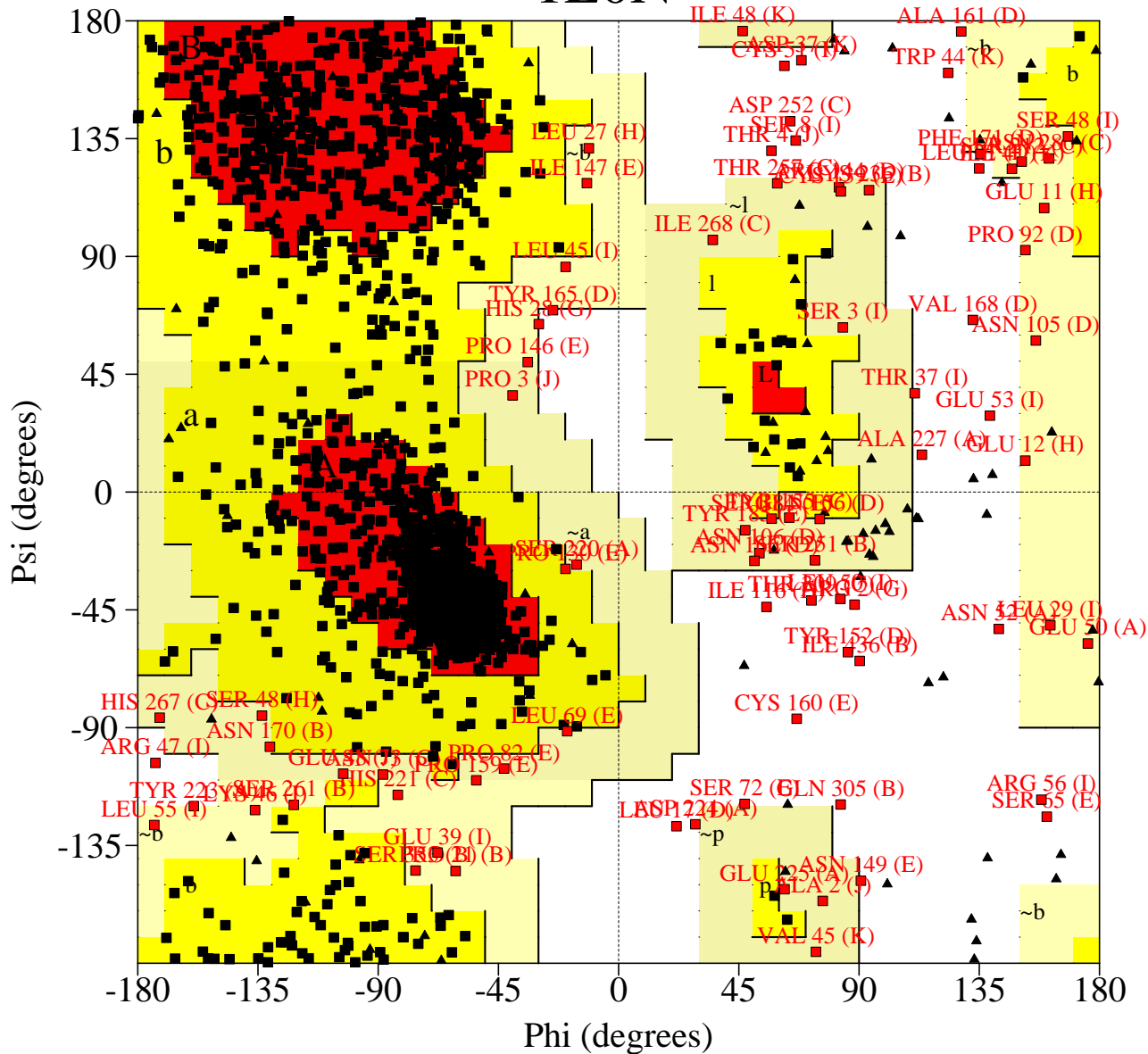


Ramachandran Plot

1LON



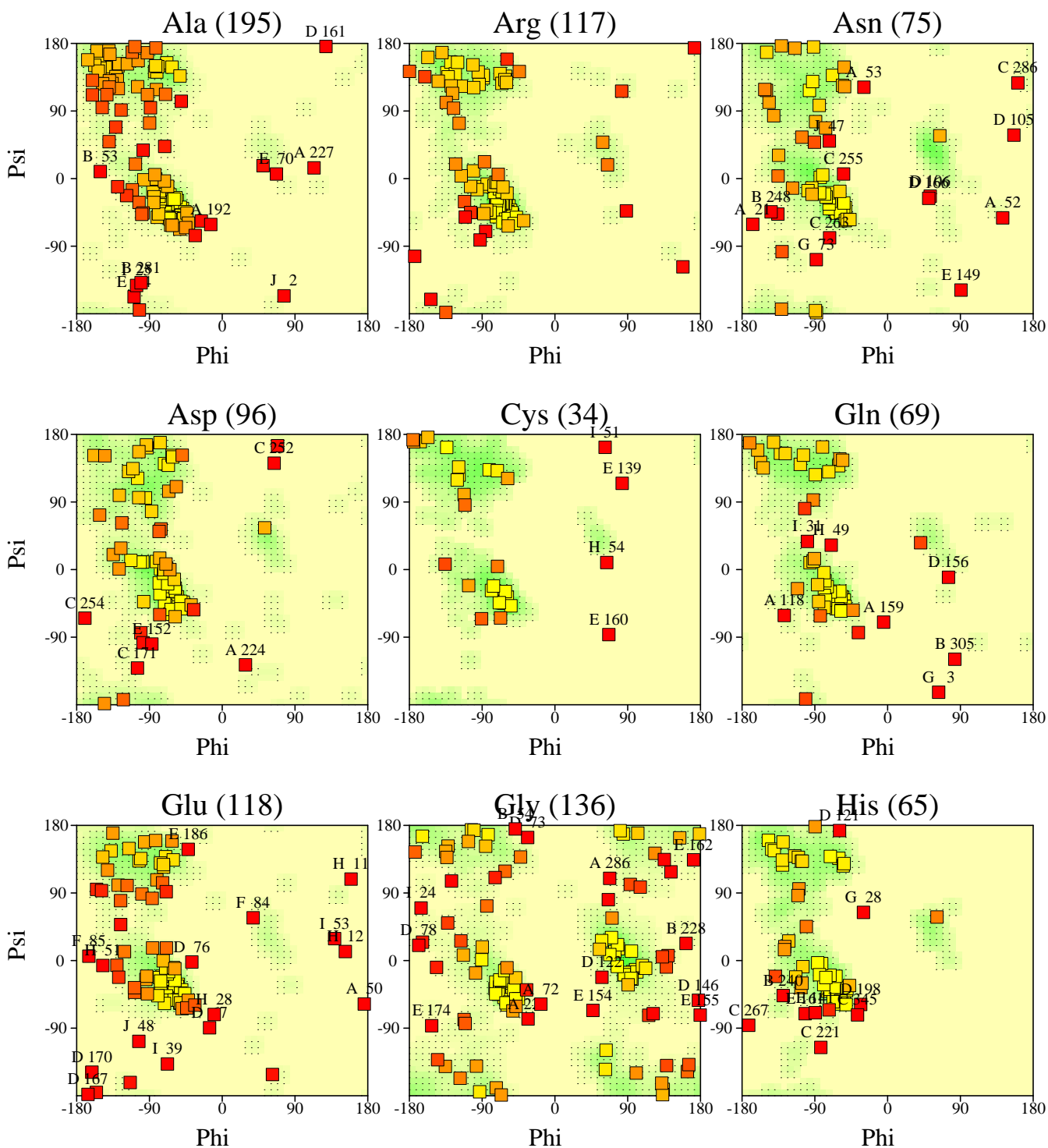
Plot statistics

Residues in most favoured regions [A,B,L]	1464	80.0%
Residues in additional allowed regions [a,b,l,p]	292	16.0%
Residues in generously allowed regions [-a,-b,-l,-p]	42	2.3%
Residues in disallowed regions	32	1.7%
Number of non-glycine and non-proline residues	1830	100.0%
Number of end-residues (excl. Gly and Pro)	19	
Number of glycine residues (shown as triangles)	139	
Number of proline residues	109	
Total number of residues	2097	

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

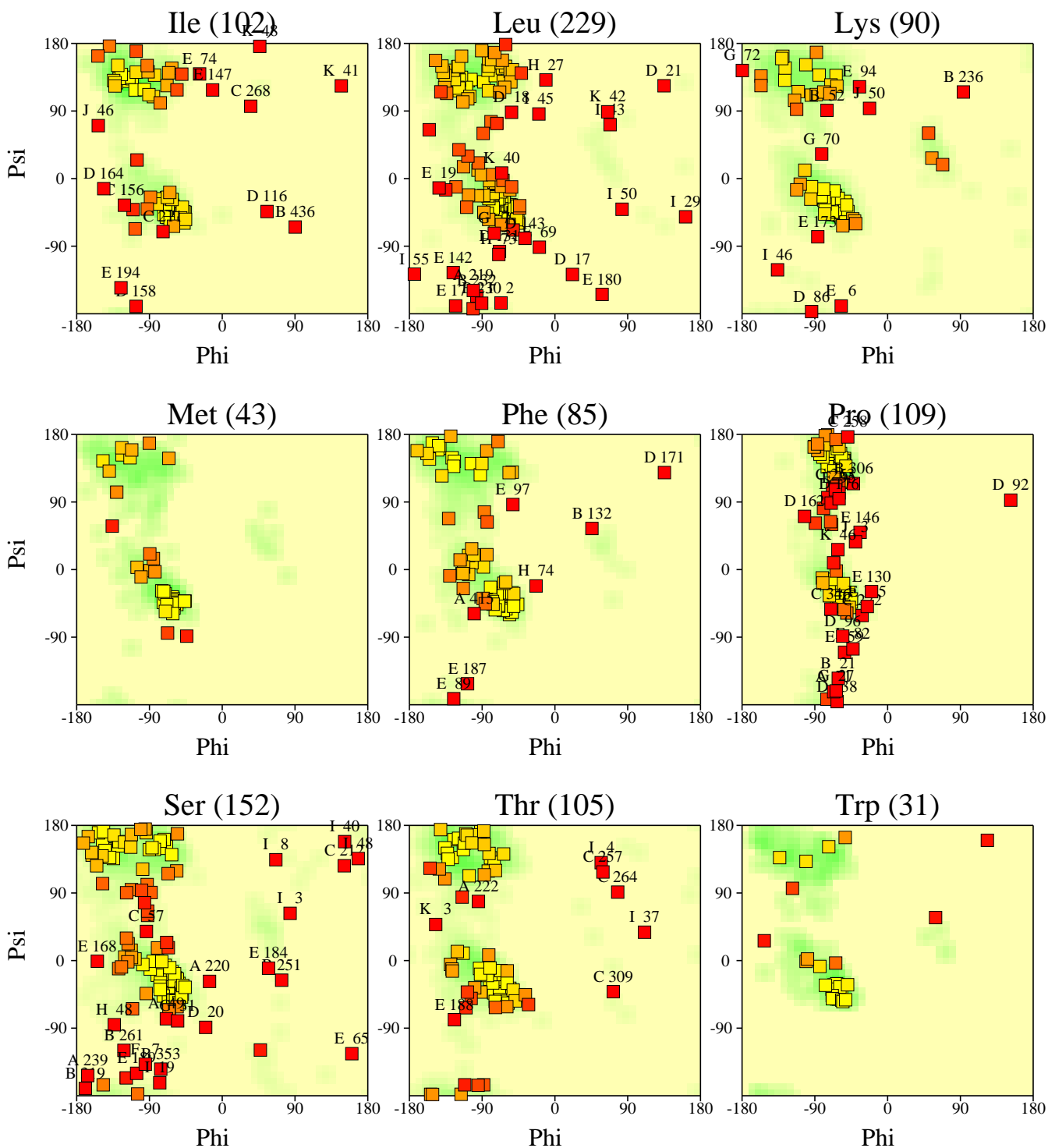
1L0N



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

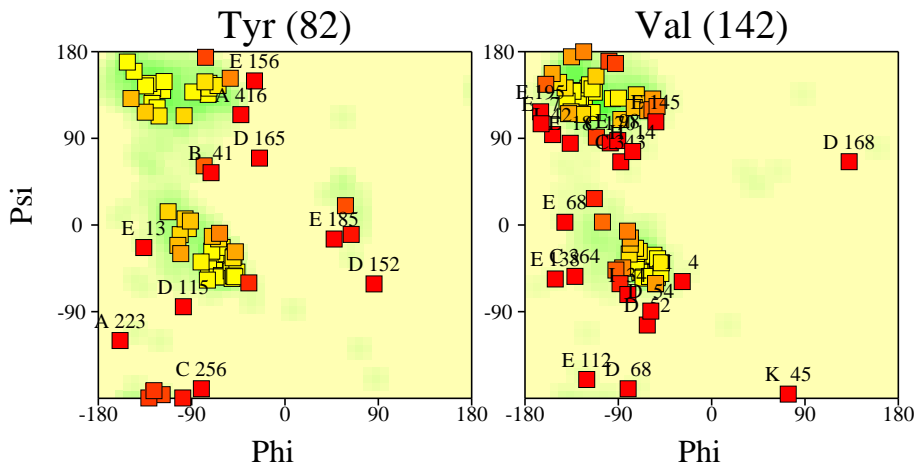
1LON



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

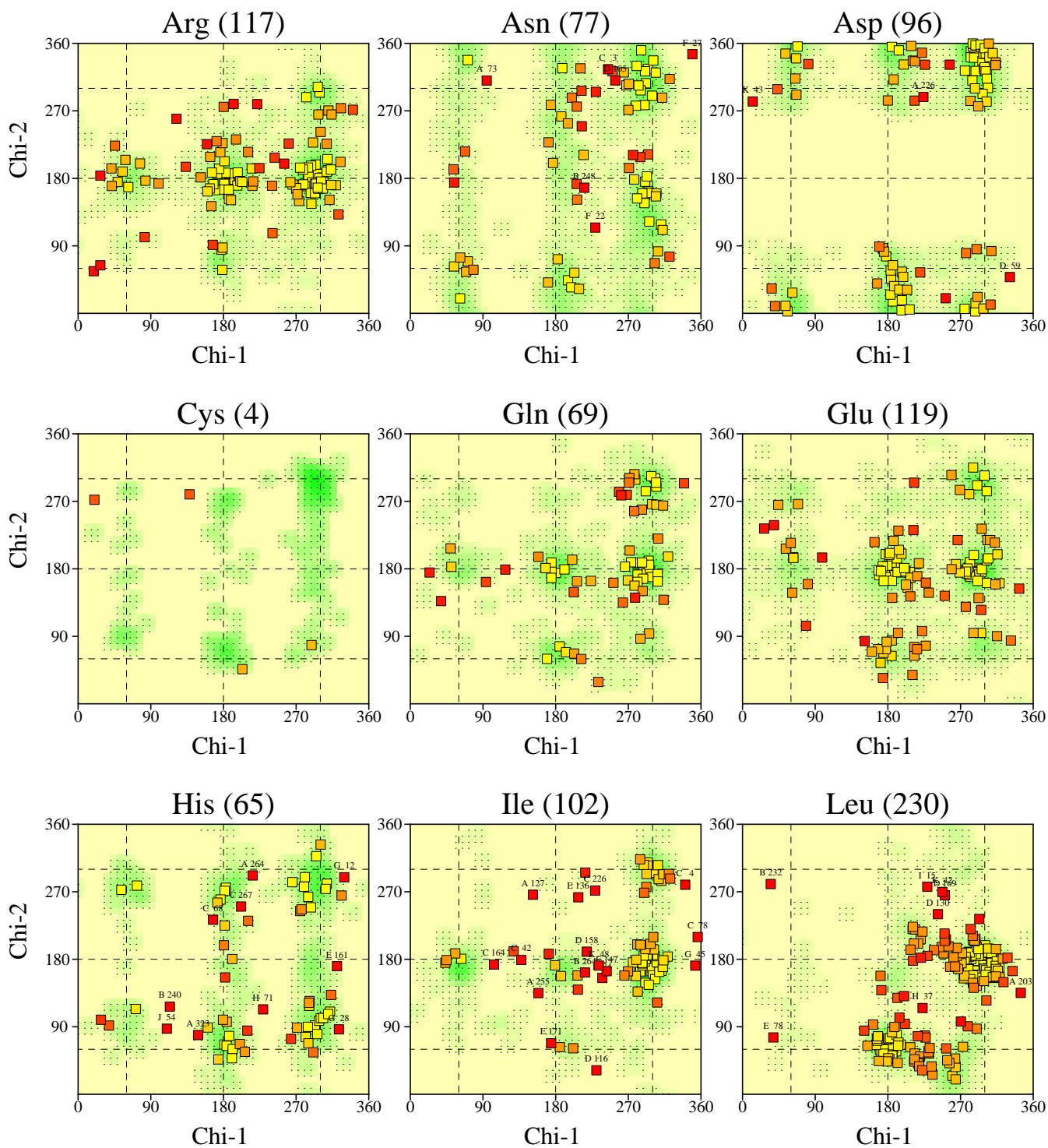
1L0N



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

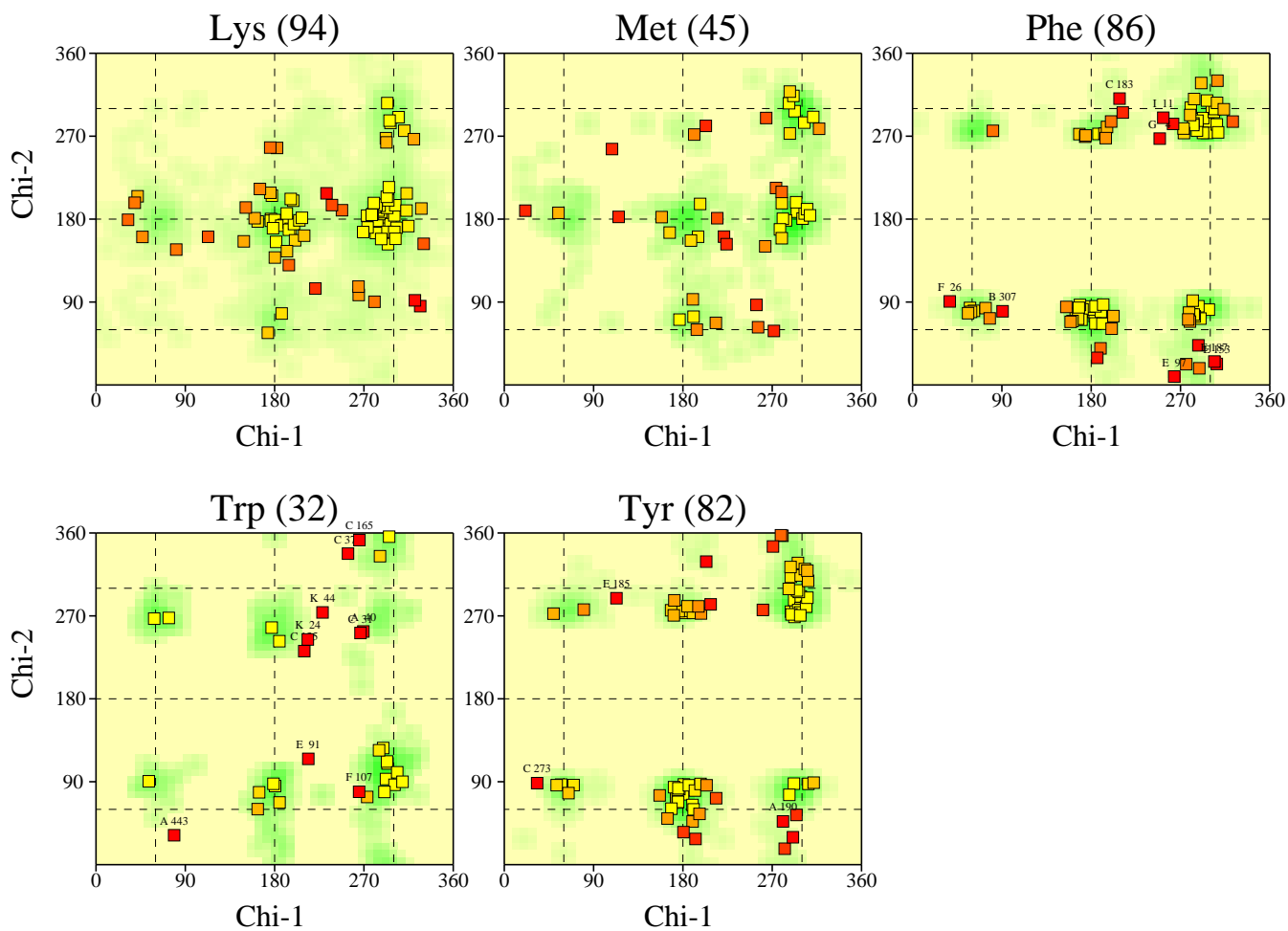
1LON



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

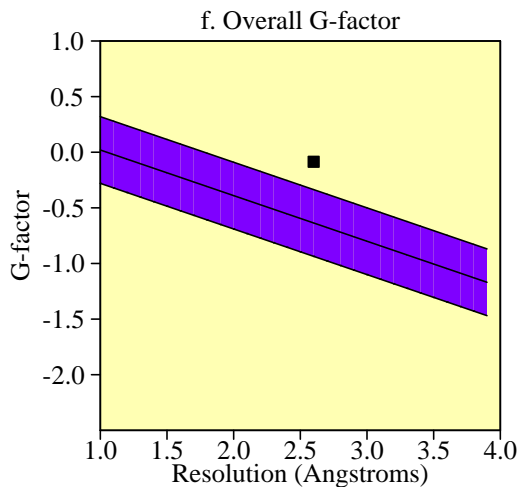
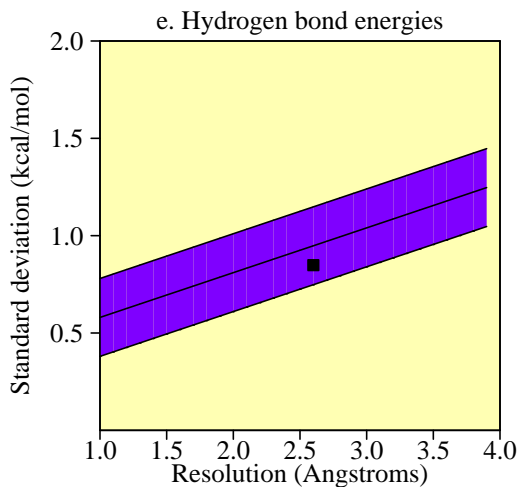
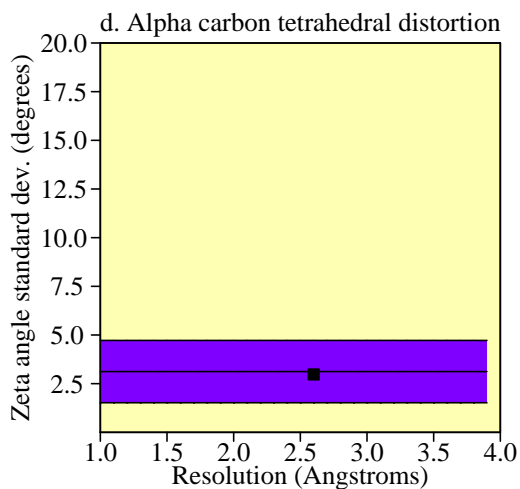
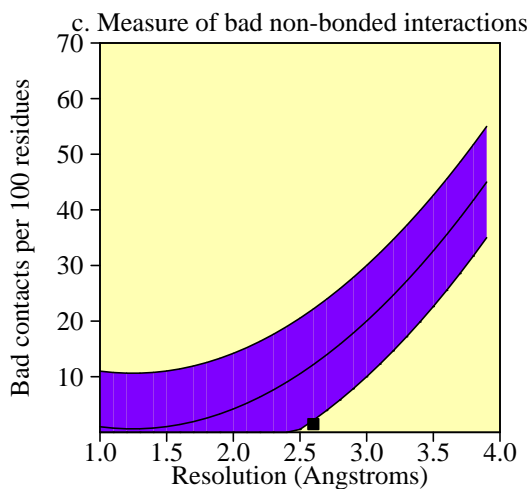
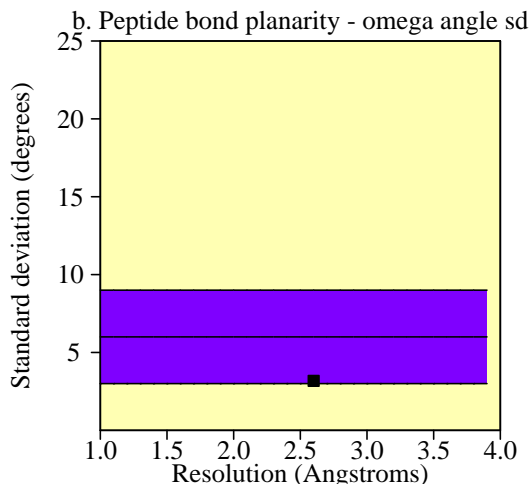
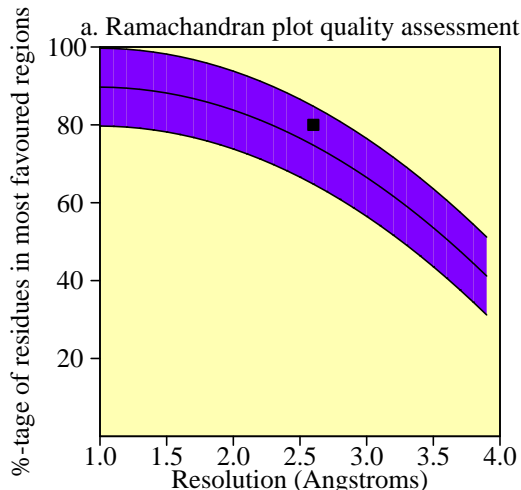
1L0N



