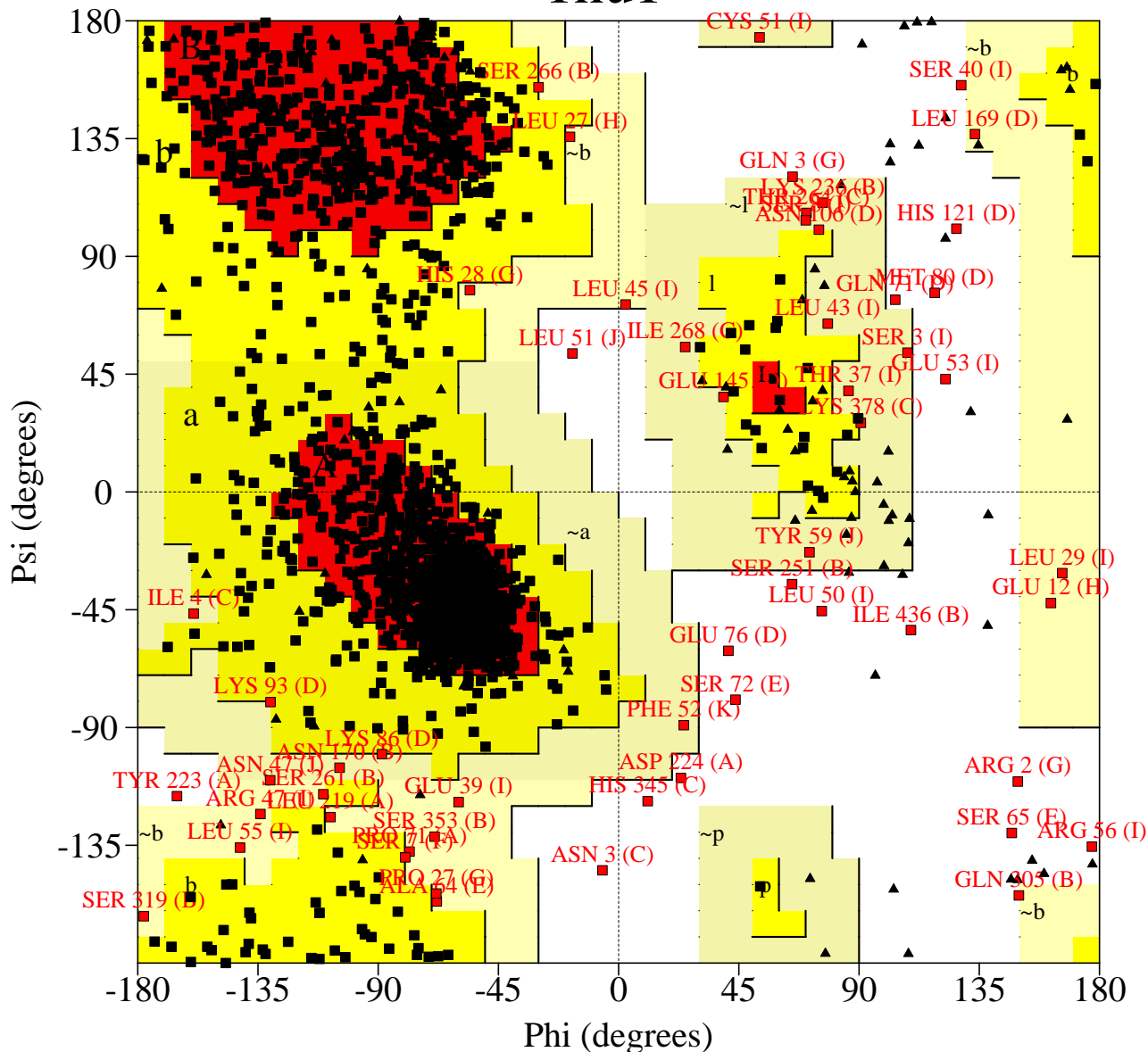


Ramachandran Plot

1nu1



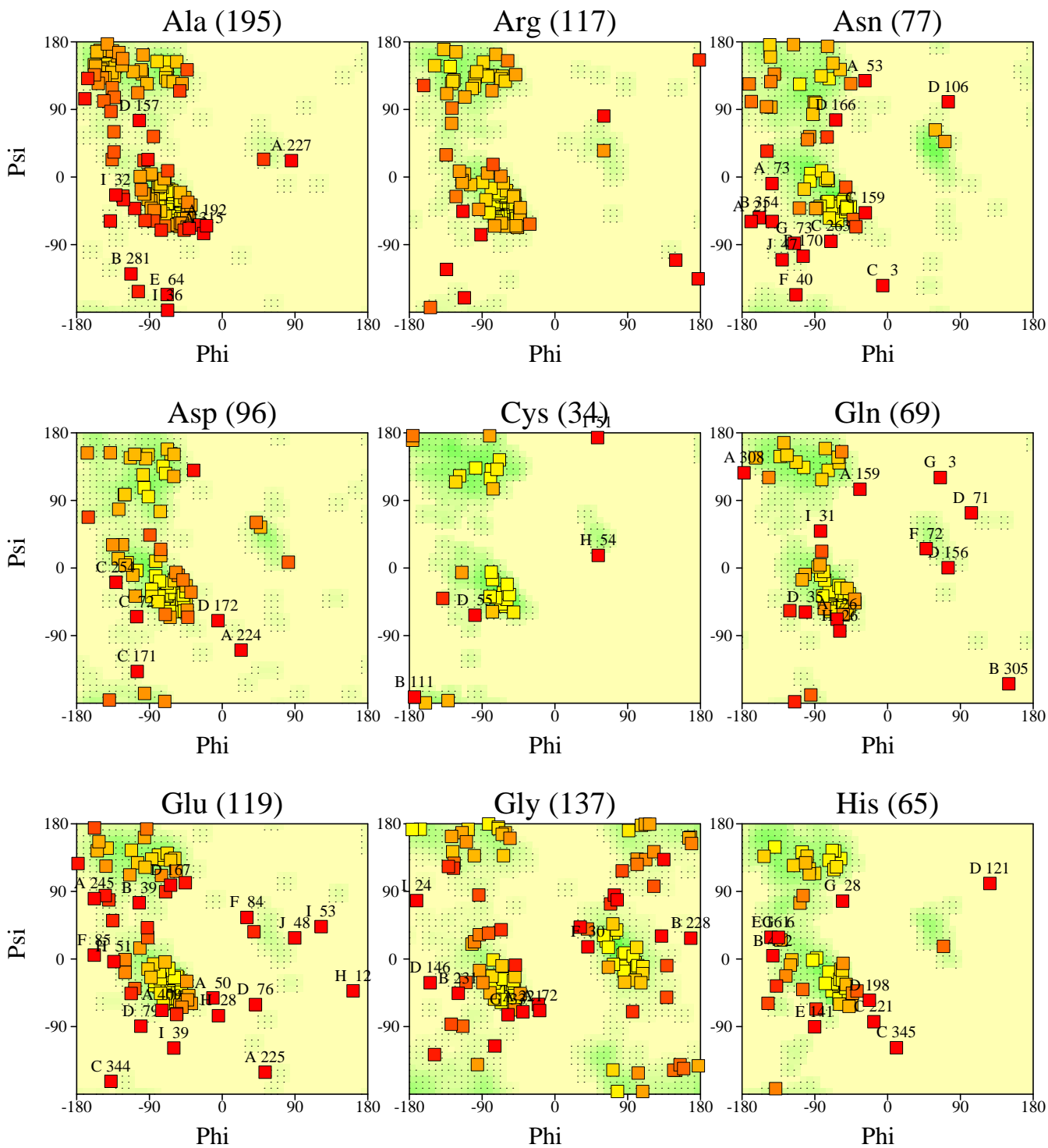
Plot statistics

Residues in most favoured regions [A,B,L]	1467	79.9%
Residues in additional allowed regions [a,b,l,p]	316	17.2%
Residues in generously allowed regions [-a,-b,-l,-p]	34	1.9%
Residues in disallowed regions	20	1.1%
Number of non-glycine and non-proline residues	1837	100.0%
Number of end-residues (excl. Gly and Pro)	19	
Number of glycine residues (shown as triangles)	140	
Number of proline residues	109	
Total number of residues	2105	

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

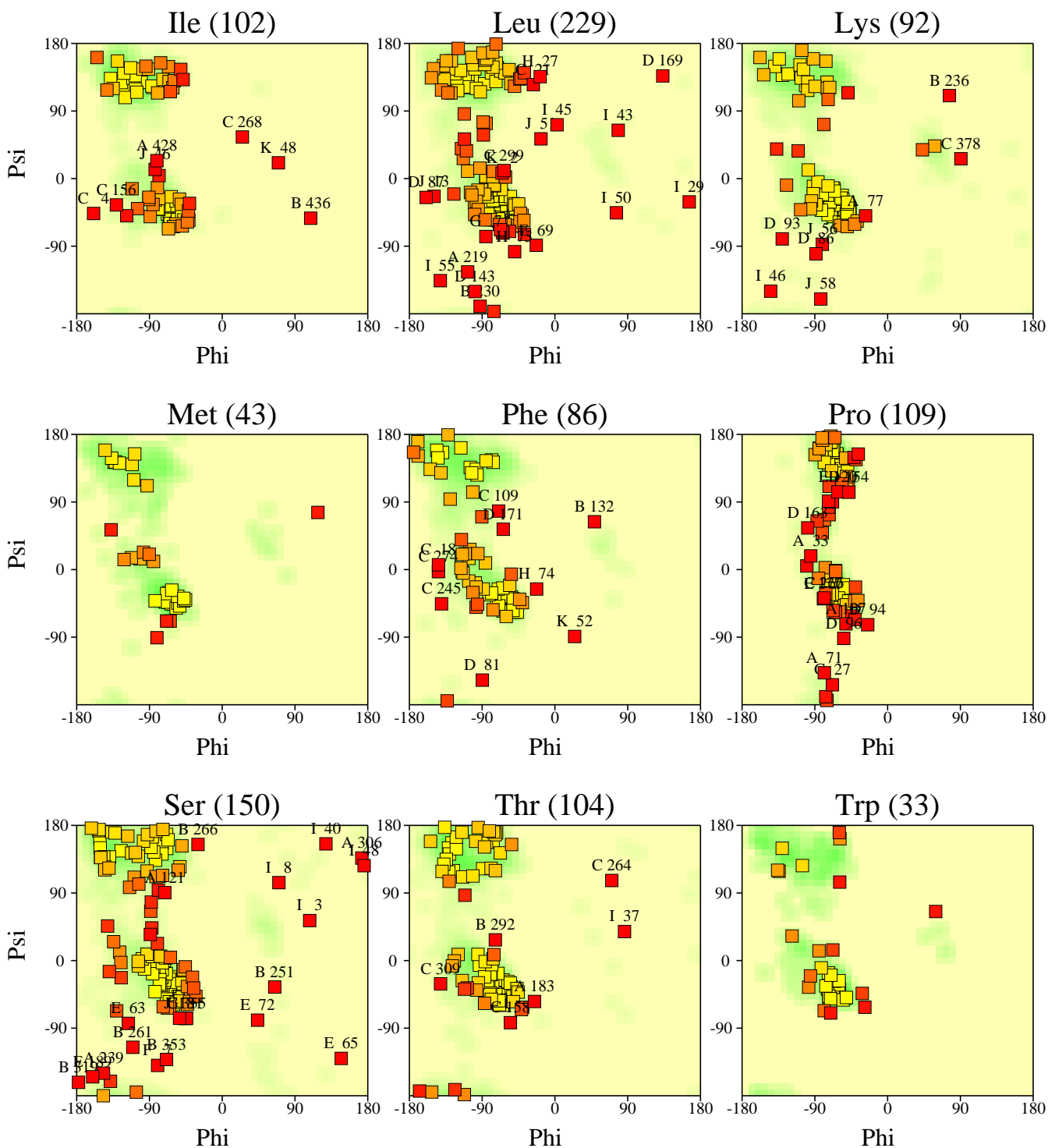
1nu1



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

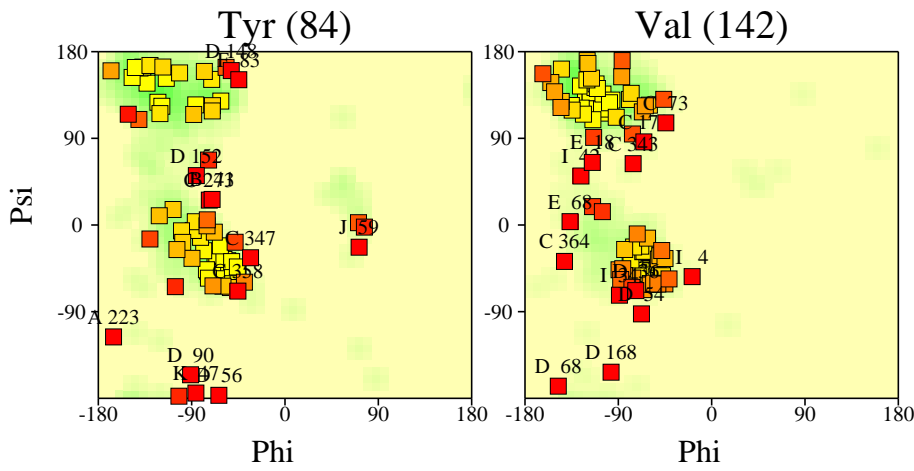
1nu1



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

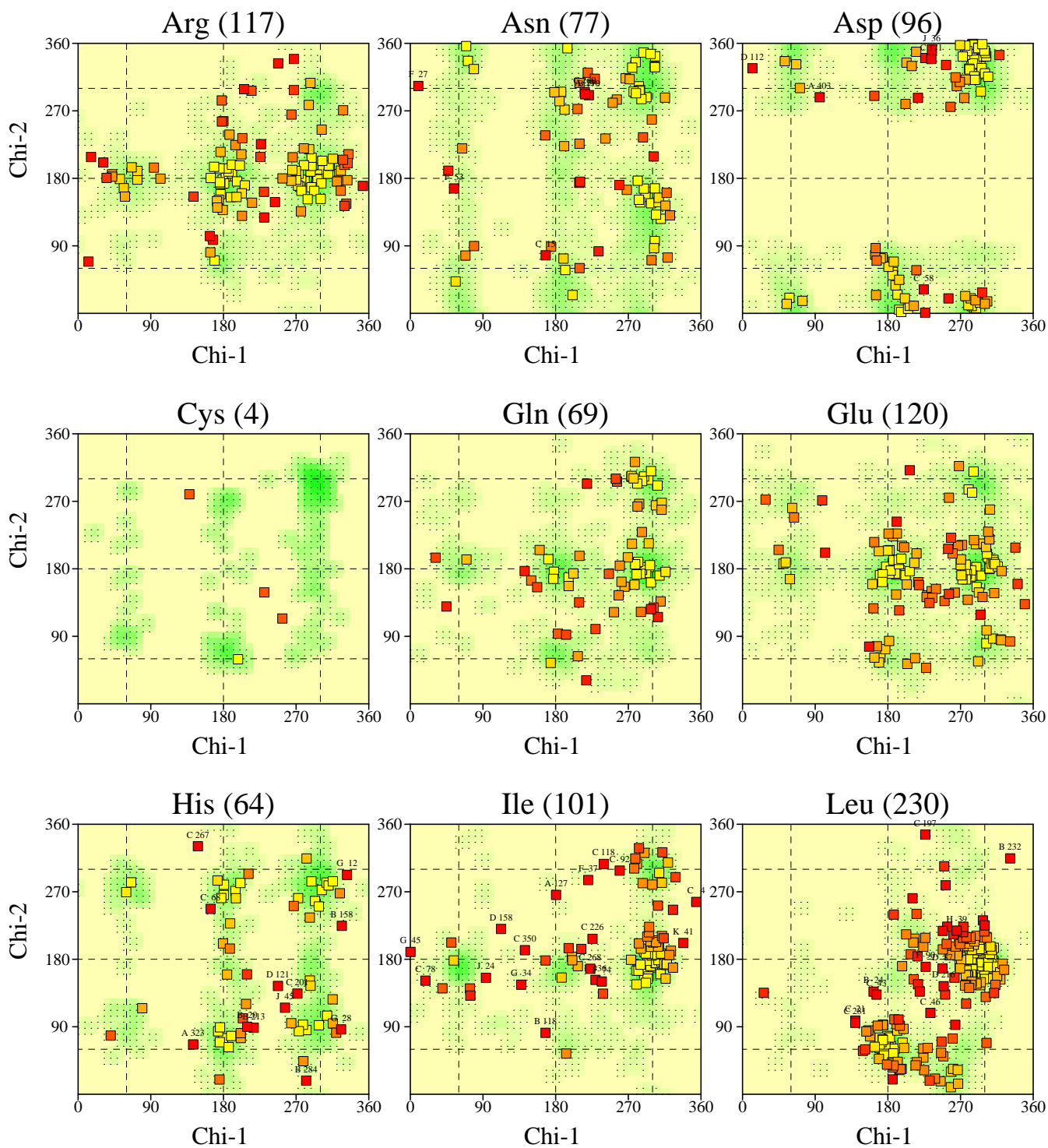
1nu1



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

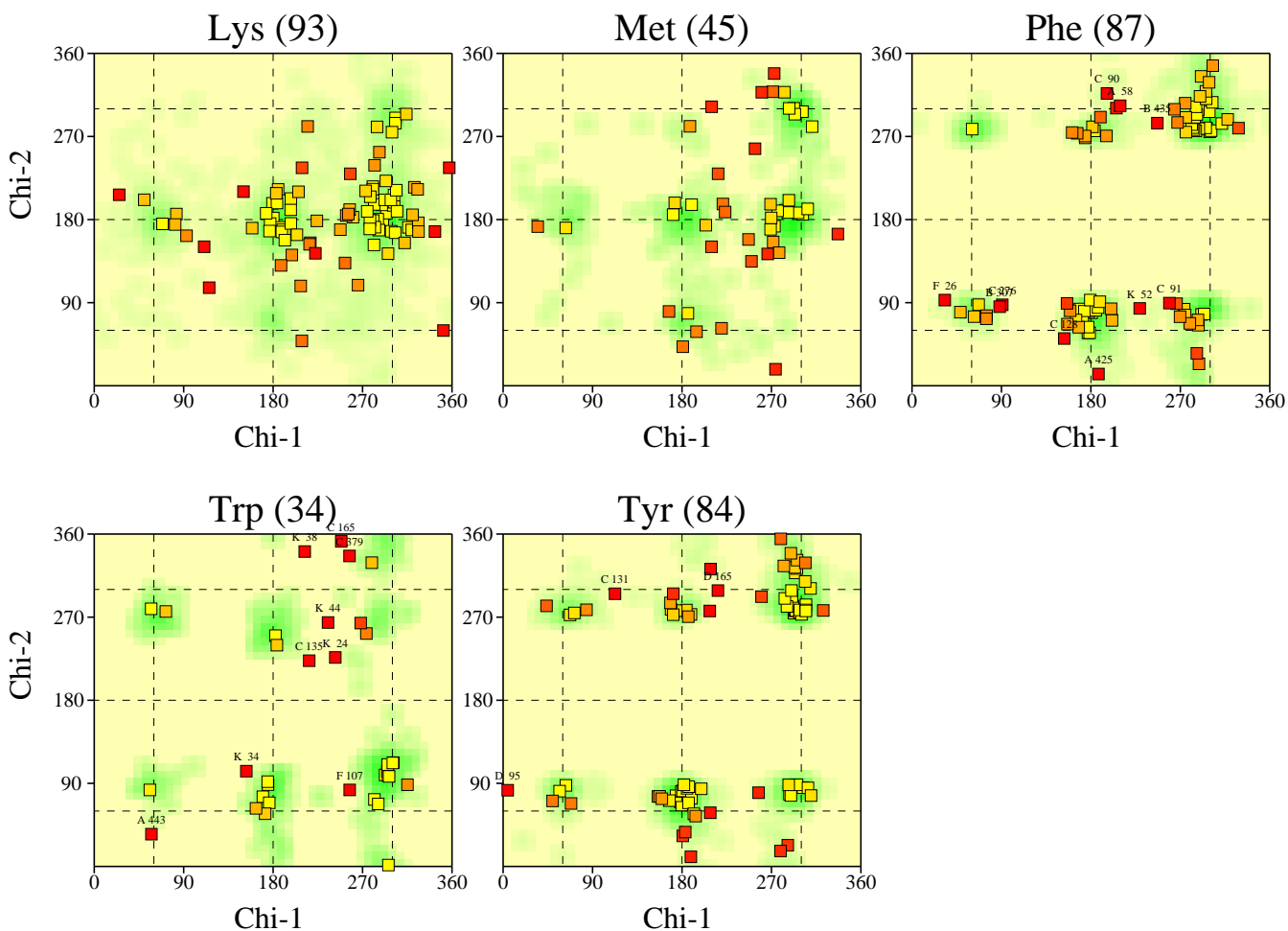
1nu1



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

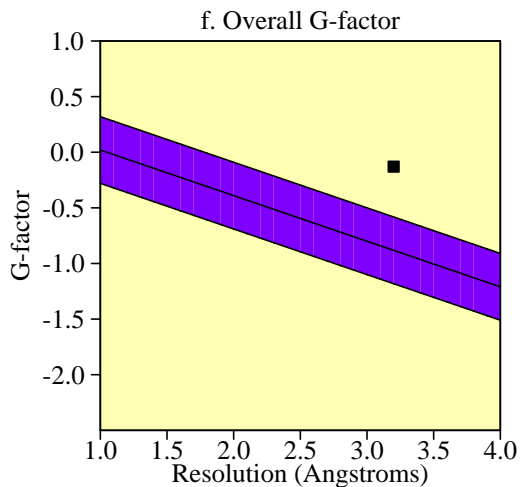
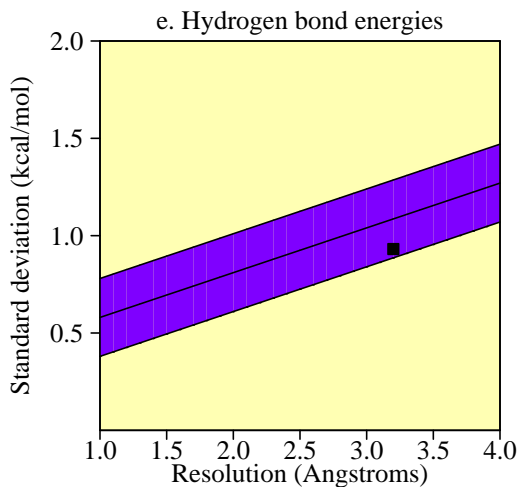
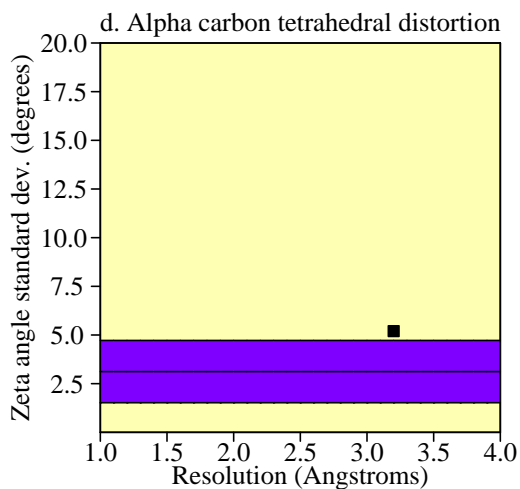
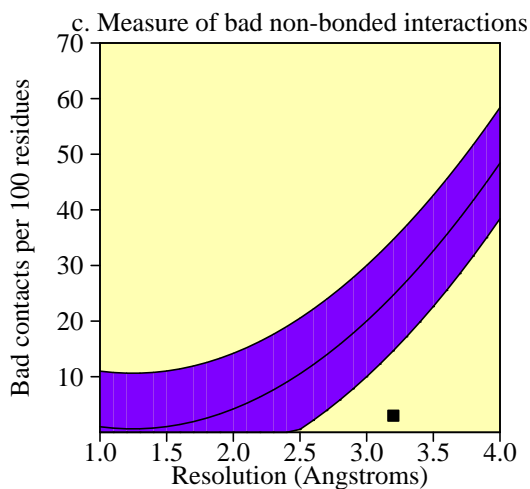
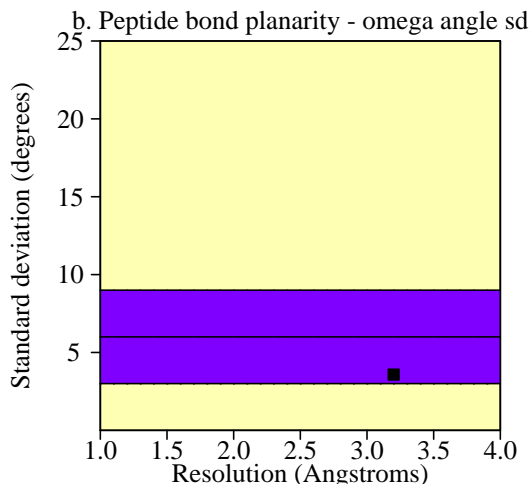
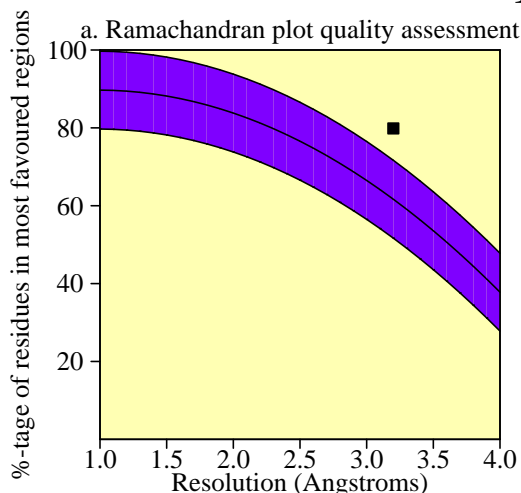
1nu1



