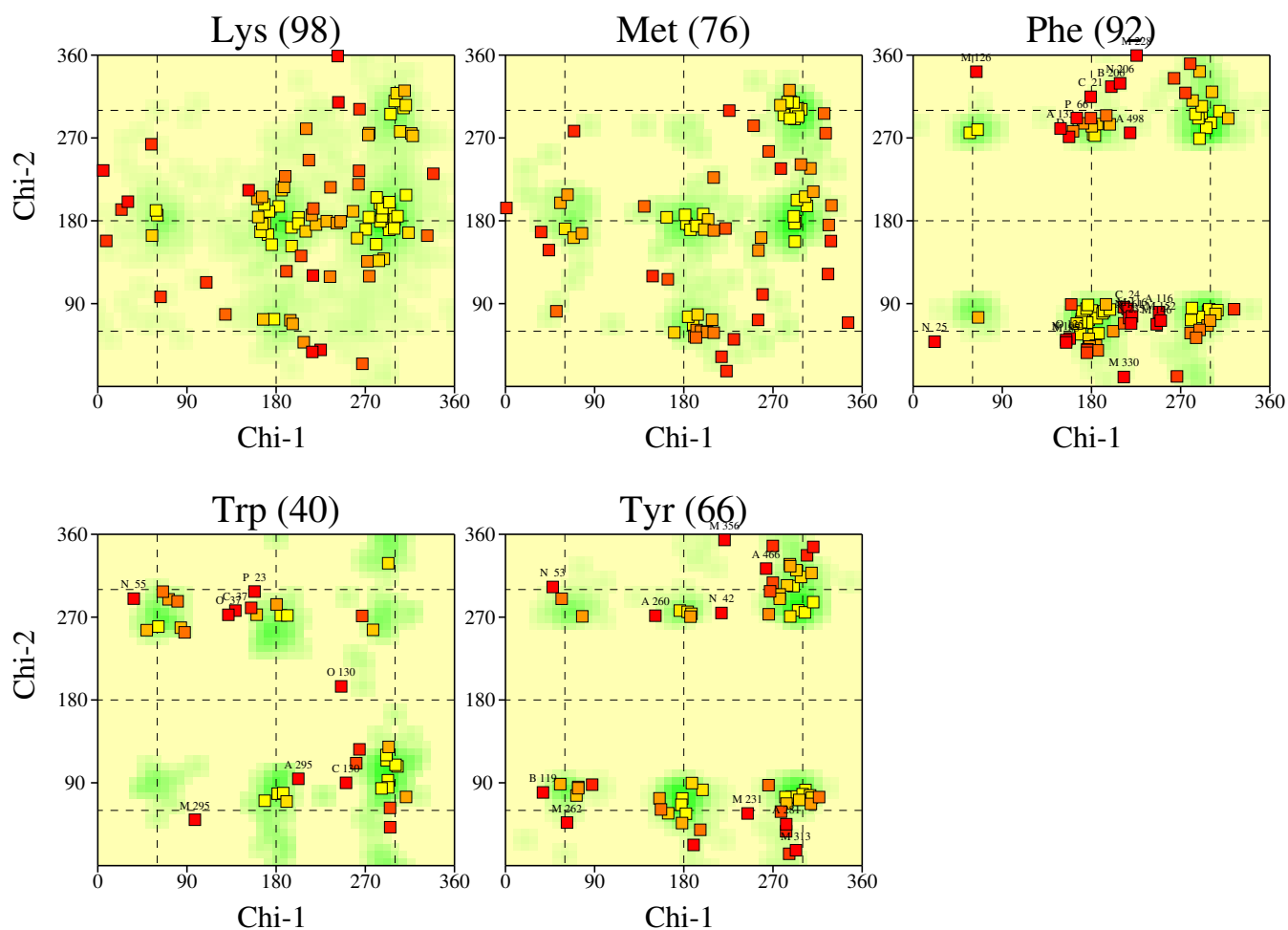
2b76



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 2.0Å or better.

Chi1-Chi2 plots

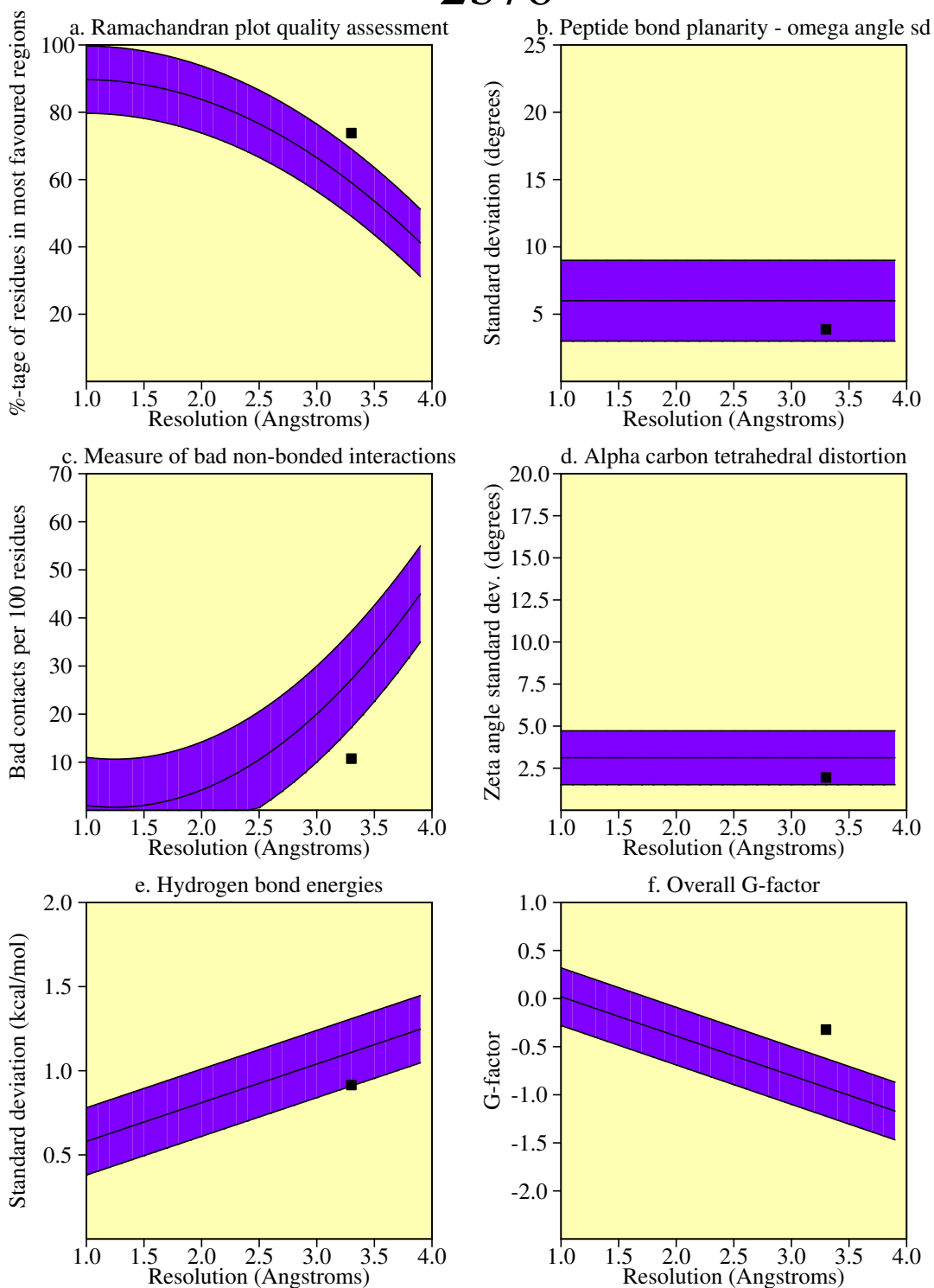
2b76



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 2.0Å or better.

Main-chain parameters

2b76

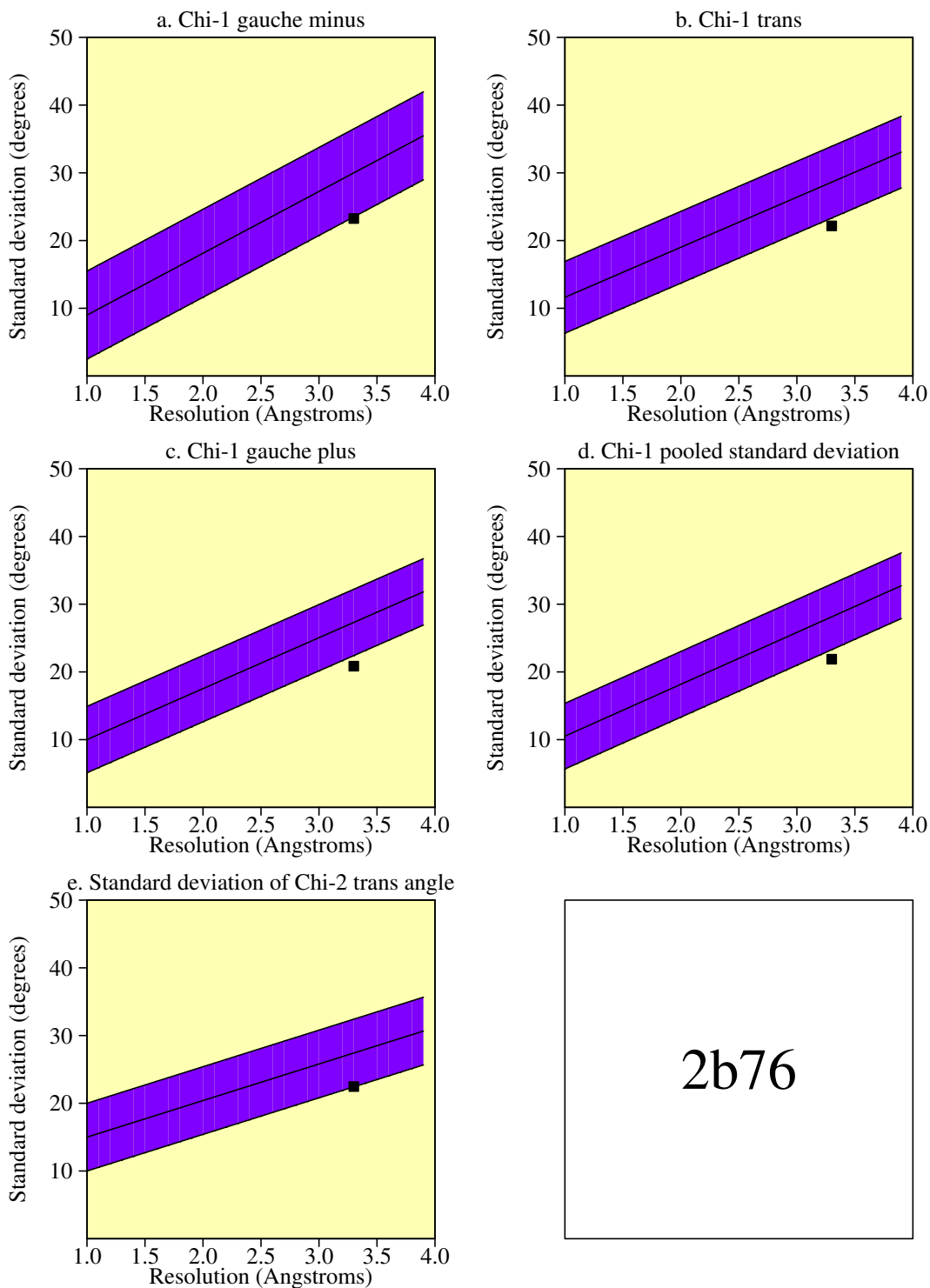


Plot statistics

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



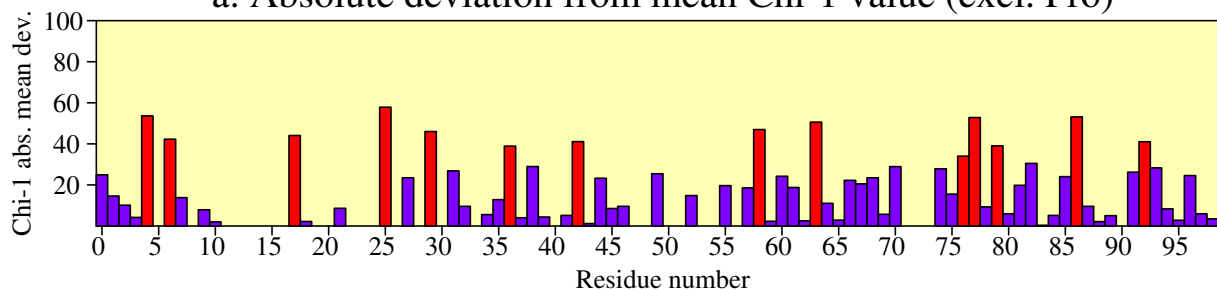
Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
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

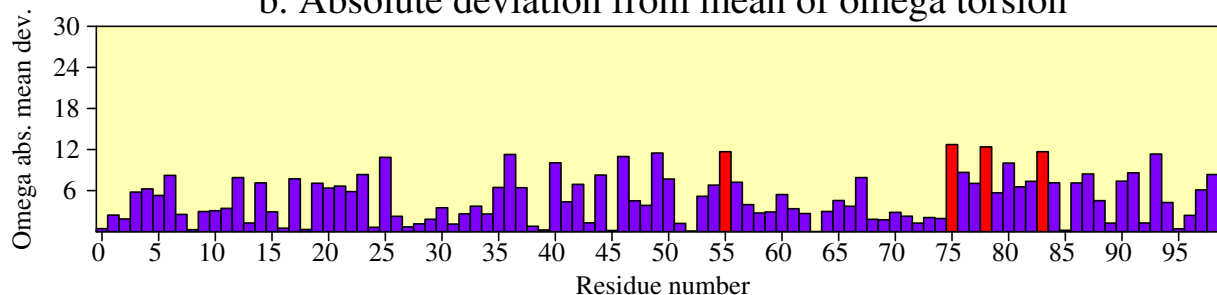
Residue properties

2b76

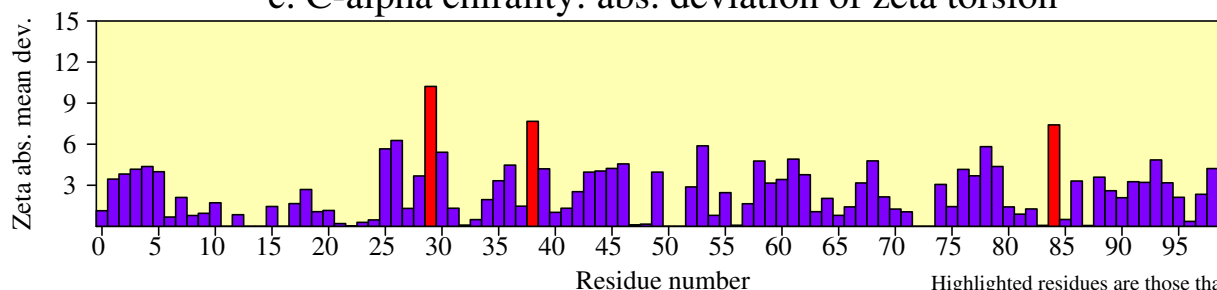
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

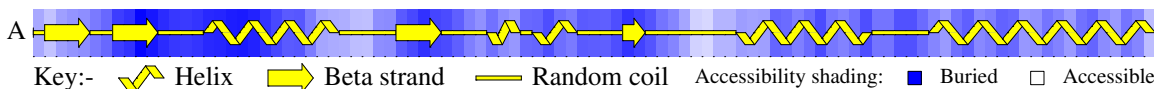


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



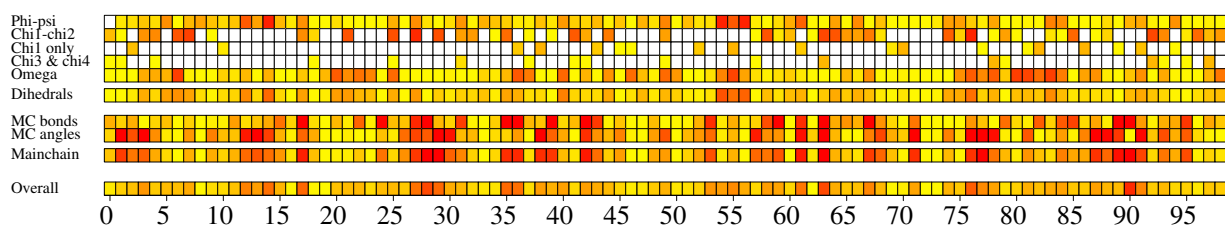
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

MQTFQADLAIVGAGGAGLRAAIAAAQANPNAKIALISKVYPMRSHTVAAQGGSAAVAQDHDSEFYHFDHDTVAGGDWLCQDQVDYFVHHCPTEMTQLELW

f. Max. deviation (see listing)



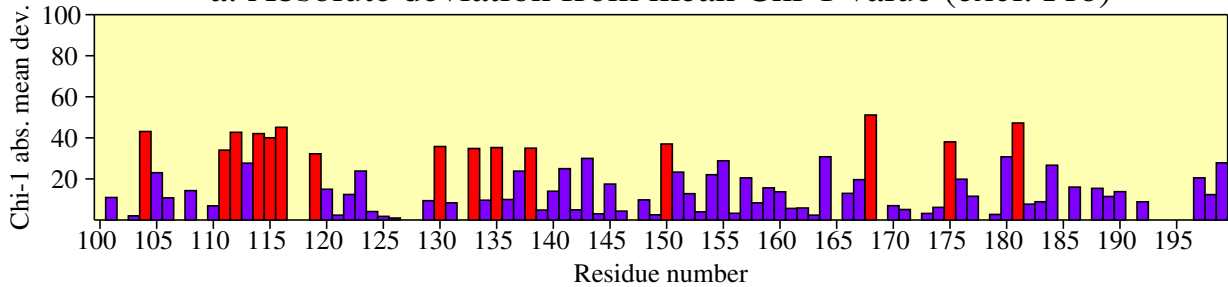
g. G-factors



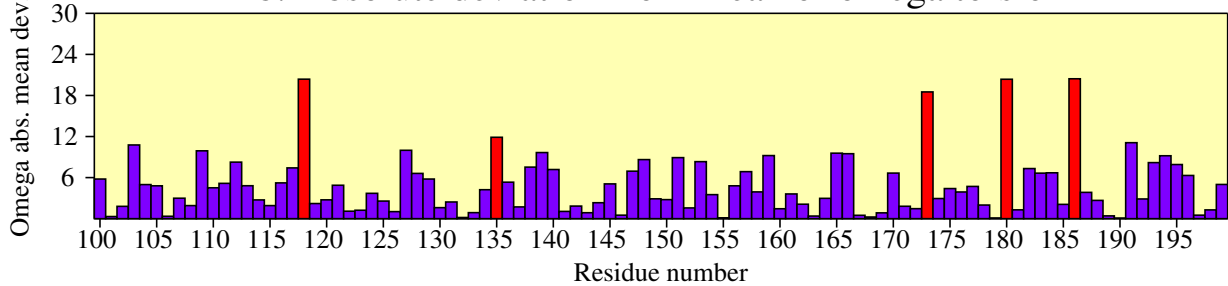
Residue properties

2b76

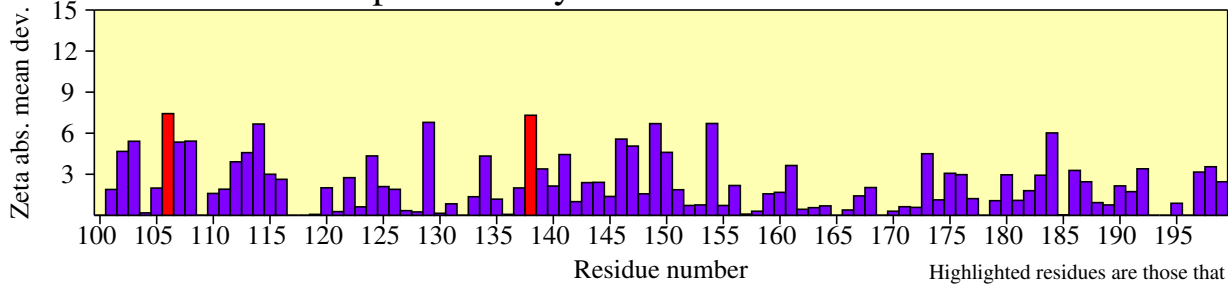
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

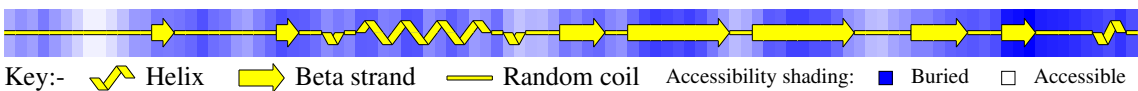


c. C-alpha chirality: abs. deviation of zeta torsion

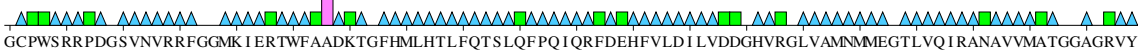


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



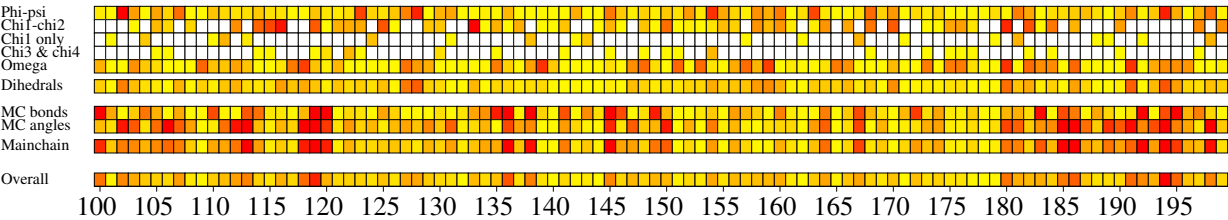
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