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

1LON

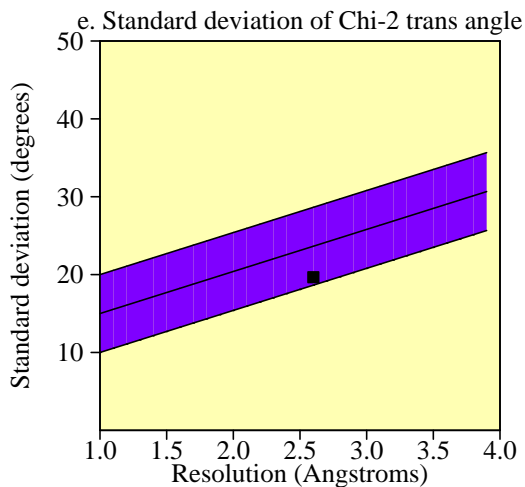
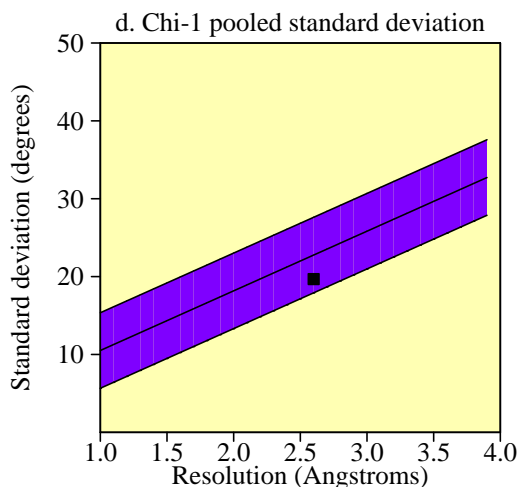
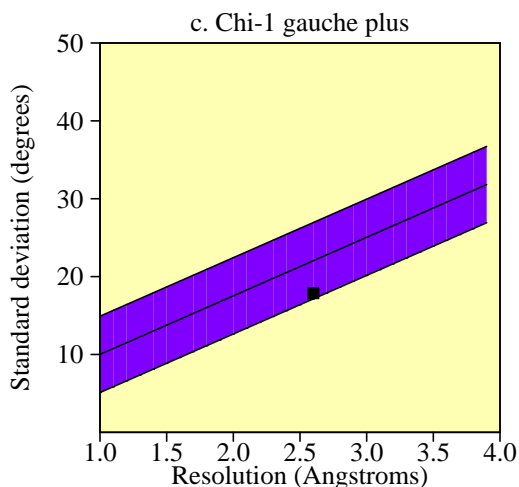
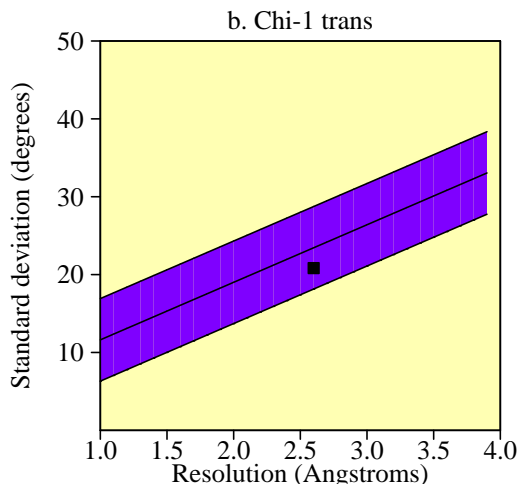
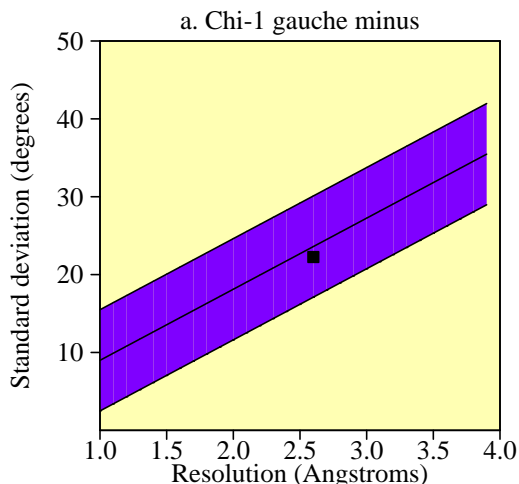


Plot statistics

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	1830	80.0	74.8	10.0	0.5	Inside
b. Omega angle st dev	2085	3.2	6.0	3.0	-0.9	Inside
c. Bad contacts / 100 residues	31	1.5	12.2	10.0	-1.1	BETTER
d. Zeta angle st dev	1958	3.0	3.1	1.6	-0.1	Inside
e. H-bond energy st dev	1340	0.8	0.9	0.2	-0.5	Inside
f. Overall G-factor	2097	-0.1	-0.6	0.3	1.8	BETTER

Side-chain parameters

1LON



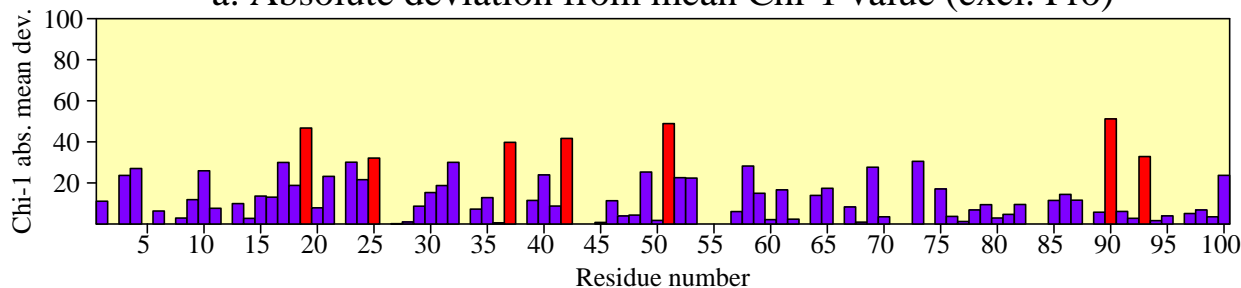
1LON

Plot statistics

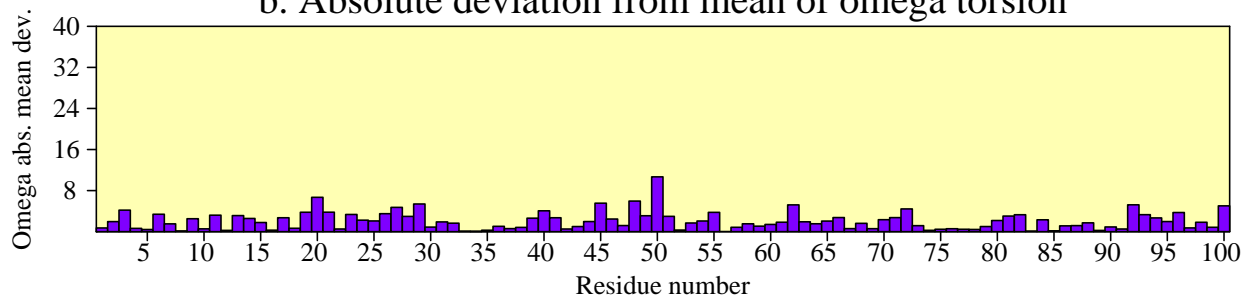
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean
			Typical value	Band width	
a. Chi-1 gauche minus st dev	228	22.3	23.6	6.5	-0.2 Inside
b. Chi-1 trans st dev	608	20.8	23.4	5.3	-0.5 Inside
c. Chi-1 gauche plus st dev	817	17.9	22.0	4.9	-0.8 Inside
d. Chi-1 pooled st dev	1653	19.7	22.8	4.8	-0.6 Inside
e. Chi-2 trans st dev	549	19.7	23.6	5.0	-0.8 Inside

Residue properties 1LON

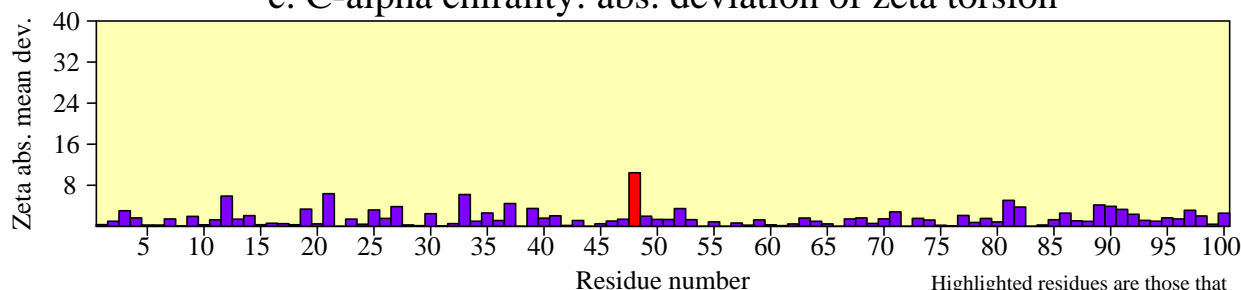
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

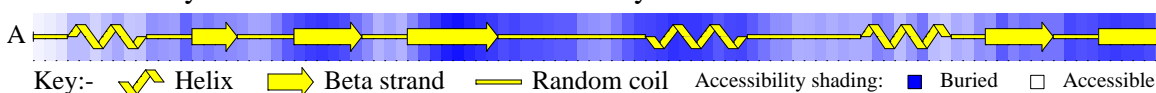


c. C-alpha chirality: abs. deviation of zeta torsion



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

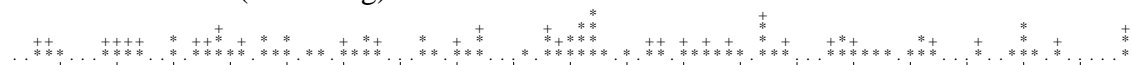
d. Secondary structure & estimated accessibility



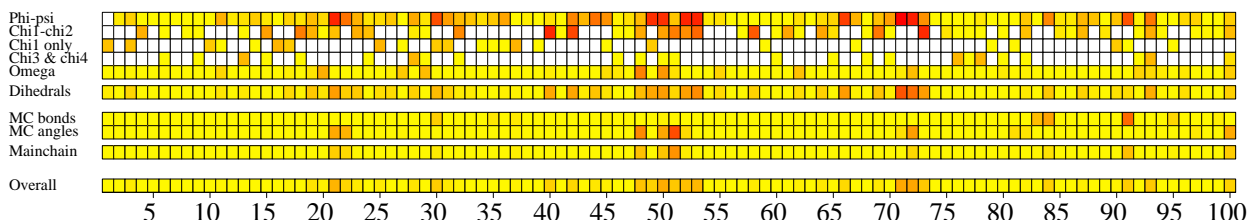
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

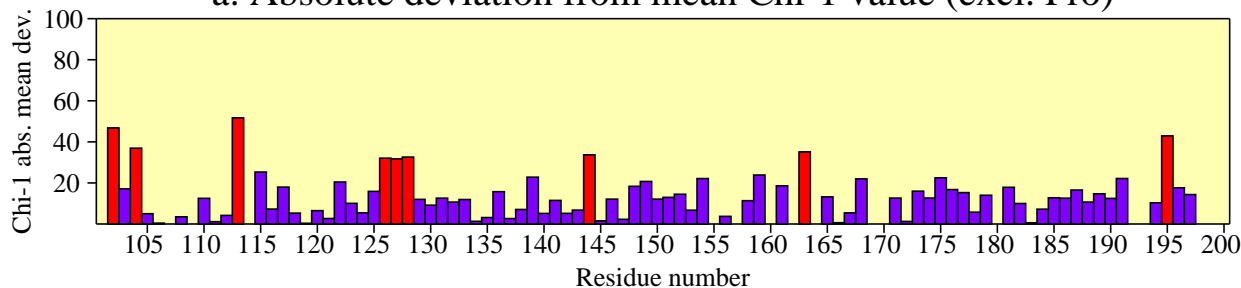


g. G-factors

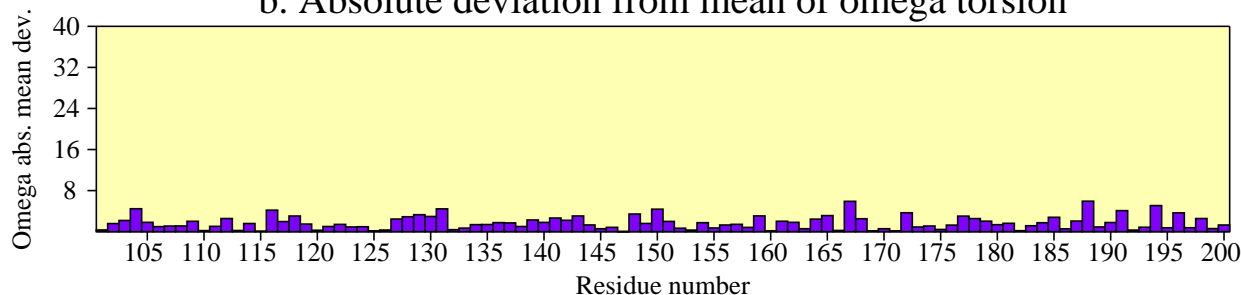


Residue properties 1LON

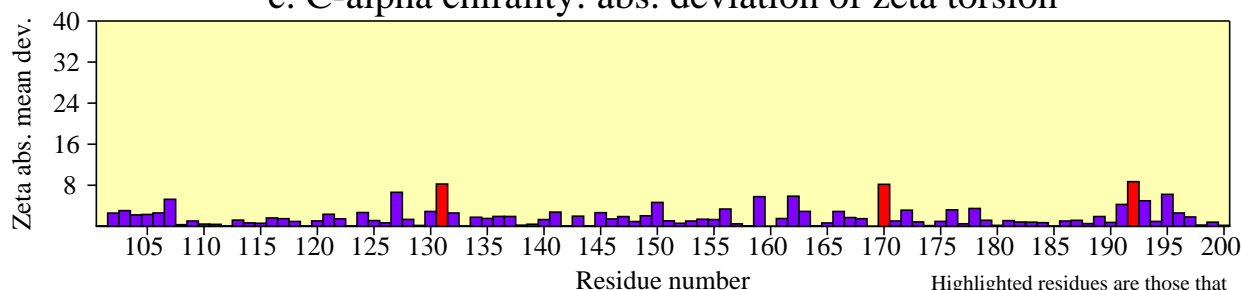
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



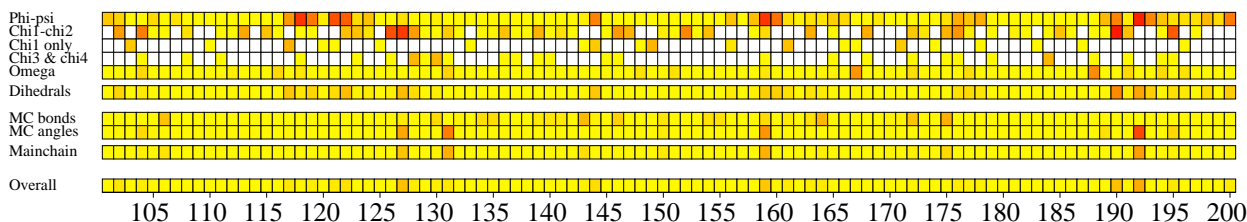
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

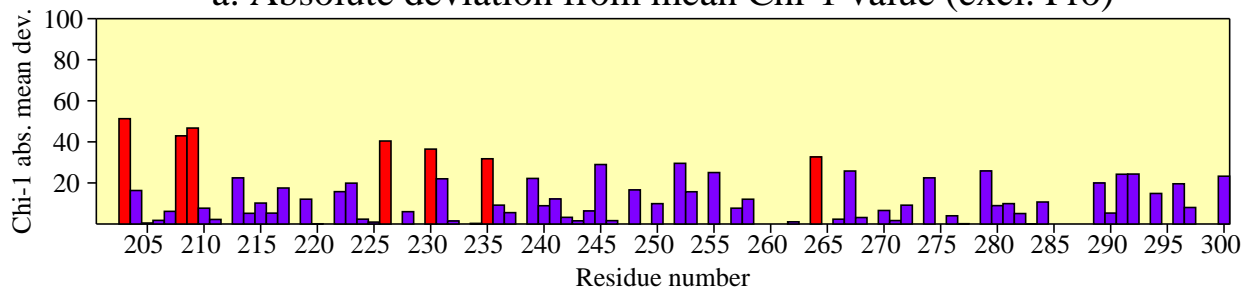


g. G-factors

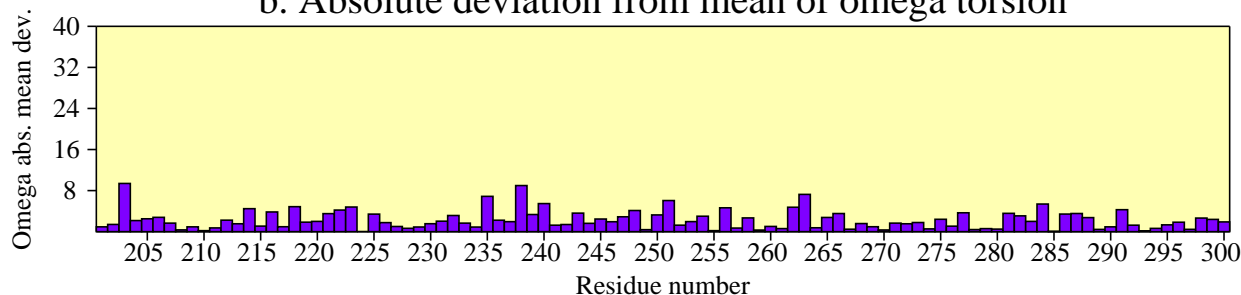


Residue properties 1LON

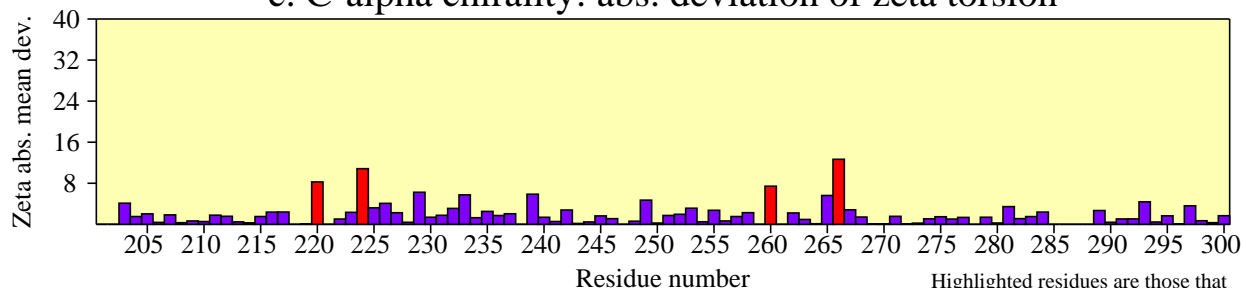
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

