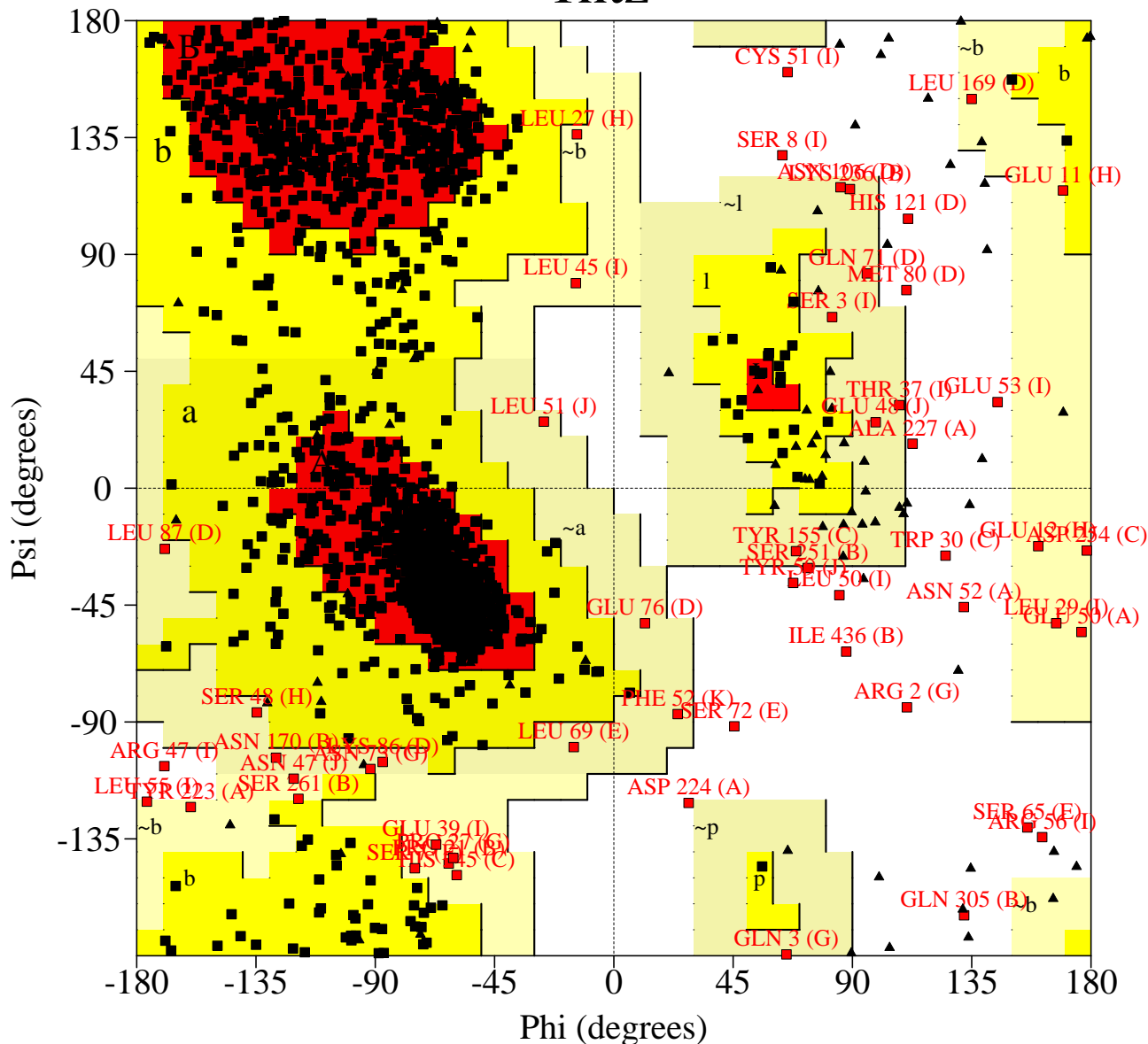


Ramachandran Plot

1ntz



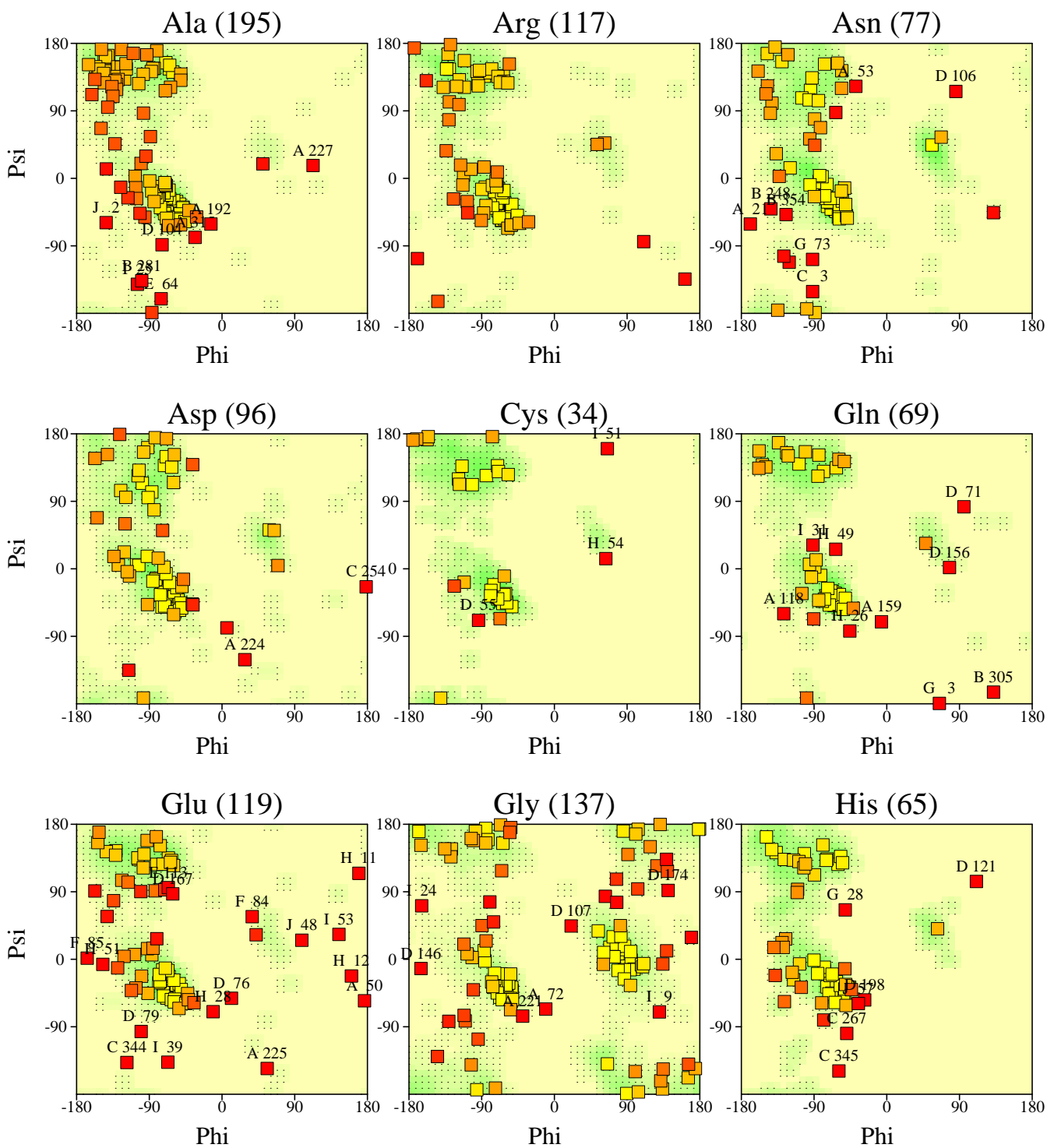
Plot statistics

Residues in most favoured regions [A,B,L]	1554	84.6%
Residues in additional allowed regions [a,b,l,p]	232	12.6%
Residues in generously allowed regions [-a,-b,-l,-p]	32	1.7%
Residues in disallowed regions	19	1.0%
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