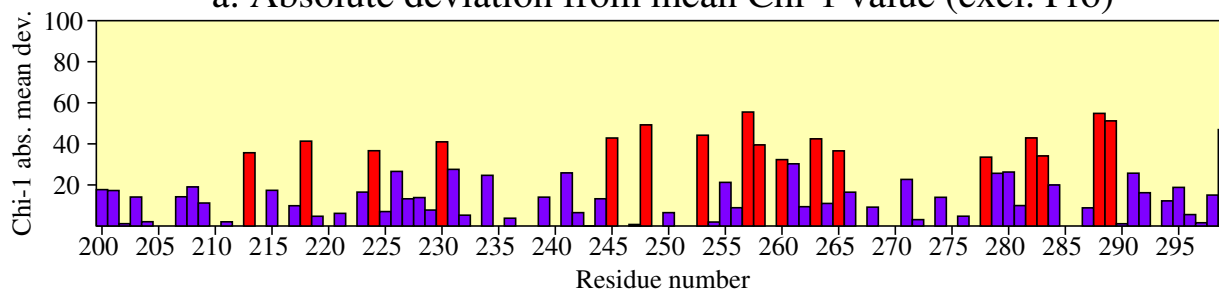
g. G-factors



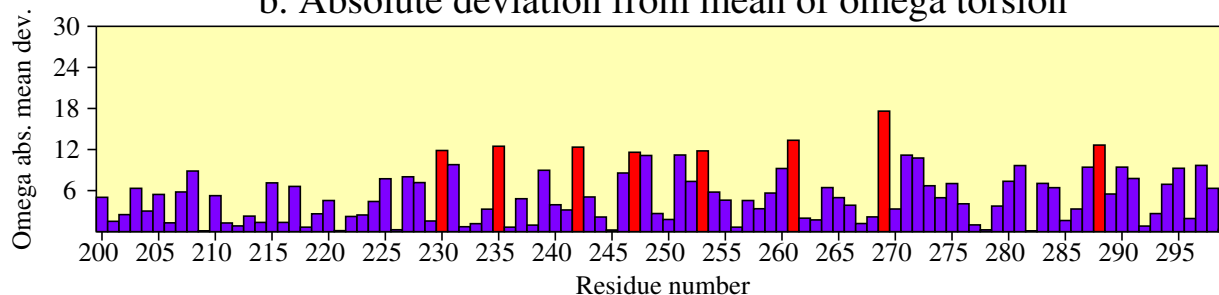
Residue properties

2b76

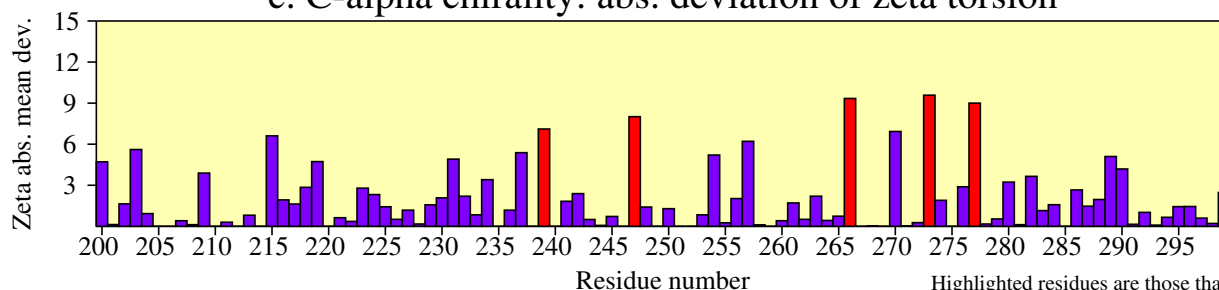
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

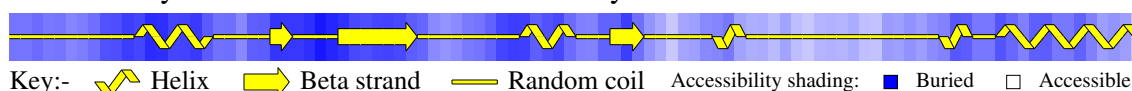


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



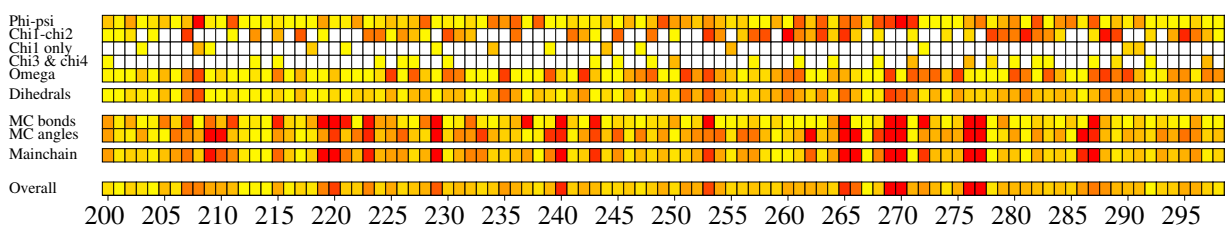
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



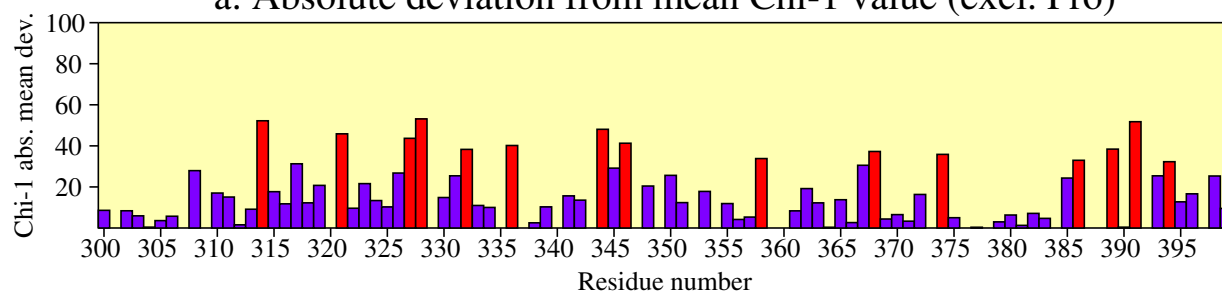
g. G-factors



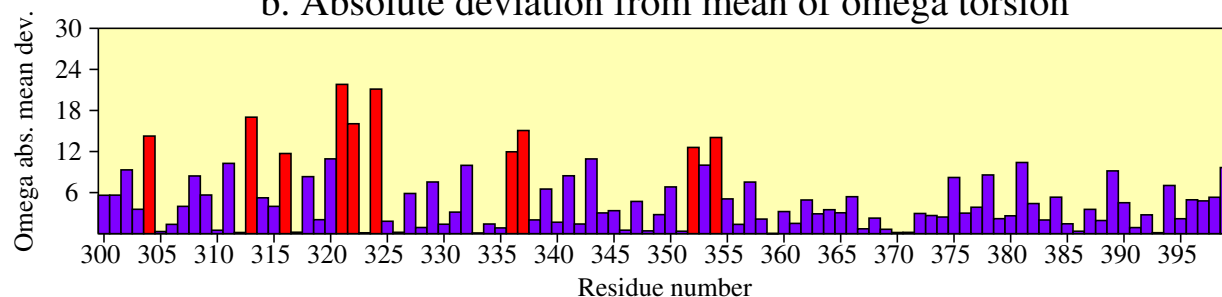
Residue properties

2b76

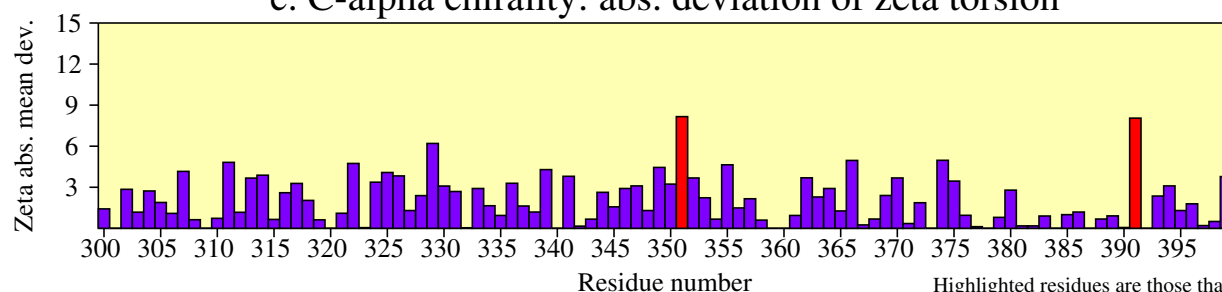
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

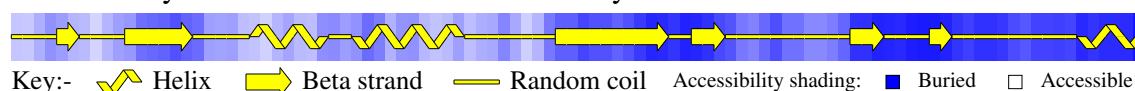


c. C-alpha chirality: abs. deviation of zeta torsion



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

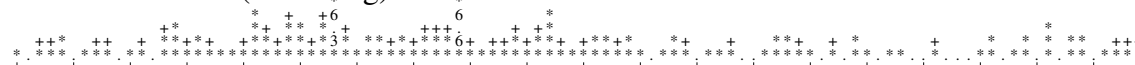
d. Secondary structure & estimated accessibility



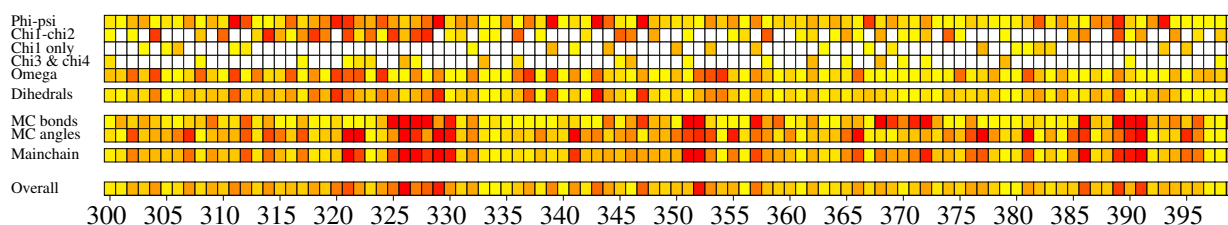
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



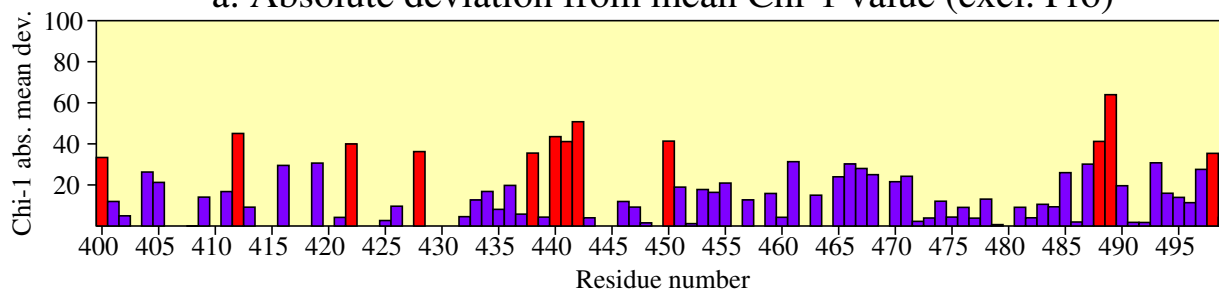
g. G-factors



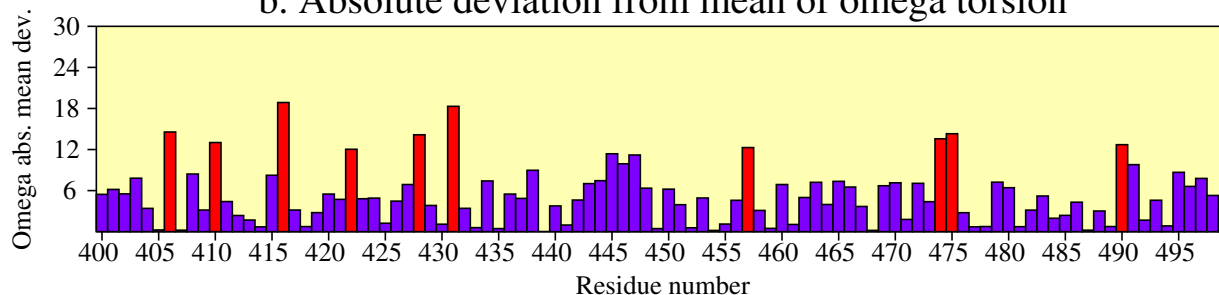
Residue properties

2b76

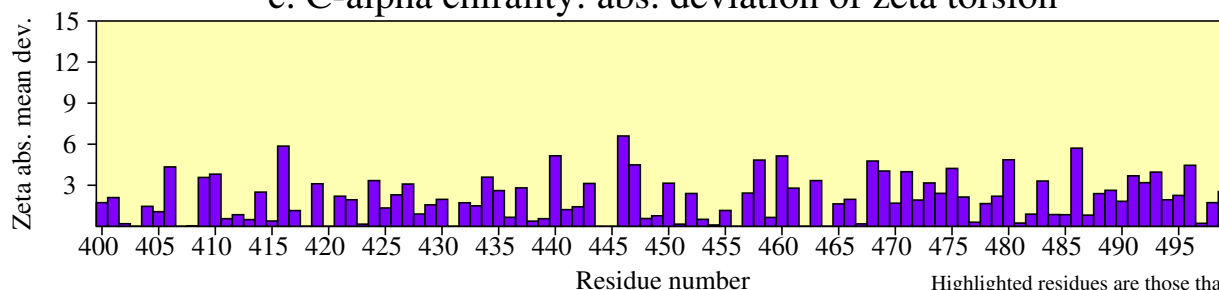
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

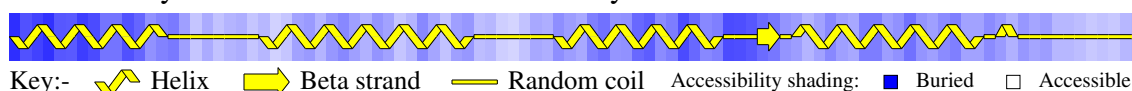


c. C-alpha chirality: abs. deviation of zeta torsion

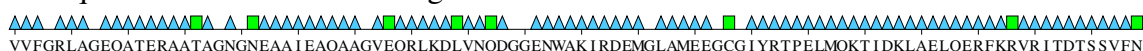


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

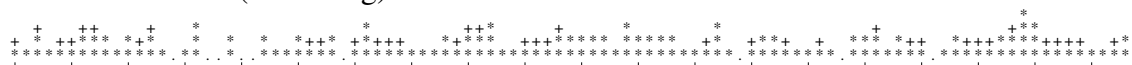
d. Secondary structure & estimated accessibility



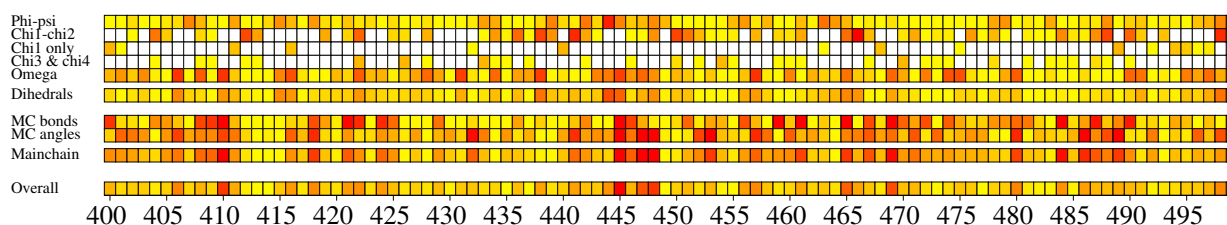
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



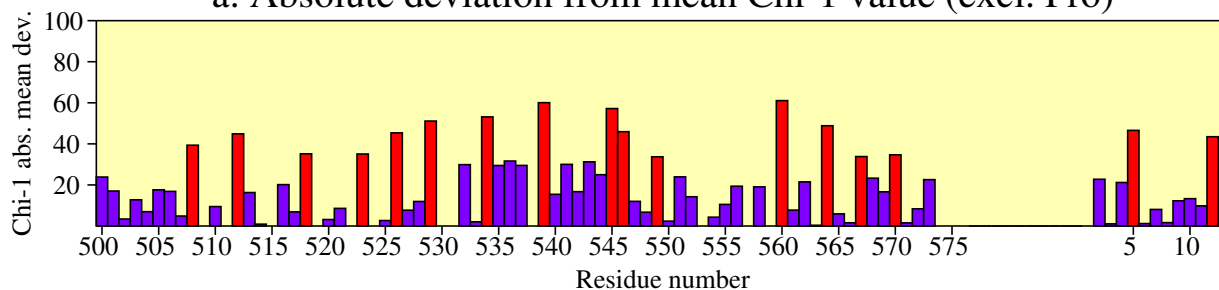
g. G-factors



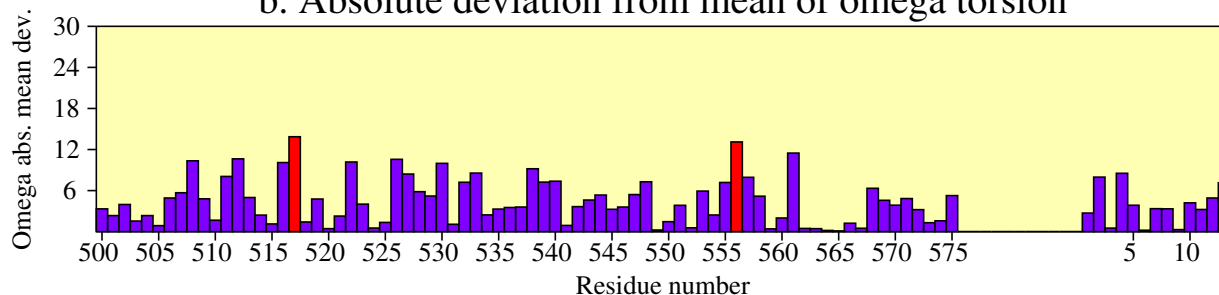
Residue properties

2b76

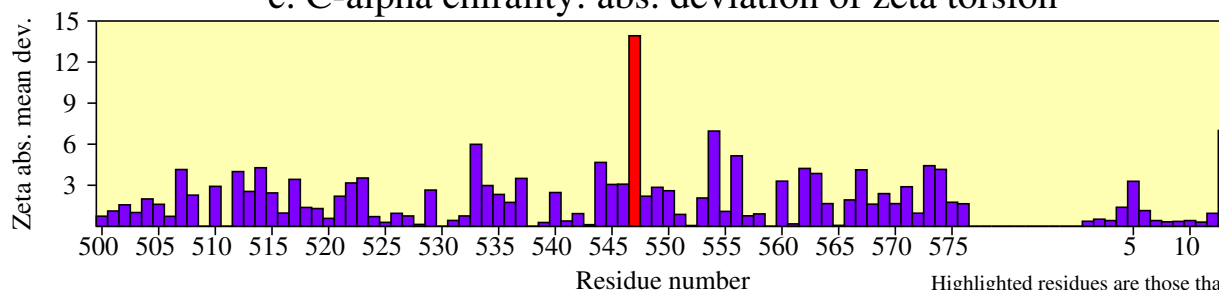
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

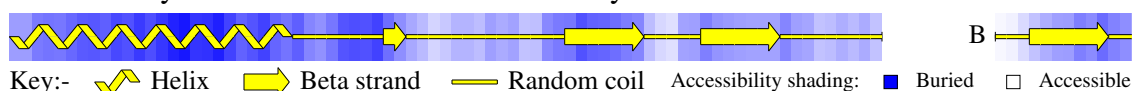


c. C-alpha chirality: abs. deviation of zeta torsion



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

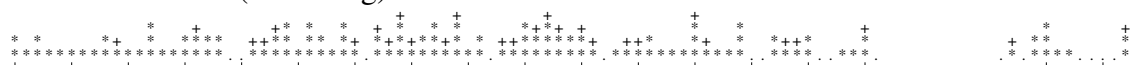
d. Secondary structure & estimated accessibility



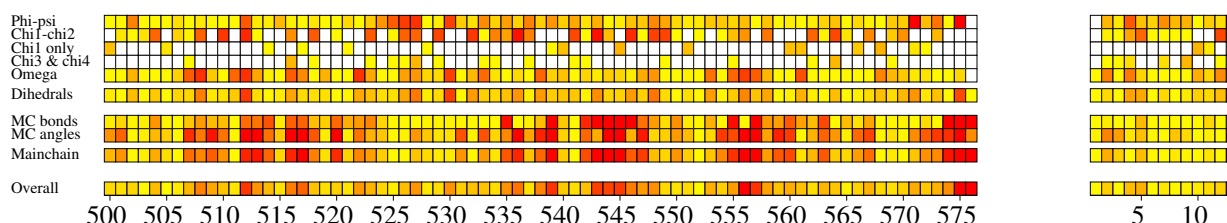
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