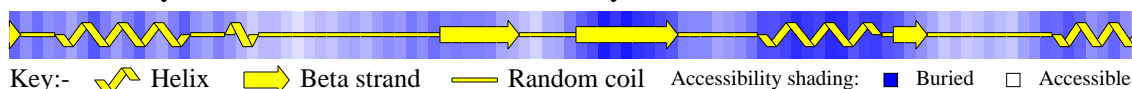


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



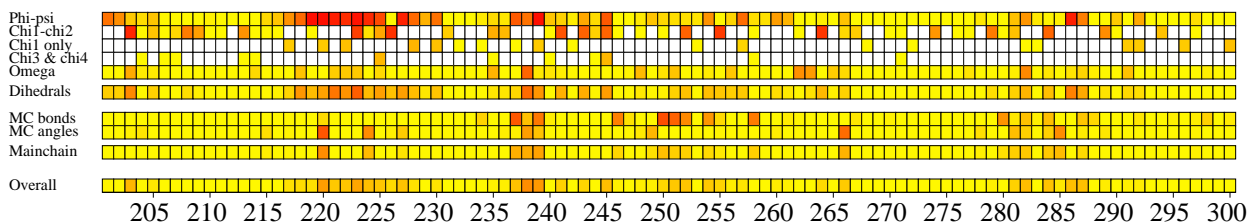
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

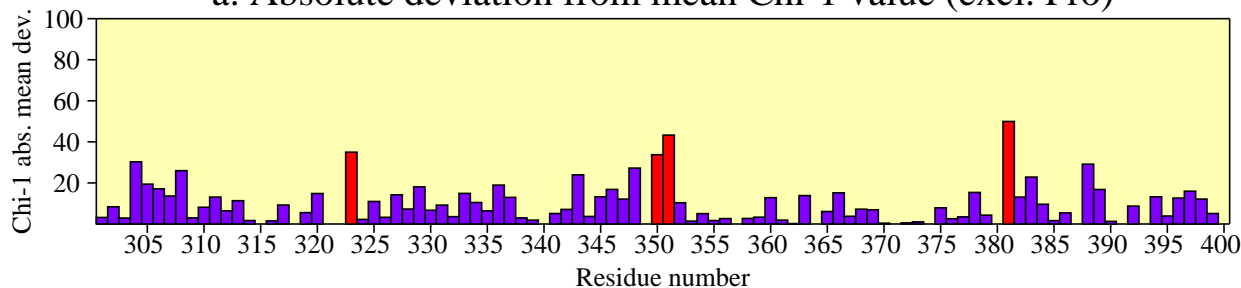


g. G-factors

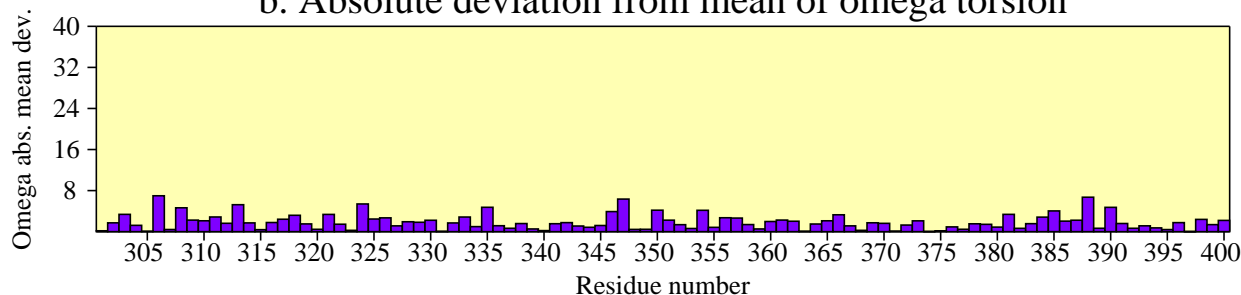


Residue properties 1LON

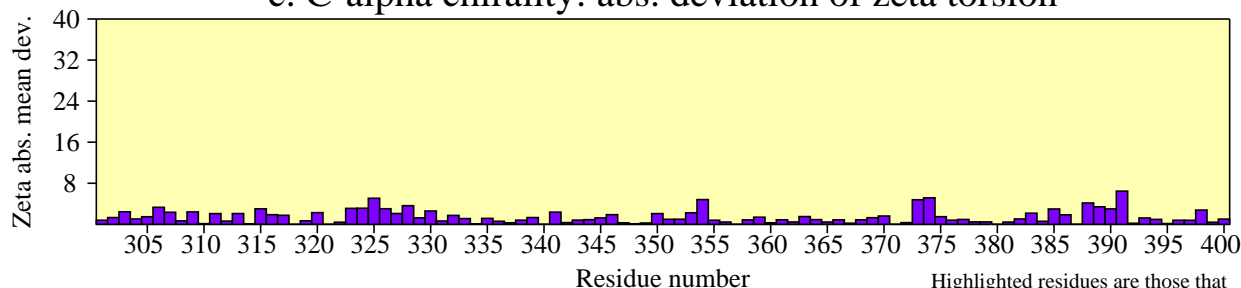
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

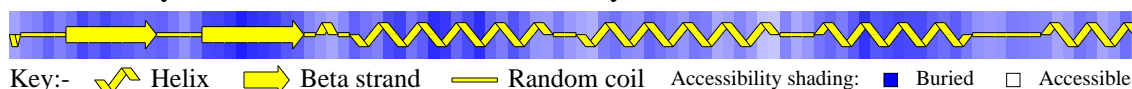


c. C-alpha chirality: abs. deviation of zeta torsion



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

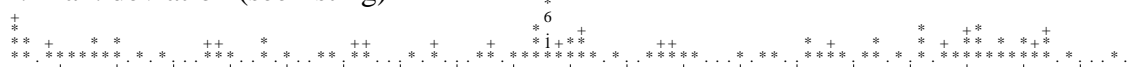
d. Secondary structure & estimated accessibility



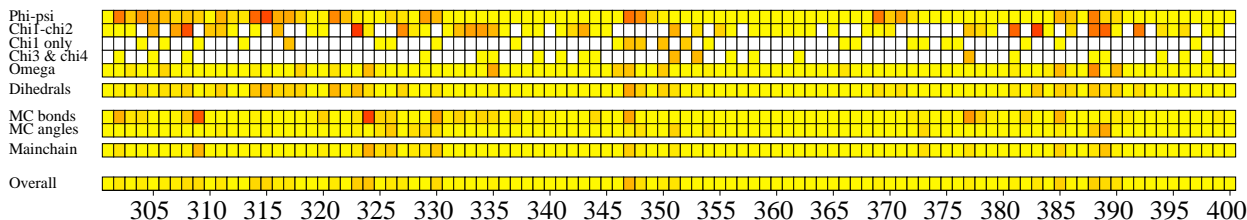
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

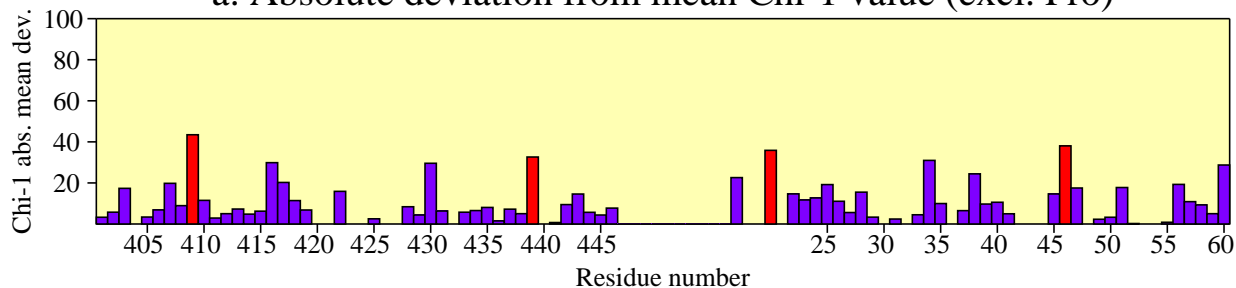


g. G-factors

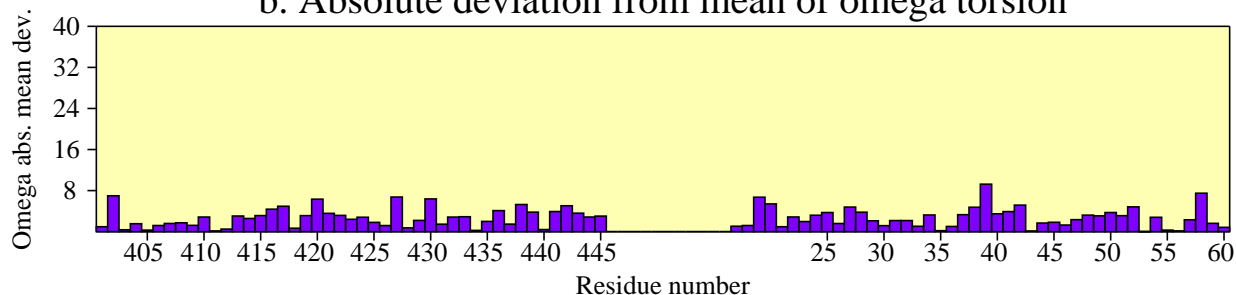


Residue properties 1LON

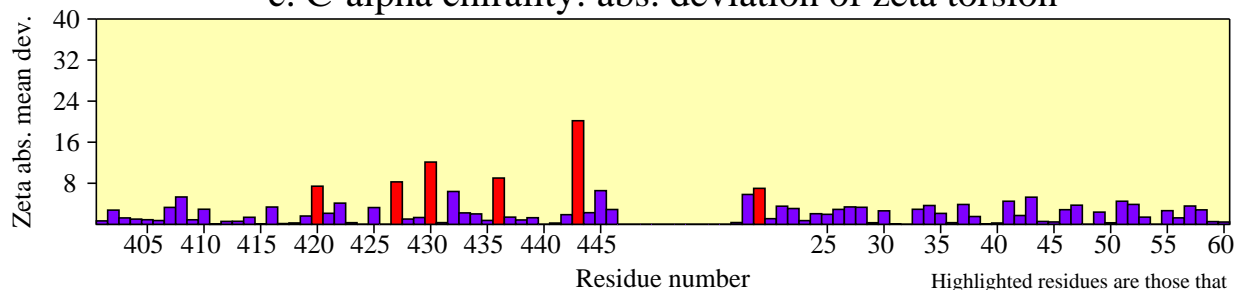
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

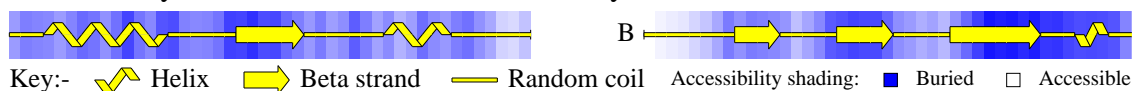


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



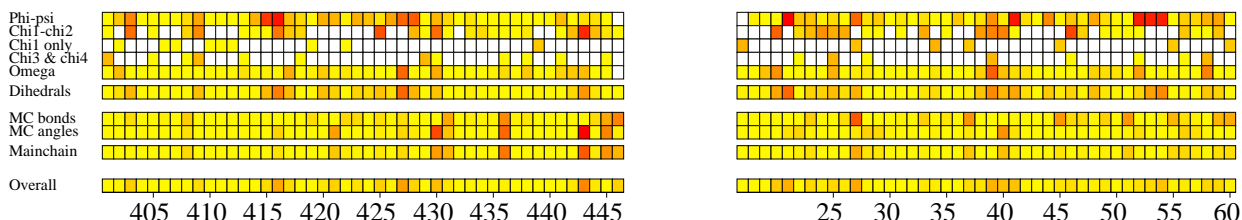
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

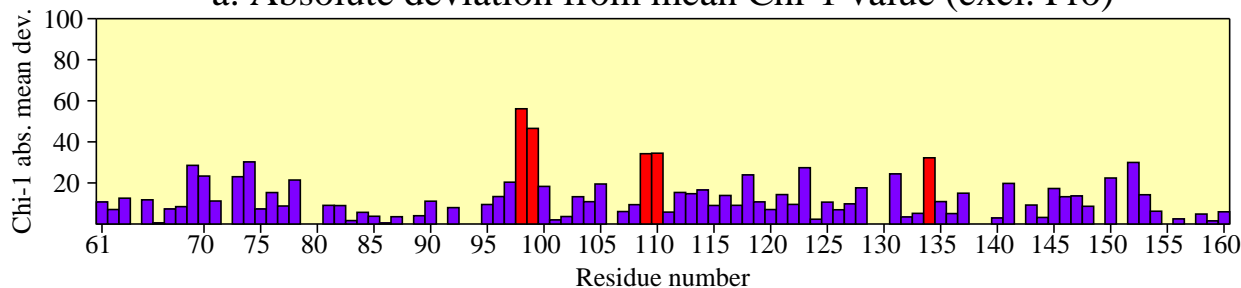


g. G-factors

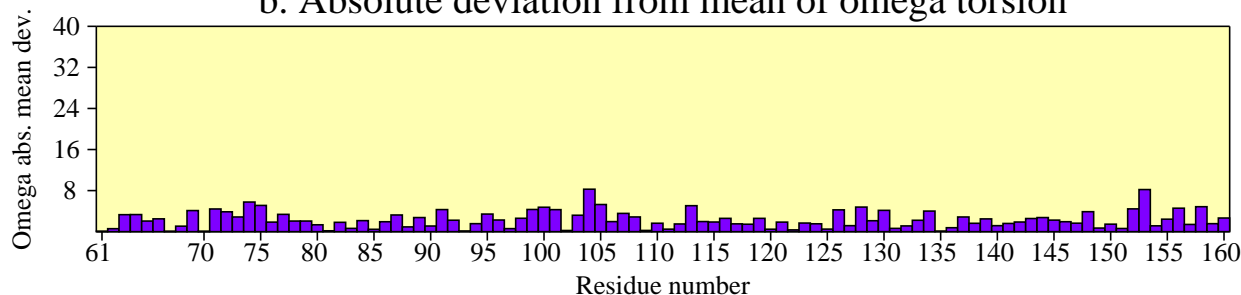


Residue properties 1LON

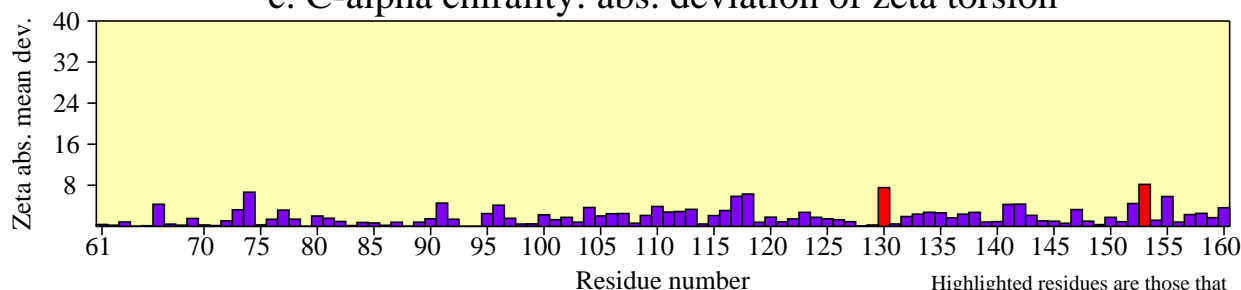
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

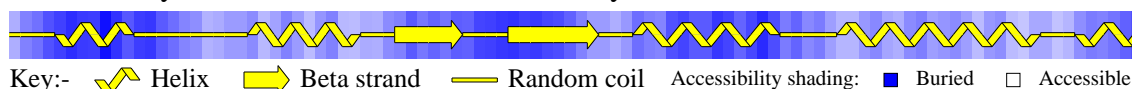


c. C-alpha chirality: abs. deviation of zeta torsion



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

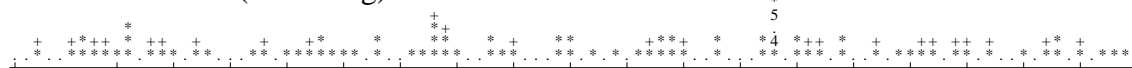
d. Secondary structure & estimated accessibility



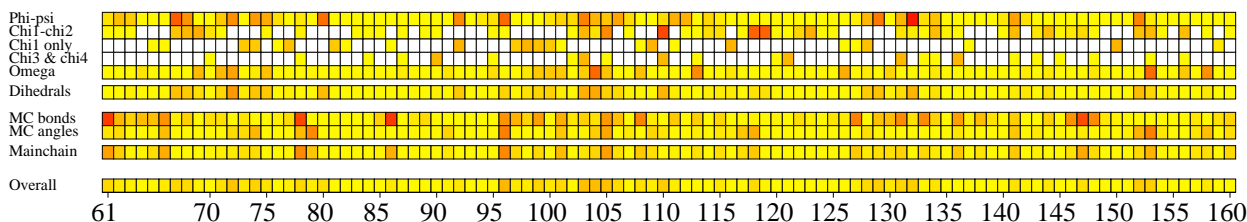
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

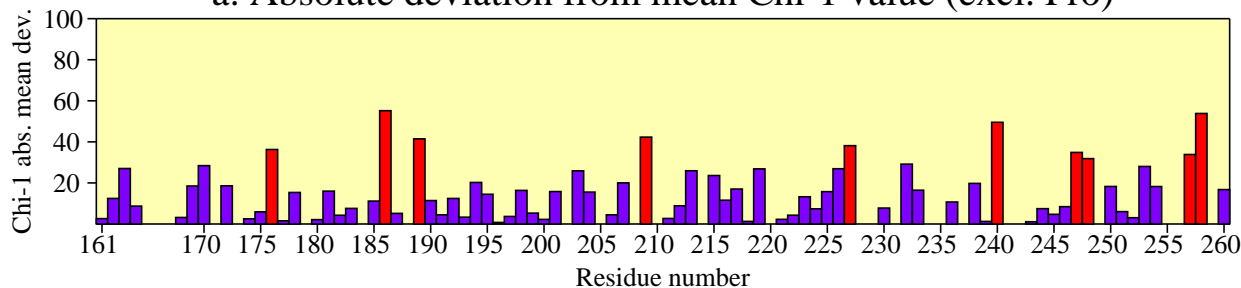


g. G-factors

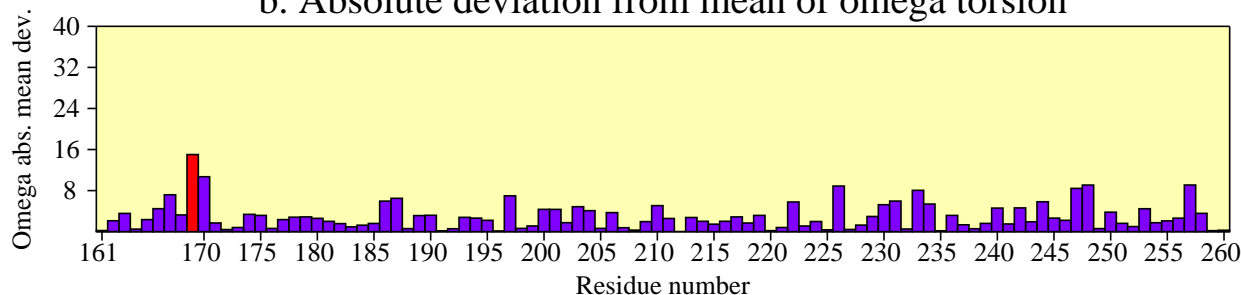


Residue properties 1LON

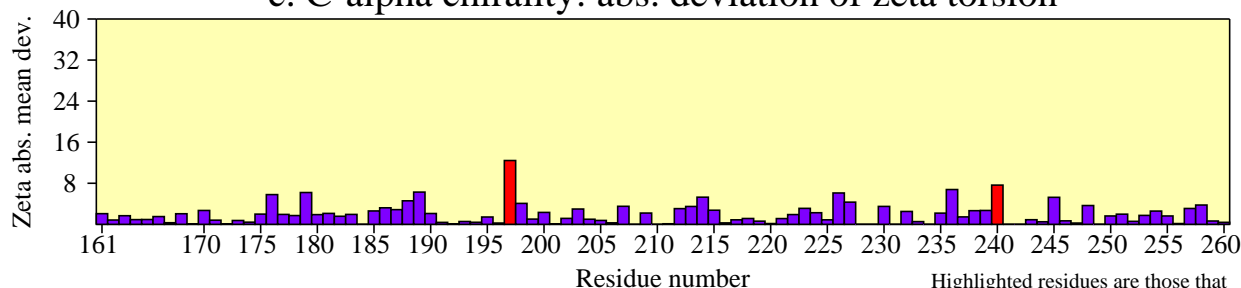
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

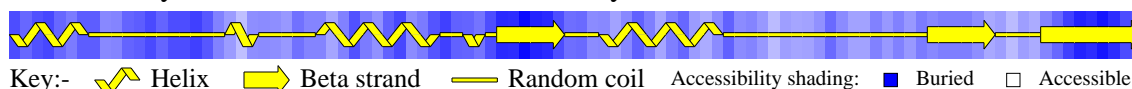


c. C-alpha chirality: abs. deviation of zeta torsion



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

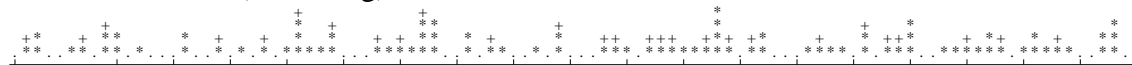
d. Secondary structure & estimated accessibility



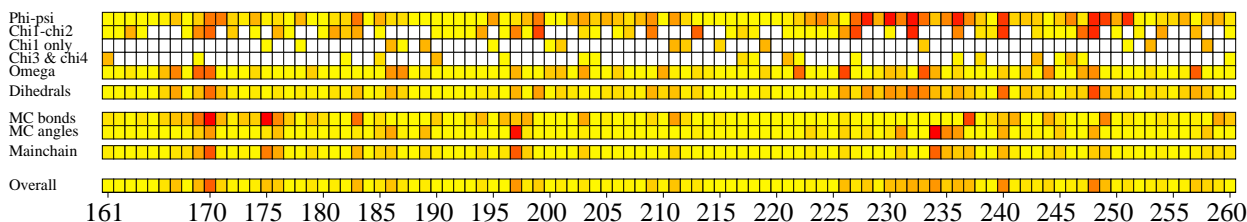
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

