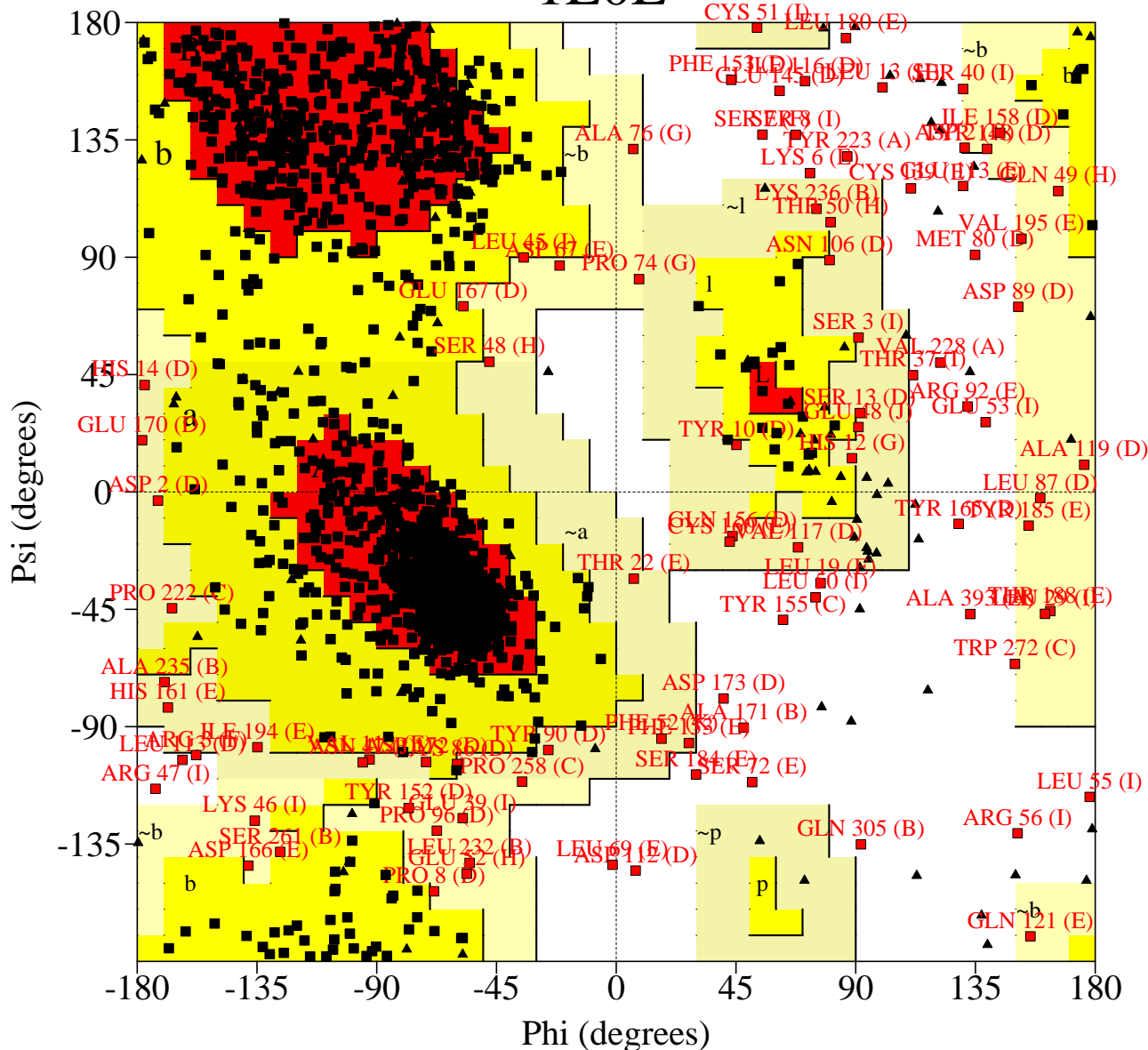


Ramachandran Plot

1LOL



Plot statistics

Residues in most favoured regions [A,B,L]	1517	82.0%
Residues in additional allowed regions [a,b,l,p]	247	13.4%
Residues in generously allowed regions [-a,-b,-l,-p]	51	2.8%
Residues in disallowed regions	34	1.8%

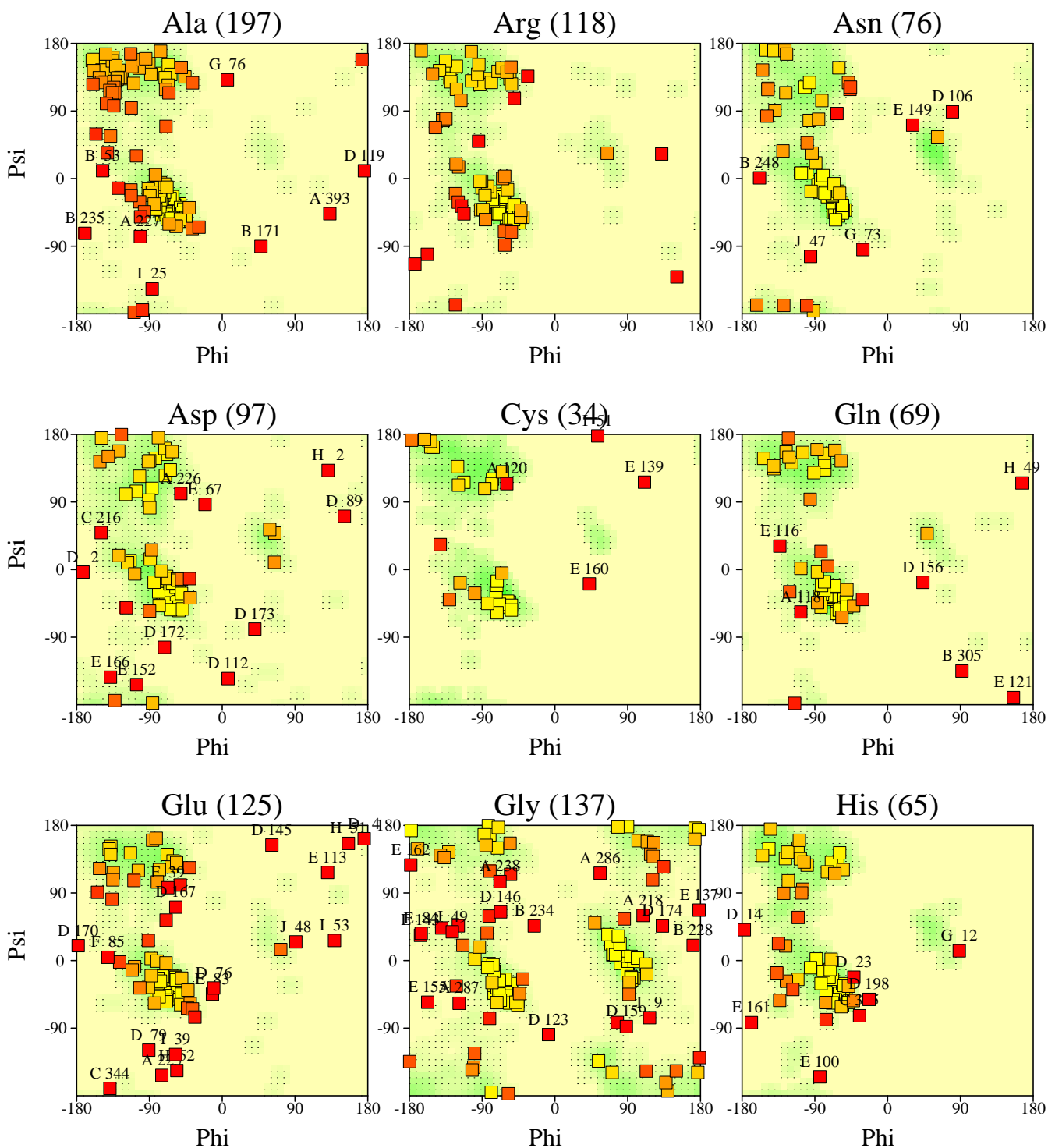
Number of non-glycine and non-proline residues	1849	100.0%
Number of end-residues (excl. Gly and Pro)	16	
Number of glycine residues (shown as triangles)	142	
Number of proline residues	111	