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

1nu1

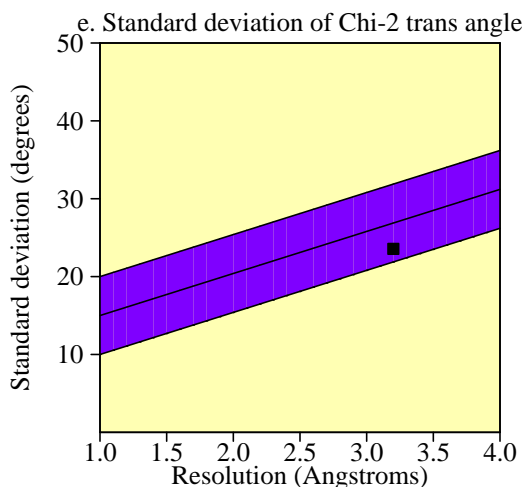
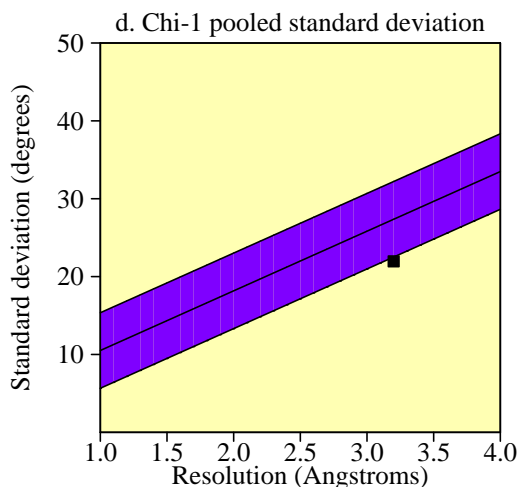
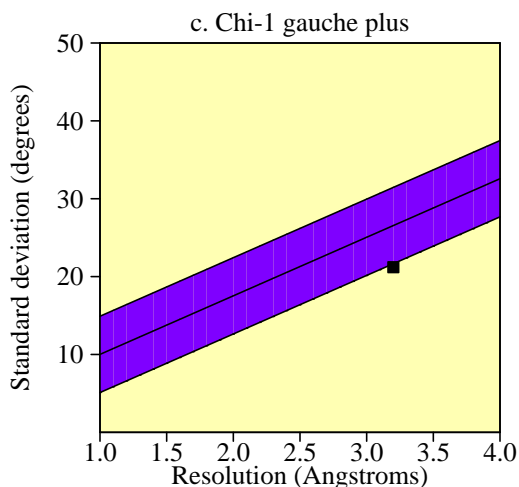
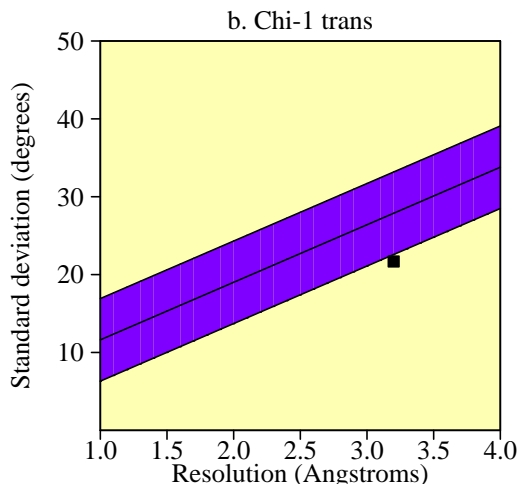
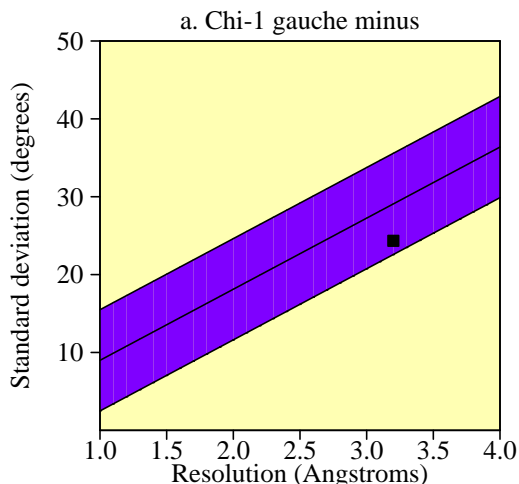


Plot statistics

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	1837	79.9	61.7	10.0	1.8	BETTER
b. Omega angle st dev	2094	3.6	6.0	3.0	-0.8	Inside
c. Bad contacts / 100 residues	63	3.0	24.7	10.0	-2.2	BETTER
d. Zeta angle st dev	1965	5.2	3.1	1.6	1.3	WORSE
e. H-bond energy st dev	1361	0.9	1.1	0.2	-0.8	Inside
f. Overall G-factor	2105	-0.1	-0.9	0.3	2.5	BETTER

Side-chain parameters

1nu1



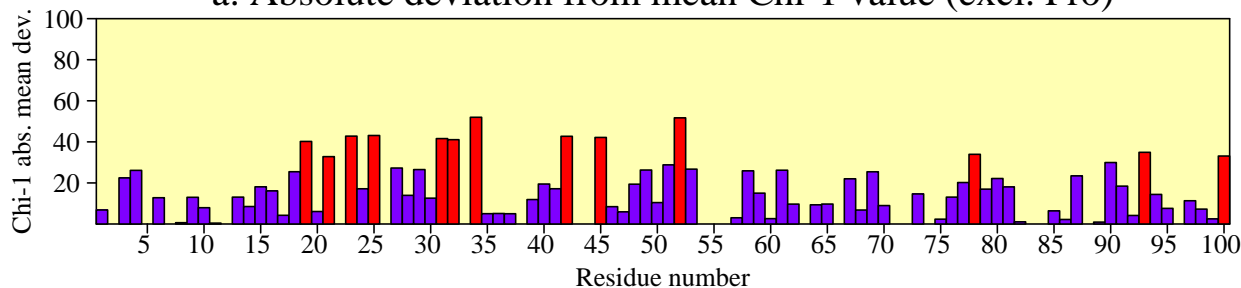
1nu1

Plot statistics

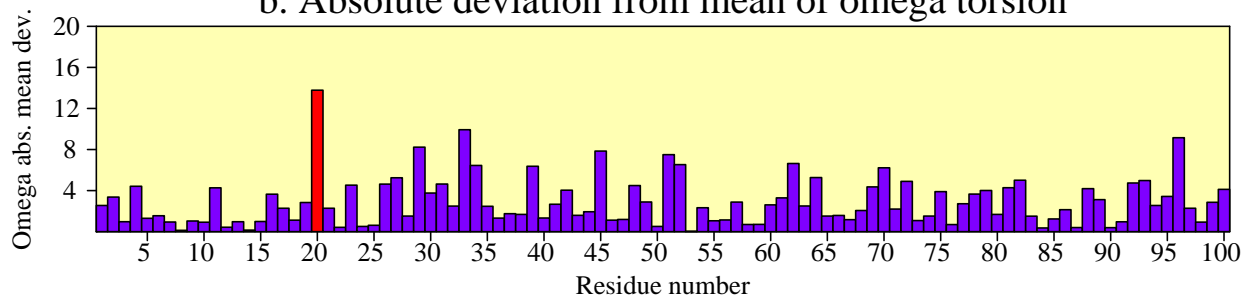
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean
			Typical value	Band width	
a. Chi-1 gauche minus st dev	214	24.3	29.1	6.5	-0.7 Inside
b. Chi-1 trans st dev	615	21.7	27.9	5.3	-1.2 BETTER
c. Chi-1 gauche plus st dev	825	21.2	26.6	4.9	-1.1 BETTER
d. Chi-1 pooled st dev	1654	22.0	27.4	4.8	-1.1 BETTER
e. Chi-2 trans st dev	569	23.6	26.9	5.0	-0.7 Inside

Residue properties 1nu1

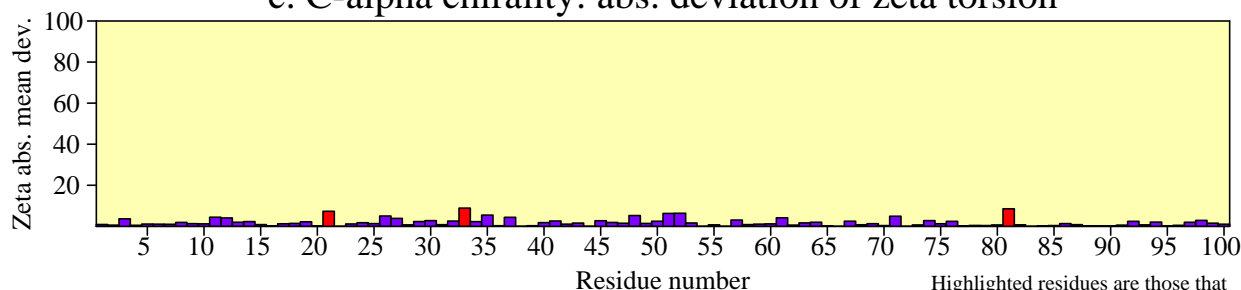
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

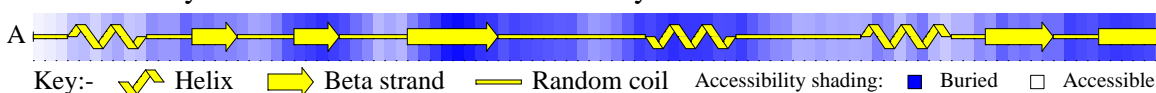


c. C-alpha chirality: abs. deviation of zeta torsion



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

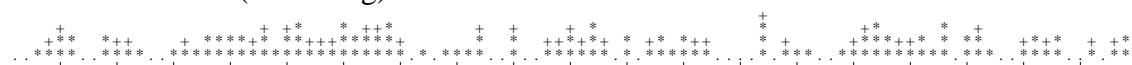
d. Secondary structure & estimated accessibility



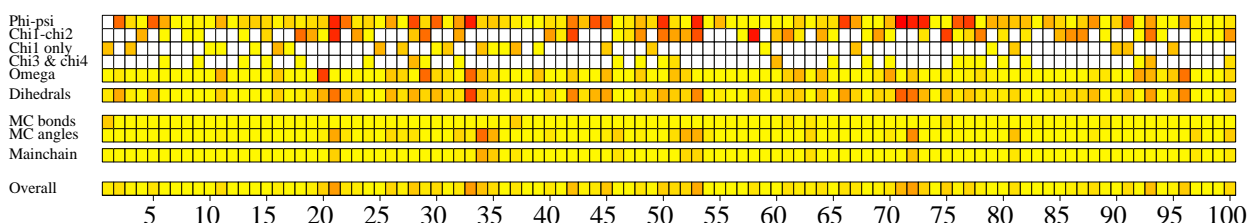
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

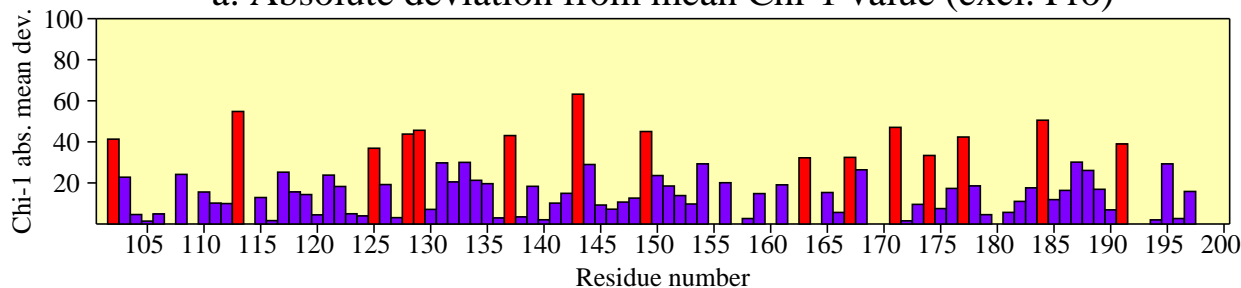


g. G-factors

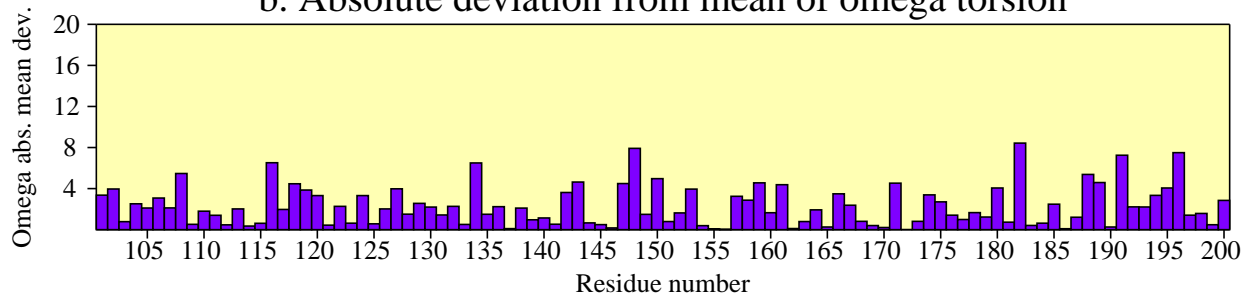


Residue properties 1nu1

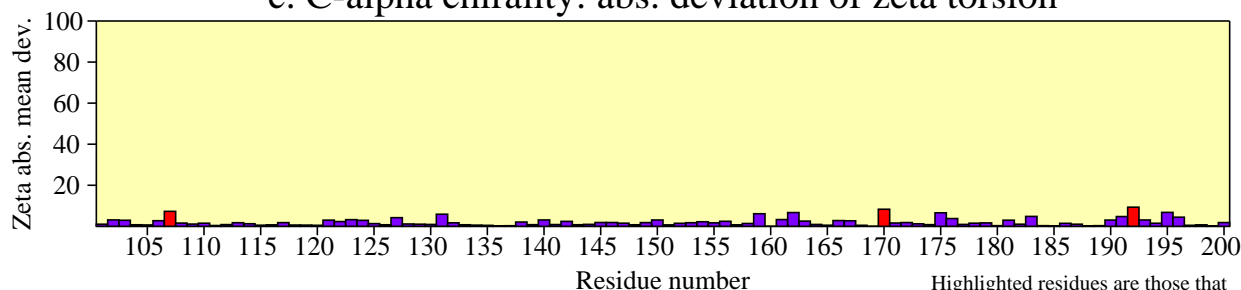
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

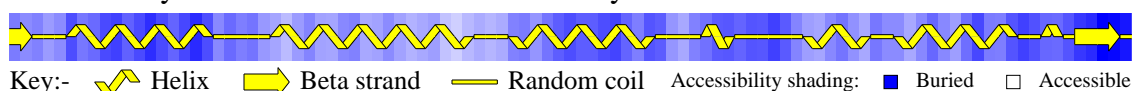


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



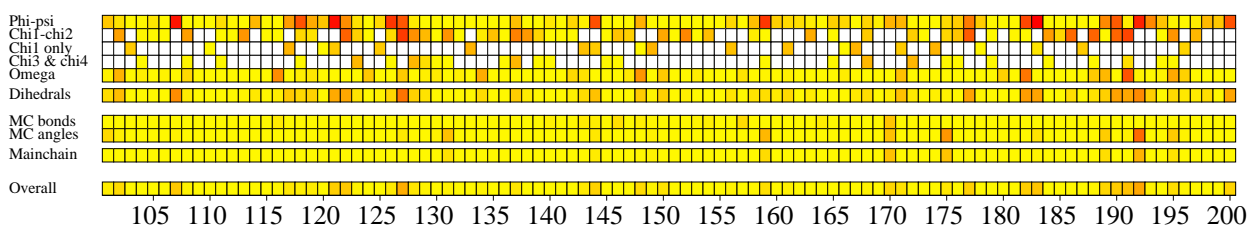
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

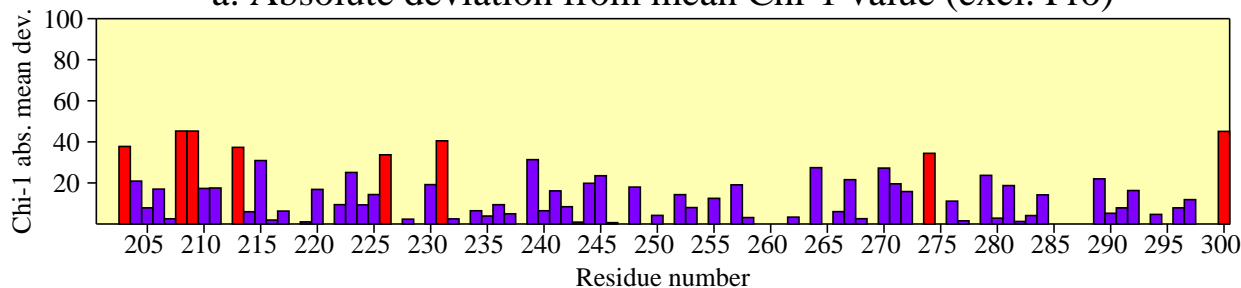


g. G-factors

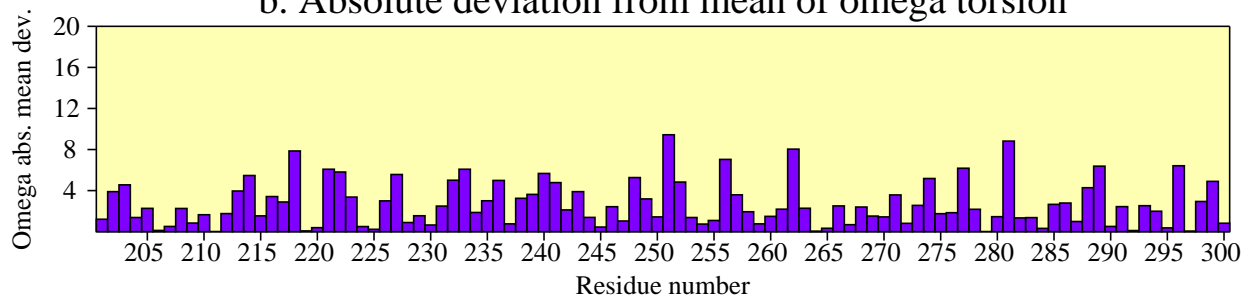


Residue properties 1nu1

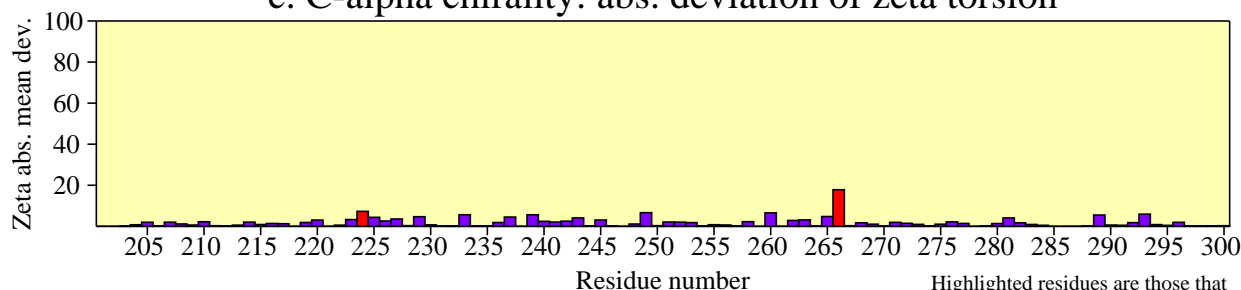
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