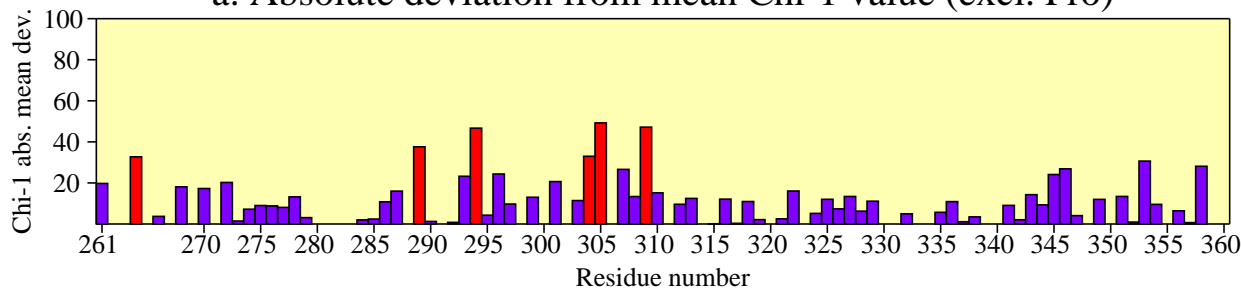


g. G-factors

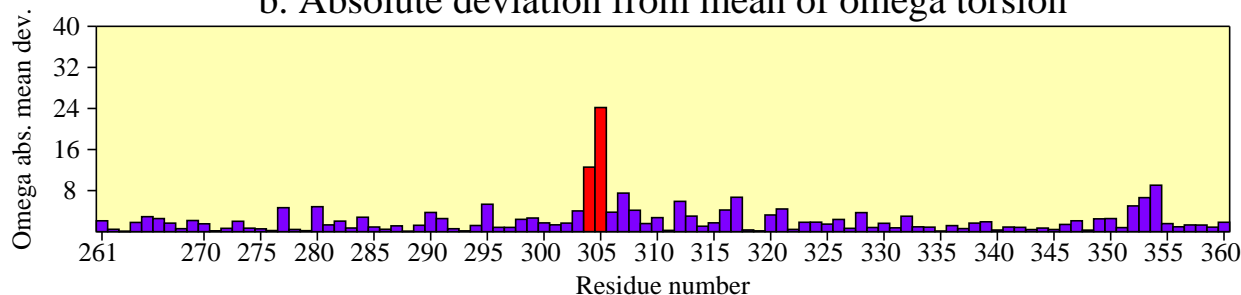


Residue properties 1LON

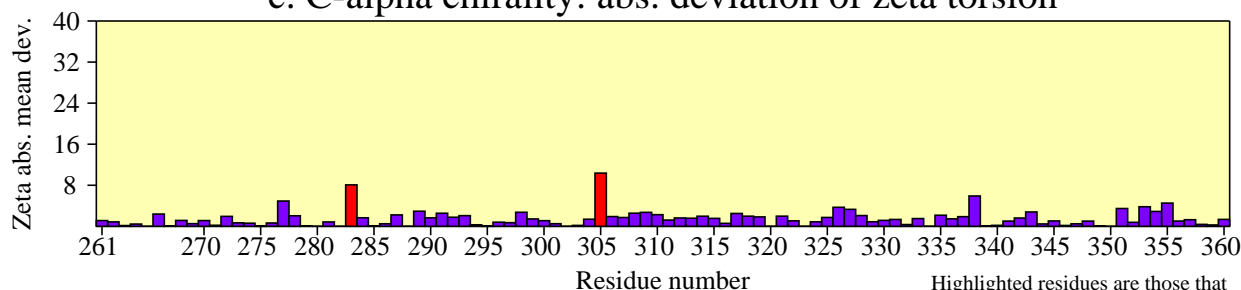
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

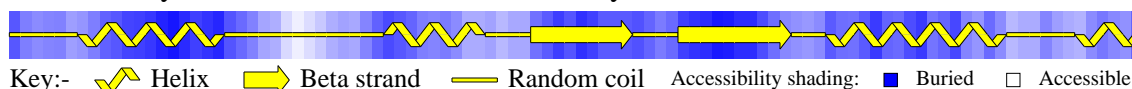


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



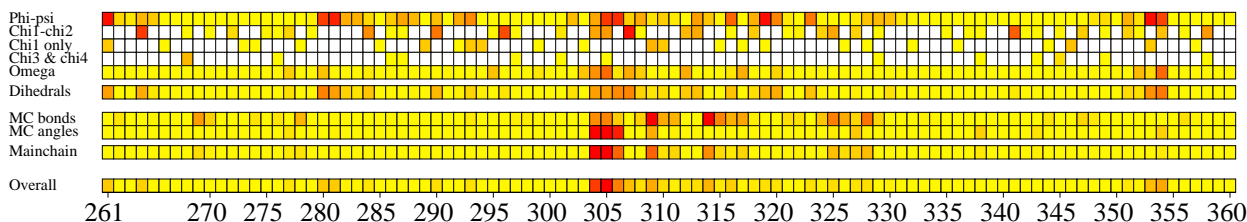
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

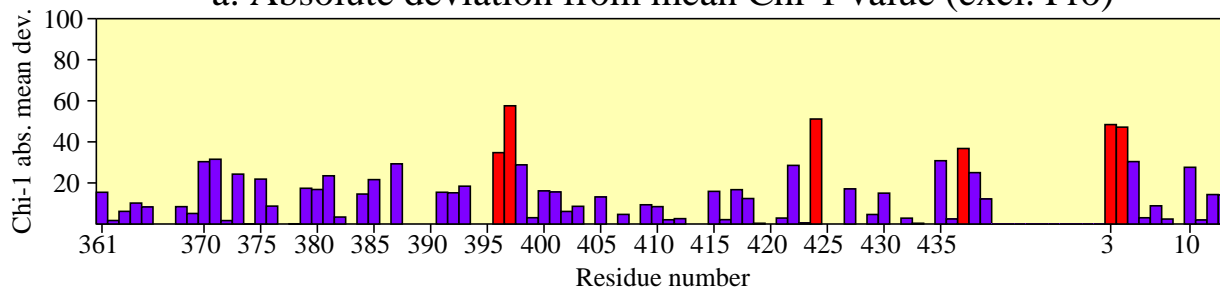


g. G-factors

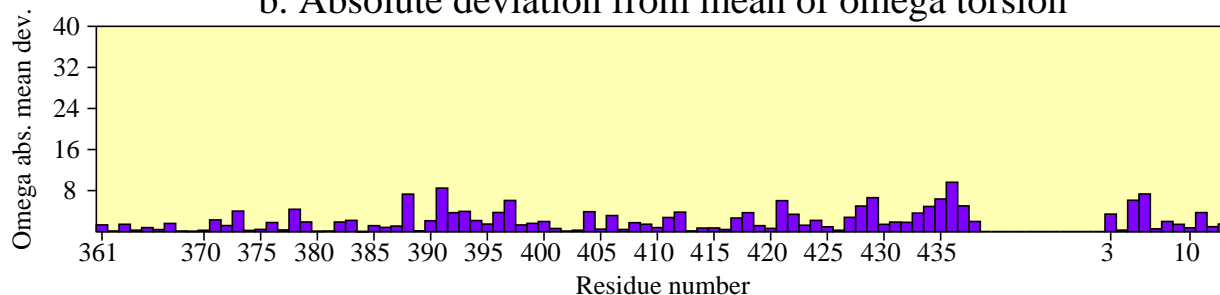


Residue properties 1LON

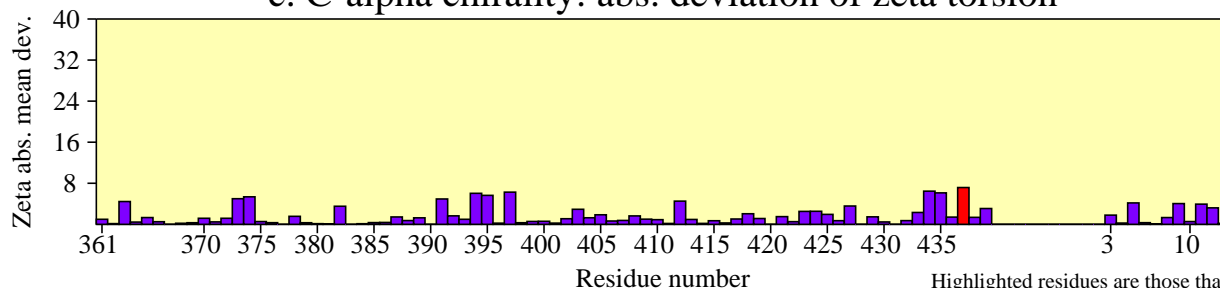
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

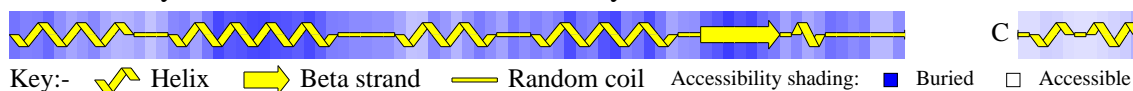


c. C-alpha chirality: abs. deviation of zeta torsion



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

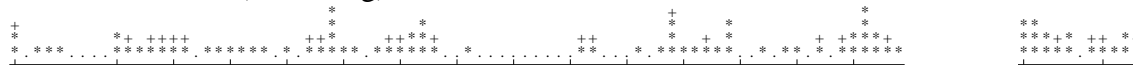
d. Secondary structure & estimated accessibility



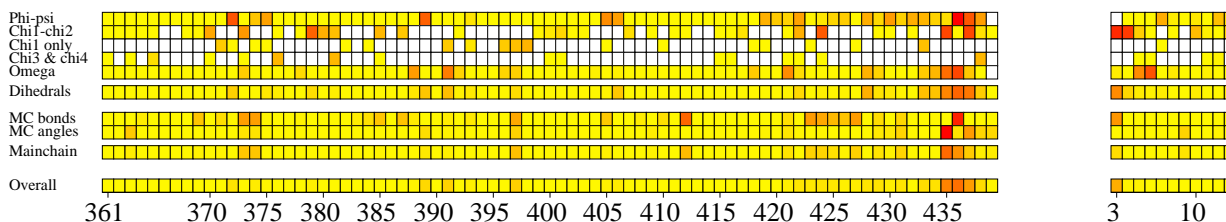
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

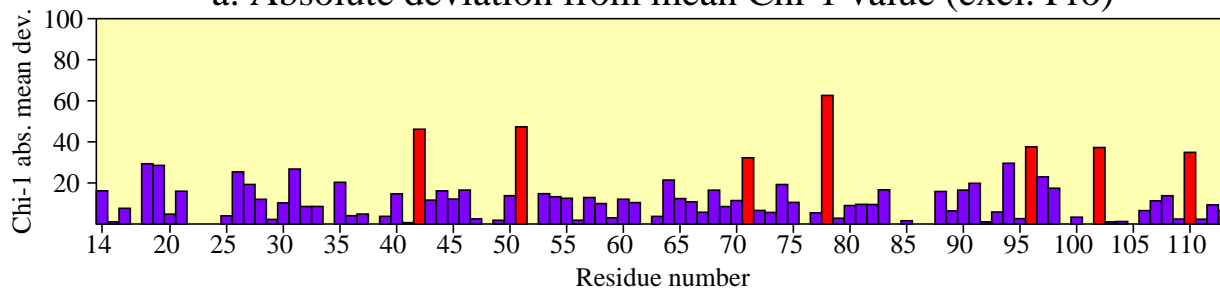


g. G-factors

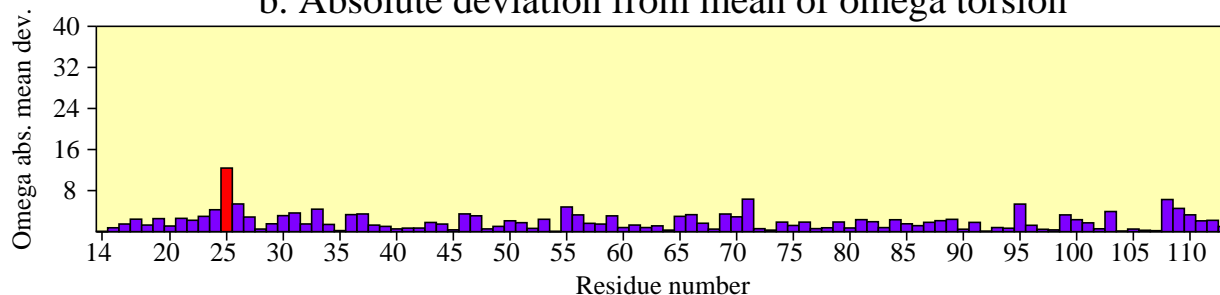


Residue properties 1LON

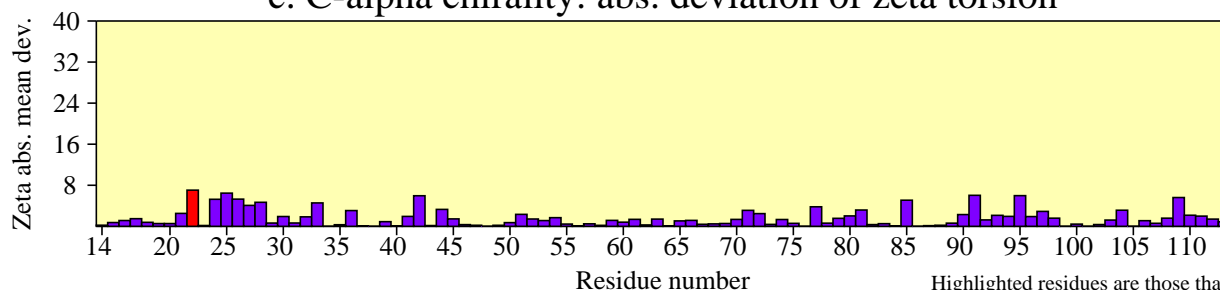
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

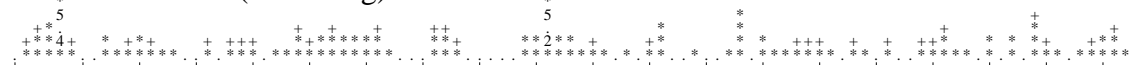
d. Secondary structure & estimated accessibility



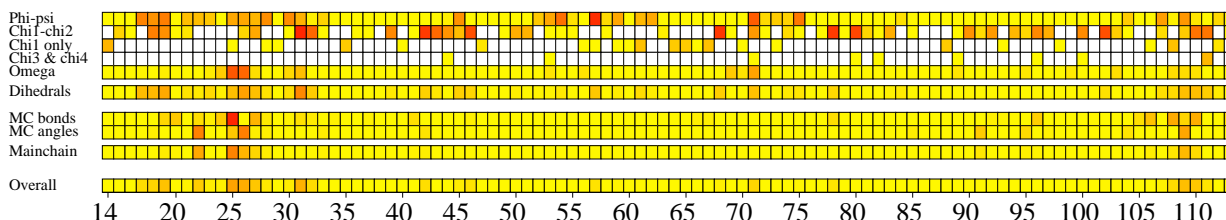
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

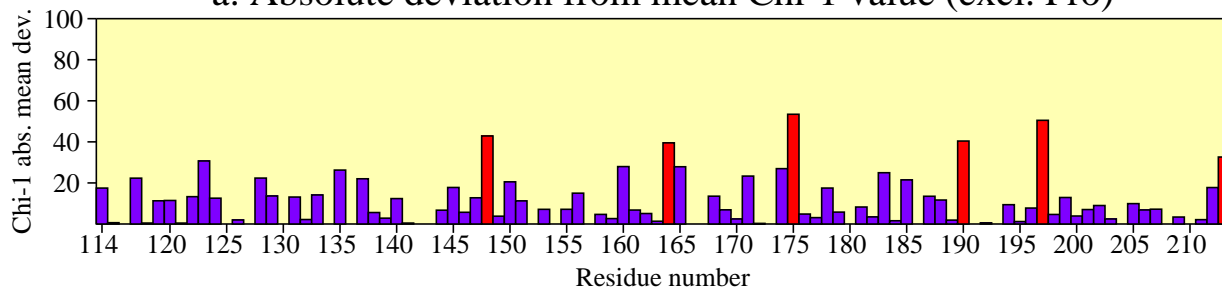


g. G-factors

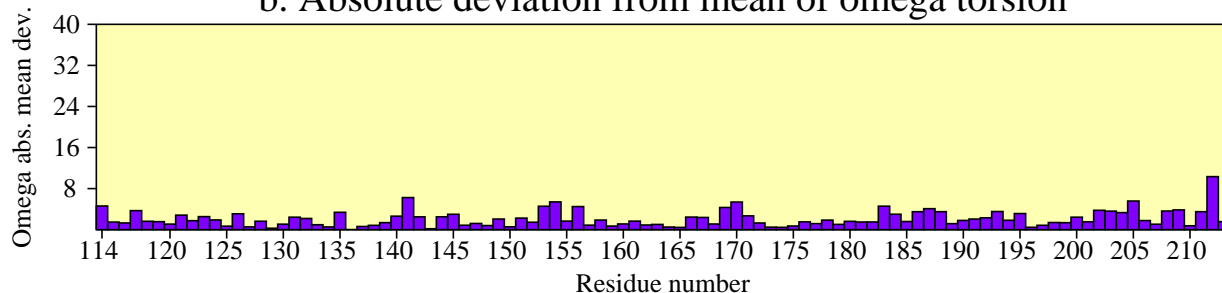


Residue properties 1LON

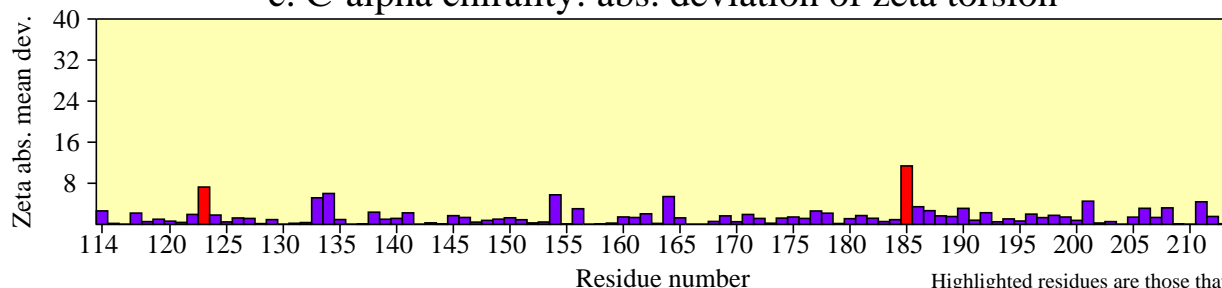
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

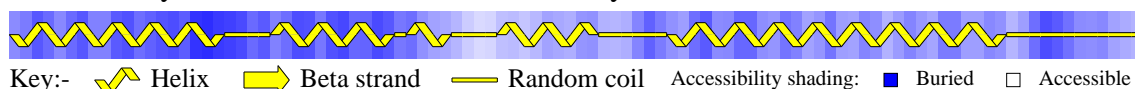


c. C-alpha chirality: abs. deviation of zeta torsion



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

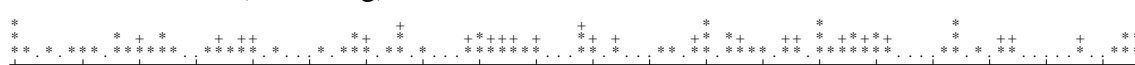
d. Secondary structure & estimated accessibility



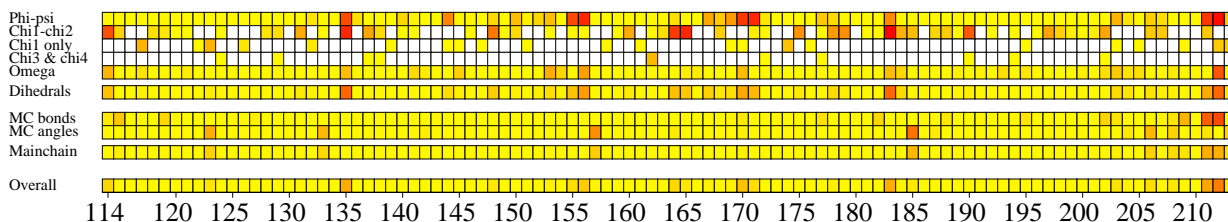
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

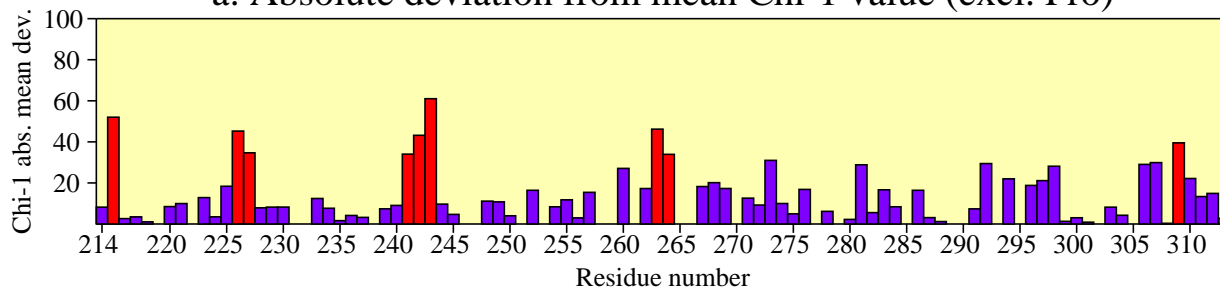


g. G-factors

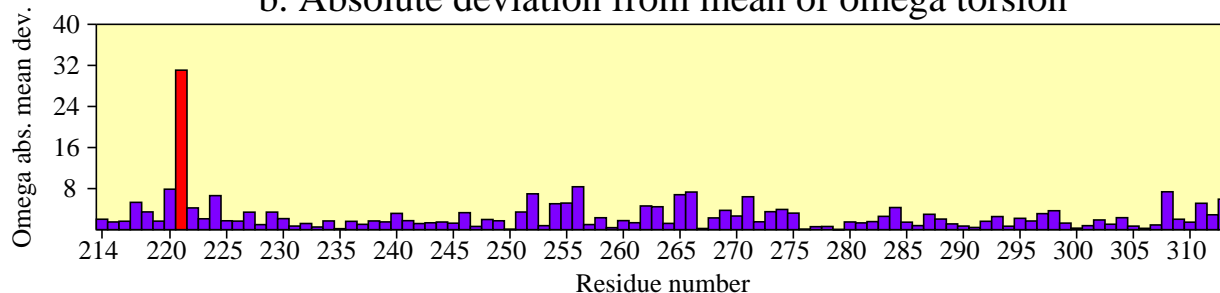


Residue properties 1LON

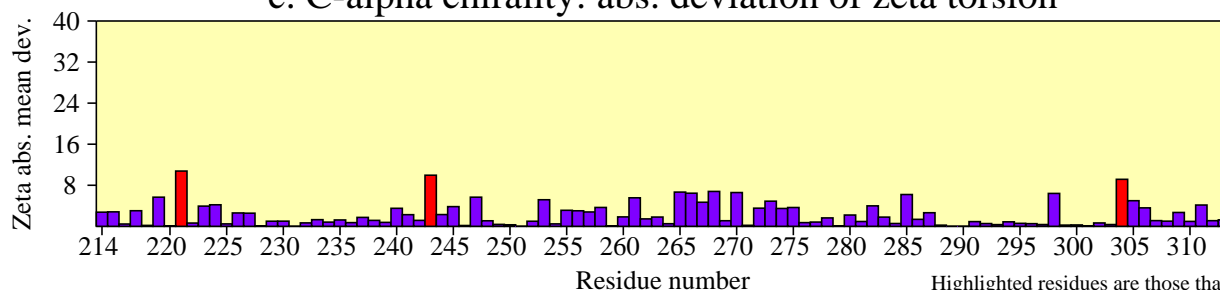
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