Total number of residues	2118	

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

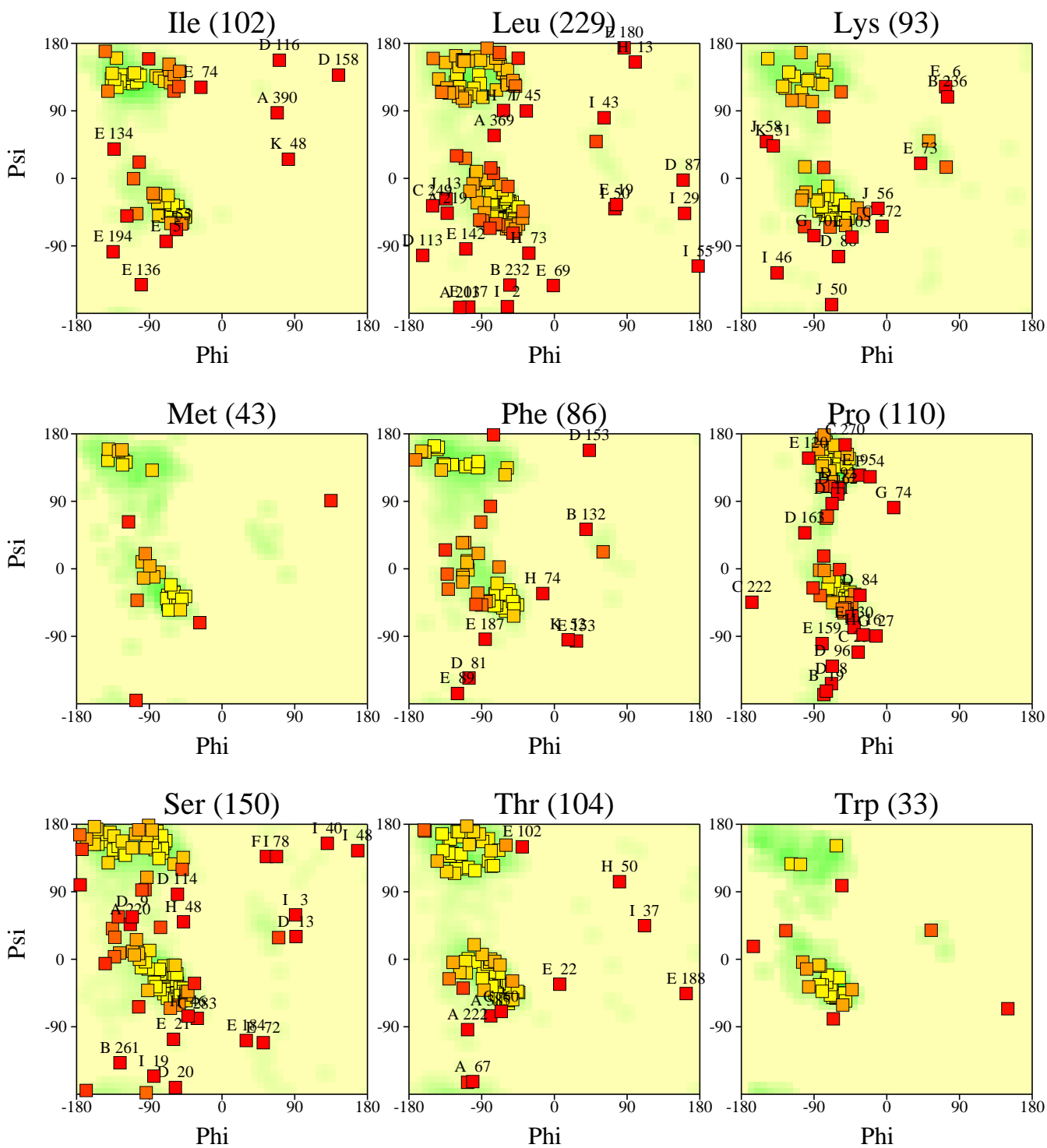
1LOL



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

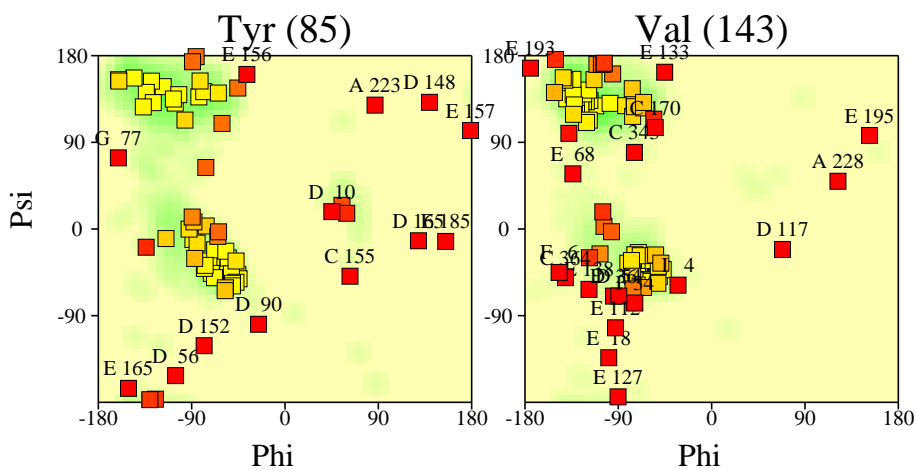
1LOL



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

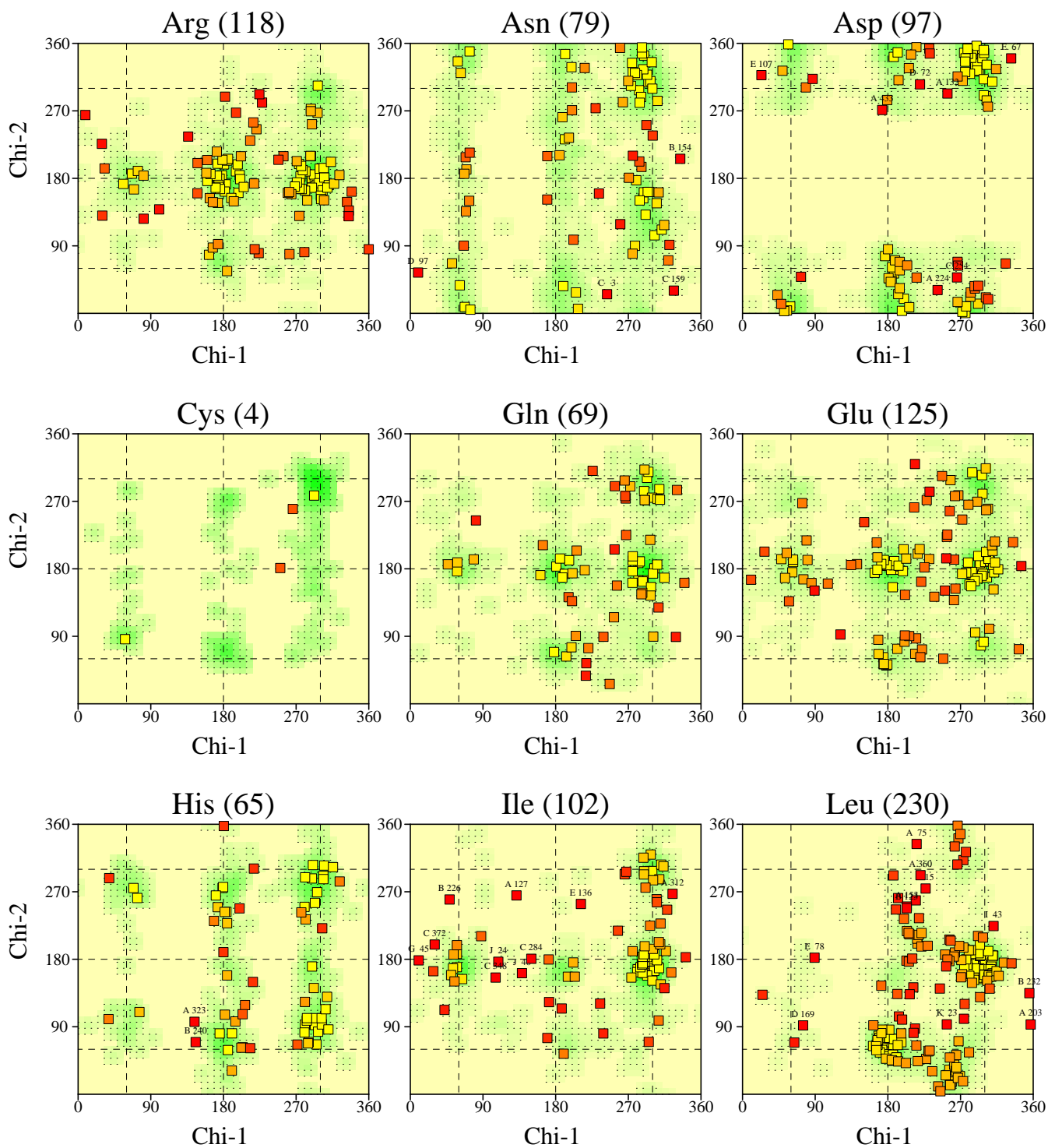
1L0L



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

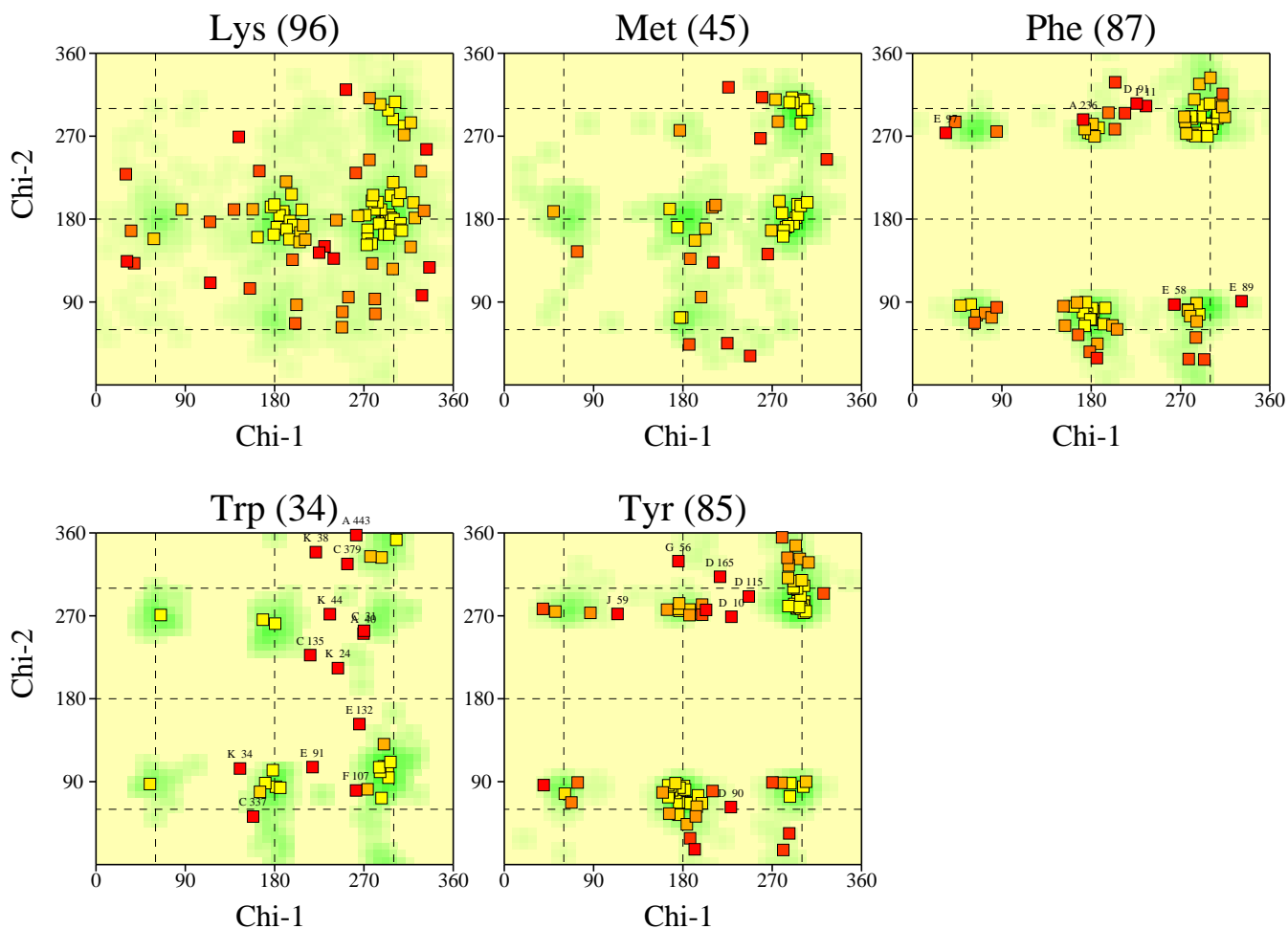
1LOL



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

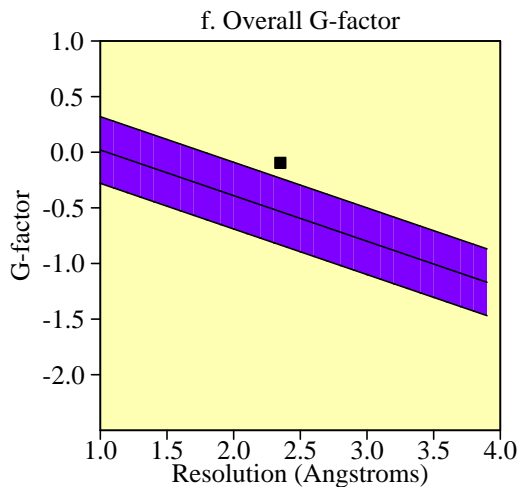
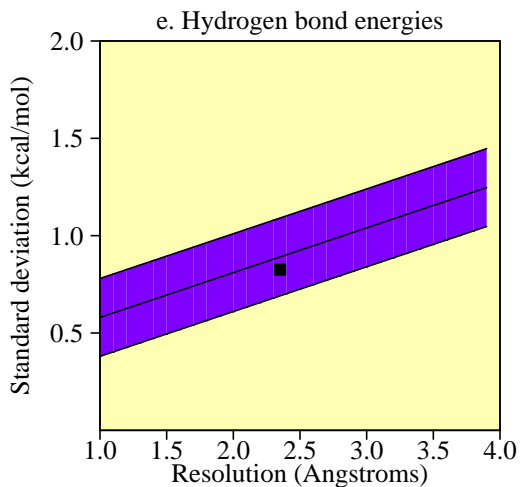
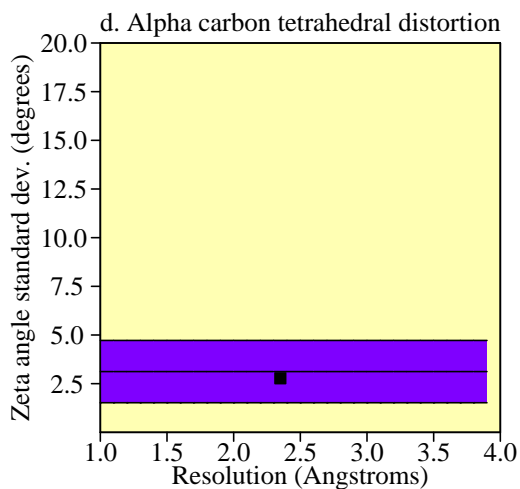
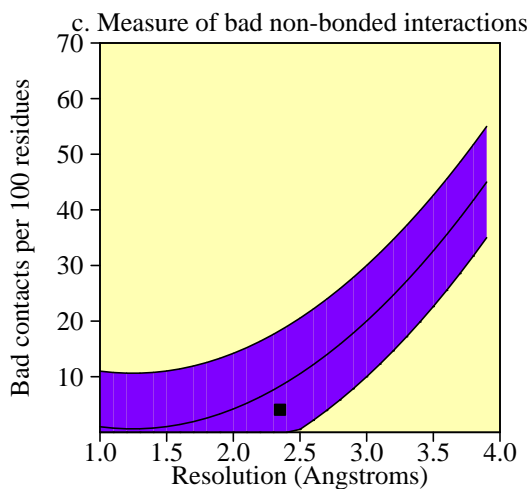
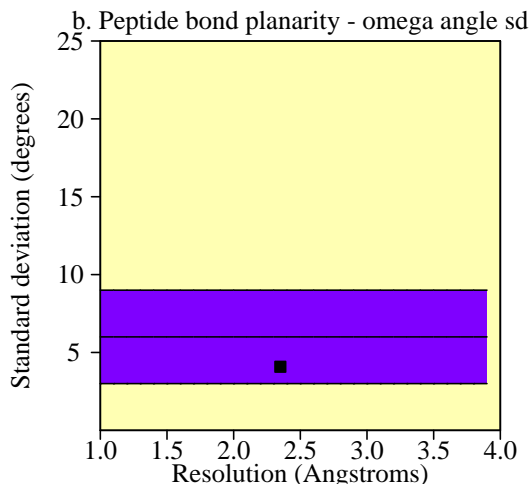
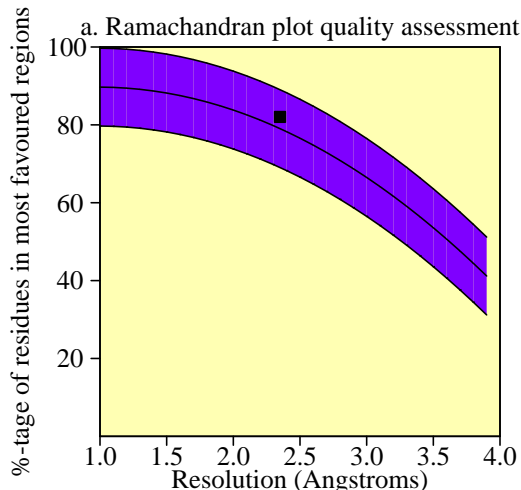
1LOL



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

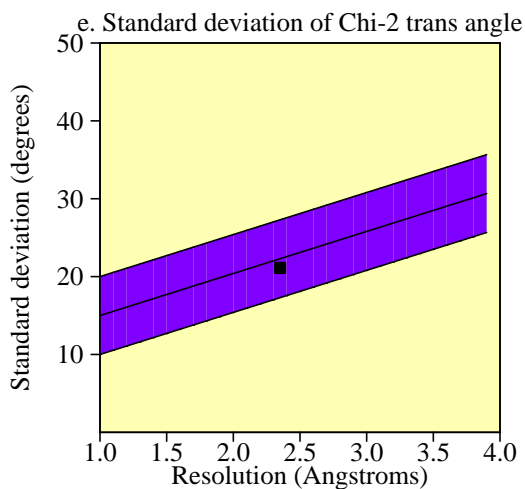
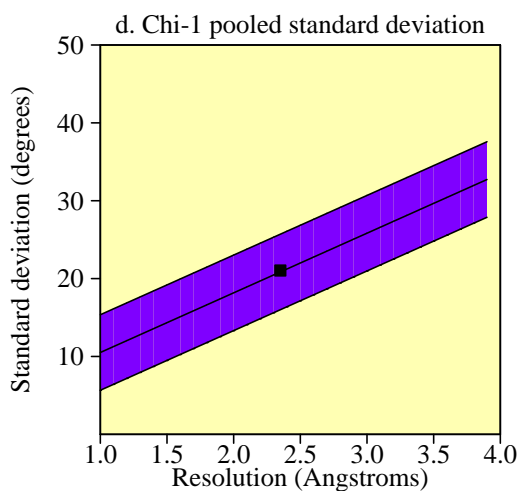
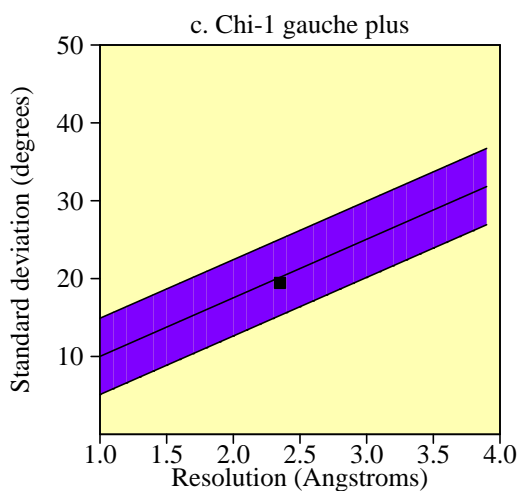
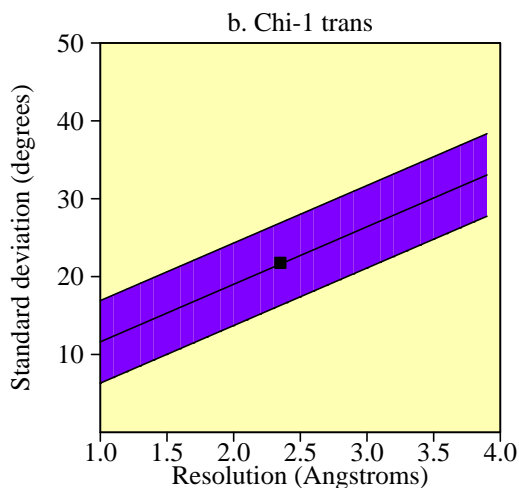
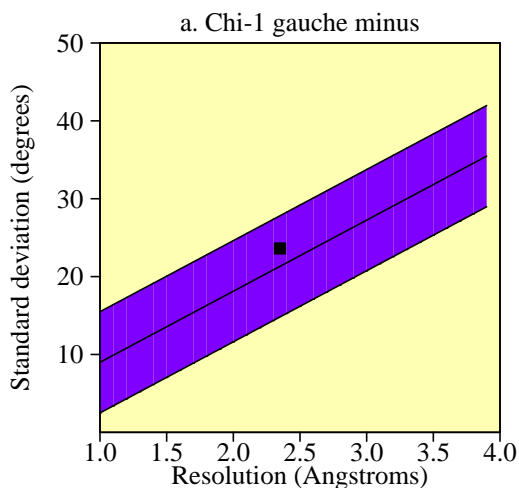
1LOL



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	1849	82.0	79.0	10.0	0.3	Inside
b. Omega angle st dev	2107	4.1	6.0	3.0	-0.6	Inside
c. Bad contacts / 100 residues	86	4.1	8.3	10.0	-0.4	Inside
d. Zeta angle st dev	1976	2.8	3.1	1.6	-0.2	Inside
e. H-bond energy st dev	1360	0.8	0.9	0.2	-0.3	Inside
f. Overall G-factor	2118	-0.1	-0.5	0.3	1.5	BETTER

Side-chain parameters 1LOL



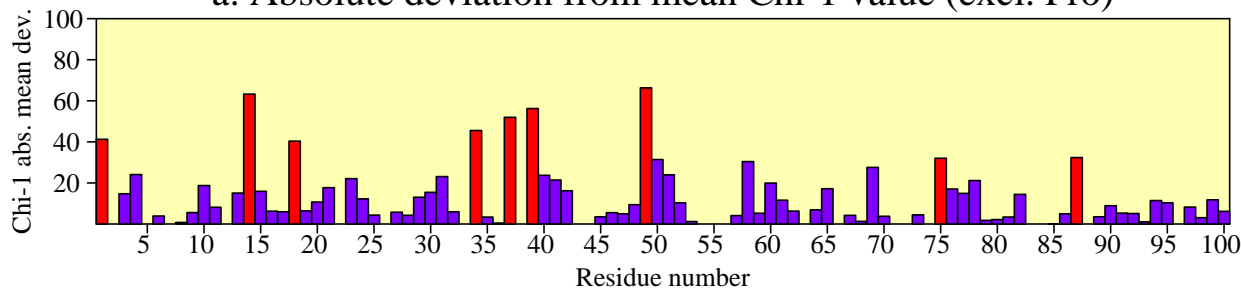
1LOL

Plot statistics

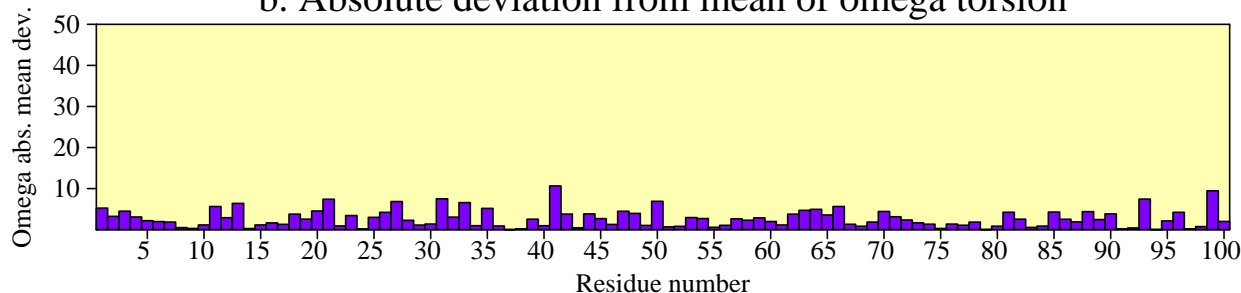
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. Chi-1 gauche minus st dev	255	23.6	21.3	6.5	0.4	Inside
b. Chi-1 trans st dev	582	21.8	21.6	5.3	0.0	Inside
c. Chi-1 gauche plus st dev	830	19.4	20.2	4.9	-0.1	Inside
d. Chi-1 pooled st dev	1667	21.0	20.9	4.8	0.0	Inside
e. Chi-2 trans st dev	527	21.1	22.3	5.0	-0.2	Inside

Residue properties 1LOL

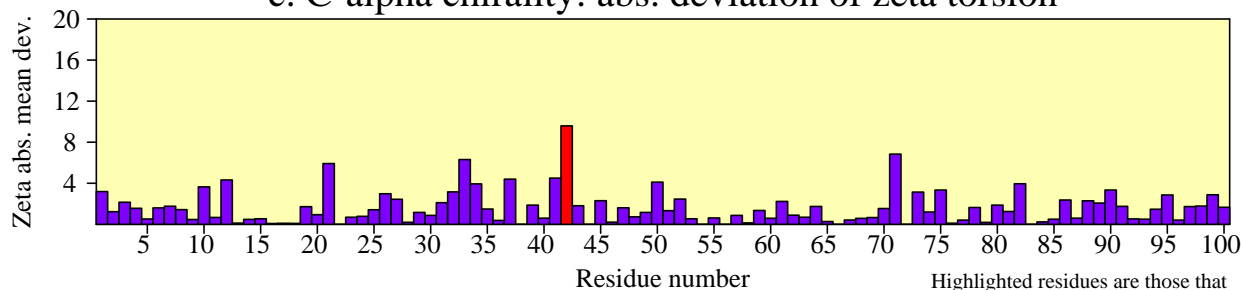
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

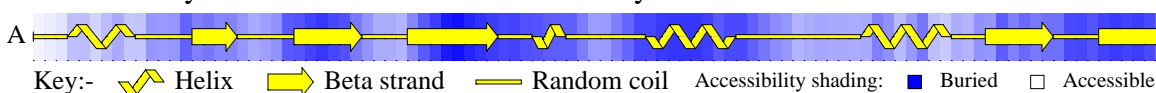


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



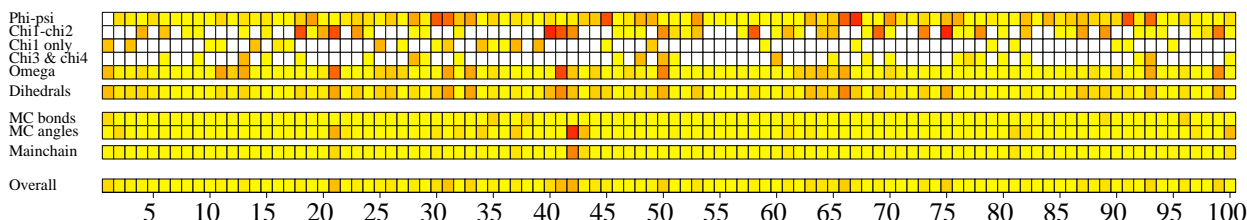
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

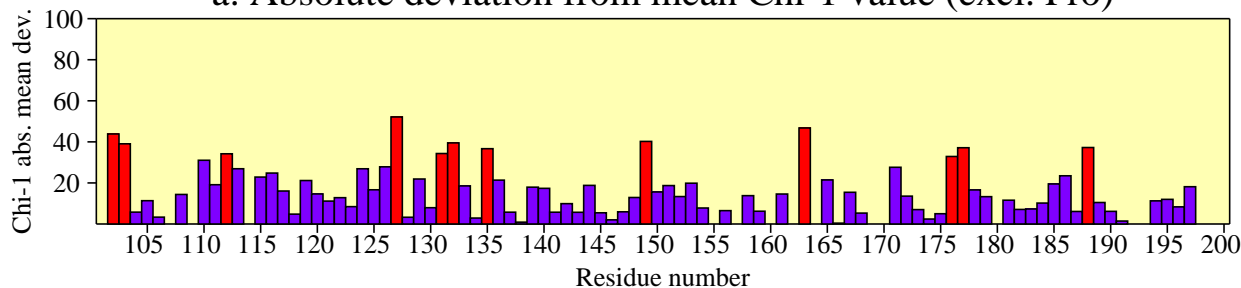


g. G-factors

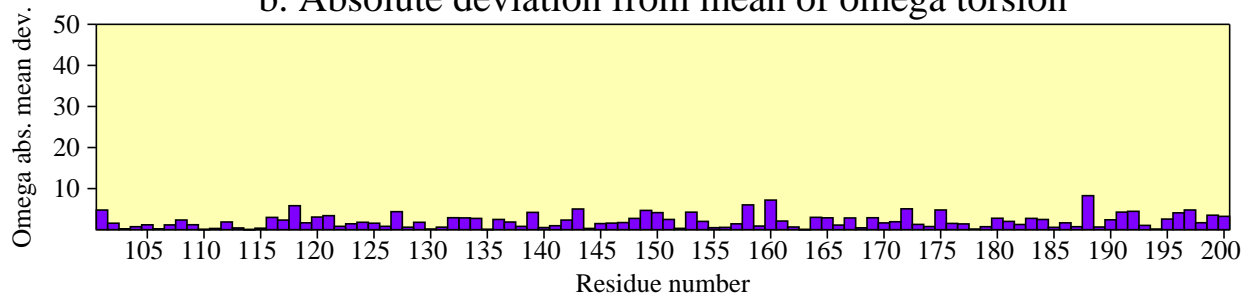


Residue properties 1LOL

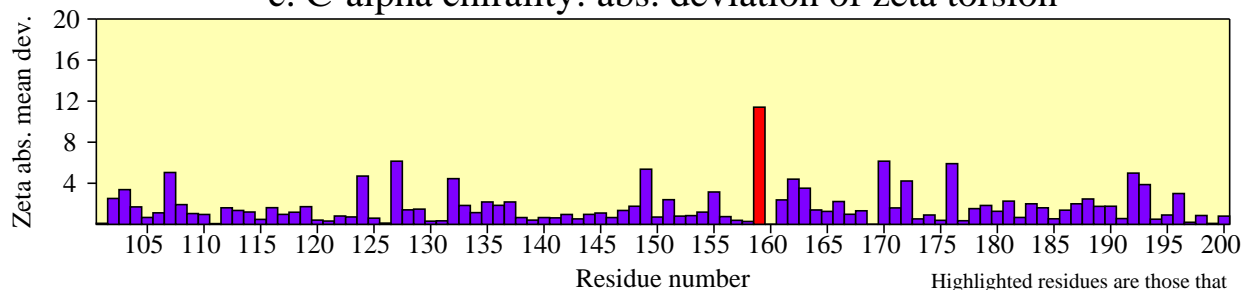
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

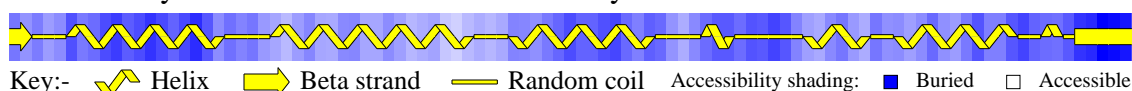


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



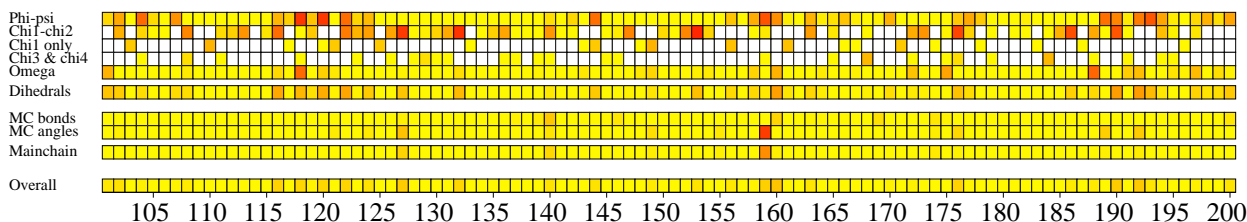
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

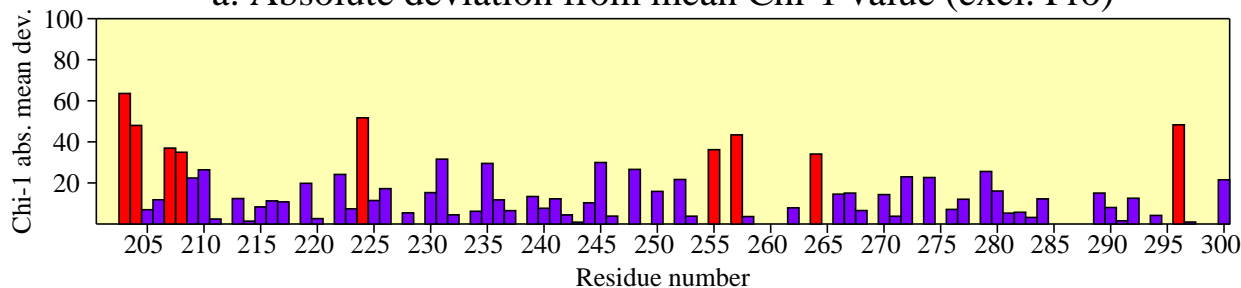


g. G-factors

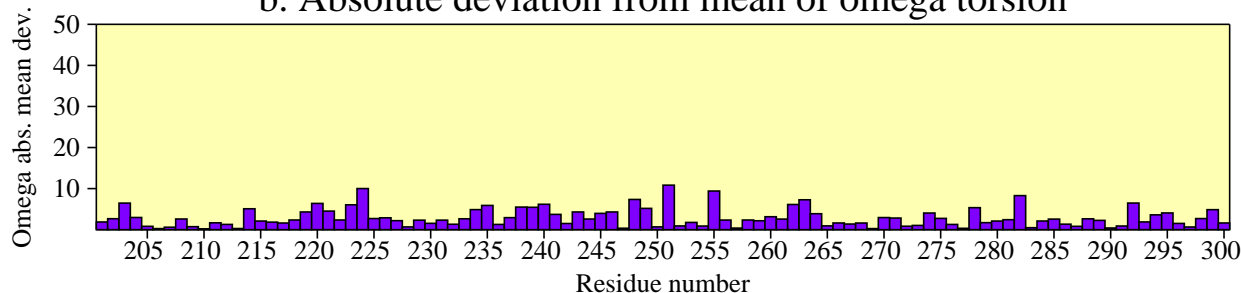


Residue properties 1LOL

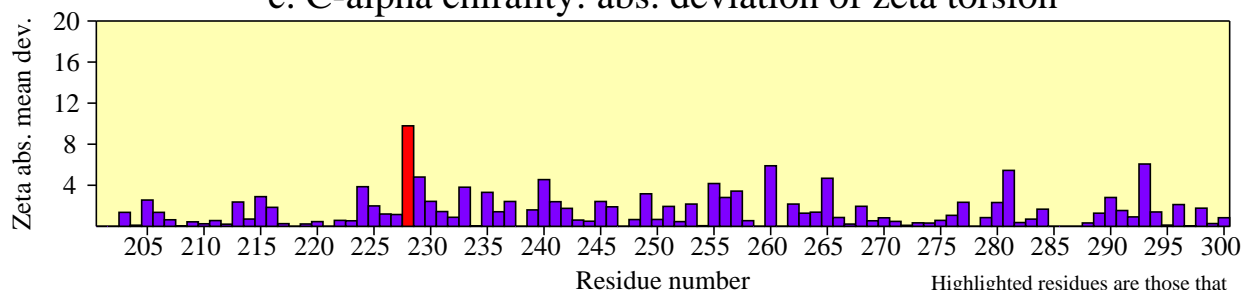
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