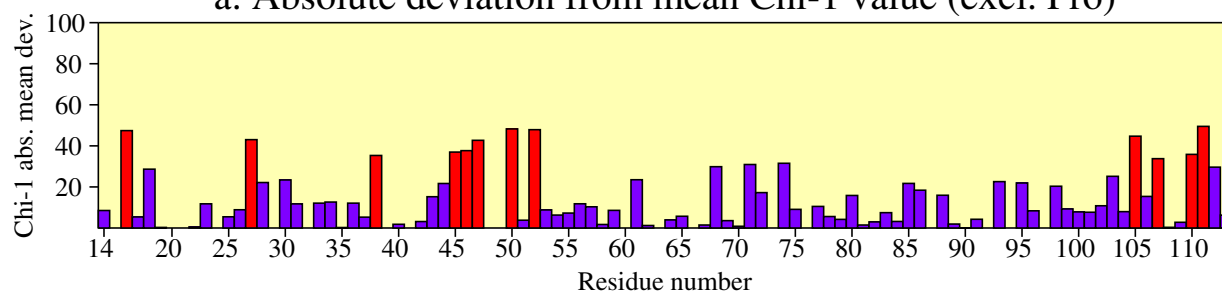
g. G-factors



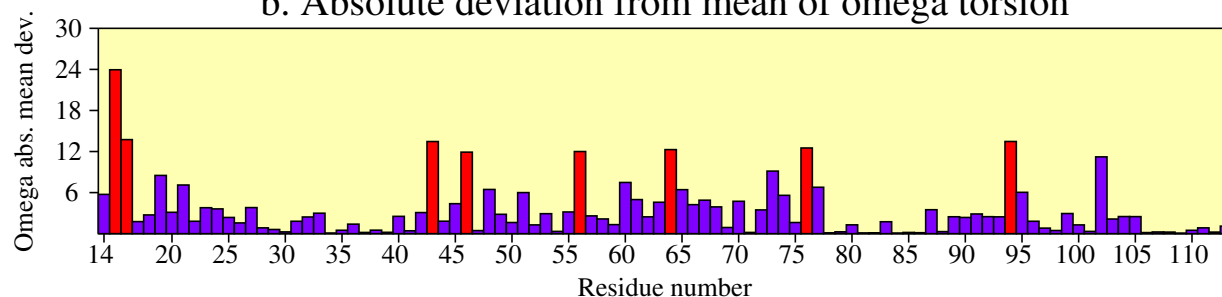
Residue properties

2b76

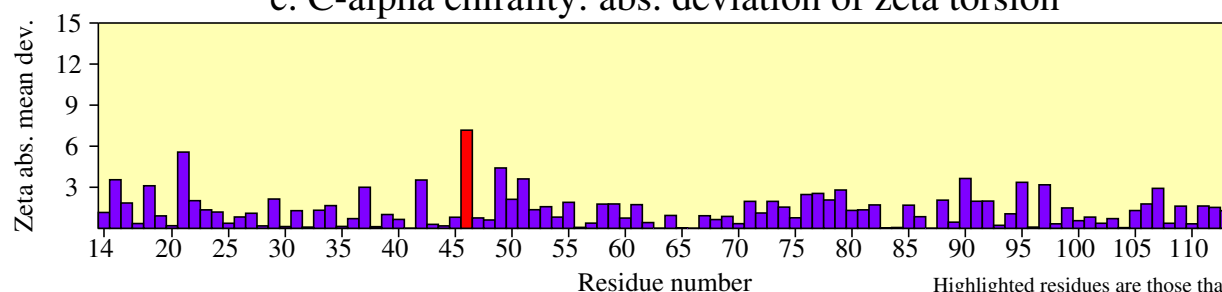
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

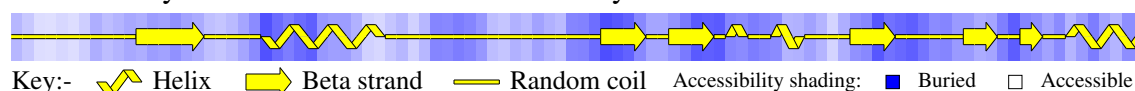


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



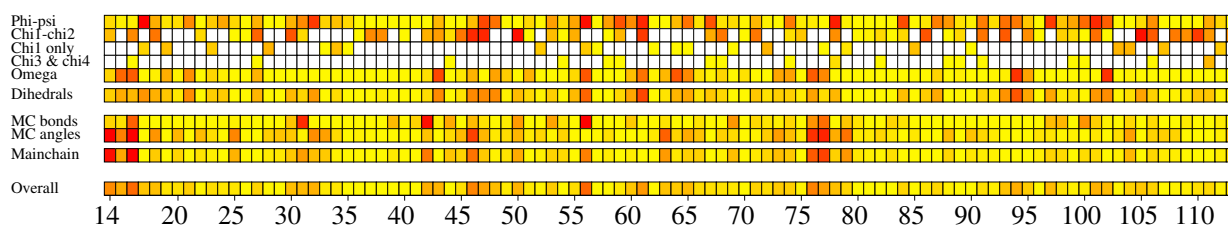
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



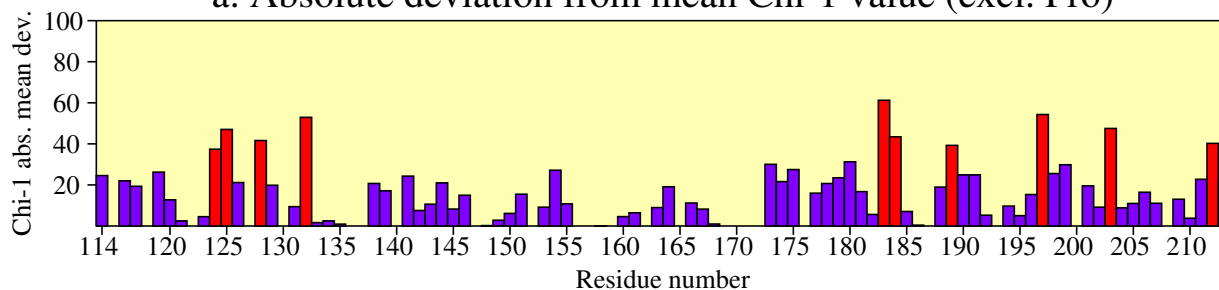
g. G-factors



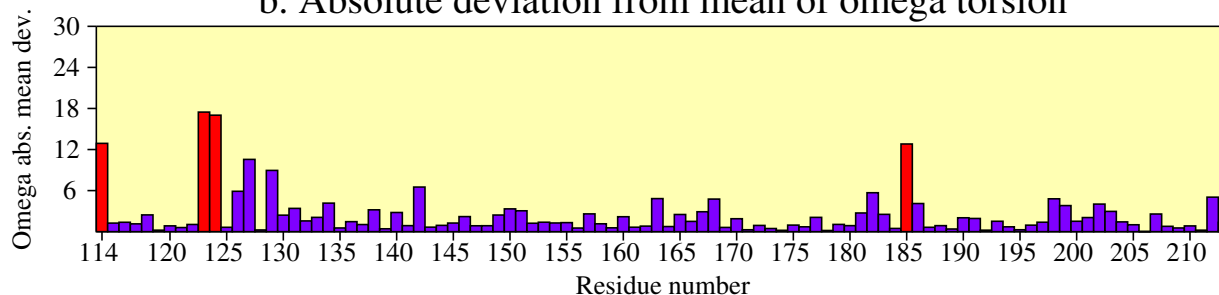
Residue properties

2b76

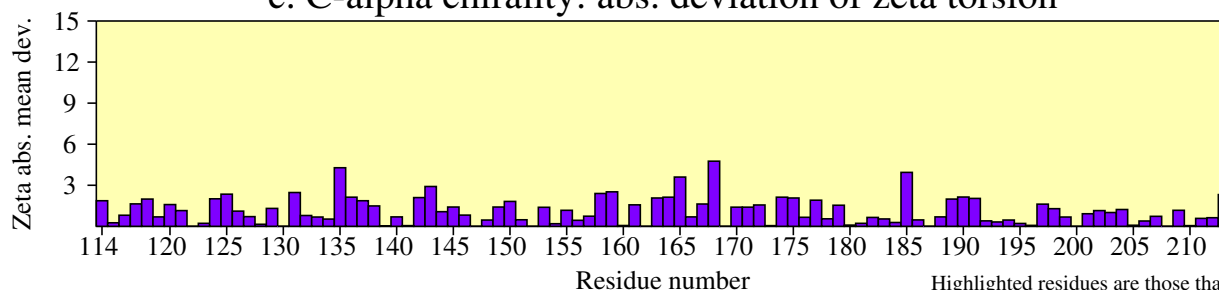
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

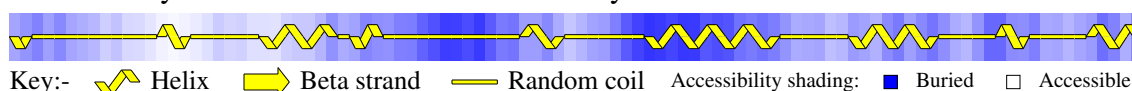


c. C-alpha chirality: abs. deviation of zeta torsion



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

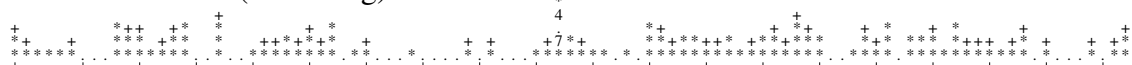
d. Secondary structure & estimated accessibility



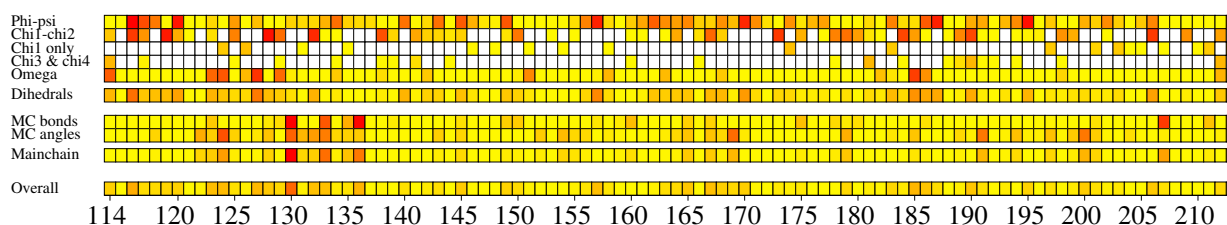
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



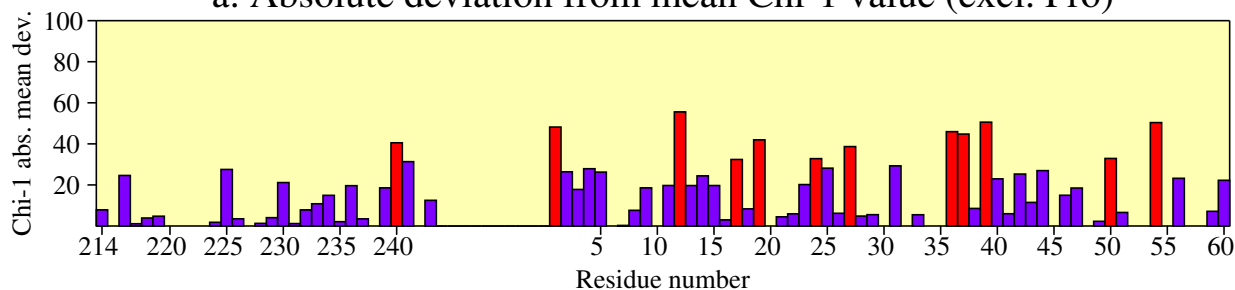
g. G-factors



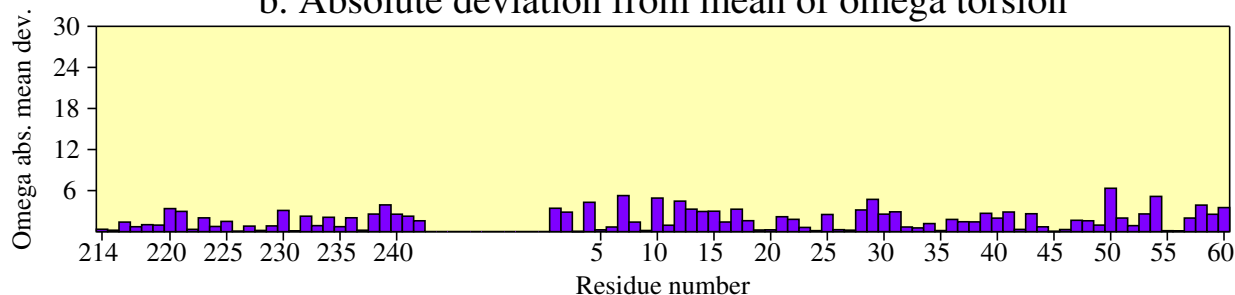
Residue properties

2b76

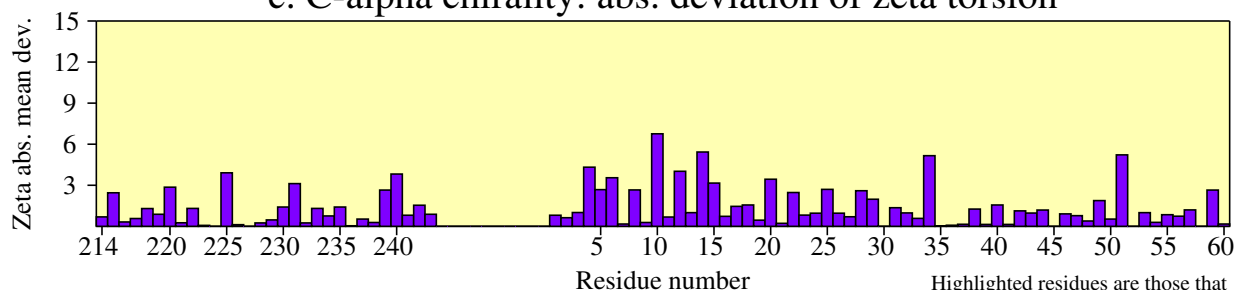
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

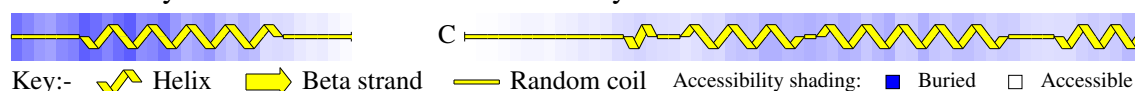


c. C-alpha chirality: abs. deviation of zeta torsion



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

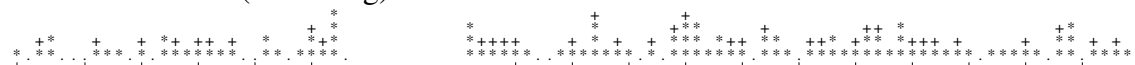
d. Secondary structure & estimated accessibility



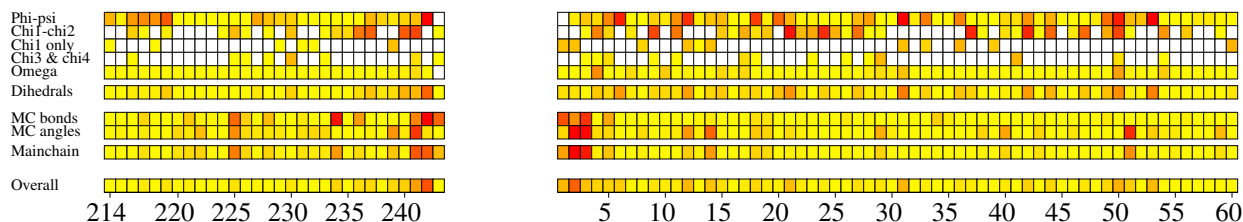
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



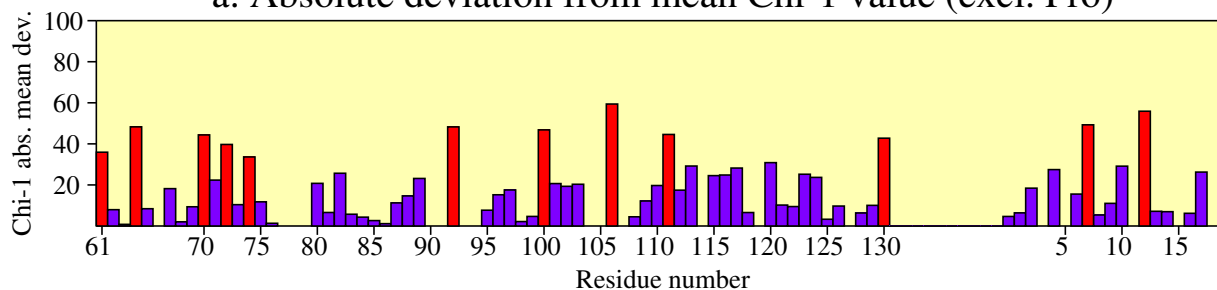
g. G-factors



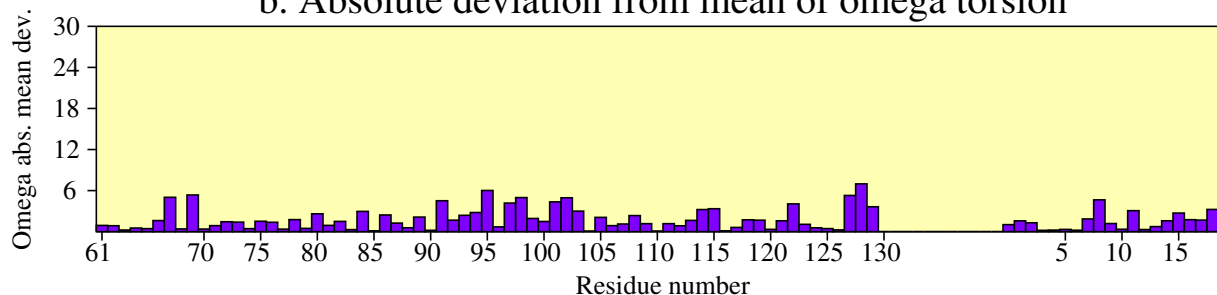
Residue properties

2b76

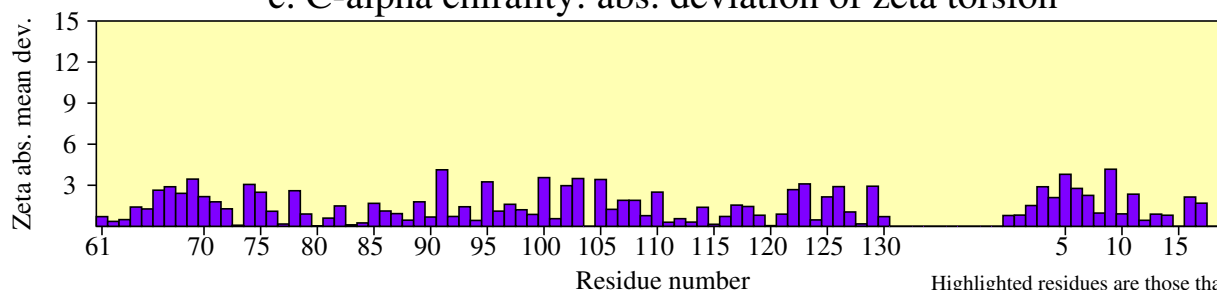
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

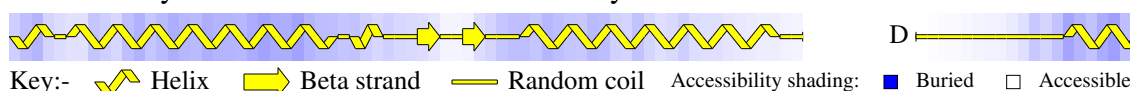


c. C-alpha chirality: abs. deviation of zeta torsion

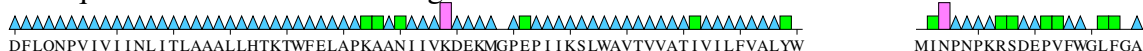


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

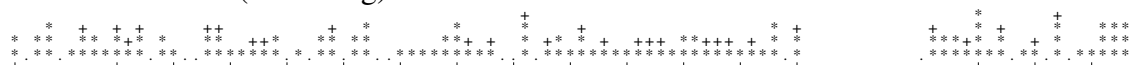
d. Secondary structure & estimated accessibility



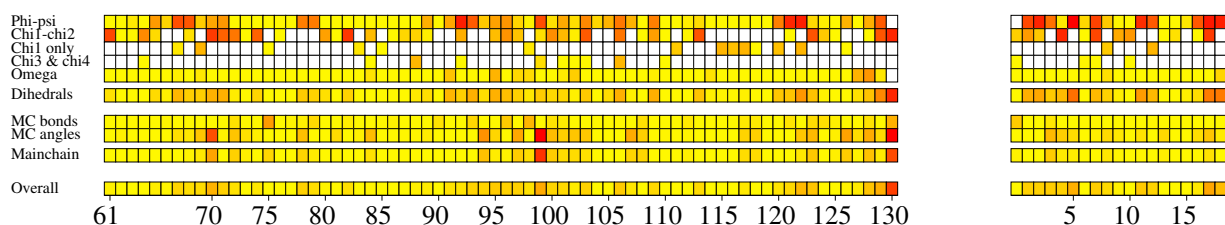
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



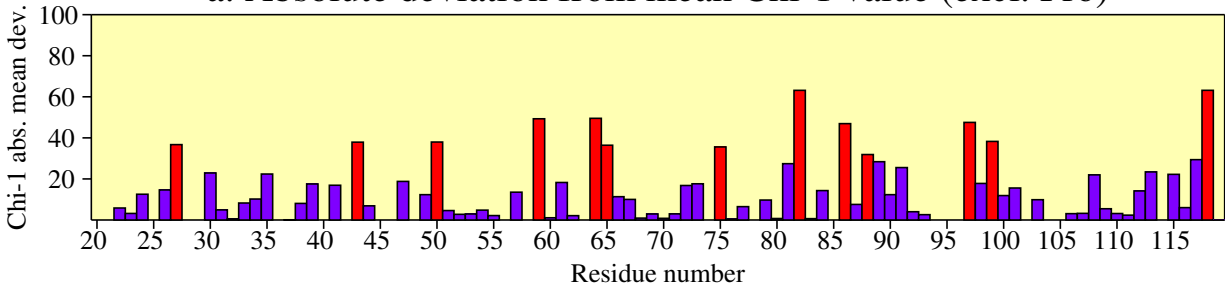
g. G-factors



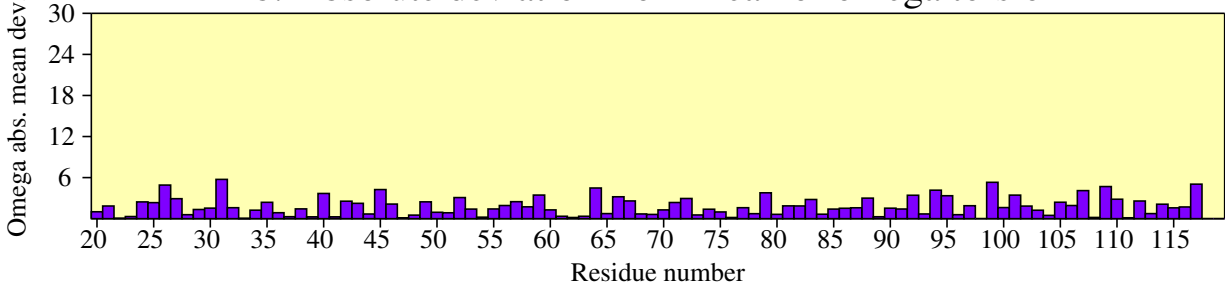
Residue properties

2b76

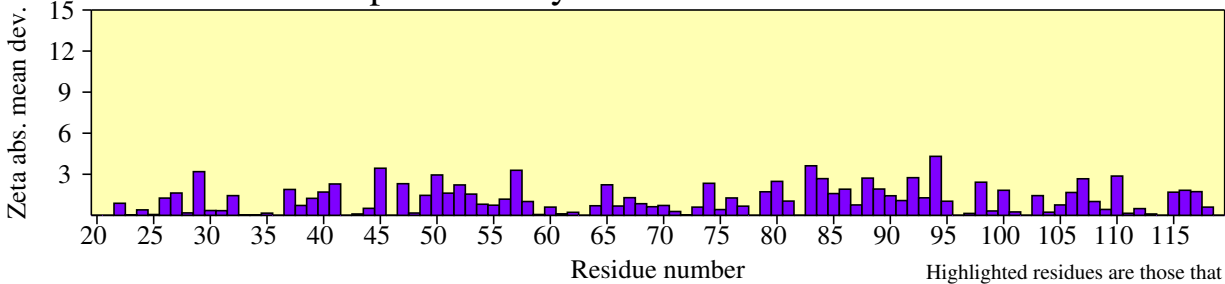
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