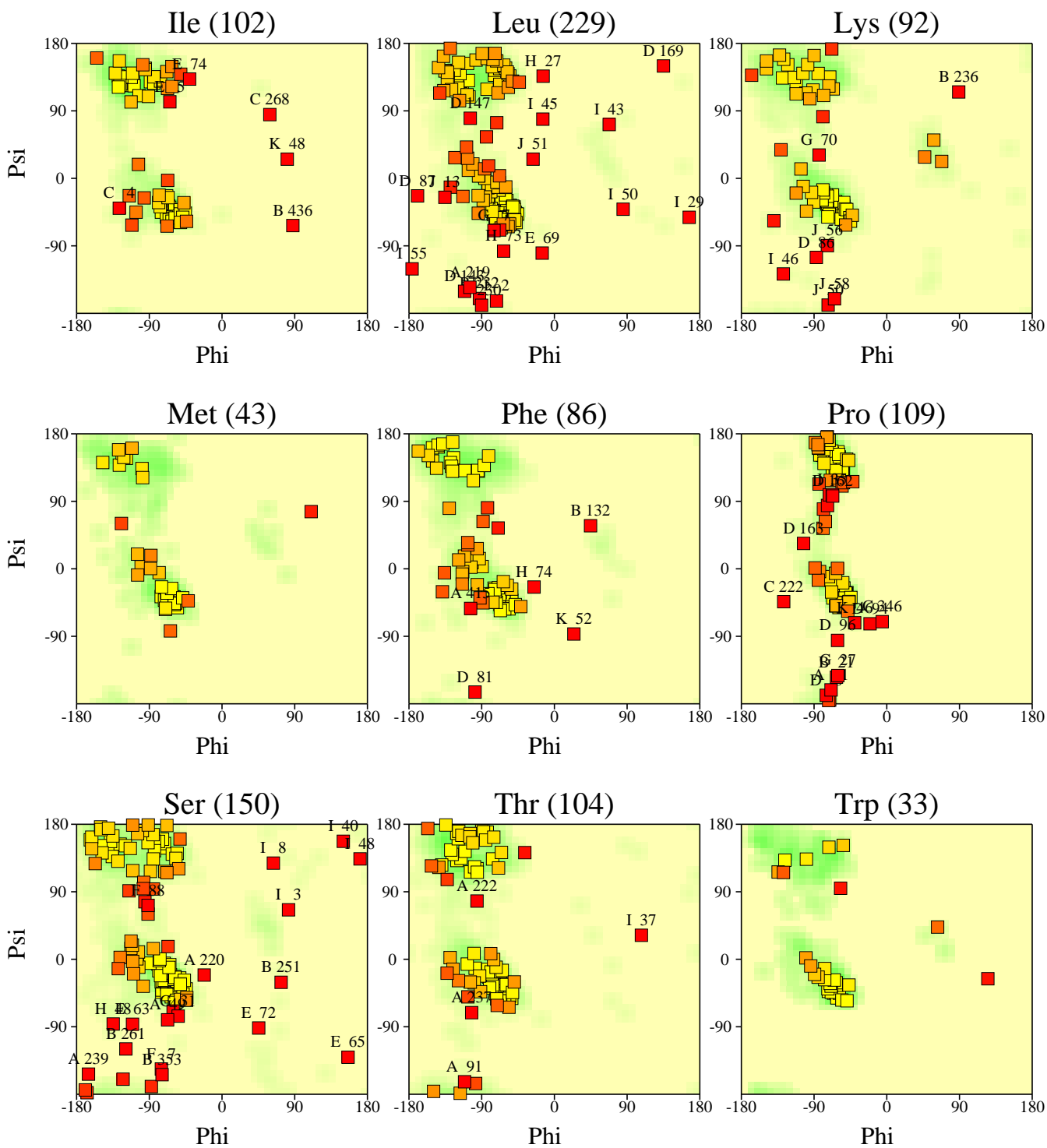
1ntz



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

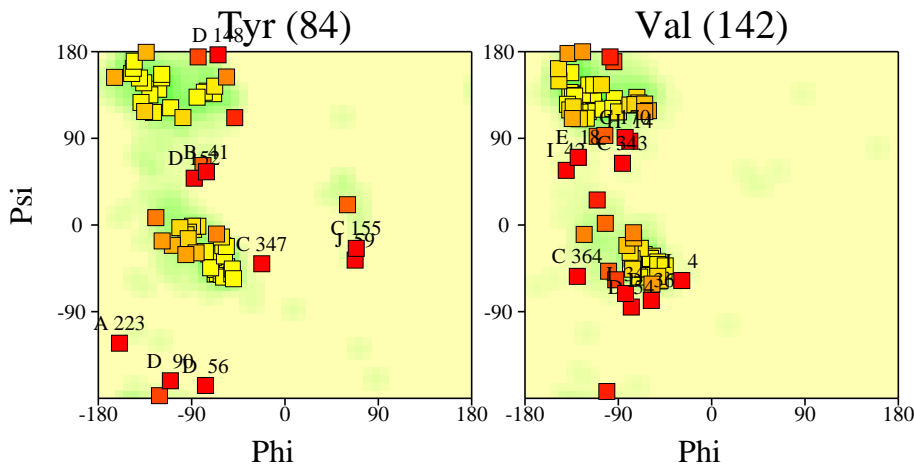
1ntz



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

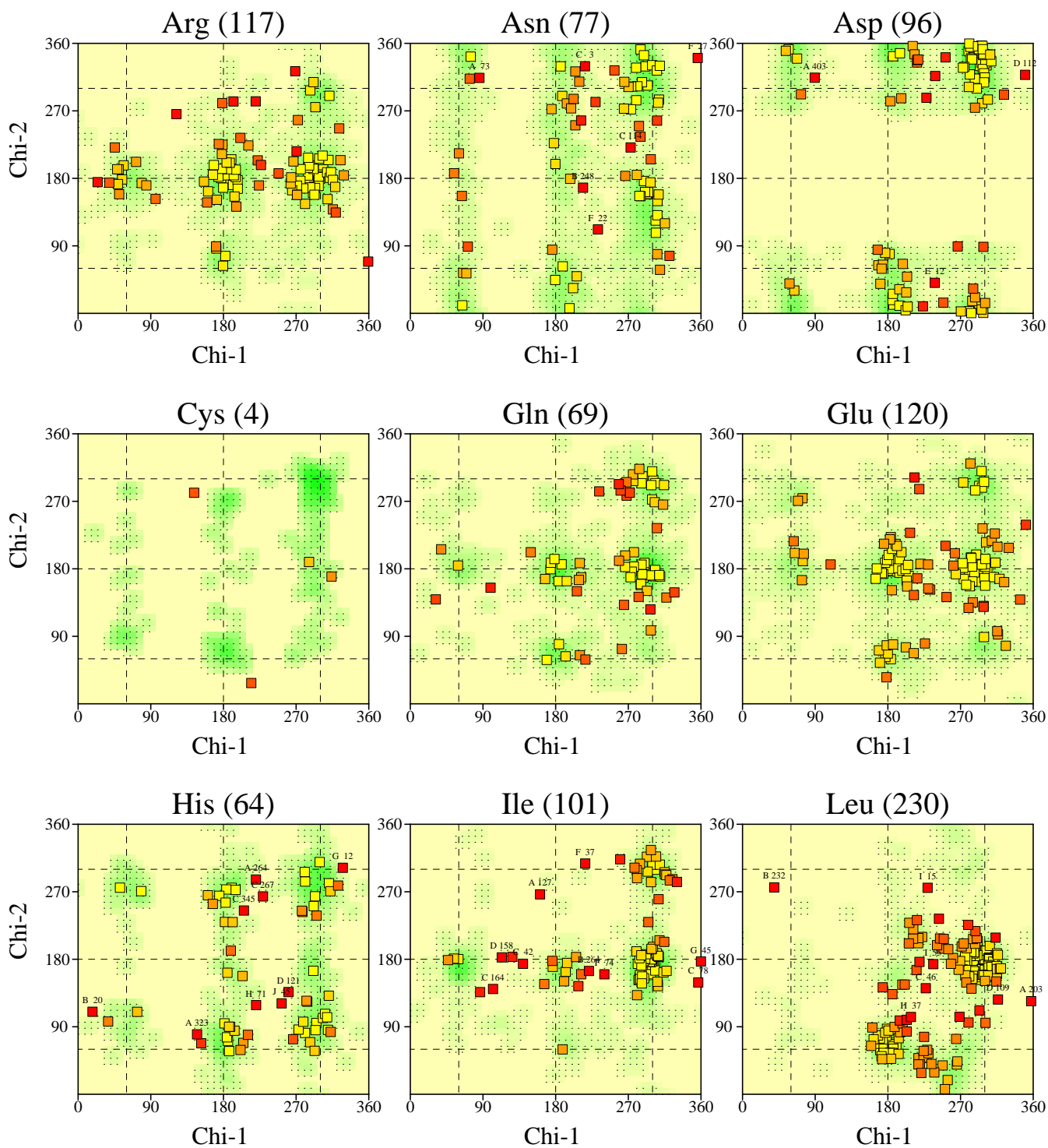
1ntz



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

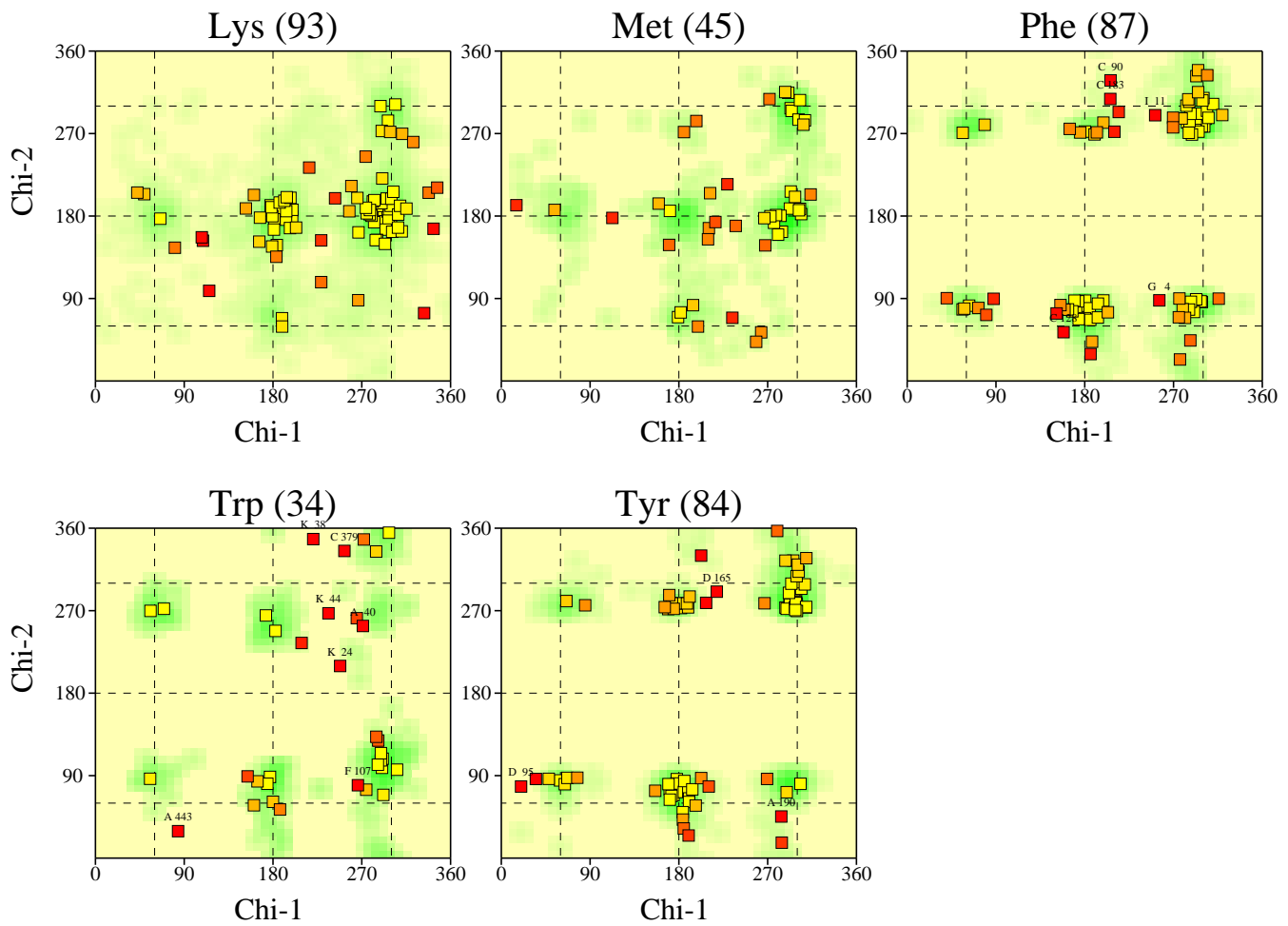
1ntz



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

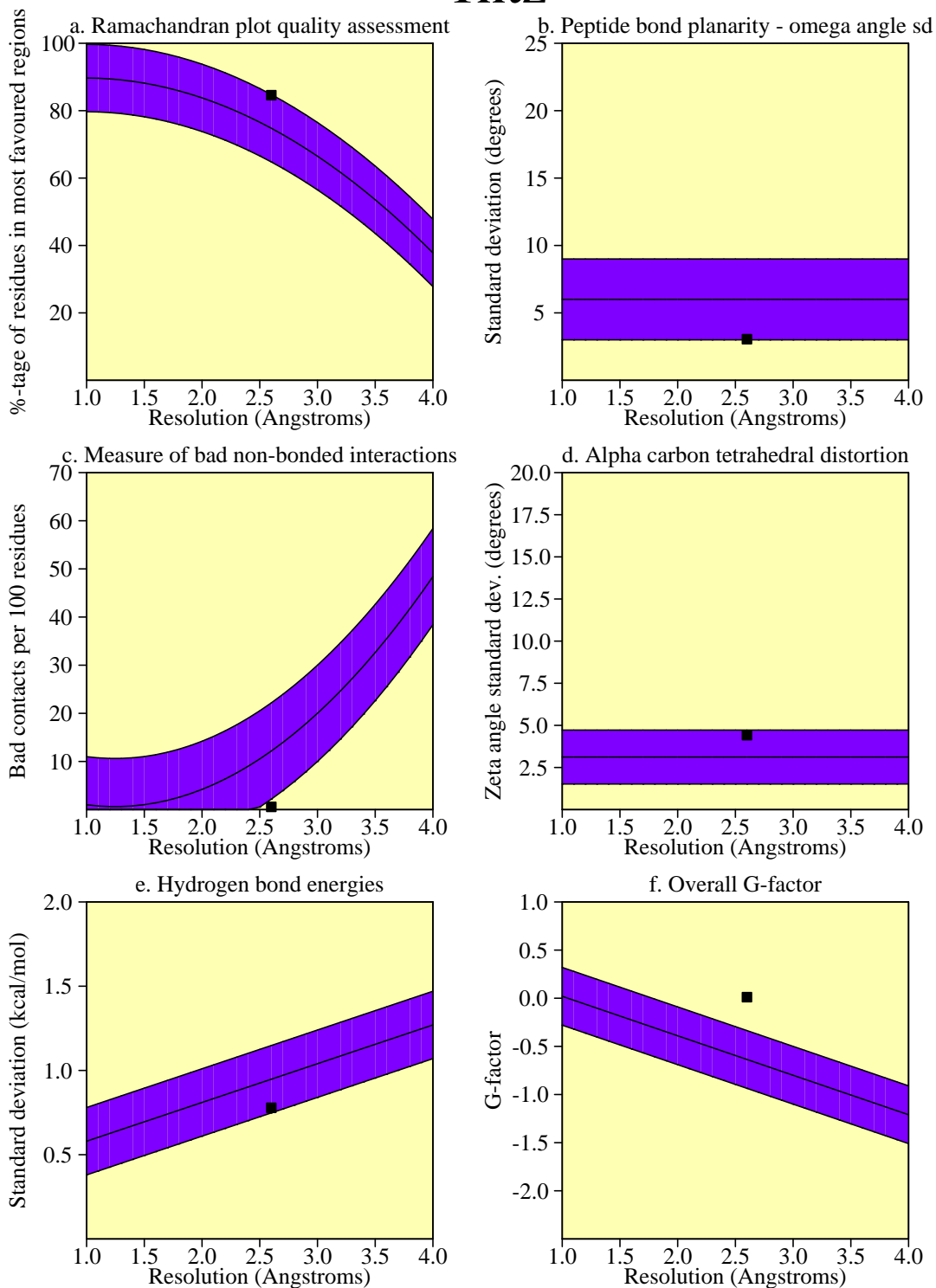
1ntz



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

1ntz

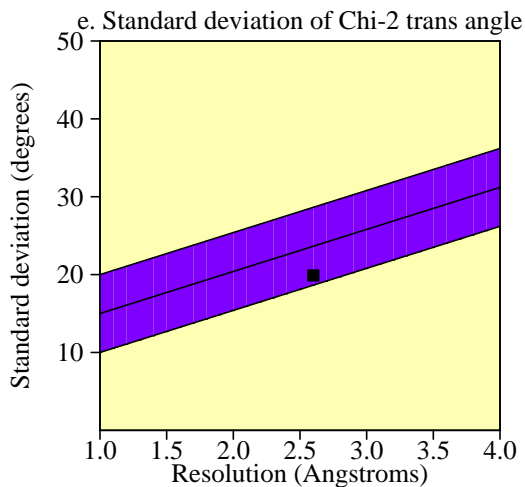
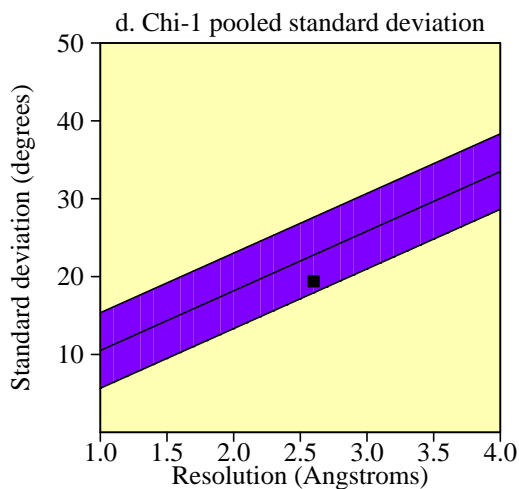
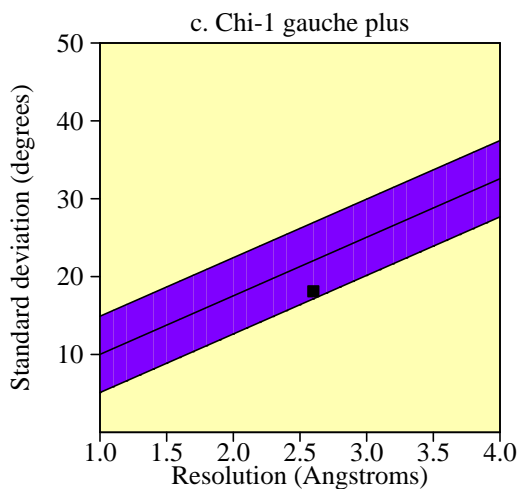
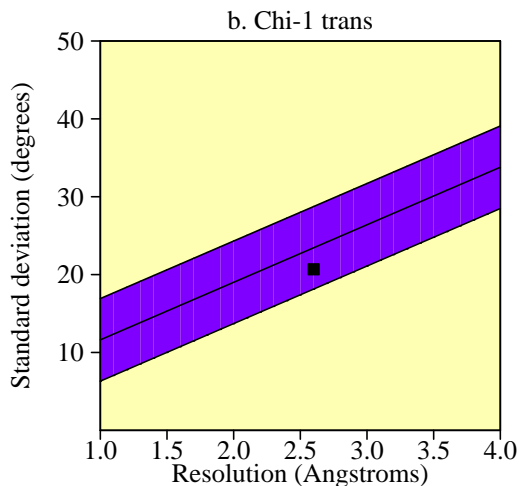
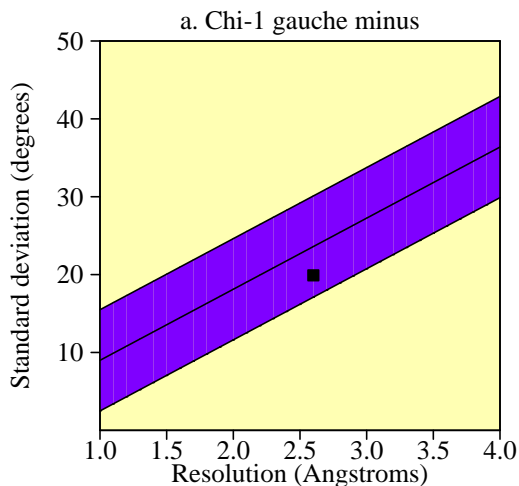


Plot statistics