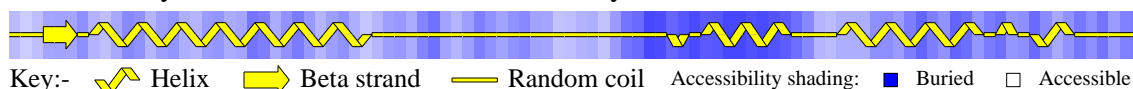


c. C-alpha chirality: abs. deviation of zeta torsion

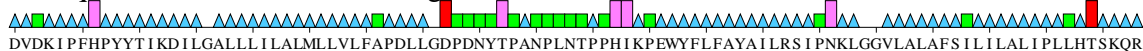


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



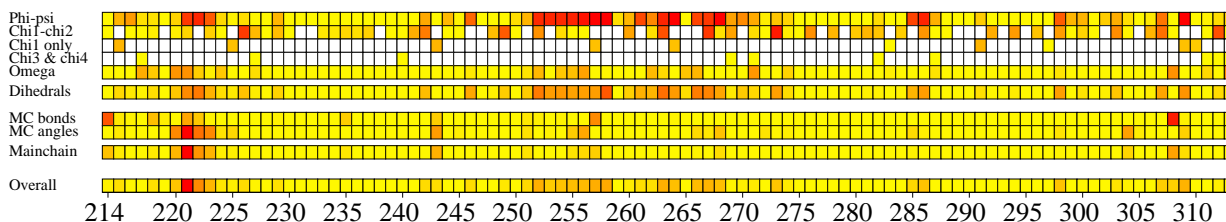
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

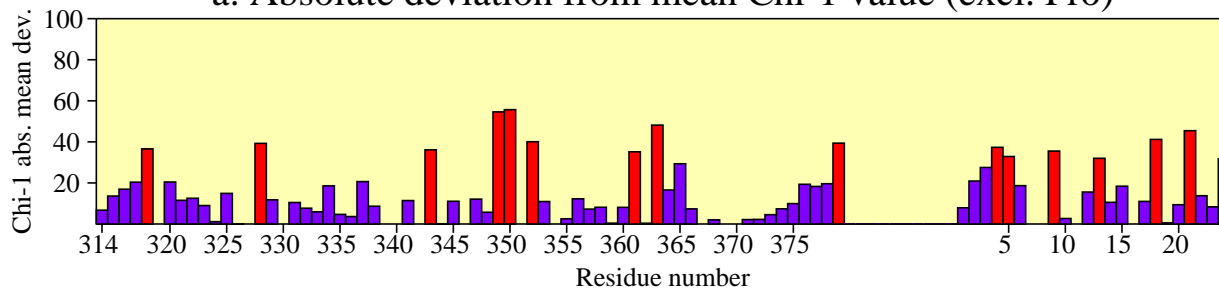


g. G-factors

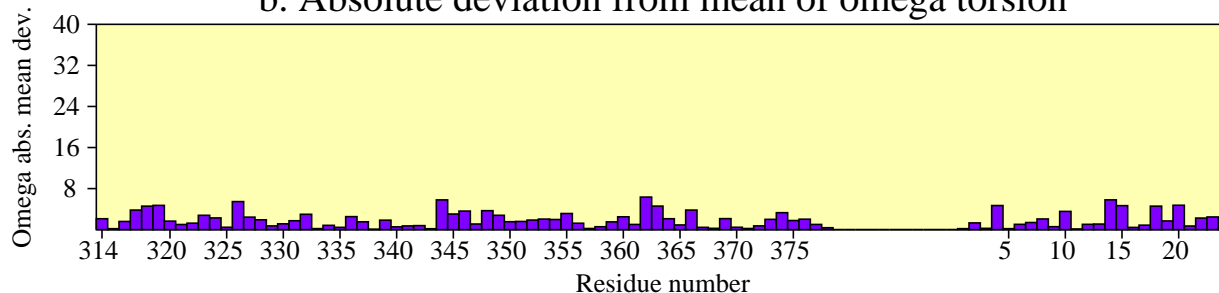


Residue properties 1LON

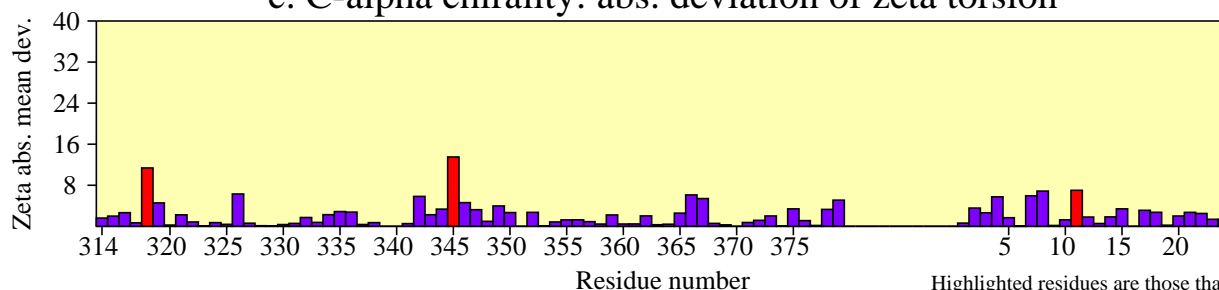
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

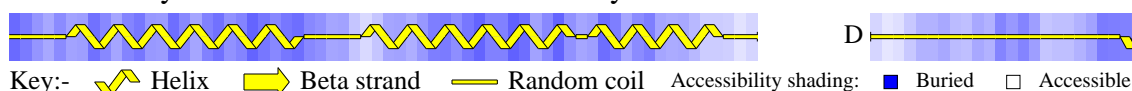


c. C-alpha chirality: abs. deviation of zeta torsion



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

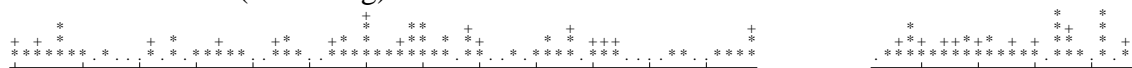
d. Secondary structure & estimated accessibility



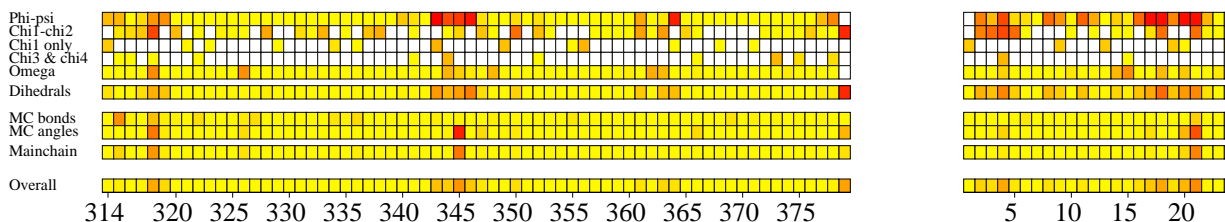
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

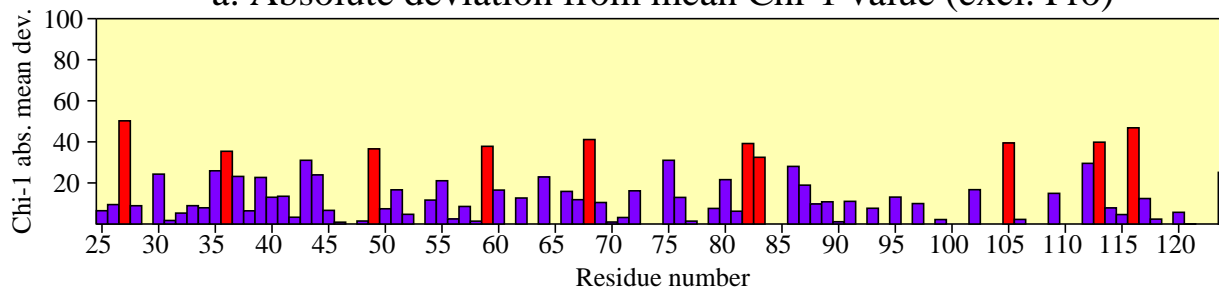


g. G-factors

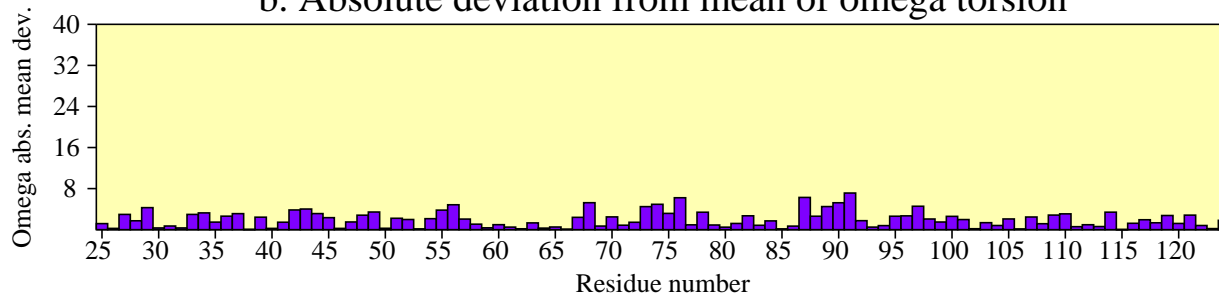


Residue properties 1LON

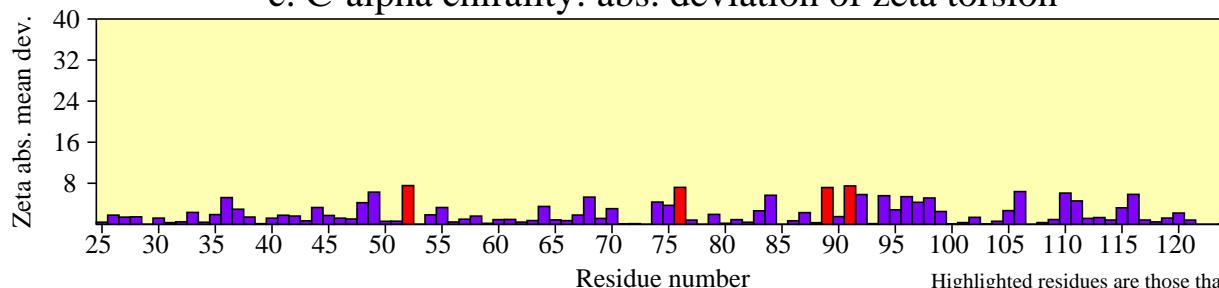
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

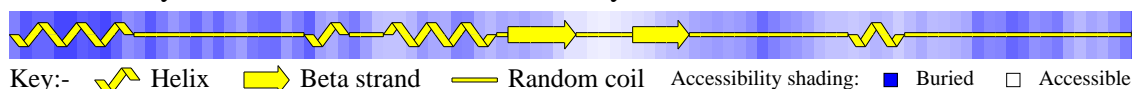


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



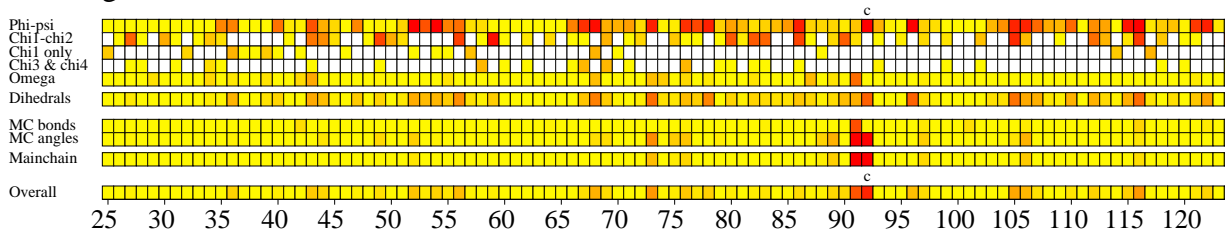
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



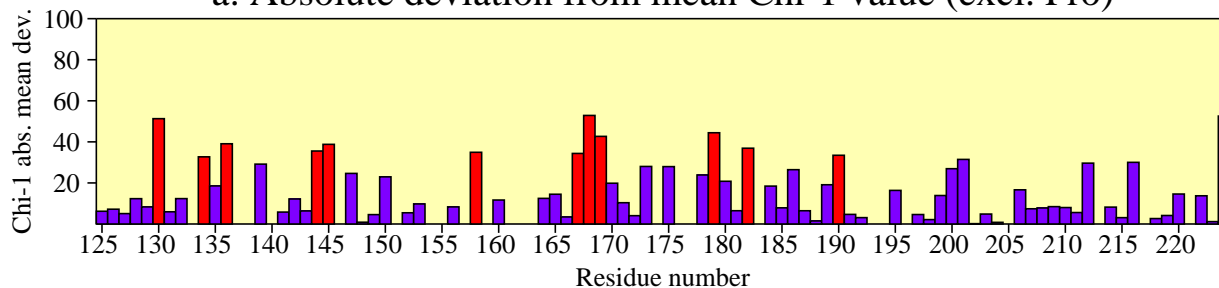
g. G-factors



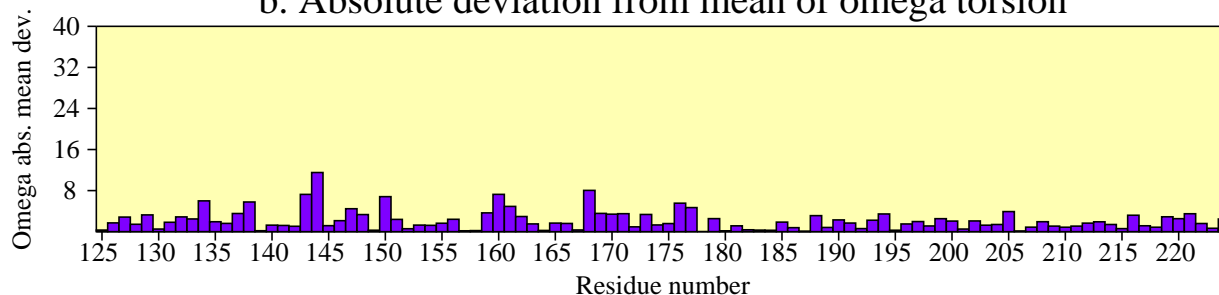
c = cis-peptide

Residue properties 1LON

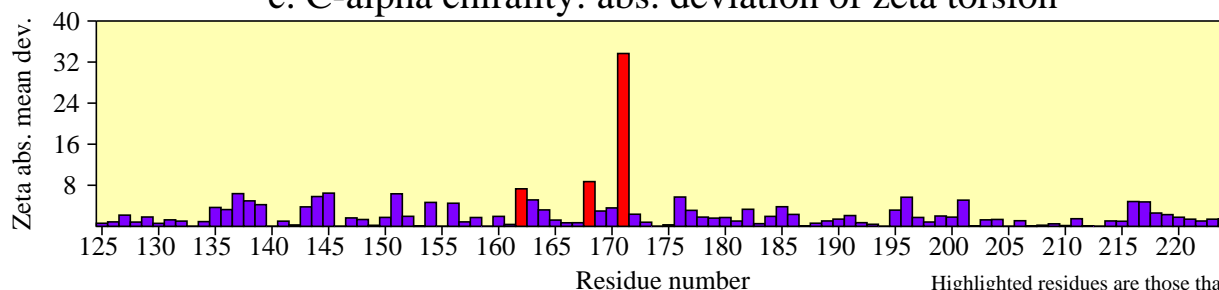
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

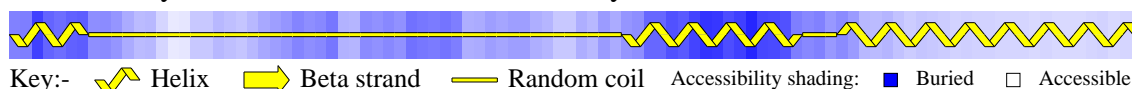


c. C-alpha chirality: abs. deviation of zeta torsion



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

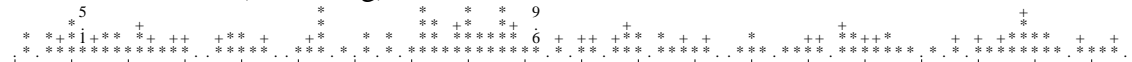
d. Secondary structure & estimated accessibility



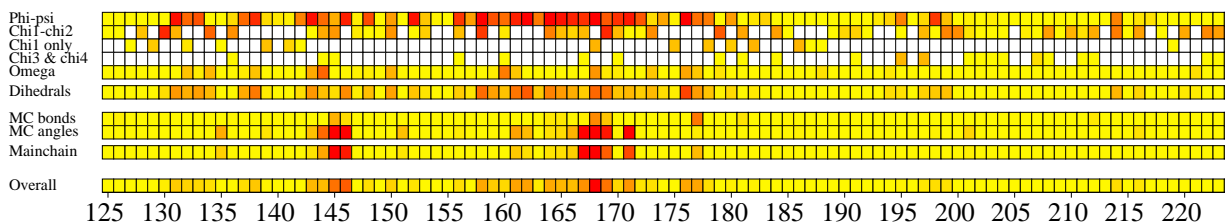
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

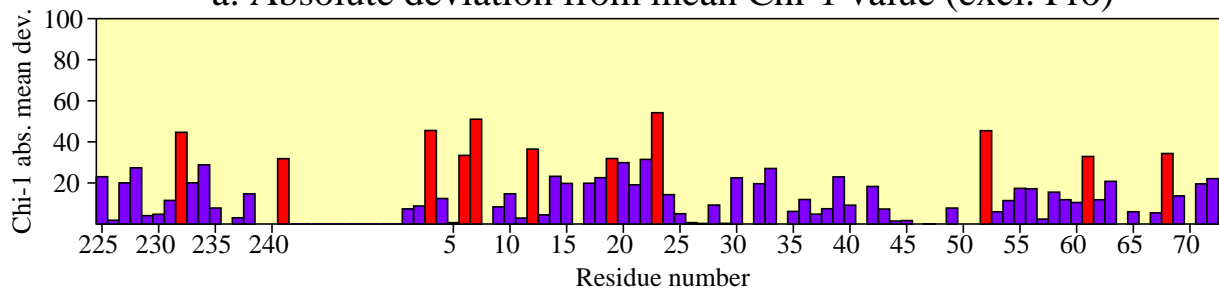


g. G-factors

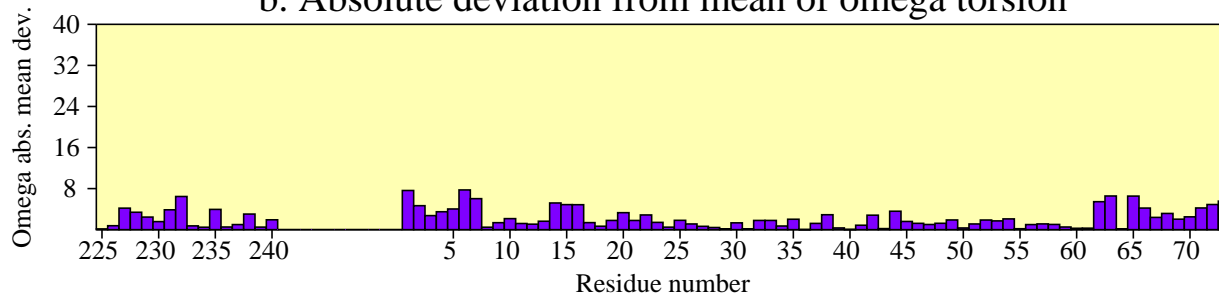


Residue properties 1LON

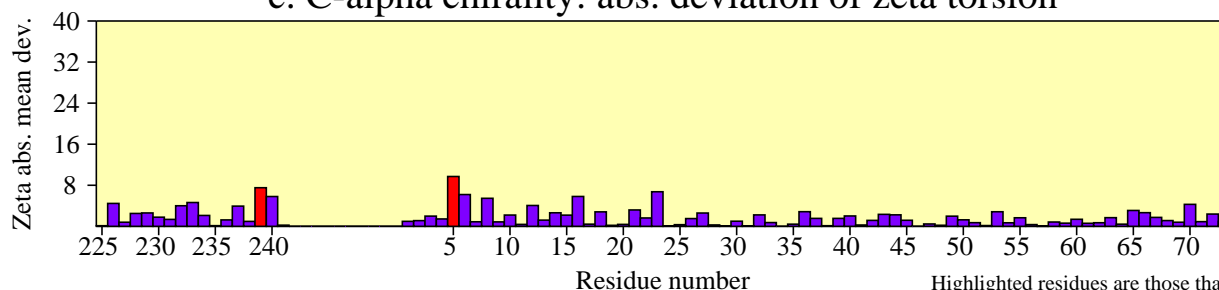
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

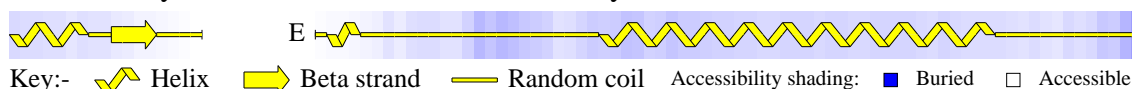


c. C-alpha chirality: abs. deviation of zeta torsion



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

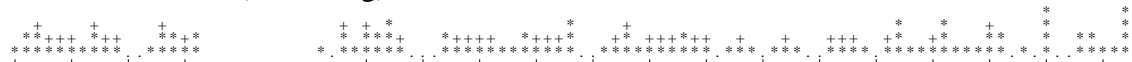
d. Secondary structure & estimated accessibility



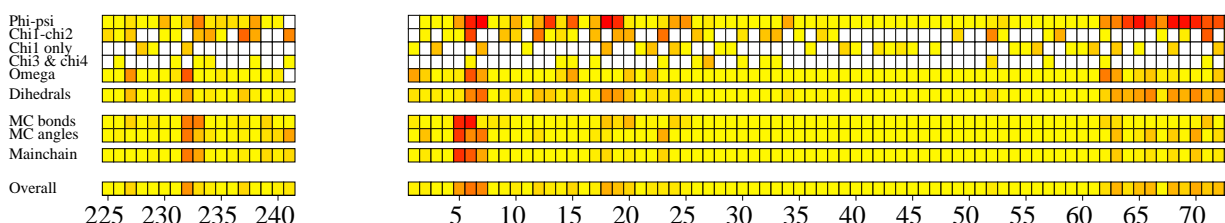
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