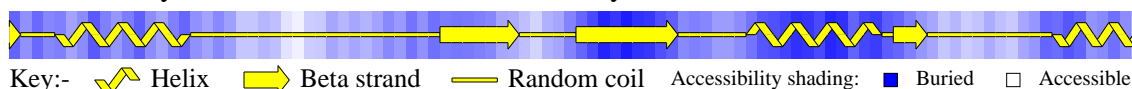


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



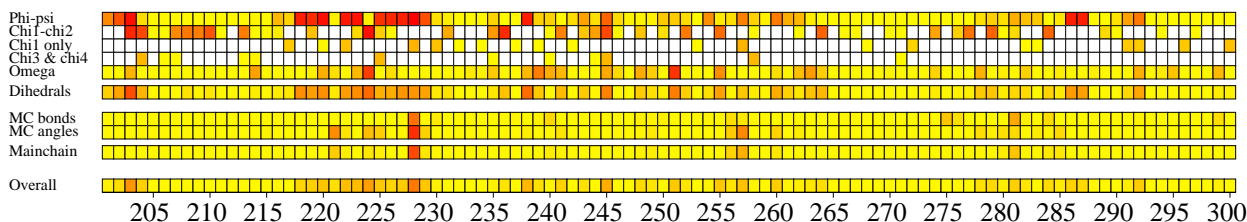
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

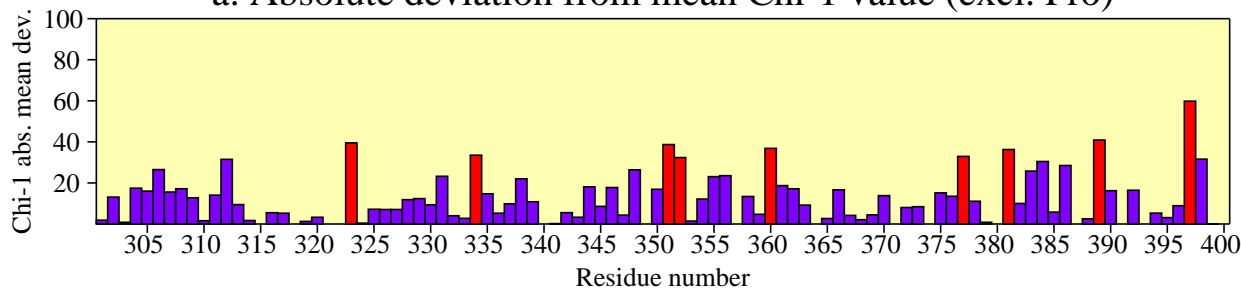


g. G-factors

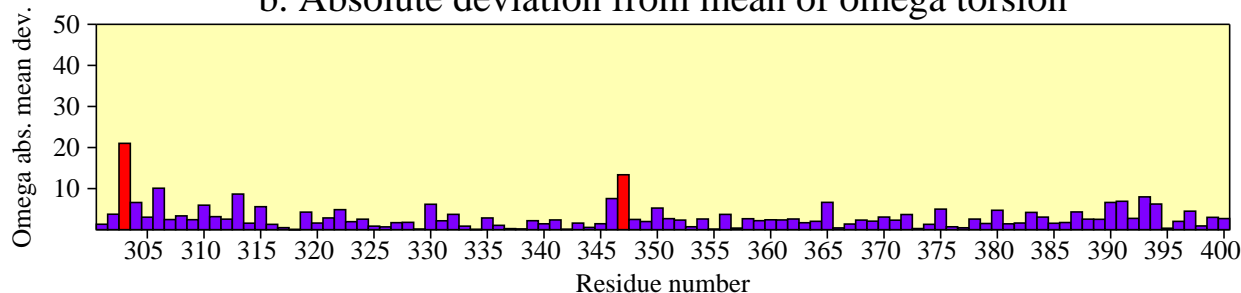


Residue properties 1L0L

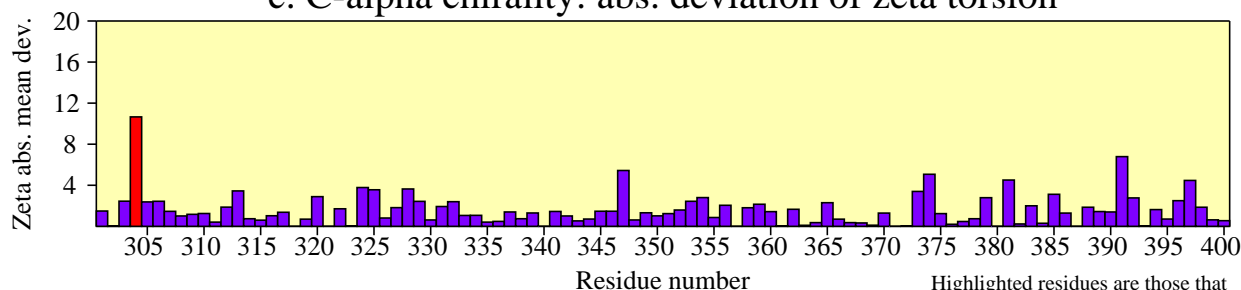
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

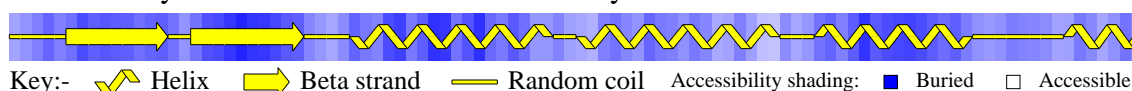


c. C-alpha chirality: abs. deviation of zeta torsion

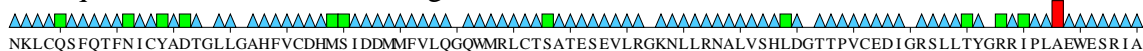


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

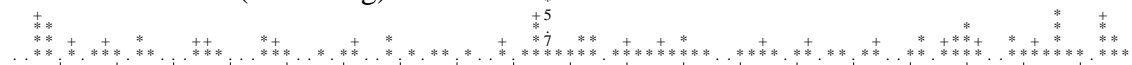
d. Secondary structure & estimated accessibility



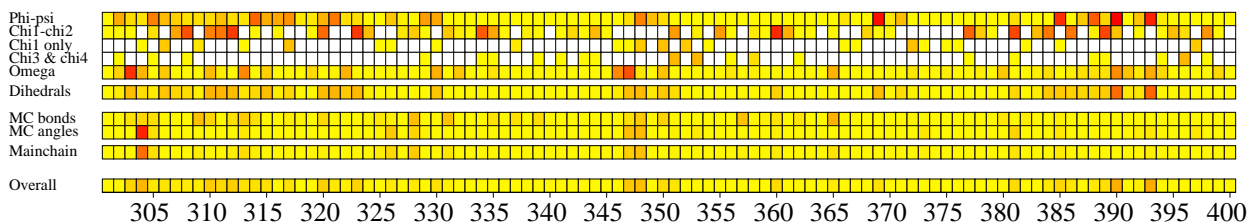
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

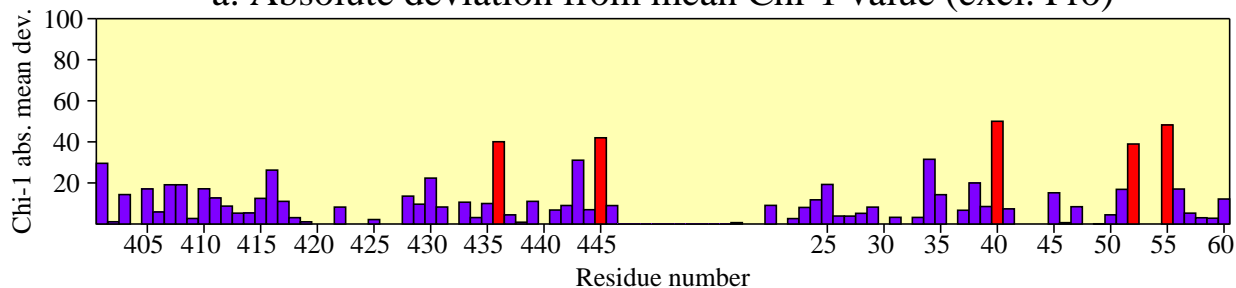


g. G-factors

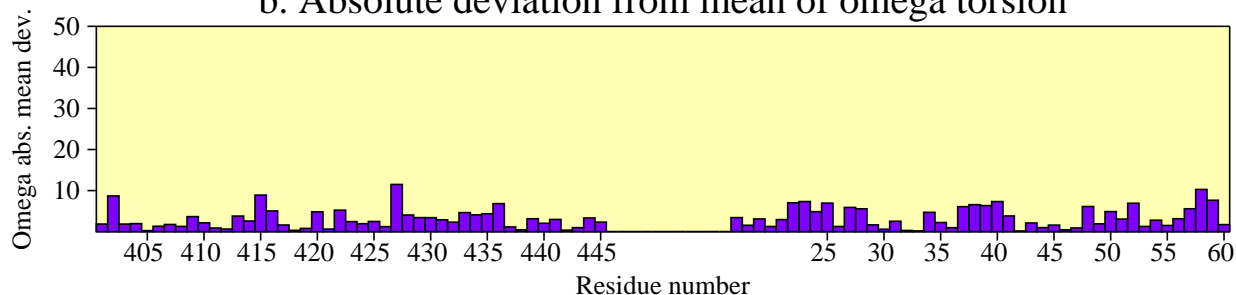


Residue properties 1LOL

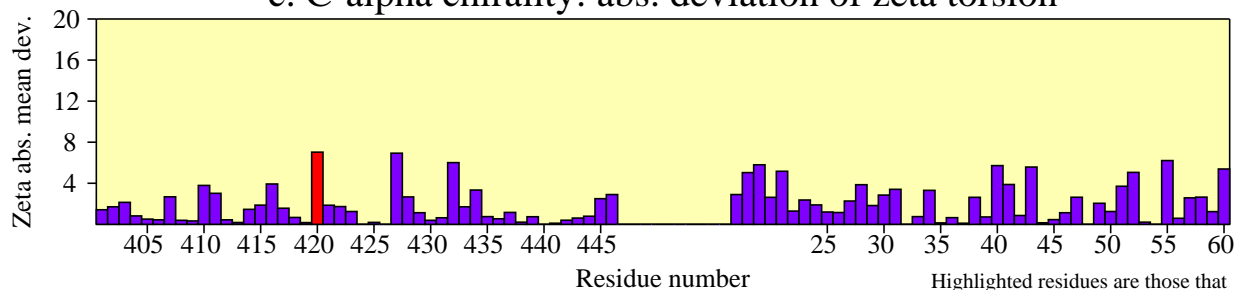
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

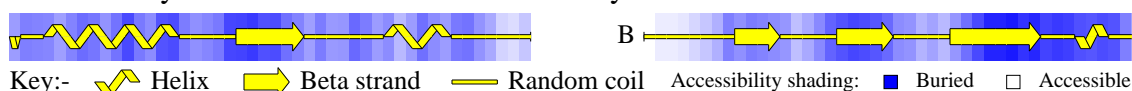


c. C-alpha chirality: abs. deviation of zeta torsion

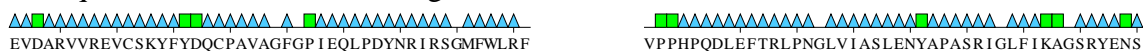


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



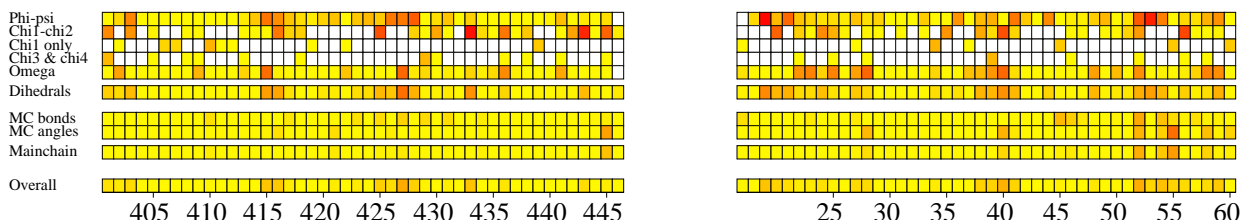
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

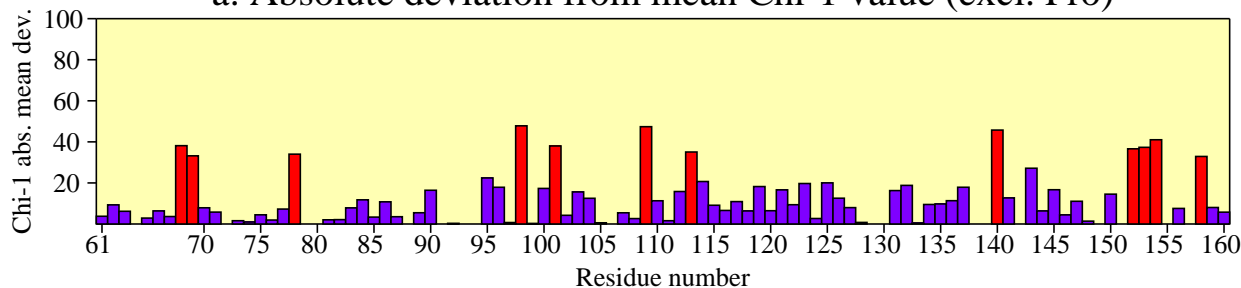


g. G-factors

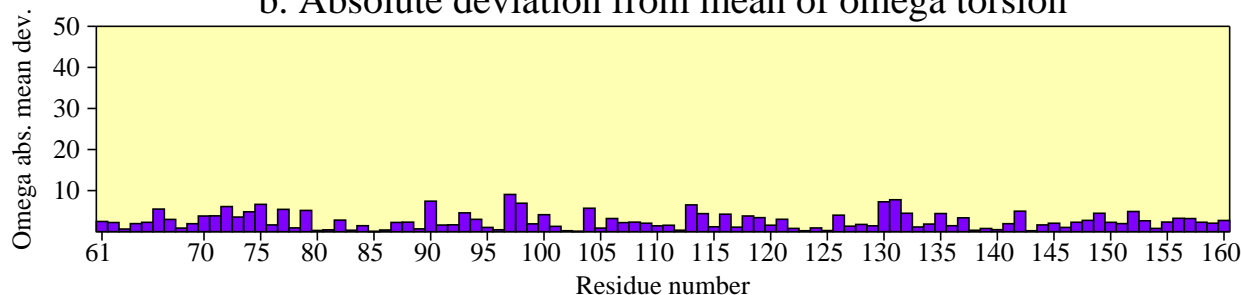


Residue properties 1L0L

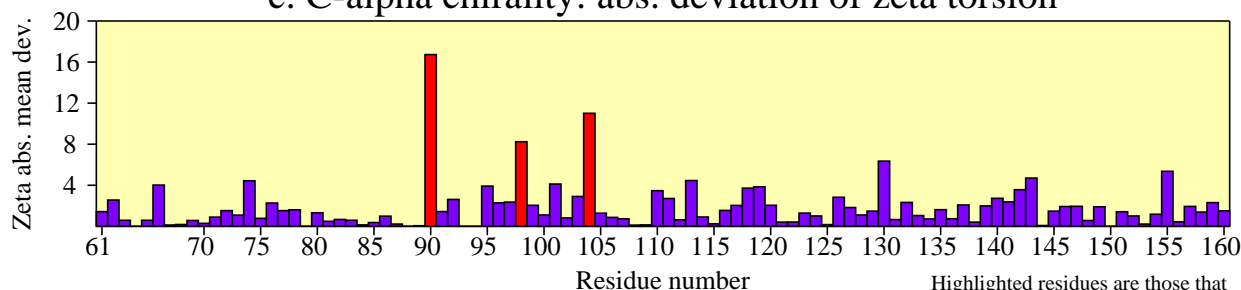
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

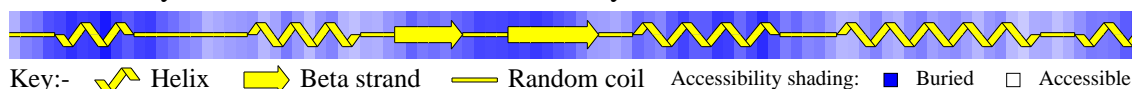


c. C-alpha chirality: abs. deviation of zeta torsion



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

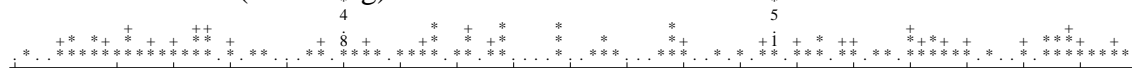
d. Secondary structure & estimated accessibility



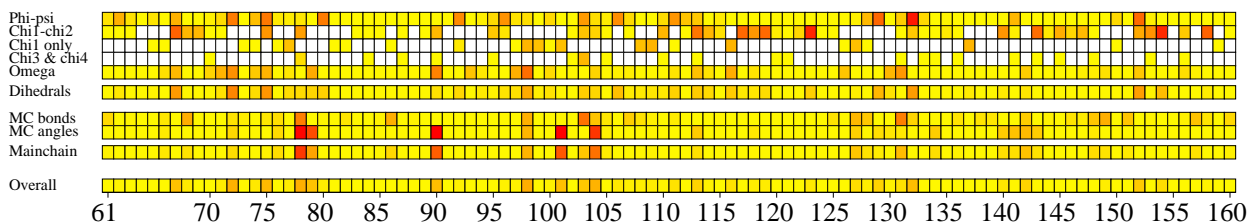
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

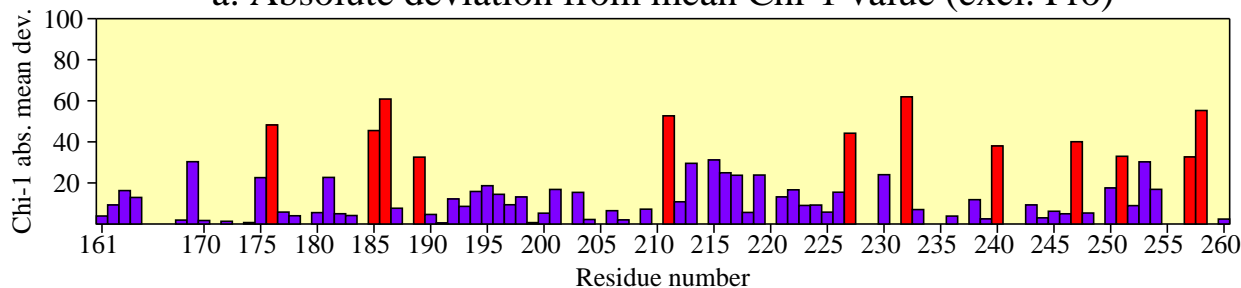


g. G-factors

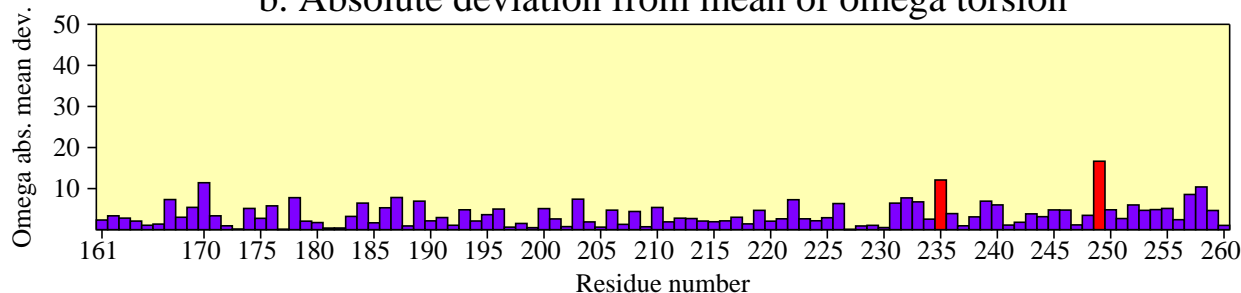


Residue properties 1LOL

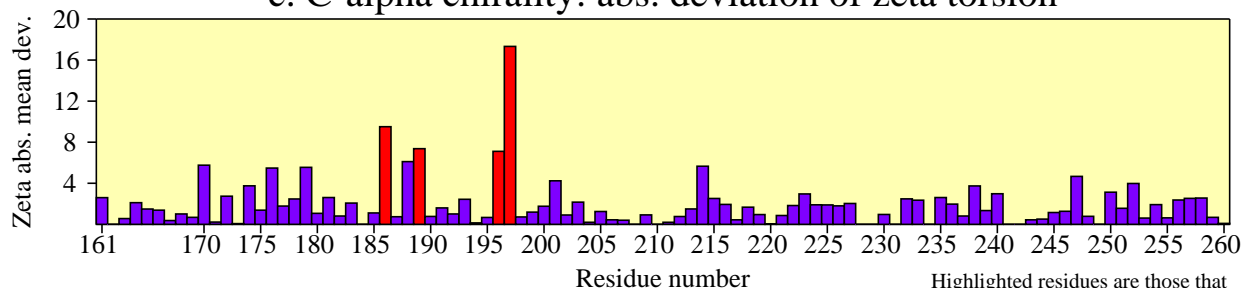
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

