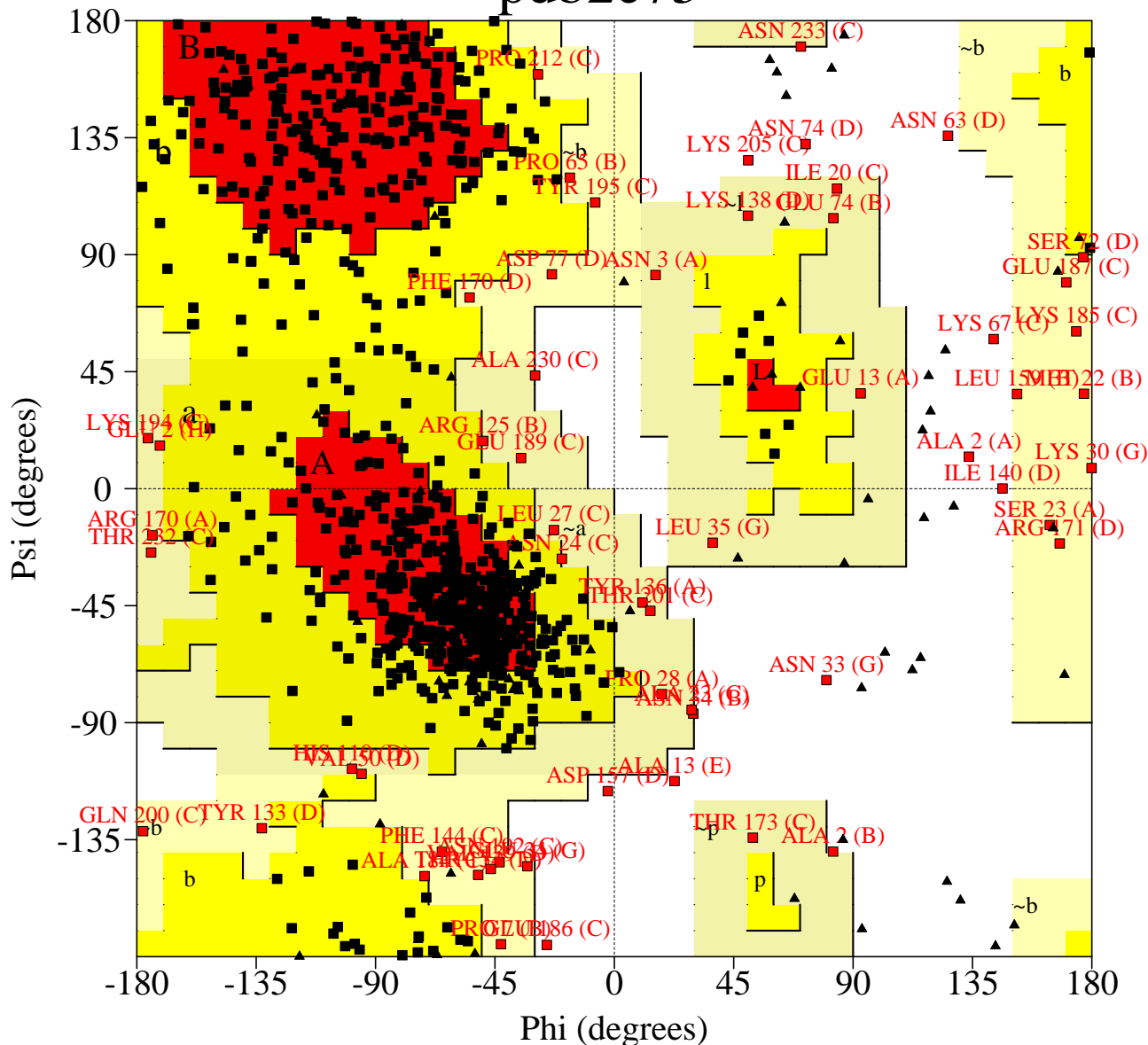


Ramachandran Plot

pdb2e75



Plot statistics

Residues in most favoured regions [A,B,L]	516	65.1%
Residues in additional allowed regions [a,b,l,p]	224	28.2%
Residues in generously allowed regions [-a,-b,-l,-p]	41	5.2%
Residues in disallowed regions	12	1.5%

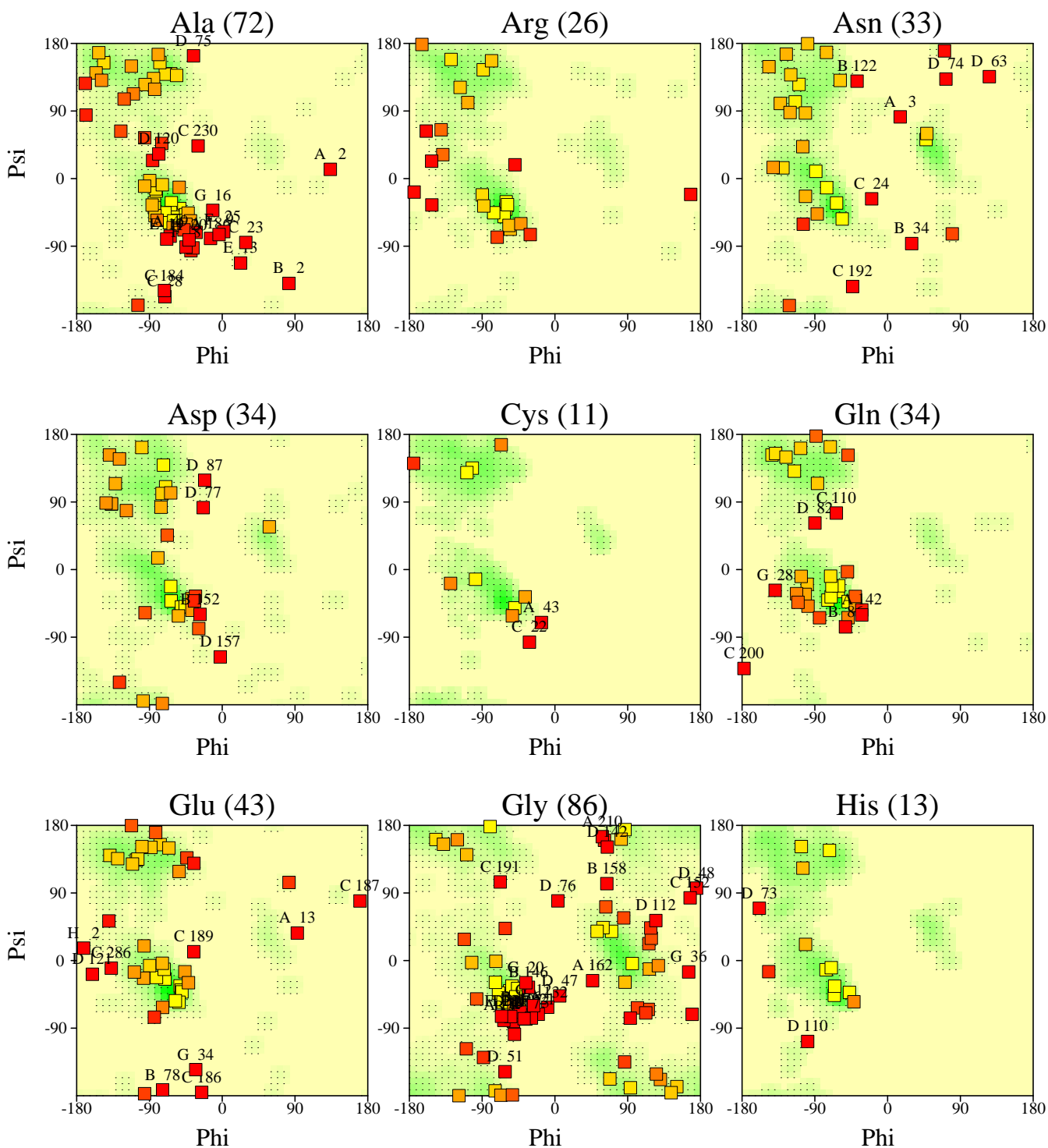
Number of non-glycine and non-proline residues	793	100.0%
Number of end-residues (excl. Gly and Pro)	17	
Number of glycine residues (shown as triangles)	87	
Number of proline residues	62	