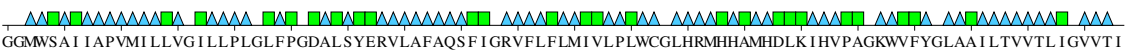


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

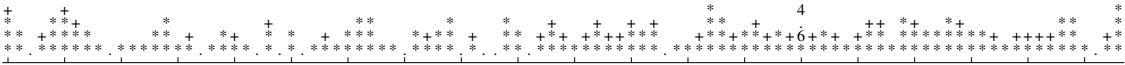
d. Secondary structure & estimated accessibility



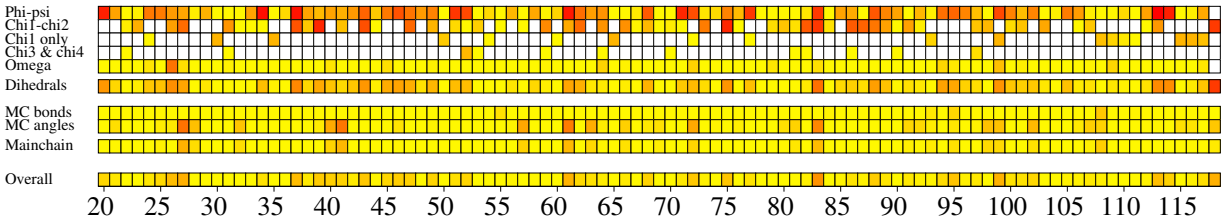
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



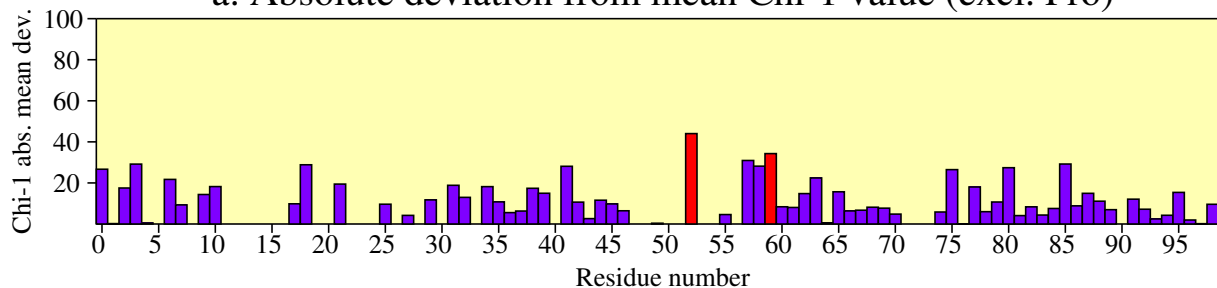
g. G-factors



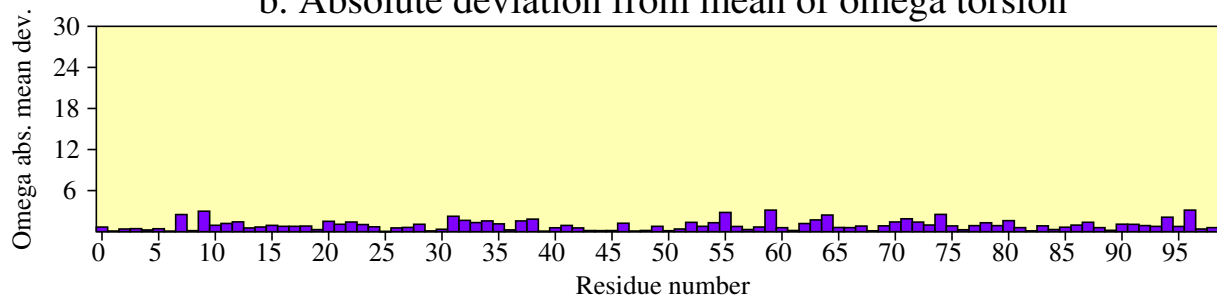
Residue properties

2b76

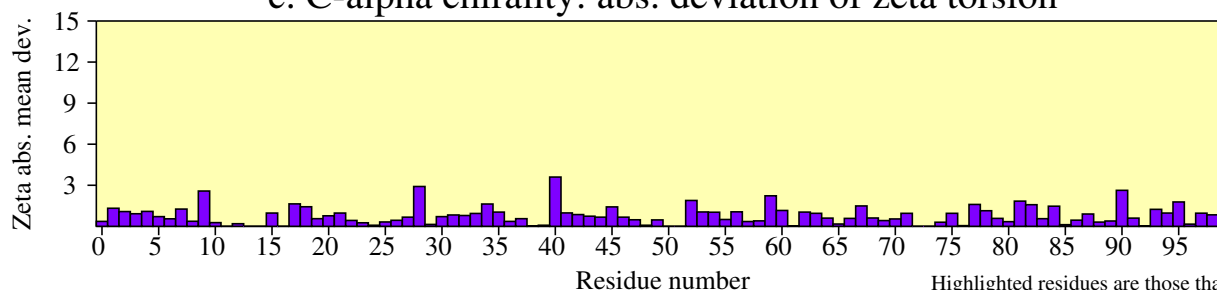
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

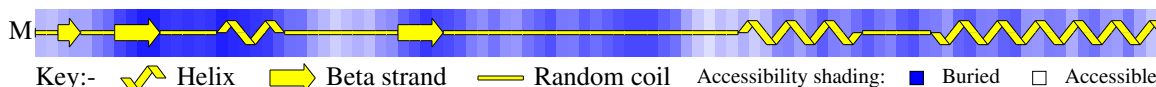


c. C-alpha chirality: abs. deviation of zeta torsion

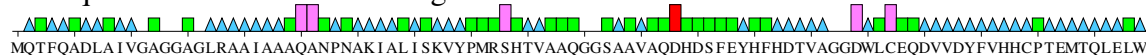


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



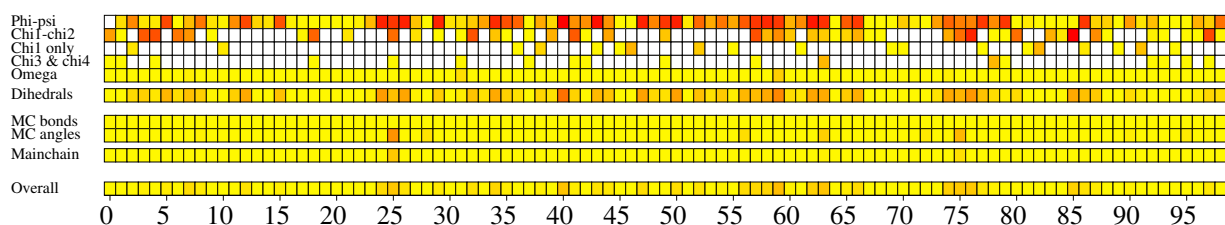
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



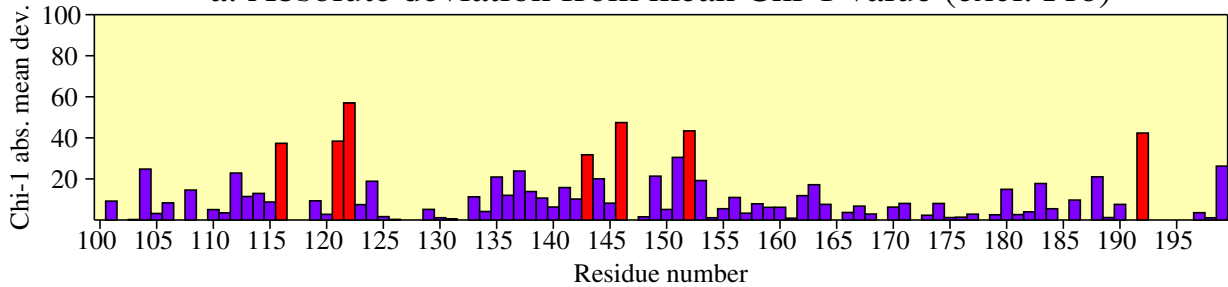
g. G-factors



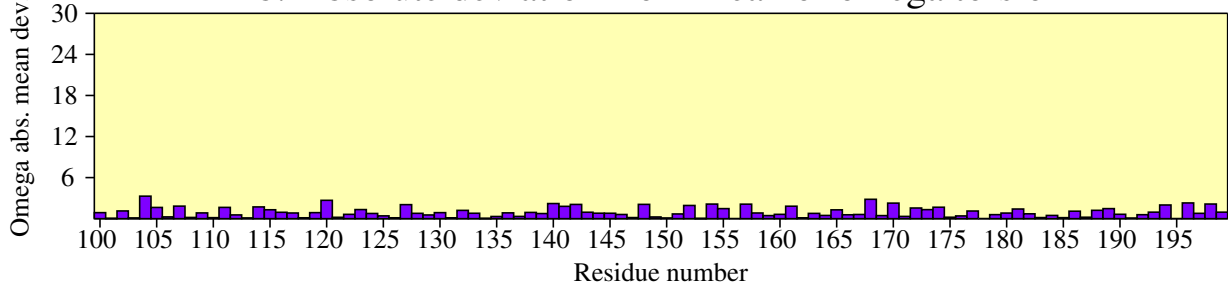
Residue properties

2b76

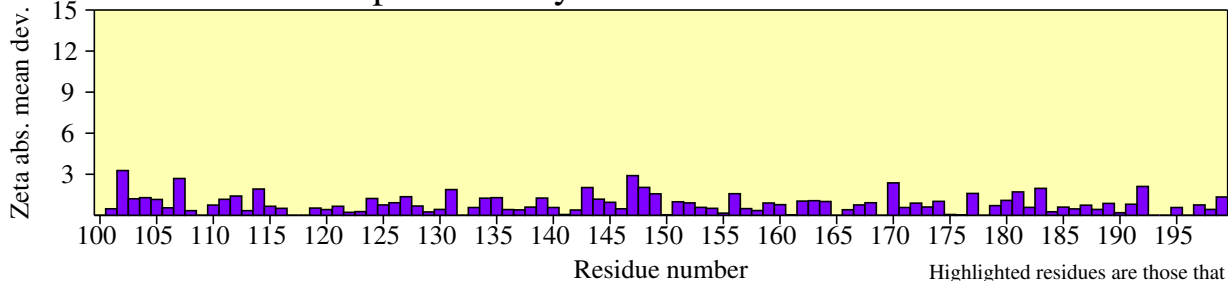
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

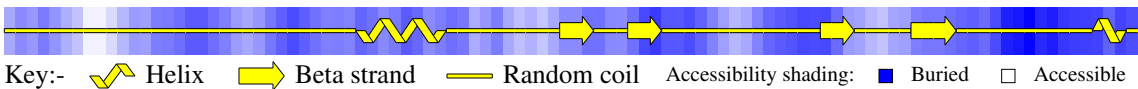


c. C-alpha chirality: abs. deviation of zeta torsion

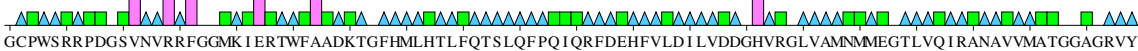


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

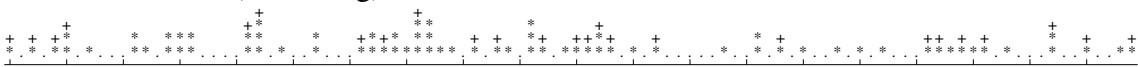
d. Secondary structure & estimated accessibility



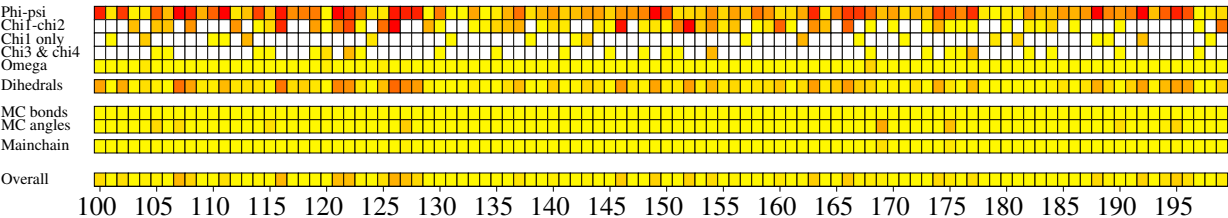
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



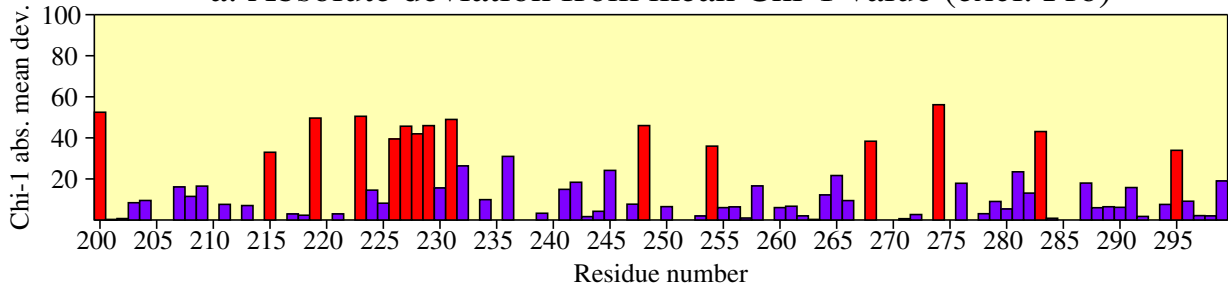
g. G-factors



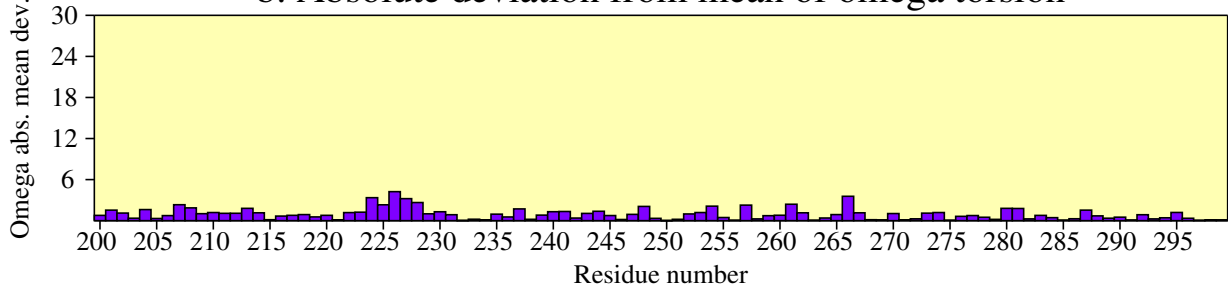
Residue properties

2b76

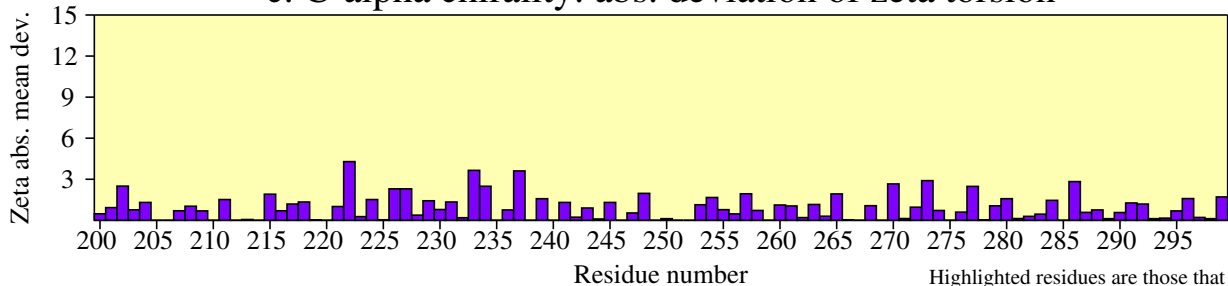
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

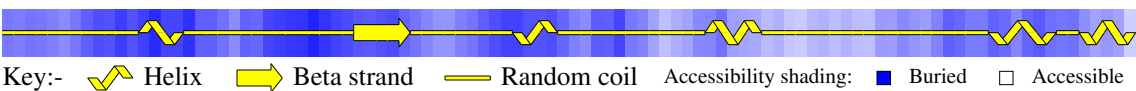


c. C-alpha chirality: abs. deviation of zeta torsion



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

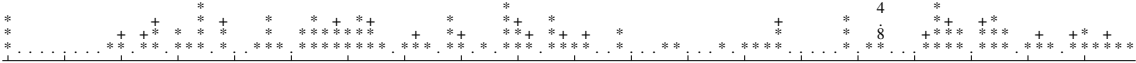
d. Secondary structure & estimated accessibility



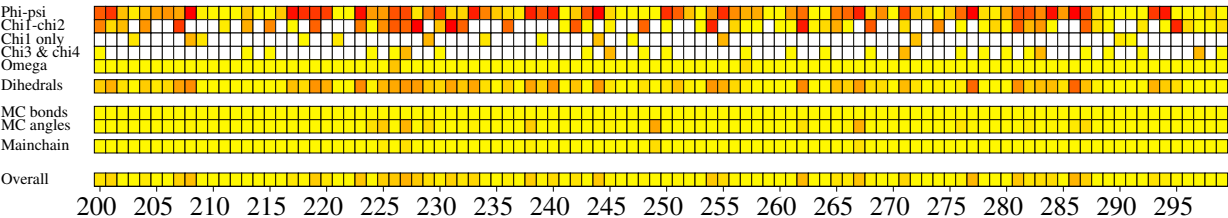
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



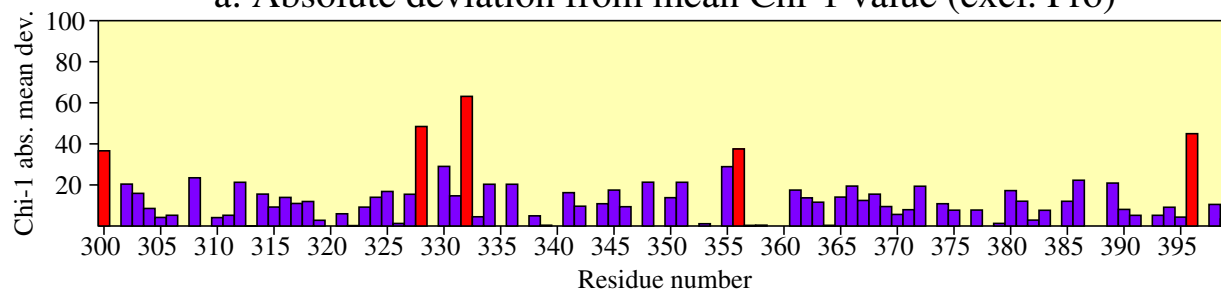
g. G-factors



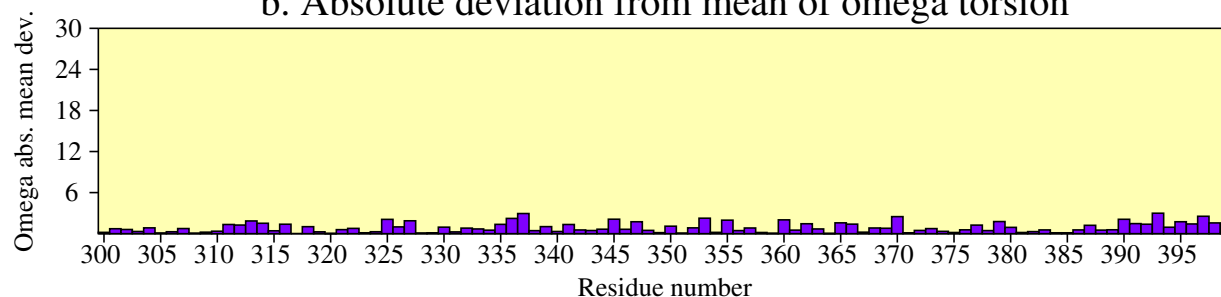
Residue properties

2b76

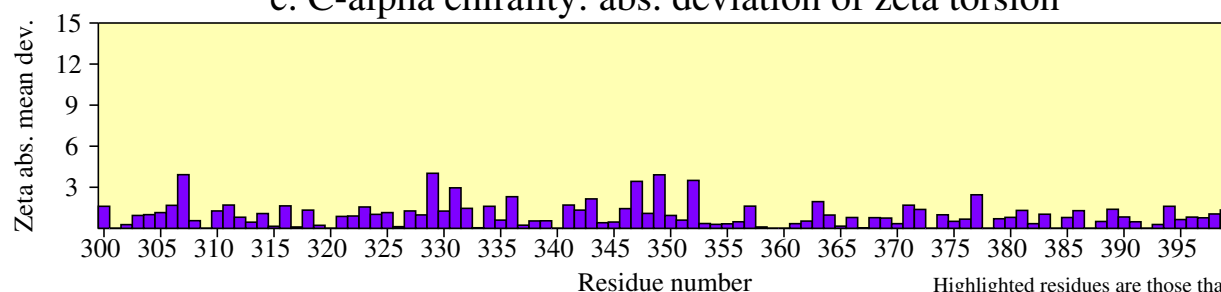
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