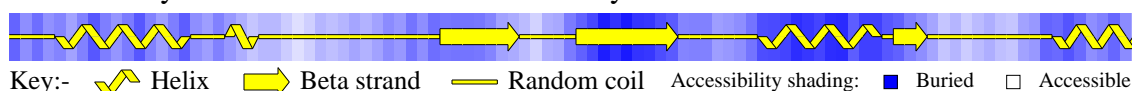


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



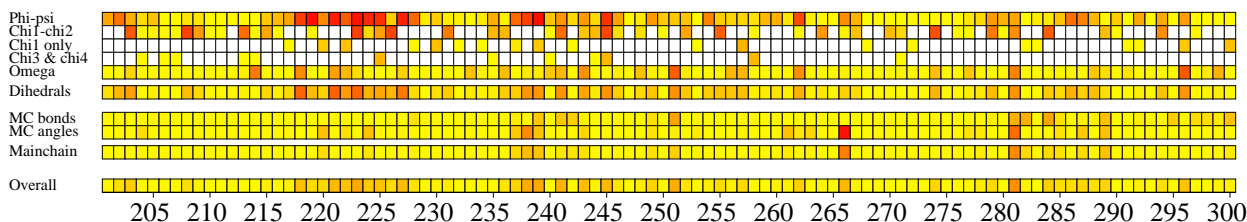
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

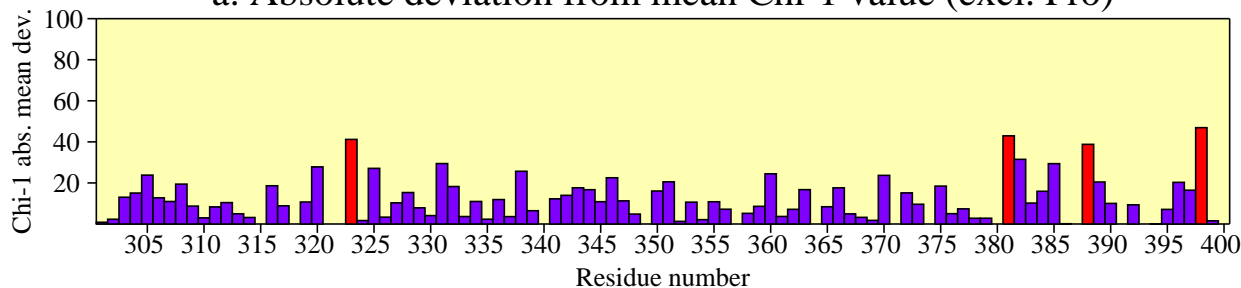


g. G-factors

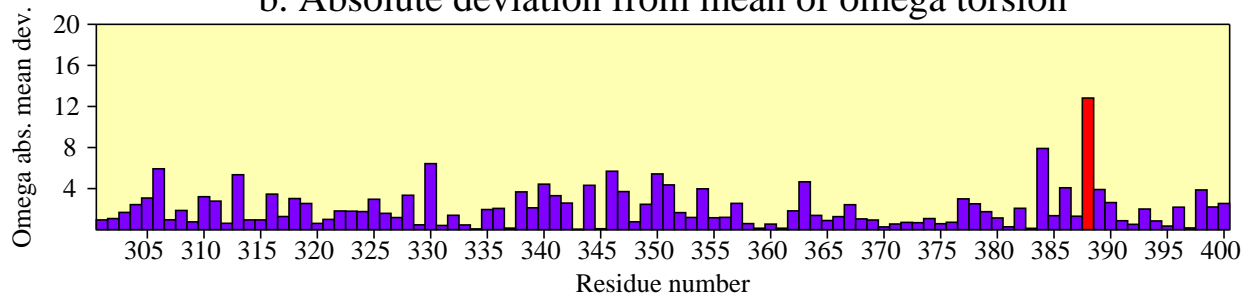


Residue properties 1nu1

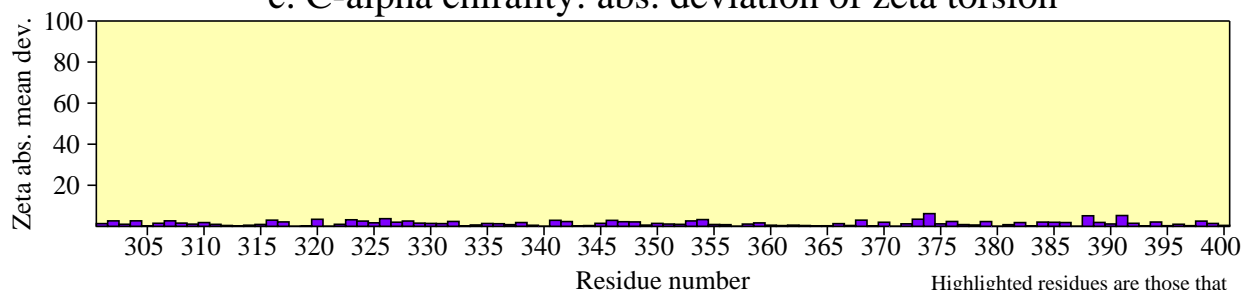
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

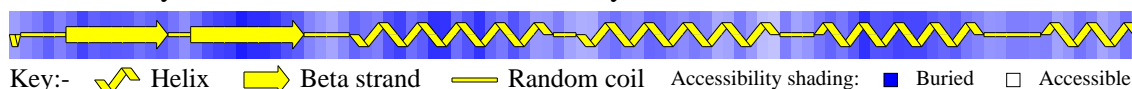


c. C-alpha chirality: abs. deviation of zeta torsion



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

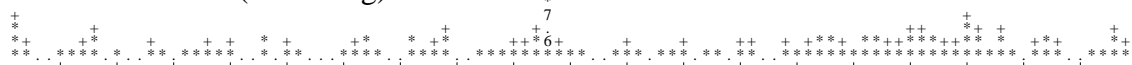
d. Secondary structure & estimated accessibility



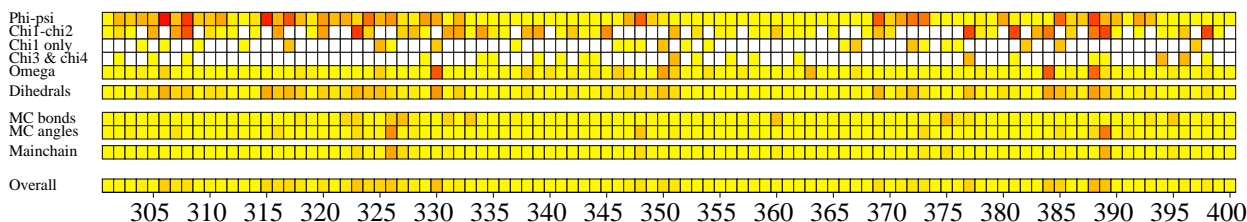
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

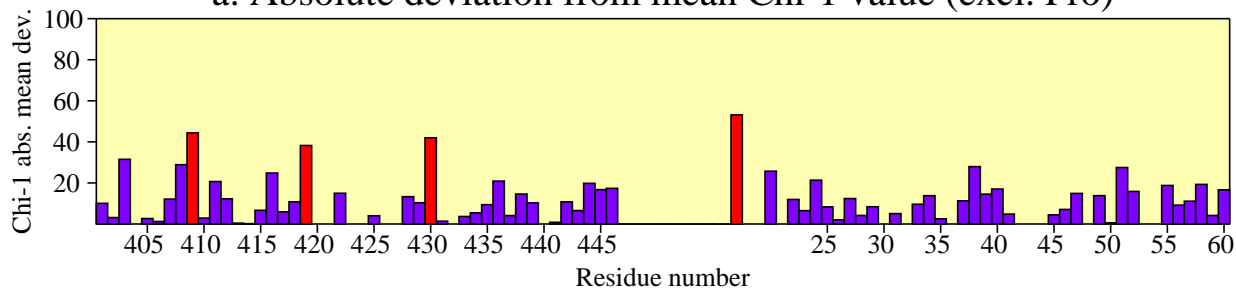


g. G-factors

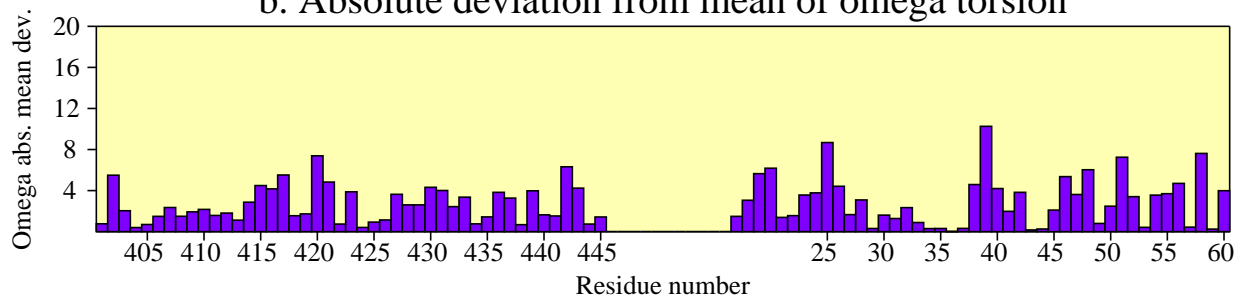


Residue properties 1nu1

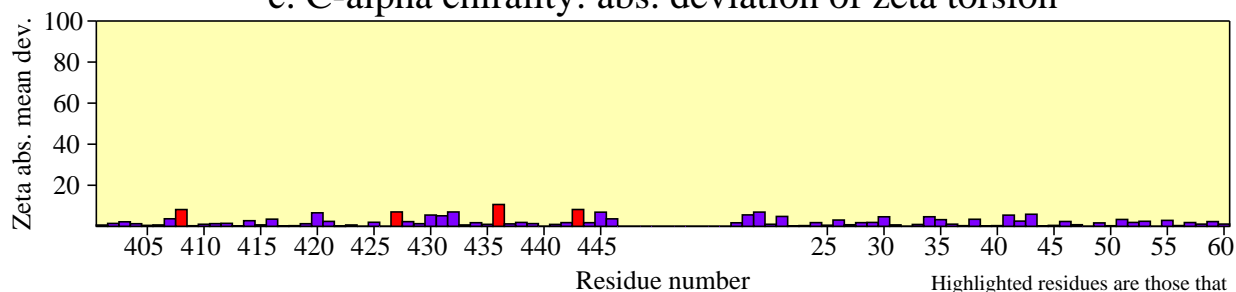
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

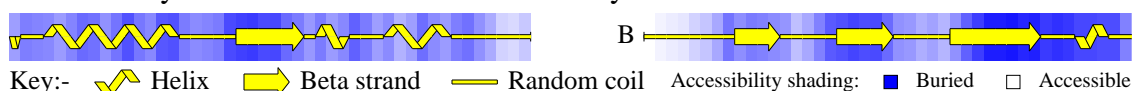


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



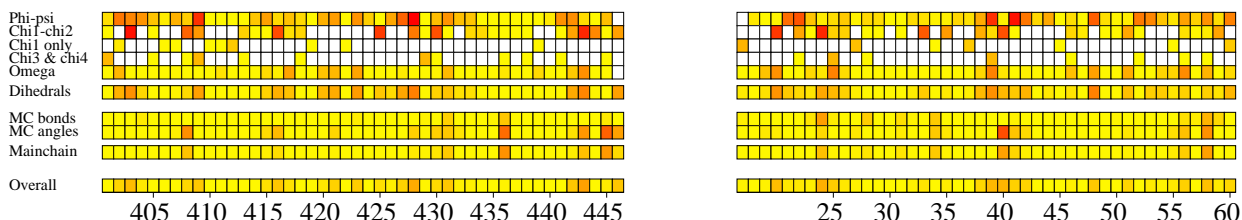
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

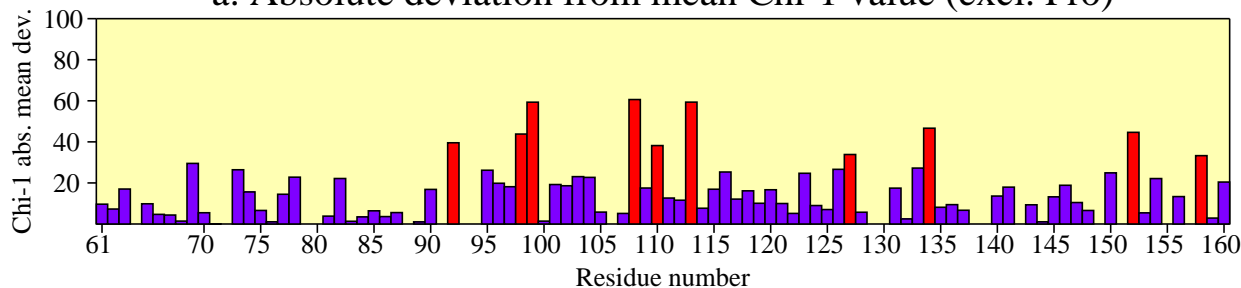


g. G-factors

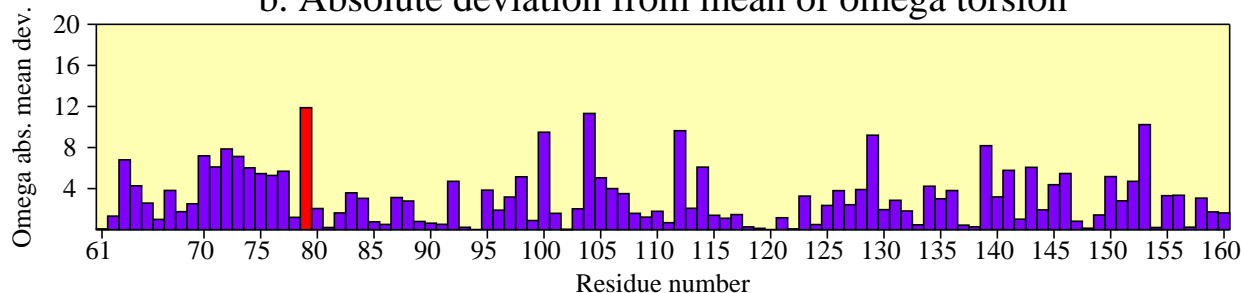


Residue properties 1nu1

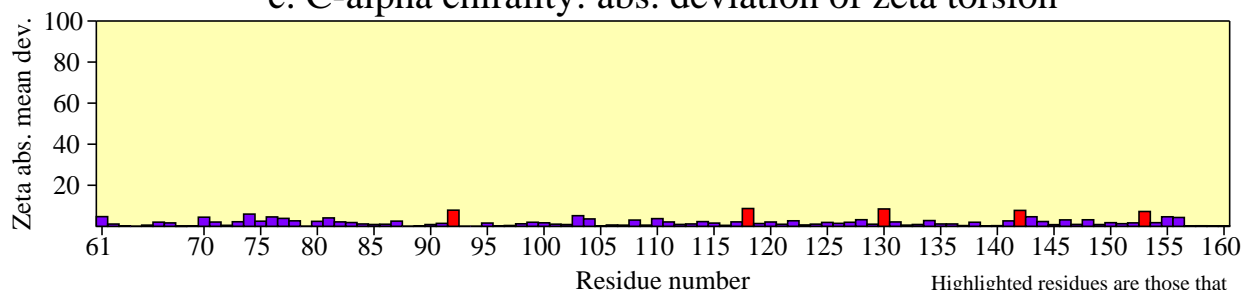
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

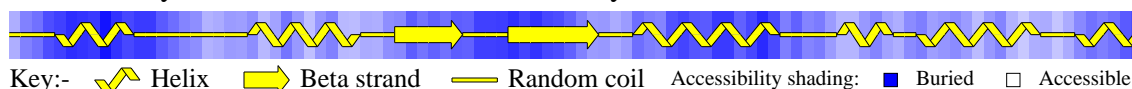


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



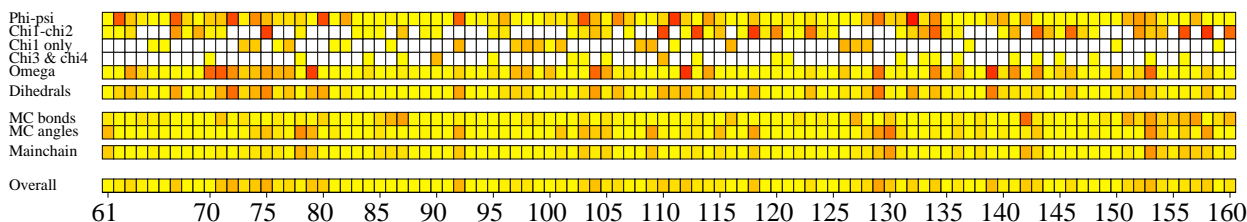
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

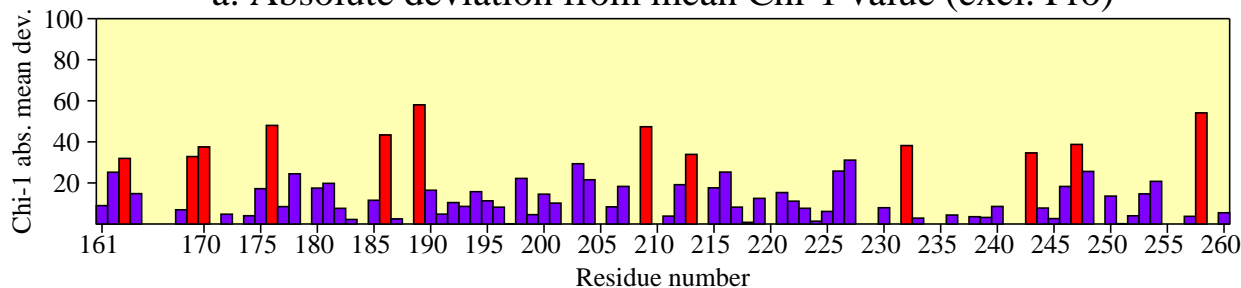


g. G-factors

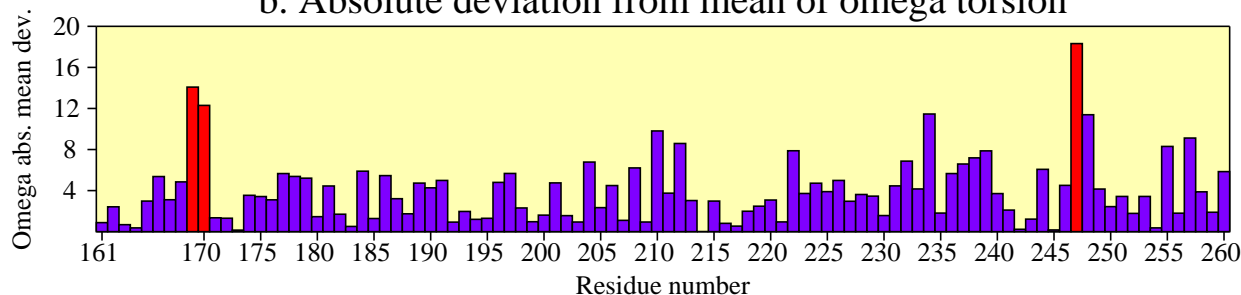


Residue properties 1nu1

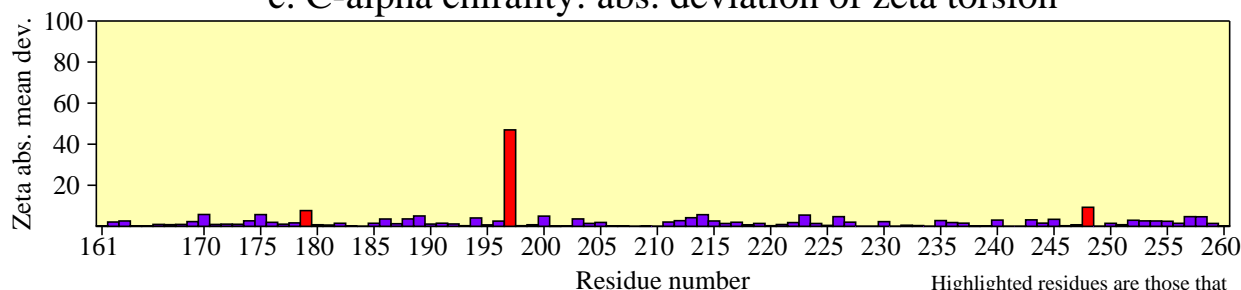
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

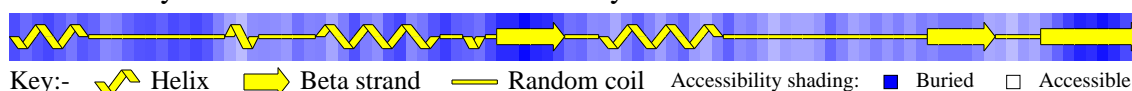


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



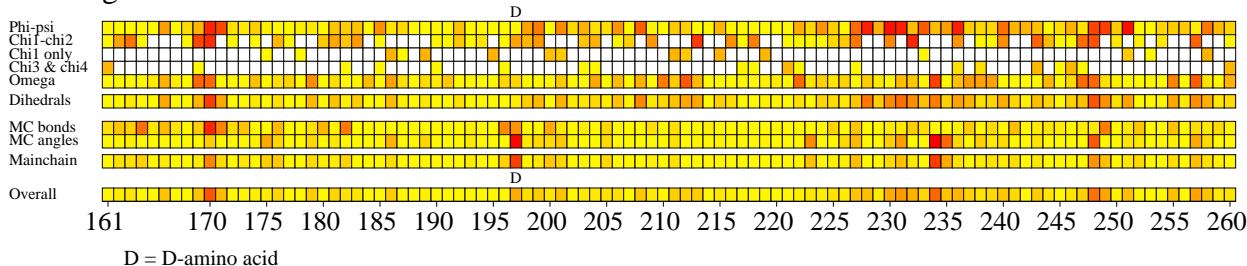
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