Total number of residues	959	

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

Ramachandran plots for all residue types

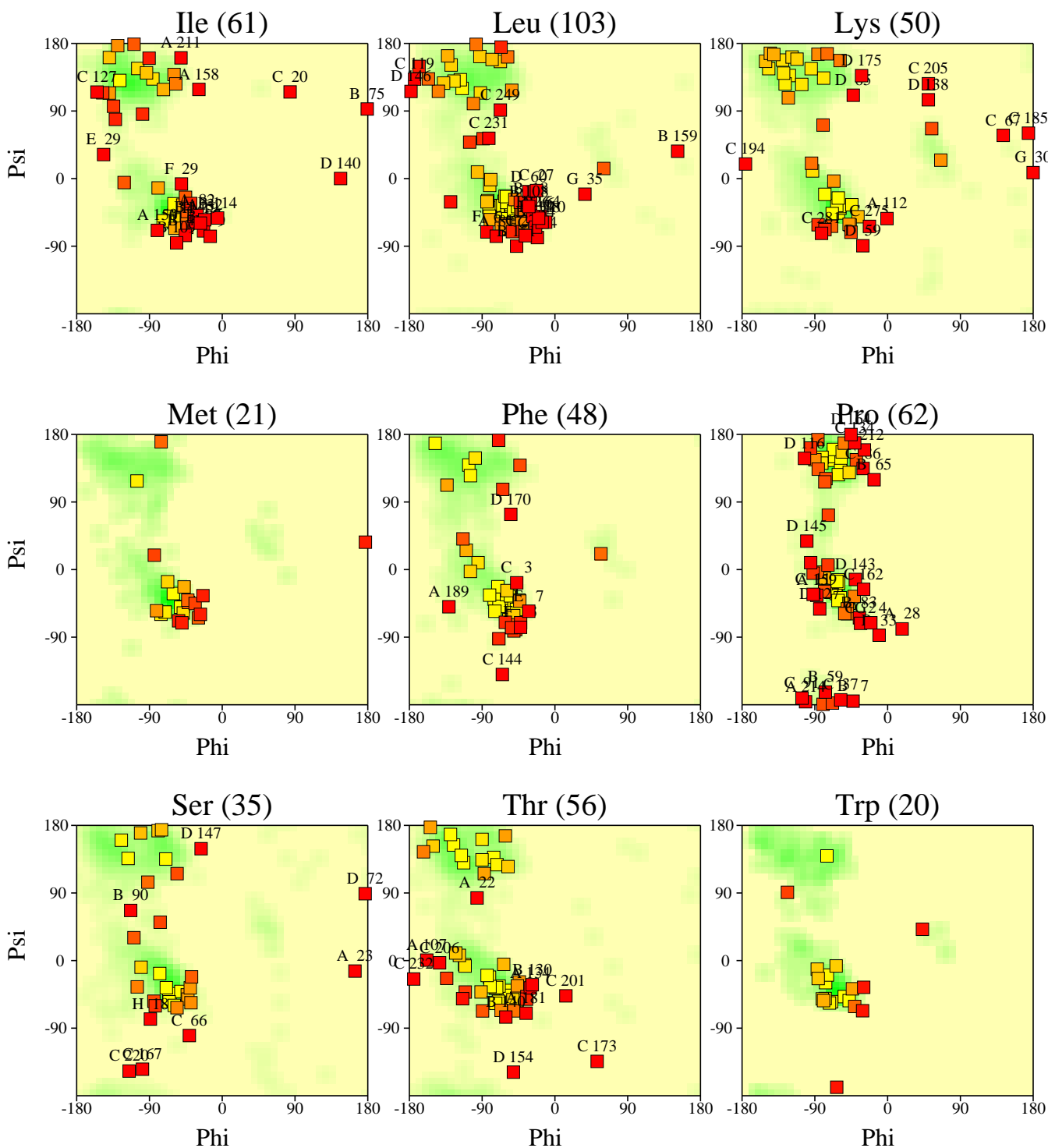
pdb2e75



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

Ramachandran plots for all residue types

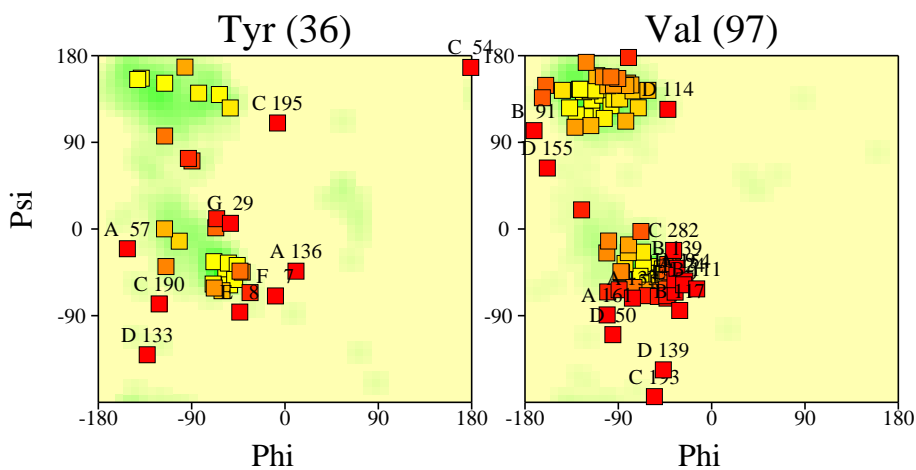
pdb2e75



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

Ramachandran plots for all residue types

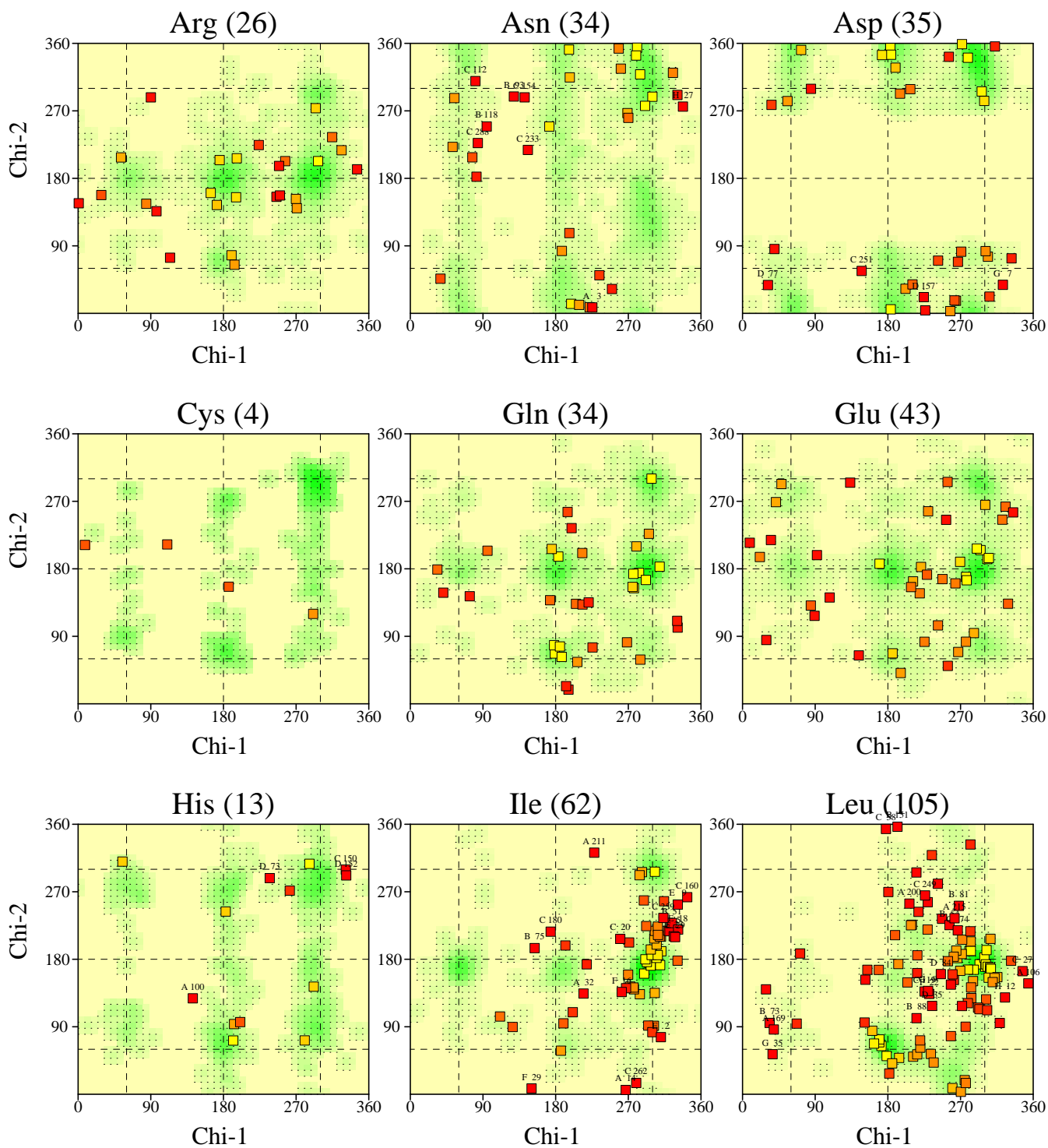
pdb2e75



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

Chi1-Chi2 plots

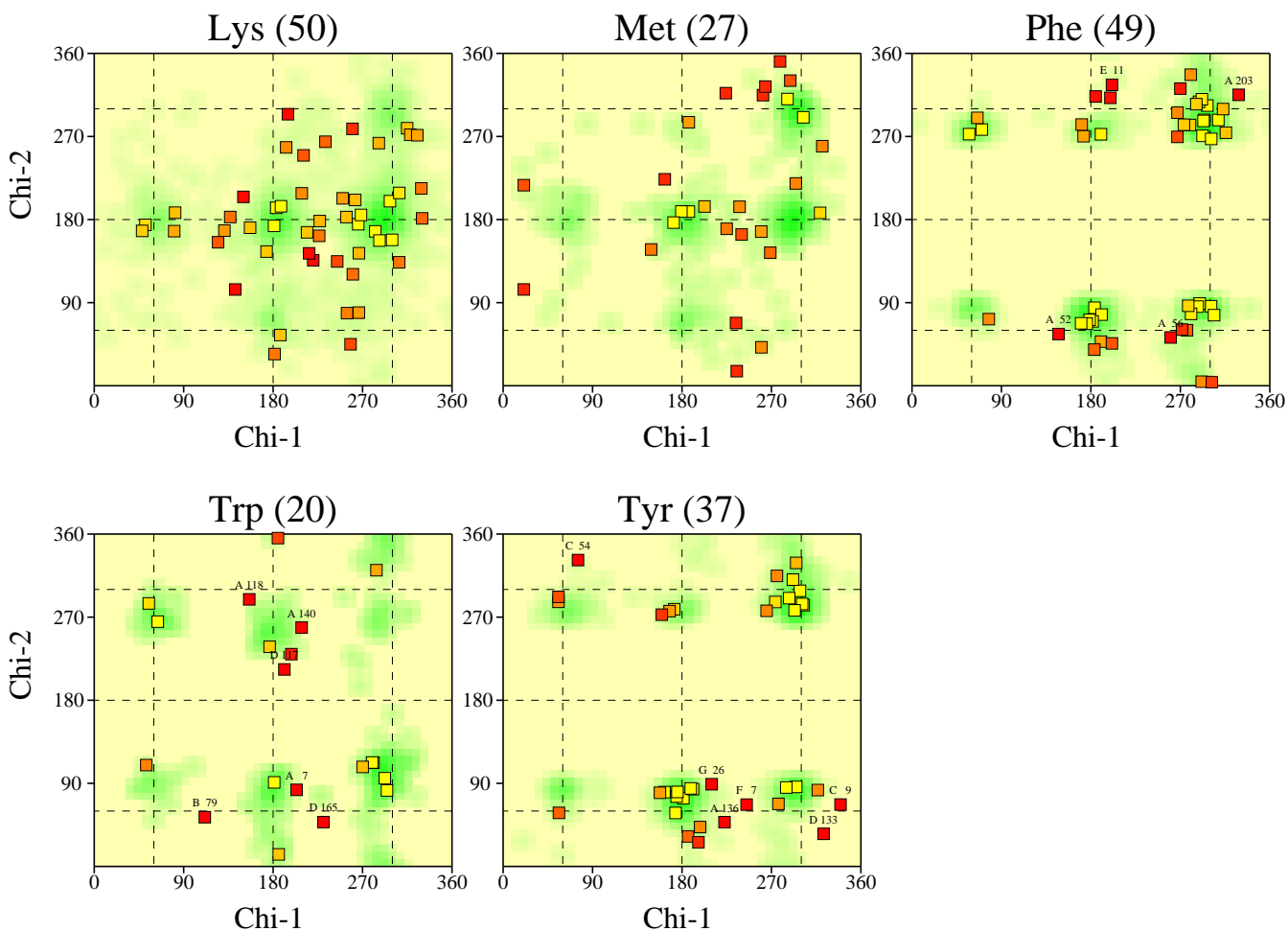
pdb2e75



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

Chi1-Chi2 plots

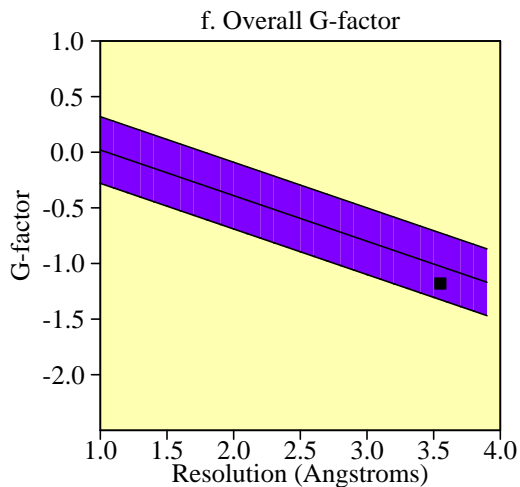
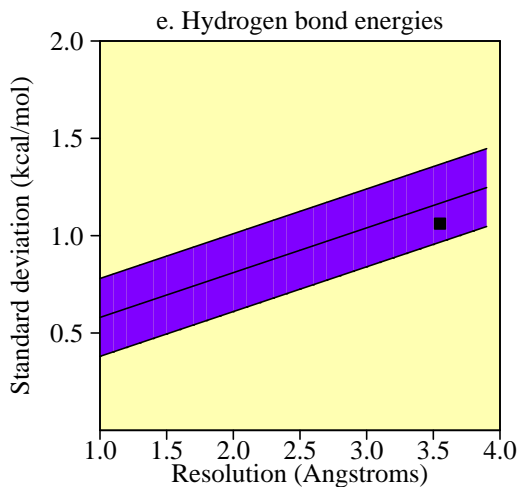
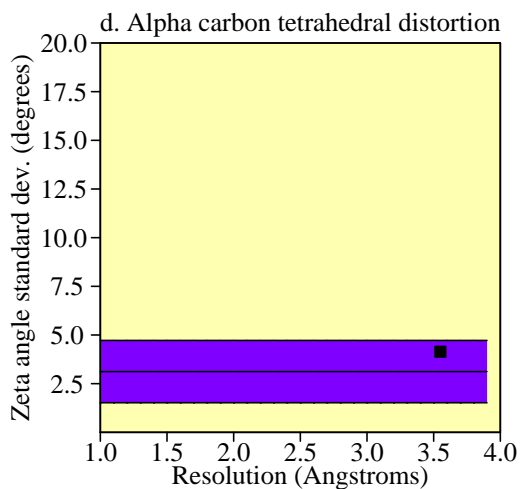
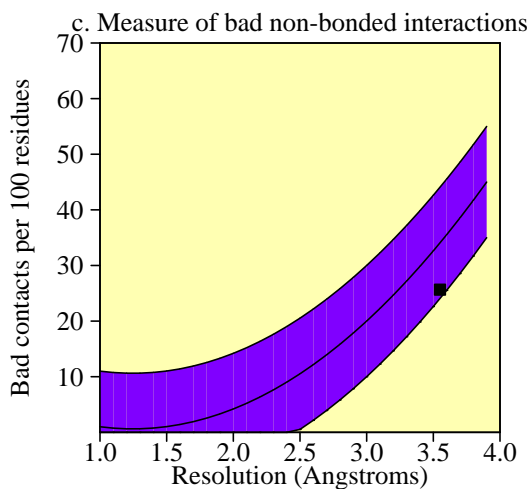
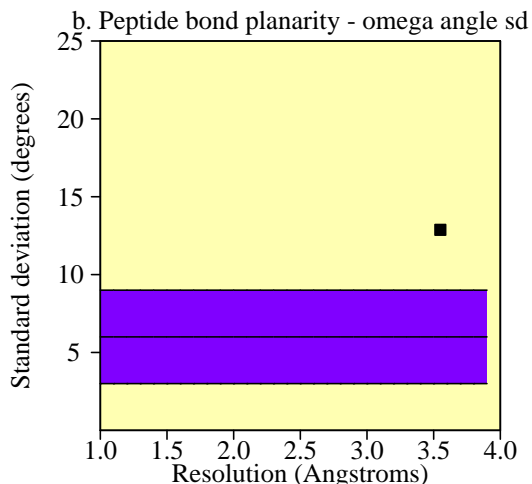
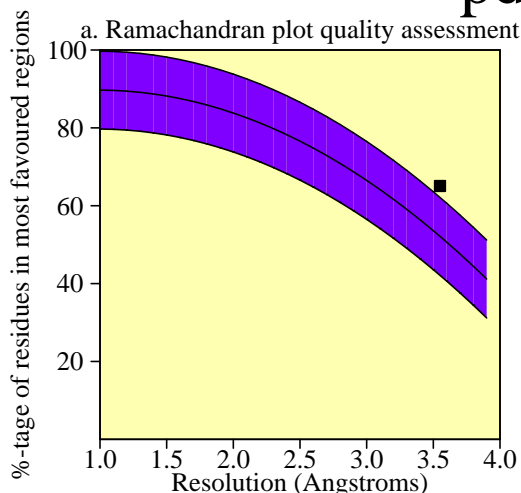
pdb2e75



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

Main-chain parameters

pdb2e75

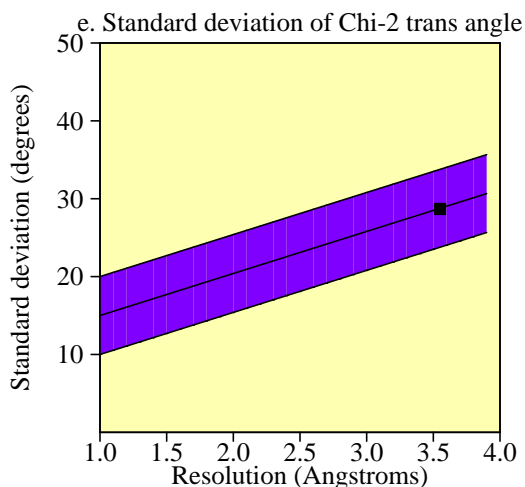
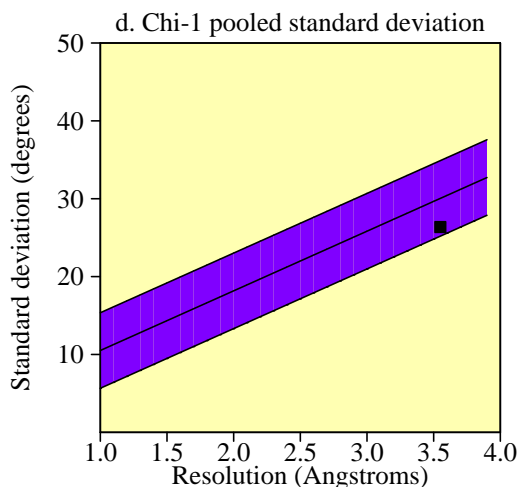
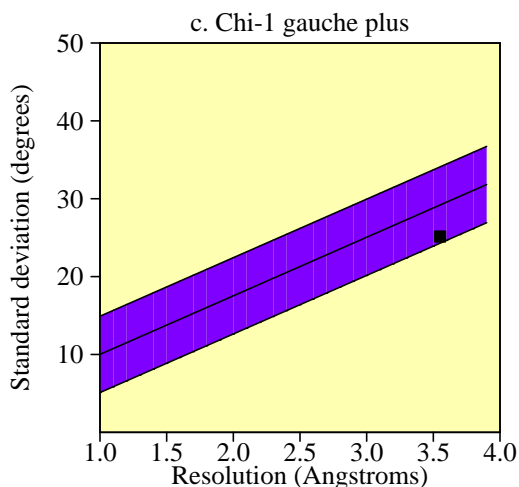
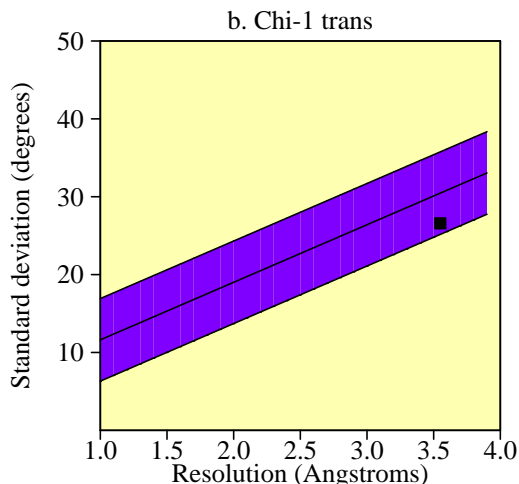
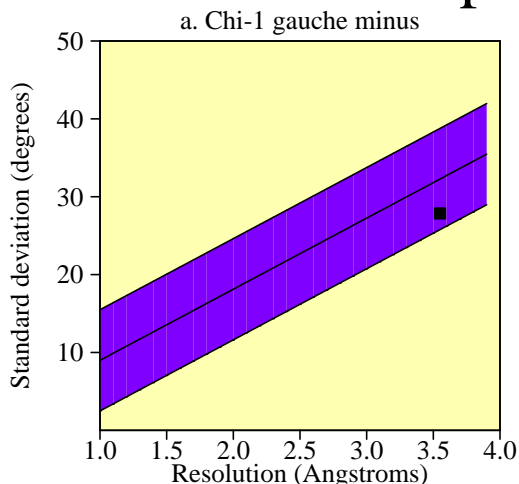


Plot statistics

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

Side-chain parameters

pdb2e75



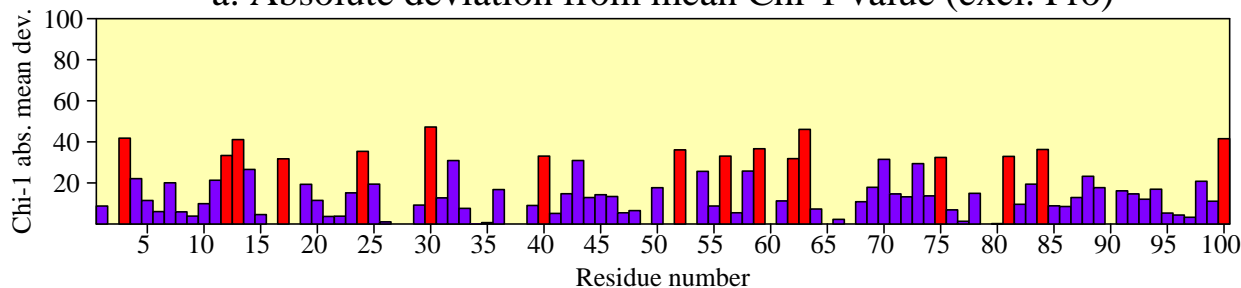
pdb2e75

Plot statistics

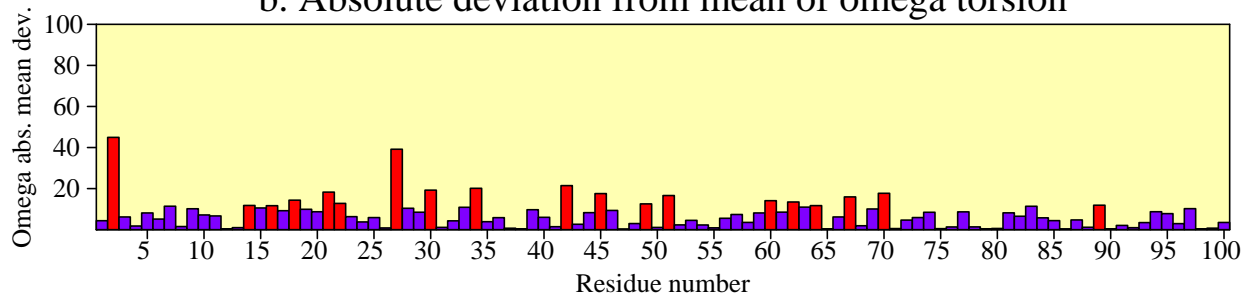
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean
			Typical value	Band width	
a. Chi-1 gauche minus st dev	109	27.9	32.3	6.5	-0.7 Inside
b. Chi-1 trans st dev	289	26.6	30.5	5.3	-0.7 Inside
c. Chi-1 gauche plus st dev	338	25.1	29.2	4.9	-0.8 Inside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

Residue properties pdb2e75

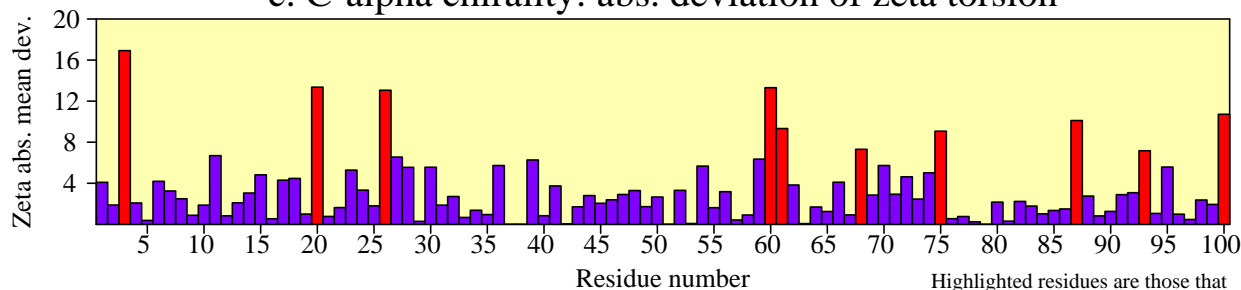
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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

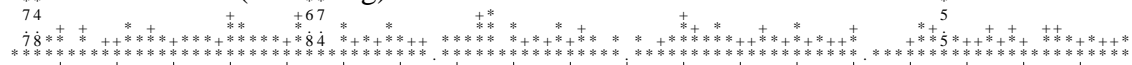
d. Secondary structure & estimated accessibility



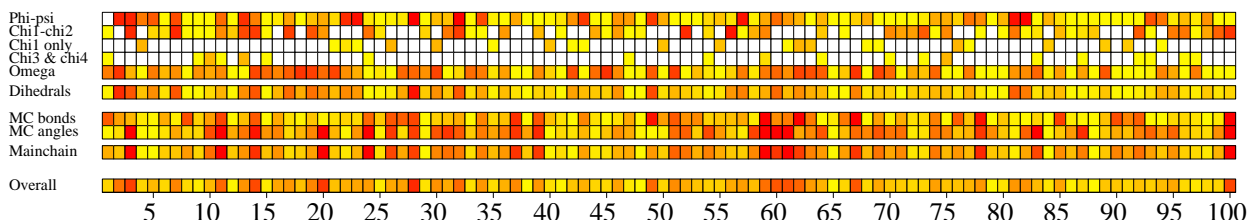
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