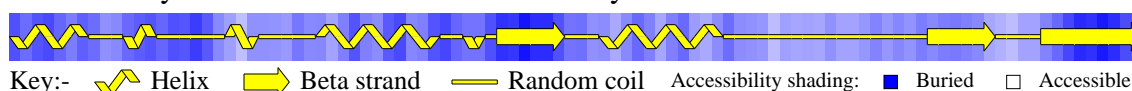


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



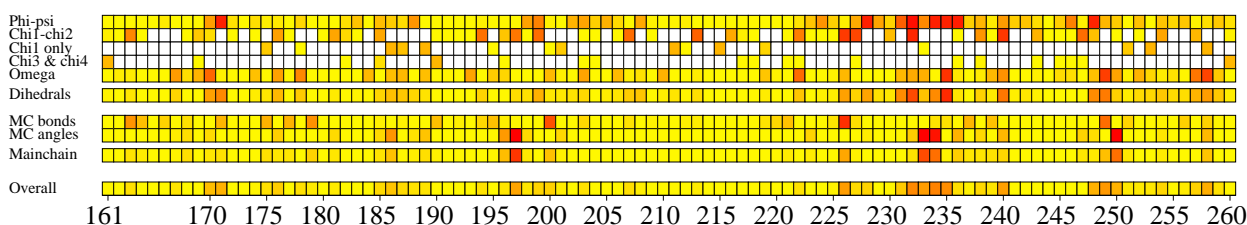
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

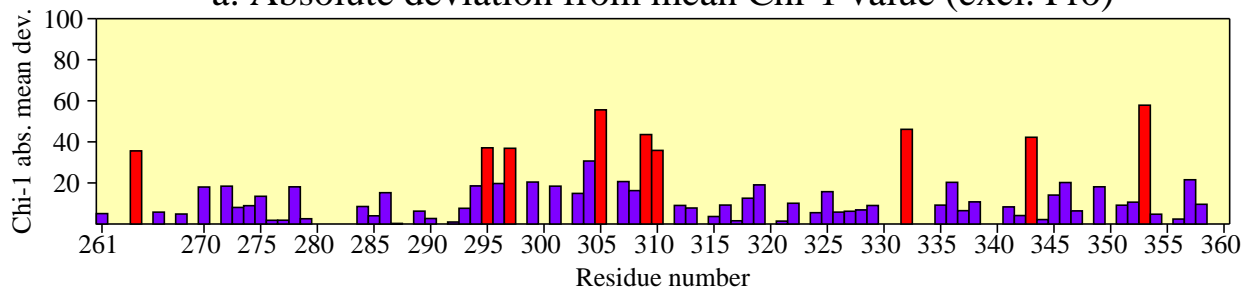


g. G-factors

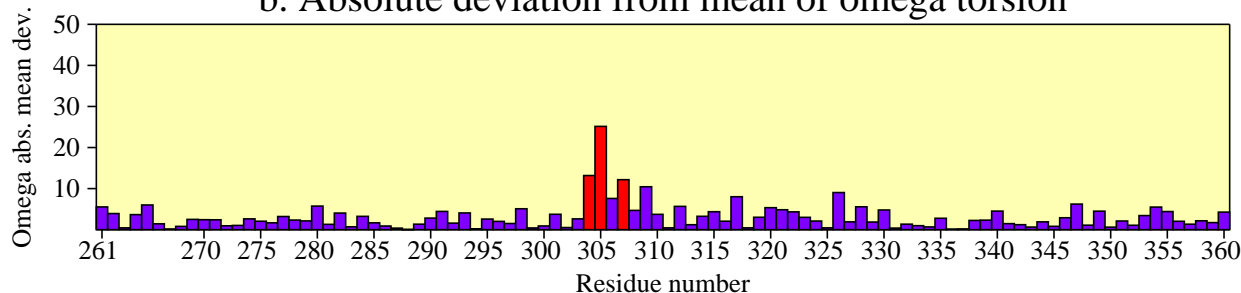


Residue properties 1L0L

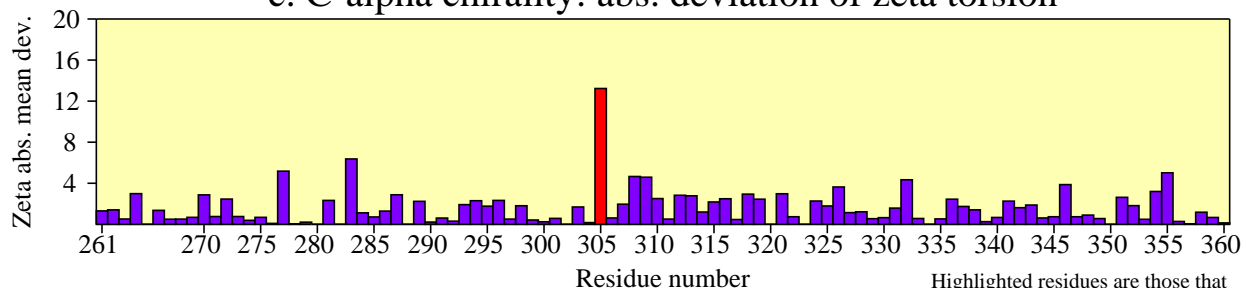
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

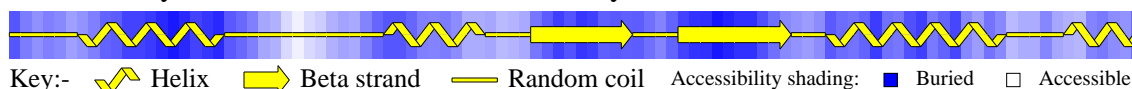


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



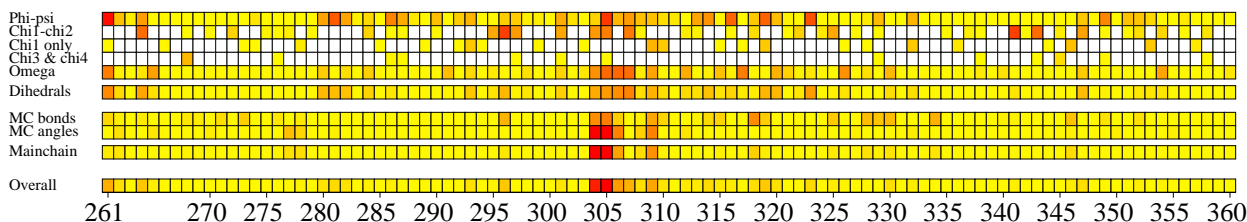
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



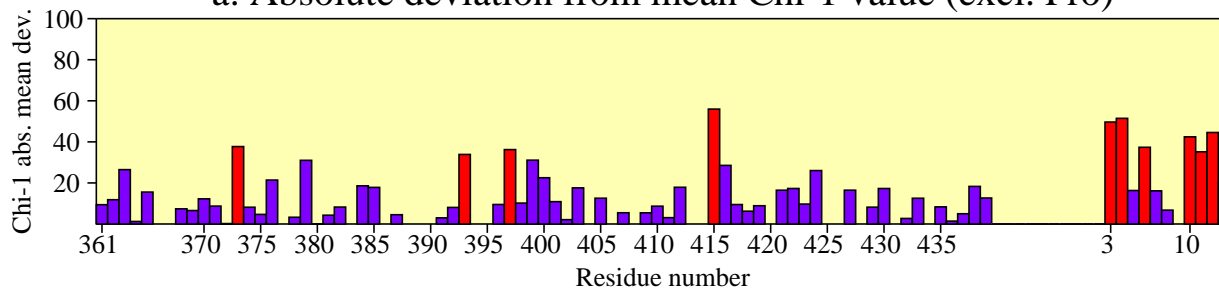
g. G-factors



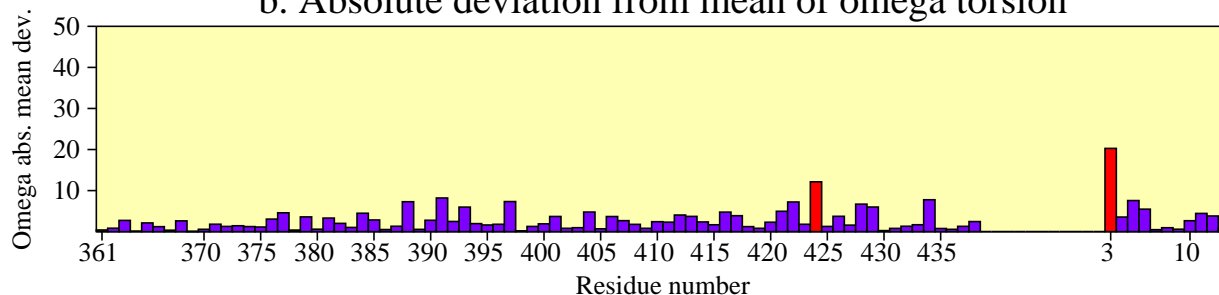
Residue properties

1L0L

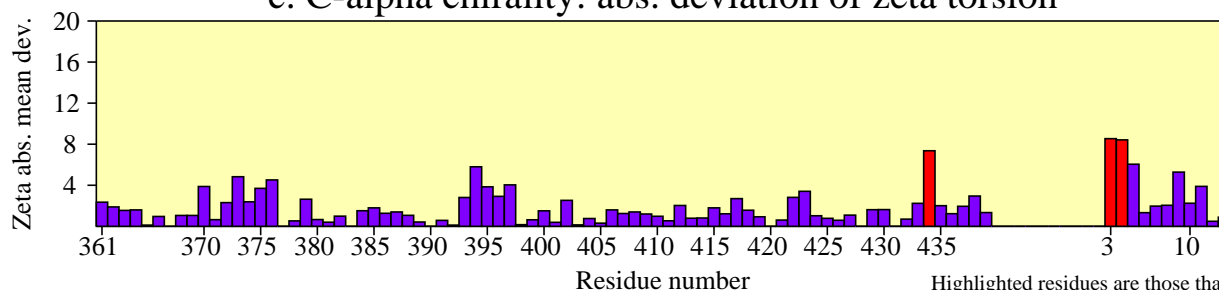
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

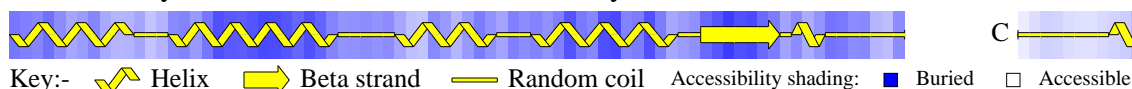


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



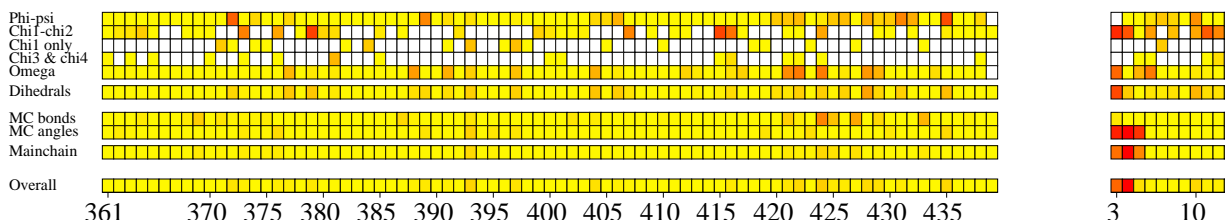
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

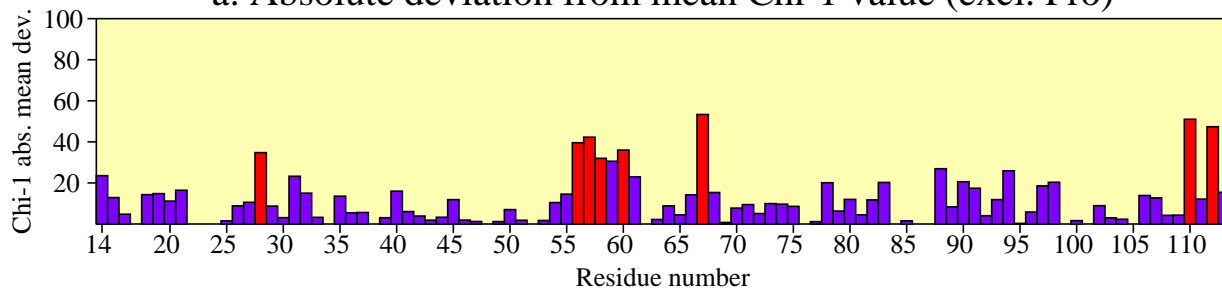


g. G-factors

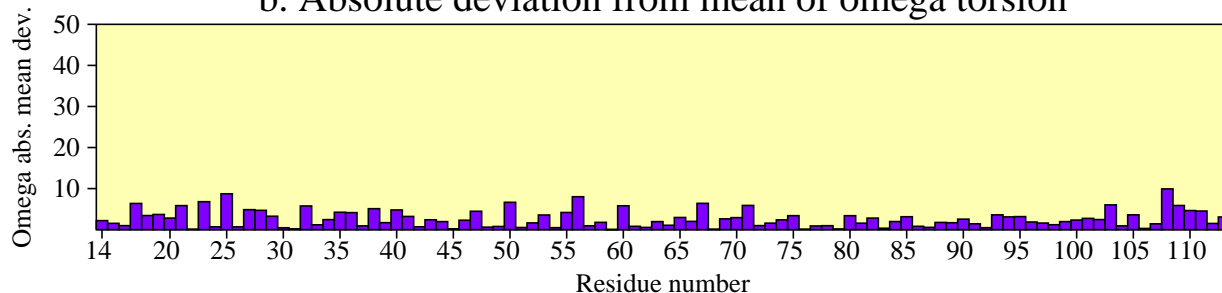


Residue properties 1LOL

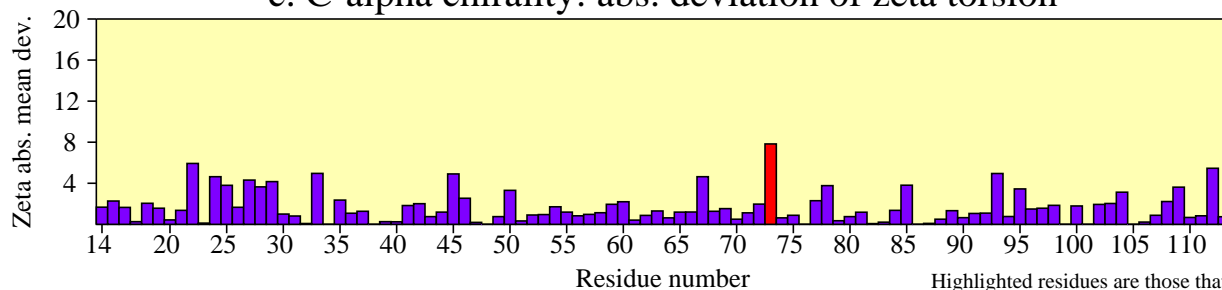
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

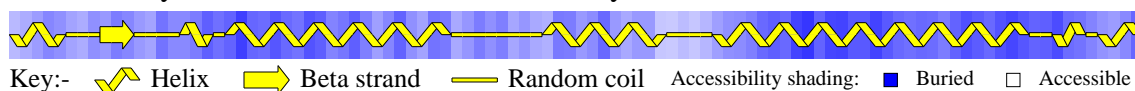


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



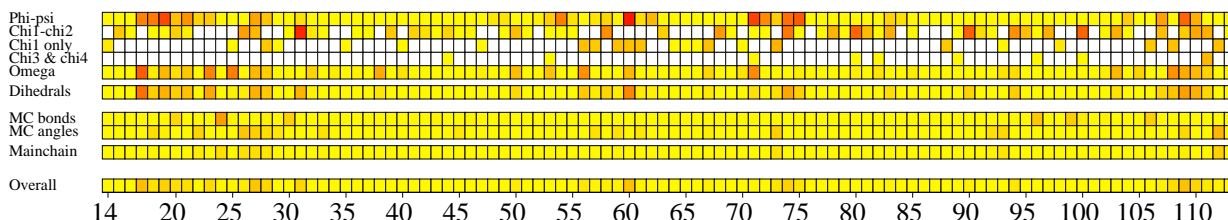
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

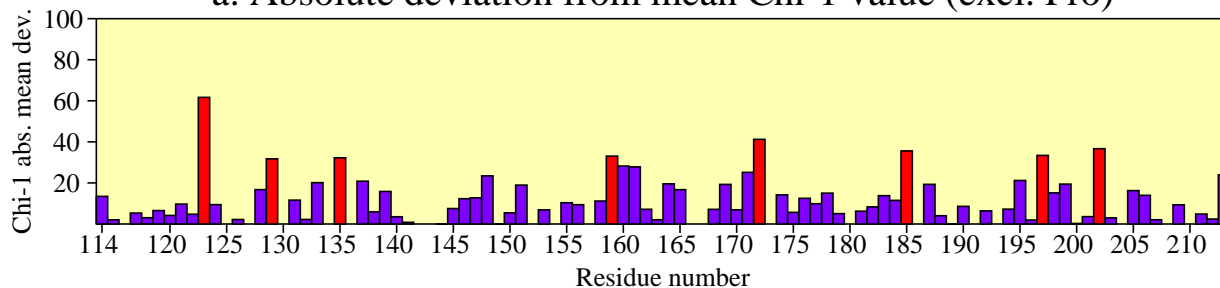


g. G-factors

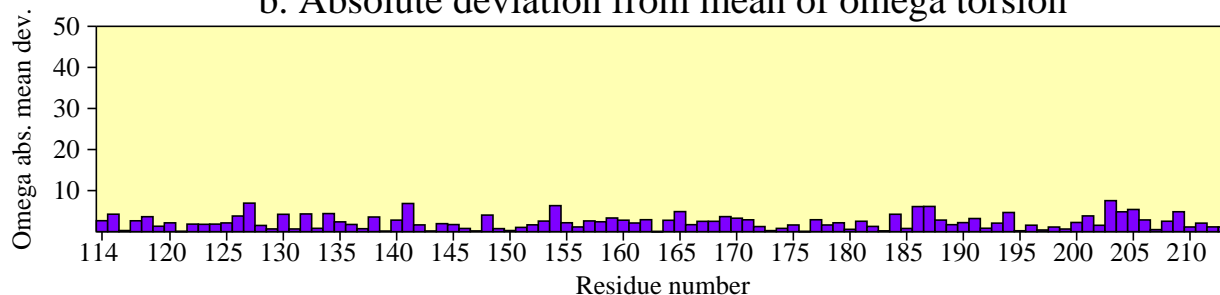


Residue properties 1LOL

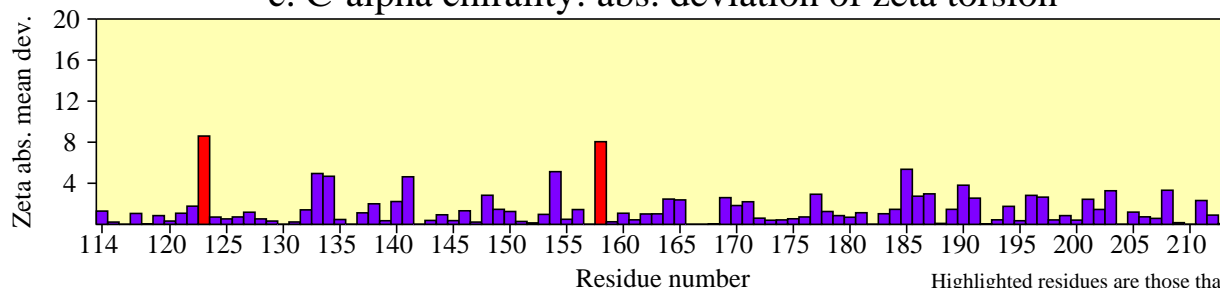
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

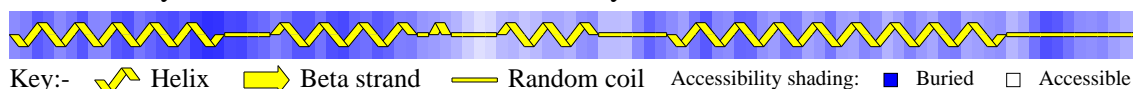


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



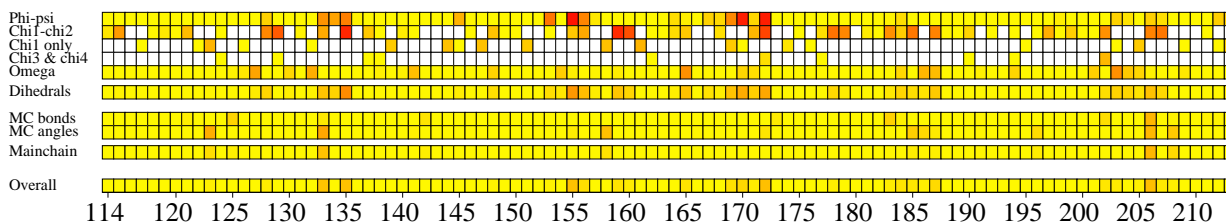
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