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	84.6	74.8	10.0	1.0	Inside
b. Omega angle st dev	2094	3.0	6.0	3.0	-1.0	Inside
c. Bad contacts / 100 residues	12	0.6	12.2	10.0	-1.2	BETTER
d. Zeta angle st dev	1965	4.4	3.1	1.6	0.8	Inside
e. H-bond energy st dev	1371	0.8	0.9	0.2	-0.8	Inside
f. Overall G-factor	2105	0.0	-0.6	0.3	2.2	BETTER

Side-chain parameters

1ntz



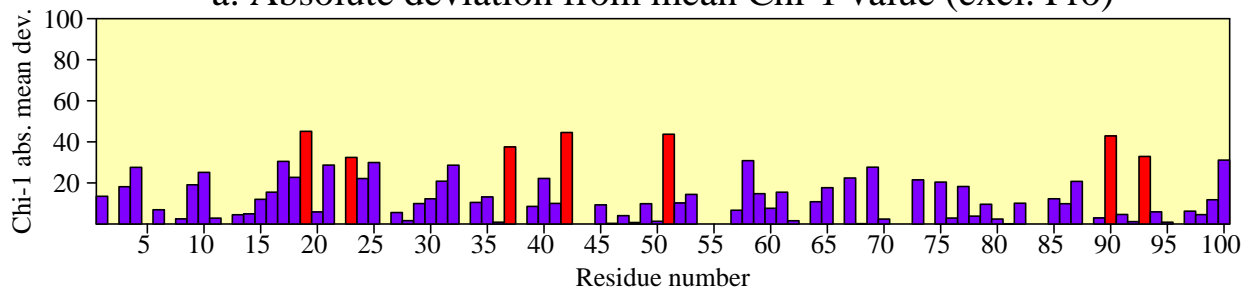
1ntz

Plot statistics

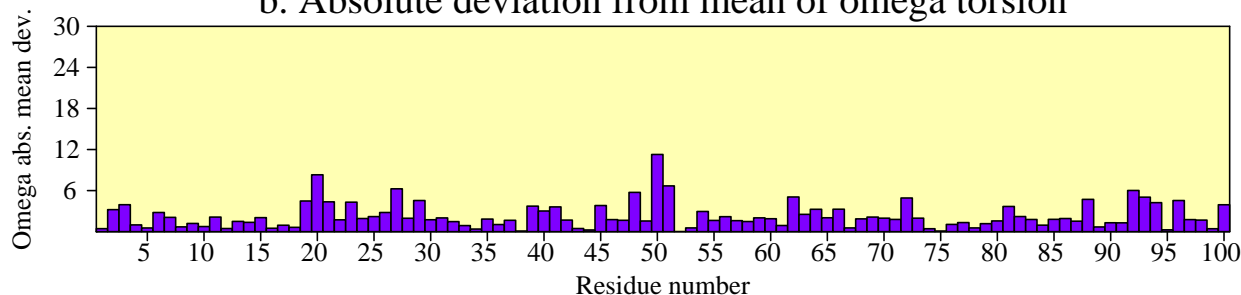
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. Chi-1 gauche minus st dev	204	19.9	23.6	6.5	-0.6	Inside
b. Chi-1 trans st dev	608	20.7	23.4	5.3	-0.5	Inside
c. Chi-1 gauche plus st dev	842	18.1	22.0	4.9	-0.8	Inside
d. Chi-1 pooled st dev	1654	19.4	22.8	4.8	-0.7	Inside
e. Chi-2 trans st dev	572	19.9	23.6	5.0	-0.7	Inside