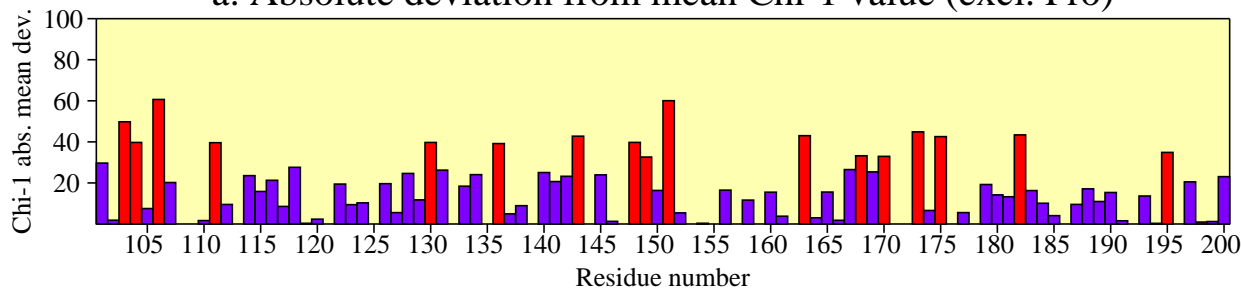


g. G-factors

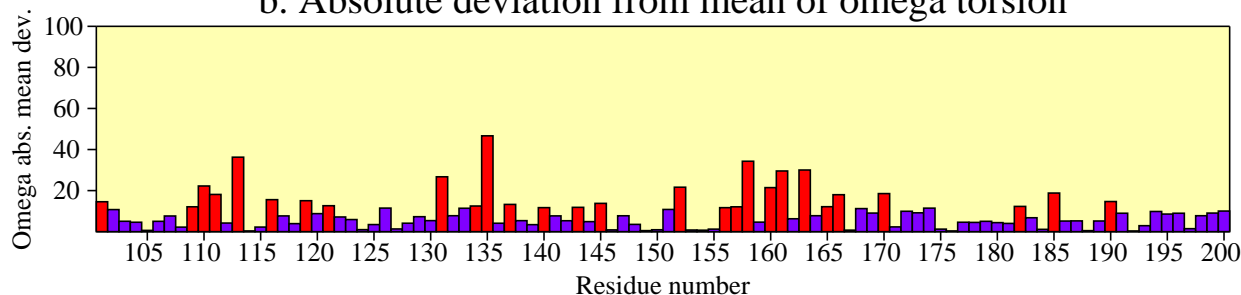


Residue properties pdb2e75

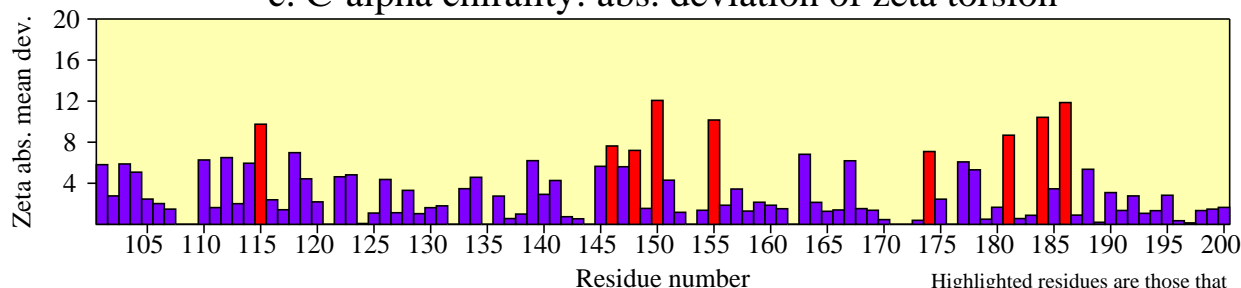
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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

d. Secondary structure & estimated accessibility



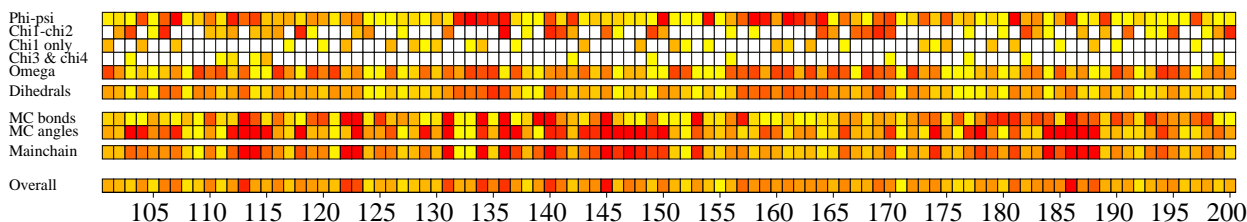
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

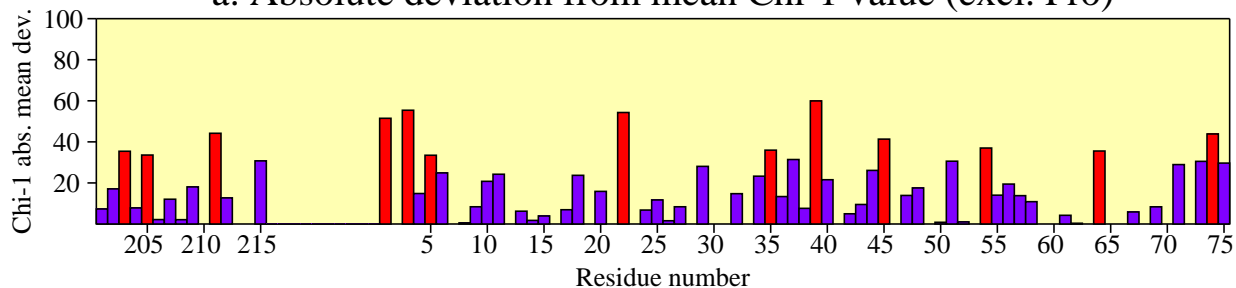


g. G-factors

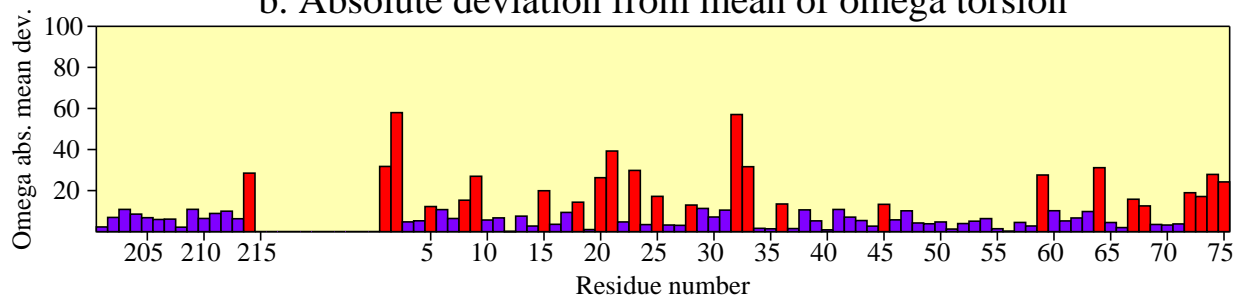


Residue properties pdb2e75

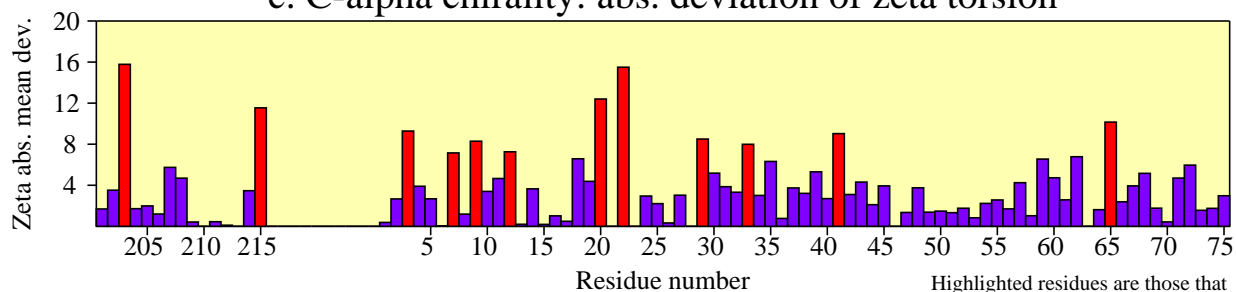
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

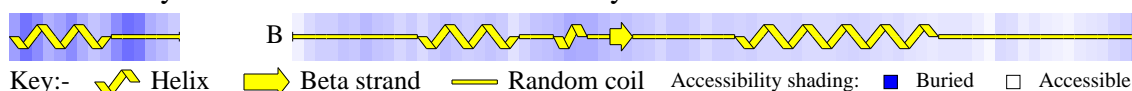


c. C-alpha chirality: abs. deviation of zeta torsion



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

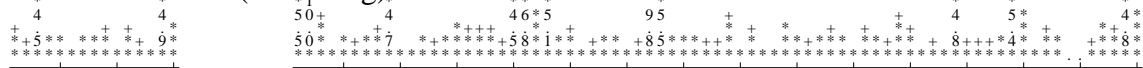
d. Secondary structure & estimated accessibility



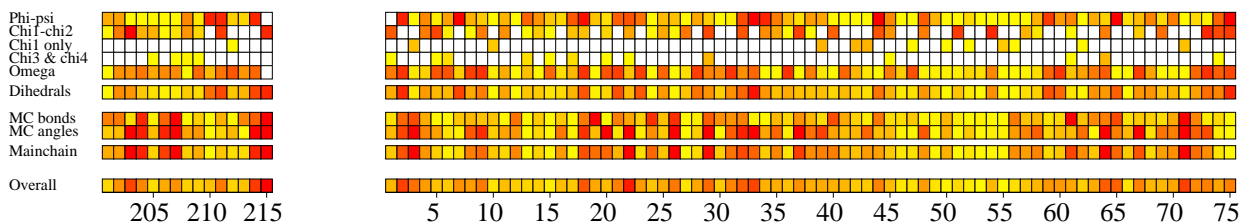
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

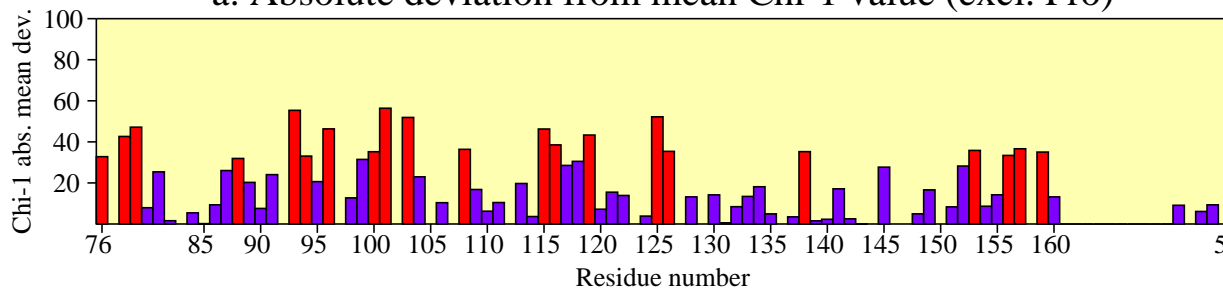


g. G-factors

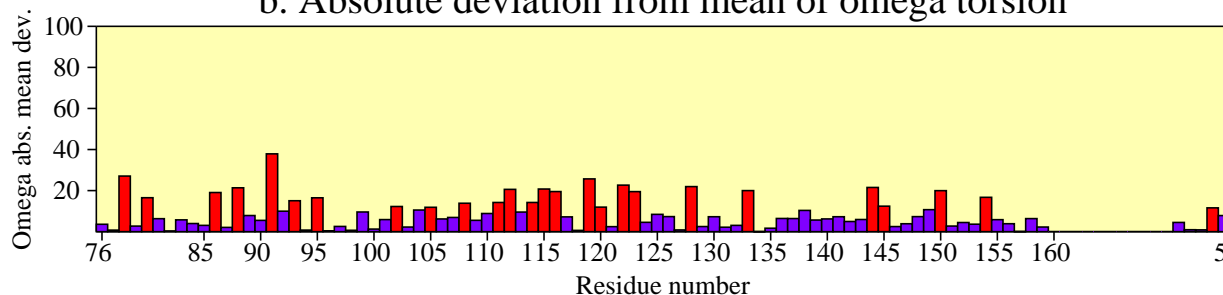


Residue properties pdb2e75

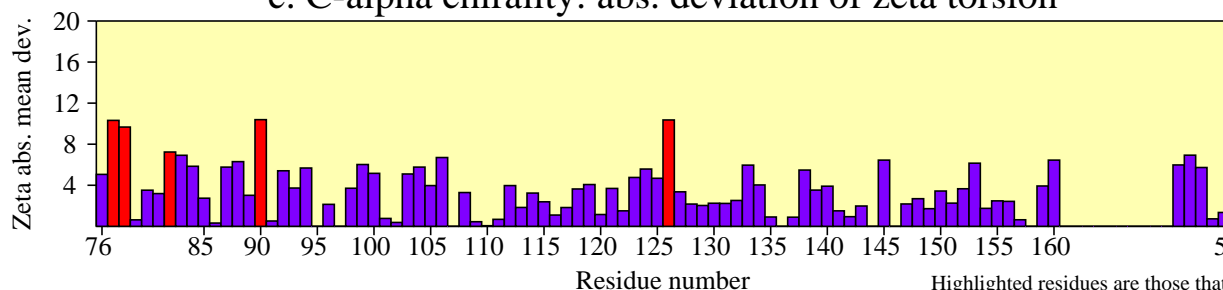
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

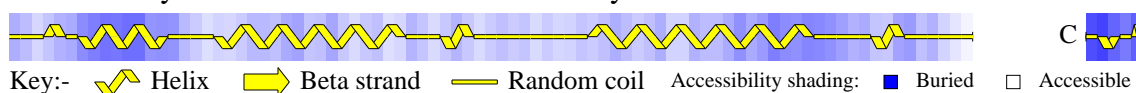


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



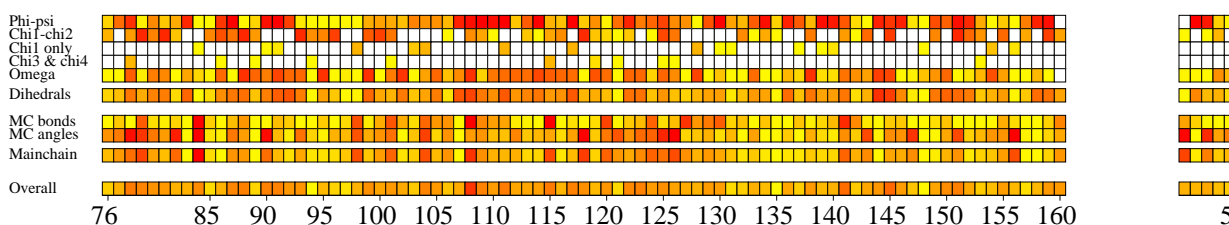
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

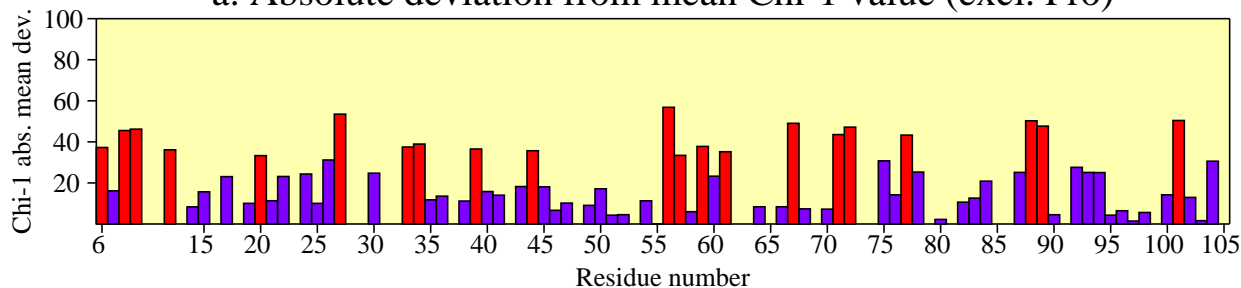


g. G-factors

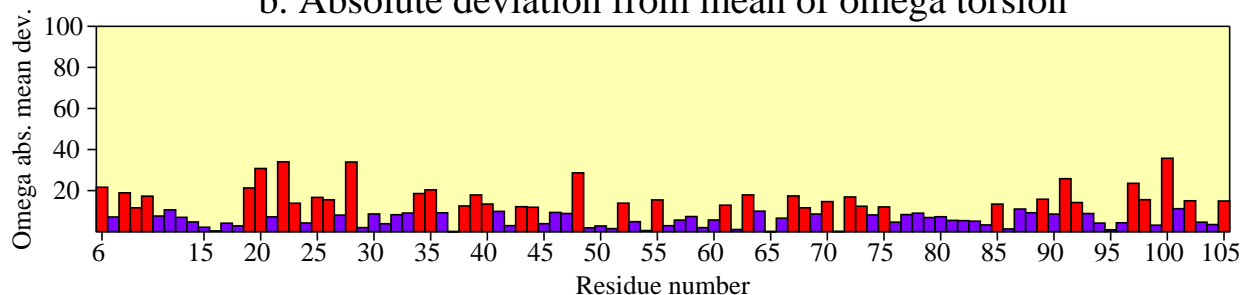


Residue properties pdb2e75

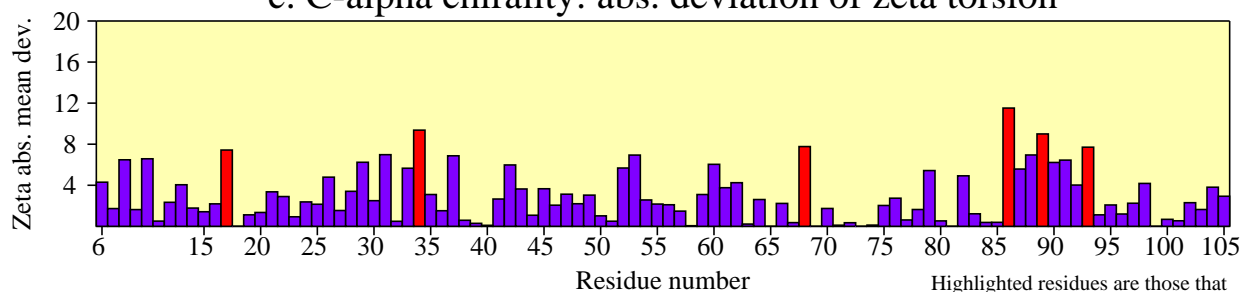
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