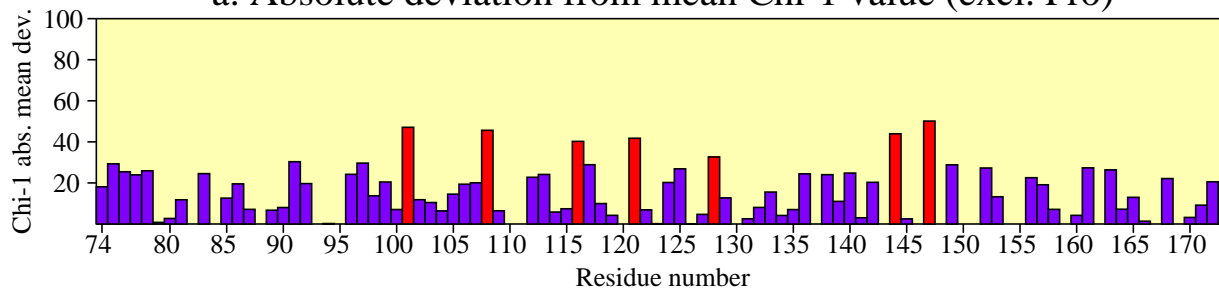


g. G-factors

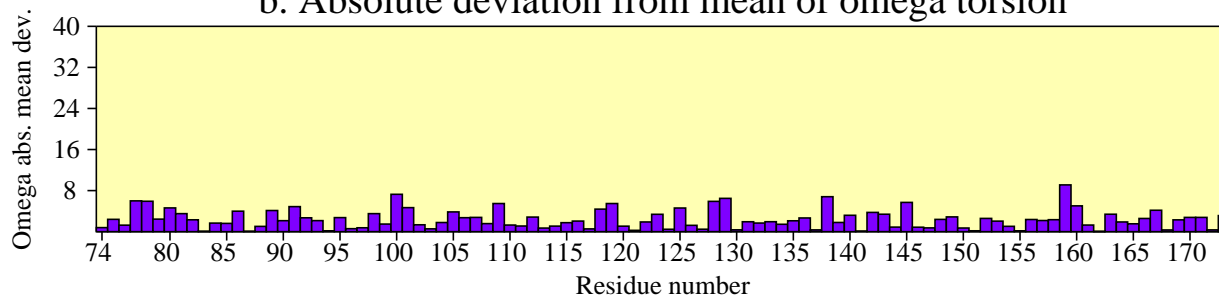


Residue properties 1LON

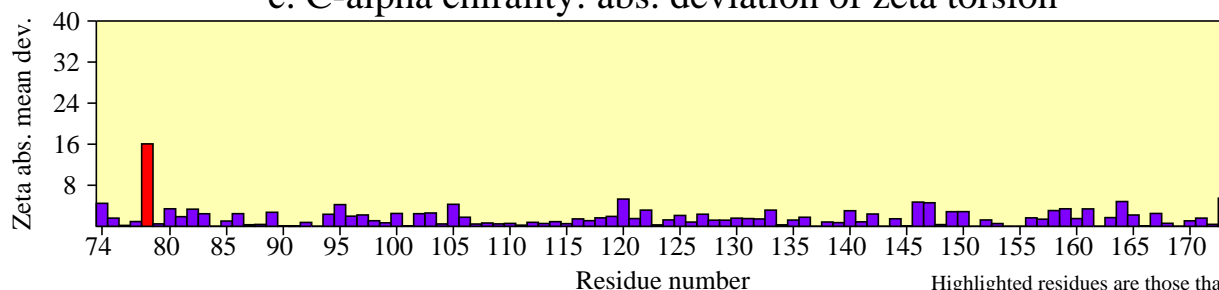
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

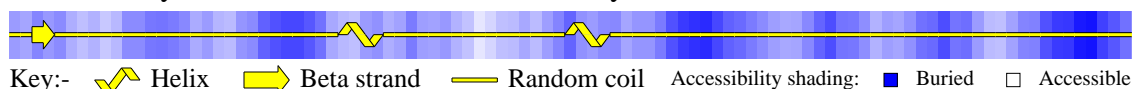


c. C-alpha chirality: abs. deviation of zeta torsion

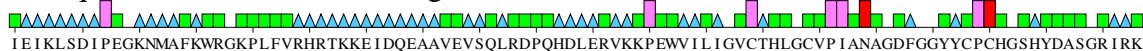


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



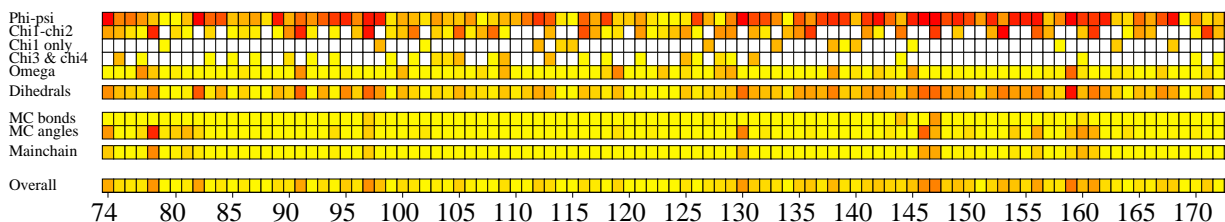
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

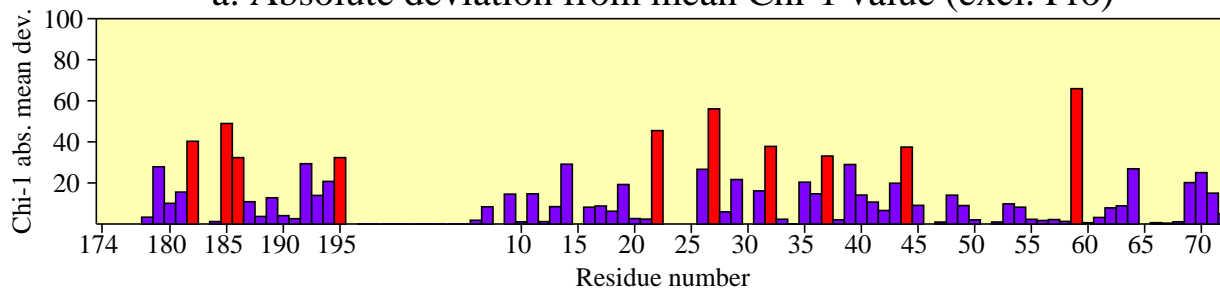


g. G-factors

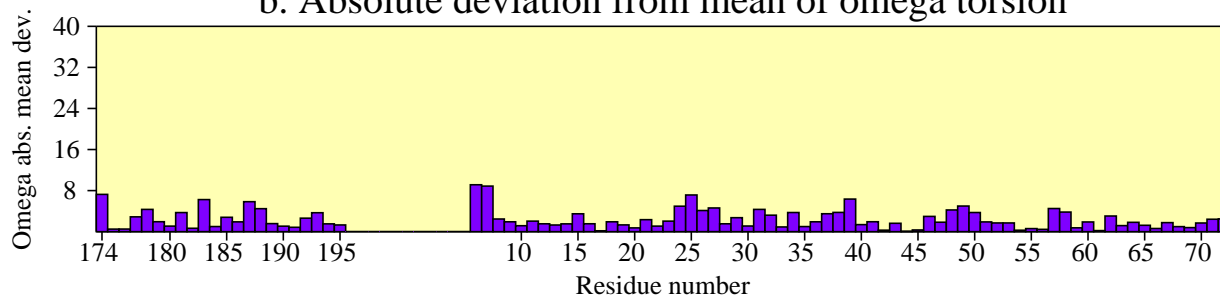


Residue properties 1LON

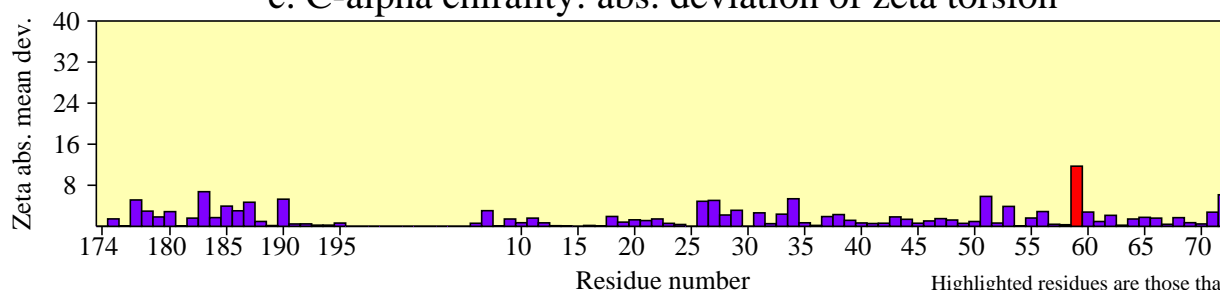
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

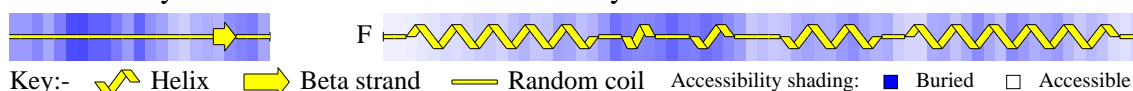


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



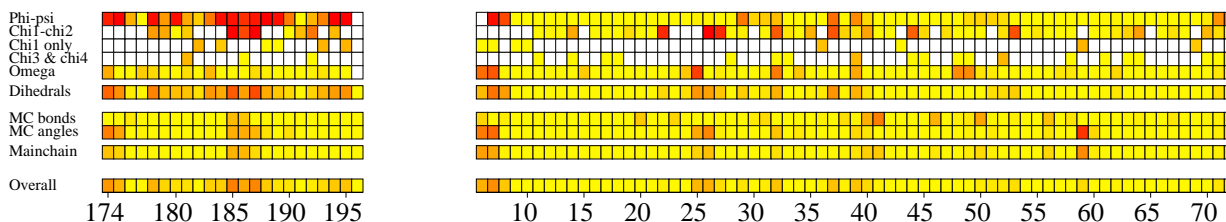
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

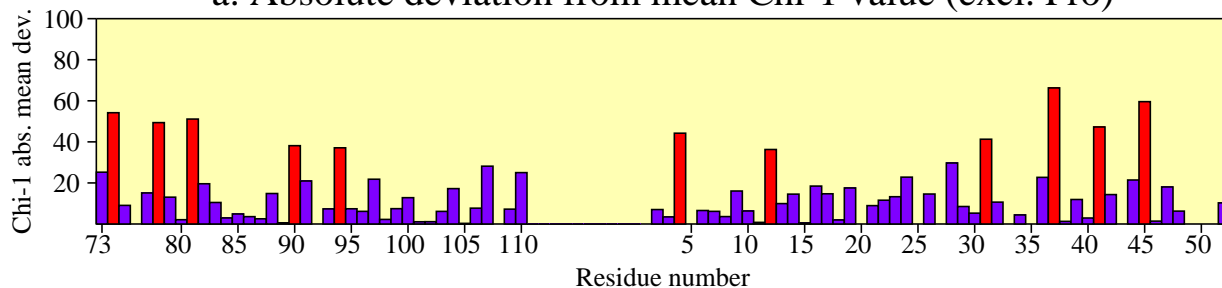


g. G-factors

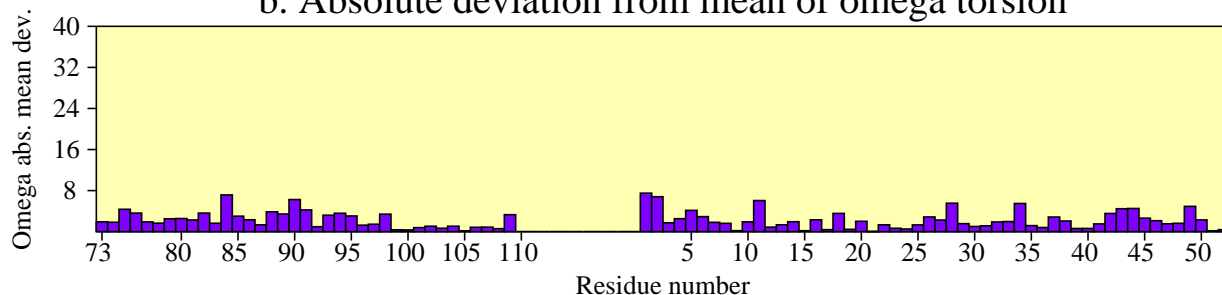


Residue properties 1LON

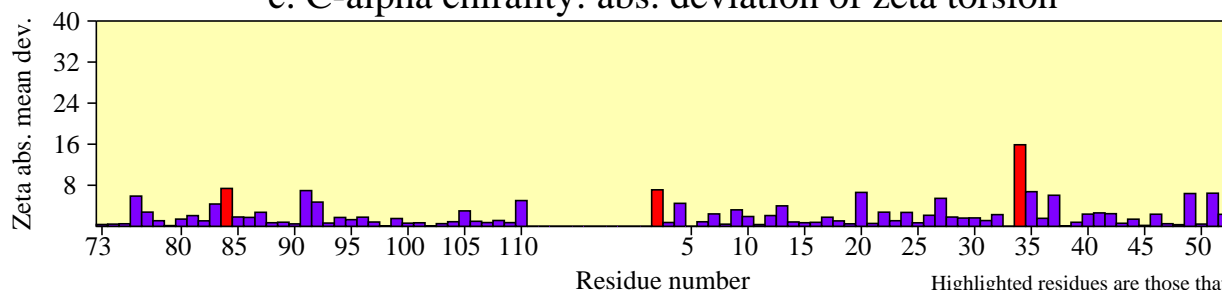
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

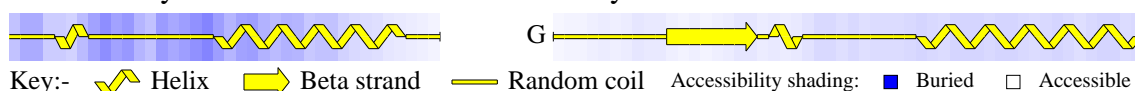


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



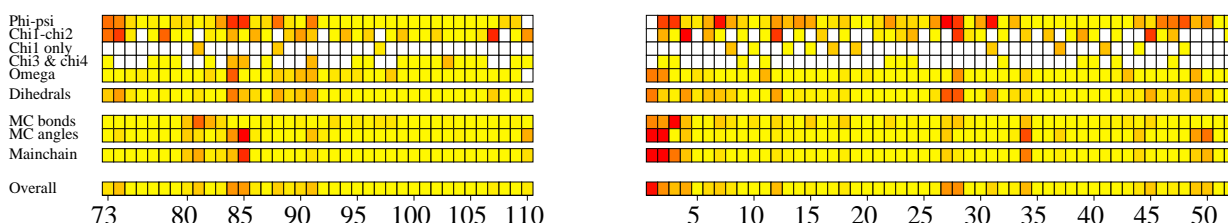
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

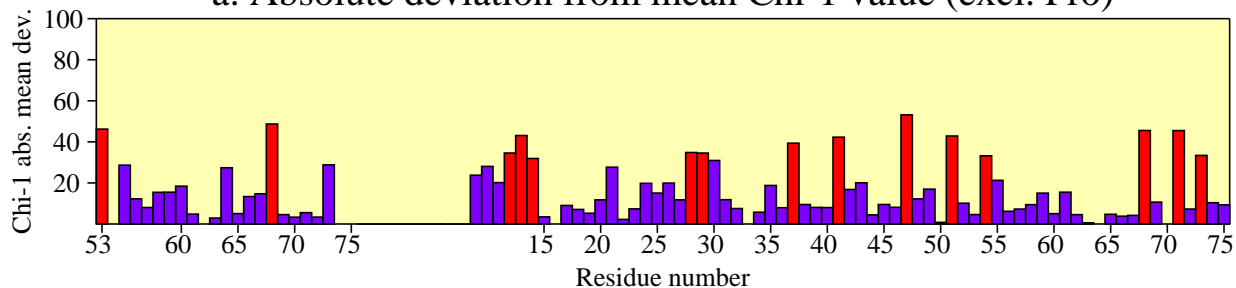


g. G-factors

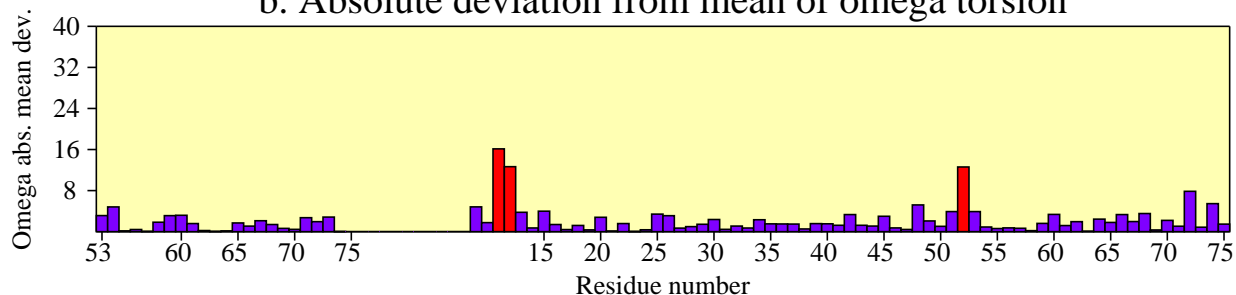


Residue properties 1LON

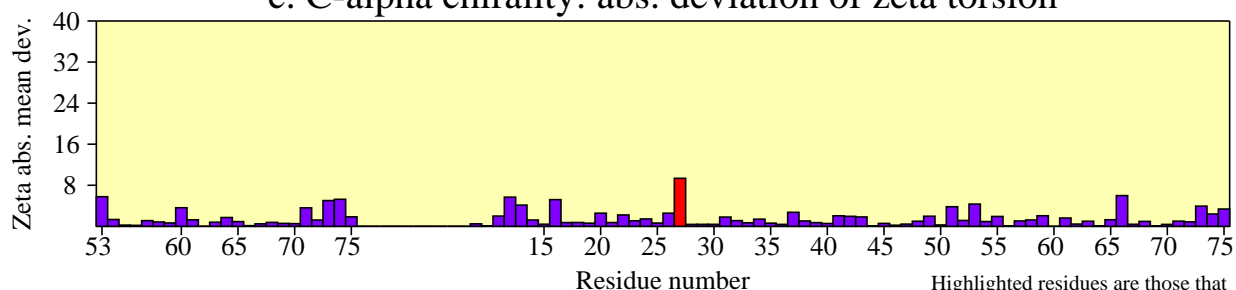
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

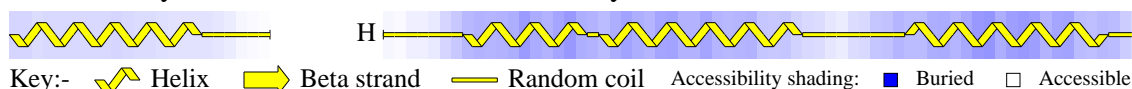


c. C-alpha chirality: abs. deviation of zeta torsion



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

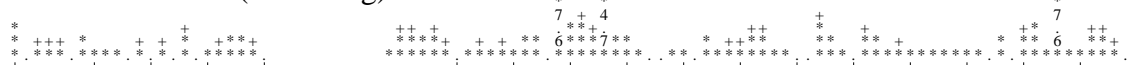
d. Secondary structure & estimated accessibility



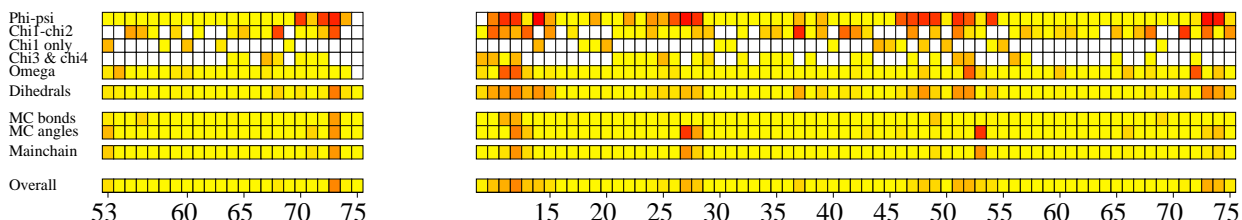
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

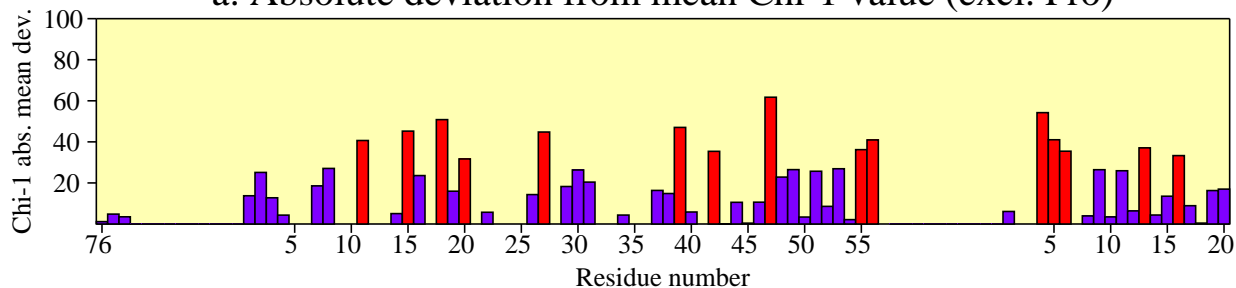


g. G-factors

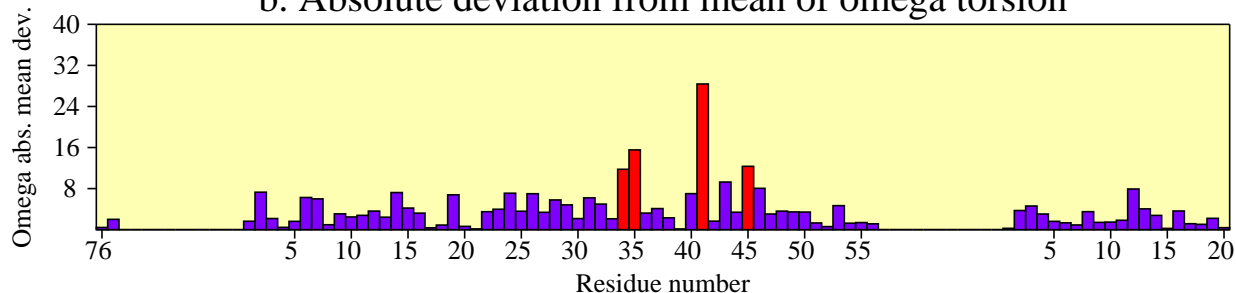


Residue properties 1LON

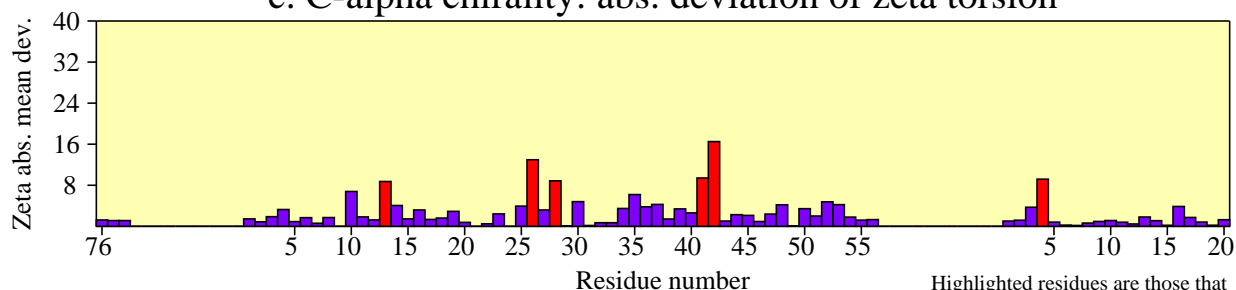
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