Residue properties 1ntz

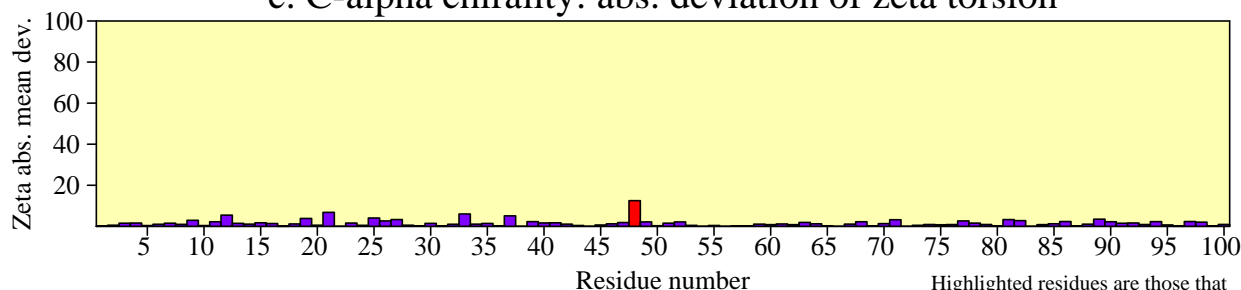
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

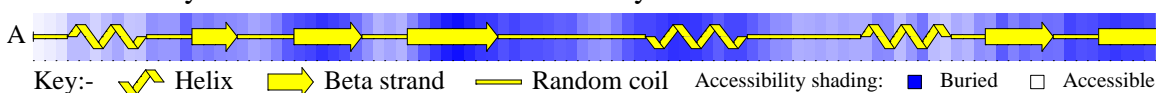


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



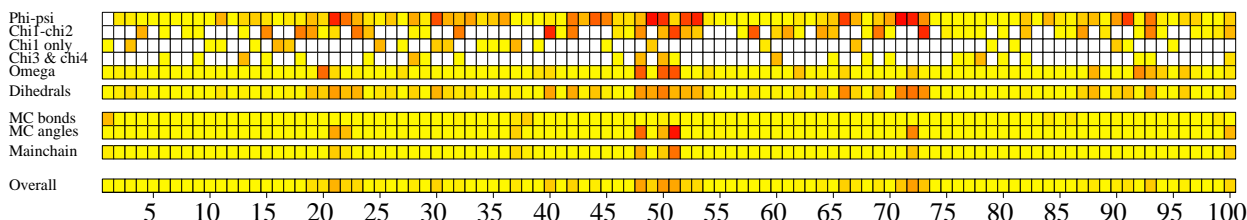
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

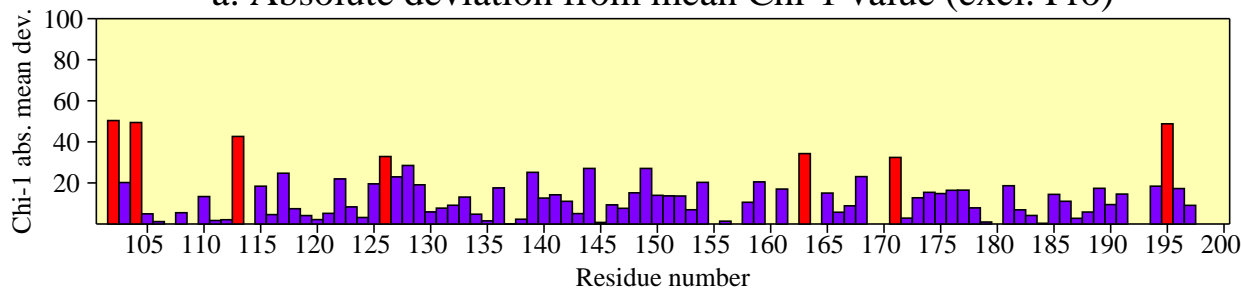


g. G-factors

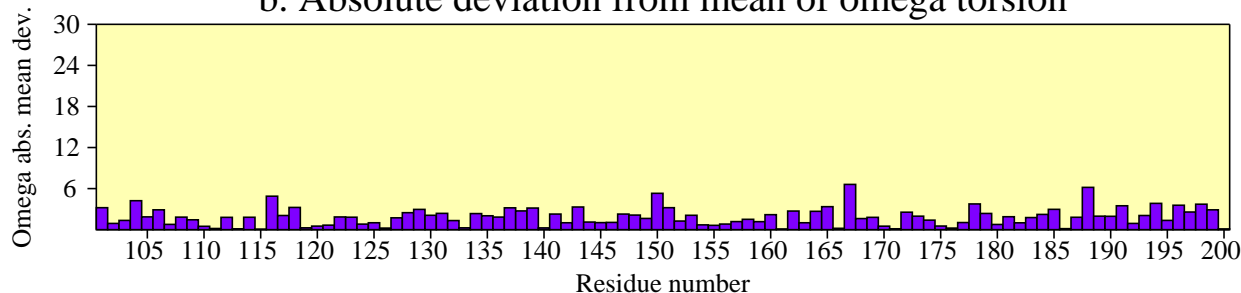


Residue properties 1ntz

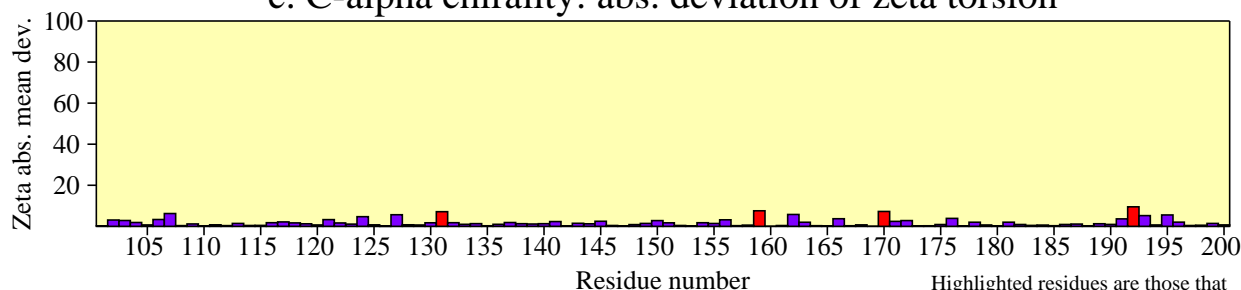
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



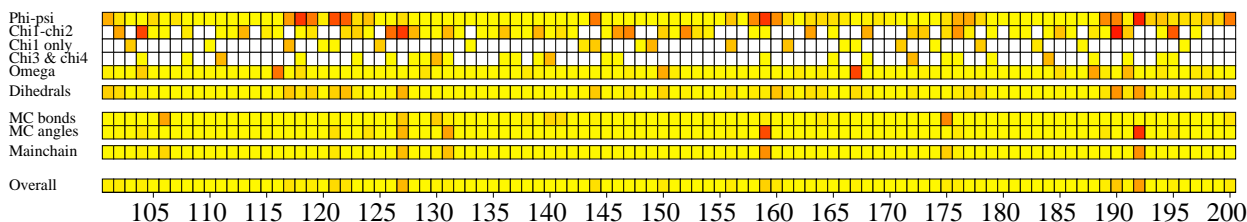
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

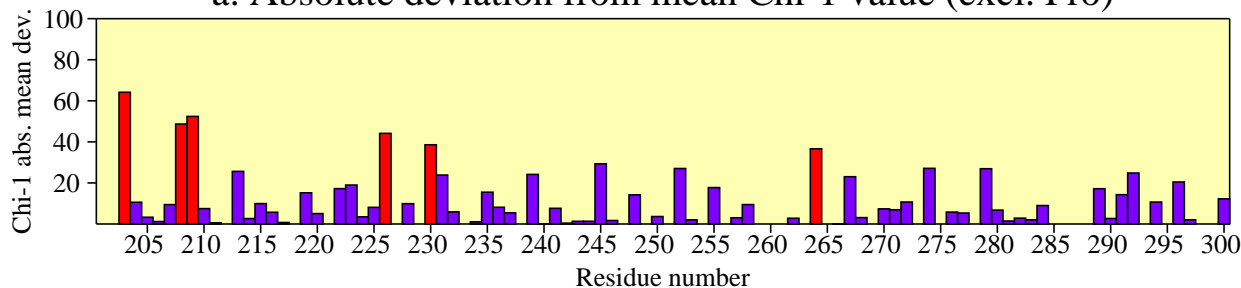


g. G-factors

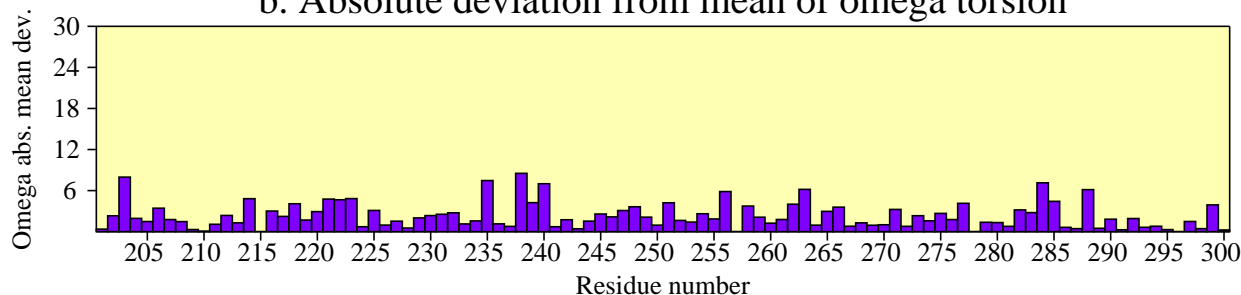


Residue properties 1ntz

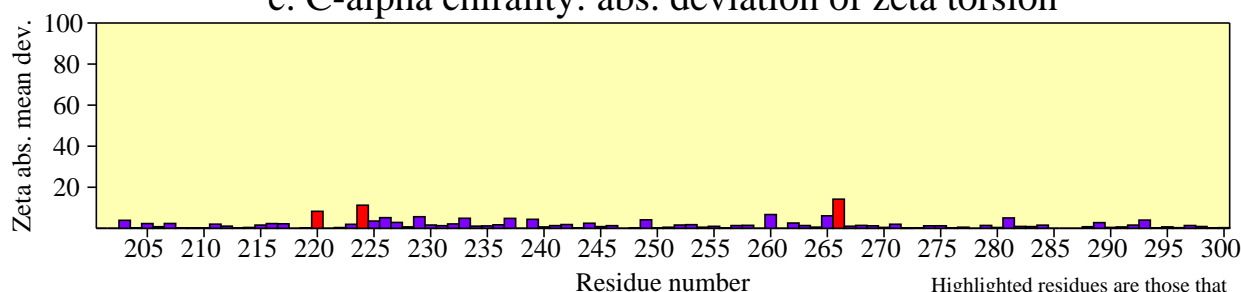
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