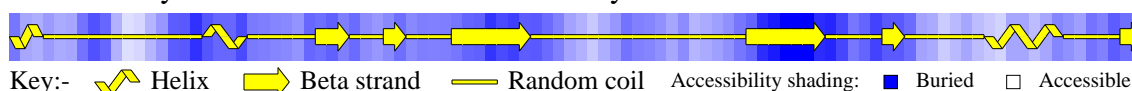


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



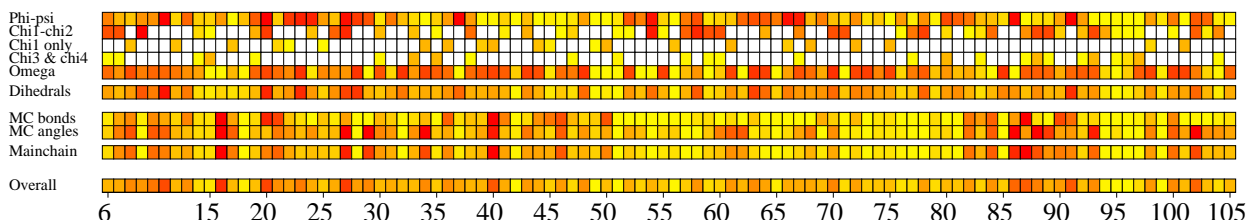
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

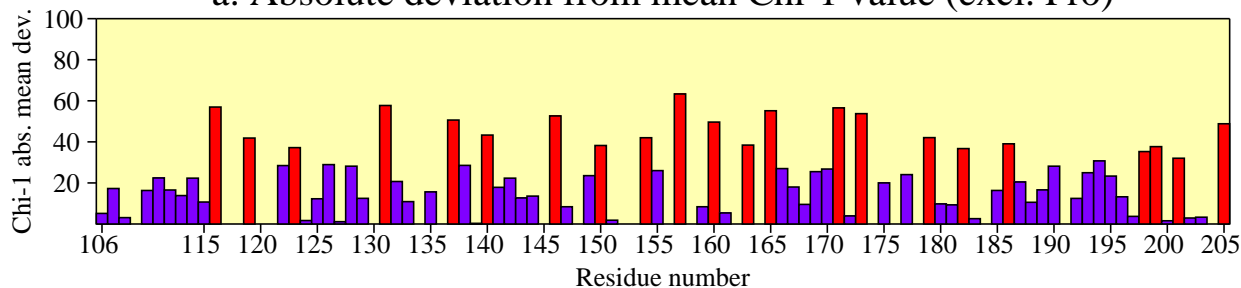


g. G-factors

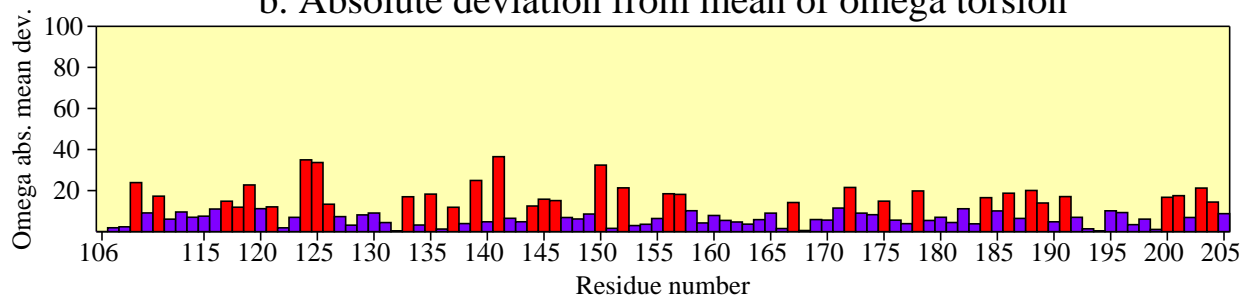


Residue properties pdb2e75

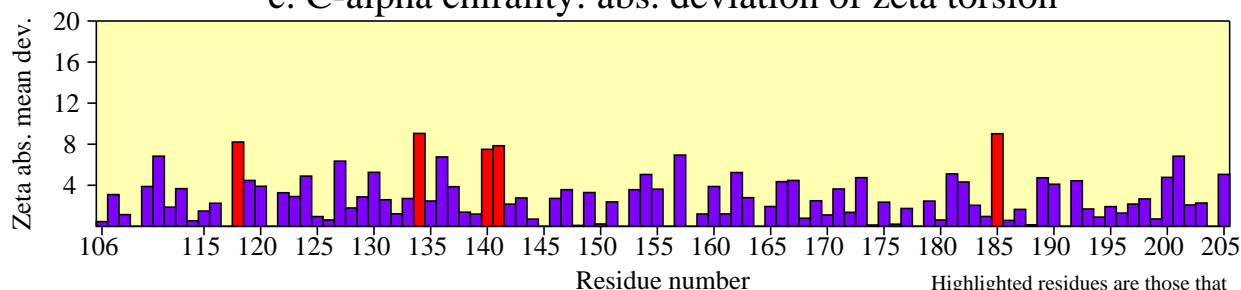
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

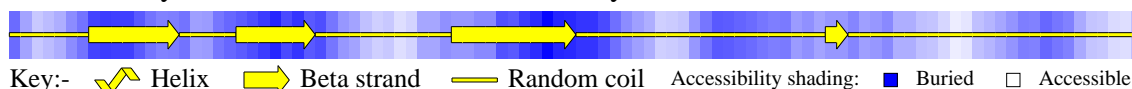


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



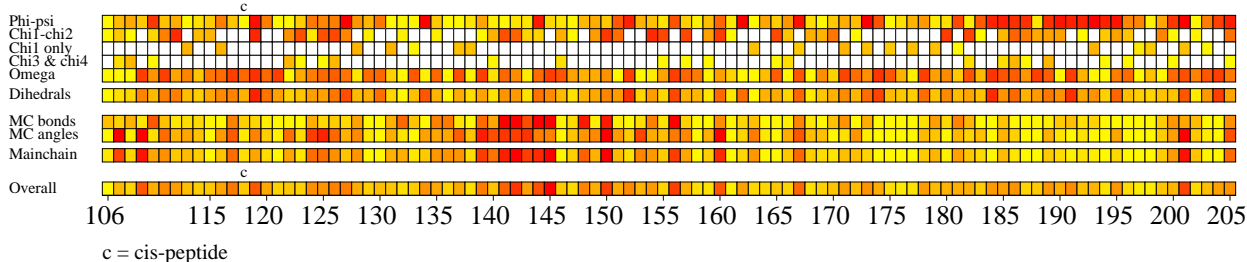
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

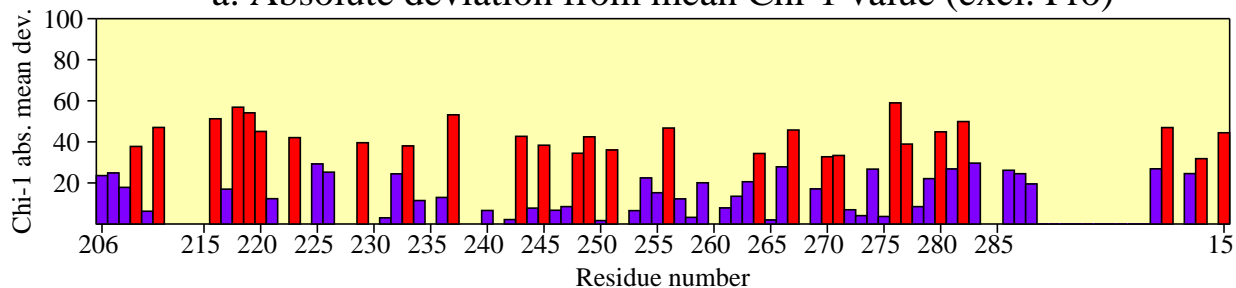


g. G-factors

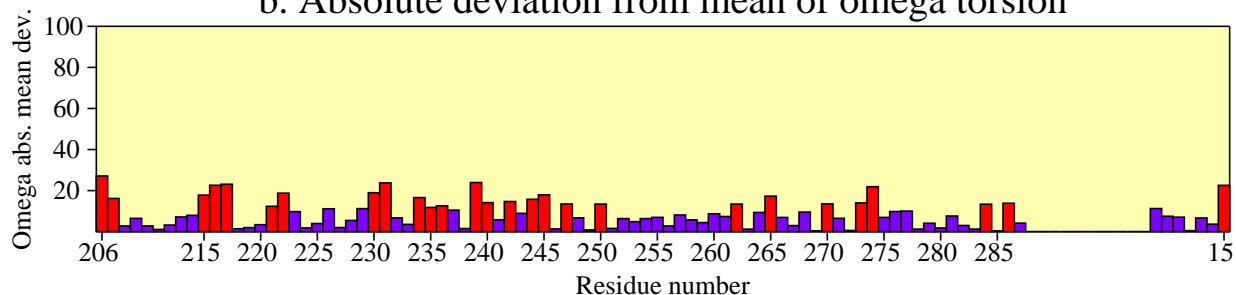


Residue properties pdb2e75

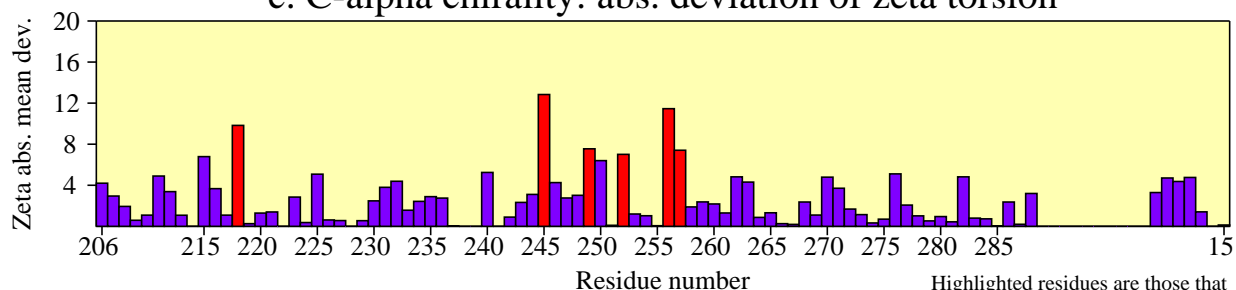
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

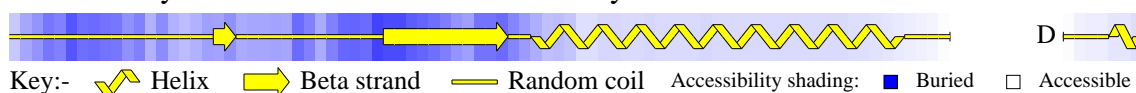


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



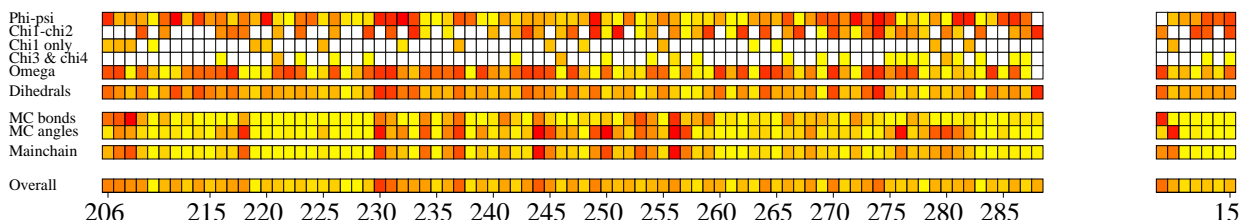
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

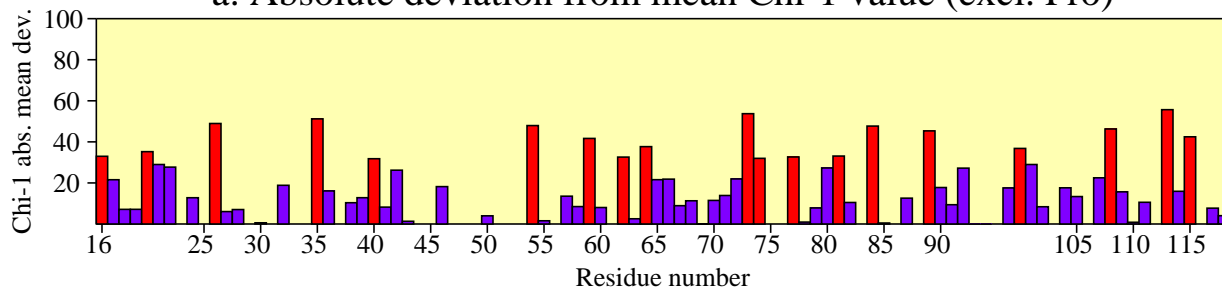


g. G-factors

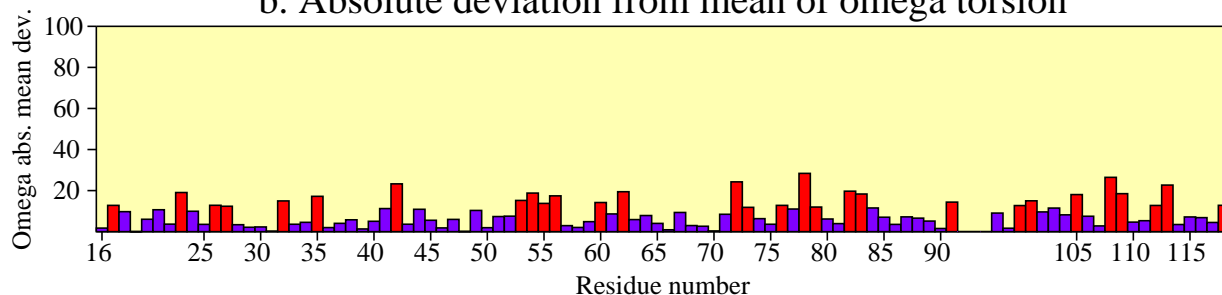


Residue properties pdb2e75

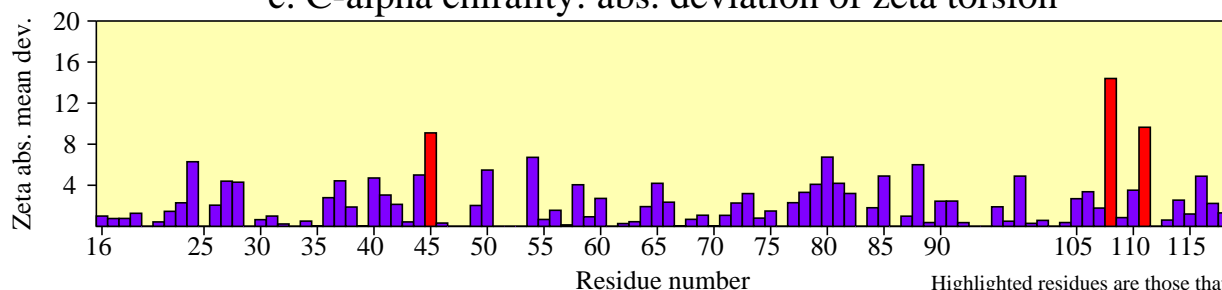
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

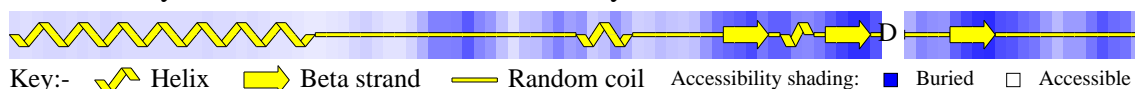


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



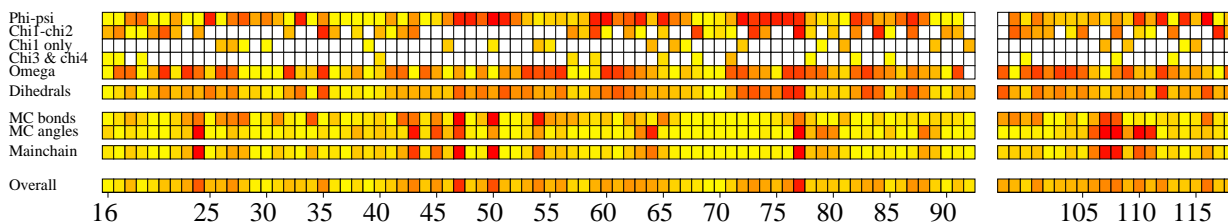
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