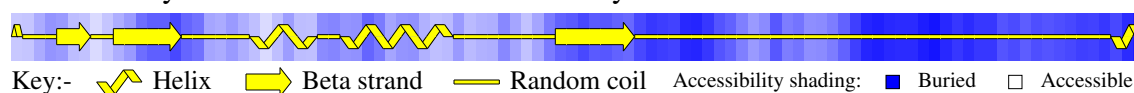


c. C-alpha chirality: abs. deviation of zeta torsion

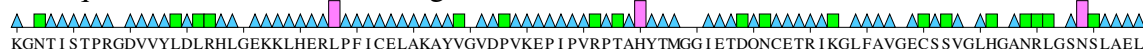


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



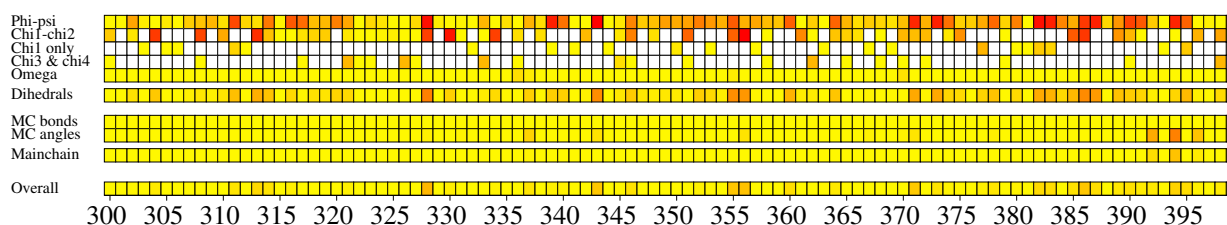
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



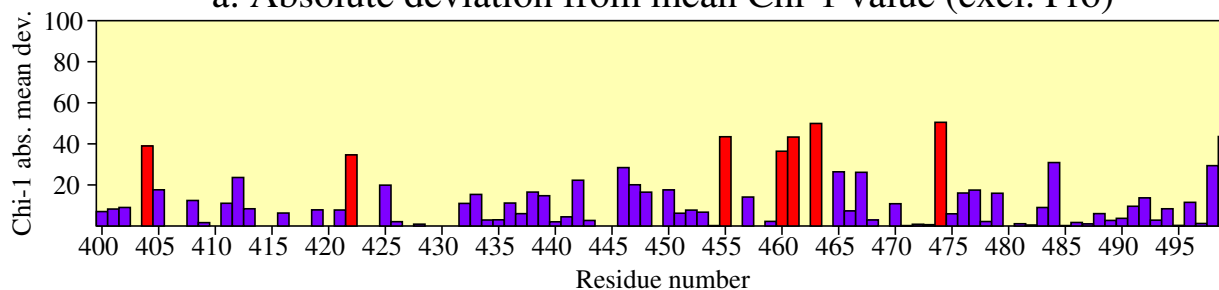
g. G-factors



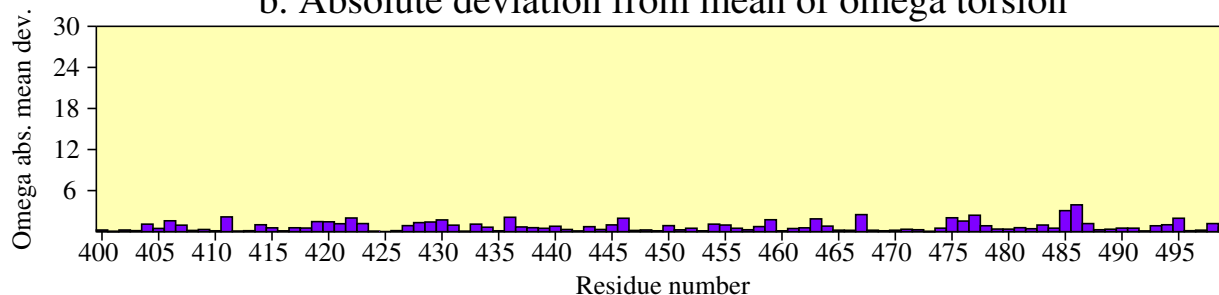
Residue properties

2b76

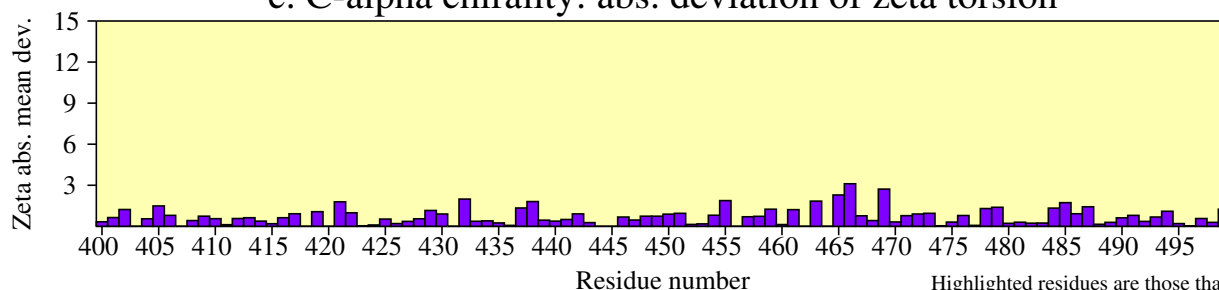
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

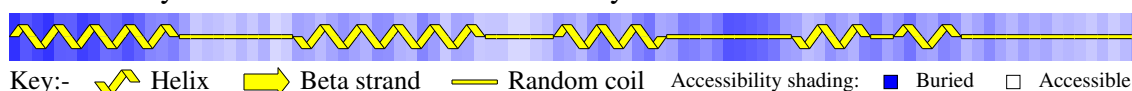


c. C-alpha chirality: abs. deviation of zeta torsion



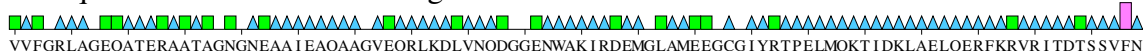
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



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

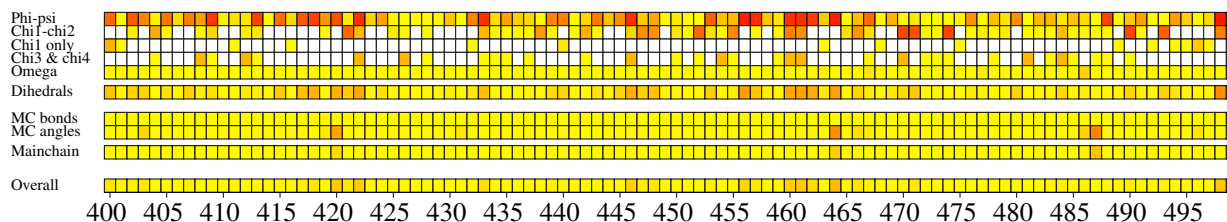
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



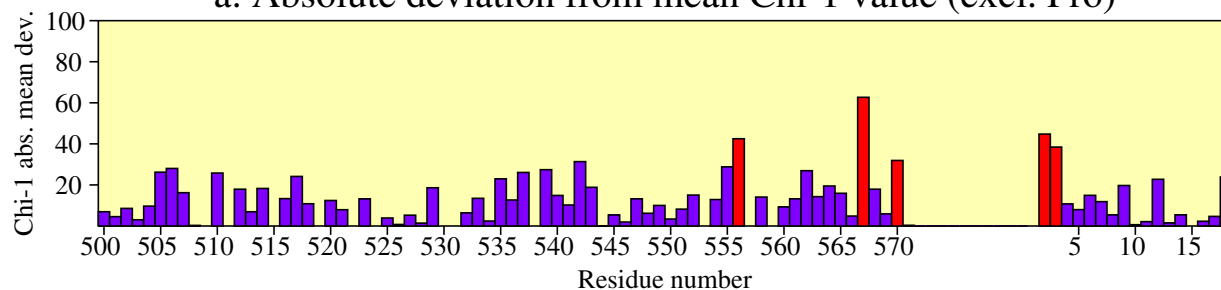
g. G-factors



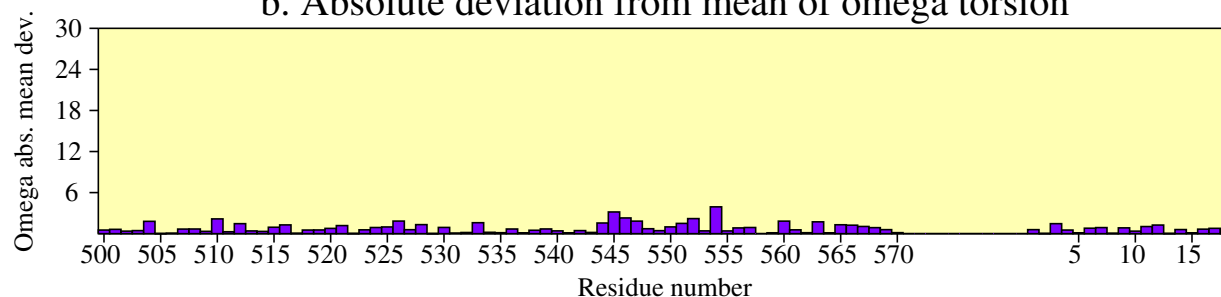
Residue properties

2b76

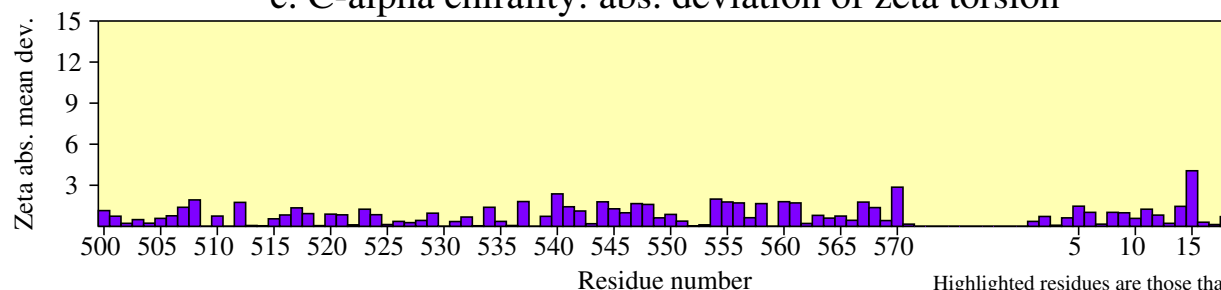
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

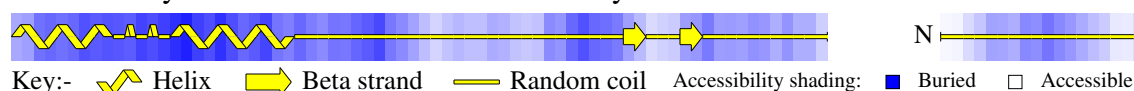


c. C-alpha chirality: abs. deviation of zeta torsion

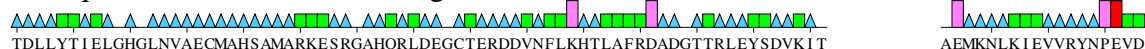


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

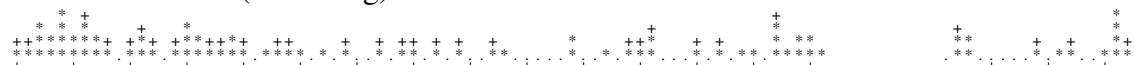
d. Secondary structure & estimated accessibility



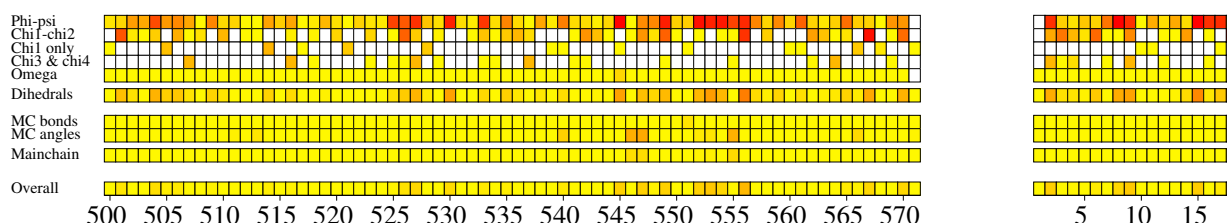
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



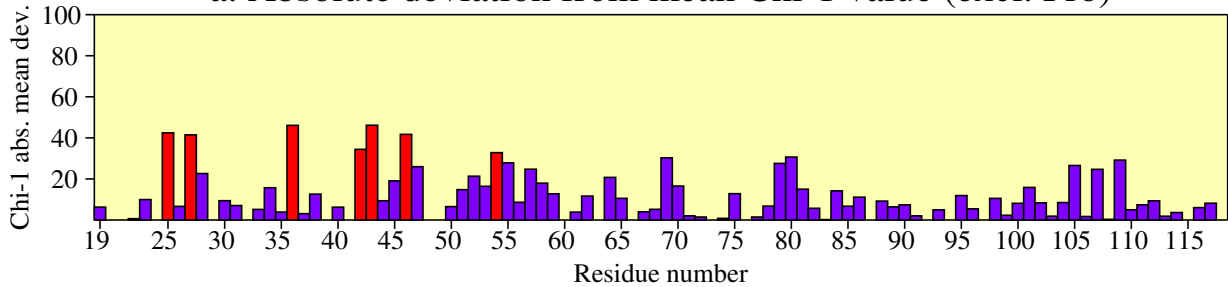
g. G-factors



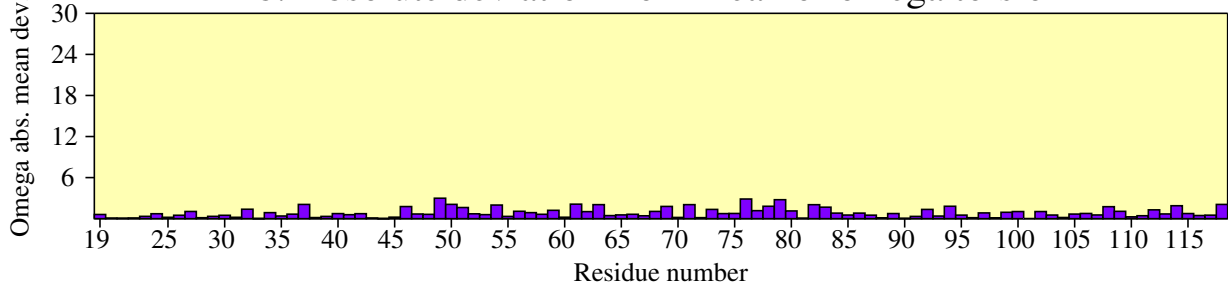
Residue properties

2b76

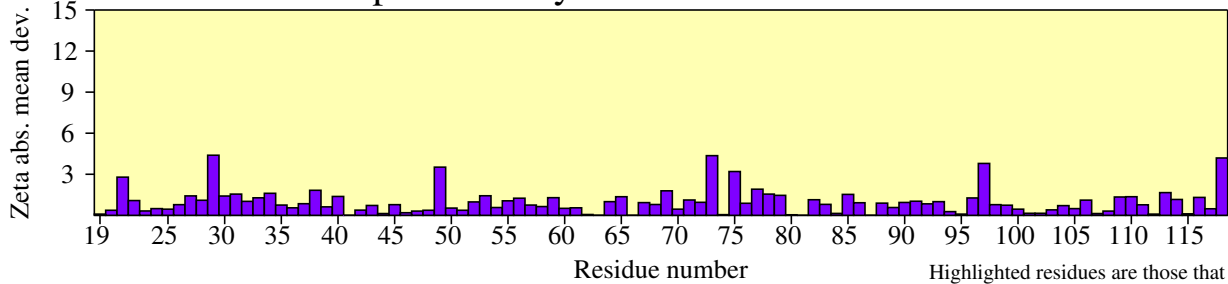
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

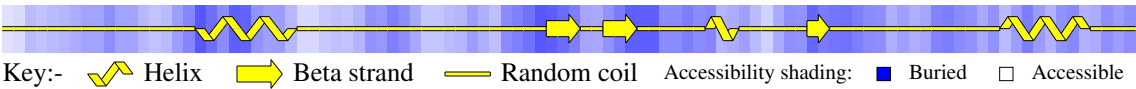


c. C-alpha chirality: abs. deviation of zeta torsion



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

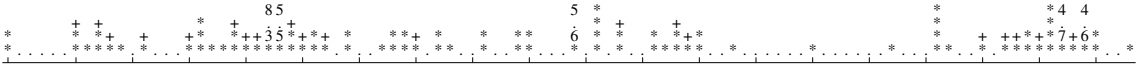
d. Secondary structure & estimated accessibility



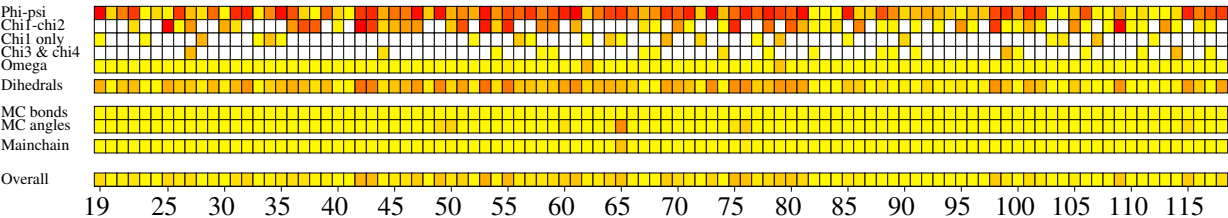
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



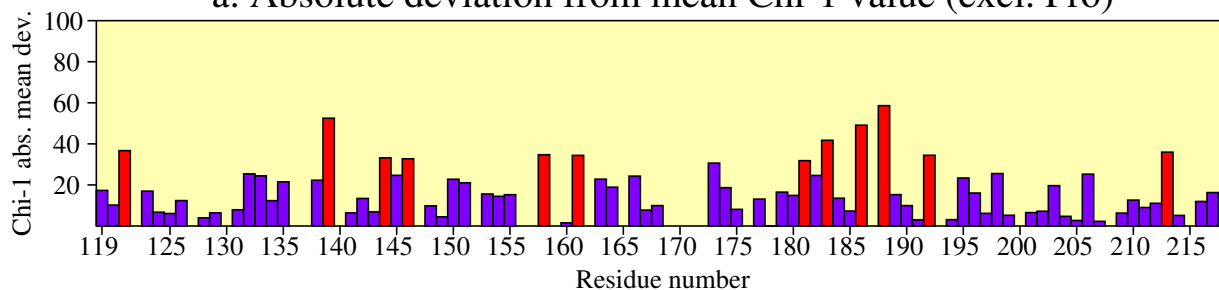
g. G-factors



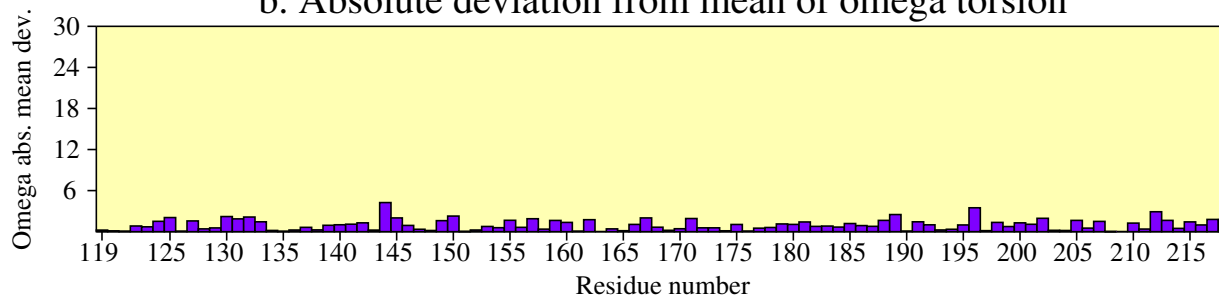
Residue properties

2b76

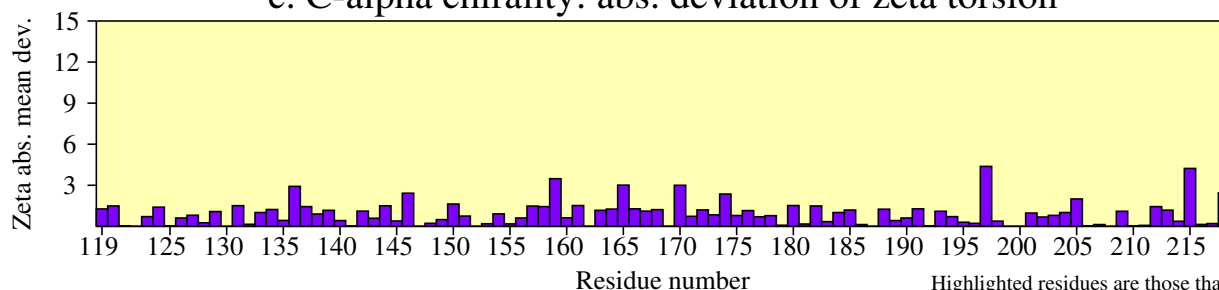
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

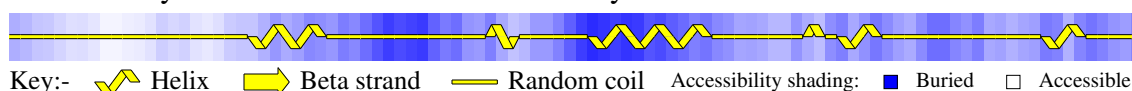


c. C-alpha chirality: abs. deviation of zeta torsion



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

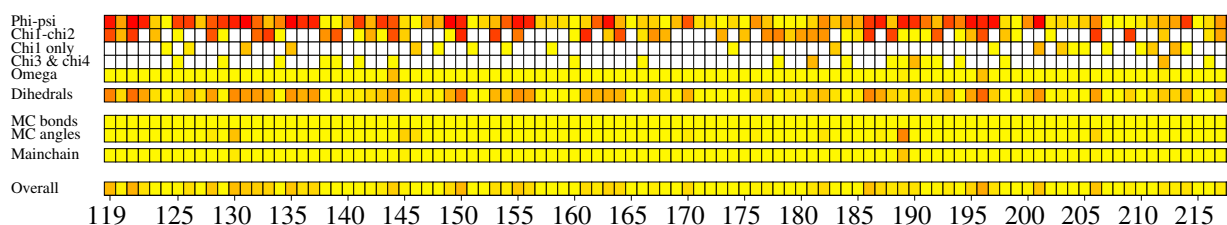
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