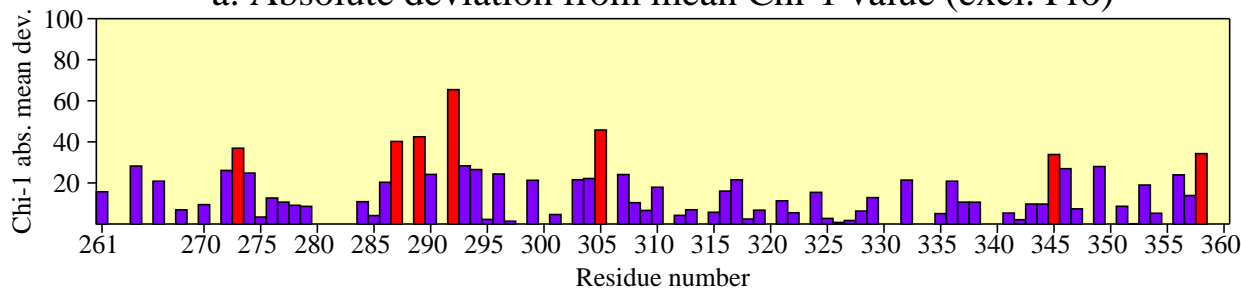


g. G-factors

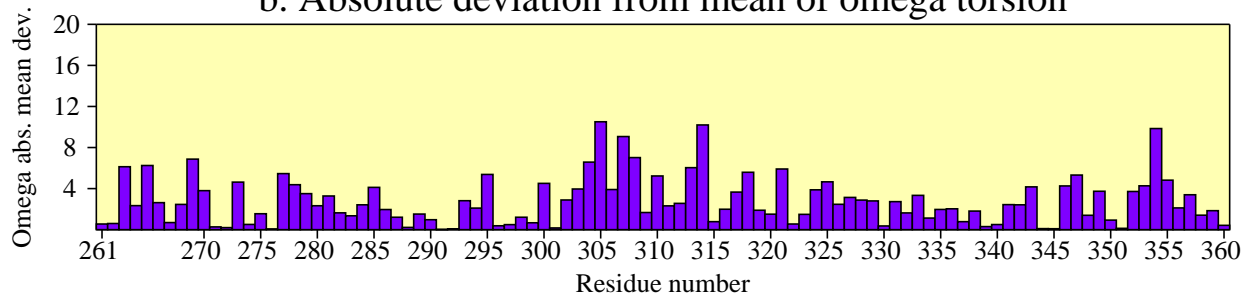


Residue properties 1nu1

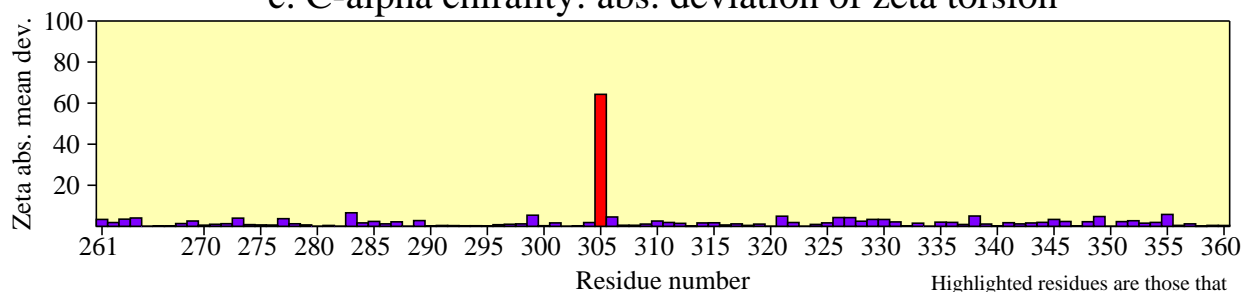
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

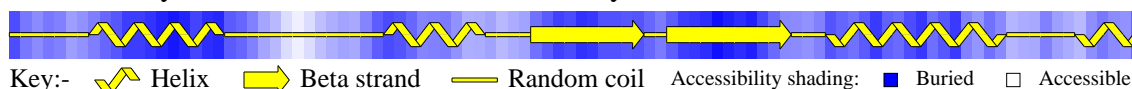


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



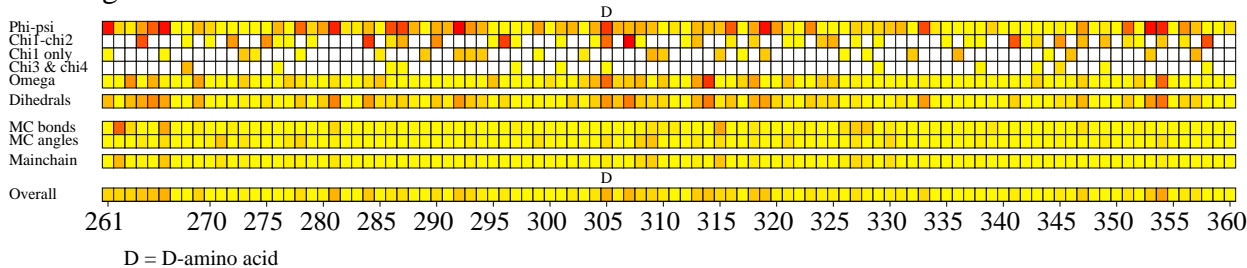
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

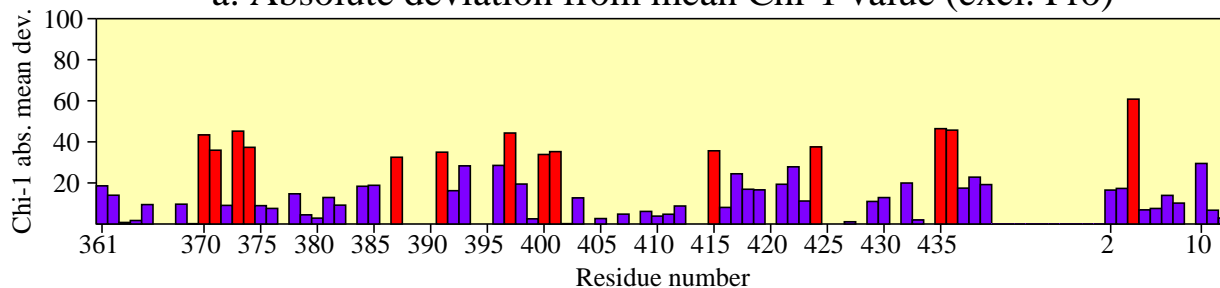


g. G-factors

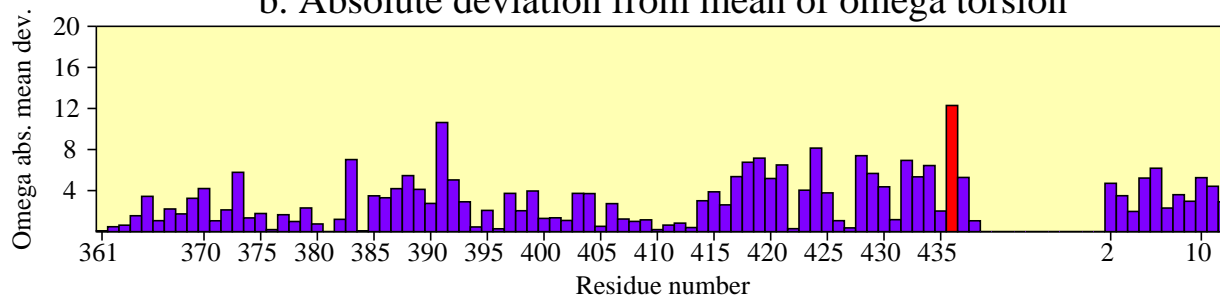


Residue properties 1nu1

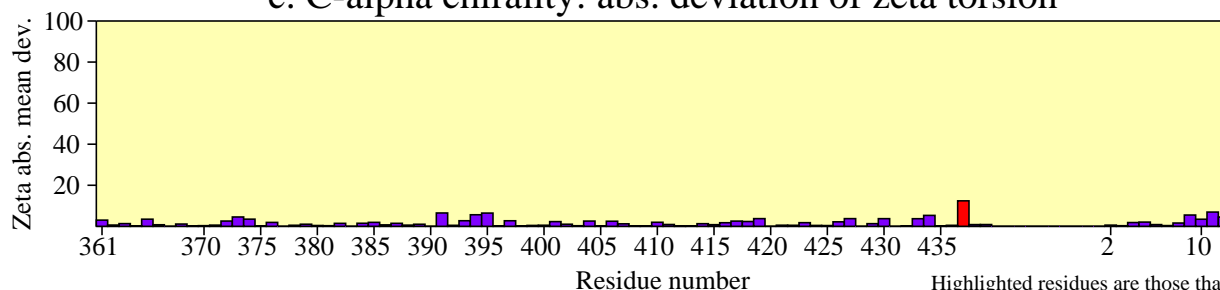
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



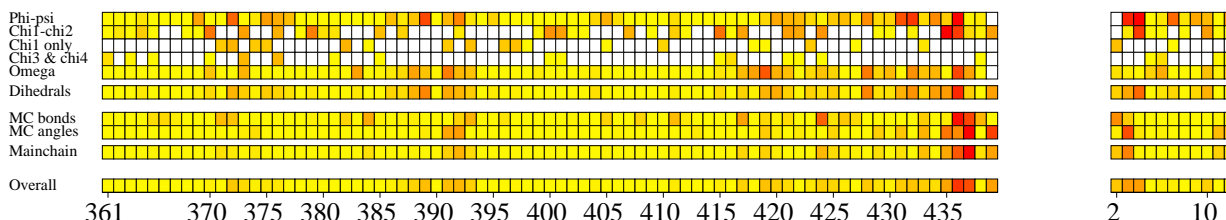
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

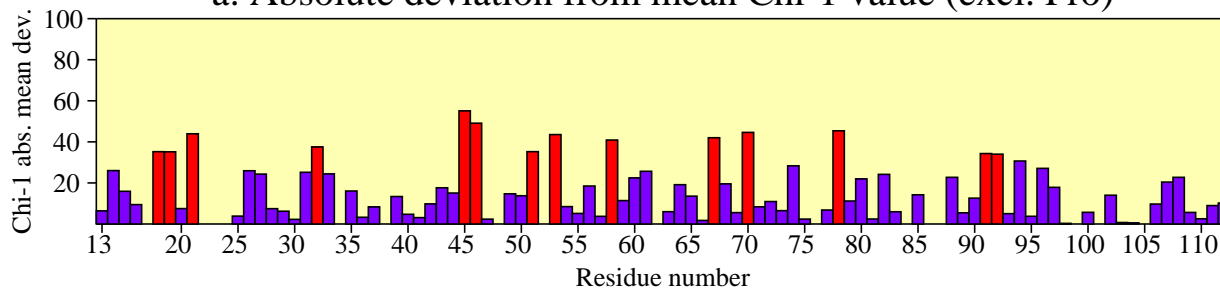


g. G-factors

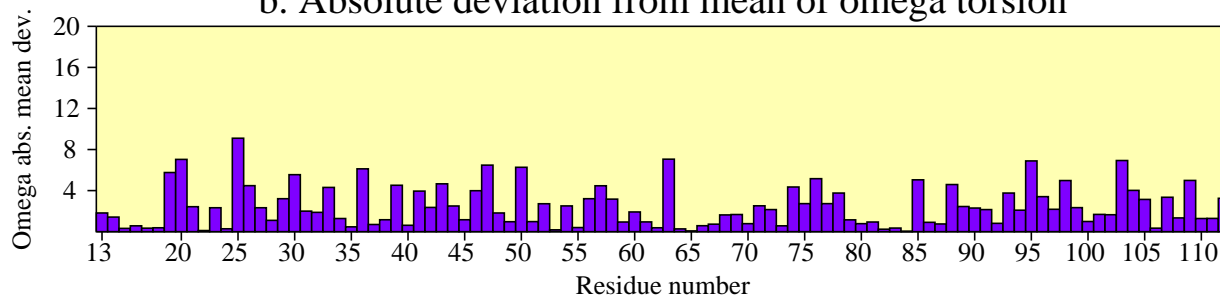


Residue properties 1nu1

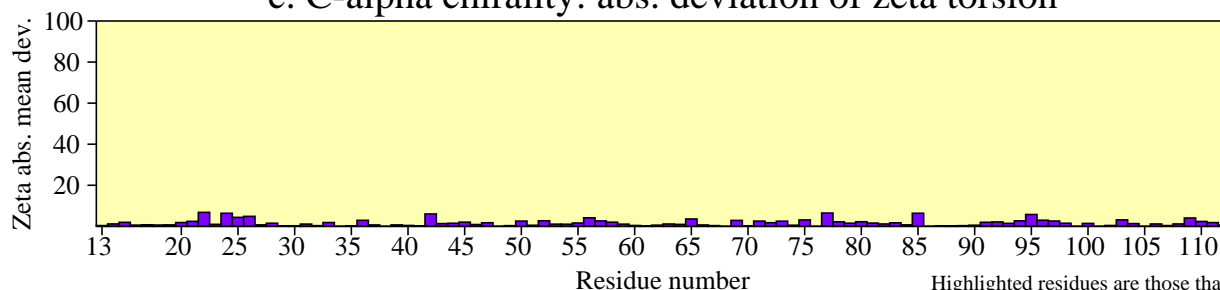
a. Absolute deviation from mean Chi-1 value (excl. Pro)



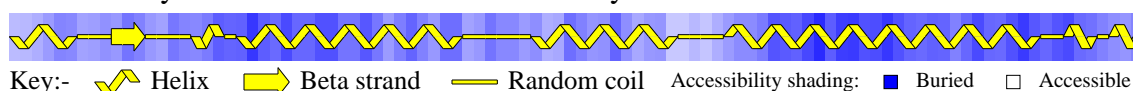
b. Absolute deviation from mean of omega torsion



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



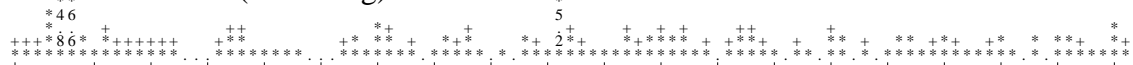
d. Secondary structure & estimated accessibility



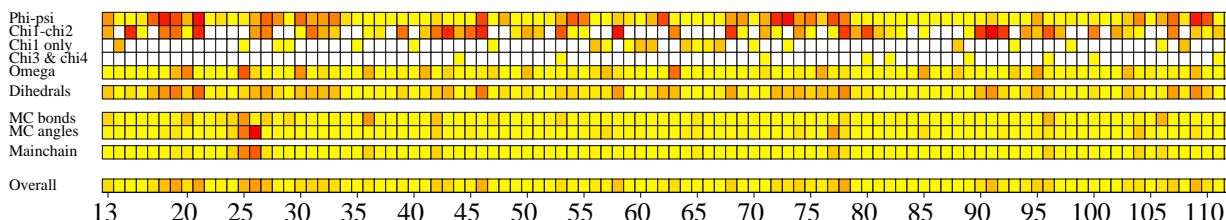
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



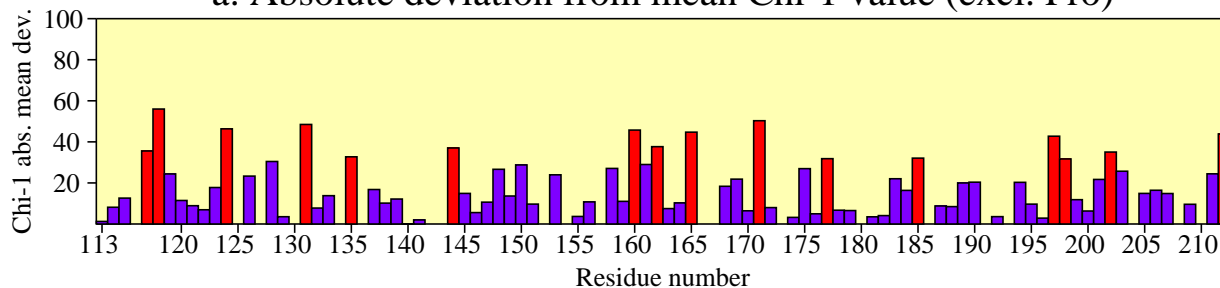
g. G-factors



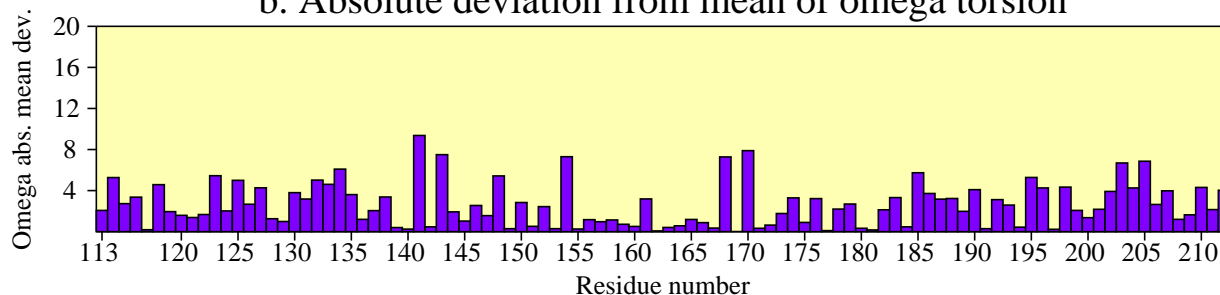
Residue properties

1nu1

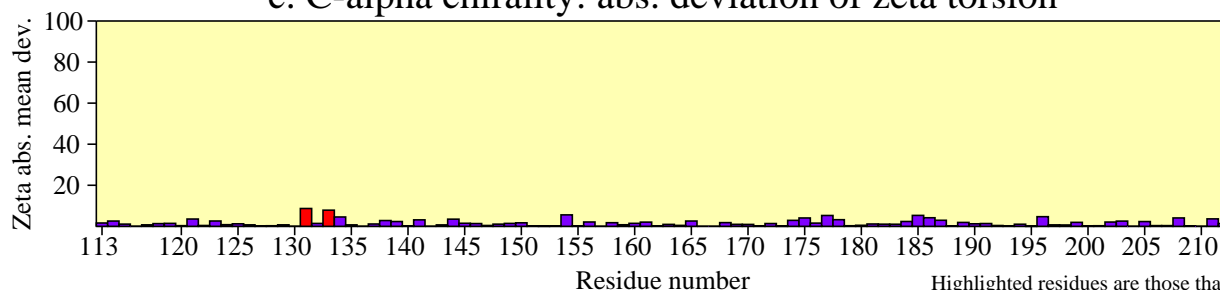
a. Absolute deviation from mean Chi-1 value (excl. Pro)



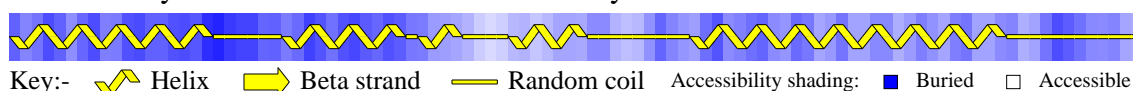
b. Absolute deviation from mean of omega torsion



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



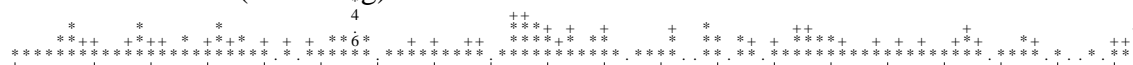
d. Secondary structure & estimated accessibility



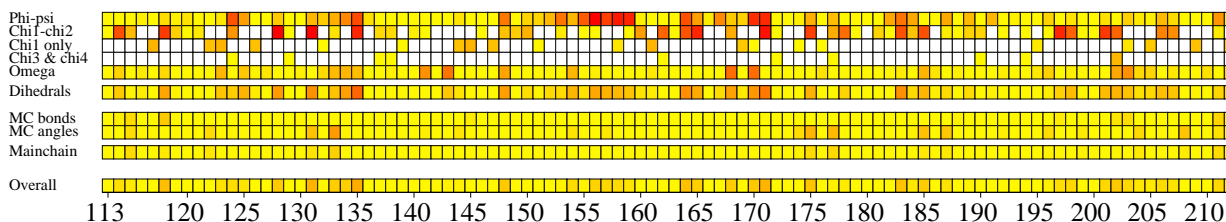
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



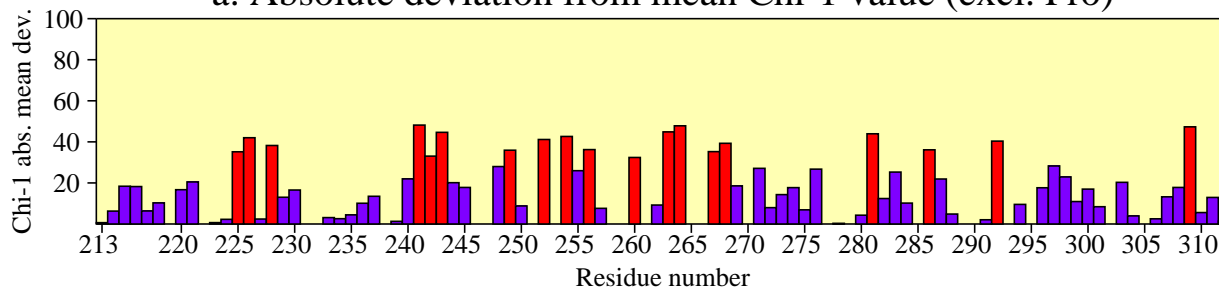
g. G-factors



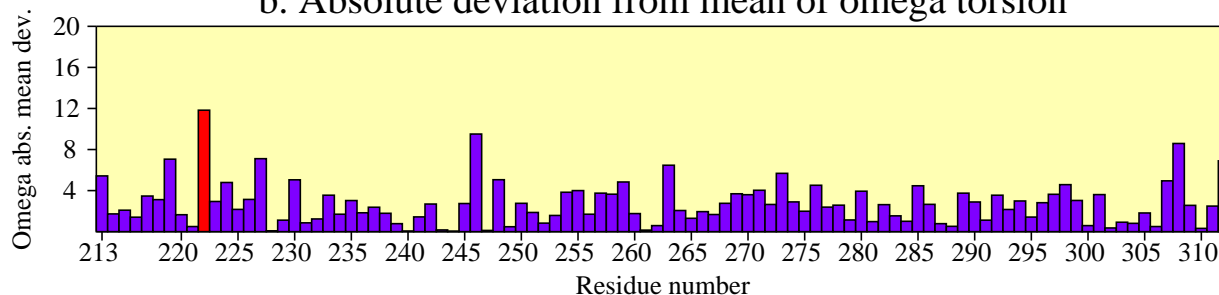
Residue properties

1nu1

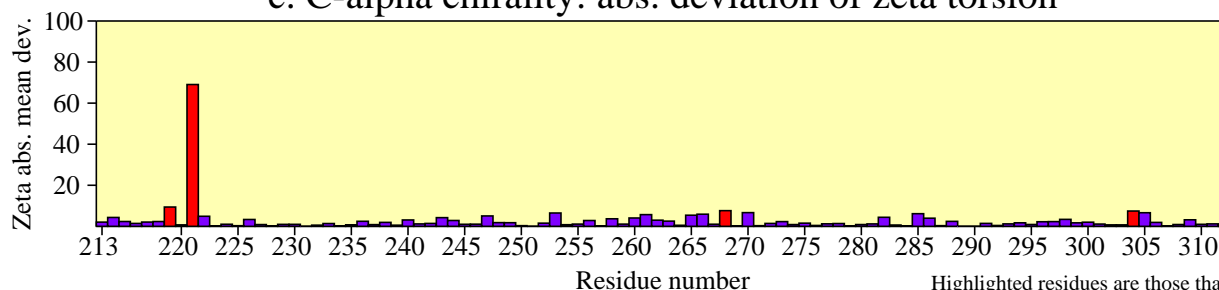
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