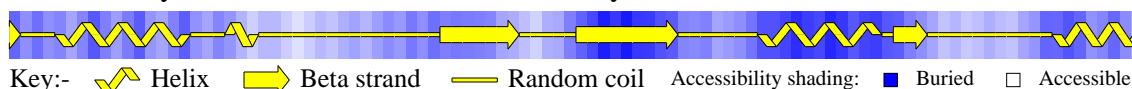


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



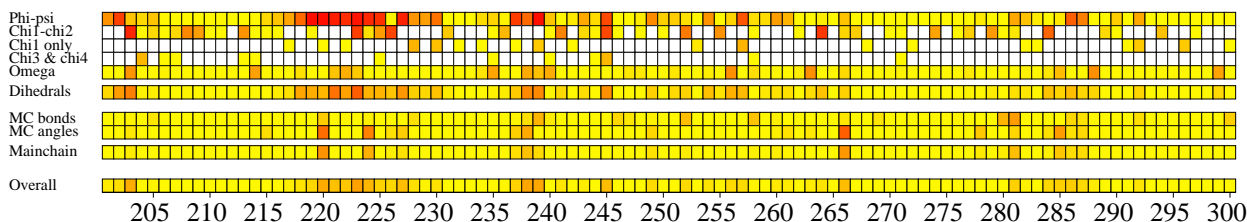
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

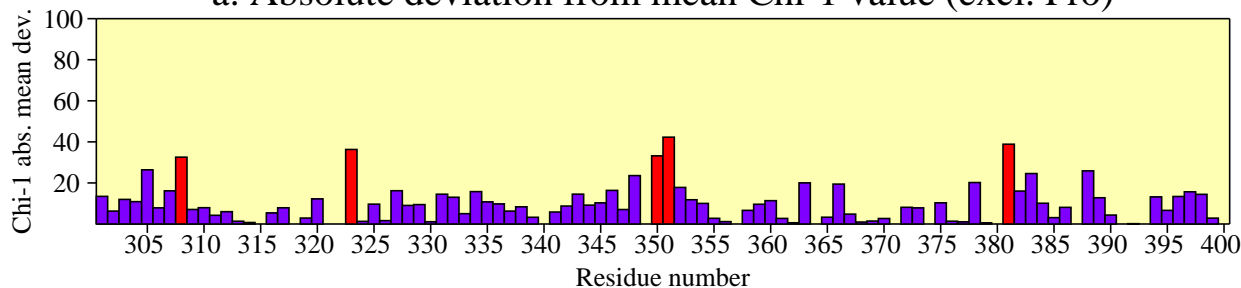


g. G-factors

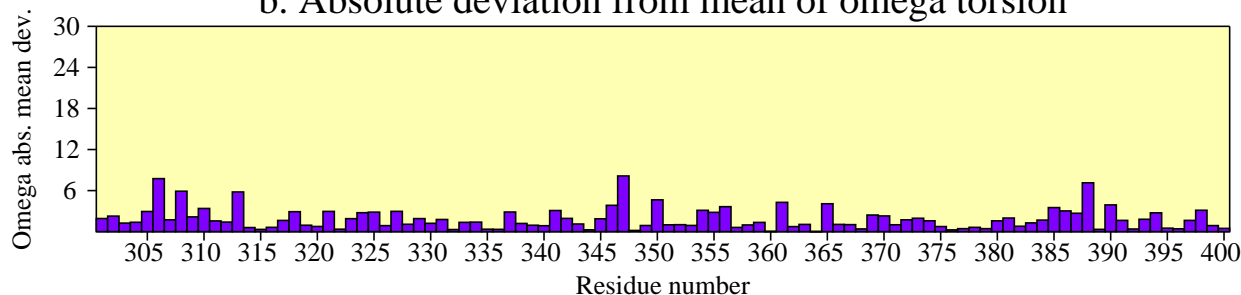


Residue properties 1ntz

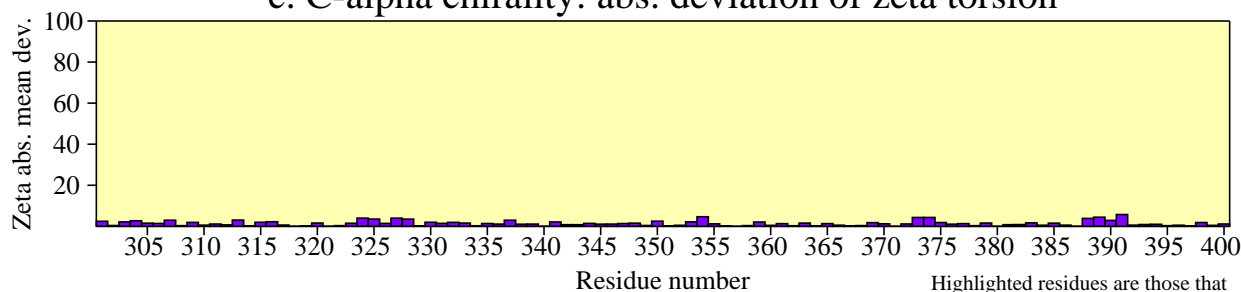
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

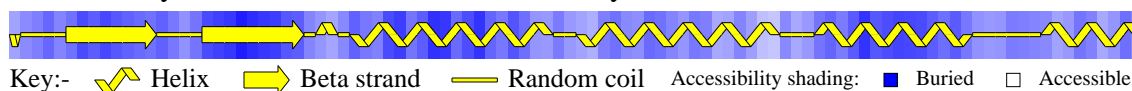


c. C-alpha chirality: abs. deviation of zeta torsion



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

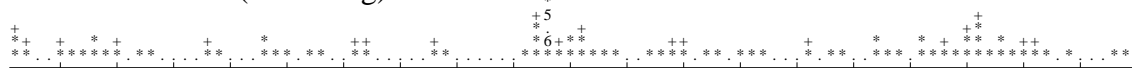
d. Secondary structure & estimated accessibility



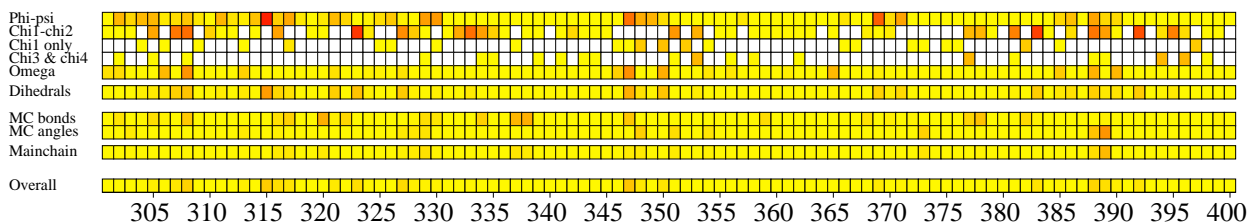
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

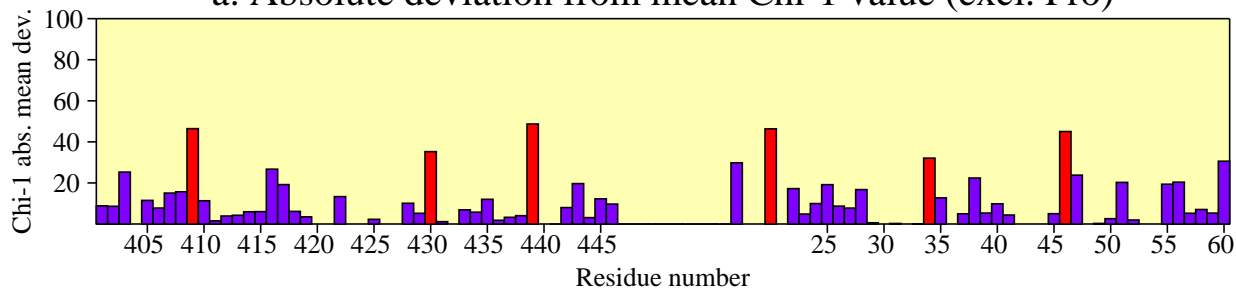


g. G-factors

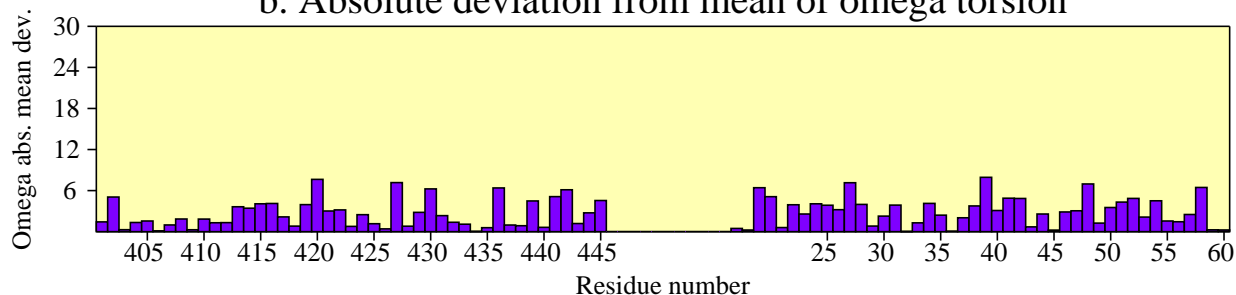


Residue properties 1ntz

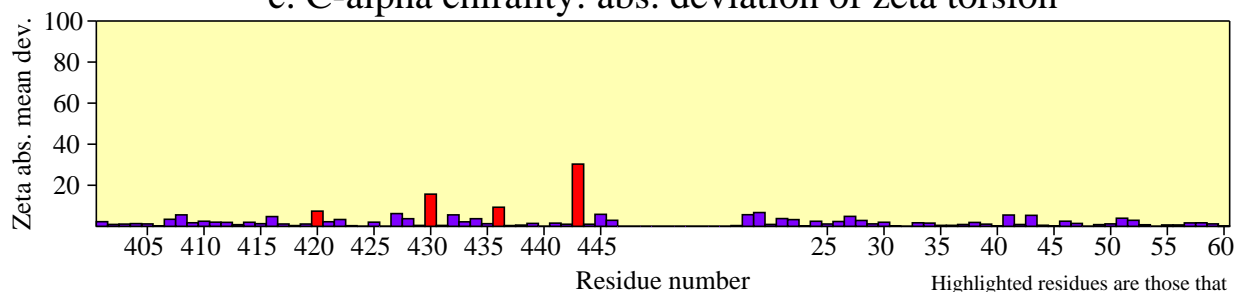
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

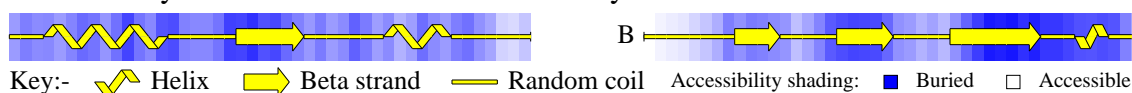


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



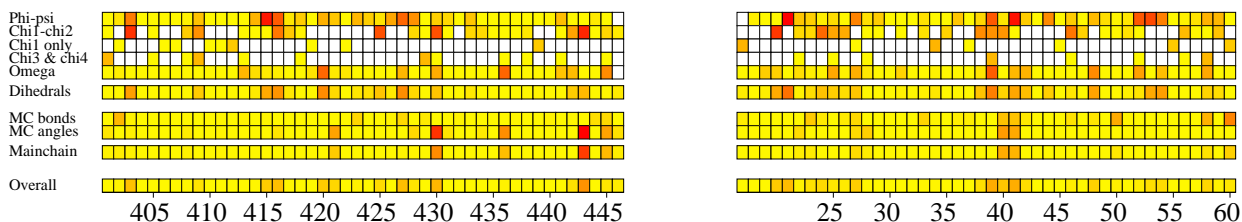
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