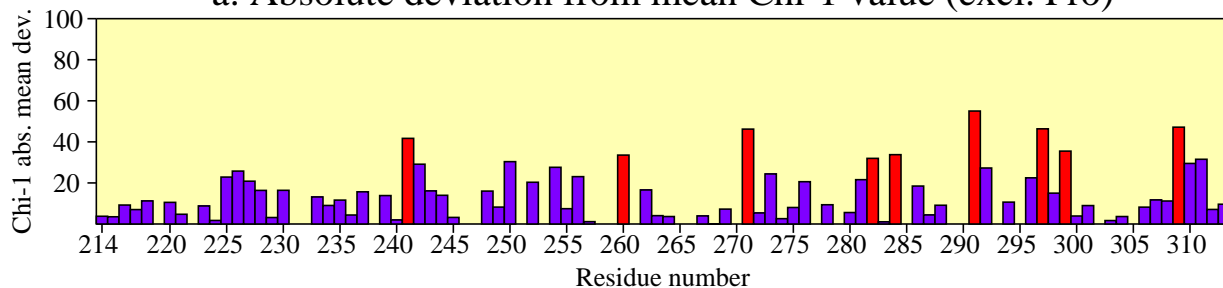


g. G-factors

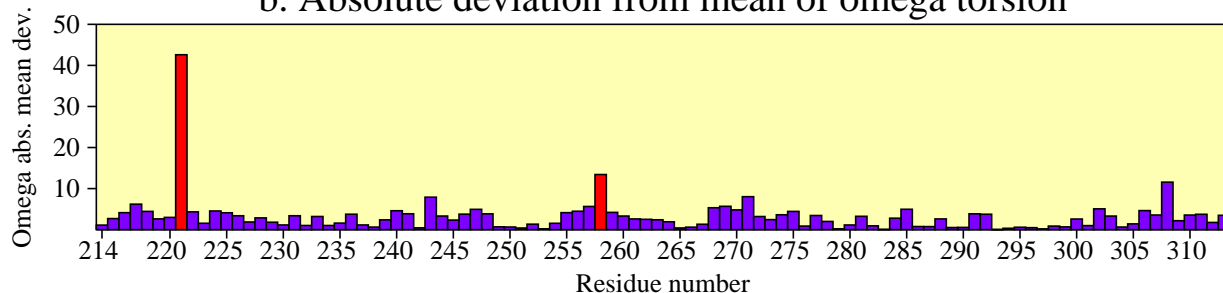


Residue properties 1LOL

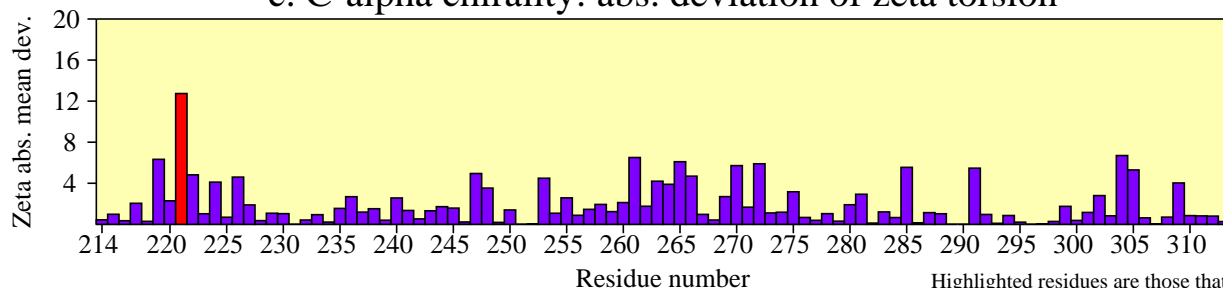
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

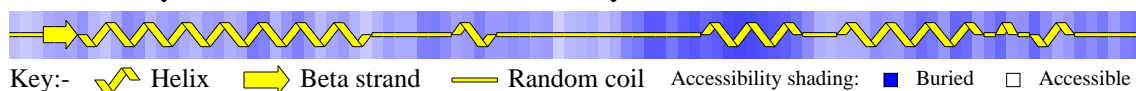


c. C-alpha chirality: abs. deviation of zeta torsion

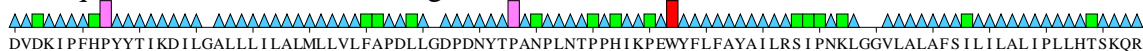


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



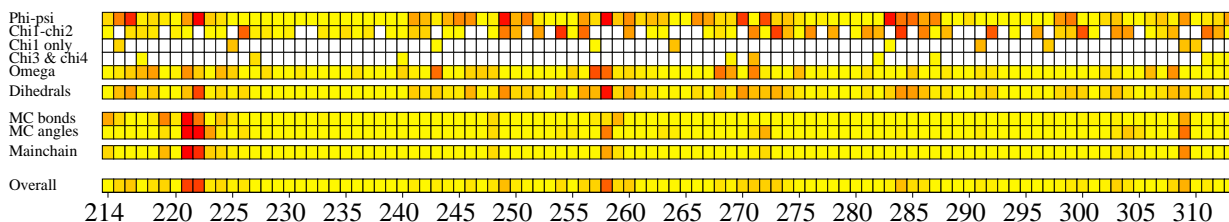
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max* deviation (see listing)

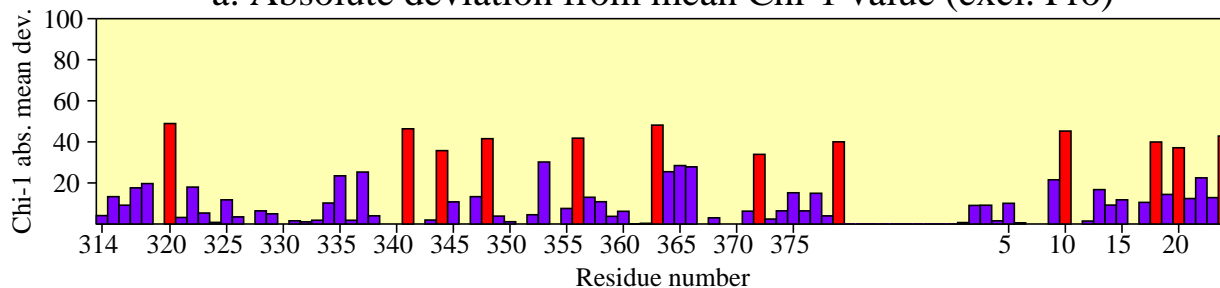


g. G-factors

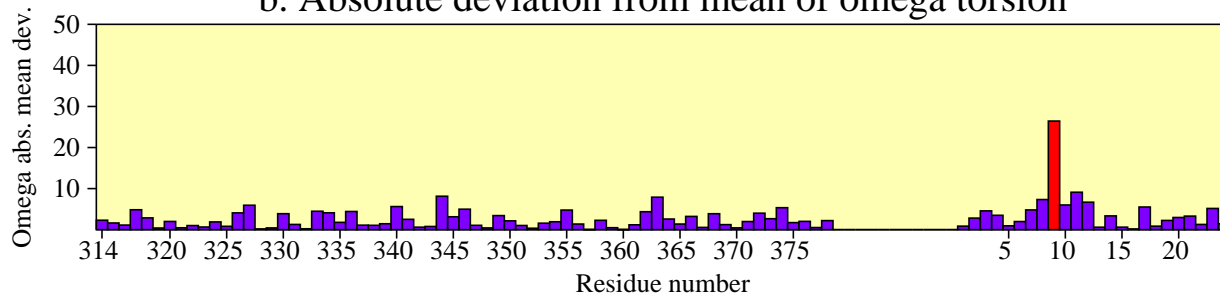


Residue properties 1LOL

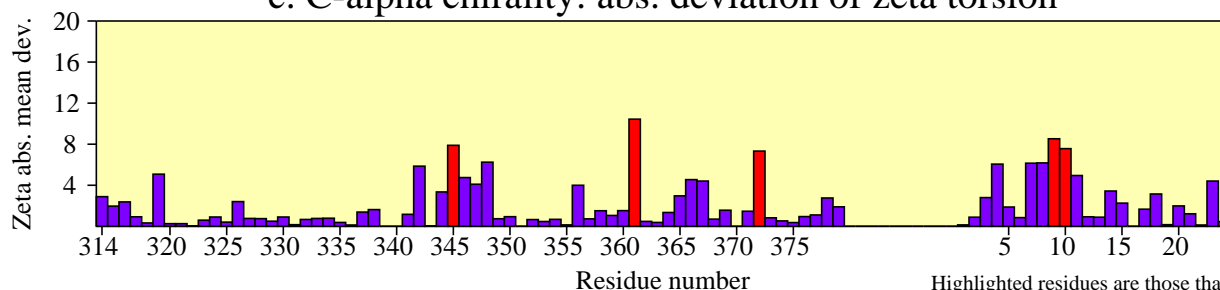
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

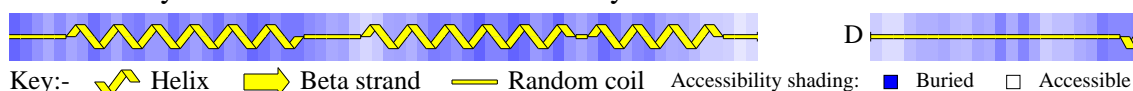


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



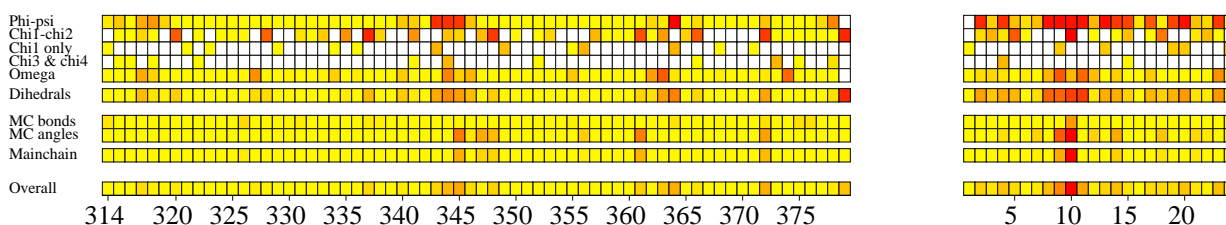
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

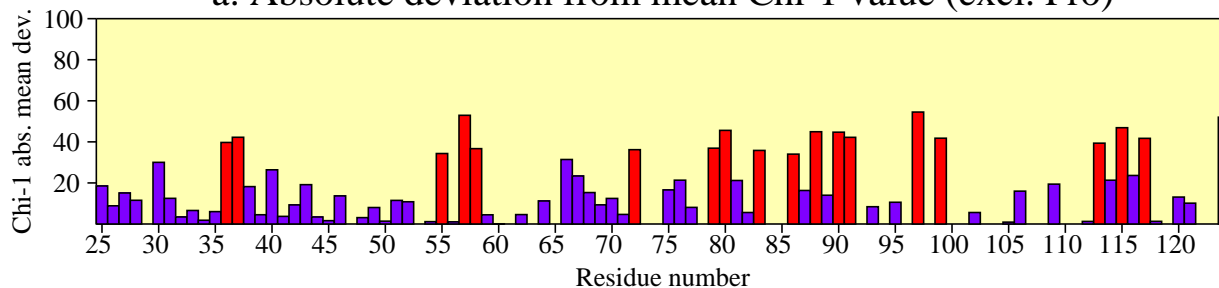


g. G-factors

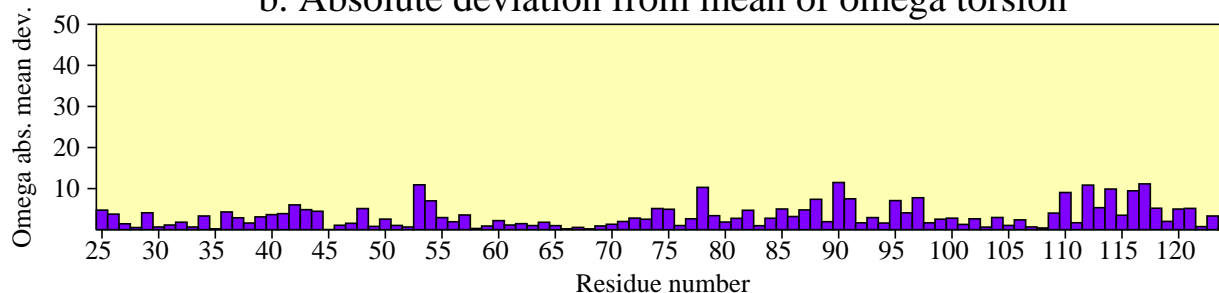


Residue properties 1L0L

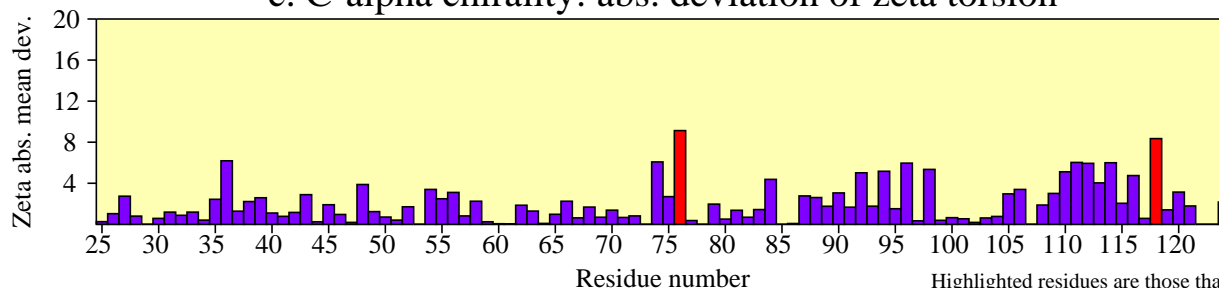
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

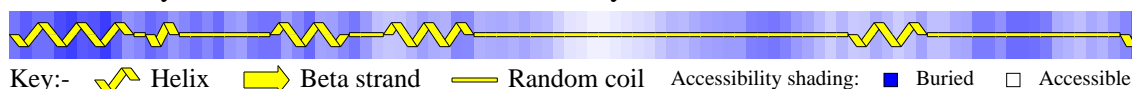


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



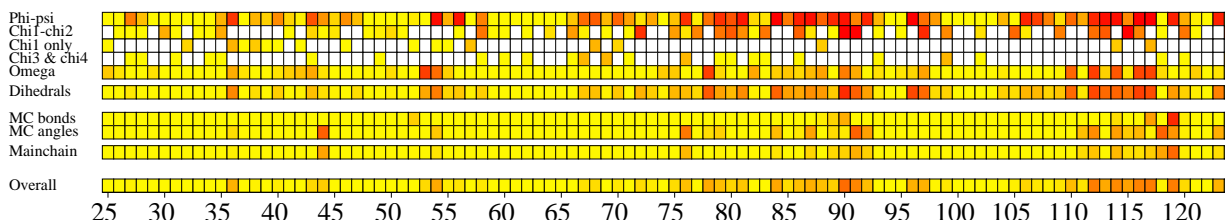
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

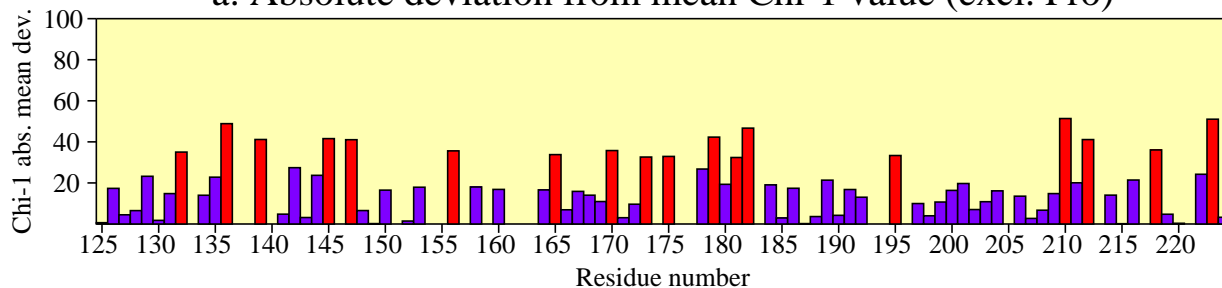


g. G-factors

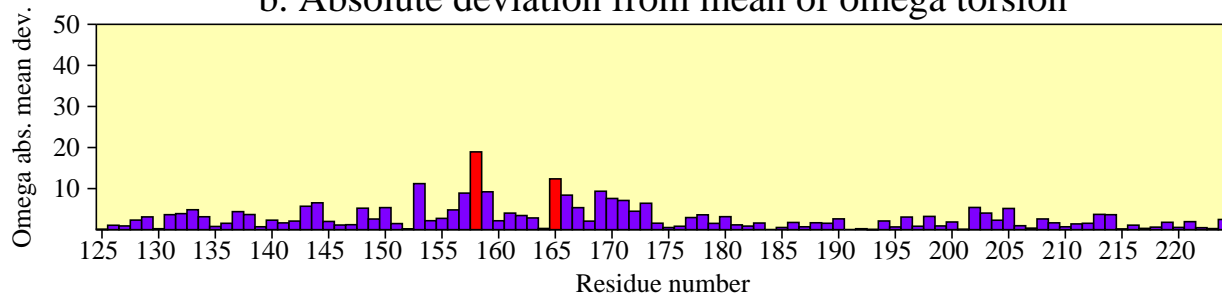


Residue properties 1L0L

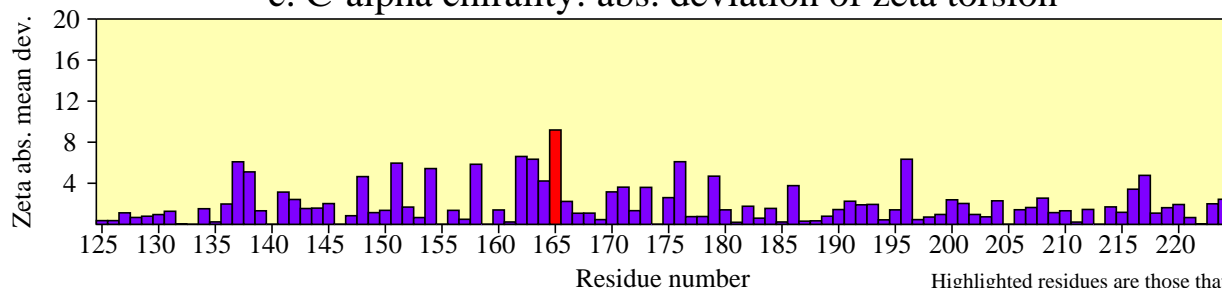
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

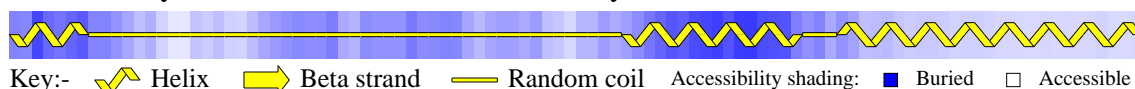


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



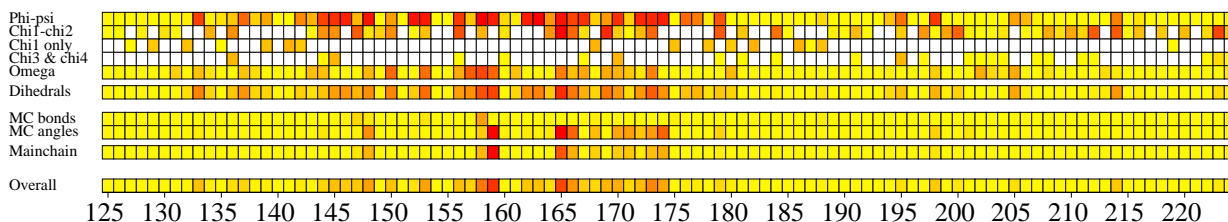
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

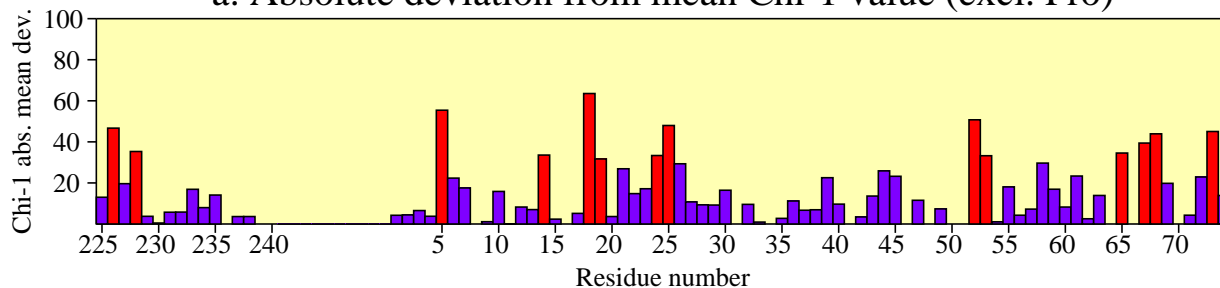


g. G-factors

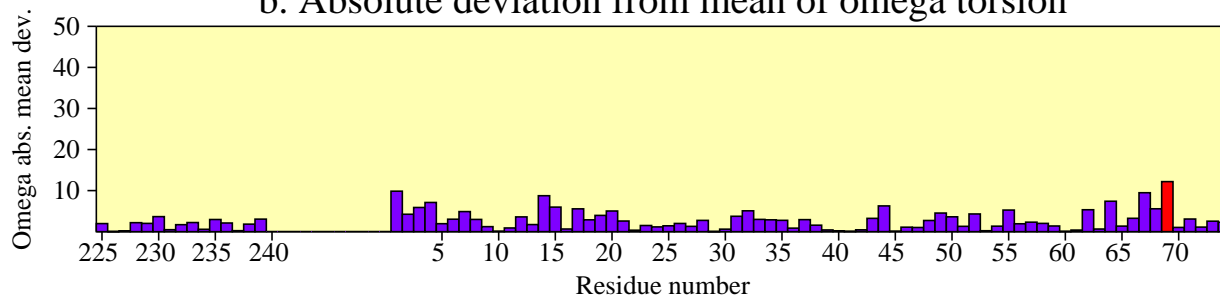


Residue properties 1LOL

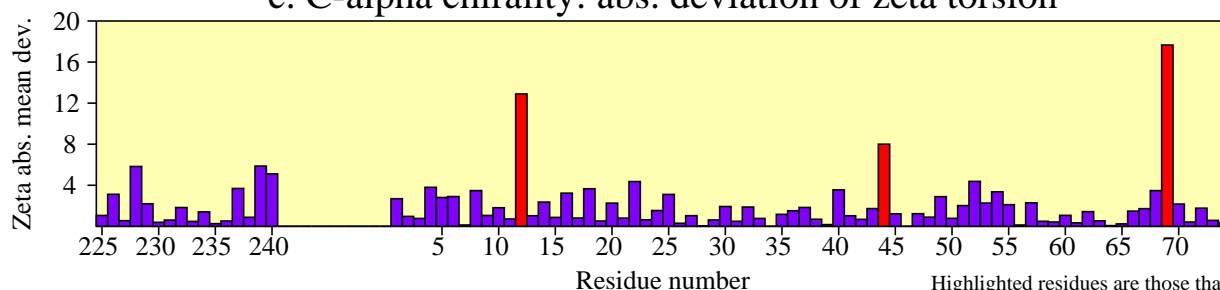
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