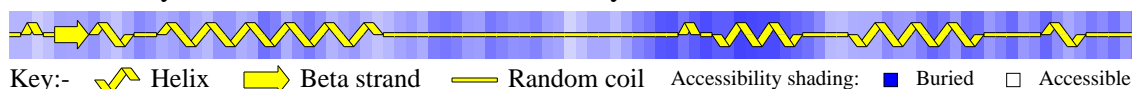


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



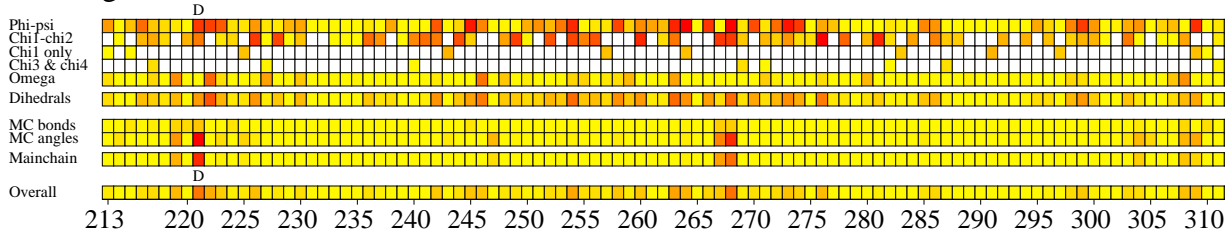
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. _i deviation (see listing)



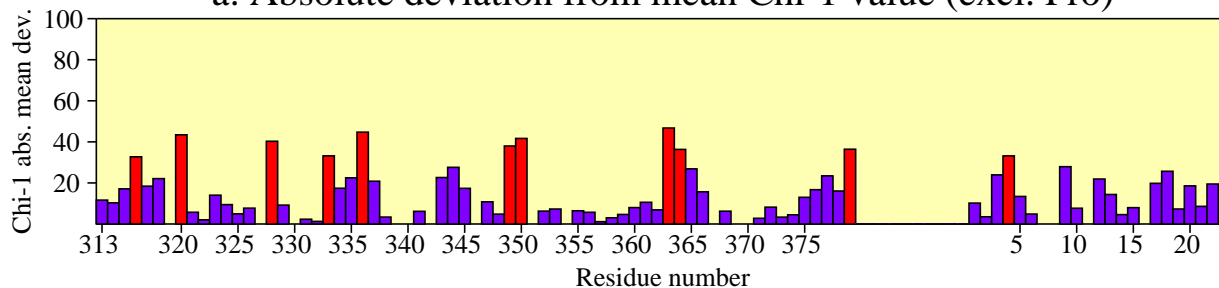
g. G-factors



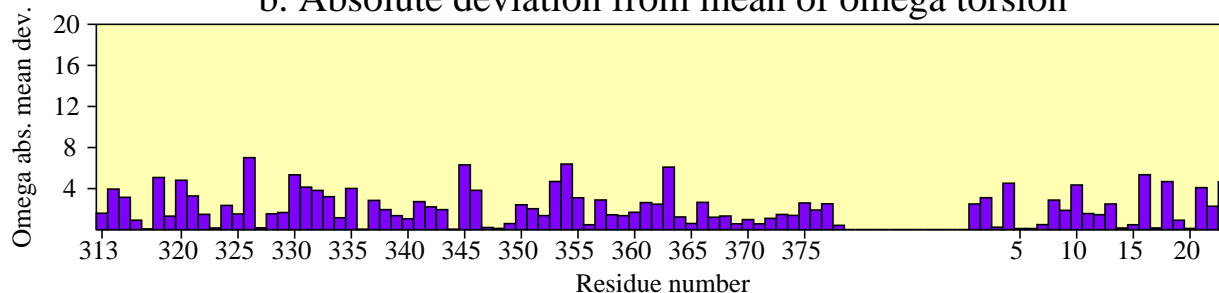
D = D-amino acid

Residue properties 1nu1

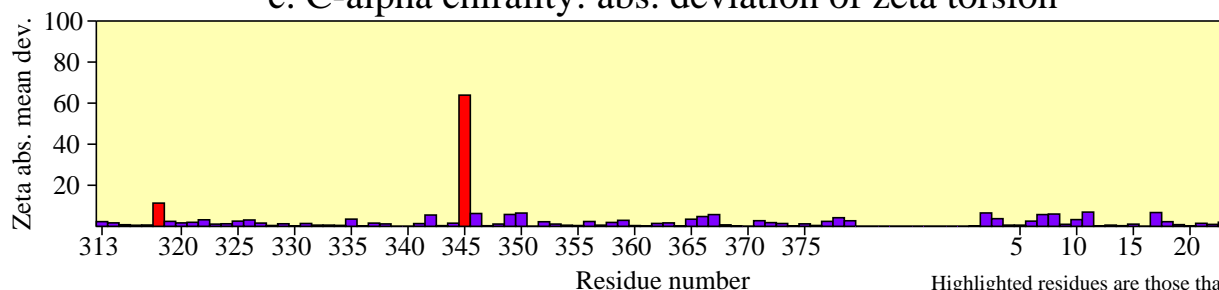
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

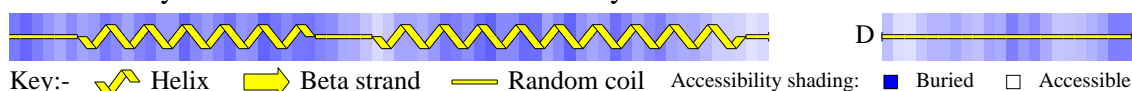


c. C-alpha chirality: abs. deviation of zeta torsion



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

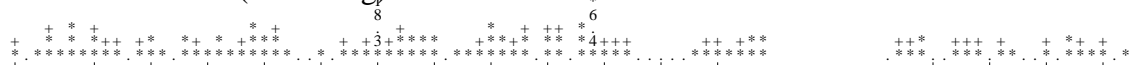
d. Secondary structure & estimated accessibility



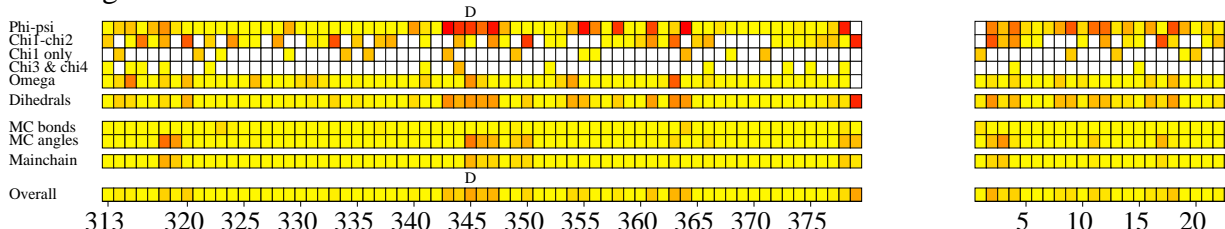
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



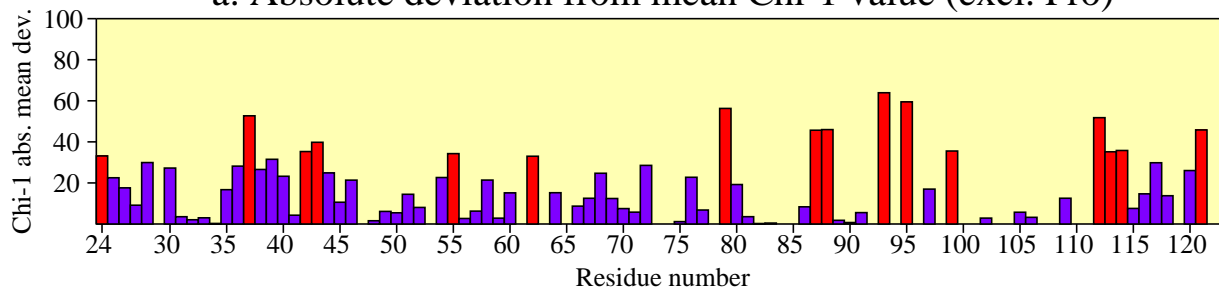
g. G-factors



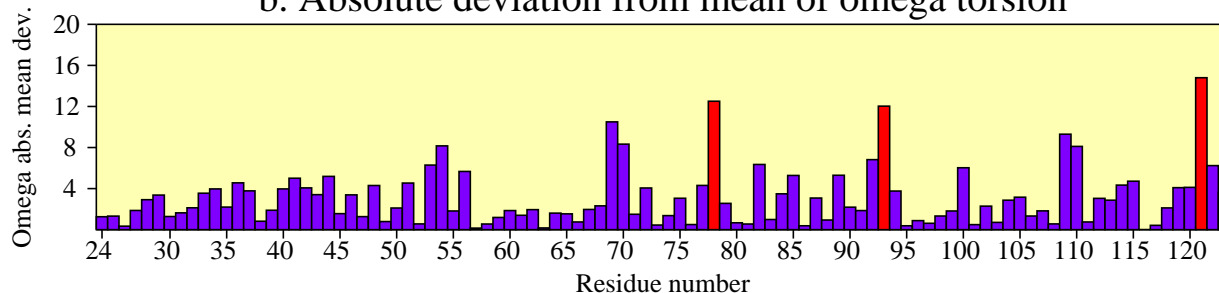
D = D-amino acid

Residue properties 1nu1

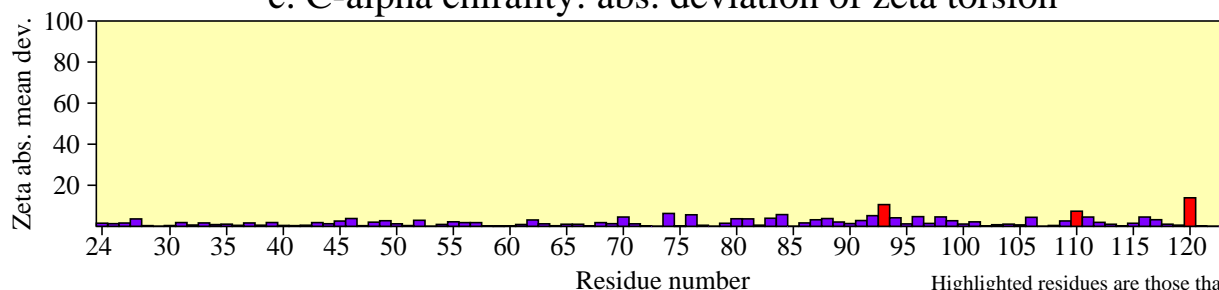
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

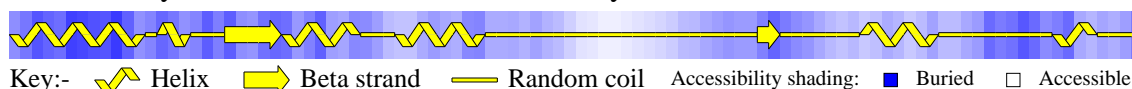


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



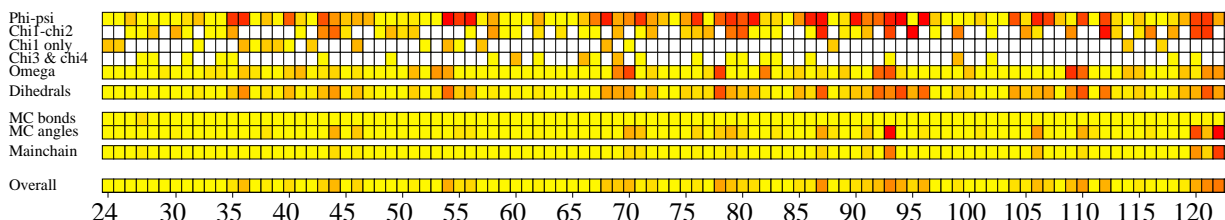
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

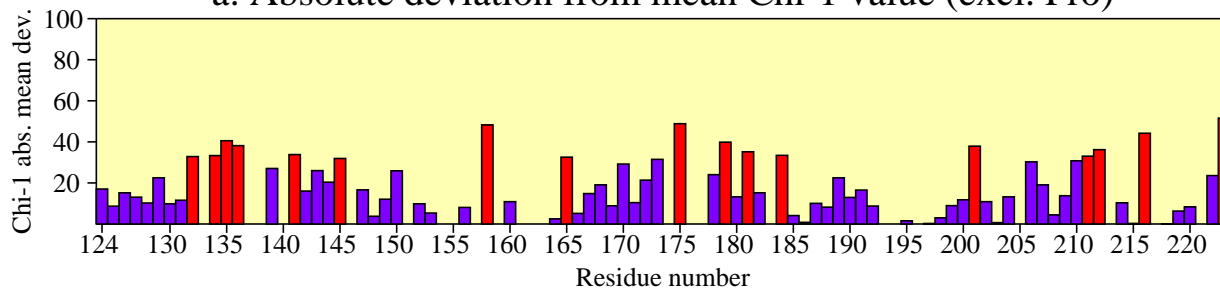


g. G-factors

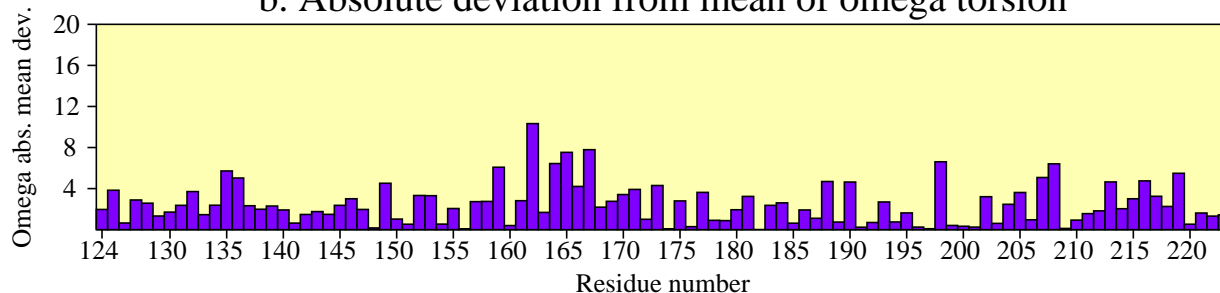


Residue properties 1nu1

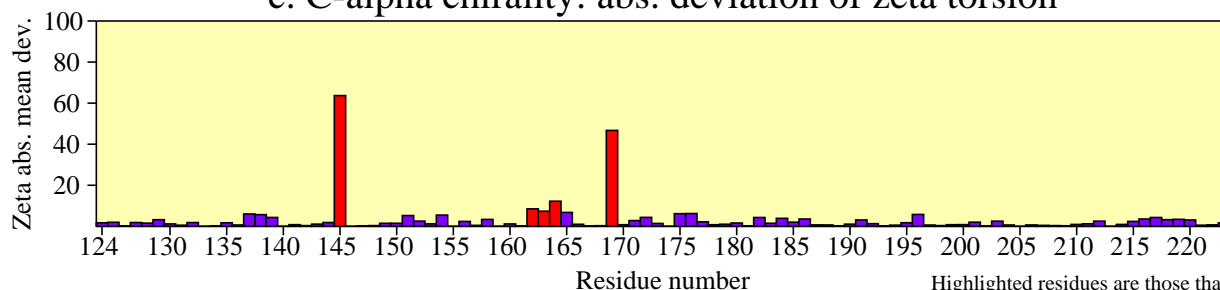
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

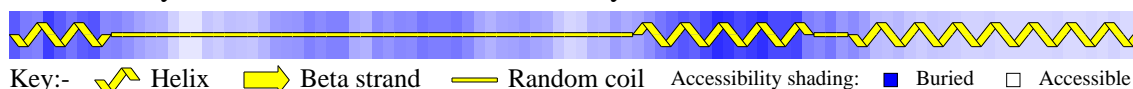


c. C-alpha chirality: abs. deviation of zeta torsion



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

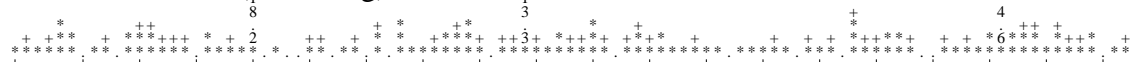
d. Secondary structure & estimated accessibility



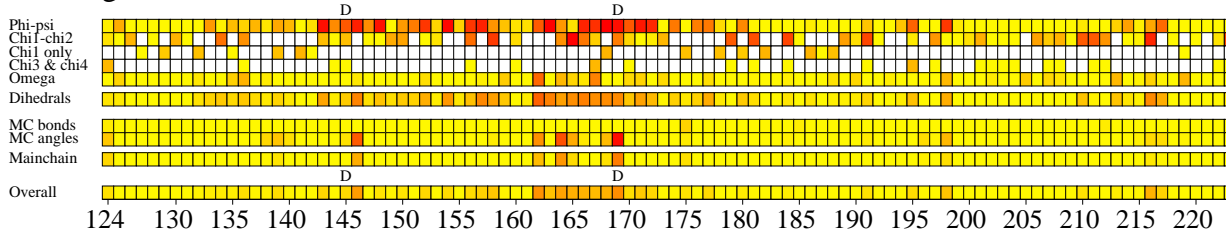
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



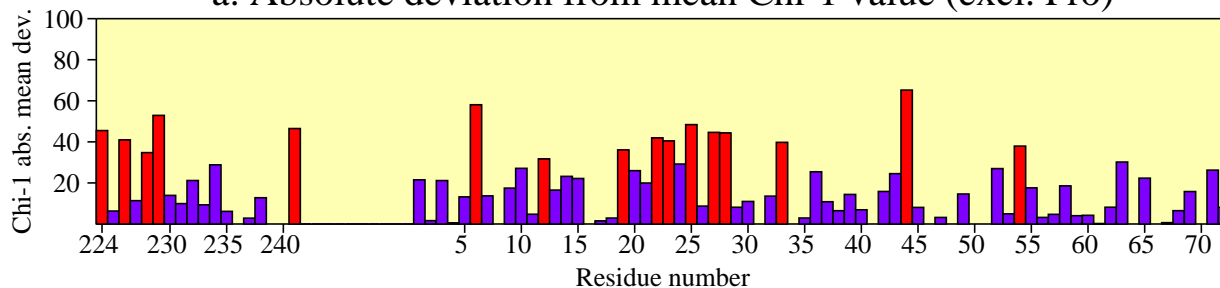
g. G-factors



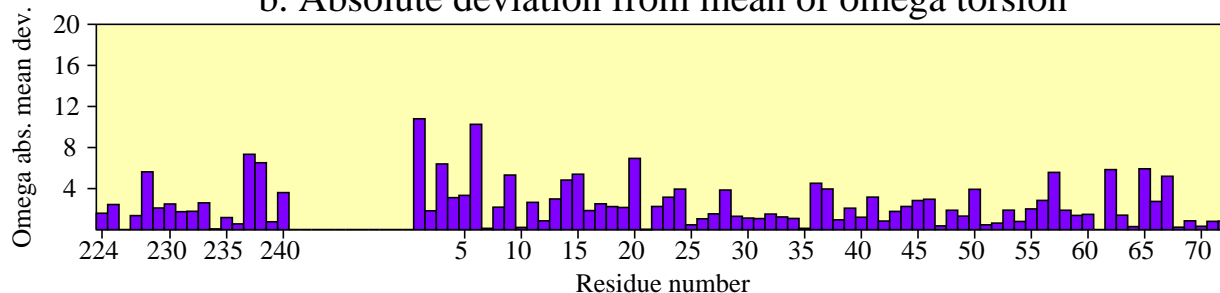
D = D-amino acid

Residue properties 1nu1

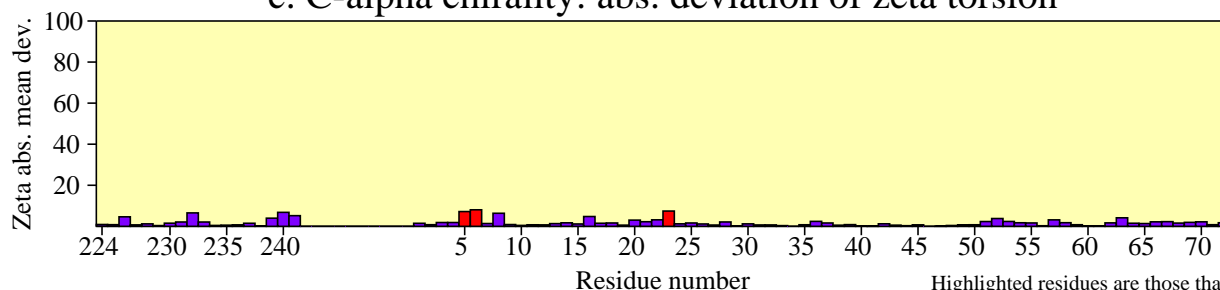
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

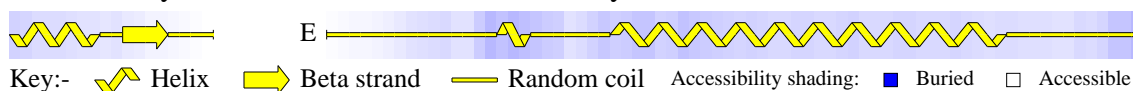


c. C-alpha chirality: abs. deviation of zeta torsion



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

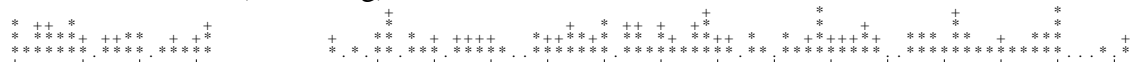
d. Secondary structure & estimated accessibility