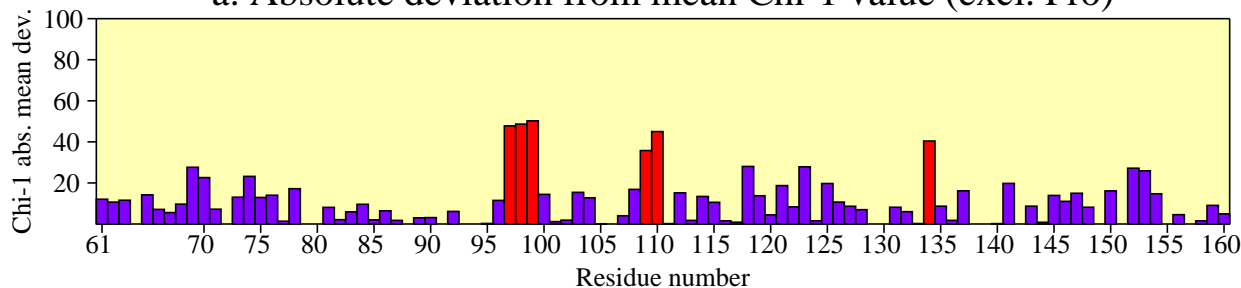


g. G-factors

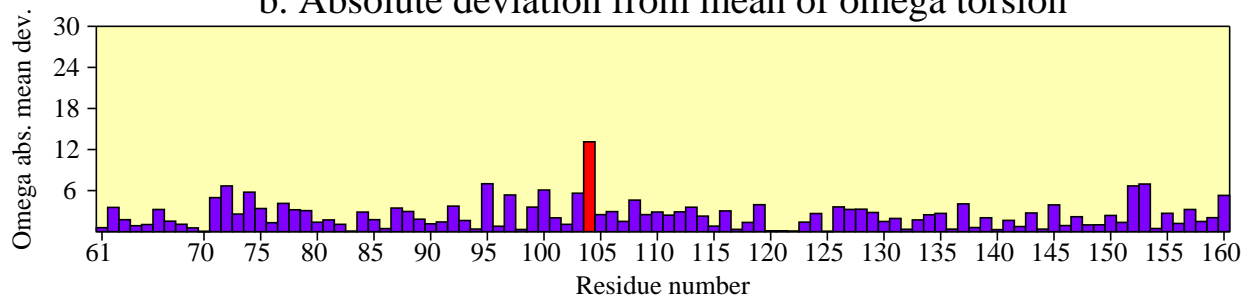


Residue properties 1ntz

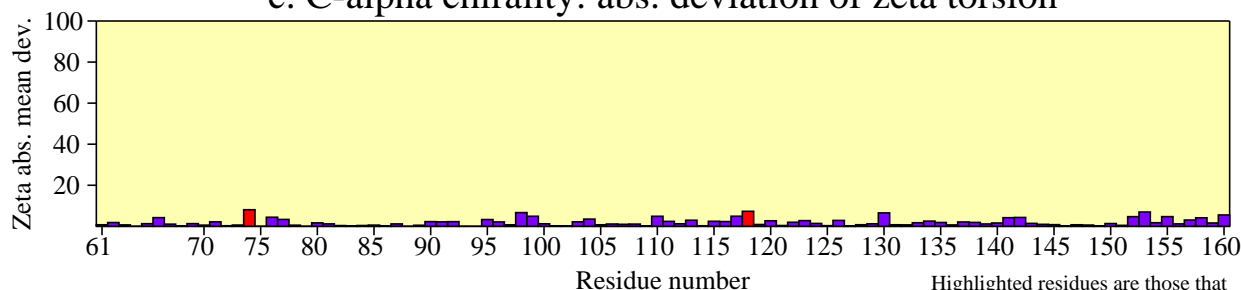
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

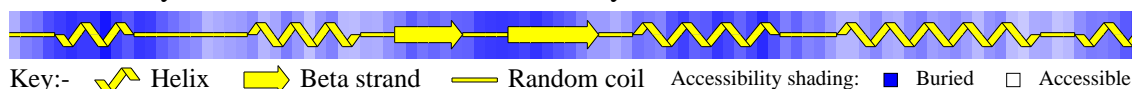


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



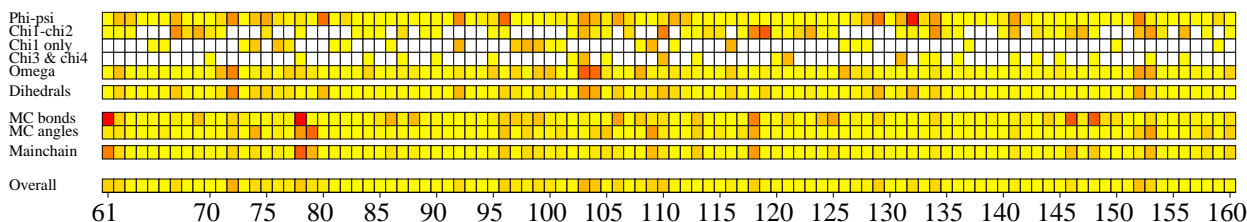
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

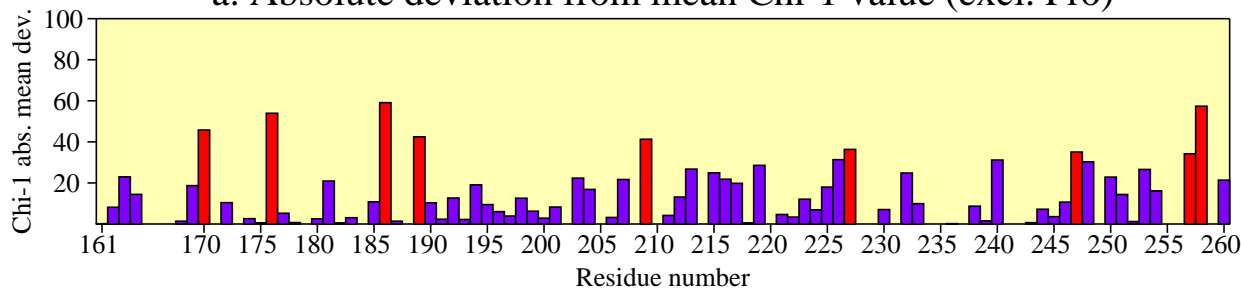


g. G-factors

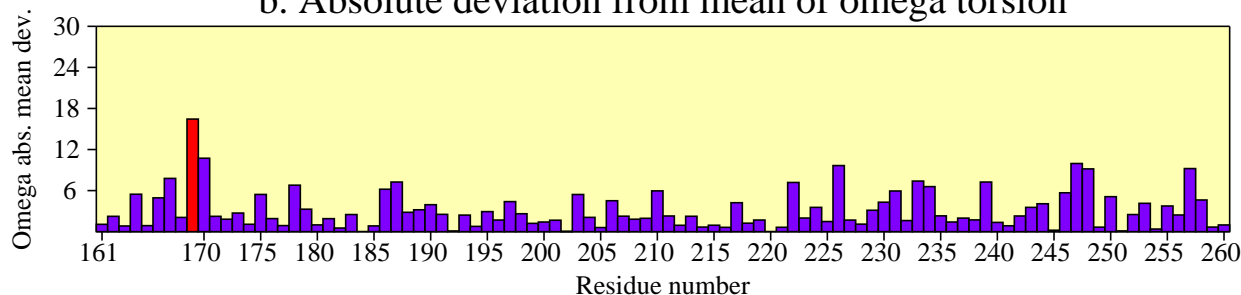


Residue properties 1ntz

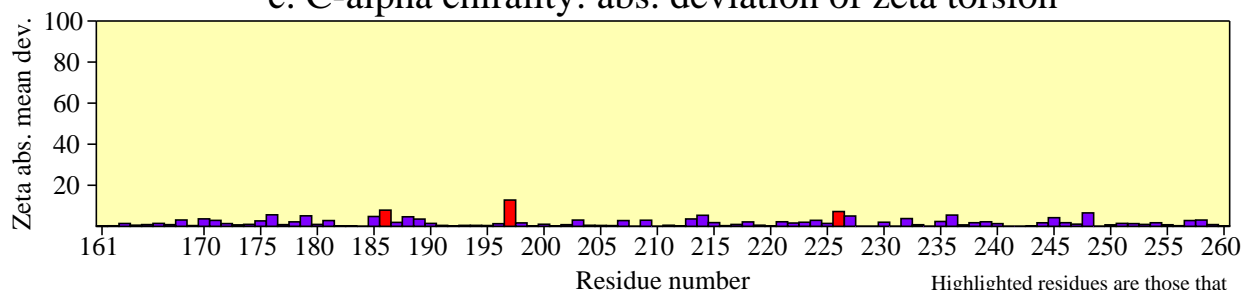
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

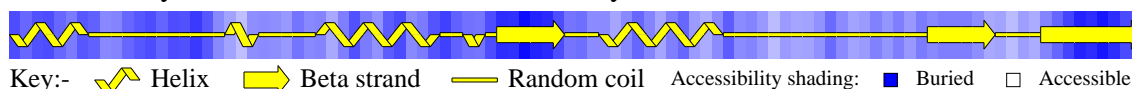


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



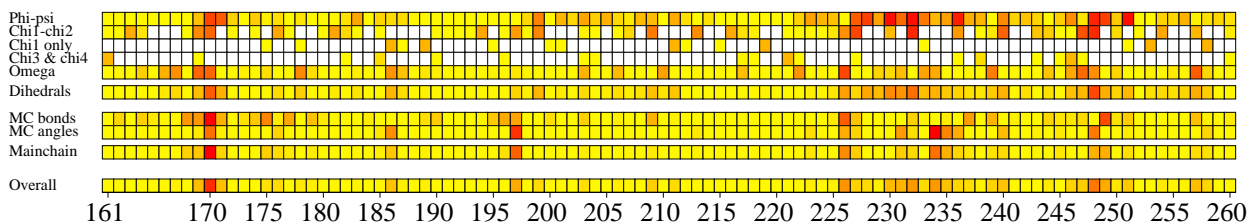
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