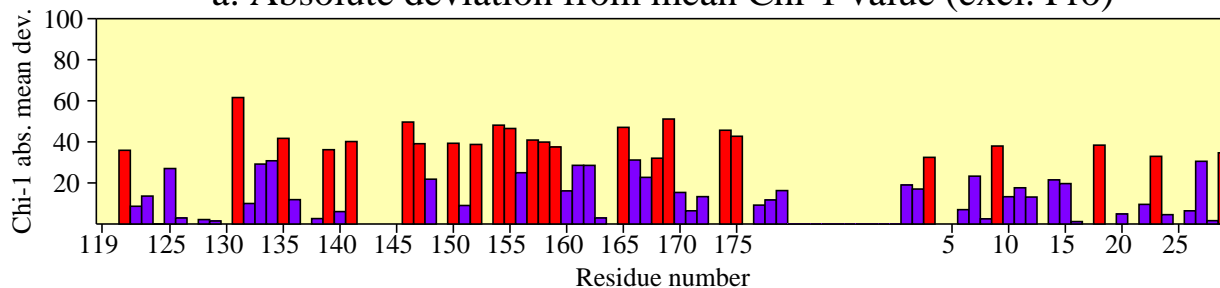


g. G-factors

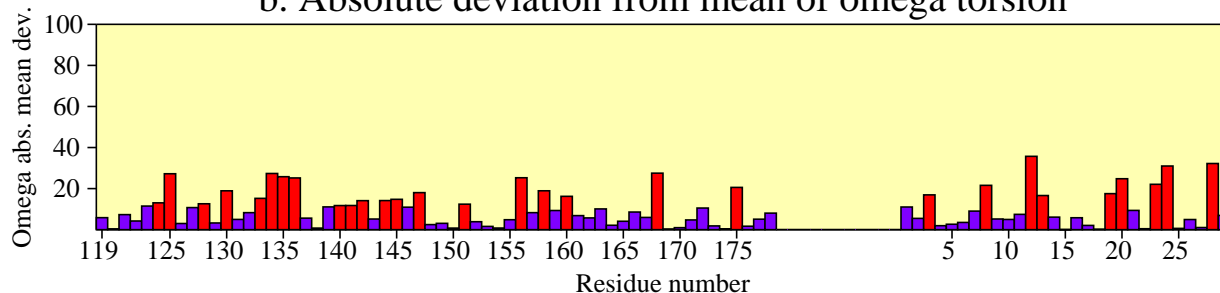


Residue properties pdb2e75

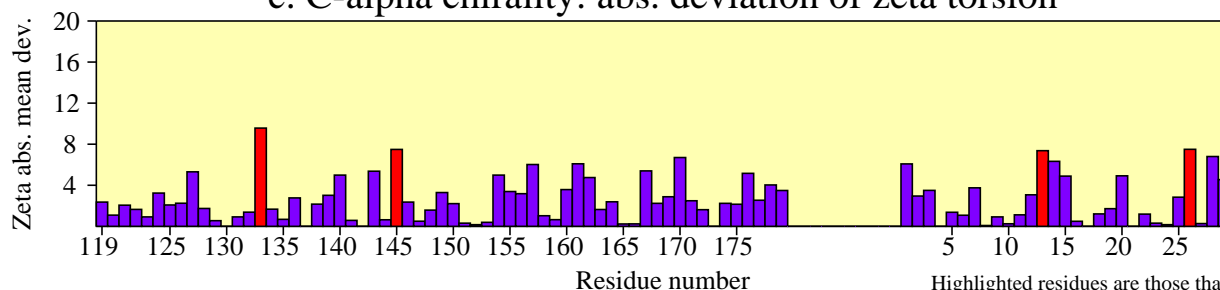
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

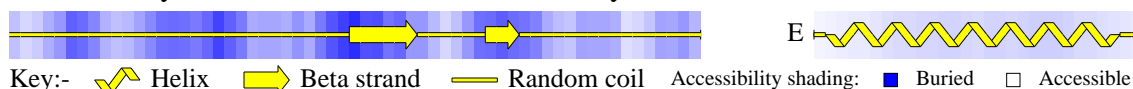


c. C-alpha chirality: abs. deviation of zeta torsion



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

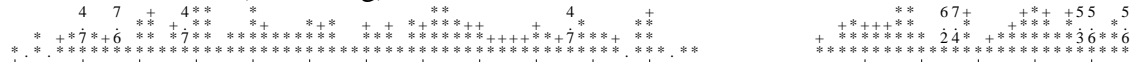
d. Secondary structure & estimated accessibility



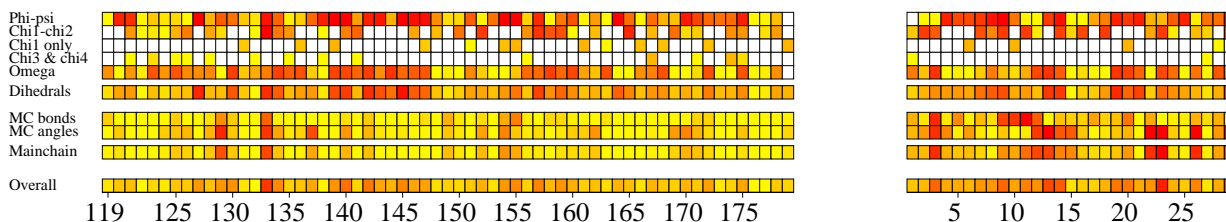
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

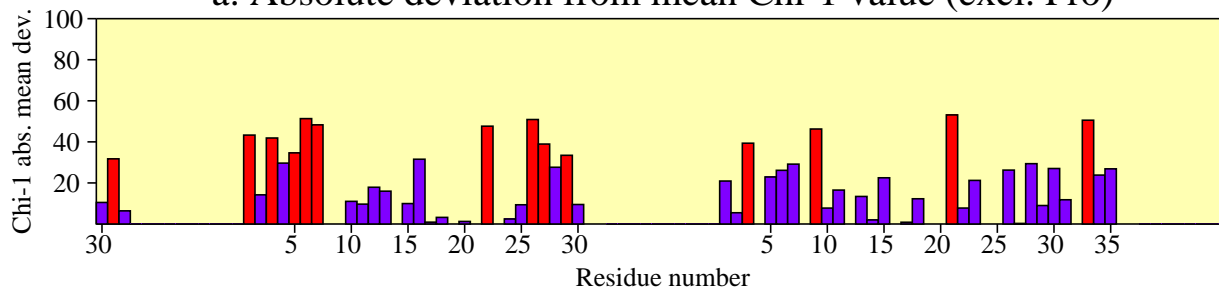


g. G-factors

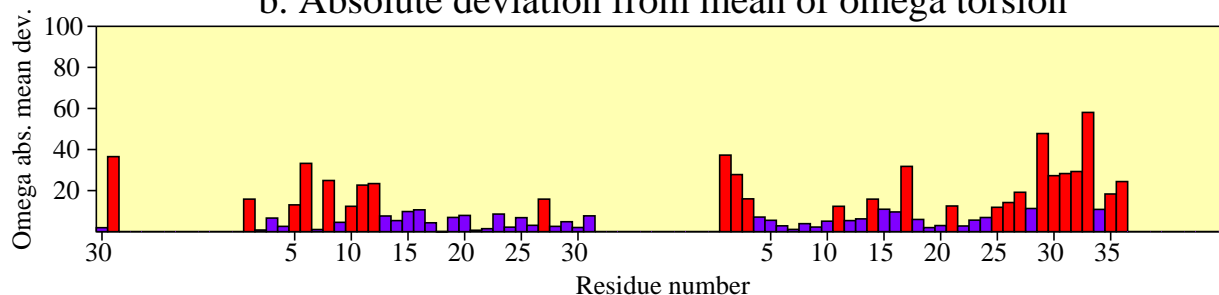


Residue properties pdb2e75

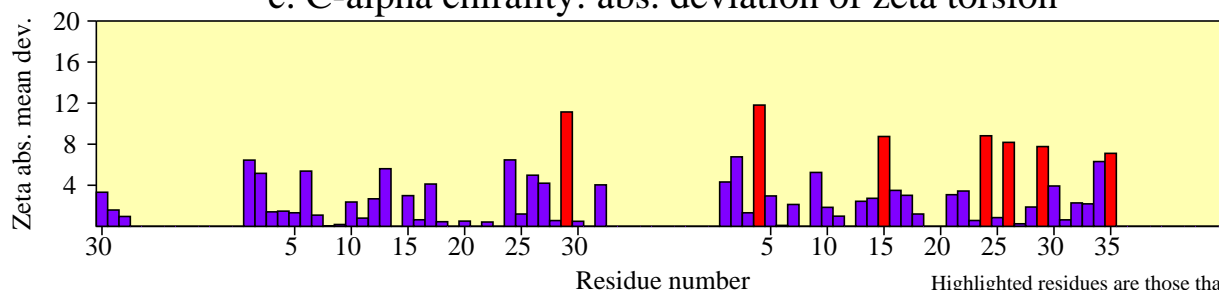
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

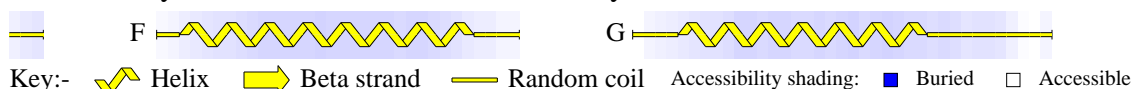


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



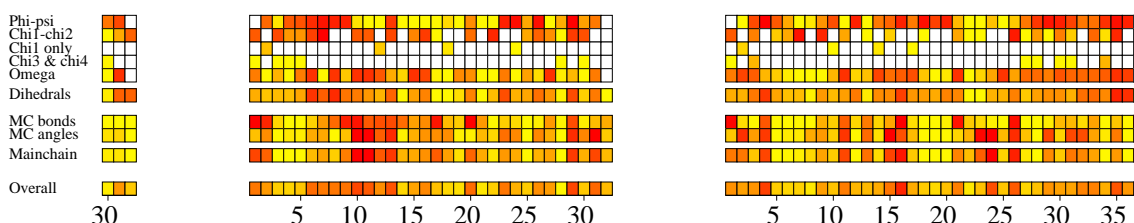
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

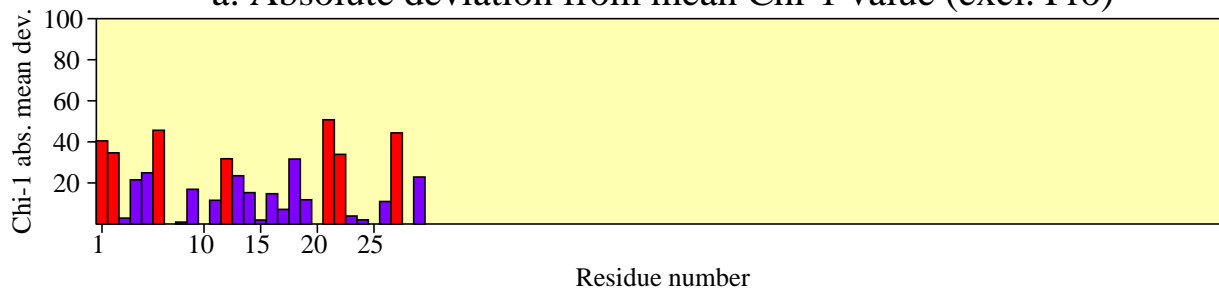


g. G-factors

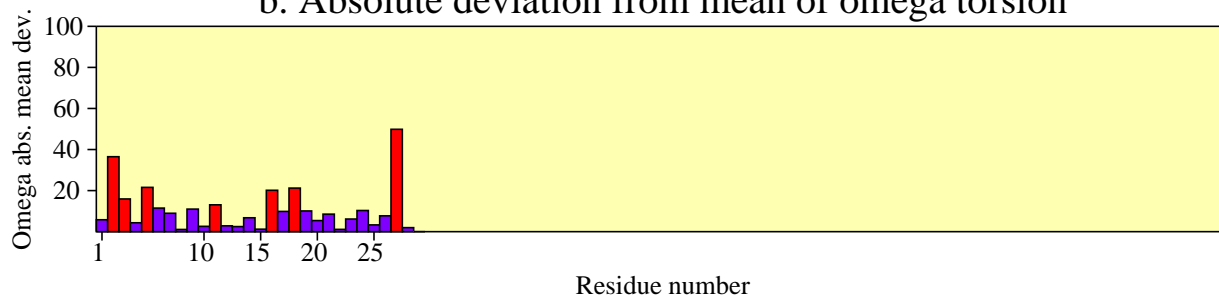


Residue properties pdb2e75

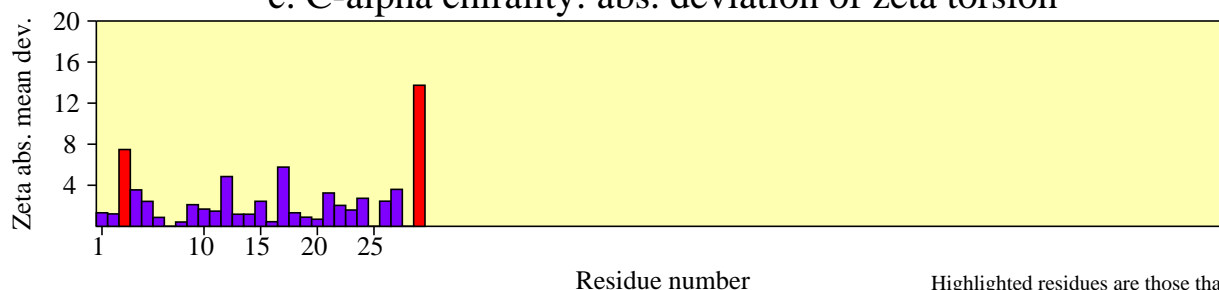
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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

d. Secondary structure & estimated accessibility

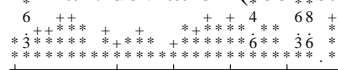


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

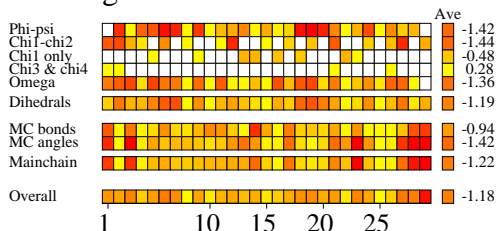
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