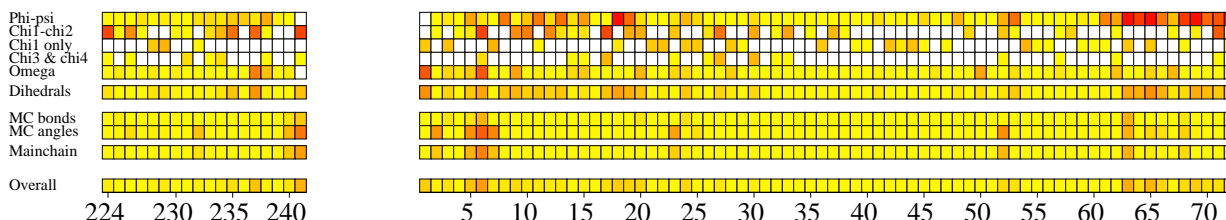
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

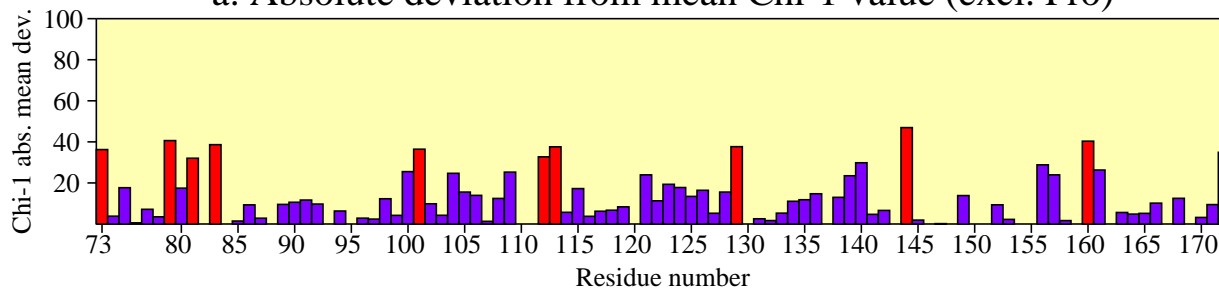


g. G-factors

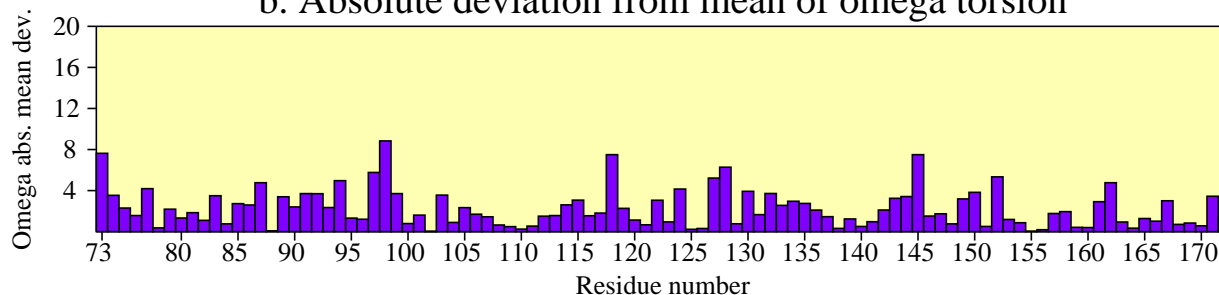


Residue properties 1nu1

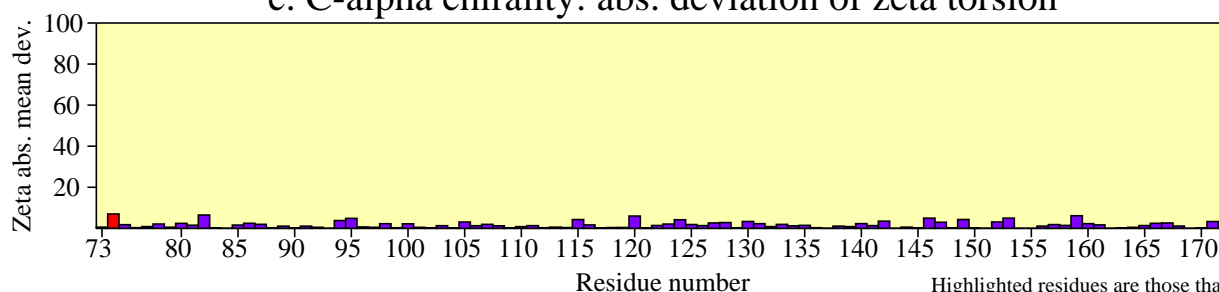
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

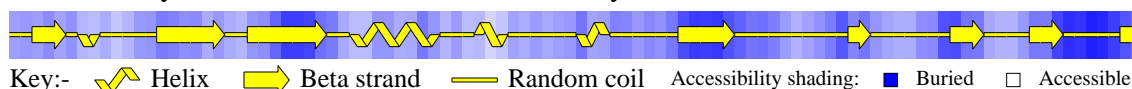


c. C-alpha chirality: abs. deviation of zeta torsion

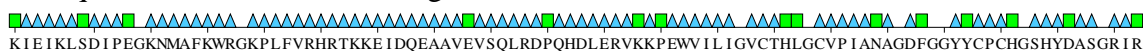


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

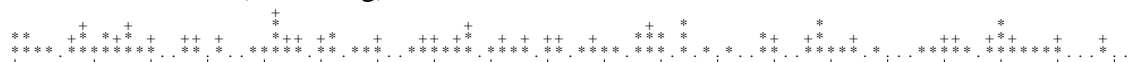
d. Secondary structure & estimated accessibility



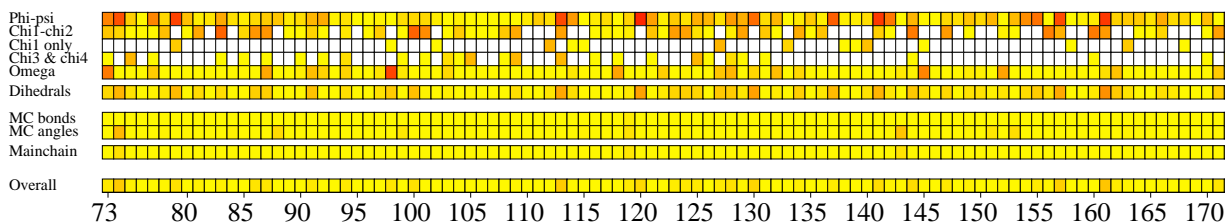
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

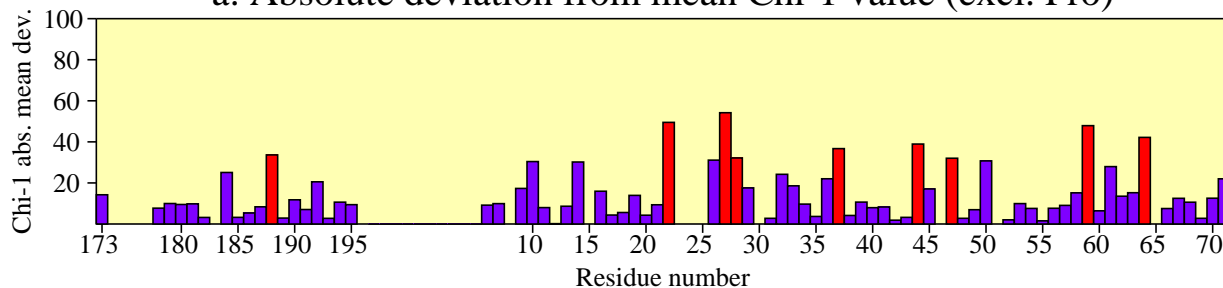


g. G-factors

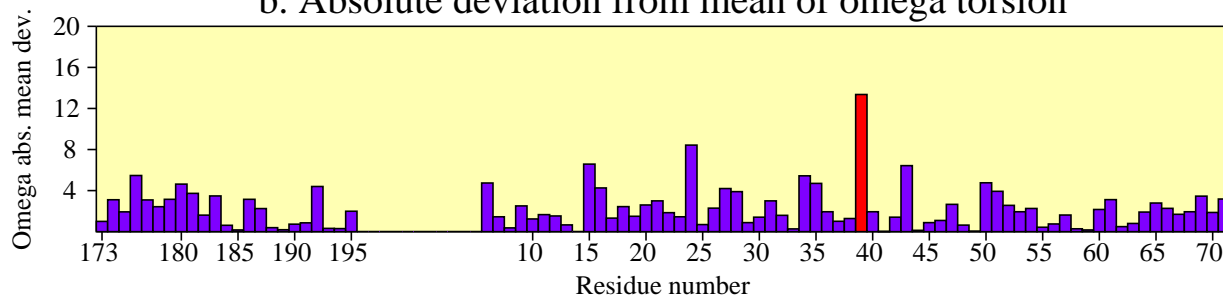


Residue properties 1nu1

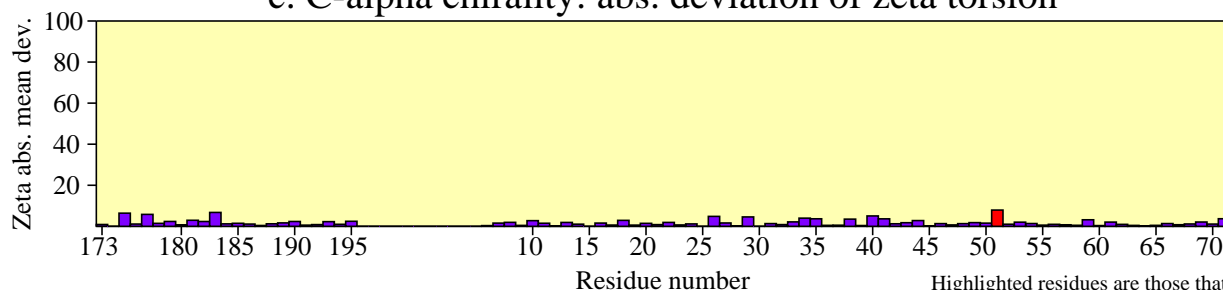
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

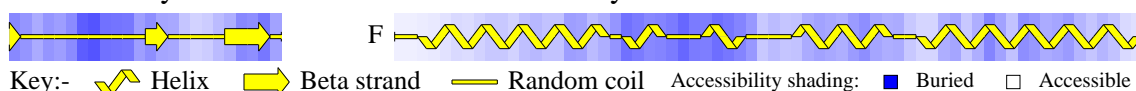


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



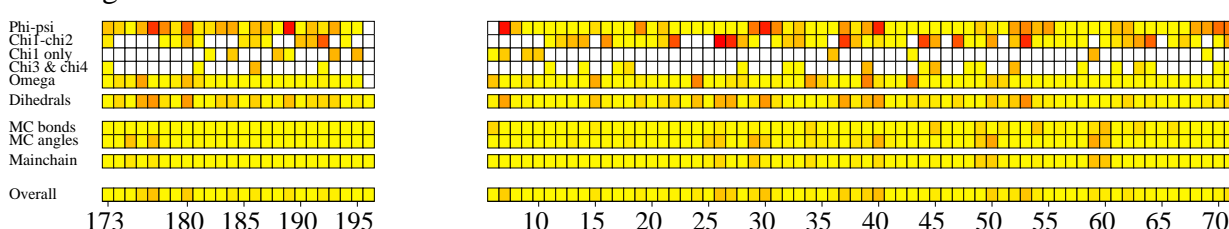
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

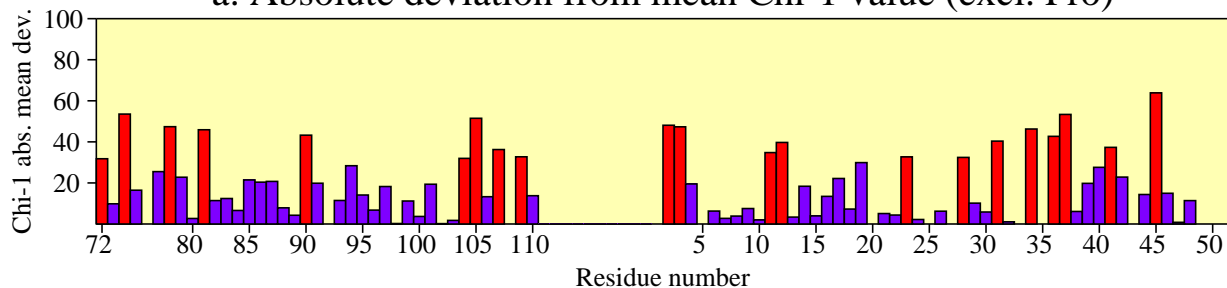


g. G-factors

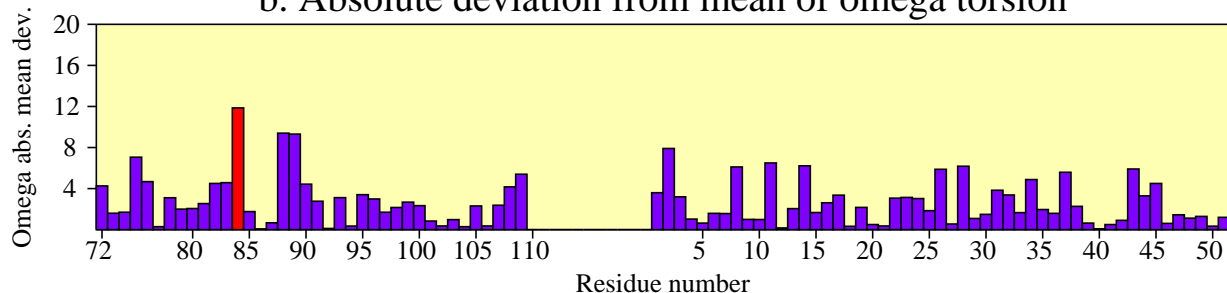


Residue properties 1nu1

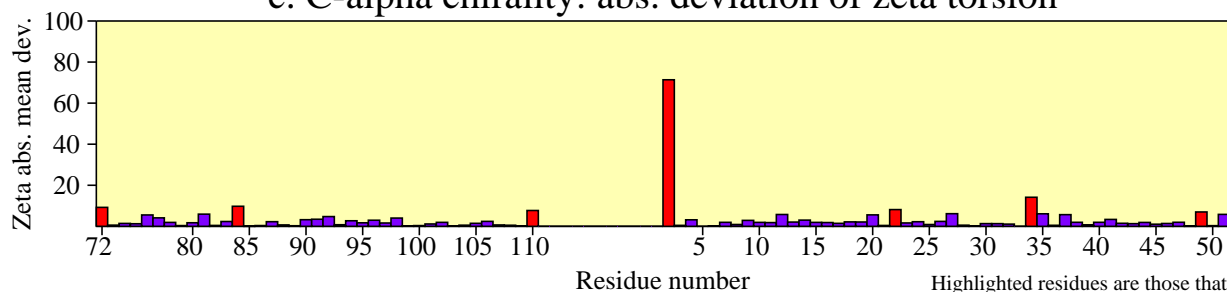
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

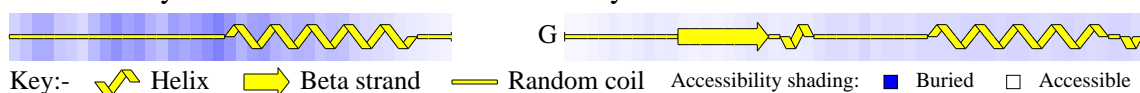


c. C-alpha chirality: abs. deviation of zeta torsion



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

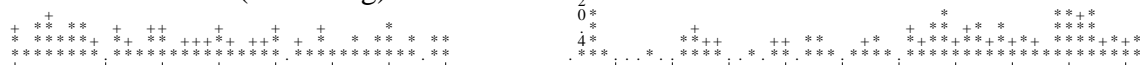
d. Secondary structure & estimated accessibility



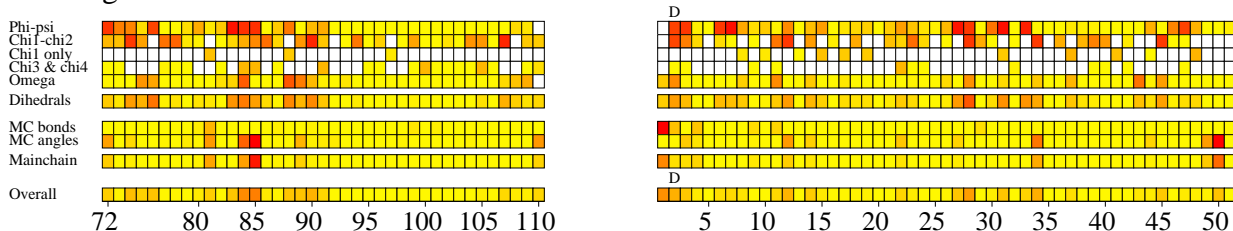
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



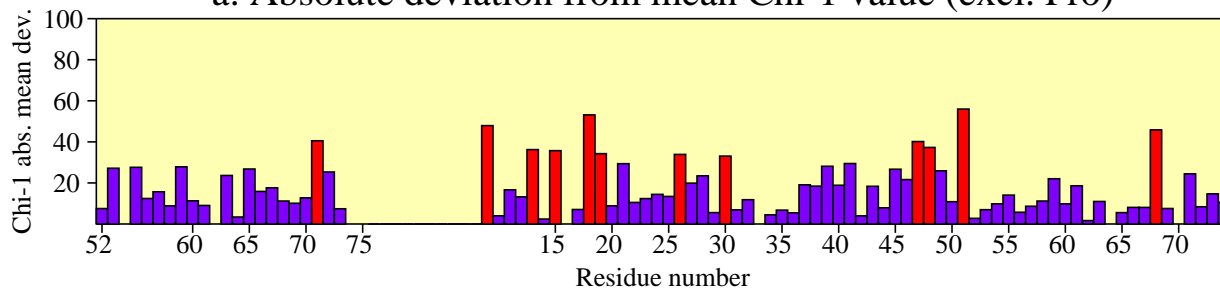
g. G-factors



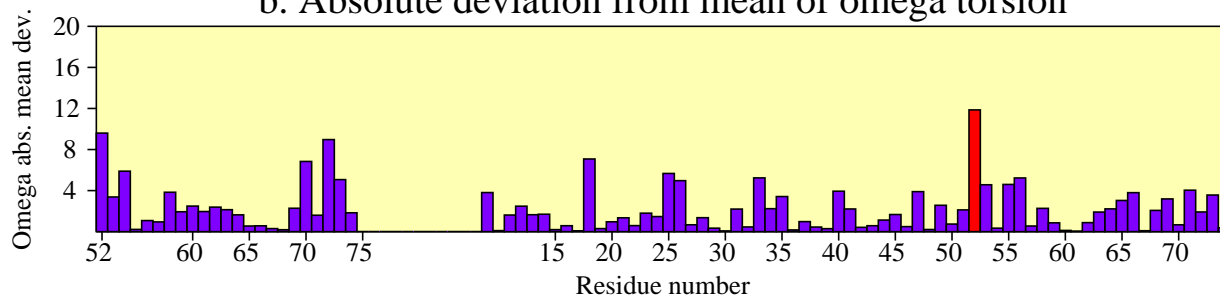
D = D-amino acid

Residue properties 1nu1

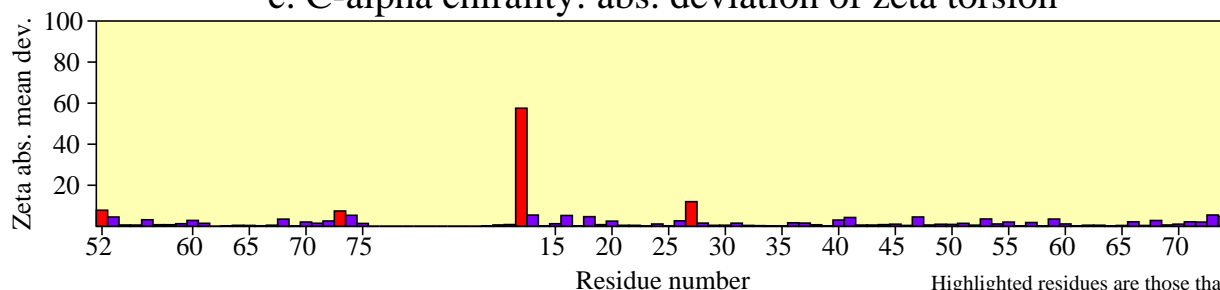
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

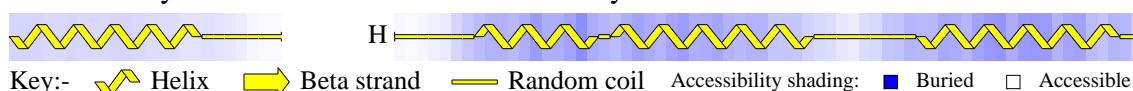


c. C-alpha chirality: abs. deviation of zeta torsion



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

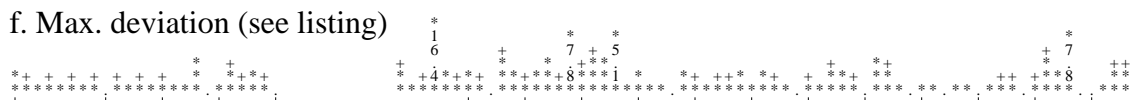
d. Secondary structure & estimated accessibility



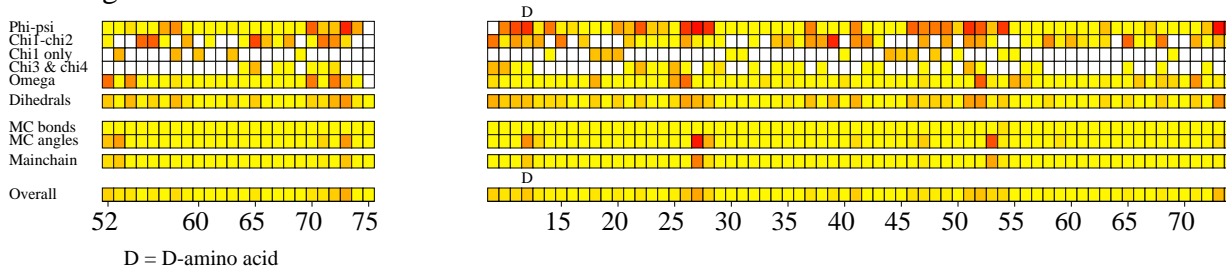
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