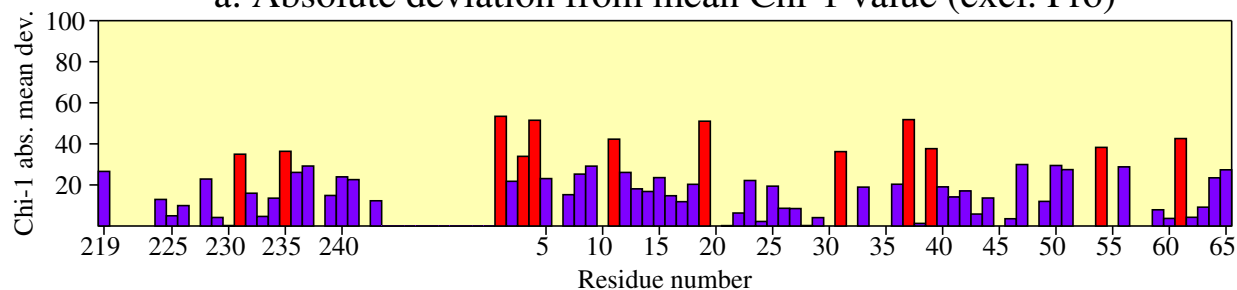
g. G-factors



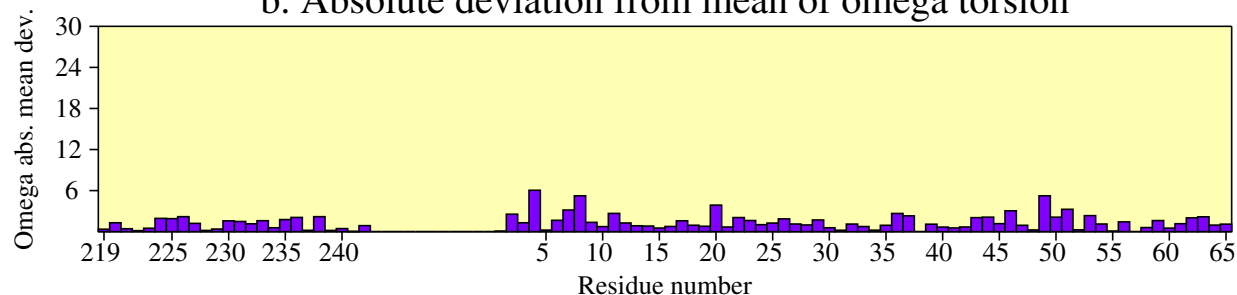
Residue properties

2b76

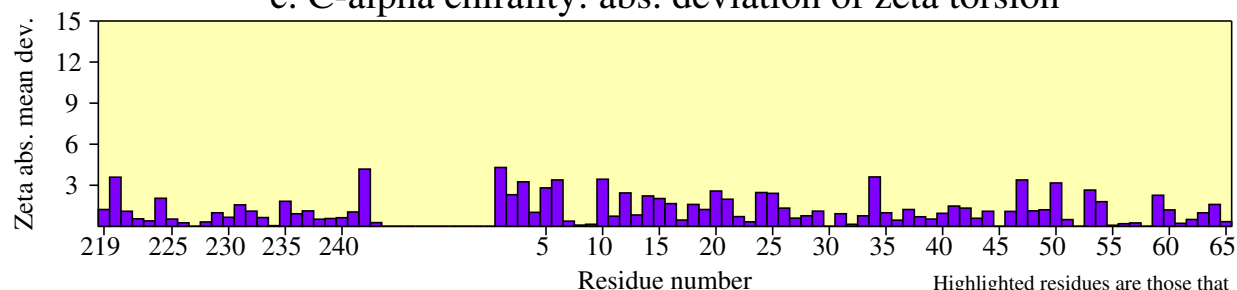
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

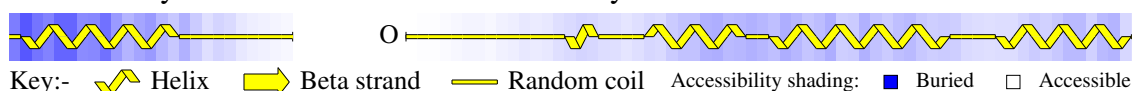


c. C-alpha chirality: abs. deviation of zeta torsion

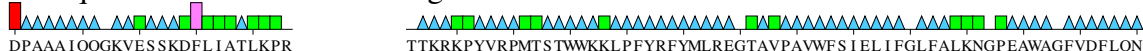


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

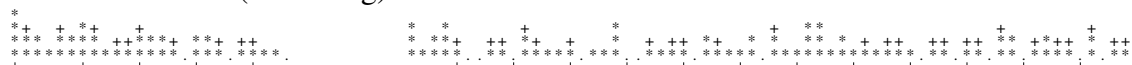
d. Secondary structure & estimated accessibility



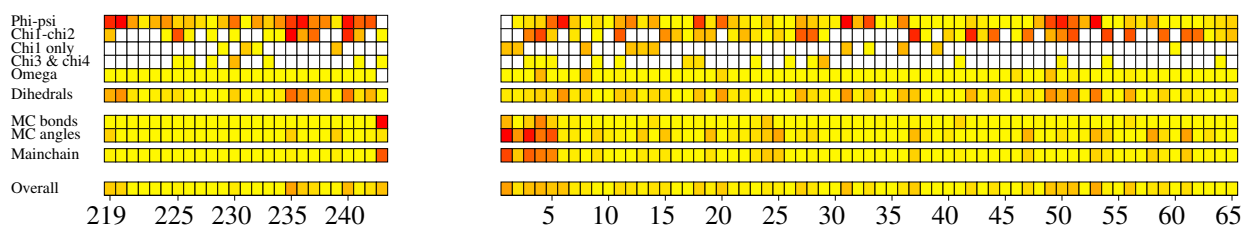
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



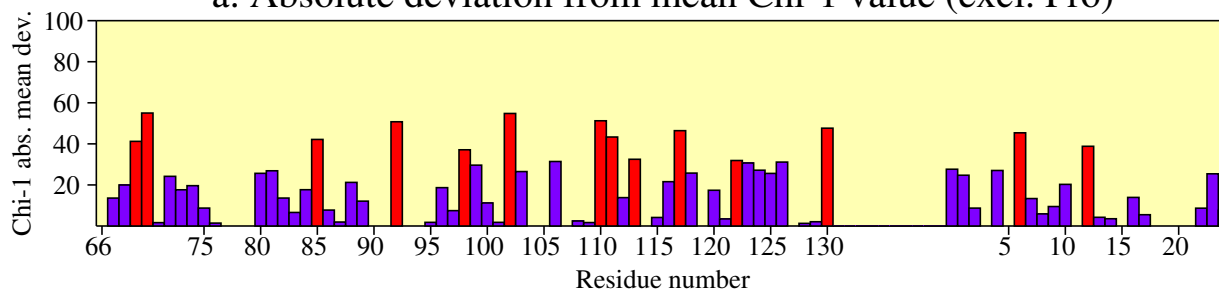
g. G-factors



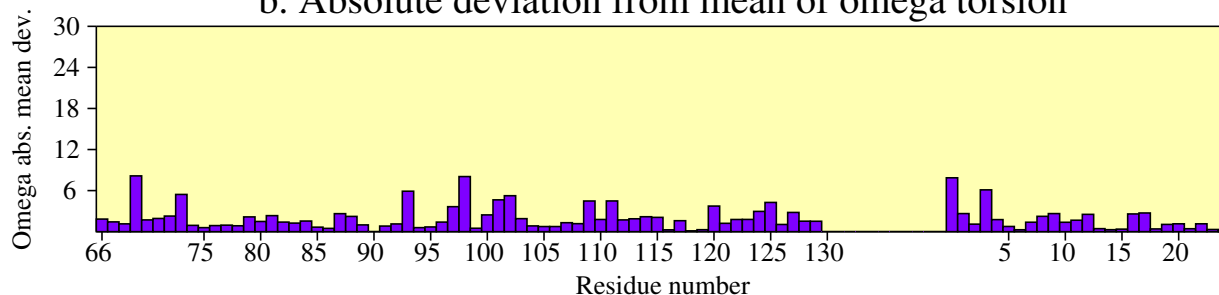
Residue properties

2b76

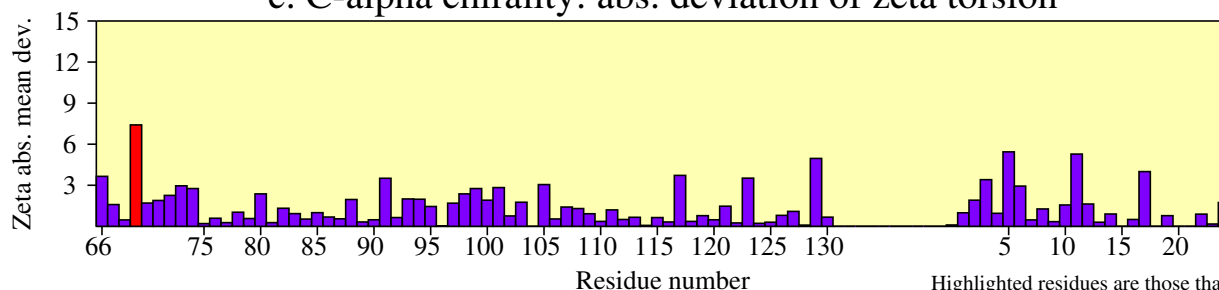
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

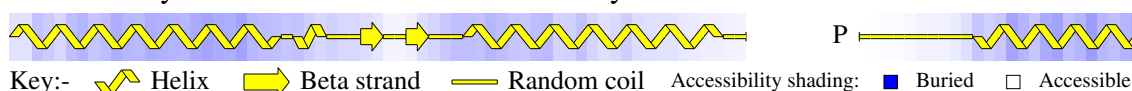


c. C-alpha chirality: abs. deviation of zeta torsion



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

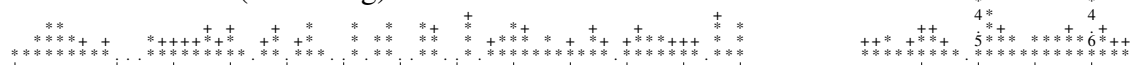
d. Secondary structure & estimated accessibility



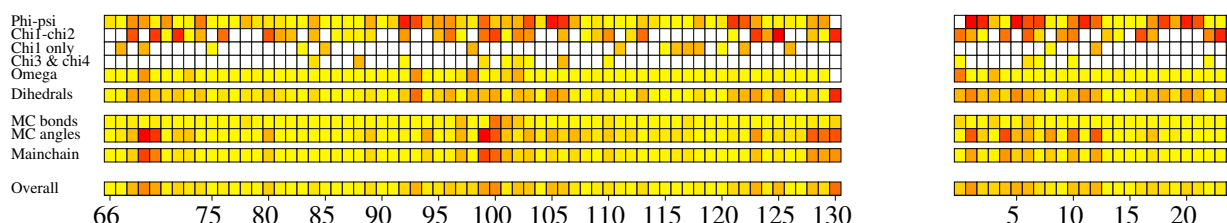
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



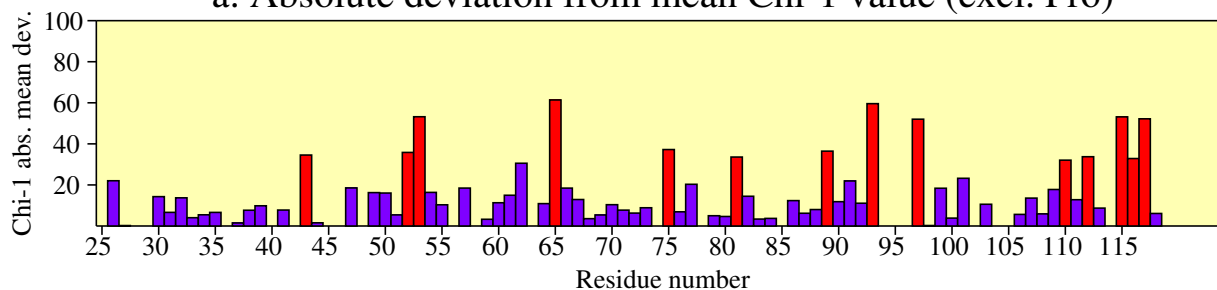
g. G-factors



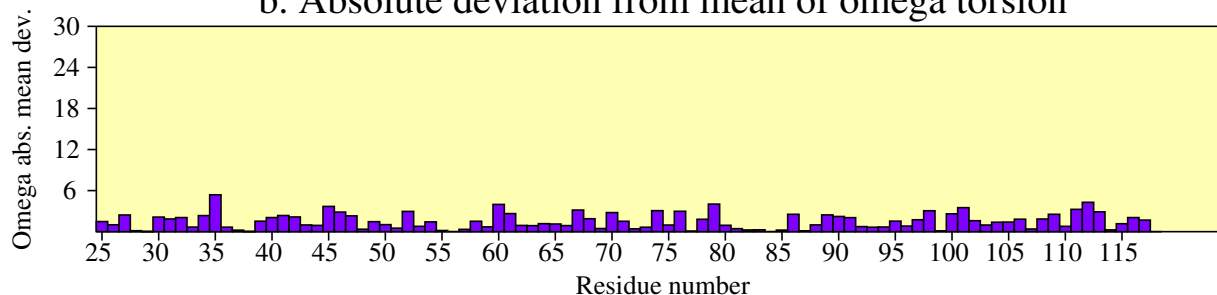
Residue properties

2b76

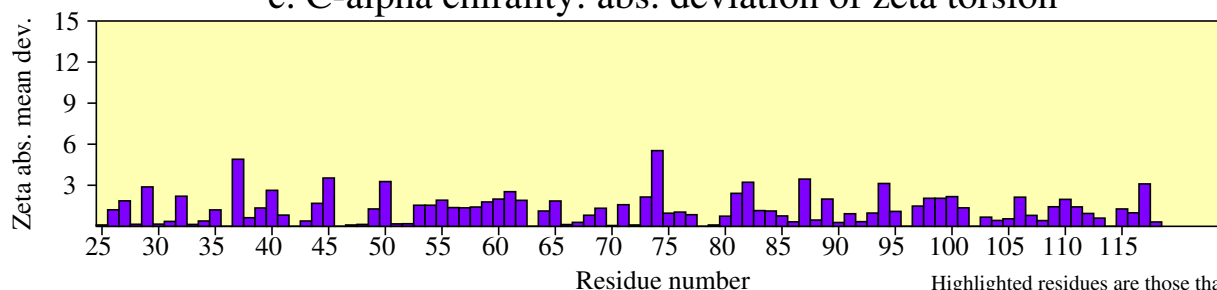
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

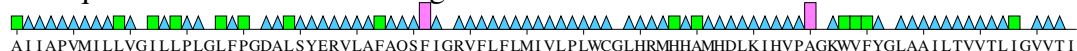


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

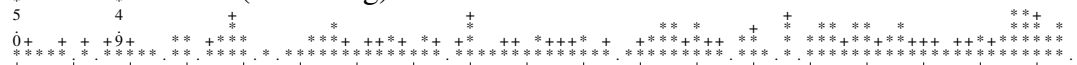
d. Secondary structure & estimated accessibility



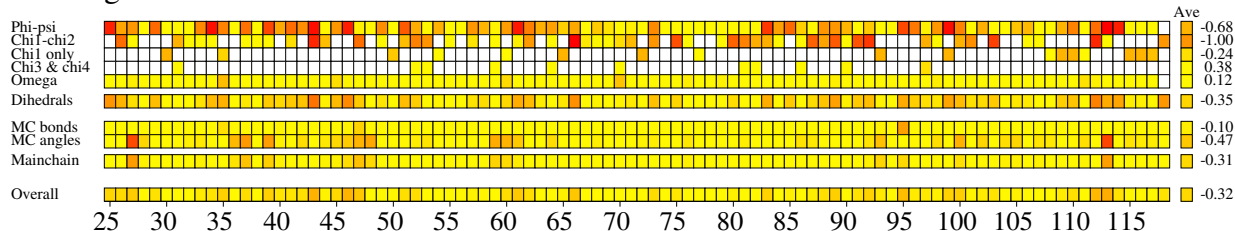
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

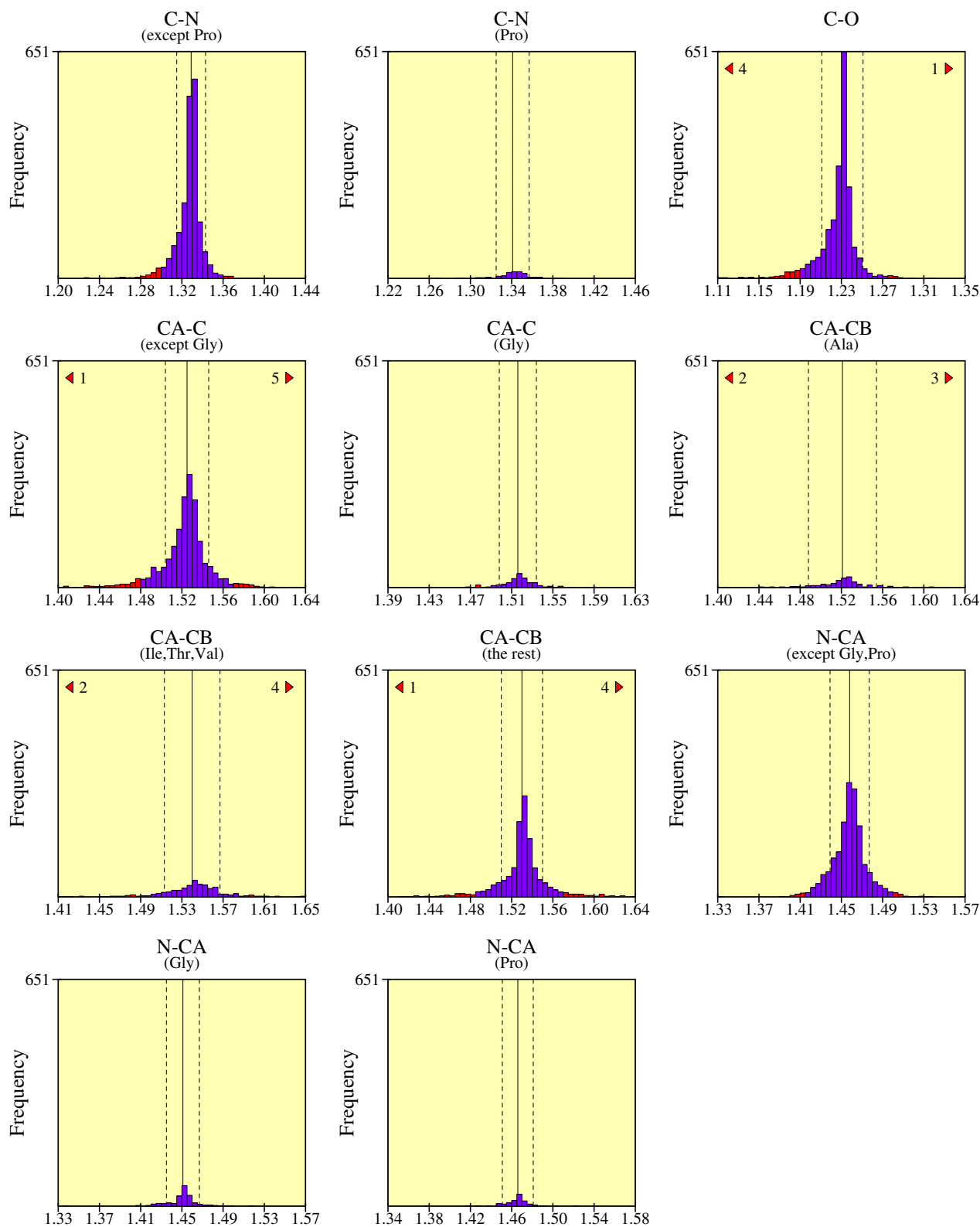


g. G-factors



Main-chain bond lengths

2b76



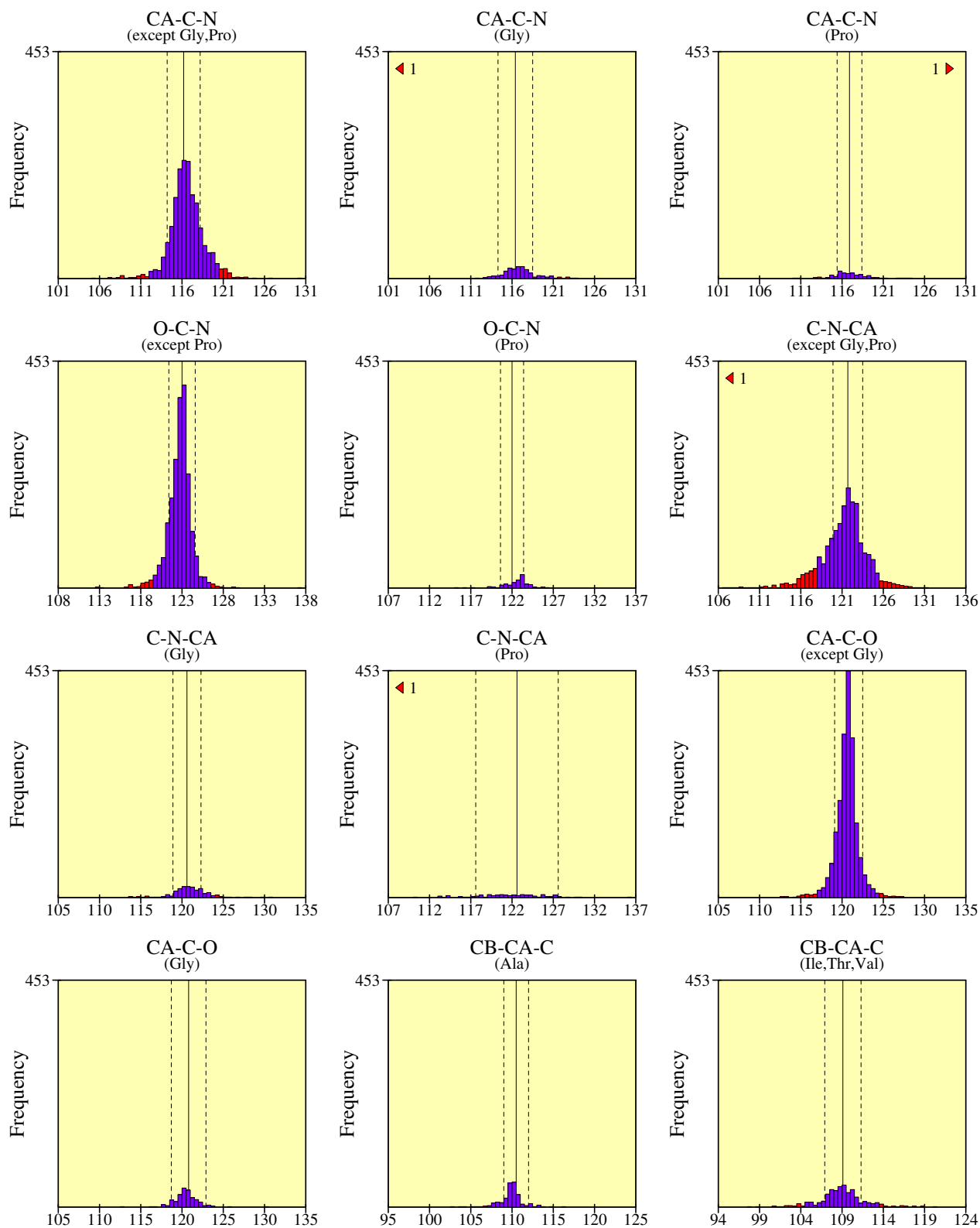
Black bars > 2.0 st. devs. from mean.