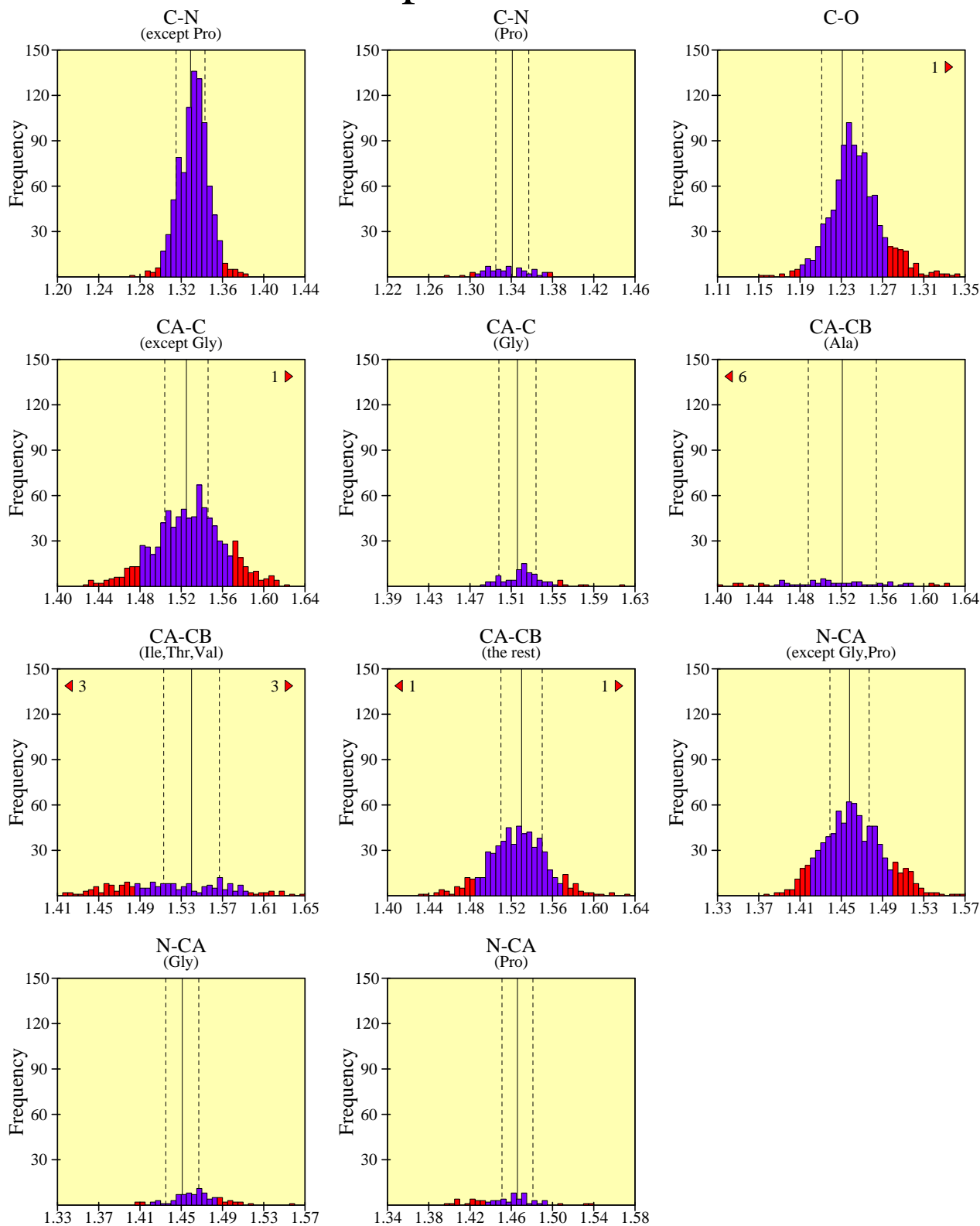


g. G-factors



Main-chain bond lengths

pdb2e75



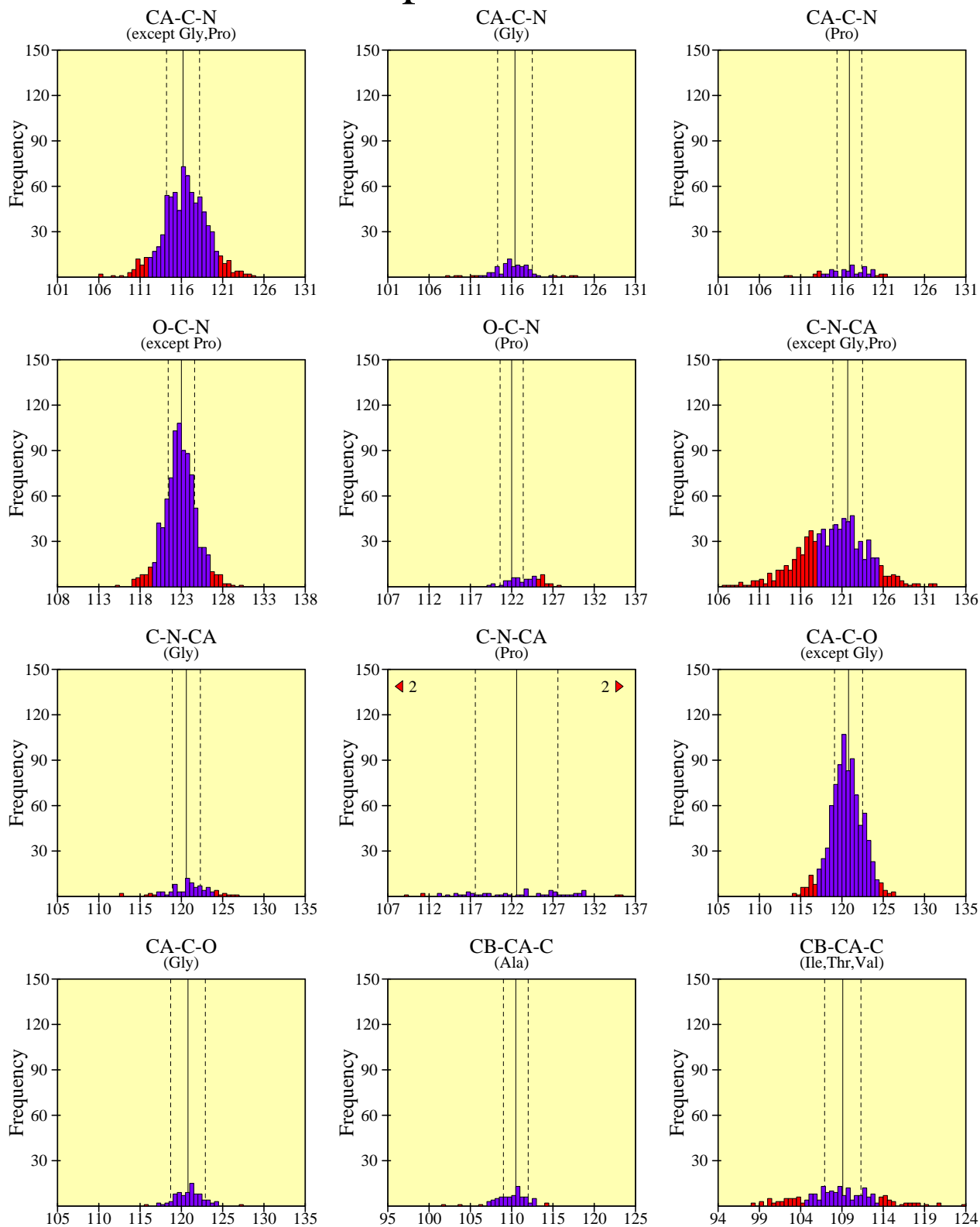
Black bars > 2.0 st. devs. from mean.

◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

pdb2e75



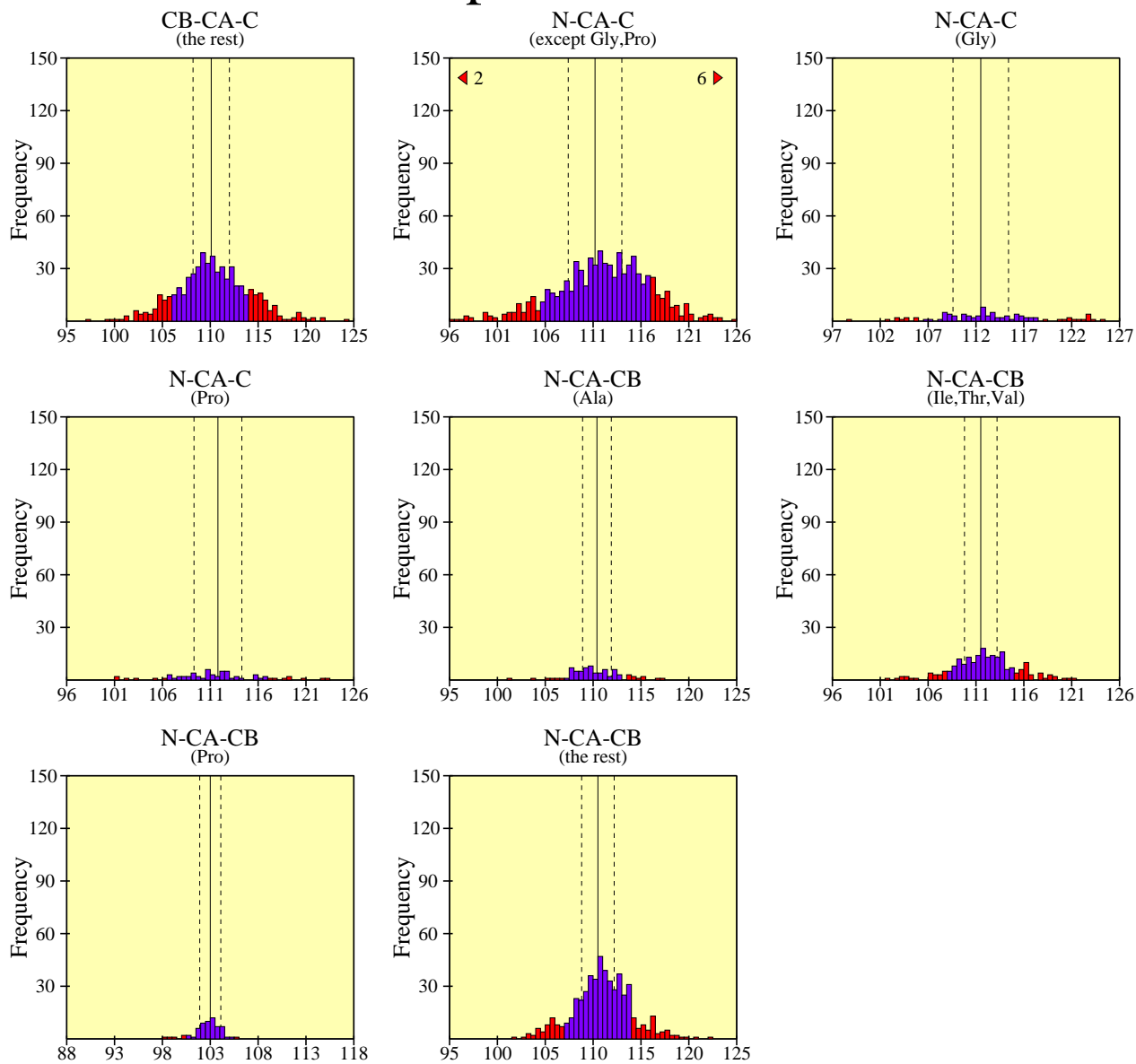
Black bars > 2.0 st. devs. from mean.

◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

pdb2e75



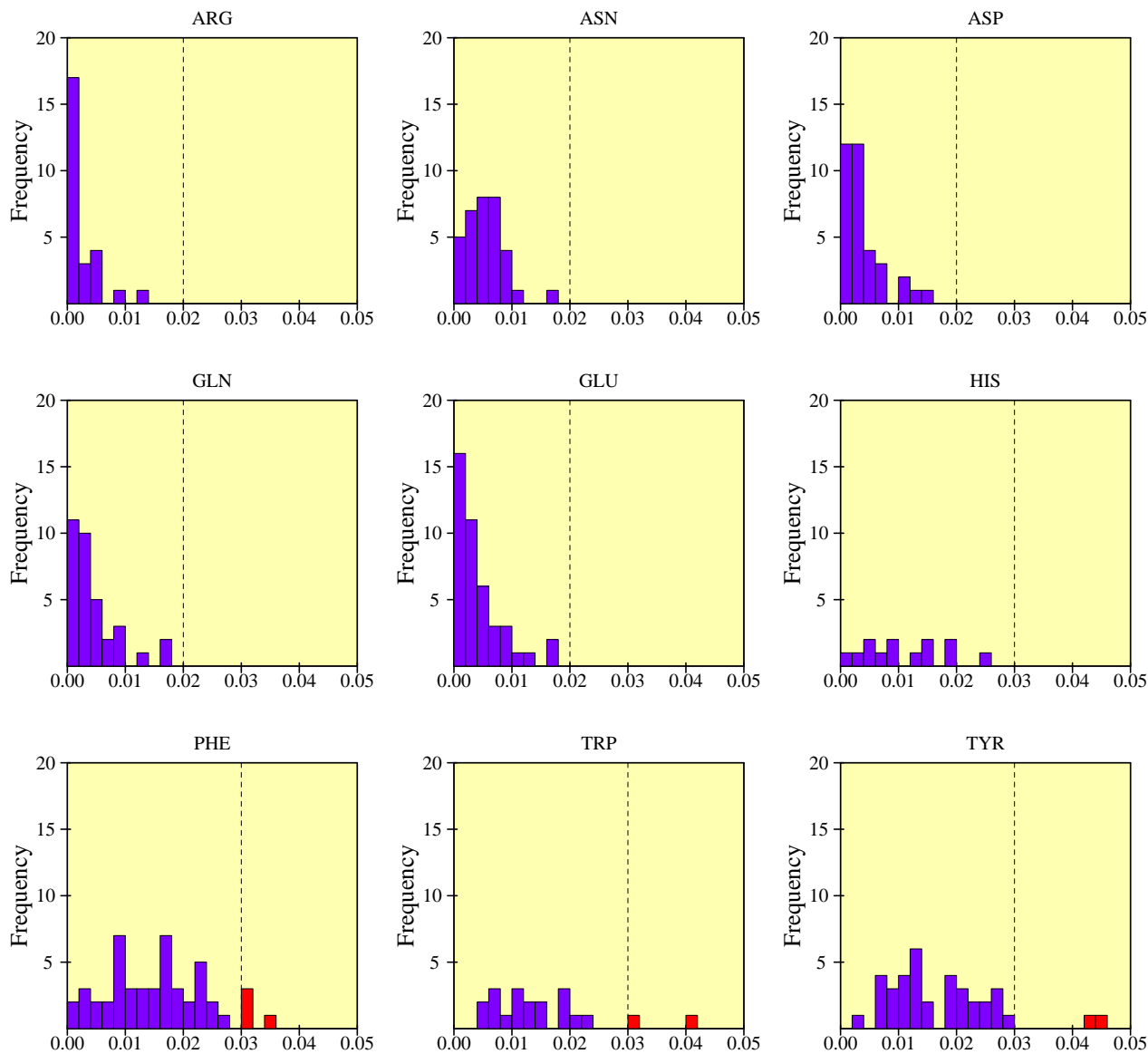
Black bars > 2.0 st. devs. from mean.

◀ or ▶ signifies data points off the graph in the direction shown.

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

RMS distances from planarity

pdb2e75



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

Distorted geometry

pdb2e75

Main-chain bond lengths

CA 1.525 C 0.063 1.588 A Met 1	N 1.458 CA 0.055 1.513 A Met 1	N 1.458 CA 0.053 1.511 A Ala 2	N 1.458 CA 0.057 1.515 A Asn 3	CA 1.525 C 0.053 1.472 A Asp 6	CA 1.530 CB 0.082 1.448 A Phe 8
CA 1.525 C 0.053 1.472 A Glu 10	C 1.231 O 0.072 1.303 A Arg 11	N 1.458 CA 0.063 1.520 A Arg 11	C 1.231 O 0.051 1.282 A Glu 13	CA 1.525 C 0.064 1.461 A Ile 14	CA 1.540 CB 0.054 1.486 A Ile 14
CA 1.521 CB 0.076 1.445 A Ala 16	CA 1.525 C 0.059 1.466 A Ser 23	C 1.231 O 0.064 1.295 A Lys 24	CA 1.525 C 0.053 1.578 A Val 26	CA 1.540 CB 0.087 1.627 A Val 26	C 1.231 O 0.051 1.281 A Pro 27
N 1.466 CA 0.067 1.399 A Pro 28	N 1.458 CA 0.061 1.519 A Ile 32	CA 1.525 C 0.068 1.593 A Tyr 34	CA 1.525 C 0.057 1.582 A Leu 36	C 1.231 O 0.063 1.293 A Gly 37	N 1.451 CA 0.055 1.506 A Gly 37
C 1.231 O 0.055 1.286 A Ile 39	CA 1.540 CB 0.097 1.443 A Ile 39	CA 1.540 CB 0.064 1.476 A Thr 40	C 1.231 O 0.056 1.287 A Cys 43	CA 1.530 CB 0.055 1.475 A Gln 47	CA 1.521 CB 0.172 1.349 A Ala 49
CA 1.540 CB 0.080 1.460 A Thr 50	C 1.231 O 0.054 1.285 A Gly 51	CA 1.525 C 0.052 1.473 A Phe 52	N 1.458 CA 0.056 1.402 A Phe 52	CA 1.525 C 0.051 1.474 A Ala 53	CA 1.521 CB 0.097 1.424 A Ala 53
CA 1.540 CB 0.066 1.474 A Thr 55	CA 1.530 CB 0.050 1.480 A Phe 56	C 1.231 O 0.060 1.291 A Tyr 57	C 1.231 O 0.077 1.154 A Lys 59	CA 1.530 CB 0.051 1.581 A Lys 59	C 1.341 N 0.064 1.277 A Lys 59 - A Pro 60
CA 1.525 C 0.058 1.583 A Pro 60	CA 1.540 CB 0.085 1.455 A Thr 61	C 1.231 O 0.051 1.180 A Val 62	CA 1.525 C 0.082 1.442 A Val 62	CA 1.540 CB 0.121 1.419 A Val 62	CA 1.540 CB 0.103 1.437 A Thr 63
CA 1.530 CB 0.071 1.459 A Tyr 66	CA 1.521 CB 0.163 1.358 A Ala 67	CA 1.540 CB 0.074 1.466 A Val 69	CA 1.530 CB 0.055 1.475 A Tyr 71	N 1.458 CA 0.061 1.397 A Asn 74	N 1.458 CA 0.069 1.527 A Val 76
CA 1.525 C 0.087 1.612 A Phe 78	N 1.458 CA 0.061 1.519 A Phe 78	CA 1.530 CB 0.056 1.474 A Trp 80	CA 1.530 CB 0.052 1.478 A Arg 83	CA 1.540 CB 0.099 1.441 A Ile 85	N 1.458 CA 0.077 1.535 A Ala 90
N 1.458 CA 0.052 1.406 A Ser 91	C 1.231 O 0.054 1.285 A Met 92	CA 1.530 CB 0.054 1.476 A Met 92	CA 1.540 CB 0.050 1.490 A Ile 98	C 1.231 O 0.059 1.290 A His 100	CA 1.525 C 0.055 1.580 A His 100

Distorted geometry

pdb2e75

Main-chain bond lengths (contd)

CA 1.530 CB 0.104 1.634 A His 100	CA 1.530 CB 0.064 1.466 A Tyr 105	CA 1.530 CB 0.081 1.449 A Phe 110	CA 1.525 C 0.056 1.581 A Pro 113	N 1.466 CA 0.068 1.534 A Pro 113	CA 1.525 C 0.057 1.582 A Arg 114
N 1.458 CA 0.057 1.515 A Arg 114	C 1.231 O 0.055 1.286 A Leu 116	C 1.231 O 0.061 1.292 A Ile 119	CA 1.525 C 0.068 1.593 A Ile 119	C 1.231 O 0.056 1.287 A Ser 120	CA 1.525 C 0.076 1.601 A Ser 120
CA 1.525 C 0.068 1.457 A Val 122	CA 1.540 CB 0.213 1.327 A Val 122	N 1.458 CA 0.051 1.407 A Val 122	C 1.231 O 0.070 1.301 A Ile 123	CA 1.525 C 0.089 1.614 A Ile 123	CA 1.521 CB 0.124 1.397 A Ala 125
N 1.458 CA 0.051 1.407 A Ala 125	CA 1.540 CB 0.064 1.476 A Val 126	CA 1.540 CB 0.085 1.455 A Ile 127	CA 1.540 CB 0.085 1.455 A Thr 128	C 1.231 O 0.110 1.341 A Phe 131	C 1.231 O 0.122 1.353 A Thr 134
C 1.231 O 0.071 1.160 A Tyr 136	C 1.329 N 0.056 1.273 A Tyr 136 - A Ser 137	C 1.231 O 0.051 1.180 A Pro 139	CA 1.525 C 0.077 1.448 A Pro 139	CA 1.530 CB 0.097 1.433 A Pro 139	C 1.231 O 0.095 1.326 A Trp 140
CA 1.530 CB 0.075 1.455 A Trp 140	C 1.231 O 0.060 1.291 A Asp 141	CA 1.525 C 0.052 1.577 A Gln 142	CA 1.525 C 0.073 1.452 A Tyr 145	CA 1.530 CB 0.138 1.392 A Tyr 145	N 1.458 CA 0.070 1.388 A Tyr 145
CA 1.525 C 0.087 1.438 A Lys 149	CA 1.516 C 0.066 1.582 A Gly 153	N 1.451 CA 0.056 1.507 A Gly 153	CA 1.525 C 0.081 1.606 A Glu 156	CA 1.521 CB 0.103 1.624 A Ala 157	N 1.458 CA 0.083 1.541 A Ala 157
CA 1.540 CB 0.053 1.487 A Ile 165	CA 1.525 C 0.056 1.469 A Ser 166	CA 1.525 C 0.061 1.464 A Asp 167	N 1.458 CA 0.062 1.396 A Leu 169	CA 1.530 CB 0.052 1.582 A Arg 170	C 1.231 O 0.061 1.291 A Gly 172
CA 1.530 CB 0.062 1.468 A Ser 173	N 1.458 CA 0.069 1.527 A Ser 174	CA 1.540 CB 0.061 1.479 A Val 175	C 1.231 O 0.051 1.282 A Gly 176	C 1.231 O 0.072 1.303 A Ala 178	CA 1.521 CB 0.057 1.464 A Ala 178
C 1.231 O 0.057 1.288 A Thr 179	CA 1.540 CB 0.111 1.429 A Thr 179	C 1.231 O 0.093 1.324 A Leu 180	C 1.231 O 0.095 1.326 A Thr 181	CA 1.530 CB 0.061 1.469 A Arg 182	N 1.458 CA 0.051 1.407 A Tyr 183
CA 1.530 CB 0.069 1.599 A Tyr 184	CA 1.525 C 0.051 1.474 A Ser 185	CA 1.525 C 0.095 1.430 A Ala 186	CA 1.521 CB 0.097 1.424 A Ala 186	C 1.231 O 0.059 1.172 A His 187	CA 1.525 C 0.071 1.454 A His 187