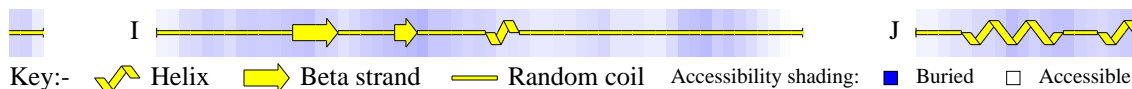


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



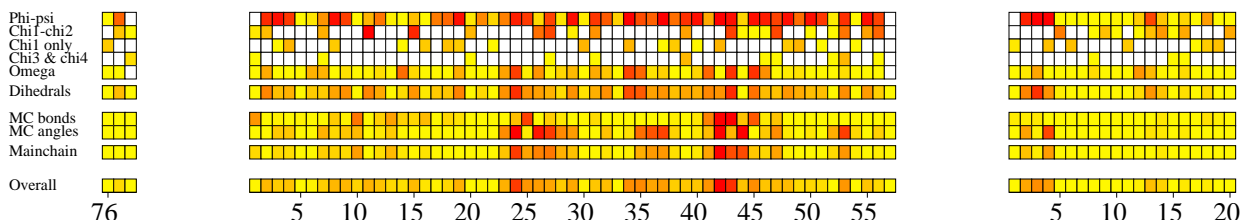
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

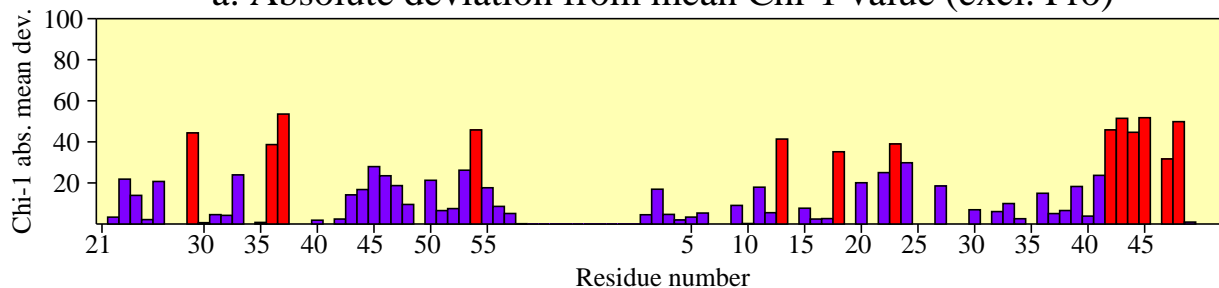


g. G-factors

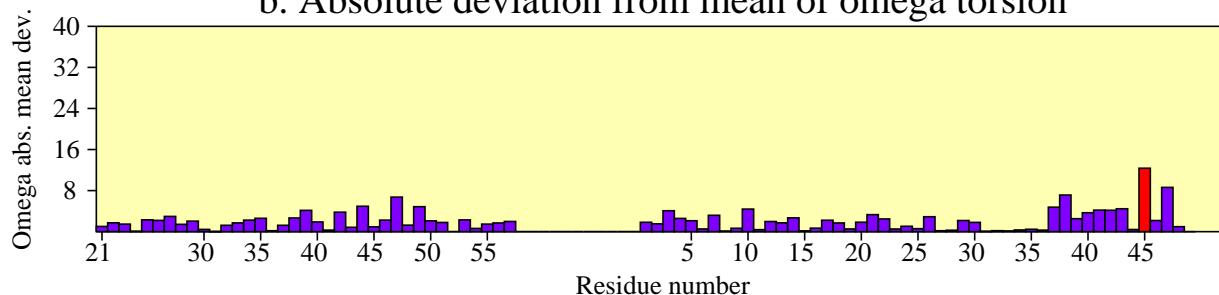


Residue properties 1LON

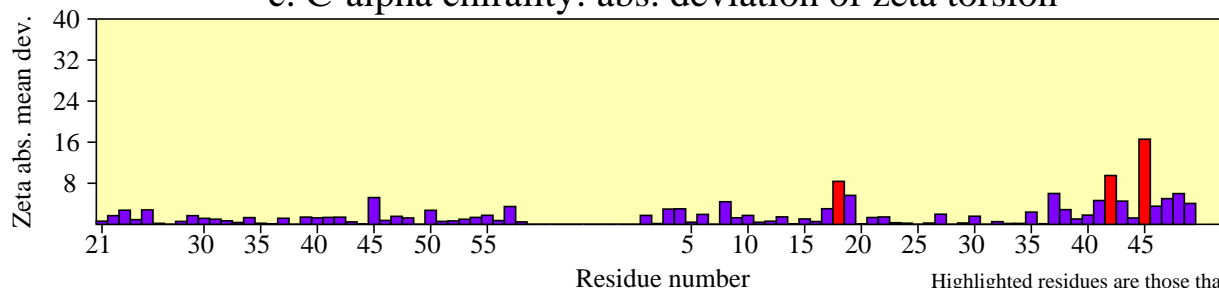
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

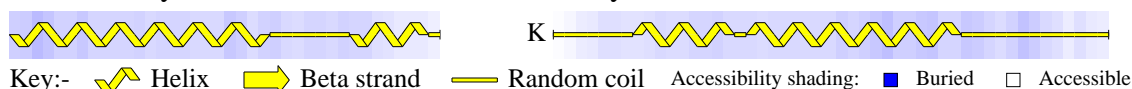


c. C-alpha chirality: abs. deviation of zeta torsion

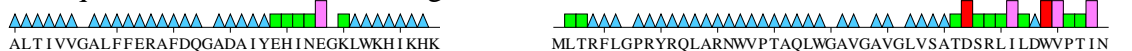


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

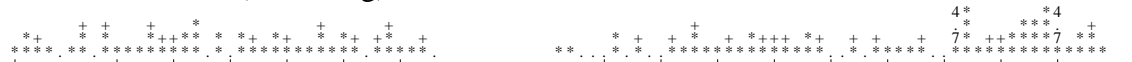
d. Secondary structure & estimated accessibility



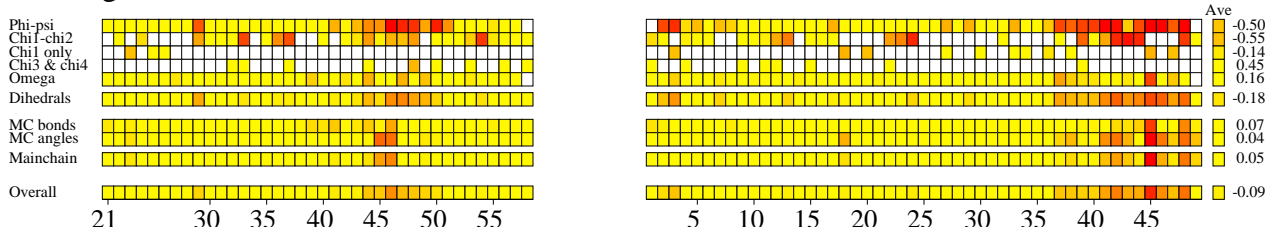
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

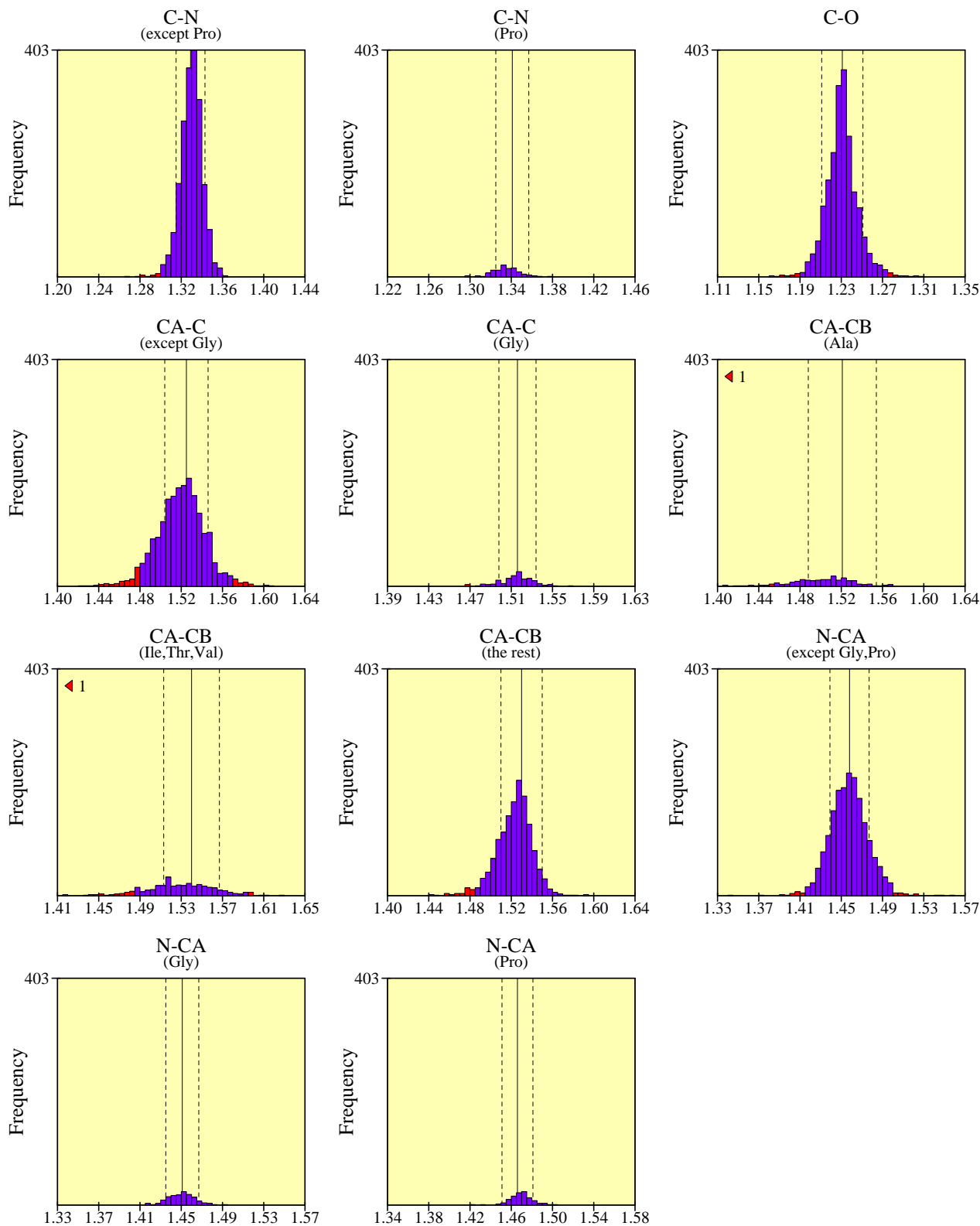


g. G-factors



Main-chain bond lengths

1L0N



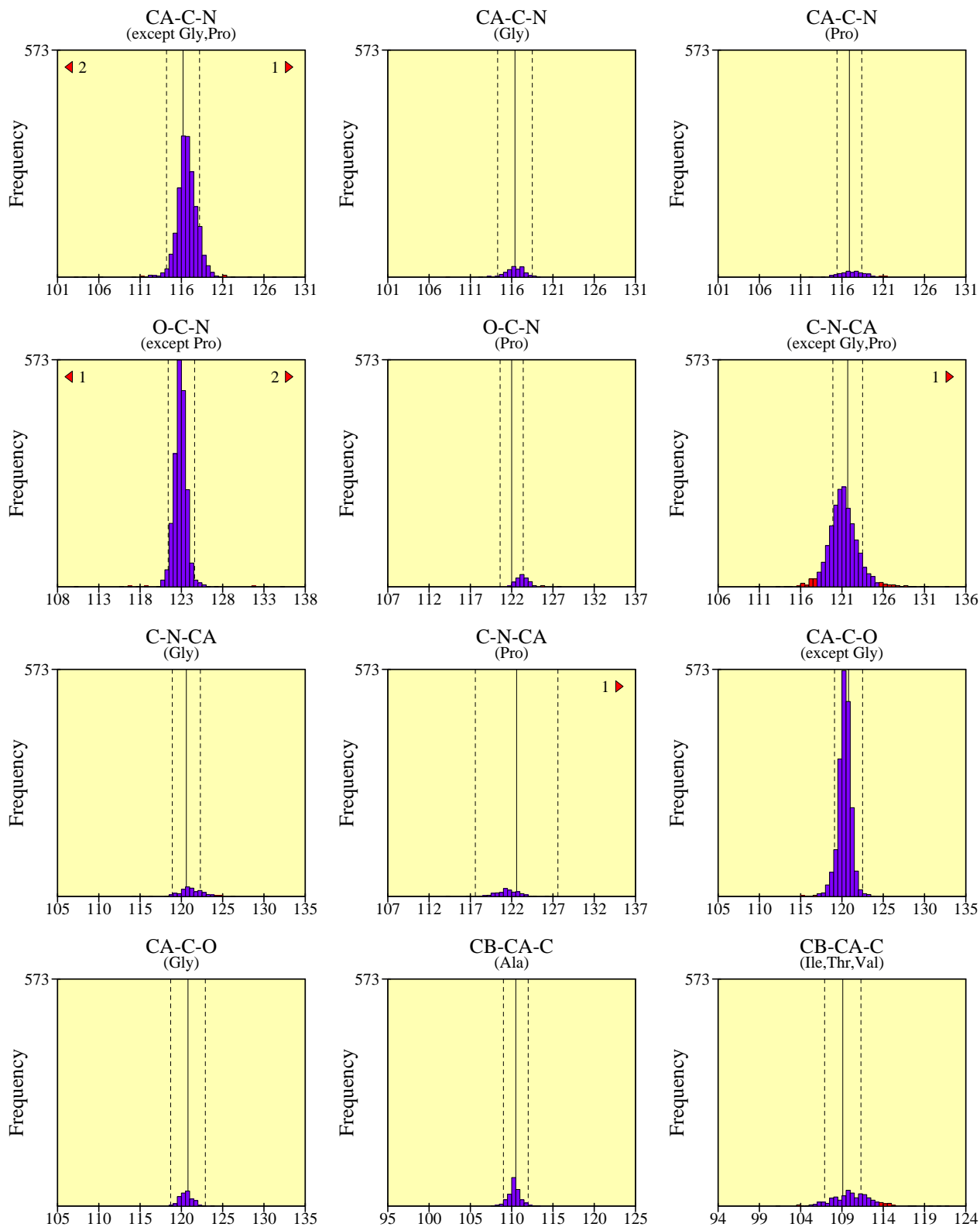
Black bars > 2.0 st. devs. from mean.

◀ 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

1L0N



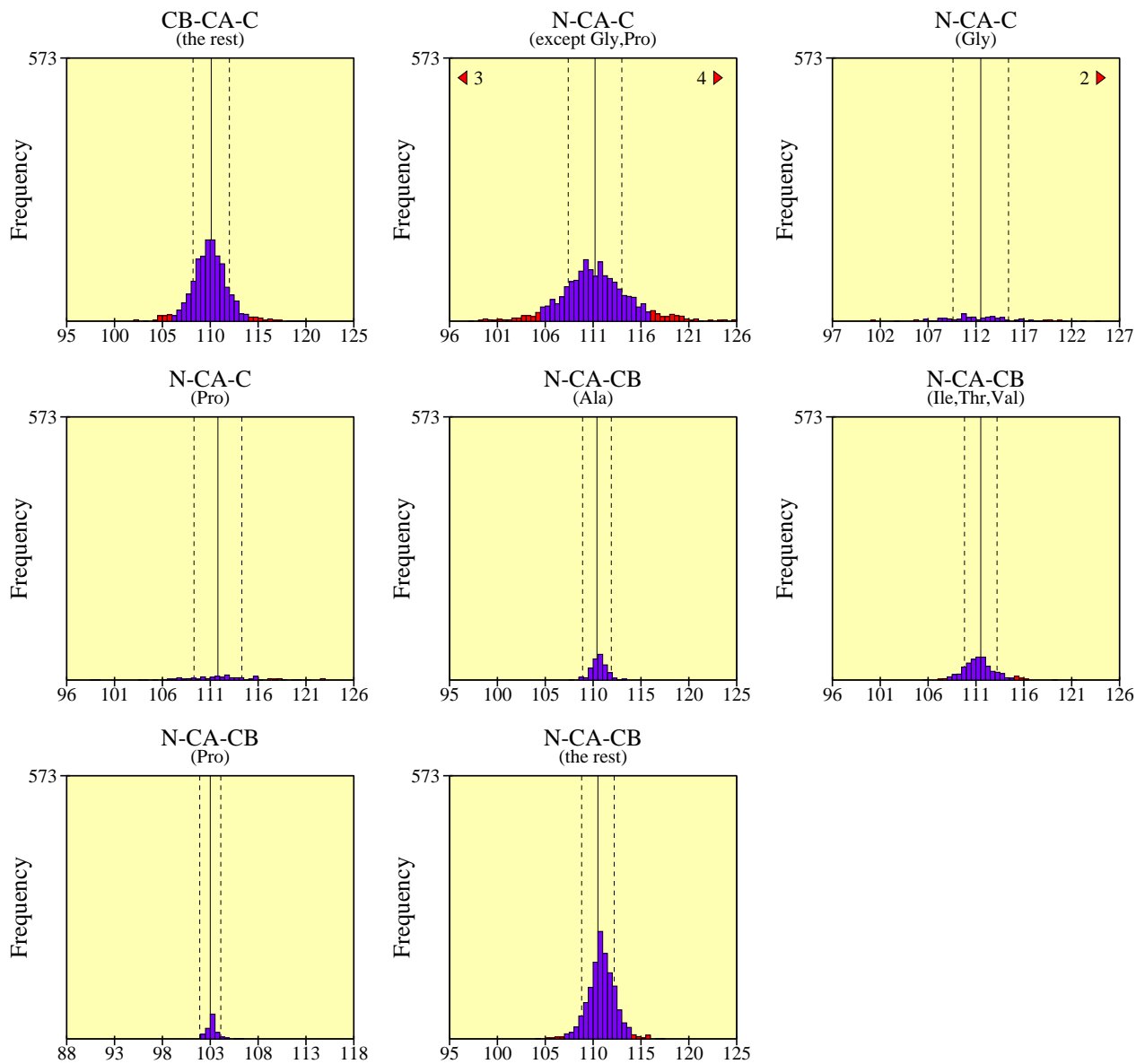
Black bars > 2.0 st. devs. from mean.

◀ 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

1LON



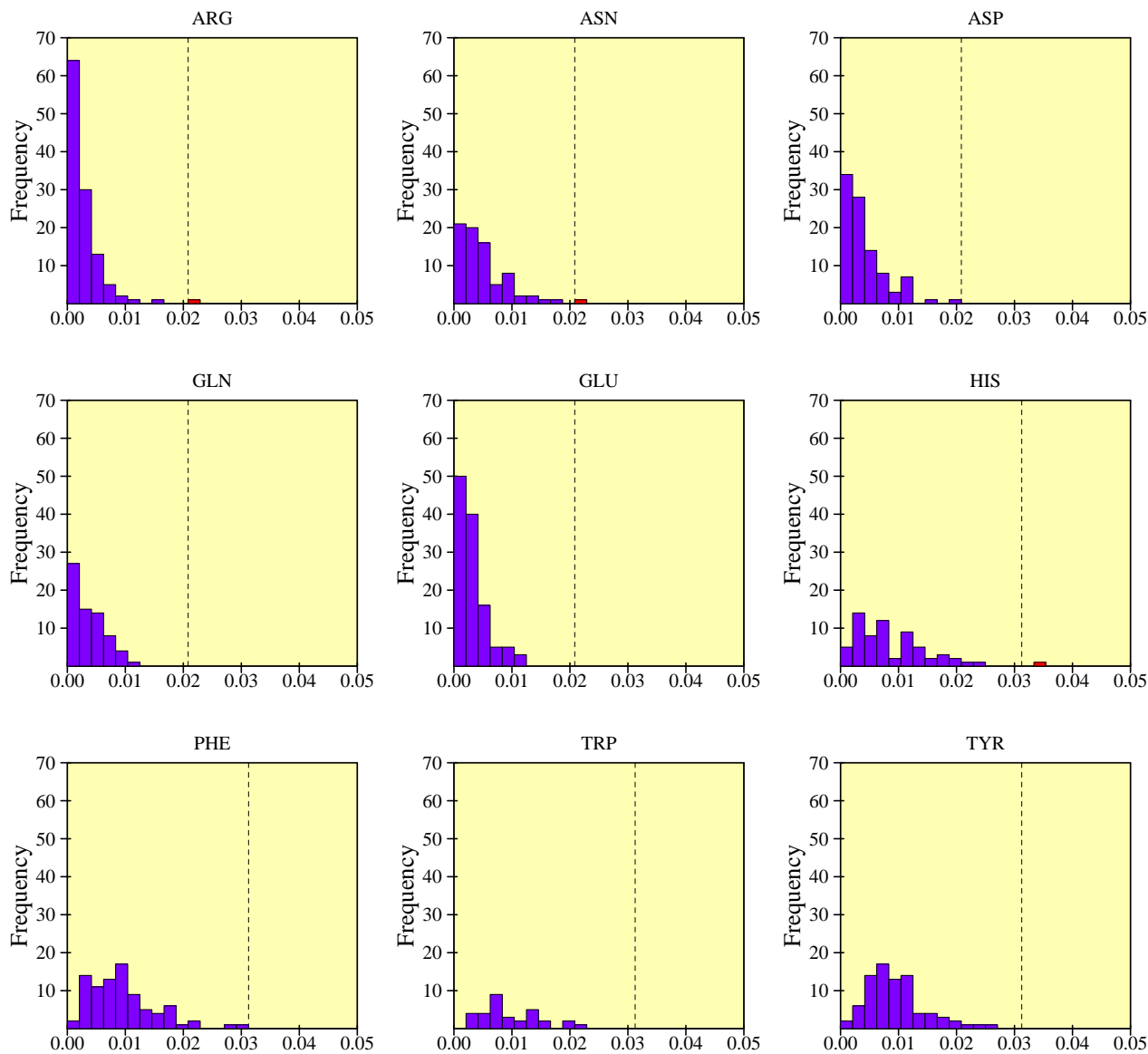
Black bars > 2.0 st. devs. from mean.