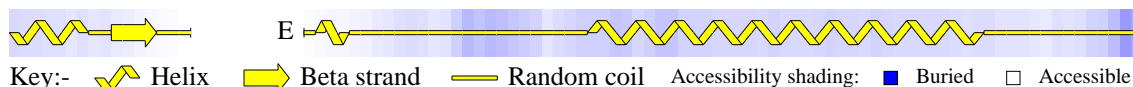


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



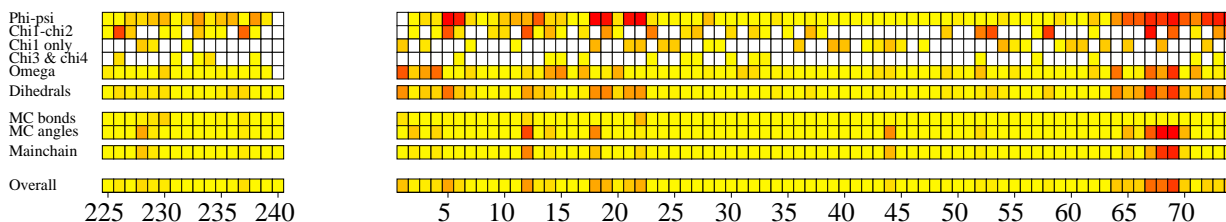
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

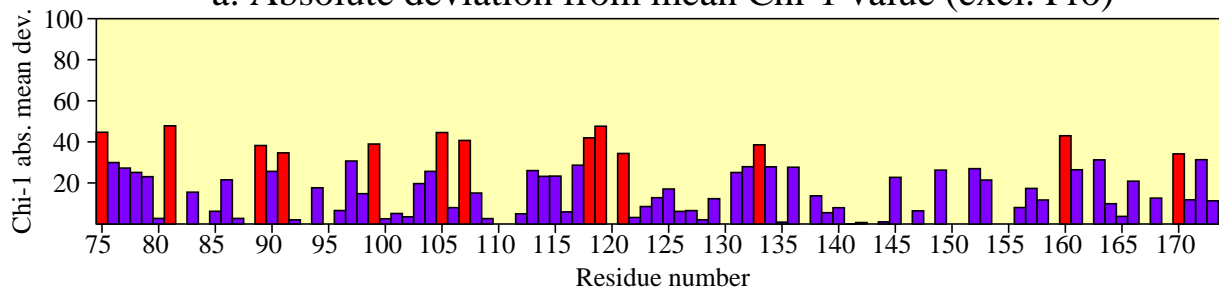


g. G-factors

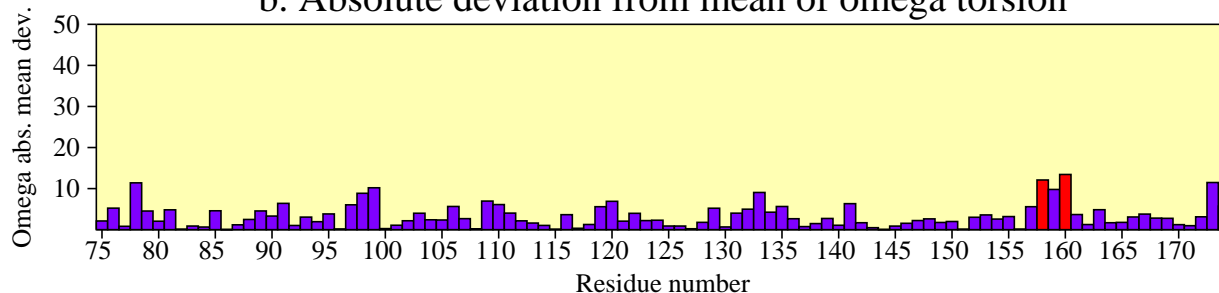


Residue properties 1LOL

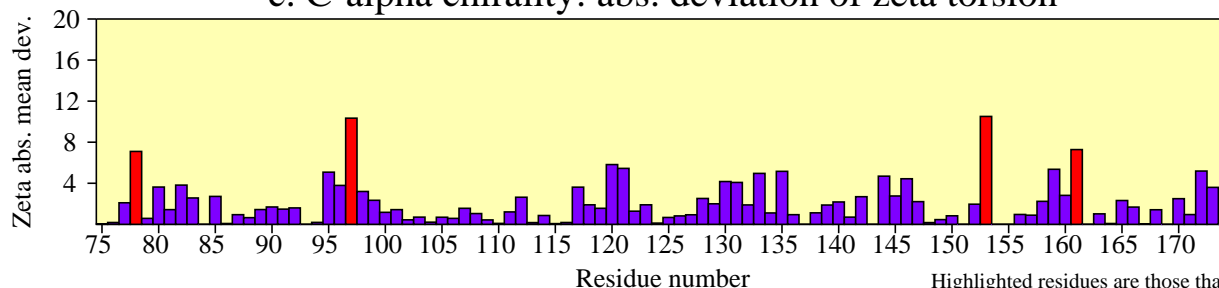
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

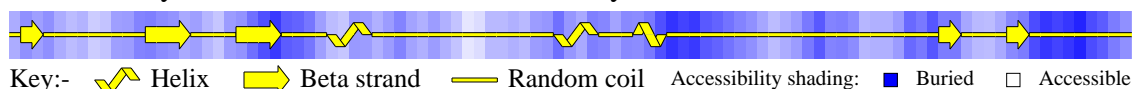


c. C-alpha chirality: abs. deviation of zeta torsion

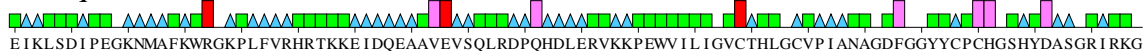


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

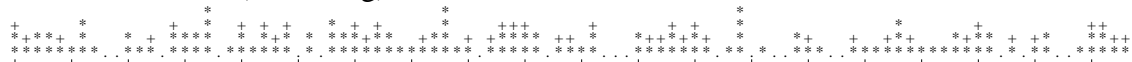
d. Secondary structure & estimated accessibility



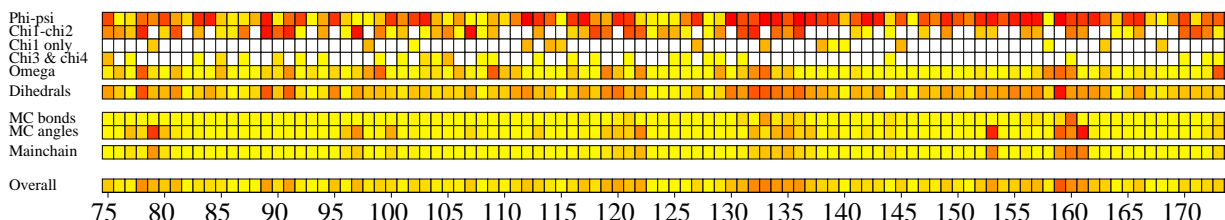
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

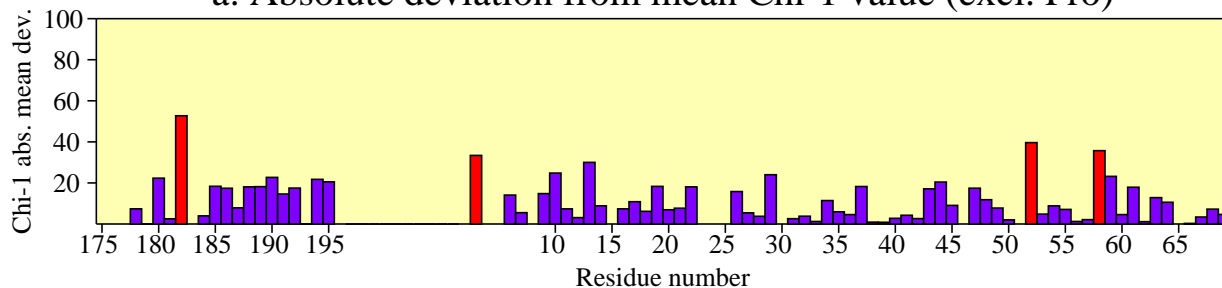


g. G-factors

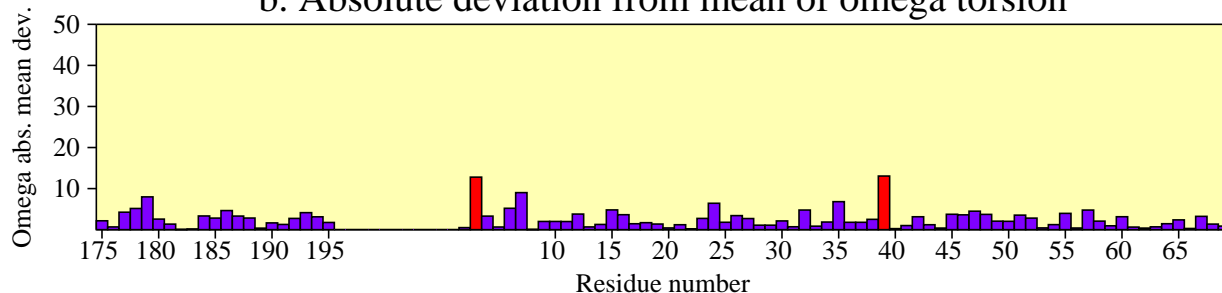


Residue properties 1LOL

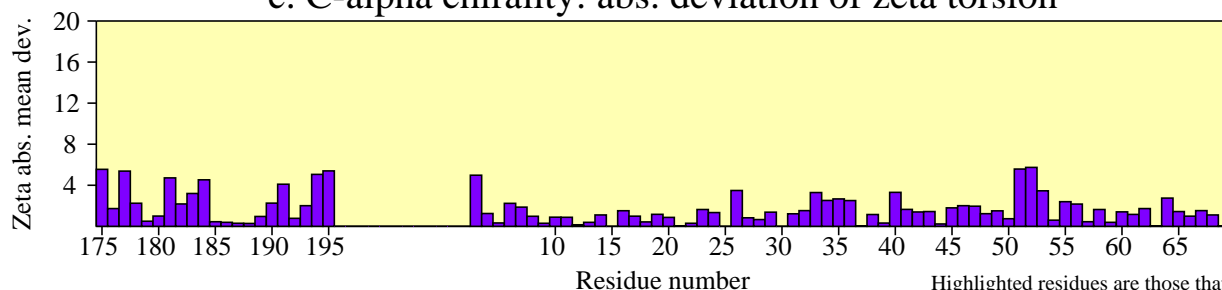
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

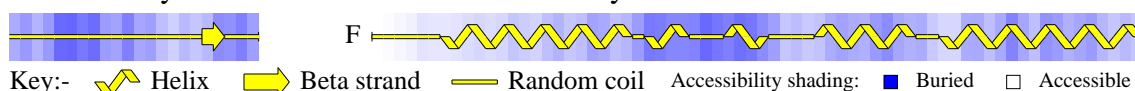


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



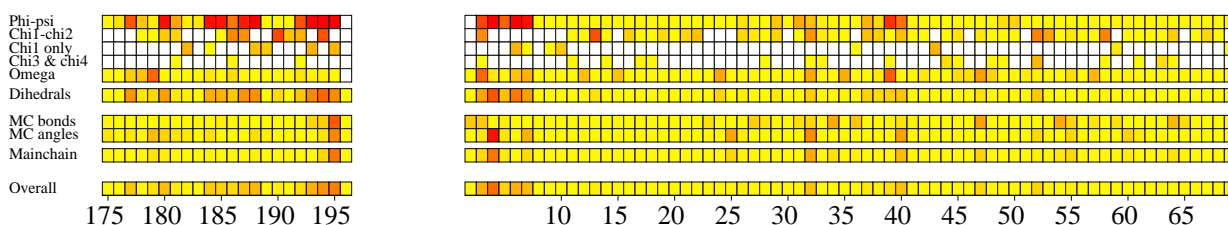
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

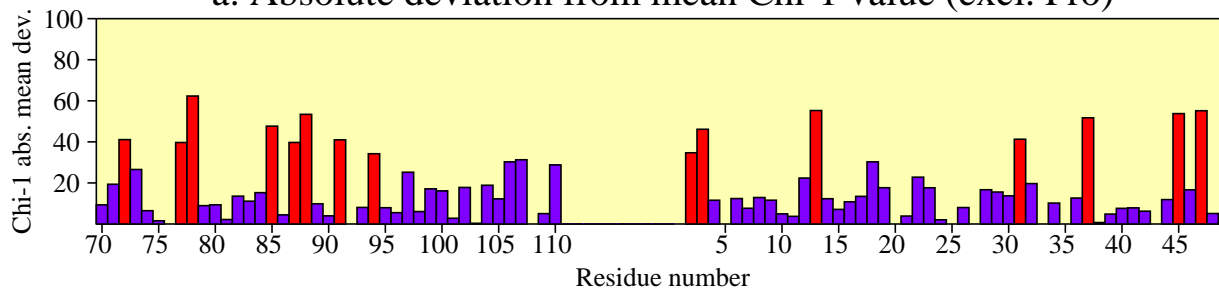


g. G-factors

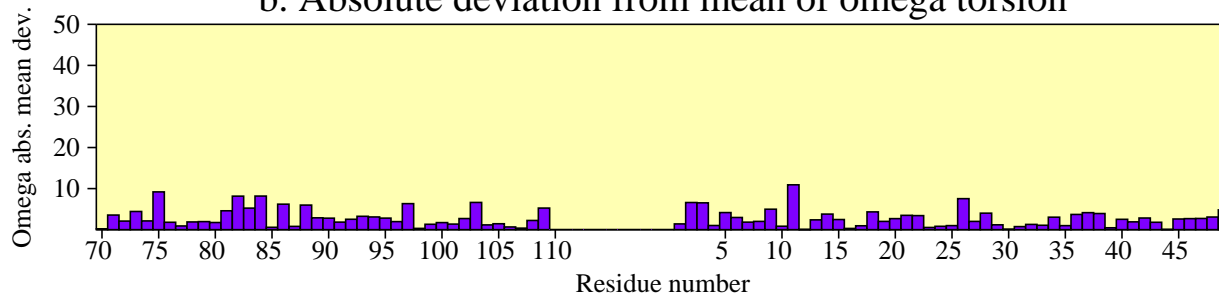


Residue properties 1L0L

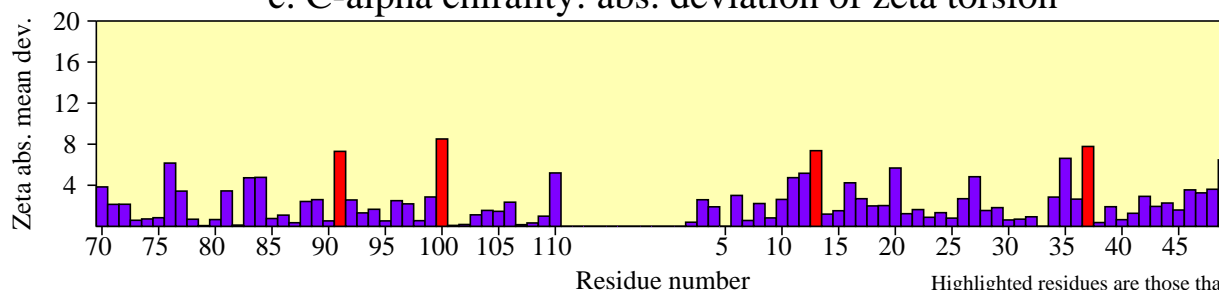
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

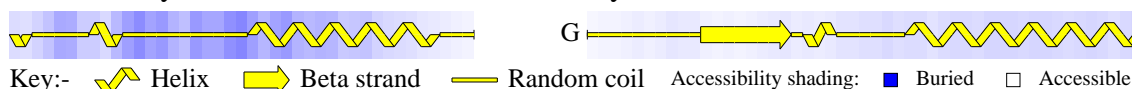


c. C-alpha chirality: abs. deviation of zeta torsion

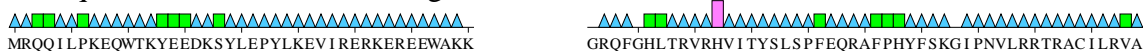


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



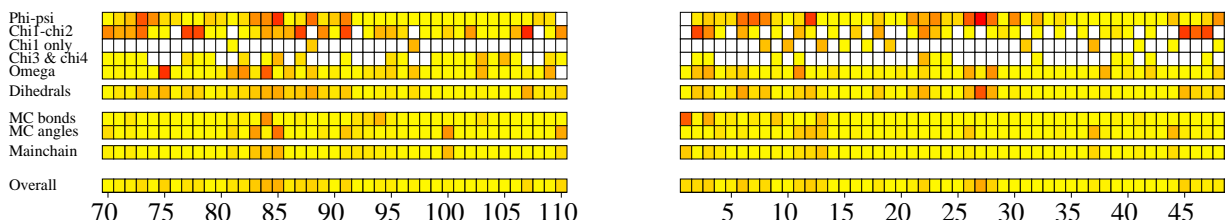
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

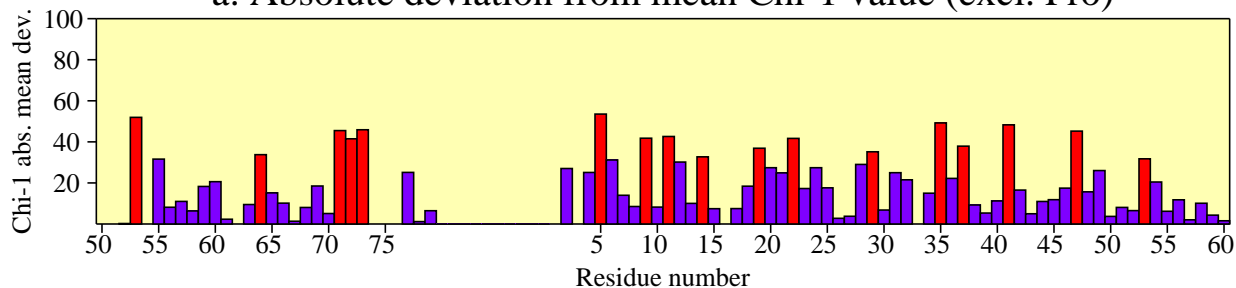


g. G-factors

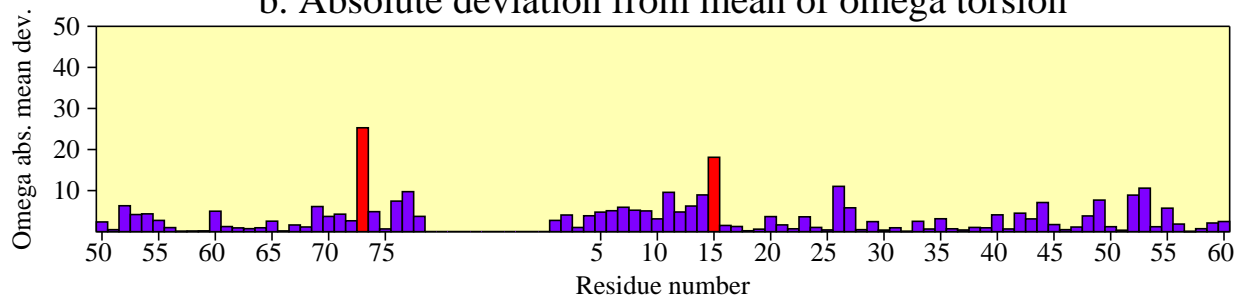


Residue properties 1LOL

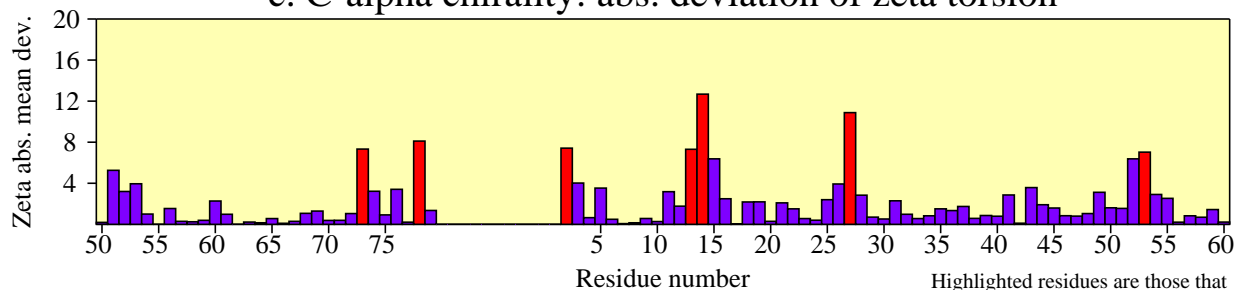
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