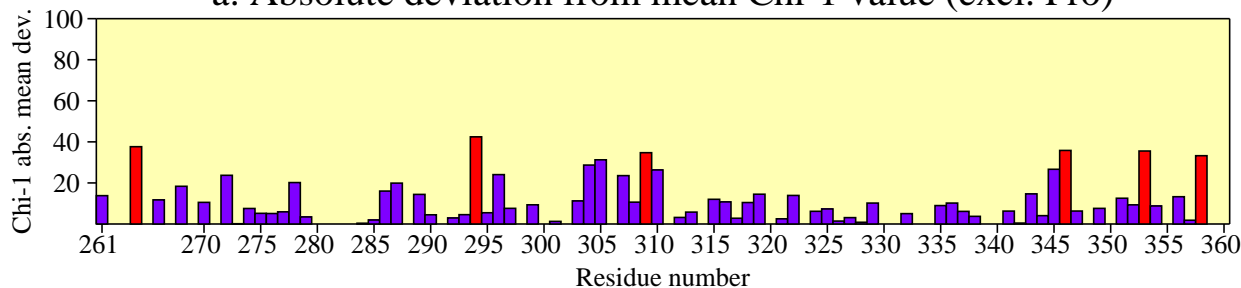


g. G-factors

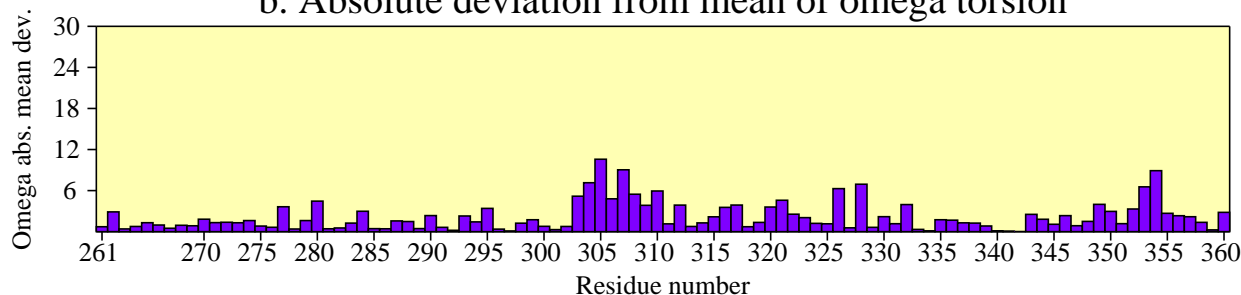


Residue properties 1ntz

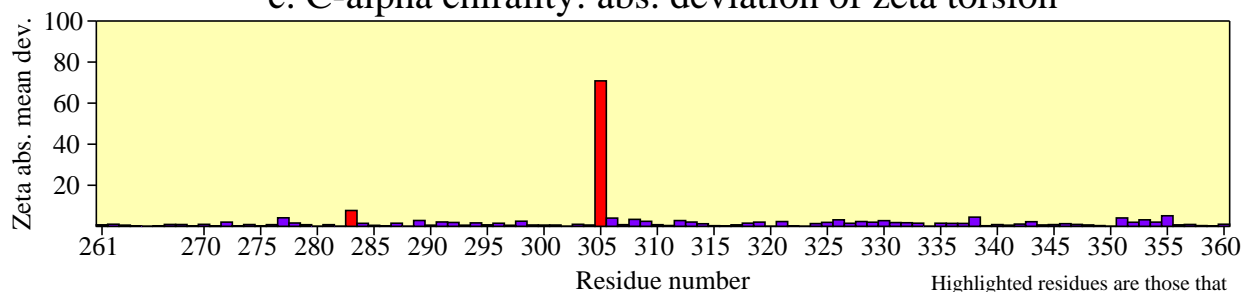
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

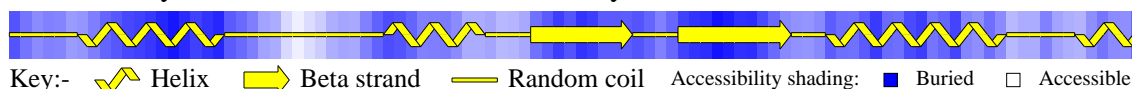


c. C-alpha chirality: abs. deviation of zeta torsion



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

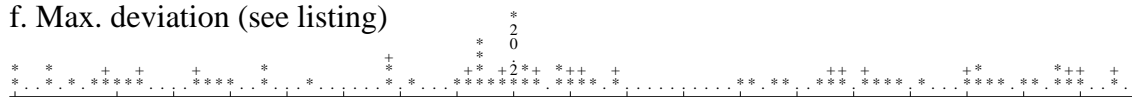
d. Secondary structure & estimated accessibility



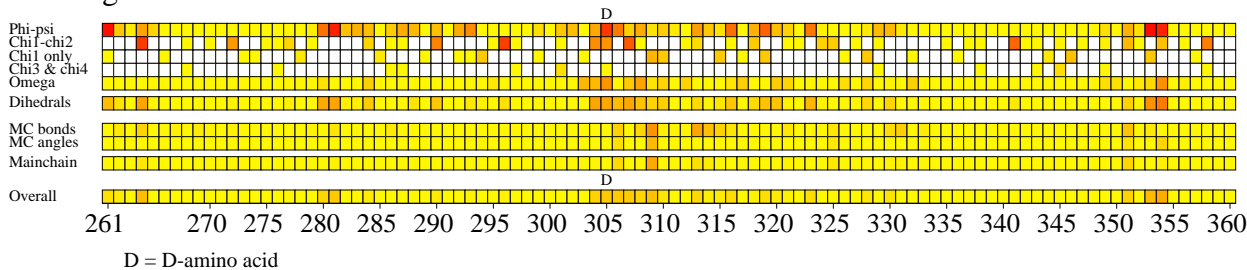
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

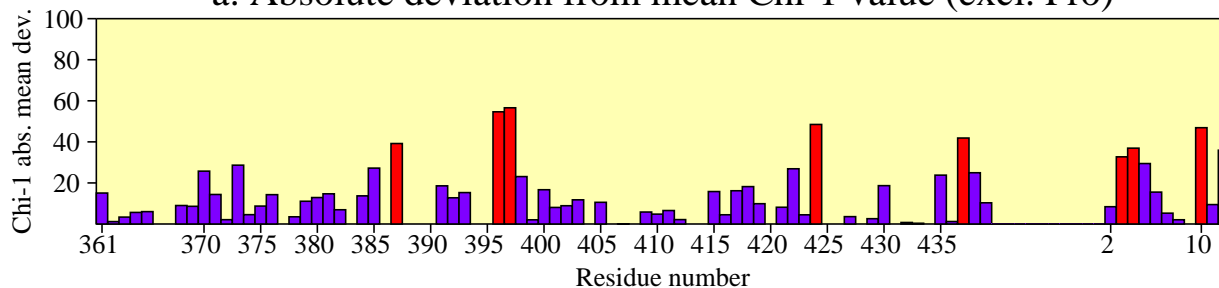


g. G-factors

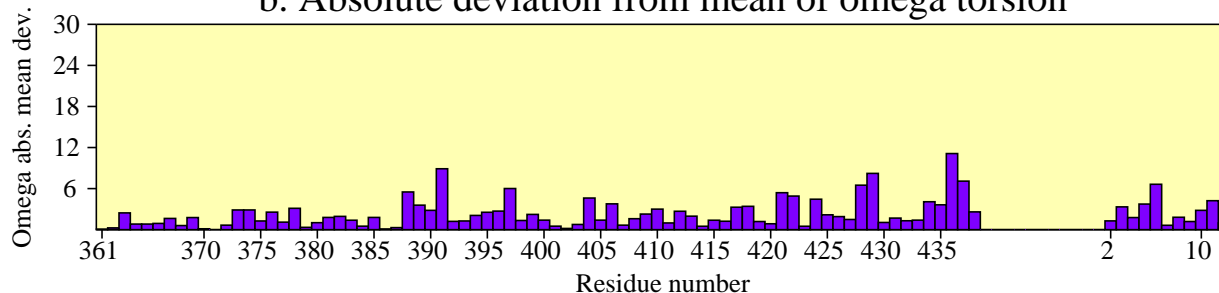


Residue properties 1ntz

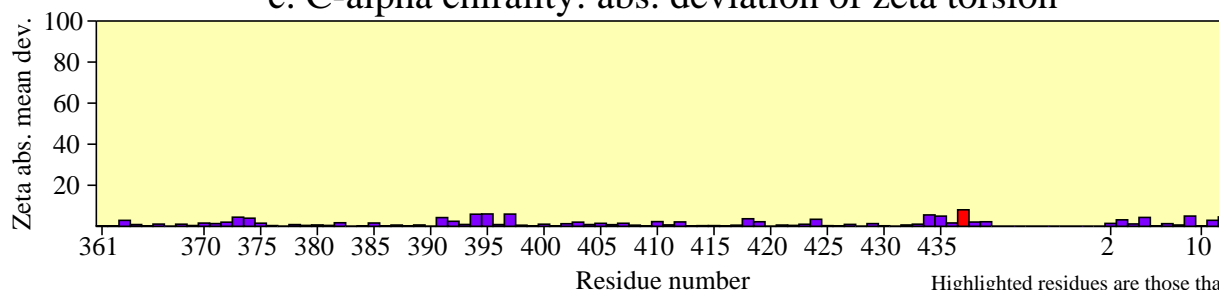
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

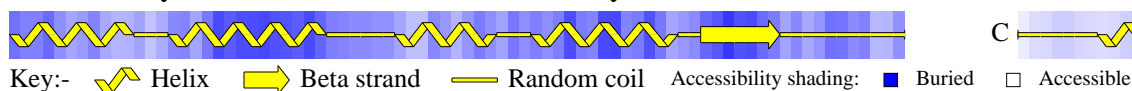


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



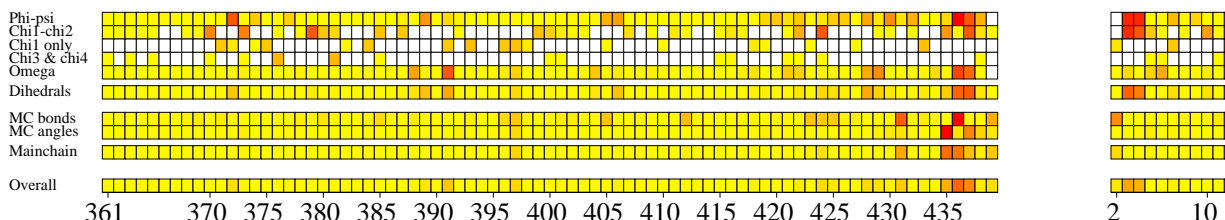
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