◀ 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



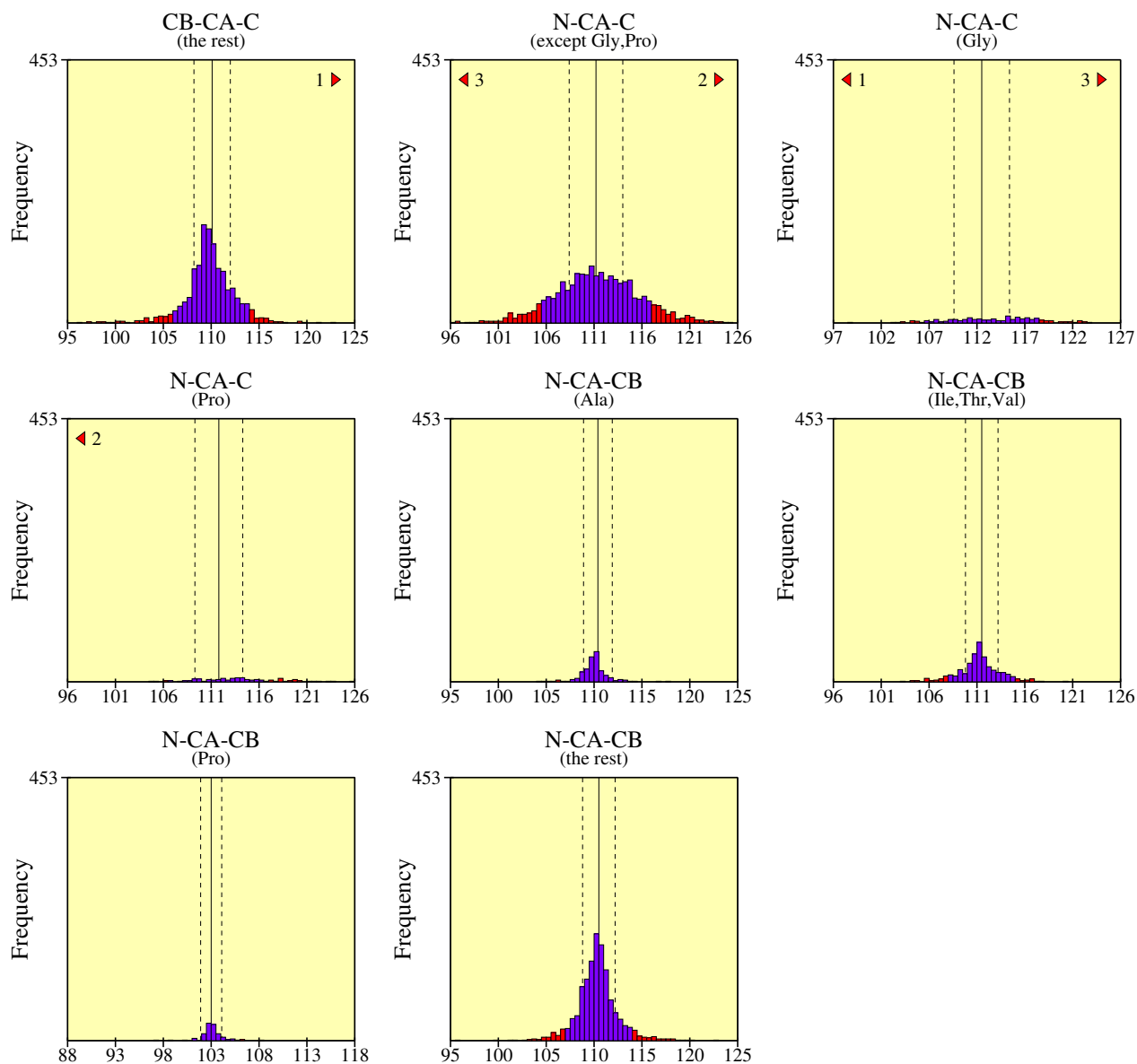
Black bars > 2.0 st. devs. from mean.

◀ 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



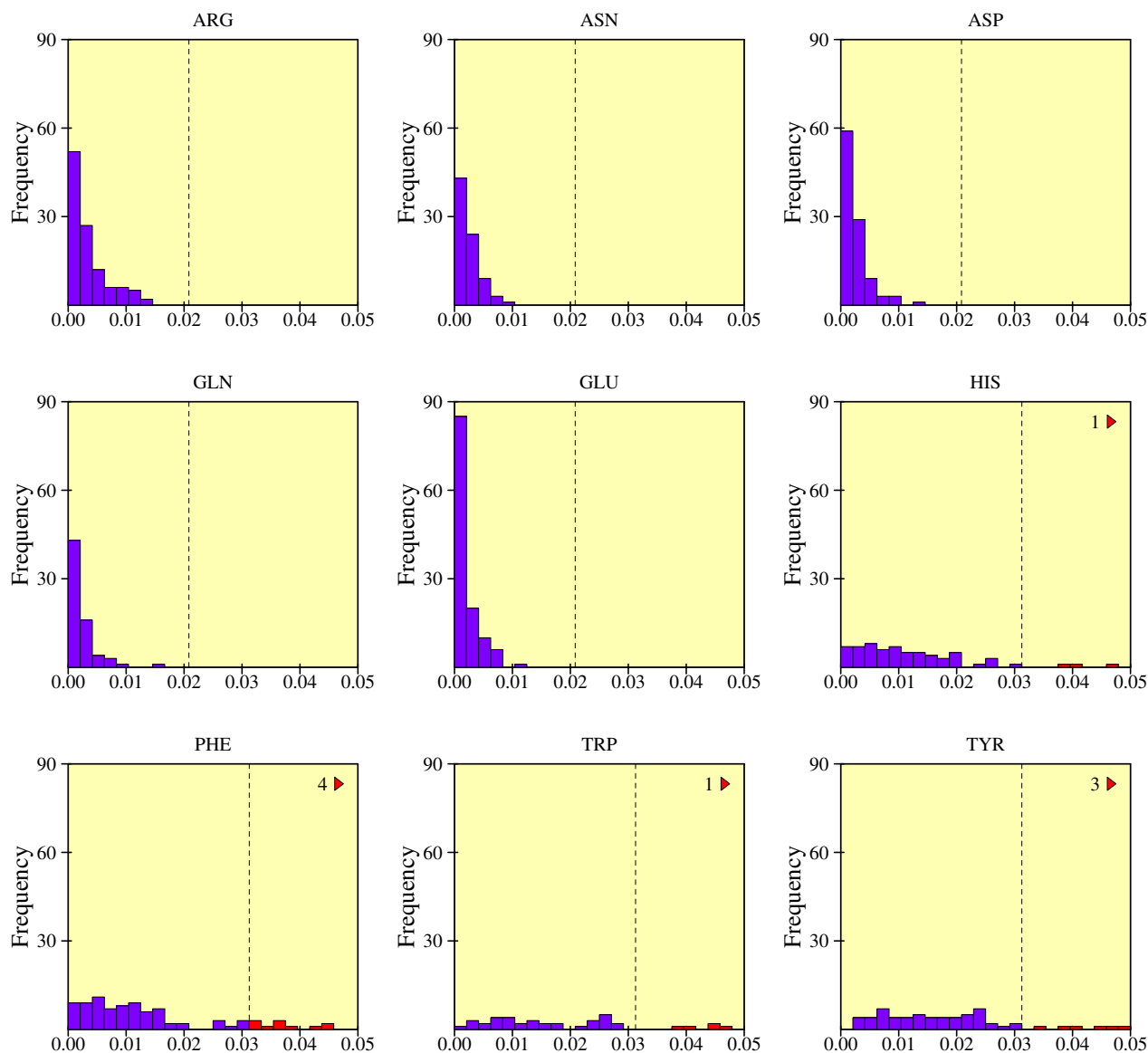
Black bars > 2.0 st. devs. from mean.

◀ 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

CA 1.530 CB 0.059 1.471 A Met 0	N 1.458 CA 0.053 1.405 A Ala 5	CA 1.525 C 0.059 1.584 A Ala 15	CA 1.521 CB 0.054 1.575 A Ala 15	CA 1.525 C 0.095 1.430 A Leu 17	CA 1.530 CB 0.070 1.460 A Leu 17
CA 1.521 CB 0.100 1.621 A Ala 20	CA 1.521 CB 0.143 1.378 A Ala 22	CA 1.525 C 0.098 1.427 A Ala 24	CA 1.521 CB 0.085 1.606 A Ala 24	CA 1.530 CB 0.063 1.467 A Gln 25	CA 1.525 C 0.051 1.474 A Asn 27
C 1.341 N 0.072 1.269 A Asn 27 - A Pro 28	CA 1.525 C 0.116 1.409 A Pro 28	N 1.466 CA 0.087 1.378 A Pro 28	CA 1.530 CB 0.067 1.597 A Asn 29	CA 1.521 CB 0.059 1.581 A Ala 30	CA 1.525 C 0.054 1.579 A Lys 31
CA 1.530 CB 0.079 1.609 A Lys 31	CA 1.530 CB 0.059 1.589 A Leu 34	C 1.231 O 0.099 1.132 A Ile 35	C 1.329 N 0.069 1.260 A Ile 35 - A Ser 36	CA 1.525 C 0.068 1.593 A Ser 36	CA 1.530 CB 0.104 1.426 A Ser 36
CA 1.525 C 0.062 1.463 A Lys 37	CA 1.540 CB 0.055 1.485 A Val 38	CA 1.525 C 0.099 1.426 A Tyr 39	CA 1.525 C 0.056 1.469 A Met 41	C 1.231 O 0.053 1.178 A Arg 42	CA 1.525 C 0.063 1.588 A Arg 42
N 1.458 CA 0.053 1.405 A Arg 42	C 1.231 O 0.053 1.178 A Ser 43	CA 1.525 C 0.064 1.589 A Ser 43	CA 1.540 CB 0.060 1.600 A Thr 45	CA 1.525 C 0.053 1.472 A Ala 48	CA 1.525 C 0.088 1.437 A Ala 53
CA 1.521 CB 0.072 1.449 A Ala 53	CA 1.521 CB 0.072 1.593 A Ala 54	CA 1.525 C 0.062 1.462 A Val 55	CA 1.525 C 0.058 1.467 A Asp 58	CA 1.530 CB 0.068 1.462 A Asp 58	CA 1.525 C 0.063 1.462 A His 59
C 1.329 N 0.060 1.269 A His 59 - A Asp 60	CA 1.530 CB 0.091 1.439 A Ser 61	C 1.231 O 0.145 1.086 A Glu 63	CA 1.530 CB 0.062 1.468 A Glu 63	CA 1.530 CB 0.055 1.585 A Tyr 64	C 1.231 O 0.059 1.172 A His 65
CA 1.525 C 0.057 1.468 A His 65	CA 1.525 C 0.052 1.473 A Phe 66	CA 1.525 C 0.055 1.470 A His 67	CA 1.530 CB 0.083 1.447 A His 67	N 1.458 CA 0.054 1.404 A His 67	N 1.458 CA 0.052 1.510 A Asp 68
C 1.231 O 0.064 1.167 A Ala 71	CA 1.525 C 0.077 1.448 A Leu 76	CA 1.525 C 0.054 1.471 A Gln 79	C 1.231 O 0.052 1.179 A Val 82	CA 1.525 C 0.066 1.459 A Val 82	CA 1.530 CB 0.089 1.619 A Tyr 84
C 1.231 O 0.056 1.175 A Phe 85	CA 1.525 C 0.057 1.468 A Phe 85	CA 1.530 CB 0.053 1.477 A His 87	CA 1.525 C 0.053 1.578 A Cys 89	CA 1.530 CB 0.099 1.629 A Cys 89	CA 1.525 C 0.117 1.408 A Pro 90

Distorted geometry

2b76

Main-chain bond lengths (contd)

CA 1.530 CB 0.135 1.395 A Pro 90	CA 1.540 CB 0.103 1.643 A Thr 91	CA 1.525 C 0.064 1.589 A Thr 94	C 1.231 O 0.051 1.180 A Gln 95	CA 1.525 C 0.063 1.462 A Gln 95	C 1.231 O 0.052 1.179 A Glu 97
CA 1.525 C 0.057 1.582 A Leu 98	C 1.231 O 0.072 1.158 A Gly 100	C 1.329 N 0.063 1.266 A Gly 100 - A Cys 101	CA 1.525 C 0.053 1.472 A Trp 103	CA 1.530 CB 0.058 1.588 A Arg 105	CA 1.525 C 0.056 1.581 A Pro 107
CA 1.530 CB 0.075 1.455 A Ser 110	CA 1.525 C 0.082 1.607 A Val 113	CA 1.540 CB 0.069 1.471 A Val 113	C 1.231 O 0.067 1.164 A Arg 114	CA 1.525 C 0.155 1.680 A Met 119	N 1.458 CA 0.067 1.525 A Met 119
C 1.329 N 0.064 1.393 A Met 119 - A Lys 120	CA 1.530 CB 0.085 1.615 A Lys 120	N 1.458 CA 0.073 1.531 A Lys 120	N 1.458 CA 0.054 1.404 A Trp 125	CA 1.530 CB 0.058 1.472 A Phe 133	CA 1.530 CB 0.066 1.596 A His 134
C 1.231 O 0.054 1.177 A Met 135	CA 1.525 C 0.081 1.444 A Met 135	C 1.231 O 0.098 1.133 A Leu 136	CA 1.525 C 0.080 1.445 A Leu 136	CA 1.530 CB 0.078 1.452 A Leu 136	C 1.231 O 0.083 1.148 A Thr 138
CA 1.540 CB 0.141 1.681 A Thr 138	CA 1.525 C 0.058 1.583 A Gln 141	CA 1.530 CB 0.079 1.609 A Gln 141	CA 1.530 CB 0.066 1.464 A Ser 143	C 1.231 O 0.122 1.109 A Gln 145	CA 1.525 C 0.066 1.459 A Phe 146
CA 1.525 C 0.061 1.464 A Ile 149	CA 1.540 CB 0.064 1.476 A Ile 149	C 1.231 O 0.050 1.181 A Phe 156	N 1.458 CA 0.050 1.508 A Val 157	CA 1.525 C 0.070 1.595 A Ile 160	CA 1.540 CB 0.054 1.594 A Ile 160
CA 1.525 C 0.056 1.581 A Asp 164	N 1.458 CA 0.060 1.398 A Asp 164	CA 1.525 C 0.085 1.440 A Val 167	CA 1.540 CB 0.079 1.461 A Val 171	CA 1.521 CB 0.132 1.389 A Ala 172	CA 1.525 C 0.066 1.591 A Asn 174
CA 1.530 CB 0.050 1.580 A Glu 177	CA 1.525 C 0.064 1.589 A Val 181	CA 1.525 C 0.066 1.459 A Ile 183	CA 1.540 CB 0.117 1.657 A Ile 183	CA 1.525 C 0.076 1.449 A Ala 185	N 1.458 CA 0.053 1.511 A Ala 185
CA 1.525 C 0.082 1.443 A Asn 186	CA 1.540 CB 0.080 1.620 A Val 188	CA 1.540 CB 0.064 1.604 A Val 189	C 1.231 O 0.080 1.151 A Thr 192	CA 1.525 C 0.118 1.407 A Thr 192	CA 1.525 C 0.092 1.617 A Ala 195
N 1.458 CA 0.071 1.529 A Ala 195	CA 1.525 C 0.079 1.446 A Arg 197	N 1.458 CA 0.051 1.407 A Val 198	CA 1.530 CB 0.059 1.471 A Arg 200	CA 1.525 C 0.053 1.578 A Tyr 201	CA 1.530 CB 0.072 1.458 A Asn 202

Distorted geometry

2b76

Main-chain bond lengths (contd)

C 1.231 O 0.051 1.180 A Gly 205	C 1.231 O 0.063 1.168 A Ile 207	CA 1.525 C 0.064 1.461 A Ile 207	C 1.329 N 0.053 1.382 A Thr 209 - A Gly 210	C 1.329 N 0.064 1.265 A Asp 211 - A Gly 212	CA 1.530 CB 0.079 1.609 A Met 215
CA 1.521 CB 0.095 1.616 A Ala 216	CA 1.525 C 0.109 1.416 A His 219	CA 1.530 CB 0.102 1.428 A His 219	C 1.231 O 0.112 1.119 A Gly 220	C 1.329 N 0.052 1.277 A Gly 220 - A Val 221	CA 1.540 CB 0.136 1.404 A Val 221
CA 1.525 C 0.073 1.452 A Leu 223	CA 1.530 CB 0.053 1.583 A Leu 223	CA 1.525 C 0.052 1.473 A Arg 224	CA 1.530 CB 0.061 1.469 A Asp 225	CA 1.525 C 0.060 1.585 A Phe 228	CA 1.530 CB 0.064 1.594 A Phe 228
C 1.231 O 0.120 1.111 A Val 229	CA 1.525 C 0.051 1.576 A Val 229	CA 1.540 CB 0.074 1.614 A Val 229	C 1.329 N 0.057 1.272 A Val 229 - A Gln 230	CA 1.530 CB 0.060 1.470 A His 232	C 1.231 O 0.066 1.165 A Pro 237
CA 1.525 C 0.059 1.466 A Pro 237	CA 1.530 CB 0.061 1.469 A Pro 237	C 1.231 O 0.134 1.097 A Gly 240	C 1.329 N 0.052 1.277 A Gly 240 - A Ile 241	C 1.231 O 0.090 1.141 A Met 243	CA 1.525 C 0.051 1.576 A Arg 248
CA 1.525 C 0.069 1.594 A Ile 253	CA 1.540 CB 0.124 1.664 A Ile 253	CA 1.530 CB 0.053 1.477 A Asp 265	C 1.329 N 0.066 1.263 A Asp 265 - A Tyr 266	N 1.451 CA 0.113 1.338 A Gly 269	C 1.341 N 0.051 1.290 A Gly 269 - A Pro 270
CA 1.525 C 0.155 1.680 A Pro 270	C 1.329 N 0.061 1.390 A Pro 270 - A Glu 271	CA 1.525 C 0.126 1.651 A Thr 272	CA 1.530 CB 0.141 1.671 A Glu 276	N 1.458 CA 0.126 1.332 A Glu 276	CA 1.525 C 0.183 1.708 A Pro 277
N 1.466 CA 0.058 1.524 A Pro 277	CA 1.530 CB 0.064 1.594 A Asn 279	C 1.231 O 0.127 1.104 A Arg 287	CA 1.525 C 0.056 1.469 A Asp 288	CA 1.525 C 0.051 1.576 A Lys 289	CA 1.525 C 0.051 1.474 A Ser 291
C 1.231 O 0.055 1.176 A His 296	CA 1.530 CB 0.099 1.629 A Arg 299	CA 1.525 C 0.060 1.585 A Asn 302	CA 1.525 C 0.056 1.581 A Thr 303	CA 1.530 CB 0.050 1.480 A Pro 307	N 1.458 CA 0.052 1.406 A Arg 308
CA 1.516 C 0.053 1.569 A Gly 309	CA 1.540 CB 0.118 1.422 A Val 312	CA 1.525 C 0.054 1.579 A Leu 314	CA 1.530 CB 0.055 1.585 A Leu 324	CA 1.525 C 0.116 1.409 A His 325	CA 1.530 CB 0.057 1.473 A Glu 326
N 1.458 CA 0.077 1.535 A Glu 326	CA 1.525 C 0.101 1.626 A Arg 327	CA 1.530 CB 0.059 1.589 A Arg 327	CA 1.525 C 0.057 1.582 A Leu 328	N 1.458 CA 0.111 1.569 A Leu 328	CA 1.525 C 0.060 1.465 A Pro 329

Distorted geometry

2b76

Main-chain bond lengths (contd)