Distorted geometry

pdb2e75

Main-chain bond lengths (contd)

CA 1.525 C 0.098 1.427 A Thr 188	C 1.231 O 0.056 1.287 A Val 190	CA 1.525 C 0.066 1.591 A Val 190	CA 1.540 CB 0.076 1.464 A Val 190	C 1.231 O 0.077 1.308 A Leu 191	C 1.231 O 0.073 1.304 A Trp 193
C 1.231 O 0.058 1.289 A Leu 194	CA 1.540 CB 0.075 1.465 A Ile 195	CA 1.521 CB 0.090 1.431 A Ala 196	C 1.231 O 0.062 1.293 A Val 197	CA 1.540 CB 0.083 1.457 A Val 197	CA 1.530 CB 0.095 1.435 A Phe 198
C 1.231 O 0.065 1.296 A Leu 201	C 1.231 O 0.071 1.302 A His 202	CA 1.525 C 0.091 1.434 A Leu 204	N 1.458 CA 0.057 1.515 A Leu 204	CA 1.525 C 0.050 1.575 A Ile 206	CA 1.540 CB 0.081 1.459 A Ile 206
C 1.231 O 0.089 1.320 A Arg 207	CA 1.525 C 0.065 1.590 A Arg 207	CA 1.530 CB 0.087 1.617 A Arg 207	CA 1.525 C 0.055 1.580 A Gln 209	C 1.231 O 0.065 1.296 A Ile 211	C 1.231 O 0.059 1.289 A Gly 213
C 1.231 O 0.062 1.293 A Pro 214	CA 1.525 C 0.120 1.645 A Leu 215	N 1.458 CA 0.099 1.557 A Leu 215	CA 1.521 CB 0.099 1.620 B Ala 2	N 1.458 CA 0.051 1.508 B Ala 2	CA 1.540 CB 0.058 1.482 B Thr 3
N 1.458 CA 0.060 1.518 B Leu 4	CA 1.525 C 0.070 1.455 B Asp 8	N 1.458 CA 0.055 1.513 B Ser 10	CA 1.525 C 0.080 1.445 B Pro 12	CA 1.530 CB 0.058 1.472 B Leu 18	CA 1.525 C 0.070 1.455 B Ala 19
N 1.458 CA 0.078 1.380 B Ala 19	CA 1.525 C 0.062 1.463 B His 24	CA 1.530 CB 0.077 1.453 B His 24	CA 1.525 C 0.053 1.472 B Asn 25	CA 1.525 C 0.089 1.436 B Tyr 26	CA 1.530 CB 0.061 1.469 B Tyr 26
CA 1.530 CB 0.077 1.607 B Glu 29	CA 1.525 C 0.067 1.458 B Asp 35	N 1.458 CA 0.070 1.388 B Leu 37	C 1.231 O 0.053 1.284 B Phe 40	CA 1.525 C 0.083 1.608 B Phe 40	CA 1.540 CB 0.064 1.476 B Val 42
CA 1.540 CB 0.064 1.476 B Val 43	CA 1.525 C 0.073 1.598 B Ile 44	CA 1.540 CB 0.066 1.474 B Thr 47	CA 1.525 C 0.054 1.579 B Cys 50	CA 1.521 CB 0.062 1.459 B Ala 53	CA 1.540 CB 0.089 1.451 B Val 56
C 1.231 O 0.088 1.319 B Met 61	C 1.329 N 0.052 1.381 B Met 61 - B Val 62	CA 1.540 CB 0.072 1.612 B Val 62	CA 1.525 C 0.056 1.469 B Glu 64	N 1.466 CA 0.061 1.405 B Pro 65	N 1.458 CA 0.059 1.517 B Asp 67
CA 1.521 CB 0.056 1.465 B Ala 70	CA 1.540 CB 0.179 1.360 B Thr 71	CA 1.525 C 0.076 1.449 B Pro 72	CA 1.525 C 0.062 1.587 B Trp 79	N 1.458 CA 0.064 1.394 B Trp 79	CA 1.525 C 0.052 1.473 B Val 84

Distorted geometry

pdb2e75

Main-chain bond lengths (contd)

CA 1.540 CB 0.155 1.385 B Val 84	N 1.458 CA 0.057 1.401 B Leu 88	C 1.231 O 0.065 1.296 B Val 98	CA 1.540 CB 0.072 1.468 B Val 98	N 1.458 CA 0.056 1.402 B Leu 100	CA 1.530 CB 0.076 1.454 B Met 101
CA 1.521 CB 0.053 1.469 B Ala 102	CA 1.530 CB 0.053 1.477 B Ser 103	C 1.231 O 0.051 1.282 B Val 104	CA 1.540 CB 0.101 1.439 B Val 104	C 1.231 O 0.054 1.285 B Pro 105	C 1.231 O 0.066 1.297 B Leu 106
C 1.231 O 0.092 1.323 B Leu 108	CA 1.525 C 0.097 1.622 B Leu 108	CA 1.540 CB 0.075 1.465 B Ile 109	CA 1.540 CB 0.052 1.488 B Val 111	C 1.231 O 0.086 1.317 B Glu 115	CA 1.525 C 0.066 1.591 B Glu 115
CA 1.530 CB 0.055 1.585 B Glu 115	C 1.231 O 0.051 1.282 B Phe 120	N 1.458 CA 0.069 1.527 B Phe 120	CA 1.525 C 0.053 1.472 B Pro 123	CA 1.525 C 0.089 1.614 B Phe 124	CA 1.525 C 0.058 1.467 B Pro 127
N 1.466 CA 0.061 1.405 B Pro 127	CA 1.540 CB 0.061 1.479 B Val 128	C 1.231 O 0.070 1.301 B Ala 129	CA 1.525 C 0.054 1.579 B Ala 129	CA 1.540 CB 0.076 1.464 B Thr 130	N 1.458 CA 0.059 1.399 B Thr 130
C 1.231 O 0.053 1.284 B Thr 131	CA 1.540 CB 0.052 1.592 B Thr 137	CA 1.540 CB 0.056 1.484 B Val 139	C 1.231 O 0.056 1.287 B Thr 140	CA 1.540 CB 0.120 1.420 B Ile 141	N 1.458 CA 0.061 1.397 B Trp 142
CA 1.540 CB 0.052 1.488 B Ile 145	N 1.458 CA 0.054 1.404 B Thr 156	CA 1.530 CB 0.050 1.580 B Leu 159	CA 1.525 C 0.050 1.575 B Phe 160	CA 1.525 C 0.057 1.468 C Gln 7	N 1.458 CA 0.066 1.524 C Thr 8
CA 1.530 CB 0.060 1.590 C Pro 11	CA 1.540 CB 0.052 1.488 C Thr 12	CA 1.525 C 0.051 1.576 C Glu 15	C 1.231 O 0.111 1.342 C Pro 16	N 1.466 CA 0.072 1.538 C Pro 16	CA 1.540 CB 0.066 1.474 C Thr 17
CA 1.525 C 0.056 1.469 C Arg 19	CA 1.525 C 0.073 1.598 C Ile 20	N 1.458 CA 0.070 1.528 C Ile 20	CA 1.525 C 0.082 1.443 C Val 21	CA 1.540 CB 0.083 1.457 C Val 21	CA 1.525 C 0.057 1.582 C Cys 22
CA 1.525 C 0.051 1.576 C Ala 23	N 1.458 CA 0.062 1.520 C Leu 27	N 1.458 CA 0.062 1.520 C Lys 30	CA 1.540 CB 0.057 1.483 C Val 34	C 1.231 O 0.069 1.162 C Val 36	CA 1.525 C 0.058 1.467 C Gln 38
CA 1.525 C 0.064 1.589 C Ser 39	CA 1.525 C 0.091 1.434 C Val 40	CA 1.540 CB 0.105 1.435 C Val 40	CA 1.525 C 0.066 1.591 C Leu 41	N 1.458 CA 0.055 1.513 C Leu 41	CA 1.540 CB 0.093 1.447 C Thr 44

Distorted geometry

pdb2e75

Main-chain bond lengths (contd)

CA 1.540 CB 0.093 1.447 C Val 45	C 1.231 O 0.052 1.283 C Phe 46	CA 1.525 C 0.074 1.451 C Phe 46	CA 1.525 C 0.054 1.471 C Lys 47	CA 1.521 CB 0.074 1.447 C Ala 48	CA 1.540 CB 0.077 1.463 C Val 49
CA 1.540 CB 0.094 1.446 C Val 50	CA 1.521 CB 0.059 1.462 C Ala 62	CA 1.521 CB 0.062 1.583 C Ala 63	N 1.458 CA 0.053 1.511 C Leu 70	CA 1.540 CB 0.054 1.485 C Val 72	CA 1.540 CB 0.058 1.482 C Val 75
C 1.231 O 0.056 1.287 C Phe 82	CA 1.525 C 0.067 1.592 C Phe 82	C 1.231 O 0.054 1.285 C Lys 83	CA 1.540 CB 0.118 1.422 C Ile 84	CA 1.530 CB 0.052 1.478 C Pro 86	CA 1.525 C 0.054 1.579 C Glu 87
CA 1.530 CB 0.116 1.646 C Glu 87	N 1.458 CA 0.105 1.563 C Glu 87	CA 1.540 CB 0.085 1.455 C Ile 90	N 1.458 CA 0.064 1.394 C Ile 90	N 1.466 CA 0.061 1.405 C Pro 91	CA 1.525 C 0.065 1.460 C Val 98
CA 1.525 C 0.071 1.596 C Asp 100	CA 1.530 CB 0.058 1.588 C Tyr 106	N 1.458 CA 0.064 1.522 C Glu 108	N 1.458 CA 0.080 1.538 C Gln 110	CA 1.530 CB 0.051 1.581 C Asp 111	CA 1.540 CB 0.058 1.482 C Val 113
CA 1.525 C 0.051 1.474 C Pro 118	CA 1.530 CB 0.070 1.460 C Tyr 124	CA 1.530 CB 0.051 1.581 C Gln 125	CA 1.525 C 0.054 1.471 C Glu 126	CA 1.525 C 0.050 1.475 C Ile 127	CA 1.540 CB 0.098 1.442 C Val 128
CA 1.525 C 0.066 1.459 C Val 131	C 1.231 O 0.068 1.299 C Leu 132	N 1.458 CA 0.052 1.406 C Leu 132	CA 1.530 CB 0.052 1.478 C Ser 133	N 1.466 CA 0.059 1.407 C Pro 136	CA 1.525 C 0.073 1.452 C Asp 139
CA 1.525 C 0.067 1.458 C Lys 140	CA 1.525 C 0.087 1.612 C Asn 141	N 1.458 CA 0.058 1.516 C Asn 141	C 1.231 O 0.105 1.336 C Ile 142	CA 1.525 C 0.062 1.587 C Ile 142	CA 1.540 CB 0.123 1.417 C Ile 142
N 1.458 CA 0.060 1.518 C His 143	N 1.458 CA 0.107 1.565 C Phe 144	CA 1.516 C 0.102 1.618 C Gly 145	N 1.451 CA 0.105 1.556 C Gly 145	CA 1.521 CB 0.156 1.365 C Ala 148	C 1.231 O 0.062 1.293 C His 150
N 1.458 CA 0.076 1.534 C Asn 154	N 1.451 CA 0.052 1.503 C Gly 156	CA 1.525 C 0.058 1.467 C Ile 160	CA 1.540 CB 0.077 1.463 C Ile 160	CA 1.525 C 0.078 1.447 C Ser 167	N 1.458 CA 0.053 1.511 C Asn 170
N 1.458 CA 0.061 1.518 C Val 171	CA 1.540 CB 0.088 1.628 C Thr 173	CA 1.540 CB 0.076 1.616 C Thr 179	CA 1.540 CB 0.074 1.614 C Thr 181	N 1.458 CA 0.054 1.512 C Thr 181	CA 1.525 C 0.052 1.577 C Gln 200

Distorted geometry

pdb2e75

Main-chain bond lengths (contd)

N 1.458 CA 0.056 1.514 C Thr 201	N 1.458 CA 0.055 1.513 C Lys 205	CA 1.525 C 0.050 1.575 C Thr 206	CA 1.540 CB 0.062 1.602 C Thr 206	N 1.458 CA 0.052 1.510 C Thr 206	CA 1.525 C 0.063 1.588 C Val 207
N 1.458 CA 0.057 1.515 C Val 207	CA 1.525 C 0.081 1.606 C Val 208	N 1.458 CA 0.066 1.524 C Val 208	N 1.458 CA 0.058 1.516 C Asp 209	CA 1.540 CB 0.054 1.594 C Ile 211	CA 1.521 CB 0.079 1.442 C Ala 213
CA 1.540 CB 0.095 1.635 C Ile 218	CA 1.525 C 0.076 1.600 C Ala 230	CA 1.521 CB 0.069 1.590 C Ala 230	N 1.458 CA 0.062 1.520 C Leu 231	C 1.231 O 0.061 1.291 C Asn 234	CA 1.525 C 0.051 1.576 C Val 237
CA 1.540 CB 0.091 1.449 C Val 237	C 1.231 O 0.051 1.282 C Asp 244	CA 1.525 C 0.055 1.470 C Pro 252	CA 1.525 C 0.056 1.469 C Asn 253	CA 1.530 CB 0.073 1.457 C Asn 253	CA 1.530 CB 0.054 1.476 C Arg 254
CA 1.530 CB 0.086 1.616 C Lys 256	CA 1.525 C 0.052 1.577 C Ile 259	CA 1.540 CB 0.080 1.620 C Ile 259	CA 1.521 CB 0.060 1.461 C Ala 260	CA 1.525 C 0.070 1.595 C Met 266	CA 1.521 CB 0.085 1.606 C Ala 268
CA 1.525 C 0.054 1.579 C Leu 272	CA 1.540 CB 0.067 1.473 C Ile 273	CA 1.525 C 0.063 1.588 C Lys 277	CA 1.540 CB 0.063 1.477 C Val 282	CA 1.525 C 0.079 1.604 D Asp 9	N 1.458 CA 0.056 1.514 D Asp 9
CA 1.530 CB 0.051 1.479 D Gln 17	CA 1.521 CB 0.059 1.580 D Ala 23	CA 1.530 CB 0.055 1.475 D Phe 24	CA 1.540 CB 0.092 1.448 D Thr 26	C 1.231 O 0.060 1.291 D Val 27	CA 1.540 CB 0.052 1.488 D Val 27
C 1.231 O 0.061 1.292 D Thr 28	CA 1.525 C 0.059 1.584 D Thr 28	CA 1.521 CB 0.105 1.416 D Ala 31	CA 1.521 CB 0.154 1.367 D Ala 34	C 1.231 O 0.052 1.283 D Phe 42	CA 1.530 CB 0.057 1.473 D Phe 42
C 1.231 O 0.060 1.291 D Ile 43	CA 1.525 C 0.060 1.465 D Pro 45	CA 1.516 C 0.060 1.576 D Gly 47	N 1.451 CA 0.069 1.520 D Gly 47	CA 1.525 C 0.080 1.605 D Val 50	CA 1.540 CB 0.140 1.680 D Val 50
N 1.458 CA 0.082 1.540 D Val 50	CA 1.525 C 0.056 1.581 D Thr 54	CA 1.540 CB 0.116 1.656 D Thr 54	CA 1.525 C 0.055 1.580 D Thr 55	CA 1.525 C 0.053 1.578 D Ala 56	CA 1.530 CB 0.058 1.588 D Leu 60
N 1.458 CA 0.054 1.512 D Asn 63	CA 1.525 C 0.068 1.593 D Lys 65	CA 1.530 CB 0.054 1.584 D Asp 77	N 1.458 CA 0.057 1.515 D Asp 77	N 1.458 CA 0.052 1.510 D Arg 78	CA 1.540 CB 0.068 1.472 D Val 81