◀ 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

1LON



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

1LON

Main-chain bond lengths

CA 1.530 CB 0.050 1.480 A Ser 30	CA 1.540 CB 0.054 1.486 A Val 39	CA 1.521 CB 0.088 1.433 A Ala 84	CA 1.540 CB 0.090 1.450 A Thr 91	N 1.458 CA 0.054 1.404 A Thr 91	CA 1.525 C 0.062 1.587 A Leu 106
CA 1.540 CB 0.057 1.597 A Ile 127	CA 1.540 CB 0.072 1.468 A Thr 143	CA 1.540 CB 0.050 1.490 A Val 149	CA 1.521 CB 0.055 1.466 A Ala 155	CA 1.540 CB 0.067 1.473 A Thr 161	CA 1.521 CB 0.073 1.448 A Ala 164
N 1.458 CA 0.062 1.520 A Glu 172	CA 1.525 C 0.052 1.473 A Arg 175	CA 1.540 CB 0.102 1.438 A Thr 237	CA 1.516 C 0.051 1.465 A Gly 238	CA 1.530 CB 0.061 1.469 A Ser 239	N 1.458 CA 0.053 1.405 A Ser 239
CA 1.530 CB 0.073 1.457 A Asp 246	N 1.458 CA 0.083 1.541 A Leu 250	CA 1.525 C 0.082 1.443 A Ala 251	C 1.231 O 0.072 1.303 A His 252	C 1.231 O 0.054 1.285 A Ala 254	CA 1.521 CB 0.090 1.431 A Ala 254
CA 1.525 C 0.077 1.448 A Glu 258	CA 1.540 CB 0.052 1.488 A Val 268	C 1.231 O 0.062 1.293 A Tyr 280	CA 1.530 CB 0.060 1.470 A Cys 282	CA 1.525 C 0.060 1.465 A Tyr 284	CA 1.521 CB 0.063 1.458 A Ala 288
CA 1.521 CB 0.066 1.455 A Ala 298	CA 1.525 C 0.065 1.460 A Lys 302	CA 1.540 CB 0.121 1.419 A Thr 309	CA 1.525 C 0.061 1.464 A Leu 320	CA 1.525 C 0.097 1.428 A Phe 324	CA 1.530 CB 0.054 1.476 A Ser 330
CA 1.530 CB 0.052 1.478 A Met 335	CA 1.540 CB 0.055 1.485 A Val 337	CA 1.540 CB 0.071 1.469 A Thr 347	CA 1.521 CB 0.056 1.465 A Ala 364	CA 1.530 CB 0.057 1.473 A Glu 377	CA 1.530 CB 0.050 1.480 A Asp 378
CA 1.540 CB 0.094 1.446 A Thr 385	CA 1.540 CB 0.055 1.485 A Ile 390	CA 1.540 CB 0.059 1.481 A Ile 399	CA 1.540 CB 0.058 1.482 A Val 406	CA 1.525 C 0.057 1.468 A Arg 408	CA 1.521 CB 0.064 1.457 A Ala 423
CA 1.525 C 0.055 1.470 A Arg 436	CA 1.540 CB 0.061 1.479 A Ile 437	CA 1.525 C 0.051 1.474 A Arg 445	CA 1.525 C 0.074 1.451 A Phe 446	CA 1.525 C 0.056 1.469 B Asp 23	CA 1.540 CB 0.123 1.417 B Thr 27
CA 1.540 CB 0.055 1.485 B Ile 35	CA 1.530 CB 0.073 1.457 B Ser 37	N 1.458 CA 0.051 1.407 B Ser 45	CA 1.540 CB 0.065 1.475 B Ile 47	CA 1.530 CB 0.059 1.471 B Leu 49	CA 1.525 C 0.053 1.472 B Ile 51
CA 1.540 CB 0.068 1.472 B Ile 51	CA 1.530 CB 0.050 1.480 B Ser 55	CA 1.530 CB 0.054 1.476 B Asn 59	CA 1.530 CB 0.054 1.476 B Ser 60	CA 1.525 C 0.065 1.460 B Asn 61	N 1.458 CA 0.051 1.407 B Asn 61

Distorted geometry

1LON

Main-chain bond lengths (contd)

CA 1.540 CB 0.056 1.484 B Thr 65	CA 1.525 C 0.071 1.454 B Ser 66	CA 1.525 C 0.056 1.581 B Leu 68	C 1.329 N 0.054 1.275 B Lys 78 - B Gly 79	CA 1.540 CB 0.132 1.408 B Thr 86	CA 1.525 C 0.076 1.449 B Leu 96
CA 1.525 C 0.070 1.455 B Ser 97	CA 1.525 C 0.066 1.459 B Thr 99	CA 1.540 CB 0.088 1.452 B Thr 101	CA 1.525 C 0.053 1.472 B Met 105	C 1.231 O 0.069 1.300 B Thr 108	CA 1.540 CB 0.053 1.593 B Ile 118
CA 1.540 CB 0.057 1.483 B Val 126	CA 1.525 C 0.083 1.442 B Thr 127	CA 1.525 C 0.080 1.605 B Glu 131	C 1.231 O 0.077 1.308 B Arg 133	CA 1.530 CB 0.056 1.474 B Arg 134	CA 1.525 C 0.063 1.462 B Glu 136
CA 1.521 CB 0.078 1.443 B Ala 138	CA 1.521 CB 0.051 1.470 B Ala 139	C 1.231 O 0.056 1.287 B Ile 146	CA 1.525 C 0.051 1.576 B Ile 146	CA 1.530 CB 0.085 1.445 B Asp 147	CA 1.540 CB 0.060 1.480 B Ile 160
CA 1.525 C 0.079 1.446 B Arg 169	CA 1.525 C 0.079 1.446 B Asn 170	N 1.458 CA 0.084 1.374 B Asn 170	CA 1.525 C 0.057 1.468 B Ala 173	CA 1.530 CB 0.084 1.446 B Ser 175	CA 1.525 C 0.053 1.578 B Leu 176
CA 1.540 CB 0.096 1.444 B Ile 183	CA 1.540 CB 0.050 1.490 B Val 186	CA 1.525 C 0.059 1.584 B Glu 190	CA 1.530 CB 0.053 1.477 B Tyr 194	N 1.458 CA 0.059 1.399 B Asn 197	CA 1.530 CB 0.061 1.469 B His 198
CA 1.525 C 0.067 1.458 B Arg 203	CA 1.521 CB 0.070 1.451 B Ala 205	CA 1.525 C 0.062 1.463 B Val 211	C 1.231 O 0.053 1.178 B Ala 237	CA 1.525 C 0.062 1.463 B Ala 237	CA 1.521 CB 0.074 1.447 B Ala 237
CA 1.525 C 0.059 1.466 B His 240	CA 1.540 CB 0.076 1.464 B Ile 244	CA 1.530 CB 0.050 1.480 B Arg 245	CA 1.516 C 0.051 1.567 B Gly 249	CA 1.521 CB 0.099 1.422 B Ala 259	C 1.231 O 0.058 1.173 B Glu 260
CA 1.521 CB 0.081 1.440 B Ala 262	CA 1.525 C 0.058 1.467 B Ala 269	CA 1.521 CB 0.070 1.451 B Ala 269	CA 1.530 CB 0.053 1.477 B Asn 270	CA 1.540 CB 0.051 1.489 B Val 274	CA 1.540 CB 0.094 1.446 B Val 278
CA 1.521 CB 0.064 1.457 B Ala 298	CA 1.525 C 0.059 1.584 B His 304	CA 1.530 CB 0.071 1.459 B Gln 305	CA 1.525 C 0.093 1.432 B Val 309	CA 1.540 CB 0.095 1.445 B Val 309	CA 1.525 C 0.086 1.439 B Ala 314
CA 1.521 CB 0.103 1.418 B Ala 314	N 1.458 CA 0.053 1.405 B Ala 314	N 1.458 CA 0.065 1.393 B Ser 315	C 1.231 O 0.051 1.179 B Ser 317	CA 1.525 C 0.063 1.588 B Tyr 325	CA 1.530 CB 0.050 1.480 B Tyr 325

Distorted geometry

1LON

Main-chain bond lengths (contd)

CA 1.540 CB 0.088 1.452 B Thr 326	CA 1.525 C 0.051 1.474 B Ile 327	CA 1.525 C 0.050 1.475 B Ser 328	CA 1.540 CB 0.061 1.479 B Val 344	CA 1.540 CB 0.052 1.488 B Val 372	CA 1.530 CB 0.058 1.472 B Glu 373
CA 1.525 C 0.055 1.470 B Ser 374	CA 1.530 CB 0.051 1.479 B Ser 374	CA 1.525 C 0.061 1.464 B Gln 385	CA 1.525 C 0.055 1.470 B Thr 397	CA 1.540 CB 0.052 1.488 B Thr 397	CA 1.540 CB 0.060 1.480 B Val 405
CA 1.521 CB 0.057 1.464 B Ala 408	CA 1.540 CB 0.060 1.480 B Val 410	CA 1.525 C 0.080 1.605 B Asn 412	CA 1.530 CB 0.062 1.468 B Ser 423	CA 1.530 CB 0.062 1.592 B Met 424	C 1.231 O 0.054 1.285 B Ala 425
CA 1.521 CB 0.056 1.465 B Ala 425	CA 1.521 CB 0.094 1.427 B Ala 426	CA 1.530 CB 0.071 1.459 B Ser 427	N 1.458 CA 0.090 1.548 B Ile 436	N 1.458 CA 0.062 1.520 C Asn 3	CA 1.540 CB 0.071 1.469 C Ile 19
CA 1.525 C 0.102 1.423 C Ser 25	CA 1.525 C 0.051 1.474 C Ile 27	CA 1.540 CB 0.060 1.480 C Ile 27	CA 1.540 CB 0.057 1.597 C Thr 67	N 1.458 CA 0.053 1.405 C Ser 106	CA 1.540 CB 0.085 1.455 C Thr 108
CA 1.540 CB 0.067 1.473 C Ile 115	CA 1.521 CB 0.063 1.458 C Ala 127	CA 1.530 CB 0.055 1.475 C His 182	CA 1.525 C 0.056 1.469 C Thr 209	CA 1.540 CB 0.079 1.461 C Ile 211	N 1.458 CA 0.063 1.395 C Ile 211
CA 1.525 C 0.063 1.462 C Ser 212	CA 1.530 CB 0.065 1.465 C Ser 212	C 1.231 O 0.069 1.162 C Asp 214	CA 1.525 C 0.053 1.472 C Asp 214	C 1.231 O 0.053 1.284 C Ile 218	CA 1.540 CB 0.055 1.485 C Ile 218
CA 1.530 CB 0.068 1.462 C His 221	CA 1.525 C 0.061 1.464 C Leu 235	N 1.458 CA 0.051 1.509 C Val 243	CA 1.540 CB 0.088 1.628 C Thr 257	CA 1.530 CB 0.088 1.442 C His 308	C 1.231 O 0.064 1.295 C Met 315
CA 1.525 C 0.064 1.589 C Arg 318	CA 1.540 CB 0.055 1.485 C Thr 334	CA 1.540 CB 0.057 1.597 C Thr 336	CA 1.540 CB 0.056 1.596 C Val 343	CA 1.521 CB 0.070 1.451 C Ala 369	CA 1.525 C 0.051 1.474 D Ser 42
CA 1.521 CB 0.053 1.468 D Ala 61	CA 1.525 C 0.059 1.584 D Phe 91	CA 1.530 CB 0.065 1.595 D Phe 91	CA 1.521 CB 0.062 1.459 D Ala 101	CA 1.540 CB 0.053 1.593 D Ile 116	N 1.458 CA 0.056 1.402 D Leu 169
CA 1.521 CB 0.115 1.406 D Ala 177	CA 1.525 C 0.089 1.436 D Ser 232	CA 1.525 C 0.071 1.454 D Arg 233	CA 1.525 C 0.052 1.473 D Pro 239	C 1.231 O 0.064 1.295 E Ile 5	CA 1.525 C 0.080 1.445 E Ile 5

Distorted geometry

1LON

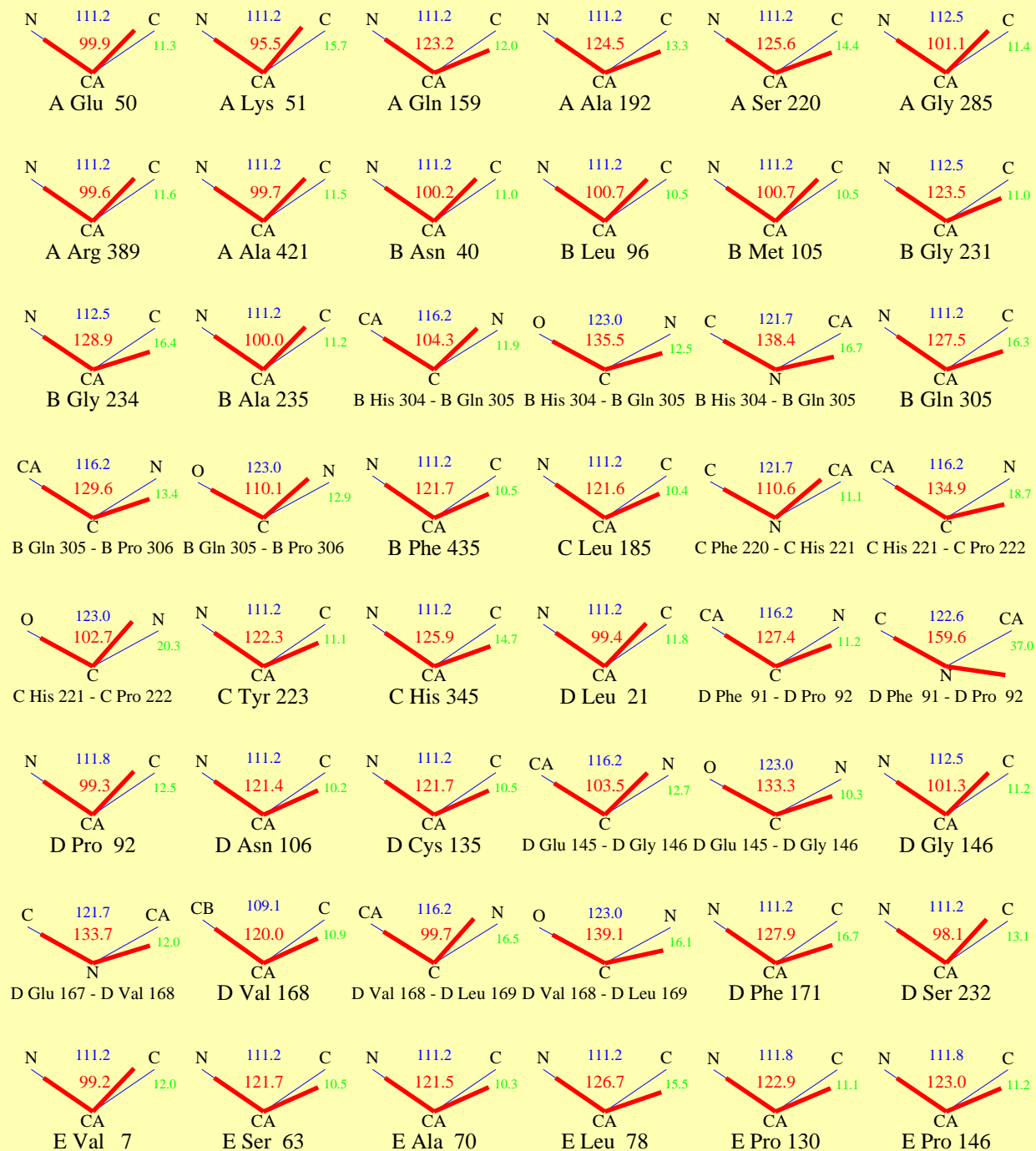
Main-chain bond lengths (contd)

N 1.458 CA 0.058 1.400 E Lys 6	CA 1.540 CB 0.050 1.490 E Val 18	N 1.458 CA 0.053 1.405 E Asp 20	CA 1.540 CB 0.055 1.595 E Thr 22	CA 1.540 CB 0.050 1.590 E Val 68	N 1.458 CA 0.059 1.517 E Met 71
CA 1.525 C 0.053 1.578 E Ile 147	CA 1.540 CB 0.059 1.599 E Ile 147	CA 1.525 C 0.066 1.591 E Tyr 185	CA 1.525 C 0.058 1.467 F Tyr 20	CA 1.521 CB 0.081 1.440 F Ala 23	CA 1.525 C 0.059 1.584 F Asn 40
CA 1.521 CB 0.111 1.410 F Ala 46	N 1.458 CA 0.056 1.514 F Leu 50	CA 1.525 C 0.059 1.466 F Thr 81	CA 1.540 CB 0.061 1.479 F Thr 81	CA 1.540 CB 0.052 1.488 F Val 97	CA 1.525 C 0.058 1.583 G Arg 2
C 1.231 O 0.060 1.171 G Gln 3	N 1.458 CA 0.099 1.557 G Gln 3	CA 1.525 C 0.062 1.463 G Leu 7	CA 1.540 CB 0.065 1.475 G Thr 8	CA 1.540 CB 0.062 1.478 G Thr 15	C 1.231 O 0.050 1.181 G Pro 27
CA 1.525 C 0.059 1.584 G His 28	CA 1.540 CB 0.069 1.609 G Ile 34	CA 1.521 CB 0.059 1.462 G Ala 43	CA 1.525 C 0.073 1.598 G Asn 73	N 1.458 CA 0.051 1.509 H Glu 12	CA 1.525 C 0.053 1.578 H Gln 49
CA 1.540 CB 0.055 1.595 H Val 69	N 1.458 CA 0.054 1.512 I Met 1	CA 1.525 C 0.052 1.473 I Ser 8	C 1.231 O 0.068 1.163 I Pro 10	CA 1.525 C 0.061 1.464 I Pro 13	CA 1.540 CB 0.051 1.489 I Val 14
CA 1.530 CB 0.054 1.476 I Leu 15	CA 1.521 CB 0.154 1.367 I Ala 25	CA 1.525 C 0.055 1.580 I Arg 27	CA 1.525 C 0.083 1.442 I Val 42	CA 1.540 CB 0.053 1.487 I Val 42	C 1.329 N 0.061 1.268 I Val 42 - I Leu 43
N 1.458 CA 0.118 1.340 I Leu 43	C 1.231 O 0.058 1.173 I Asp 44	CA 1.525 C 0.063 1.588 I Leu 45	N 1.458 CA 0.063 1.521 I Leu 45	CA 1.530 CB 0.052 1.582 I Arg 47	CA 1.521 CB 0.065 1.456 J Ala 39
C 1.231 O 0.063 1.168 J Ala 41	N 1.458 CA 0.053 1.511 J Glu 44	CA 1.540 CB 0.051 1.591 J Ile 55	N 1.458 CA 0.051 1.509 K Trp 44	CA 1.525 C 0.077 1.602 K Val 45	CA 1.540 CB 0.074 1.614 K Val 45
CA 1.525 C 0.053 1.578 K Ile 48	CA 1.540 CB 0.053 1.593 K Ile 48				

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

Distorted geometry 1LON

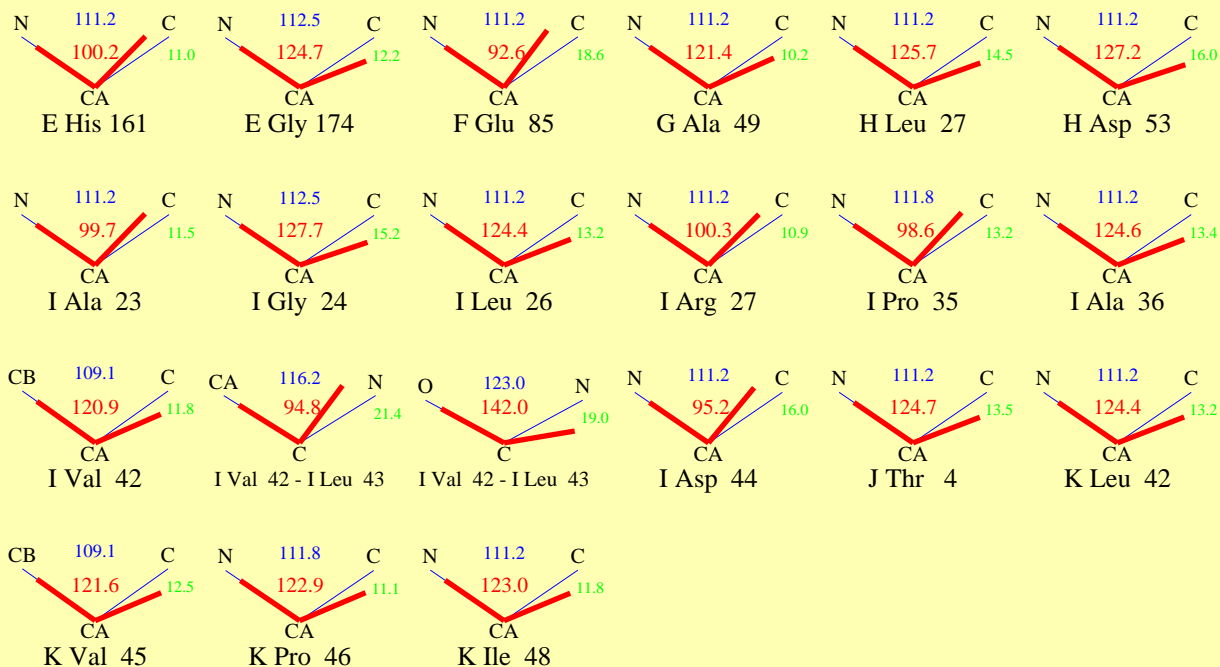
Main-chain bond angles



Distorted geometry

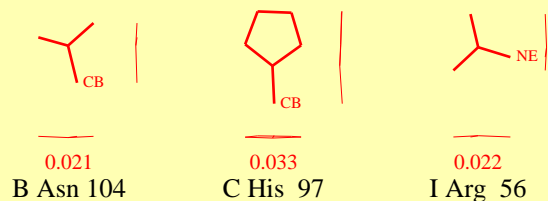
1LON

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.