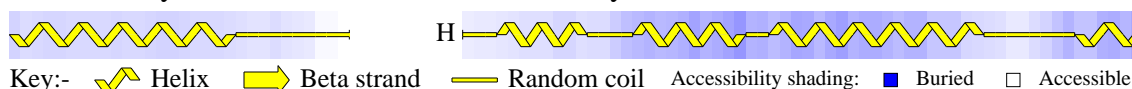


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



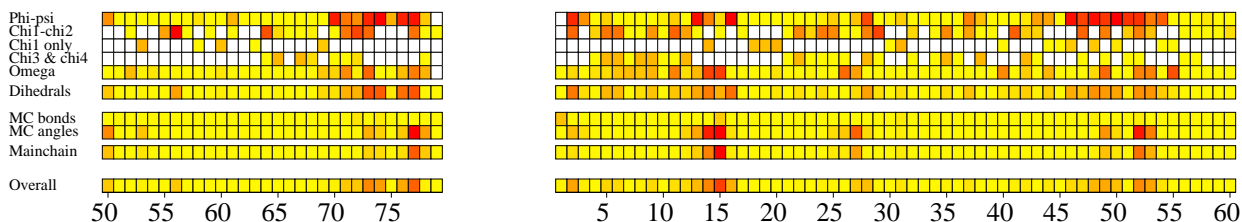
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

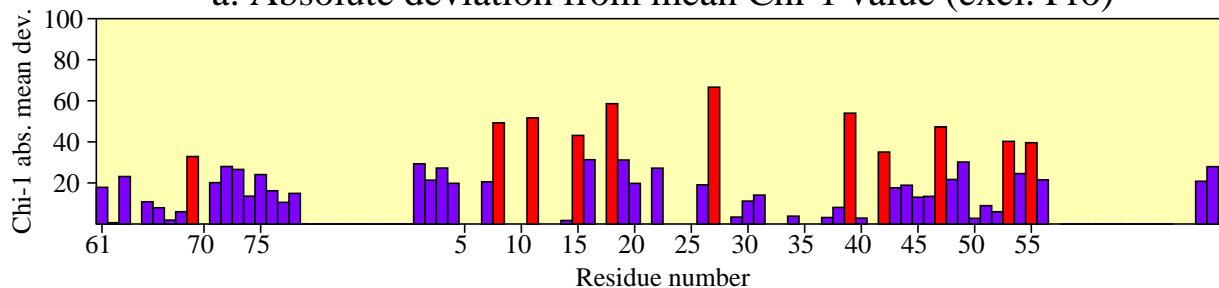


g. G-factors

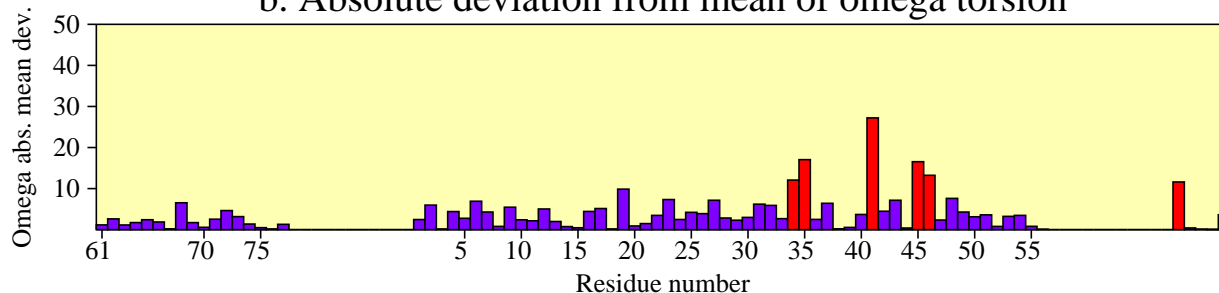


Residue properties 1LOL

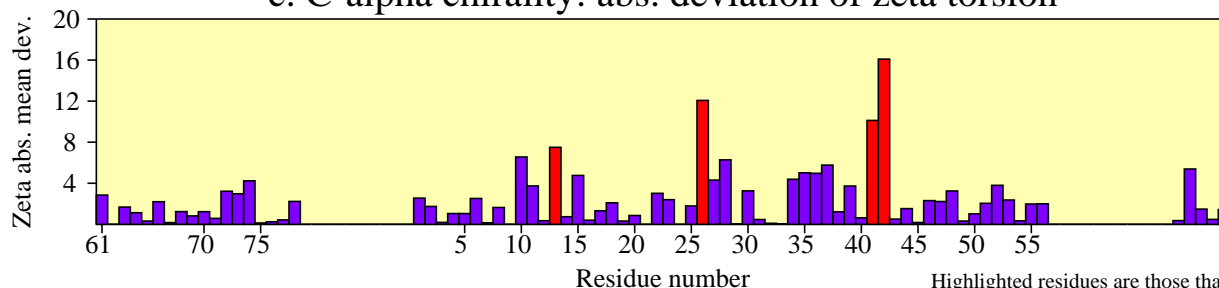
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

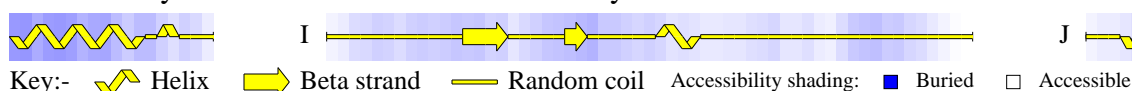


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



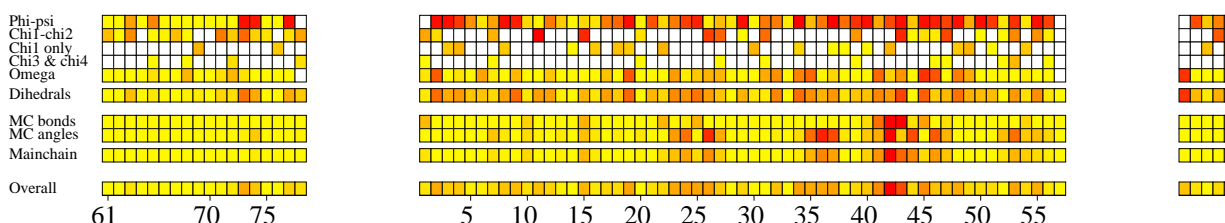
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

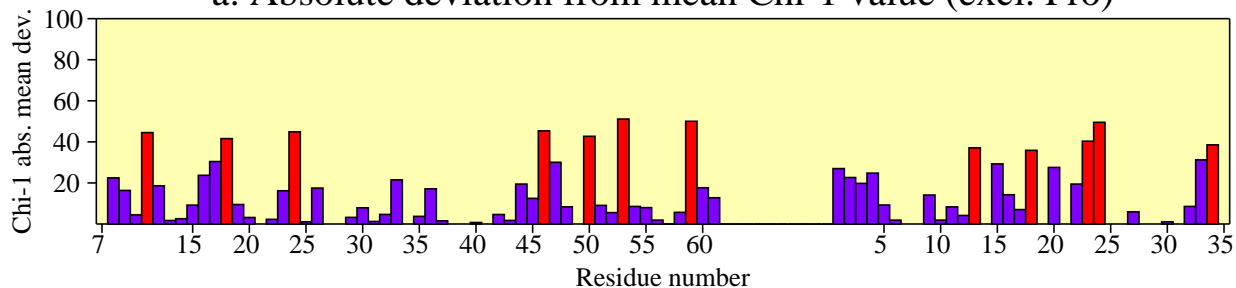


g. G-factors

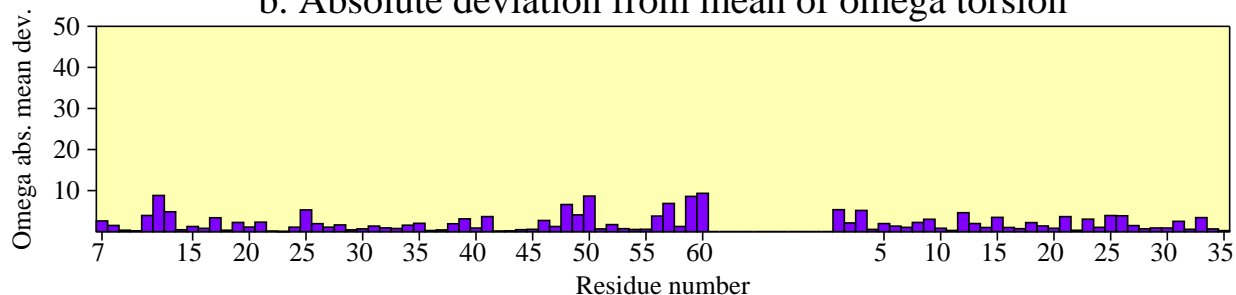


Residue properties 1LOL

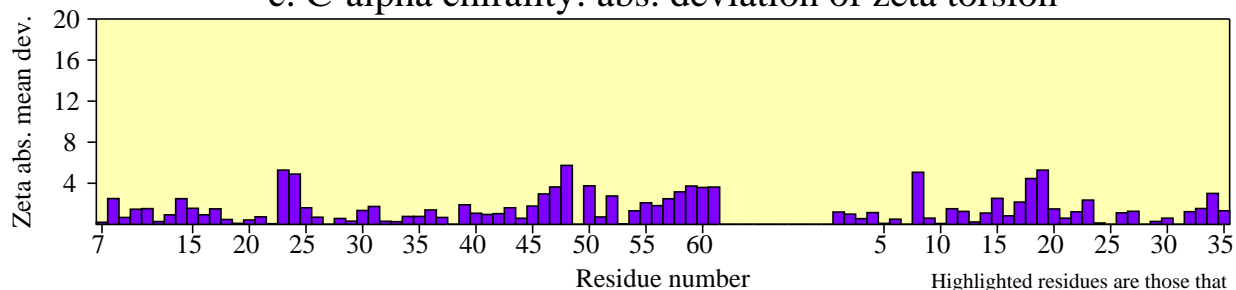
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

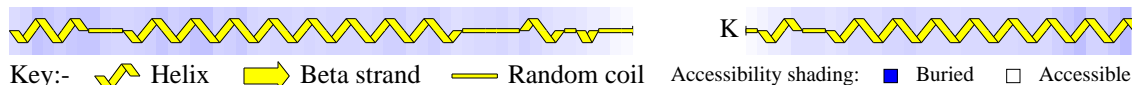


c. C-alpha chirality: abs. deviation of zeta torsion



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

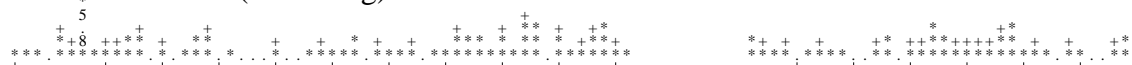
d. Secondary structure & estimated accessibility



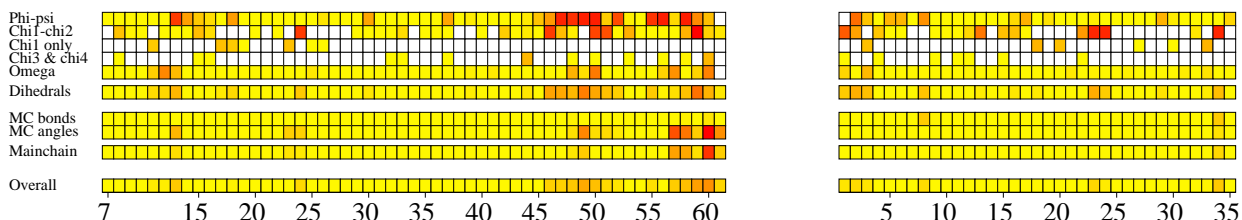
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

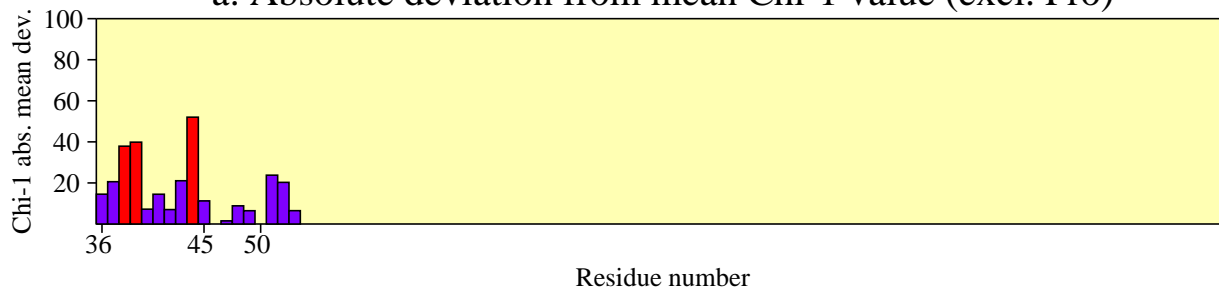


g. G-factors

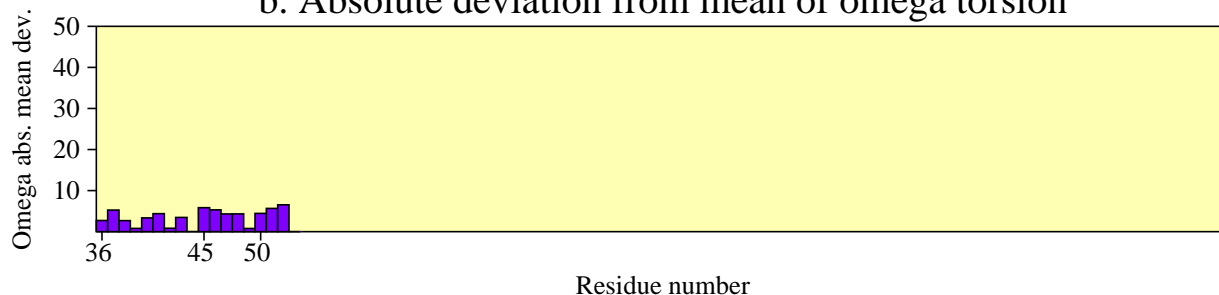


Residue properties 1LOL

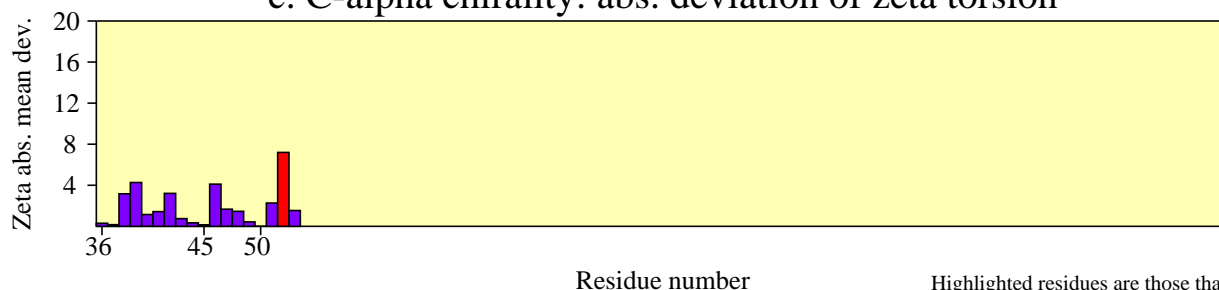
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

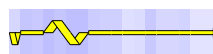


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



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

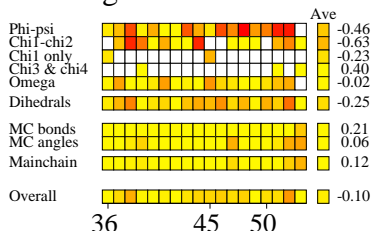
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