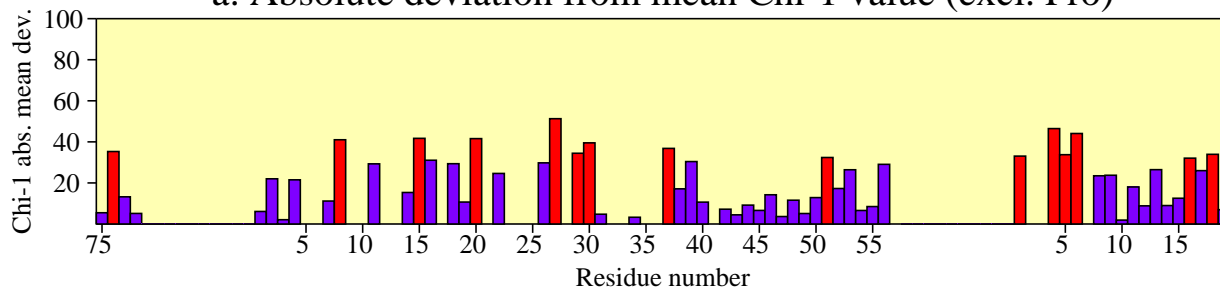


g. G-factors

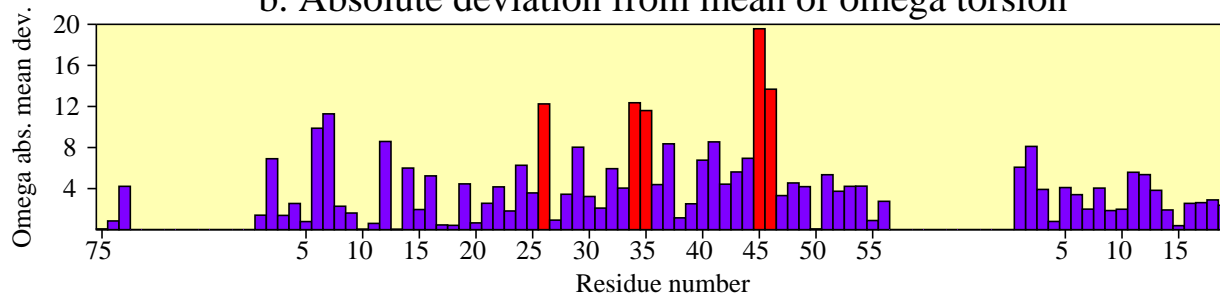


Residue properties 1nu1

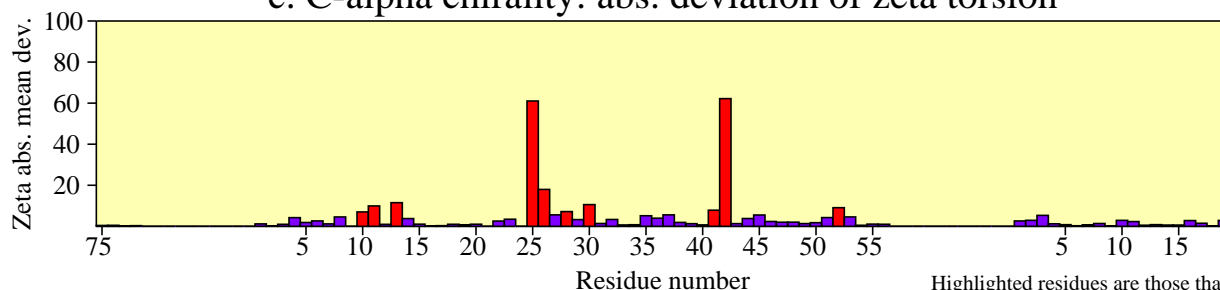
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

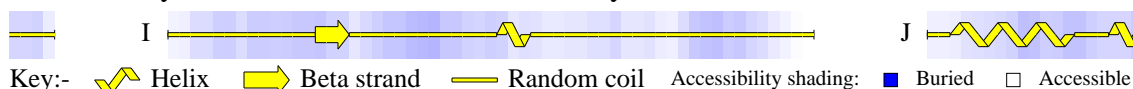


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



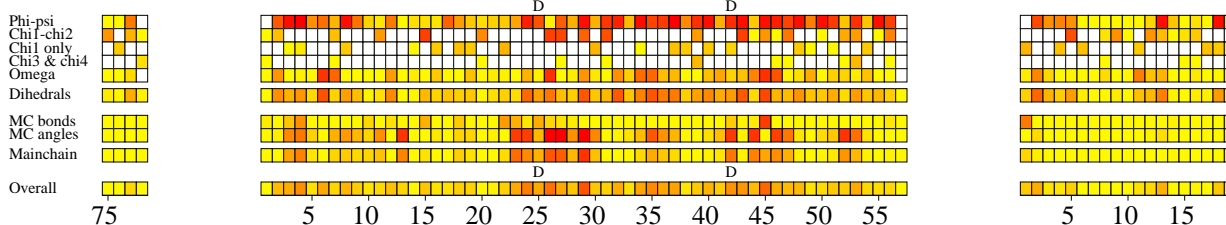
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



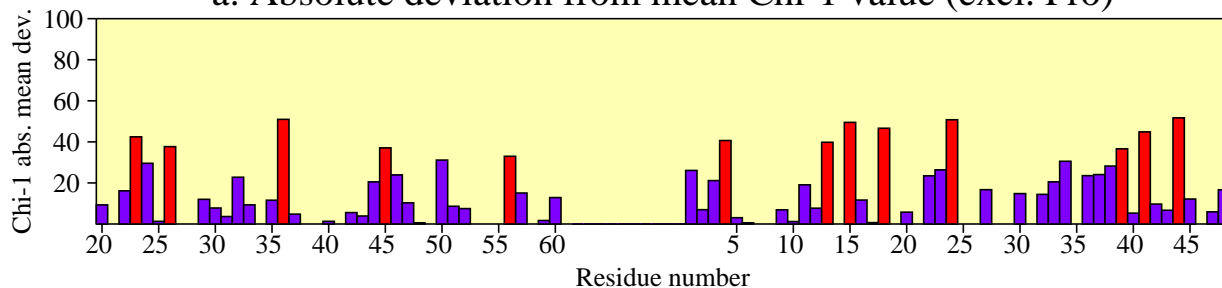
g. G-factors



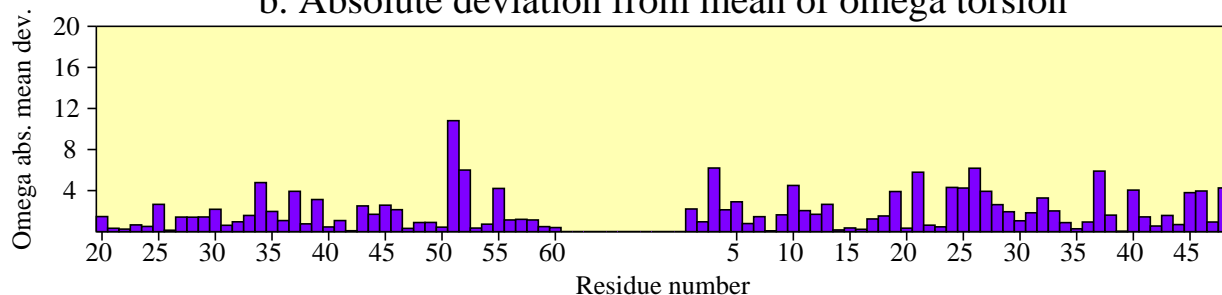
D = D-amino acid

Residue properties 1nu1

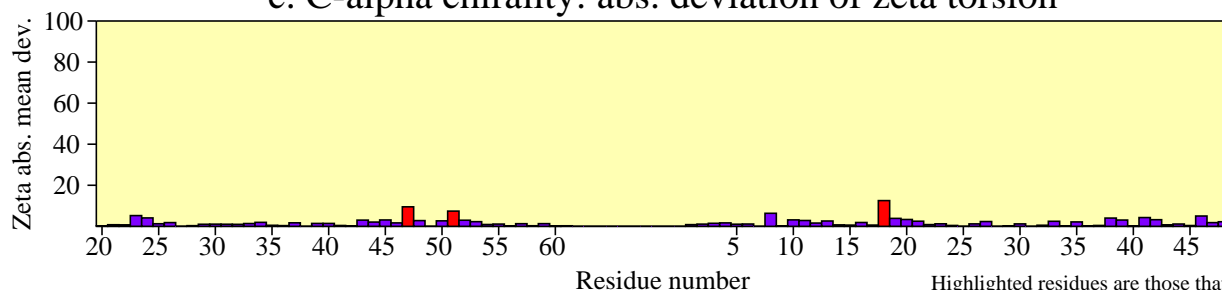
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

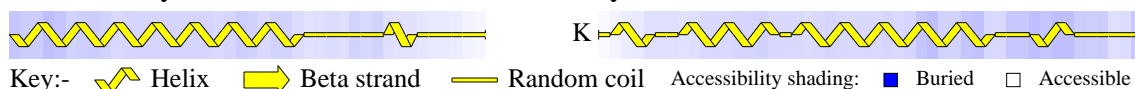


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



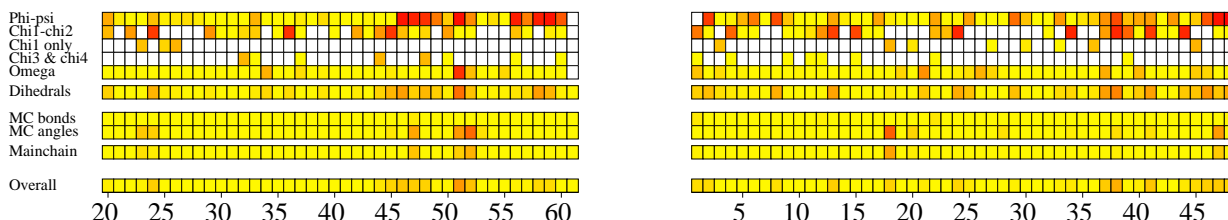
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



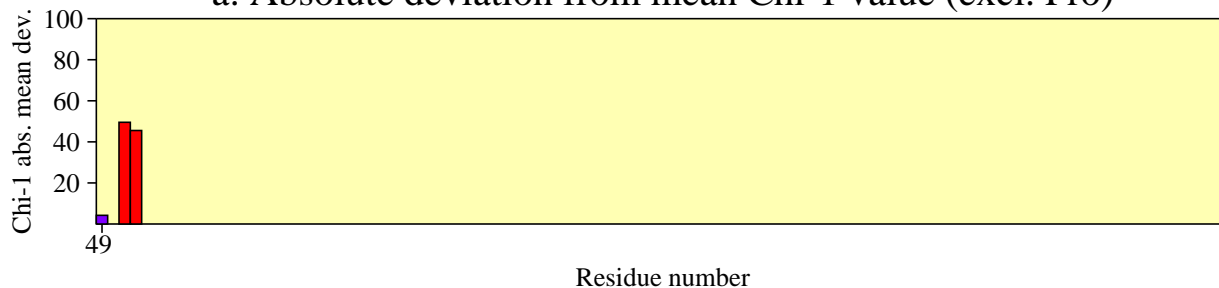
g. G-factors



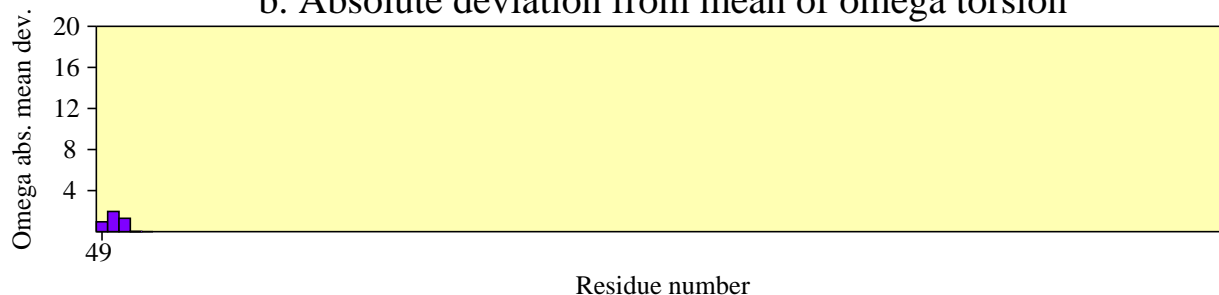
Residue properties

1nu1

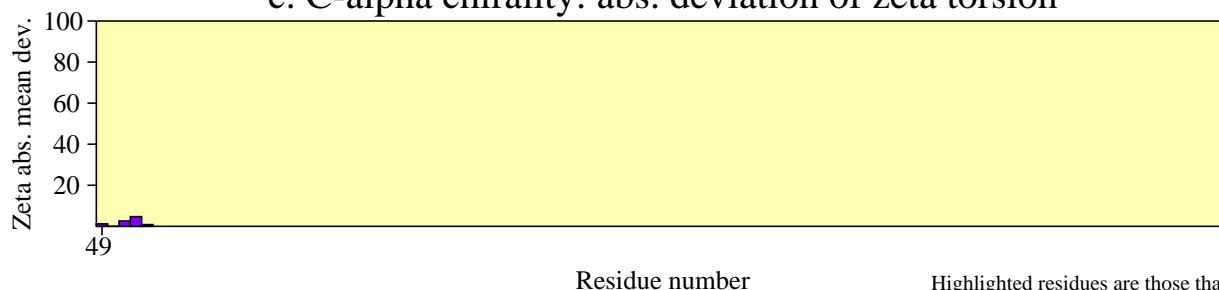
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

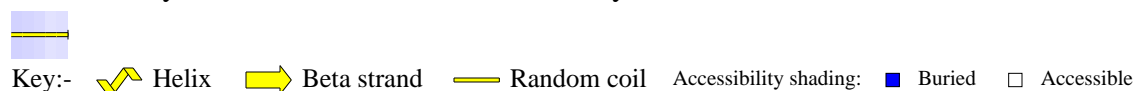


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



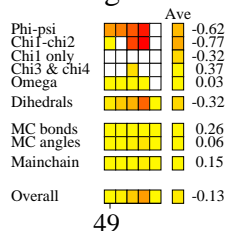
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