CA 1.530 CB 0.054 1.584 A Pro 329	CA 1.530 CB 0.106 1.636 A Phe 330	CA 1.540 CB 0.066 1.606 A Ile 331	CA 1.525 C 0.062 1.587 A Cys 332	CA 1.521 CB 0.057 1.464 A Ala 335	CA 1.525 C 0.072 1.597 A Val 344
CA 1.530 CB 0.066 1.595 A Glu 346	CA 1.525 C 0.083 1.608 A Pro 347	C 1.231 O 0.051 1.281 A Ile 348	CA 1.525 C 0.089 1.614 A Arg 351	CA 1.530 CB 0.096 1.626 A Arg 351	CA 1.525 C 0.159 1.684 A Pro 352
CA 1.525 C 0.055 1.470 A Thr 353	CA 1.525 C 0.052 1.577 A Thr 357	CA 1.540 CB 0.127 1.413 A Thr 357	CA 1.525 C 0.062 1.463 A Met 358	C 1.231 O 0.050 1.281 A Gly 359	CA 1.540 CB 0.060 1.480 A Ile 361
CA 1.530 CB 0.053 1.582 A Glu 362	CA 1.525 C 0.071 1.596 A Gln 365	CA 1.525 C 0.063 1.462 A Asn 366	CA 1.530 CB 0.108 1.422 A Glu 368	CA 1.540 CB 0.110 1.650 A Thr 369	CA 1.525 C 0.074 1.451 A Arg 370
CA 1.540 CB 0.134 1.674 A Ile 371	C 1.231 O 0.076 1.155 A Lys 372	CA 1.525 C 0.062 1.587 A Lys 372	CA 1.530 CB 0.079 1.609 A Lys 372	CA 1.521 CB 0.077 1.444 A Ala 376	C 1.231 O 0.114 1.117 A His 386
CA 1.530 CB 0.083 1.447 A His 386	C 1.329 N 0.056 1.273 A His 386 - A Gly 387	CA 1.521 CB 0.074 1.595 A Ala 388	C 1.231 O 0.064 1.167 A Asn 389	CA 1.530 CB 0.099 1.431 A Asn 389	C 1.231 O 0.061 1.170 A Arg 390
CA 1.525 C 0.094 1.431 A Arg 390	C 1.231 O 0.093 1.138 A Leu 391	CA 1.530 CB 0.113 1.417 A Leu 391	C 1.231 O 0.057 1.174 A Ser 393	CA 1.525 C 0.052 1.473 A Ser 395	CA 1.530 CB 0.093 1.623 A Leu 396
CA 1.525 C 0.081 1.444 A Leu 399	CA 1.540 CB 0.107 1.433 A Val 400	N 1.458 CA 0.052 1.406 A Val 400	C 1.231 O 0.050 1.181 A Val 401	CA 1.530 CB 0.077 1.453 A Arg 404	CA 1.530 CB 0.061 1.469 A Glu 408
CA 1.525 C 0.091 1.434 A Gln 409	C 1.231 O 0.109 1.122 A Ala 410	CA 1.525 C 0.066 1.459 A Ala 410	CA 1.525 C 0.062 1.463 A Thr 411	C 1.231 O 0.053 1.178 A Asn 419	CA 1.525 C 0.077 1.448 A Asn 421
CA 1.530 CB 0.067 1.597 A Asn 421	C 1.231 O 0.095 1.136 A Glu 422	CA 1.521 CB 0.137 1.658 A Ala 424	CA 1.540 CB 0.107 1.647 A Ile 425	CA 1.525 C 0.080 1.605 A Ala 429	CA 1.521 CB 0.060 1.581 A Ala 429
CA 1.525 C 0.056 1.581 A Val 432	N 1.458 CA 0.066 1.392 A Leu 436	CA 1.525 C 0.054 1.579 A Asn 441	CA 1.525 C 0.057 1.582 A Gln 442	C 1.329 N 0.101 1.228 A Gly 445 - A Glu 446	C 1.329 N 0.053 1.276 A Glu 446 - A Asn 447

Distorted geometry

2b76

Main-chain bond lengths (contd)

CA 1.525 C 0.055 1.580 A Asn 447	CA 1.525 C 0.066 1.459 A Ile 451	CA 1.540 CB 0.072 1.467 A Ile 451	C 1.231 O 0.058 1.173 A Asp 453	CA 1.530 CB 0.056 1.474 A Glu 454	C 1.231 O 0.056 1.175 A Gly 456
CA 1.530 CB 0.090 1.440 A Met 459	C 1.231 O 0.059 1.172 A Glu 461	CA 1.530 CB 0.118 1.648 A Glu 461	C 1.231 O 0.056 1.175 A Ile 465	CA 1.540 CB 0.146 1.394 A Ile 465	CA 1.525 C 0.094 1.431 A Arg 467
CA 1.525 C 0.132 1.393 A Pro 469	CA 1.530 CB 0.057 1.587 A Leu 471	CA 1.525 C 0.066 1.459 A Met 472	CA 1.530 CB 0.061 1.469 A Met 472	CA 1.530 CB 0.085 1.615 A Lys 474	CA 1.525 C 0.073 1.452 A Thr 475
C 1.231 O 0.052 1.179 A Lys 478	CA 1.530 CB 0.051 1.479 A Leu 479	CA 1.525 C 0.090 1.435 A Ala 480	CA 1.530 CB 0.075 1.605 A Glu 481	C 1.231 O 0.069 1.162 A Glu 484	CA 1.525 C 0.121 1.404 A Glu 484
CA 1.530 CB 0.074 1.604 A Glu 484	C 1.231 O 0.054 1.285 A Phe 486	CA 1.530 CB 0.086 1.616 A Lys 487	CA 1.525 C 0.072 1.453 A Val 489	CA 1.540 CB 0.059 1.599 A Val 489	CA 1.530 CB 0.102 1.428 A Arg 490
C 1.231 O 0.072 1.159 A Thr 494	CA 1.530 CB 0.064 1.594 A Asn 499	CA 1.540 CB 0.052 1.592 A Thr 500	C 1.231 O 0.060 1.171 A Tyr 504	C 1.231 O 0.056 1.175 A Glu 507	CA 1.530 CB 0.060 1.590 A Leu 508
C 1.231 O 0.057 1.174 A His 510	C 1.231 O 0.071 1.160 A Leu 512	CA 1.530 CB 0.051 1.581 A Leu 512	C 1.231 O 0.058 1.173 A Asn 513	CA 1.540 CB 0.110 1.430 A Val 514	CA 1.530 CB 0.078 1.608 A Glu 516
CA 1.530 CB 0.053 1.477 A Cys 517	CA 1.525 C 0.055 1.580 A Met 518	CA 1.521 CB 0.053 1.574 A Ala 519	CA 1.530 CB 0.072 1.458 A His 520	CA 1.525 C 0.055 1.470 A Ser 521	CA 1.521 CB 0.119 1.640 A Ala 522
CA 1.530 CB 0.072 1.602 A Met 523	C 1.231 O 0.053 1.178 A Leu 535	CA 1.525 C 0.088 1.437 A Leu 535	CA 1.525 C 0.099 1.426 A Cys 539	C 1.329 N 0.069 1.260 A Cys 539 - A Thr 540	CA 1.525 C 0.075 1.450 A Arg 542
CA 1.530 CB 0.062 1.468 A Arg 542	CA 1.530 CB 0.159 1.689 A Asp 543	C 1.231 O 0.096 1.135 A Asp 544	C 1.231 O 0.087 1.144 A Val 545	CA 1.525 C 0.066 1.459 A Val 545	CA 1.540 CB 0.069 1.609 A Val 545
CA 1.530 CB 0.113 1.643 A Asn 546	CA 1.530 CB 0.089 1.619 A Phe 547	CA 1.530 CB 0.066 1.464 A Leu 548	CA 1.530 CB 0.053 1.477 A His 550	CA 1.521 CB 0.078 1.443 A Ala 553	C 1.329 N 0.072 1.257 A Arg 555 - A Asp 556

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)

CA 1.540 CB 0.063 1.477 D Val 93	CA 1.521 CB 0.089 1.610 D Ala 95	CA 1.540 CB 0.071 1.611 D Thr 108	C 1.231 O 0.125 1.355 O Thr 1	C 1.231 O 0.069 1.300 O Arg 4	C 1.231 O 0.055 1.176 O Lys 5
CA 1.540 CB 0.056 1.484 O Val 8	CA 1.540 CB 0.058 1.597 O Thr 14	CA 1.540 CB 0.059 1.599 O Ile 97	C 1.231 O 0.053 1.284 O Asp 100	CA 1.530 CB 0.052 1.582 O Asp 100	CA 1.530 CB 0.057 1.587 O Lys 102
C 1.231 O 0.052 1.283 O Trp 130	CA 1.530 CB 0.057 1.587 P Lys 6	CA 1.540 CB 0.055 1.485 P Ile 37	CA 1.521 CB 0.115 1.406 P Ala 95		

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

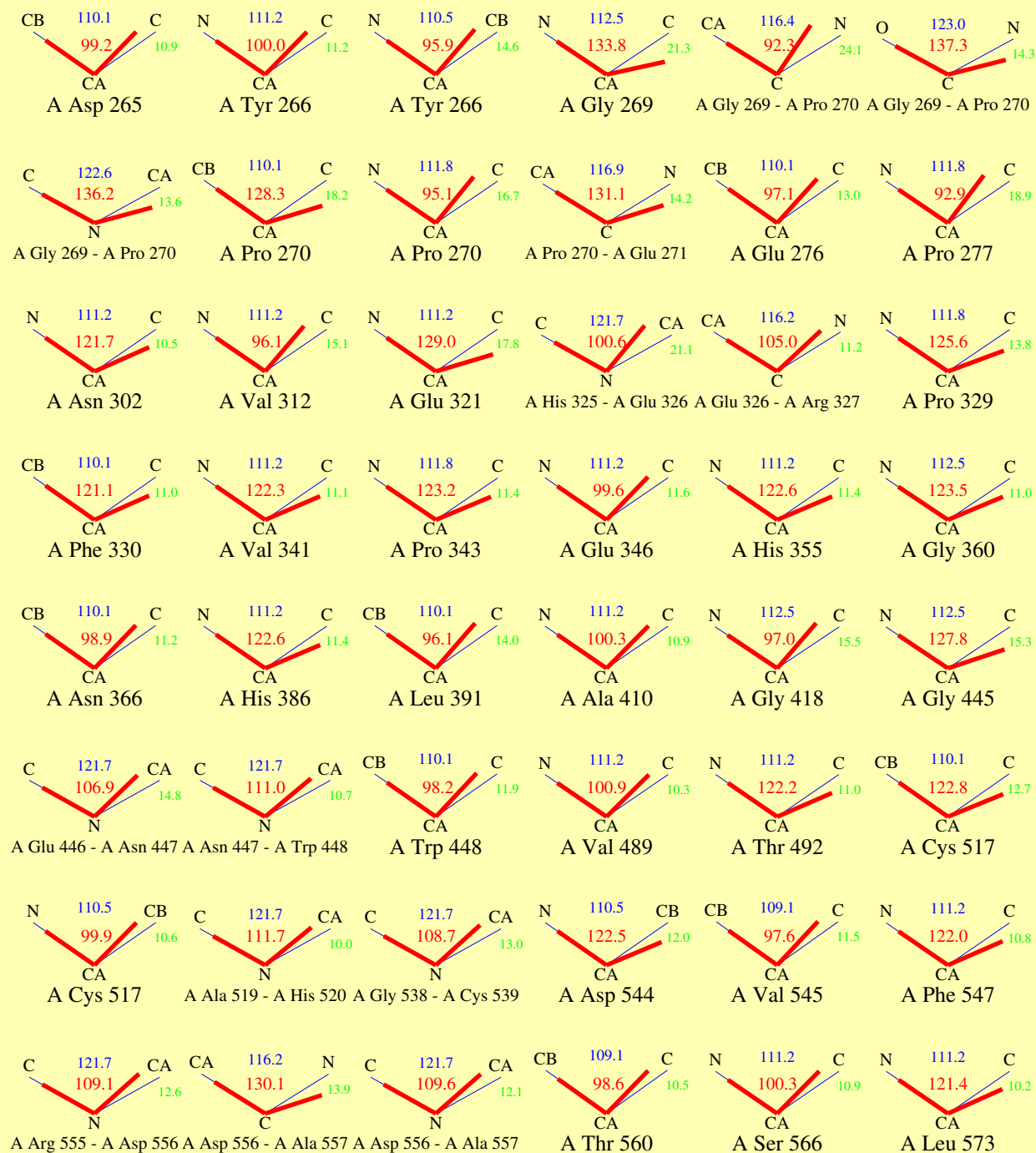
Main-chain bond angles

N 111.2 C 96.5 14.7 CA A Gln 1	N 111.2 C 97.9 13.3 CA A Phe 3	N 111.2 C 101.1 10.1 CA A Gln 4	N 111.2 C 124.7 13.5 CA A Ala 12	N 112.5 C 98.7 13.8 CA A Gly 13	C 121.7 CA 107.0 14.7 N A Pro 28 - A Asn 29
N 111.2 C 121.3 10.1 CA A Ala 30	CB 110.1 C 98.9 11.2 CA A Ser 61	CB 110.1 C 99.9 10.2 CA A Asp 68	C 121.7 CA 111.6 10.1 N A Leu 76 - A Cys 77	N 111.2 C 123.3 12.1 CA A Arg 105	CB 110.1 C 97.2 12.9 CA A Arg 106
CB 109.1 C 120.3 11.2 CA A Val 113	O 123.0 N 112.9 10.1 C A Gly 118 - A Met 119	C 121.7 CA 111.2 10.5 N A Gly 118 - A Met 119	N 111.2 C 100.7 10.5 CA A Ala 127	N 111.2 C 123.2 12.0 CA A Thr 131	N 111.2 C 101.0 10.2 CA A Val 167
N 111.2 C 99.4 11.8 CA A Val 189	C 120.6 CA 130.8 10.2 N A Gly 193 - A Gly 194	N 112.5 C 129.4 16.9 CA A Gly 194	C 121.7 CA 110.3 11.4 N A Arg 197 - A Val 198	N 112.5 C 122.7 10.2 CA A Gly 206	N 111.8 C 121.9 10.1 CA A Pro 222
N 111.2 C 94.9 16.3 CA A Leu 223	O 123.0 N 112.6 10.4 C A Val 229 - A Gln 230	N 111.8 C 123.9 12.1 CA A Pro 233	N 111.2 C 99.4 11.8 CA A Met 243	N 112.5 C 123.0 10.5 CA A Gly 249	N 111.2 C 126.1 14.9 CA A Tyr 262

Distorted geometry

2b76

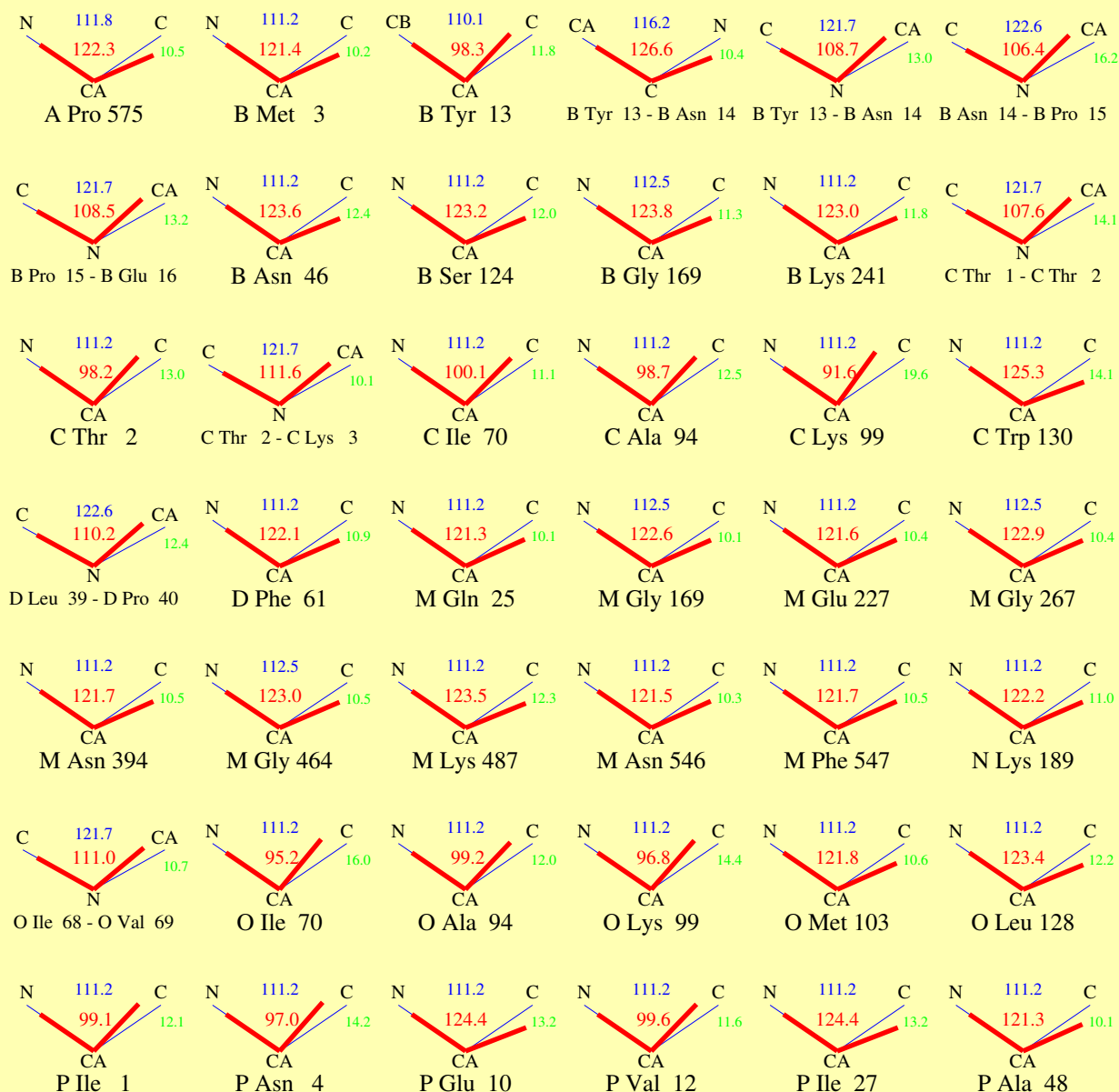
Main-chain bond angles (contd)



Distorted geometry

2b76

Main-chain bond angles (contd)

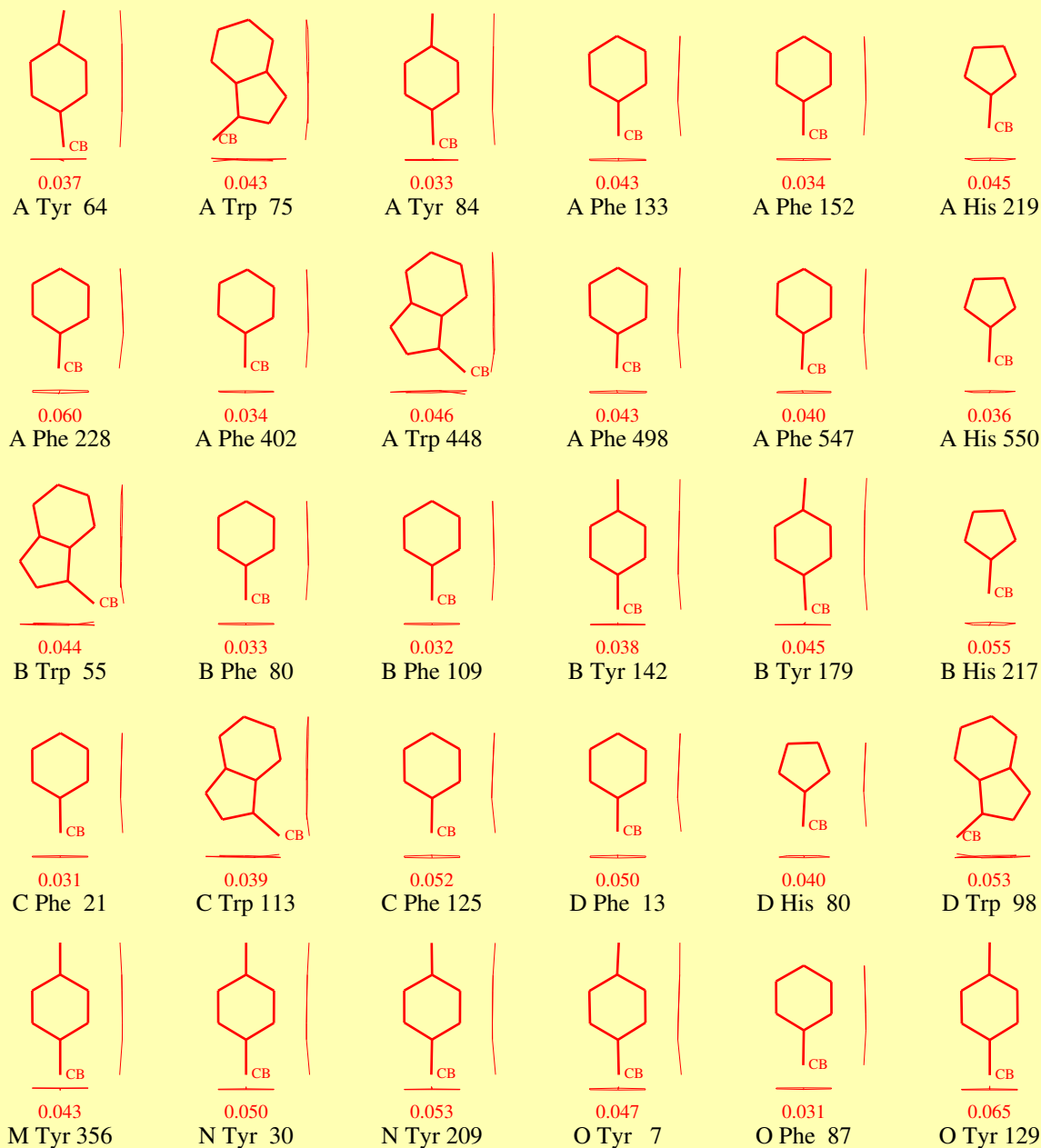


Bond angles differing by > 10.0 degrees from small-molec values. Values shown: "ideal", actual, diff.

Distorted geometry

2b76

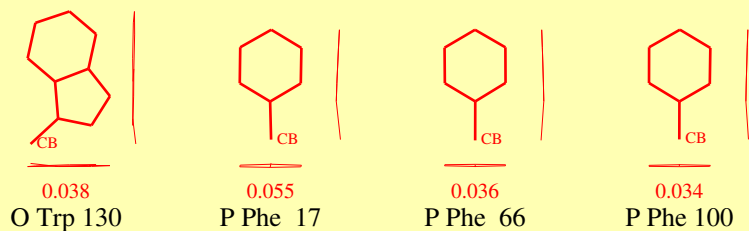
Planar groups



Distorted geometry

2b76

Planar groups (contd)



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