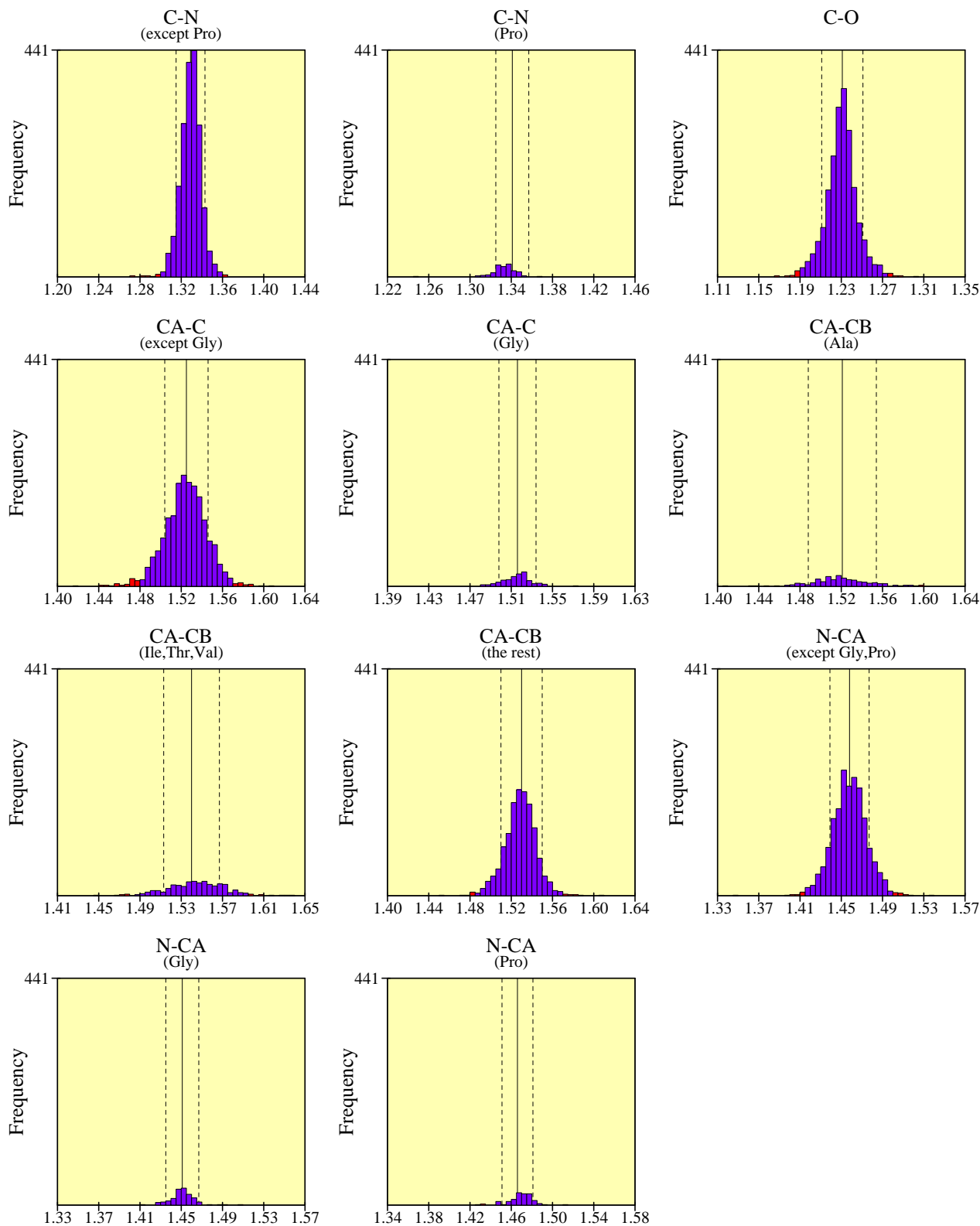


g. G-factors



Main-chain bond lengths

1L0L

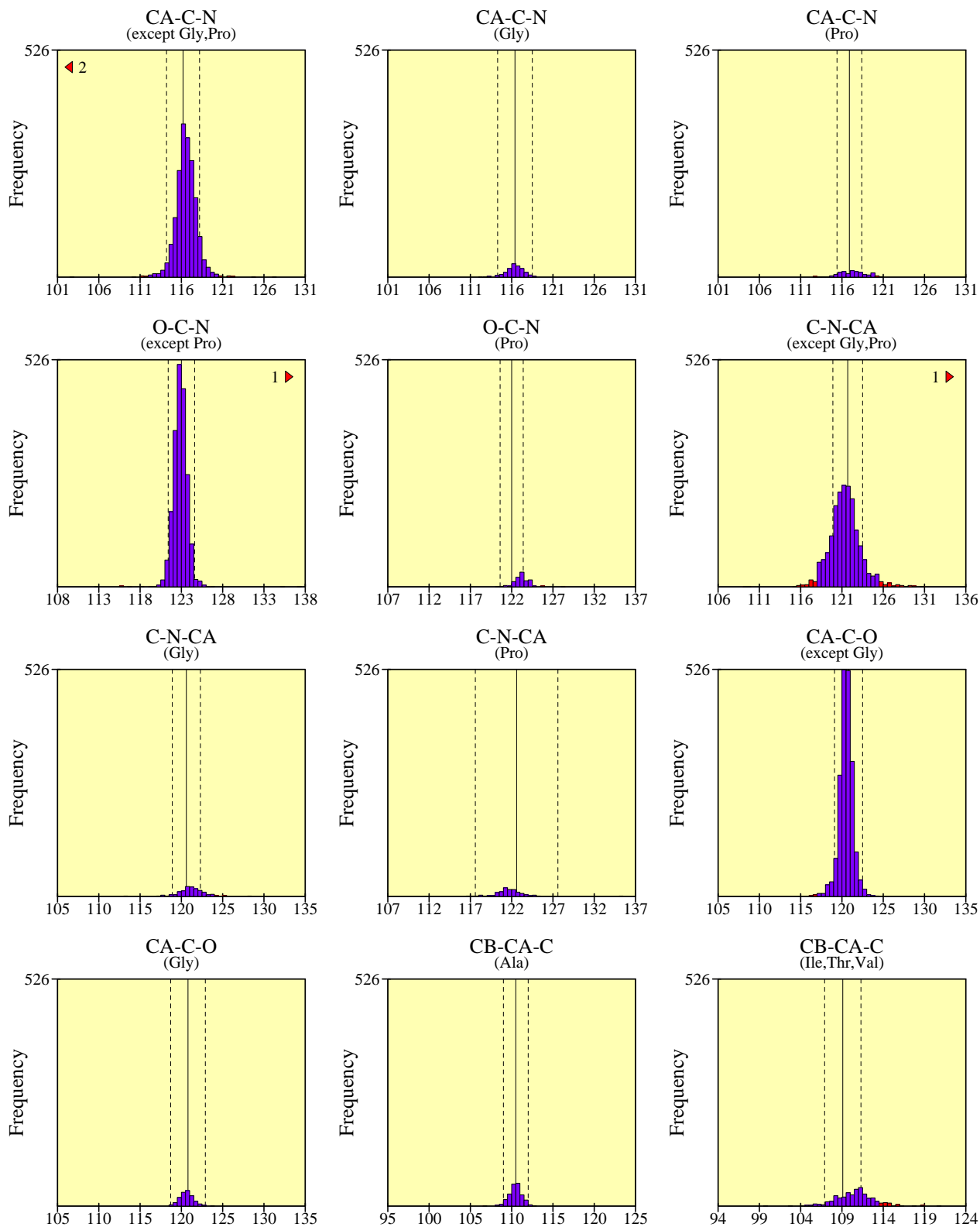


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

1L0L



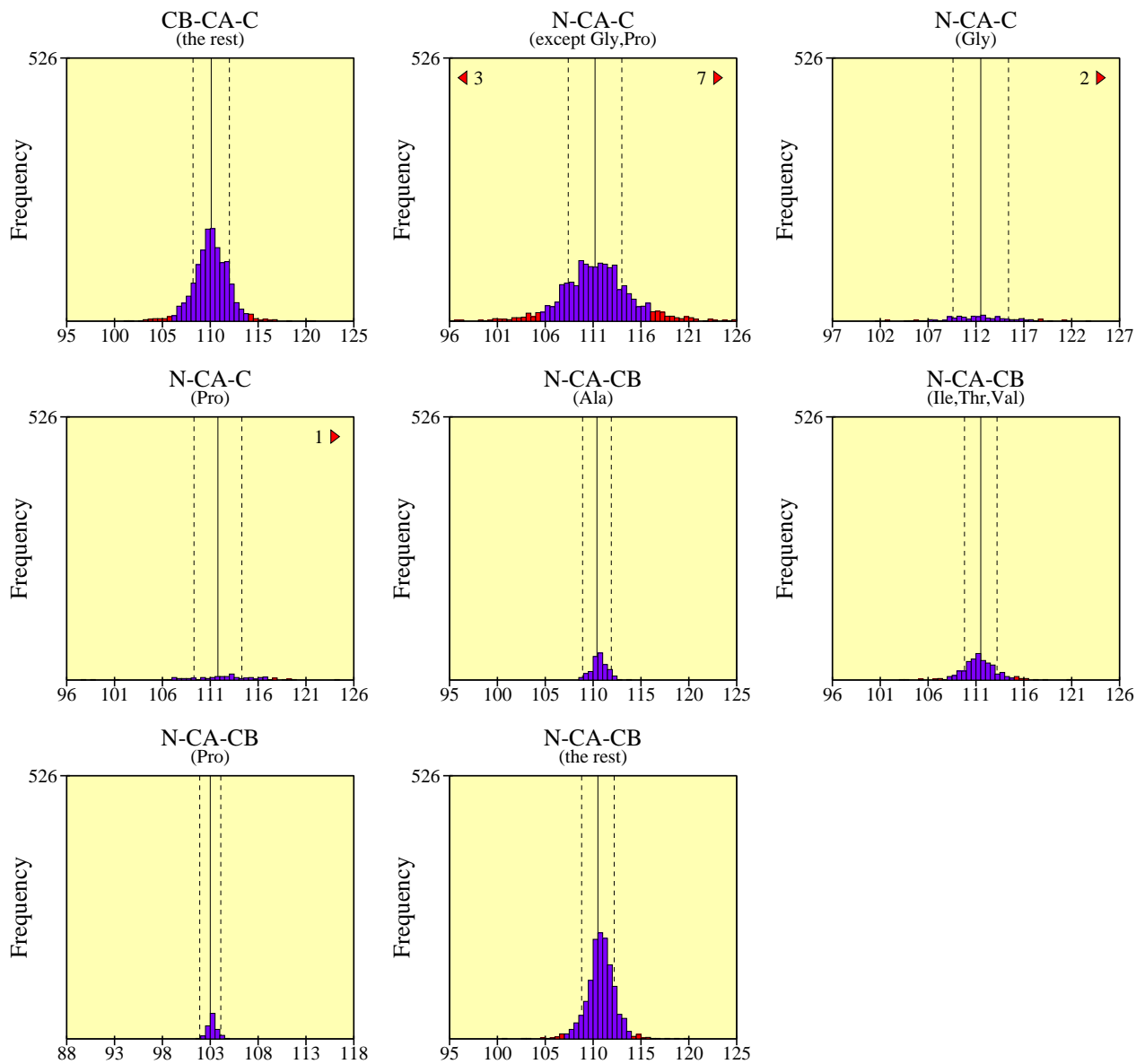
Black bars > 2.0 st. devs. from mean.

◀ 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

1LOL

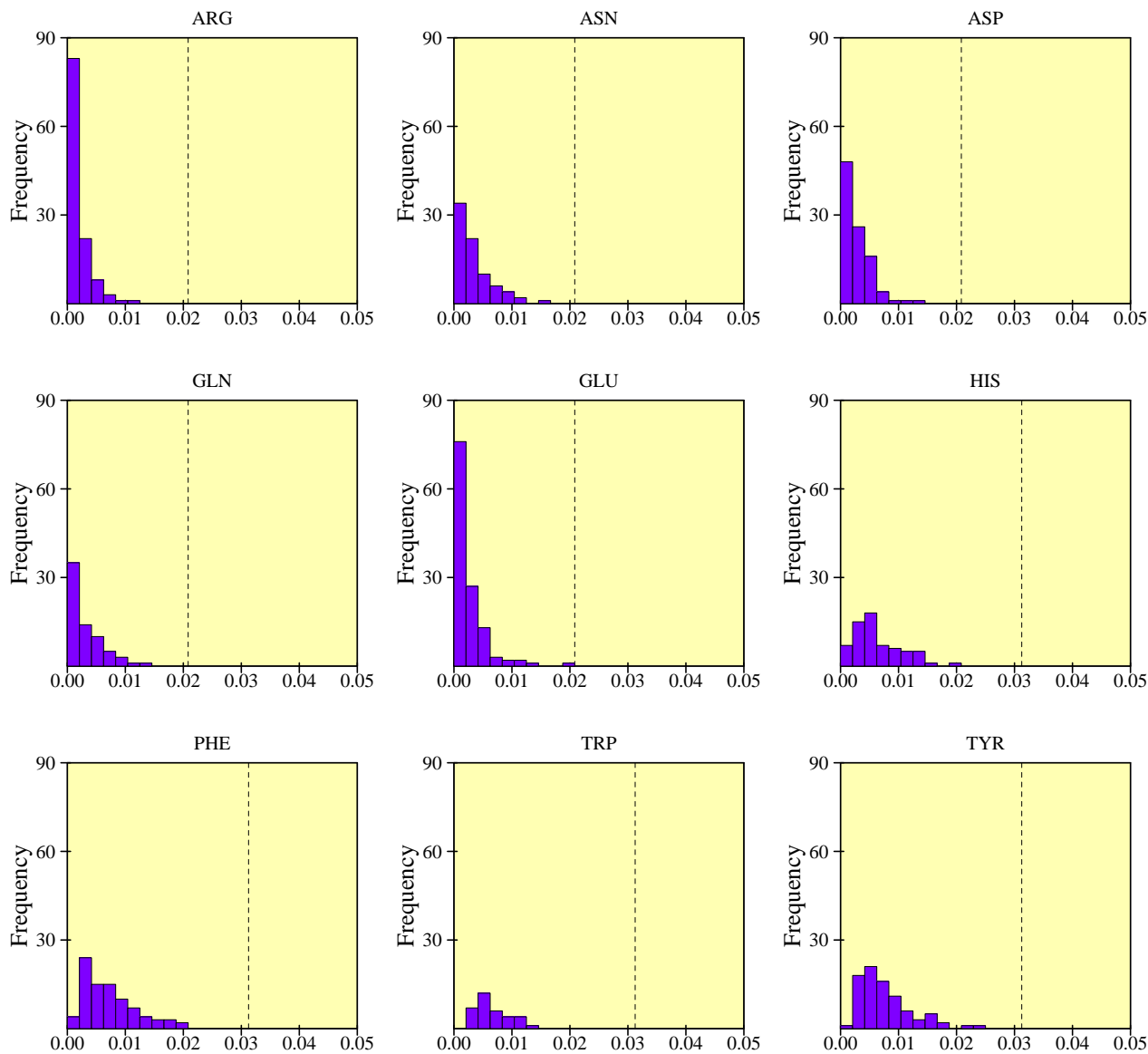


Black bars > 2.0 st. devs. from mean.

◀ 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 1LOL



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

1LOL

Main-chain bond lengths

CA 1.521 CB 0.068 1.589 A Ala 200	CA 1.540 CB 0.088 1.628 A Val 228	N 1.458 CA 0.051 1.509 A Val 228	CA 1.521 CB 0.062 1.459 A Ala 254	CA 1.521 CB 0.078 1.599 A Ala 275	N 1.458 CA 0.058 1.400 A Asp 281
CA 1.540 CB 0.067 1.473 A Thr 309	CA 1.525 C 0.051 1.474 A Phe 310	CA 1.540 CB 0.067 1.607 A Ile 312	CA 1.525 C 0.055 1.470 A Cys 313	CA 1.525 C 0.067 1.458 A Ile 331	CA 1.540 CB 0.062 1.478 A Val 337
CA 1.540 CB 0.071 1.469 A Thr 347	CA 1.525 C 0.060 1.585 A Ser 348	CA 1.540 CB 0.056 1.596 A Val 354	CA 1.525 C 0.054 1.579 A Arg 362	CA 1.525 C 0.054 1.471 A Leu 365	CA 1.521 CB 0.076 1.445 A Ala 423
CA 1.540 CB 0.064 1.476 B Thr 27	CA 1.525 C 0.051 1.474 B Ser 45	N 1.458 CA 0.053 1.405 B Arg 46	CA 1.540 CB 0.064 1.476 B Ile 47	CA 1.525 C 0.062 1.587 B Leu 68	C 1.329 N 0.056 1.273 B Lys 78 - B Gly 79
CA 1.521 CB 0.056 1.465 B Ala 80	CA 1.540 CB 0.093 1.447 B Thr 86	C 1.231 O 0.055 1.286 B Val 98	CA 1.525 C 0.084 1.441 B Glu 103	C 1.231 O 0.052 1.179 B Thr 127	CA 1.540 CB 0.051 1.489 B Thr 127
N 1.458 CA 0.052 1.510 B Thr 128	CA 1.525 C 0.084 1.609 B Glu 131	CA 1.521 CB 0.062 1.583 B Ala 138	CA 1.521 CB 0.059 1.580 B Ala 139	C 1.231 O 0.065 1.166 B Ala 149	CA 1.521 CB 0.070 1.591 B Ala 157
CA 1.525 C 0.075 1.450 B Leu 163	CA 1.525 C 0.053 1.472 B His 164	CA 1.525 C 0.051 1.474 B Tyr 177	CA 1.525 C 0.062 1.463 B Val 195	CA 1.525 C 0.068 1.457 B Thr 200	CA 1.525 C 0.054 1.471 B Ile 207
CA 1.530 CB 0.053 1.583 B Glu 221	CA 1.525 C 0.085 1.440 B Ile 226	C 1.231 O 0.064 1.167 B Ala 237	CA 1.516 C 0.055 1.571 B Gly 249	CA 1.521 CB 0.088 1.433 B Ala 256	CA 1.540 CB 0.053 1.487 B Val 258
CA 1.525 C 0.054 1.470 B Tyr 296	CA 1.530 CB 0.077 1.452 B Gln 305	CA 1.525 C 0.071 1.454 B Val 309	CA 1.525 C 0.056 1.469 B Ala 314	C 1.231 O 0.070 1.301 B Asp 318	CA 1.525 C 0.063 1.462 B Ser 319
CA 1.525 C 0.053 1.578 B Tyr 325	CA 1.525 C 0.060 1.465 B Ser 328	CA 1.530 CB 0.054 1.584 B Gln 329	CA 1.521 CB 0.077 1.598 B Ala 330	N 1.458 CA 0.051 1.407 B Gln 349	C 1.231 O 0.052 1.179 B Arg 421
CA 1.530 CB 0.077 1.607 B Met 424	CA 1.521 CB 0.086 1.435 B Ala 425	CA 1.525 C 0.068 1.457 C Pro 24	CA 1.525 C 0.054 1.471 C Ala 125	CA 1.525 C 0.055 1.580 C Phe 183	CA 1.521 CB 0.053 1.574 C Ala 191

Distorted geometry

1LOL

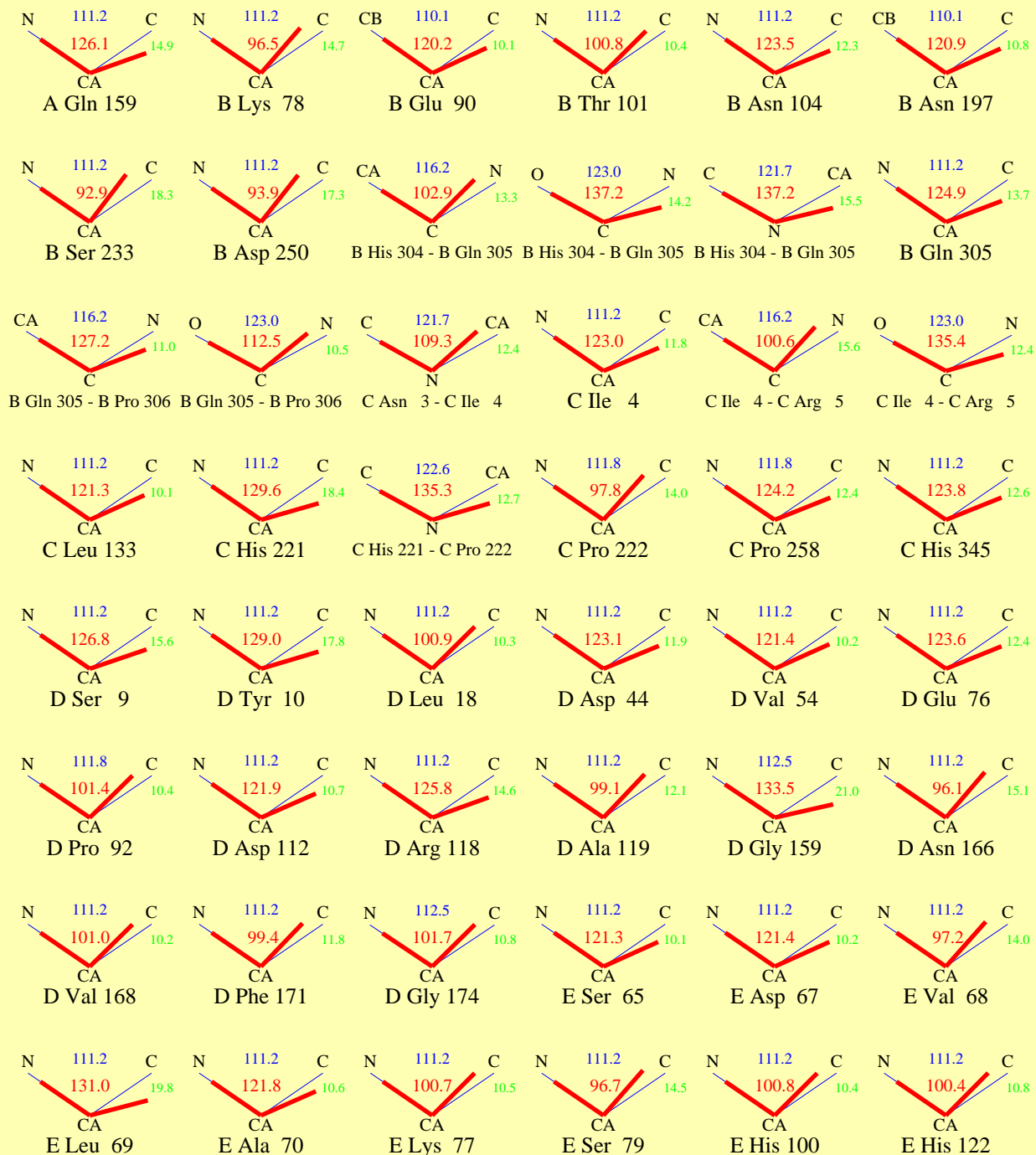
Main-chain bond lengths (contd)

N 1.458 CA 0.058 1.516 C Asp 214	C 1.231 O 0.052 1.283 C Pro 219	CA 1.525 C 0.057 1.468 C His 221	C 1.341 N 0.094 1.247 C His 221 - C Pro 222	CA 1.525 C 0.074 1.599 C Pro 222	CA 1.525 C 0.055 1.470 C Tyr 224
CA 1.525 C 0.051 1.474 C Asp 248	CA 1.525 C 0.055 1.470 C Ala 259	CA 1.521 CB 0.068 1.589 C Ala 259	N 1.458 CA 0.055 1.403 C Thr 309	CA 1.521 CB 0.057 1.578 C Ala 327	CA 1.540 CB 0.051 1.591 C Val 364
CA 1.525 C 0.058 1.583 D Tyr 10	N 1.458 CA 0.054 1.512 D Tyr 90	CA 1.540 CB 0.099 1.639 D Val 117	CA 1.525 C 0.108 1.417 D Ala 119	CA 1.540 CB 0.091 1.631 D Ile 158	CA 1.540 CB 0.058 1.598 D Thr 175
CA 1.540 CB 0.076 1.616 E Thr 22	CA 1.540 CB 0.052 1.592 E Val 45	CA 1.540 CB 0.051 1.591 E Val 68	N 1.458 CA 0.056 1.514 E Val 133	CA 1.530 CB 0.058 1.472 E Cys 160	CA 1.540 CB 0.053 1.593 E Val 195
N 1.458 CA 0.078 1.536 E Val 195	CA 1.525 C 0.059 1.584 F Arg 3	CA 1.530 CB 0.052 1.478 F Asn 27	CA 1.525 C 0.058 1.583 F Asp 34	CA 1.525 C 0.052 1.473 F Thr 36	CA 1.525 C 0.051 1.576 F Asn 40
CA 1.540 CB 0.067 1.607 F Ile 47	CA 1.525 C 0.067 1.458 F Leu 54	CA 1.540 CB 0.052 1.592 F Val 59	CA 1.530 CB 0.057 1.587 F Glu 84	CA 1.525 C 0.050 1.575 F Pro 92	N 1.451 CA 0.056 1.507 G Gly 1
CA 1.525 C 0.056 1.469 G Gln 3	CA 1.525 C 0.053 1.472 G Val 13	CA 1.525 C 0.051 1.474 G Lys 72	CA 1.525 C 0.060 1.585 H Asp 15	CA 1.540 CB 0.060 1.600 H Val 31	CA 1.525 C 0.064 1.589 I Val 22
CA 1.521 CB 0.115 1.406 I Ala 25	CA 1.525 C 0.067 1.458 I Pro 41	CA 1.525 C 0.079 1.446 I Val 42	CA 1.540 CB 0.066 1.474 I Val 42	C 1.329 N 0.055 1.274 I Val 42 - I Leu 43	N 1.458 CA 0.108 1.350 I Leu 43
N 1.458 CA 0.051 1.509 I Leu 45	CA 1.525 C 0.054 1.579 I Arg 47	CA 1.525 C 0.051 1.576 K Pro 8	CA 1.521 CB 0.052 1.469 K Ala 26	N 1.458 CA 0.052 1.406 K Trp 34	C 1.231 O 0.056 1.287 K Lys 53

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

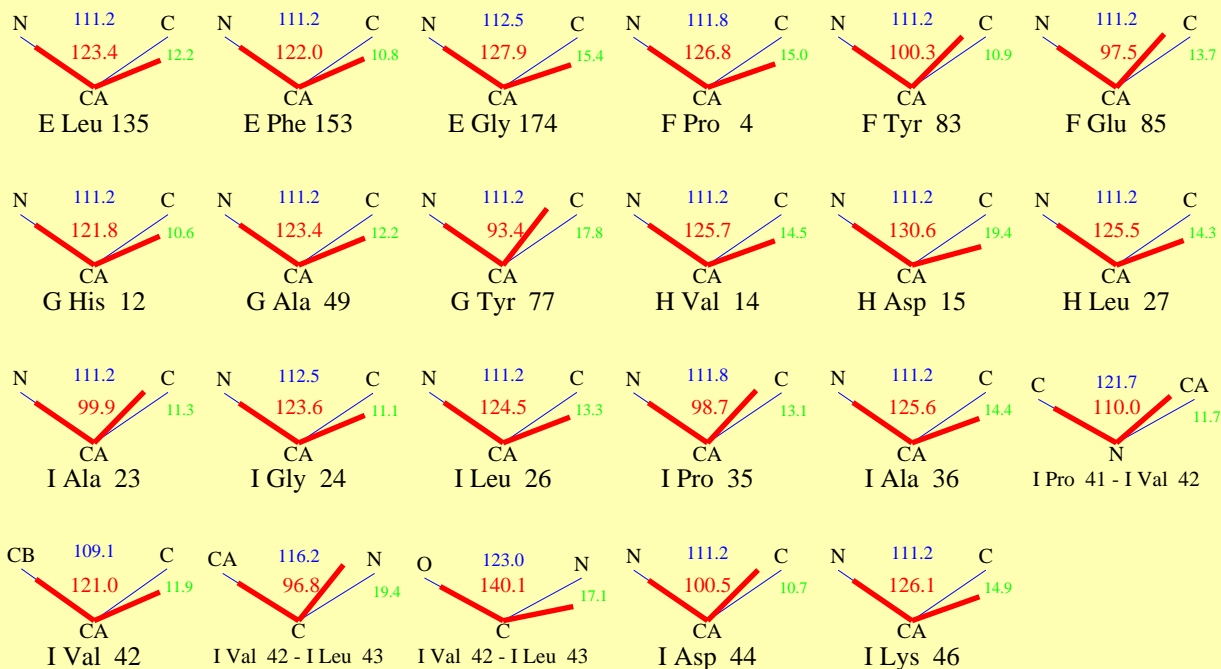
Distorted geometry 1L0L

Main-chain bond angles



Distorted geometry 1L0L

Main-chain bond angles (contd)



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