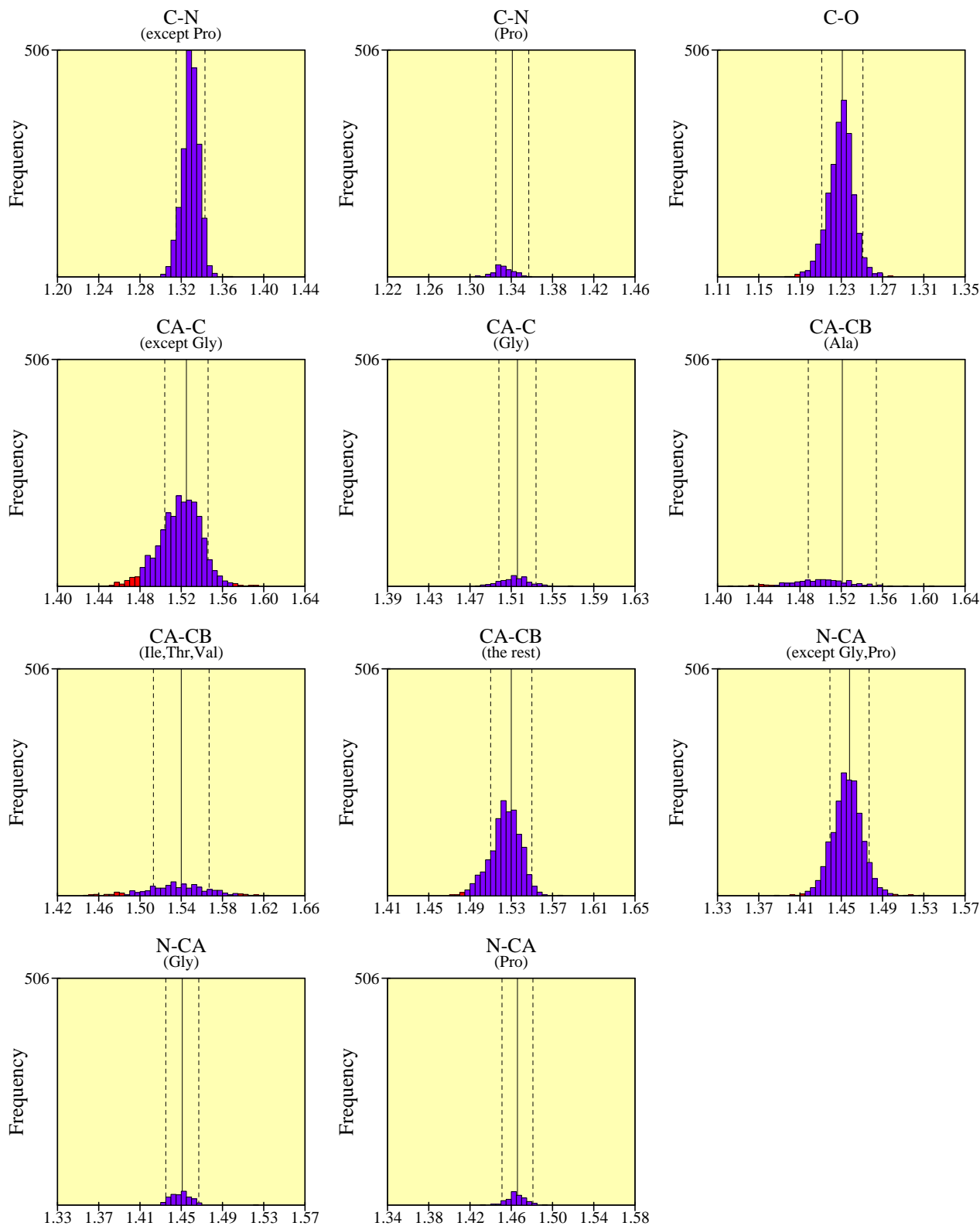


g. G-factors



Main-chain bond lengths

1nu1

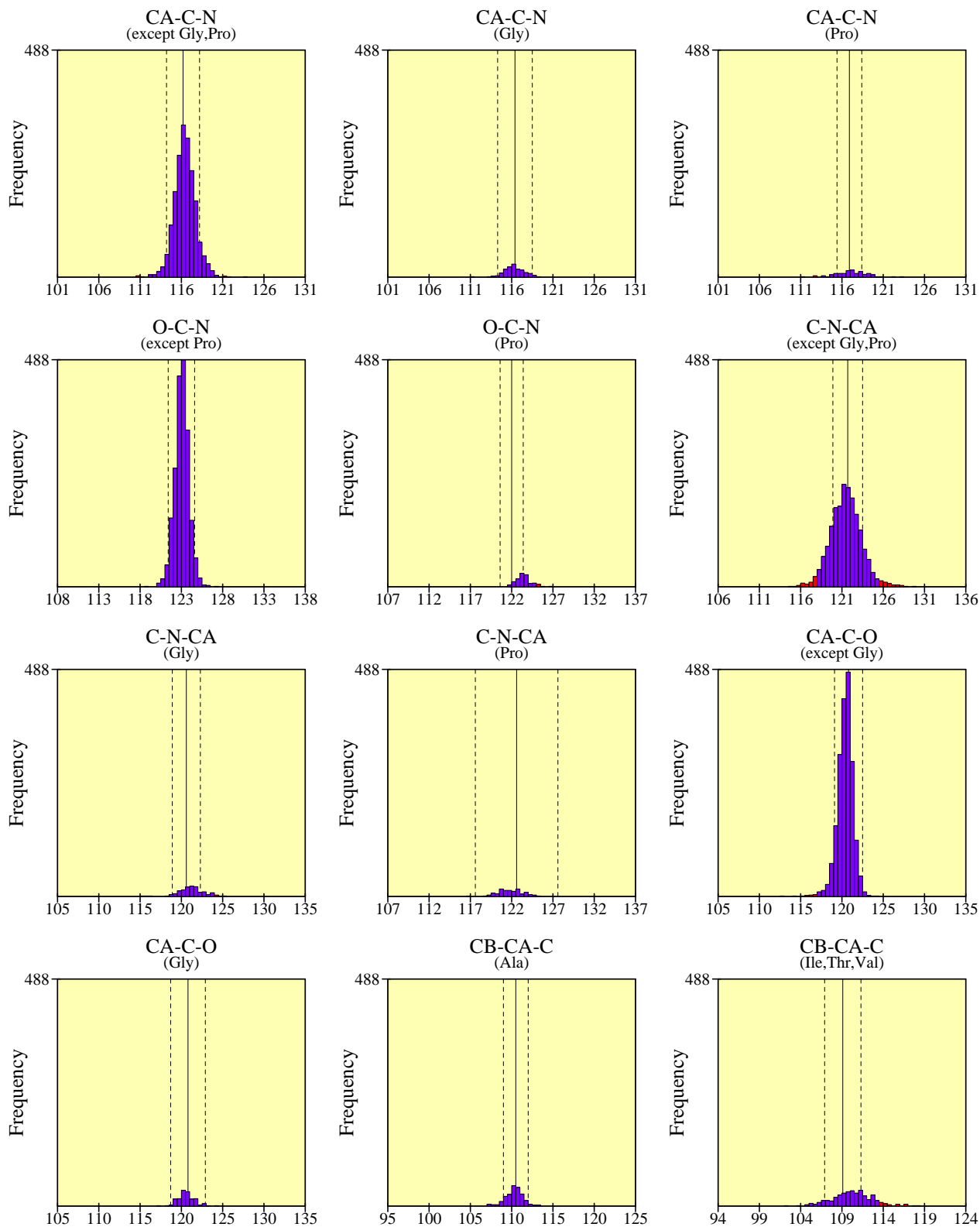


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

1nu1

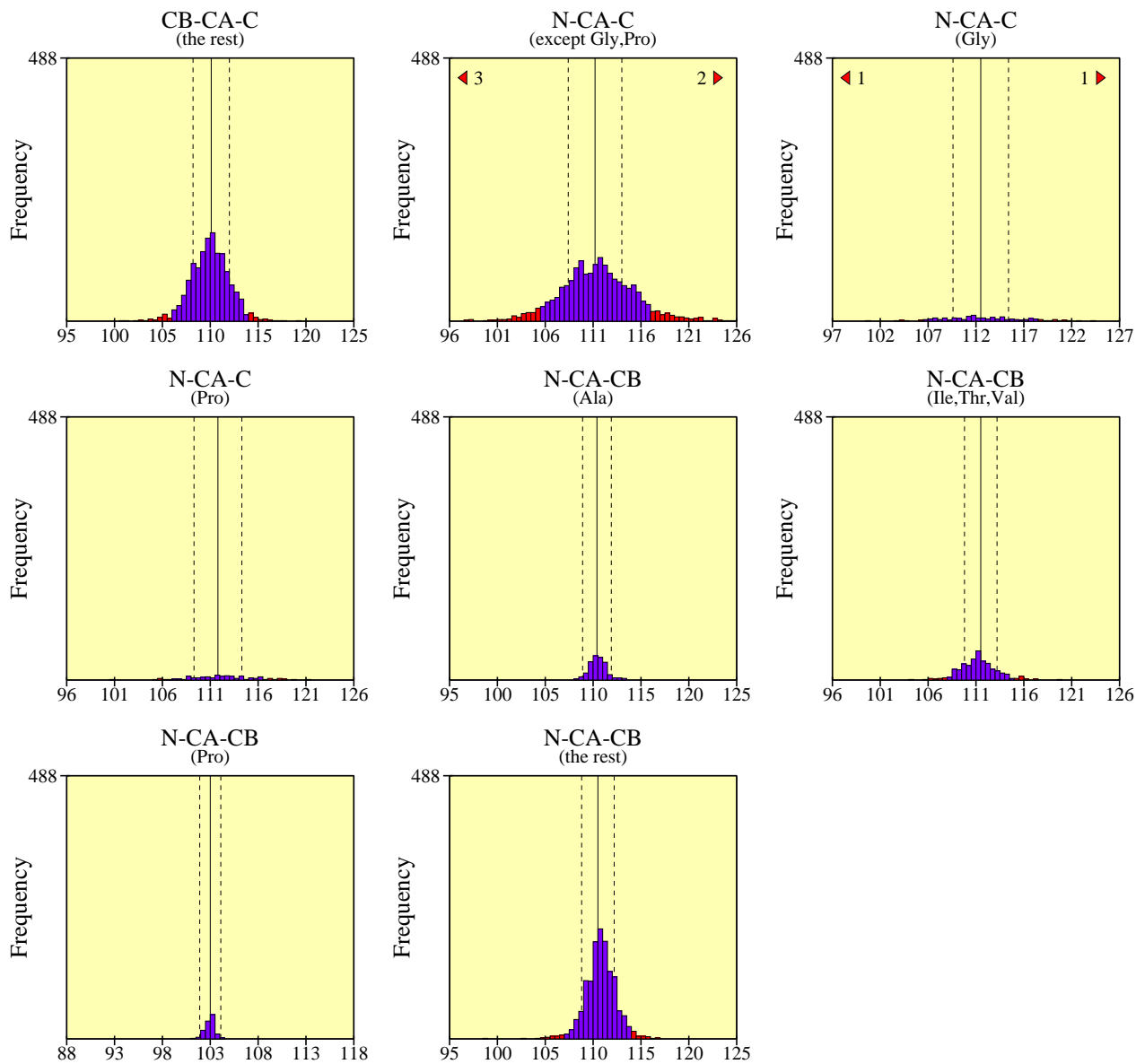


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

1nu1



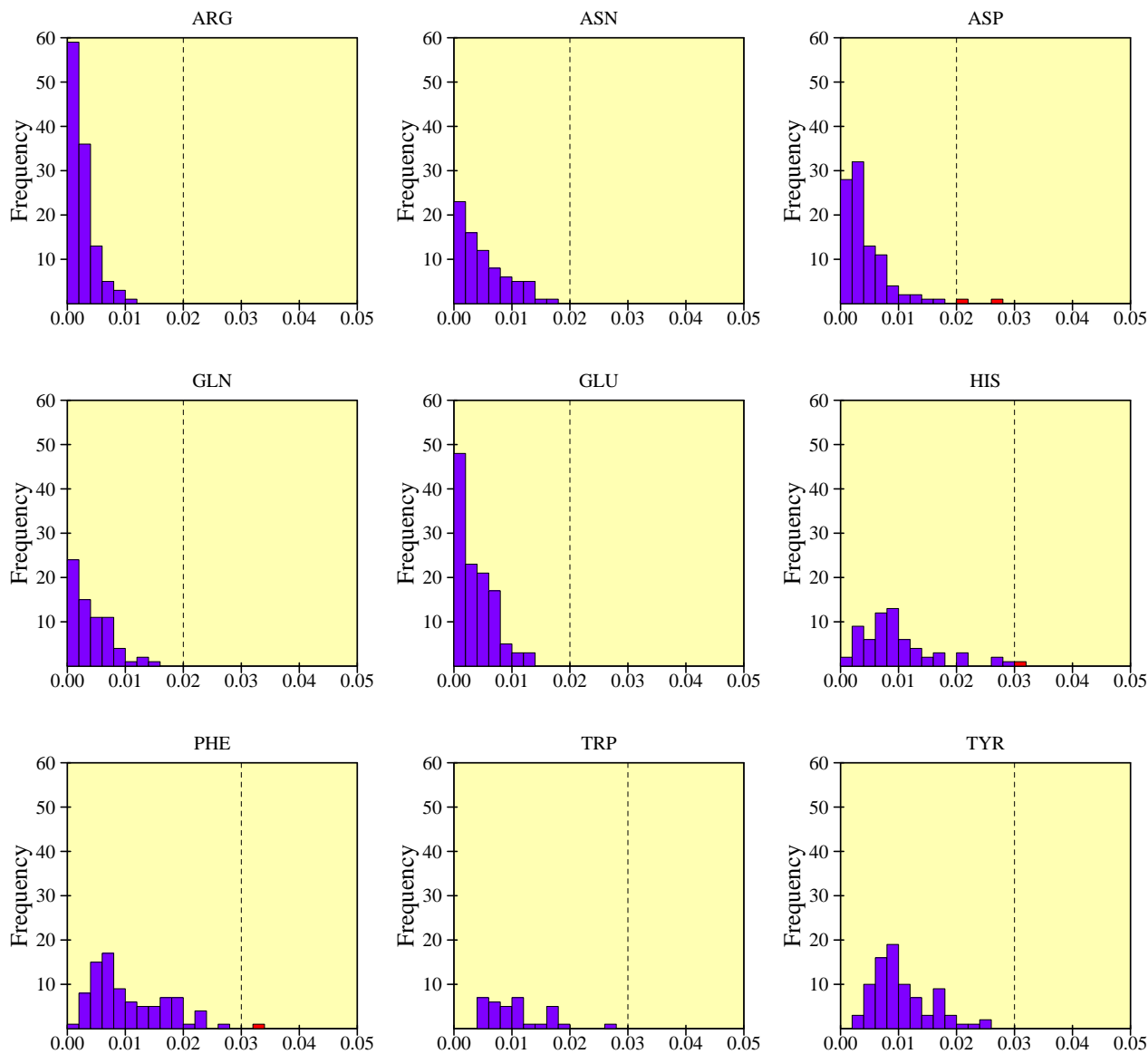
Black bars > 2.0 st. devs. from mean.

◀ 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

1nu1



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

1nu1

Main-chain bond lengths

N 1.458 CA 0.052 1.510 A Thr 1	CA 1.521 CB 0.051 1.470 A Ala 43	CA 1.521 CB 0.077 1.444 A Ala 63	CA 1.540 CB 0.059 1.481 A Thr 143	CA 1.521 CB 0.058 1.463 A Ala 155	CA 1.525 C 0.061 1.464 A Pro 170
CA 1.540 CB 0.056 1.596 A Val 228	CA 1.540 CB 0.063 1.477 A Ile 241	CA 1.525 C 0.055 1.470 A Cys 242	CA 1.525 C 0.053 1.472 A Ala 251	CA 1.525 C 0.051 1.474 A Asp 281	CA 1.525 C 0.051 1.474 A Cys 282
CA 1.525 C 0.060 1.465 A Tyr 284	CA 1.521 CB 0.050 1.471 A Ala 288	CA 1.530 CB 0.054 1.476 A His 289	CA 1.525 C 0.057 1.468 A Ile 297	CA 1.525 C 0.056 1.469 A Thr 300	CA 1.525 C 0.055 1.470 A Asp 327
CA 1.540 CB 0.058 1.482 A Ile 331	CA 1.540 CB 0.054 1.486 A Val 337	CA 1.521 CB 0.066 1.455 A Ala 393	CA 1.521 CB 0.076 1.445 A Ala 404	CA 1.521 CB 0.060 1.461 A Ala 423	N 1.458 CA 0.055 1.403 A Arg 436
CA 1.525 C 0.052 1.473 B Leu 24	CA 1.525 C 0.055 1.470 B Asn 31	CA 1.525 C 0.054 1.471 B Glu 58	CA 1.540 CB 0.058 1.482 B Thr 65	CA 1.521 CB 0.051 1.470 B Ala 72	CA 1.525 C 0.056 1.469 B Ser 73
CA 1.540 CB 0.063 1.603 B Thr 76	CA 1.521 CB 0.075 1.446 B Ala 80	CA 1.525 C 0.057 1.468 B Ile 85	CA 1.540 CB 0.085 1.455 B Thr 86	CA 1.540 CB 0.061 1.601 B Val 92	CA 1.540 CB 0.057 1.483 B Val 98
CA 1.540 CB 0.084 1.456 B Val 116	CA 1.525 C 0.066 1.459 B Thr 127	CA 1.521 CB 0.052 1.469 B Ala 138	CA 1.530 CB 0.057 1.473 B Pro 142	CA 1.521 CB 0.052 1.469 B Ala 149	CA 1.525 C 0.059 1.466 B Ala 151
CA 1.521 CB 0.076 1.445 B Ala 151	C 1.231 O 0.050 1.181 B Gln 153	CA 1.530 CB 0.052 1.478 B Gln 156	CA 1.521 CB 0.101 1.420 B Ala 157	CA 1.540 CB 0.066 1.474 B Val 159	CA 1.540 CB 0.075 1.465 B Ile 160
CA 1.525 C 0.053 1.472 B Leu 163	CA 1.525 C 0.070 1.455 B His 164	CA 1.521 CB 0.056 1.465 B Ala 165	CA 1.521 CB 0.051 1.470 B Ala 166	CA 1.521 CB 0.051 1.470 B Ala 167	CA 1.525 C 0.067 1.457 B Asn 170
N 1.458 CA 0.070 1.388 B Asn 170	CA 1.525 C 0.059 1.466 B Ala 171	CA 1.521 CB 0.079 1.442 B Ala 171	CA 1.521 CB 0.088 1.433 B Ala 173	CA 1.525 C 0.065 1.460 B Asp 180	CA 1.525 C 0.065 1.460 B Arg 182
CA 1.525 C 0.071 1.454 B Gln 196	CA 1.525 C 0.052 1.473 B Asn 197	CA 1.540 CB 0.094 1.446 B Thr 200	CA 1.521 CB 0.058 1.463 B Ala 202	CA 1.521 CB 0.066 1.455 B Ala 205	CA 1.540 CB 0.063 1.477 B Val 211

Distorted geometry

1nu1

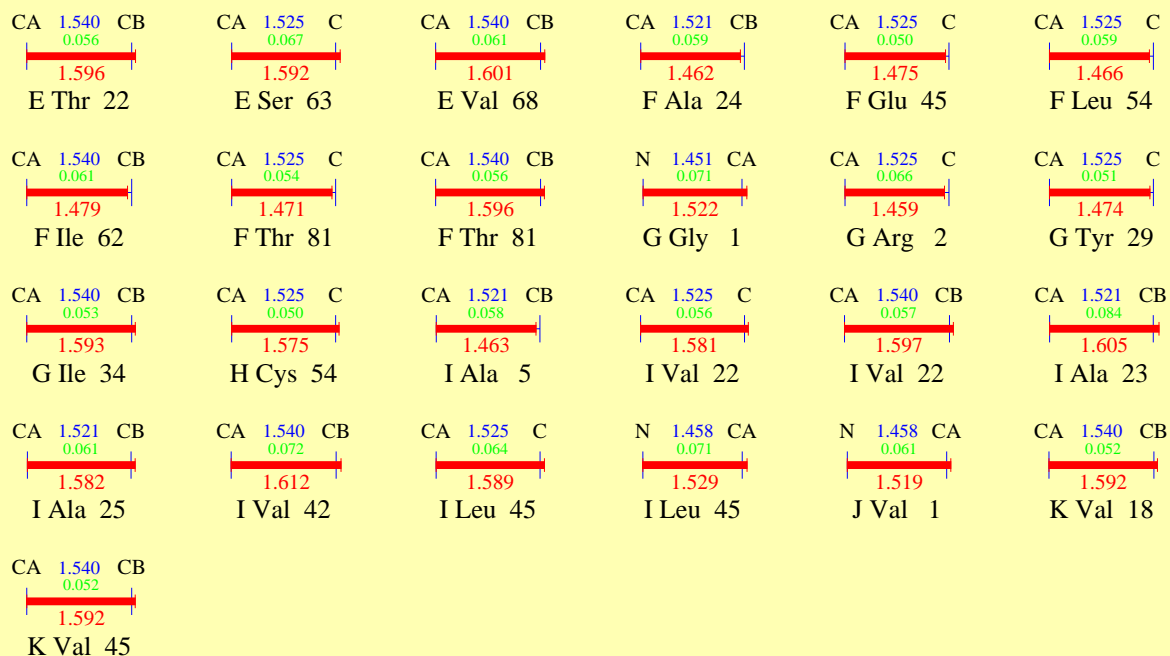
Main-chain bond lengths (contd)

CA 1.525 C 0.064 1.461 B Arg 227	CA 1.525 C 0.050 1.475 B Ala 237	C 1.231 O 0.053 1.178 B Gly 241	CA 1.540 CB 0.066 1.474 B Ile 244	CA 1.516 C 0.053 1.569 B Gly 249	CA 1.525 C 0.050 1.475 B Ser 251
CA 1.525 C 0.063 1.462 B Ala 255	CA 1.525 C 0.066 1.459 B Ala 262	CA 1.521 CB 0.111 1.410 B Ala 262	CA 1.521 CB 0.086 1.435 B Ala 263	CA 1.525 C 0.063 1.588 B Ser 266	CA 1.521 CB 0.060 1.461 B Ala 269
CA 1.521 CB 0.076 1.445 B Ala 281	CA 1.521 CB 0.061 1.461 B Ala 291	CA 1.521 CB 0.052 1.469 B Ala 298	CA 1.525 C 0.055 1.470 B Ser 315	CA 1.540 CB 0.065 1.475 B Thr 326	CA 1.525 C 0.060 1.465 B Ile 327
CA 1.530 CB 0.058 1.472 B Ser 328	CA 1.521 CB 0.051 1.470 B Ala 331	CA 1.540 CB 0.072 1.468 B Ile 347	CA 1.540 CB 0.086 1.454 B Val 372	CA 1.540 CB 0.057 1.483 B Val 382	CA 1.525 C 0.074 1.451 B Ser 384
CA 1.525 C 0.051 1.474 B Tyr 392	CA 1.525 C 0.053 1.472 B Ser 396	CA 1.540 CB 0.062 1.478 B Ile 402	CA 1.540 CB 0.072 1.468 B Val 405	CA 1.540 CB 0.083 1.457 B Ile 411	CA 1.525 C 0.069 1.456 B Phe 417
CA 1.525 C 0.079 1.446 B Met 424	CA 1.521 CB 0.056 1.465 B Ala 425	CA 1.521 CB 0.081 1.441 B Ala 426	CA 1.540 CB 0.064 1.476 B Thr 433	CA 1.525 C 0.064 1.461 B Ile 436	N 1.458 CA 0.072 1.530 B Ile 436
CA 1.525 C 0.058 1.467 B Asp 437	N 1.458 CA 0.056 1.402 B Asp 437	CA 1.525 C 0.056 1.469 B Glu 438	N 1.458 CA 0.062 1.520 C Thr 2	CA 1.525 C 0.051 1.474 C Ile 13	CA 1.521 CB 0.063 1.458 C Ala 23
CA 1.525 C 0.081 1.444 C Ser 25	CA 1.525 C 0.052 1.473 C Ile 27	CA 1.525 C 0.067 1.458 C Leu 36	CA 1.540 CB 0.075 1.615 C Ile 42	CA 1.540 CB 0.063 1.477 C Thr 47	CA 1.521 CB 0.052 1.469 C Ala 87
CA 1.525 C 0.067 1.592 C Met 96	CA 1.540 CB 0.089 1.451 C Thr 112	CA 1.540 CB 0.057 1.483 C Ile 115	CA 1.540 CB 0.066 1.606 C Ile 118	CA 1.540 CB 0.054 1.486 C Val 145	CA 1.525 C 0.050 1.475 C Thr 203
CA 1.540 CB 0.068 1.472 C Ile 211	CA 1.525 C 0.055 1.470 C Pro 219	CA 1.525 C 0.054 1.579 C His 267	CA 1.521 CB 0.062 1.459 C Ala 327	CA 1.540 CB 0.054 1.594 C Thr 349	CA 1.521 CB 0.050 1.471 C Ala 354
CA 1.540 CB 0.080 1.620 C Val 364	CA 1.525 C 0.052 1.473 D Arg 27	CA 1.540 CB 0.050 1.590 D Val 68	CA 1.540 CB 0.076 1.616 D Thr 175	CA 1.540 CB 0.063 1.477 E Thr 3	N 1.458 CA 0.050 1.408 E Lys 6

Distorted geometry

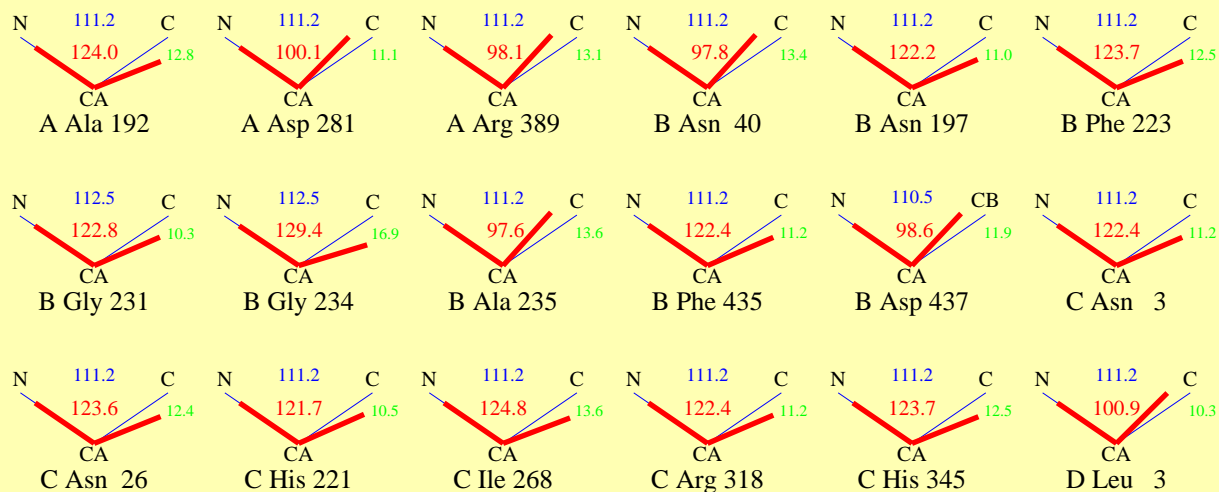
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Main-chain bond lengths (contd)



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

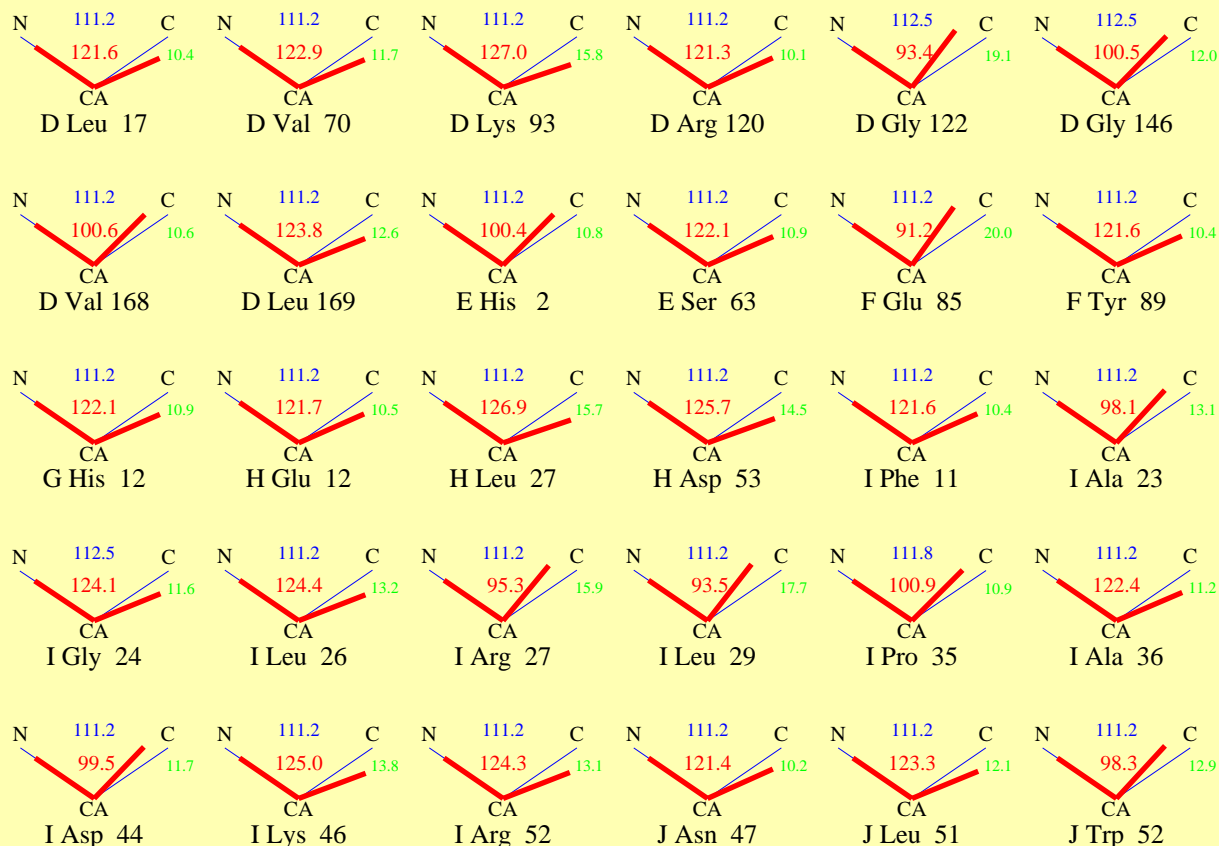
Main-chain bond angles



Distorted geometry

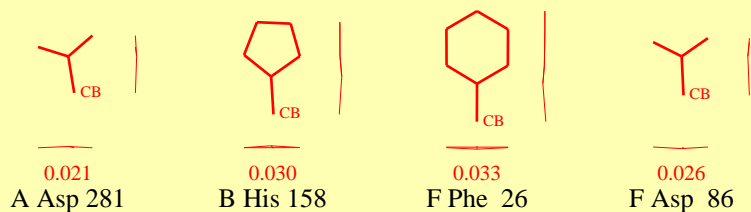
1nu1

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.