Distorted geometry

pdb2e75

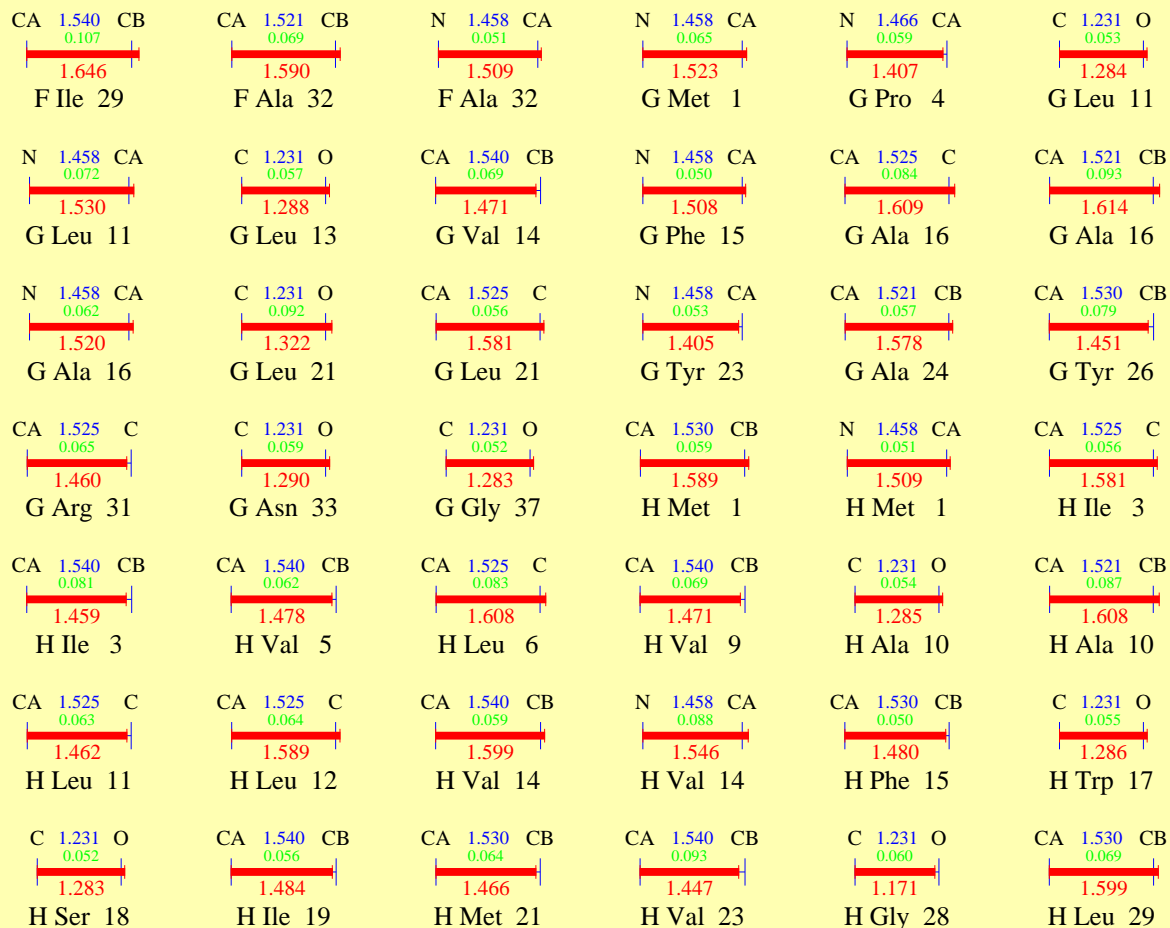
Main-chain bond lengths (contd)

CA 1.525 C 0.056 1.469 D Leu 84	CA 1.540 CB 0.067 1.607 D Thr 89	CA 1.540 CB 0.054 1.594 D Ile 91	CA 1.525 C 0.053 1.578 D Ala 98	CA 1.540 CB 0.056 1.596 D Ile 99	N 1.458 CA 0.059 1.517 D Ile 99
CA 1.530 CB 0.060 1.590 D Asp 101	CA 1.540 CB 0.064 1.476 D Ile 104	N 1.458 CA 0.073 1.531 D Val 107	CA 1.530 CB 0.072 1.602 D Cys 108	N 1.458 CA 0.051 1.509 D Cys 108	CA 1.525 C 0.068 1.593 D Pro 116
CA 1.525 C 0.051 1.474 D Trp 117	N 1.458 CA 0.055 1.513 D Ala 119	CA 1.525 C 0.062 1.463 D Lys 125	N 1.458 CA 0.064 1.522 D His 129	CA 1.525 C 0.085 1.610 D Tyr 133	CA 1.525 C 0.062 1.587 D Ala 149
CA 1.540 CB 0.069 1.609 D Thr 154	CA 1.540 CB 0.088 1.628 D Val 155	N 1.458 CA 0.050 1.508 D Thr 172	N 1.458 CA 0.053 1.511 E Met 1	C 1.231 O 0.072 1.303 E Leu 3	CA 1.525 C 0.072 1.597 E Leu 3
CA 1.521 CB 0.104 1.417 E Ala 5	C 1.231 O 0.056 1.287 E Ile 9	CA 1.525 C 0.077 1.602 E Ile 9	C 1.231 O 0.085 1.316 E Val 10	CA 1.525 C 0.056 1.581 E Val 10	C 1.231 O 0.102 1.333 E Phe 11
C 1.329 N 0.052 1.381 E Phe 11 - E Ile 12	C 1.231 O 0.063 1.294 E Ile 12	CA 1.540 CB 0.076 1.464 E Ile 12	CA 1.530 CB 0.061 1.469 E Leu 14	CA 1.525 C 0.053 1.578 E Ile 18	C 1.231 O 0.055 1.286 E Ala 19
CA 1.521 CB 0.060 1.461 E Ala 19	CA 1.540 CB 0.109 1.431 E Val 20	C 1.231 O 0.060 1.291 E Ile 22	CA 1.540 CB 0.075 1.615 E Ile 26	CA 1.530 CB 0.052 1.582 E Ser 28	CA 1.525 C 0.084 1.609 F Met 1
N 1.458 CA 0.064 1.522 F Met 1	CA 1.540 CB 0.117 1.657 F Thr 2	N 1.458 CA 0.056 1.514 F Thr 2	CA 1.521 CB 0.120 1.401 F Ala 8	CA 1.521 CB 0.135 1.386 F Ala 9	CA 1.525 C 0.093 1.432 F Leu 10
N 1.458 CA 0.057 1.515 F Leu 10	C 1.231 O 0.071 1.302 F Leu 11	C 1.231 O 0.080 1.311 F Ser 12	CA 1.525 C 0.067 1.592 F Phe 13	CA 1.530 CB 0.052 1.478 F Phe 13	C 1.231 O 0.074 1.305 F Gly 14
C 1.231 O 0.061 1.292 F Leu 15	CA 1.540 CB 0.096 1.444 F Ile 16	C 1.231 O 0.077 1.308 F Phe 17	CA 1.530 CB 0.076 1.454 F Phe 17	C 1.231 O 0.053 1.283 F Gly 19	C 1.231 O 0.103 1.334 F Trp 20
CA 1.525 C 0.053 1.578 F Trp 20	C 1.231 O 0.062 1.293 F Gly 21	C 1.231 O 0.052 1.283 F Gly 23	CA 1.540 CB 0.074 1.466 F Val 24	CA 1.530 CB 0.053 1.477 F Leu 27	CA 1.525 C 0.057 1.582 F Ile 29

Distorted geometry

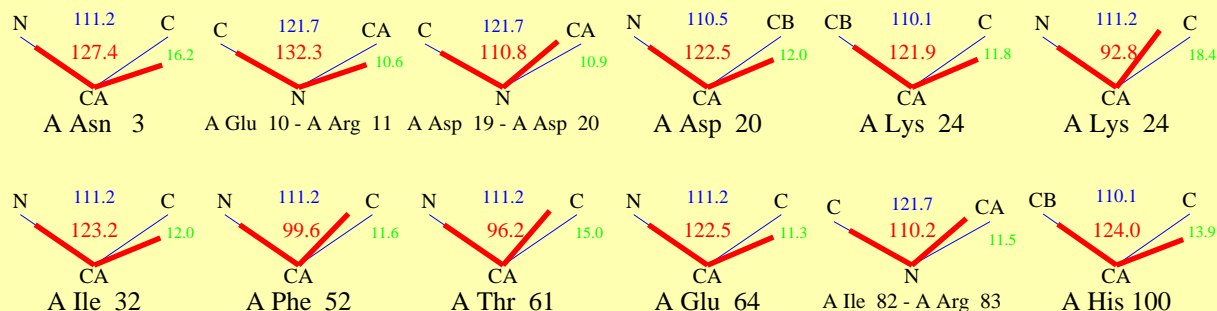
pdb2e75

Main-chain bond lengths (contd)



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

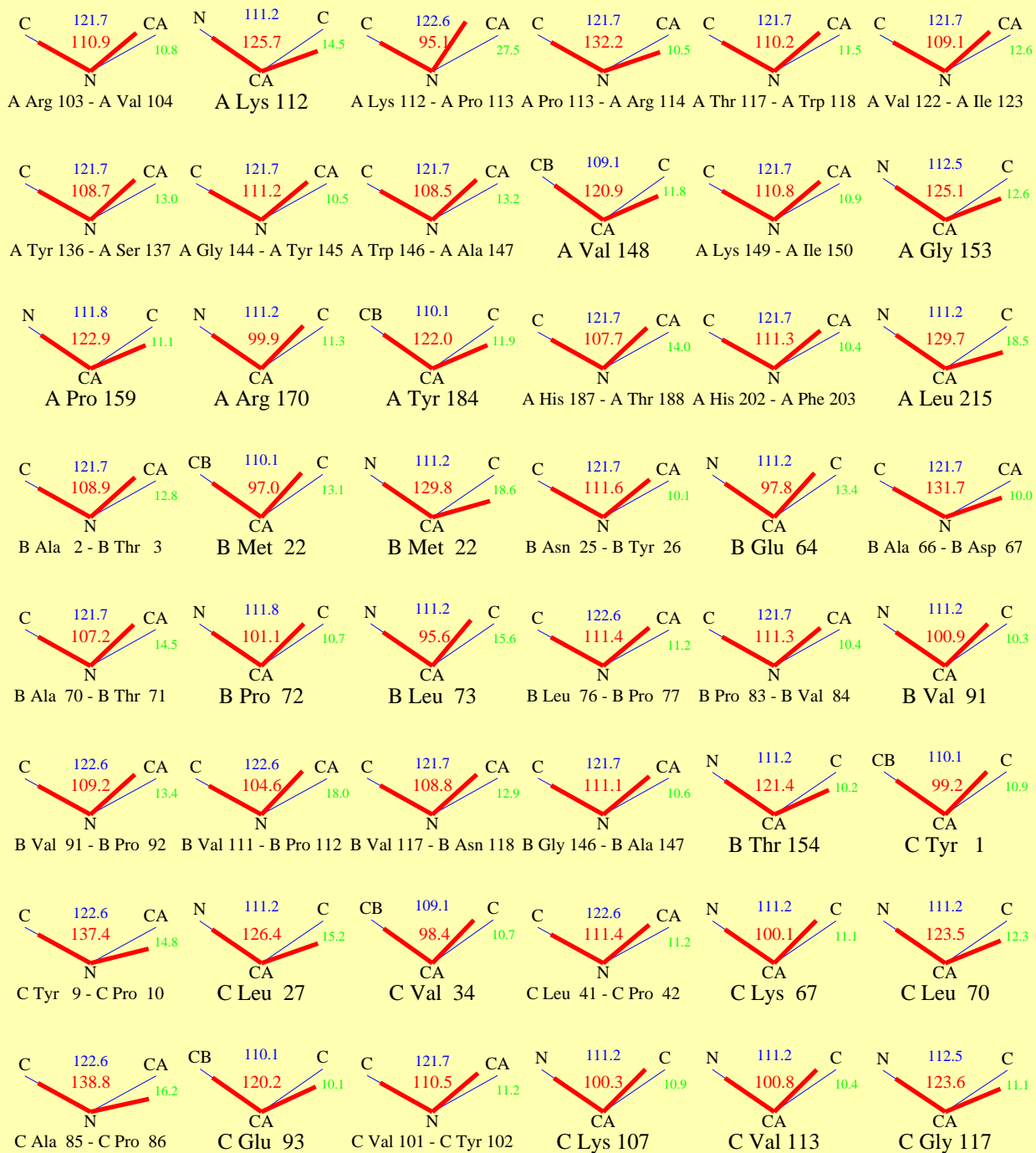
Main-chain bond angles



Distorted geometry

pdb2e75

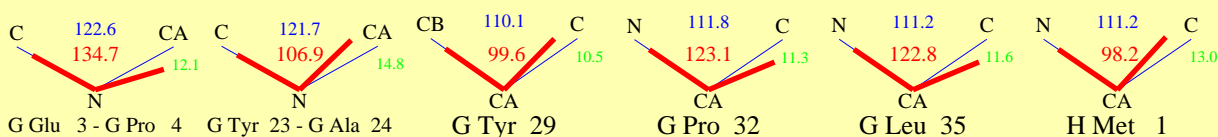
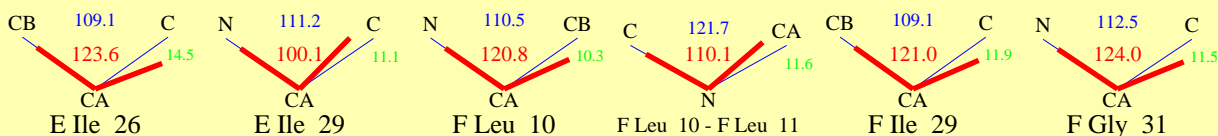
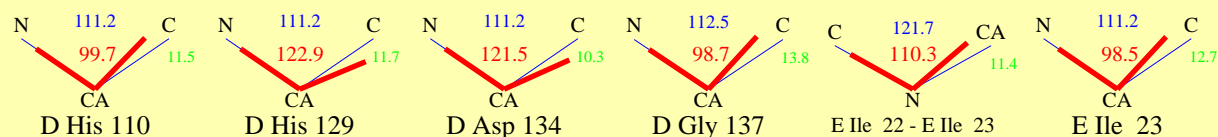
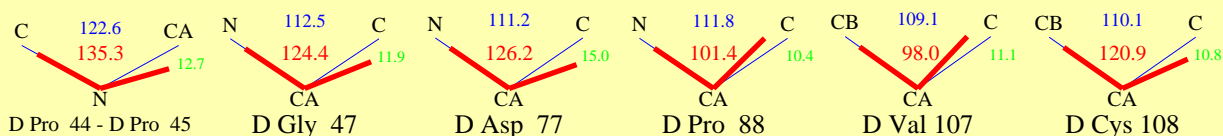
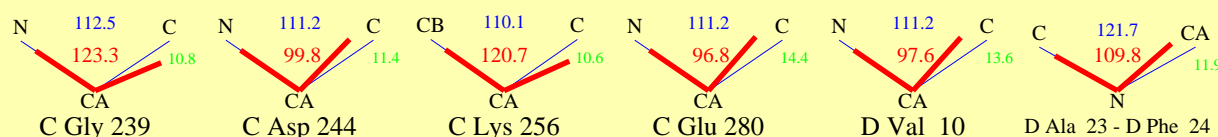
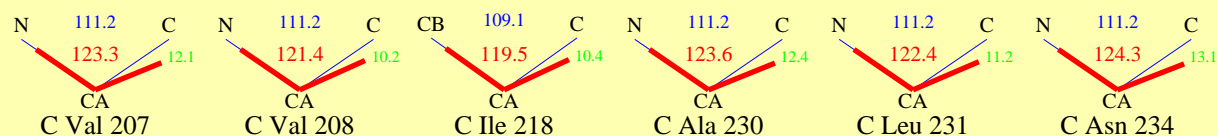
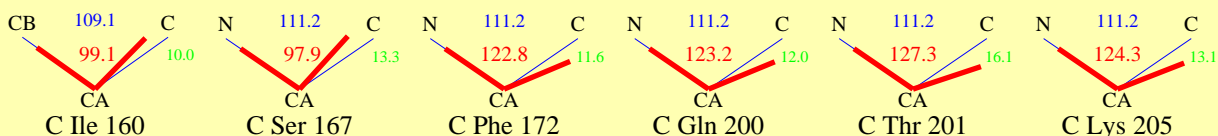
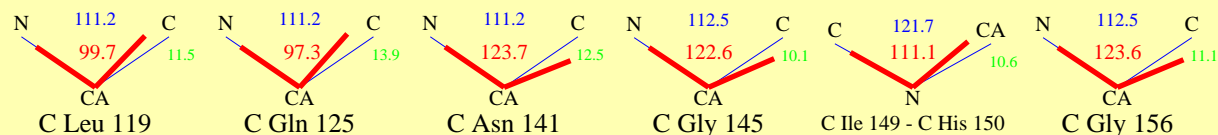
Main-chain bond angles (contd)



Distorted geometry

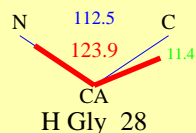
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Main-chain bond angles (contd)



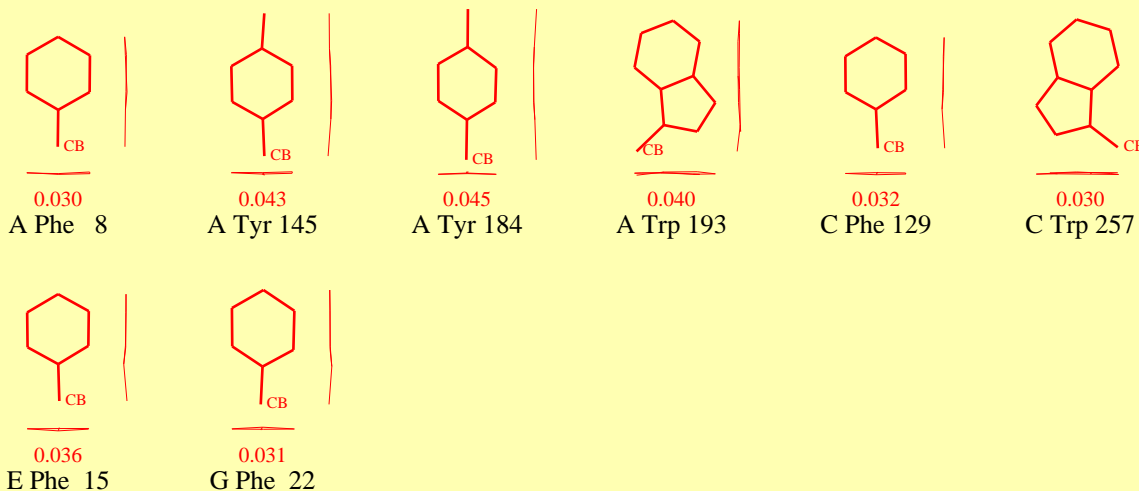
Distorted geometry pdb2e75

Main-chain bond angles (contd)



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

Planar groups



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