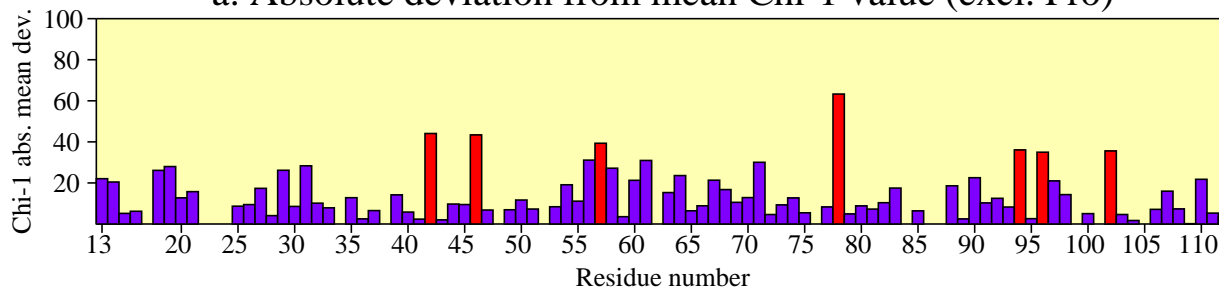


g. G-factors

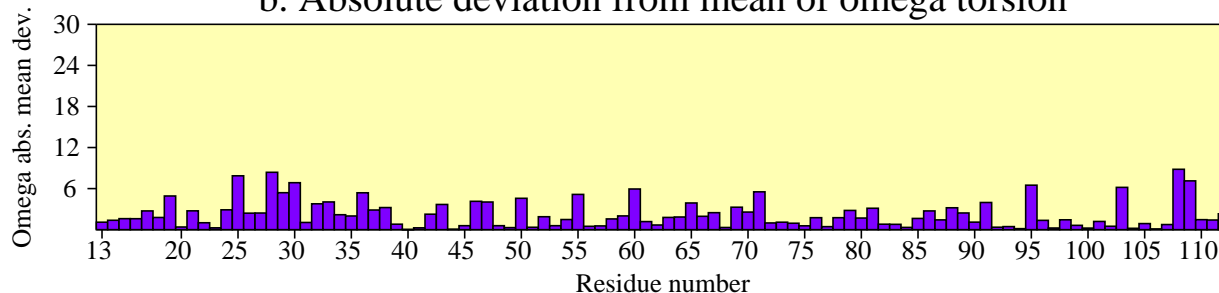


Residue properties 1ntz

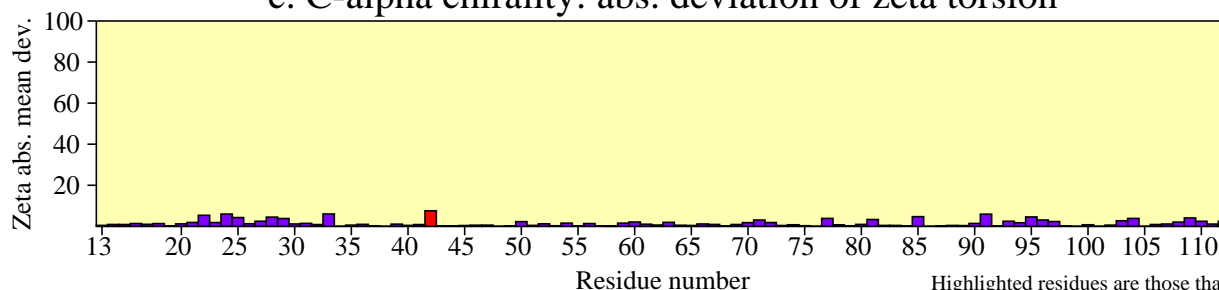
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

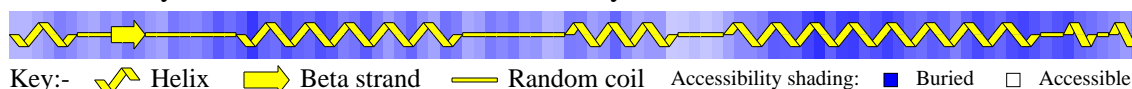


c. C-alpha chirality: abs. deviation of zeta torsion



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

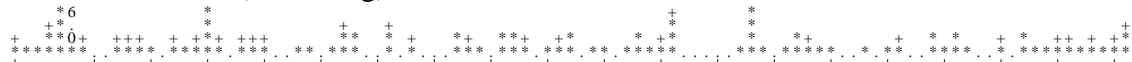
d. Secondary structure & estimated accessibility



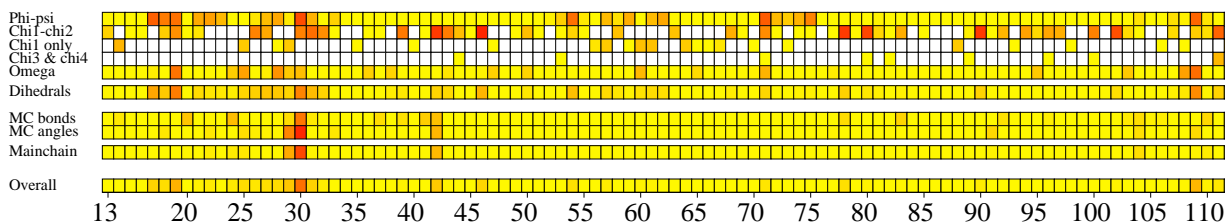
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



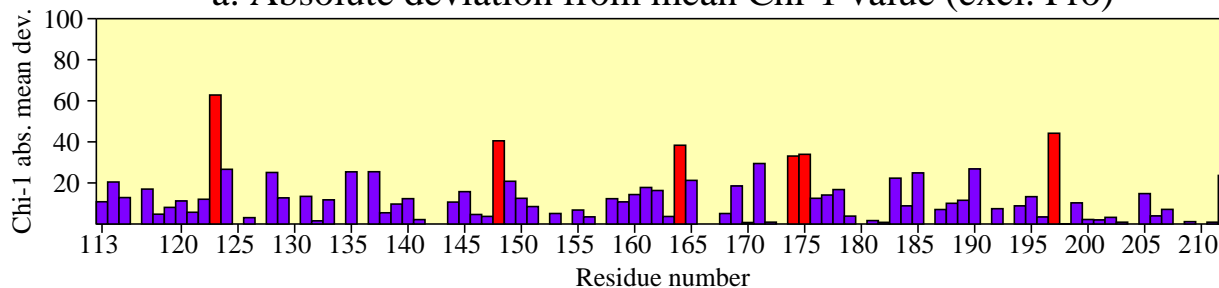
g. G-factors



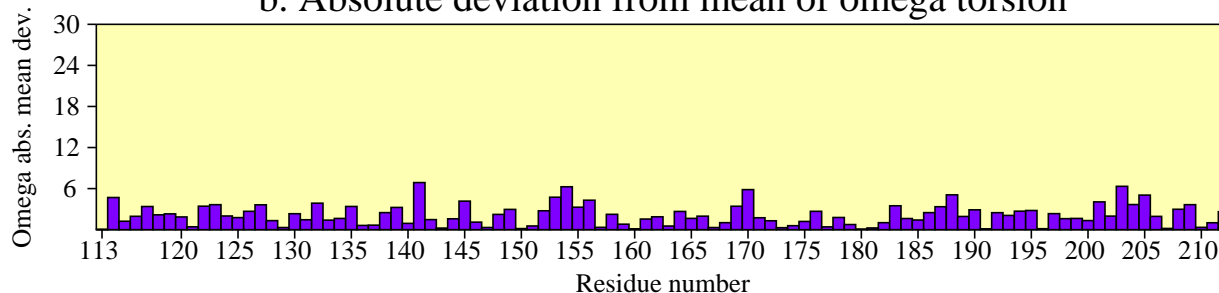
Residue properties

1ntz

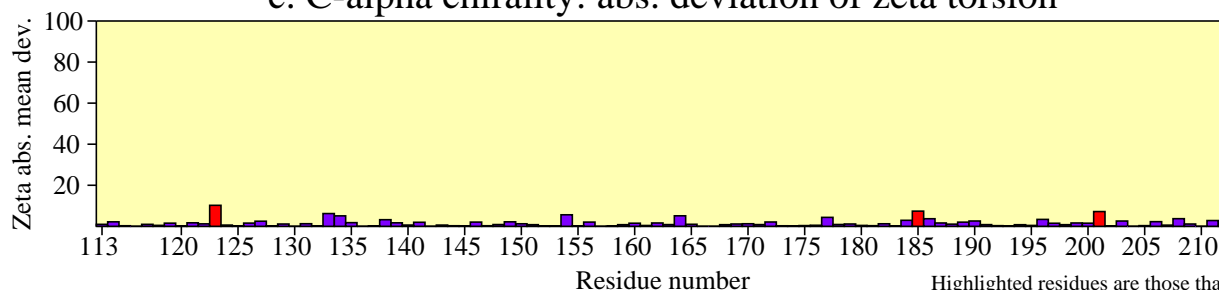
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

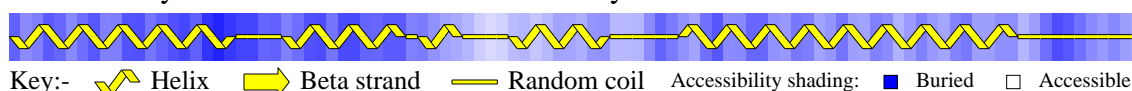


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



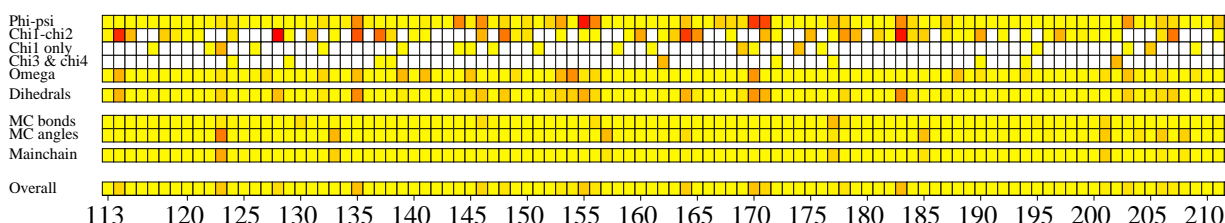
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

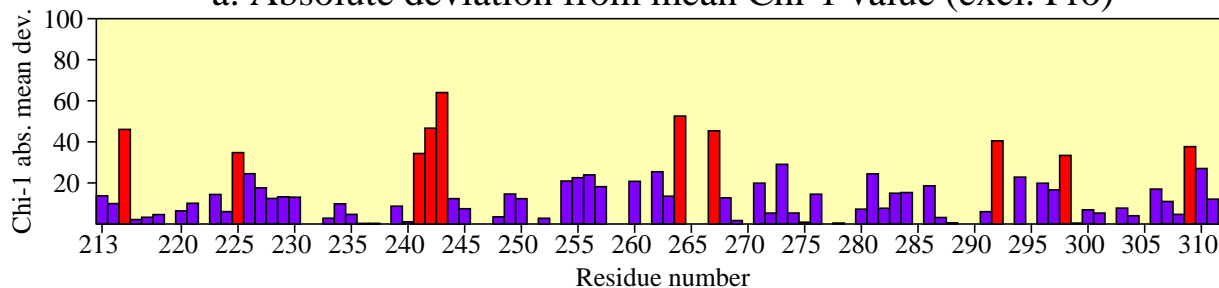


g. G-factors

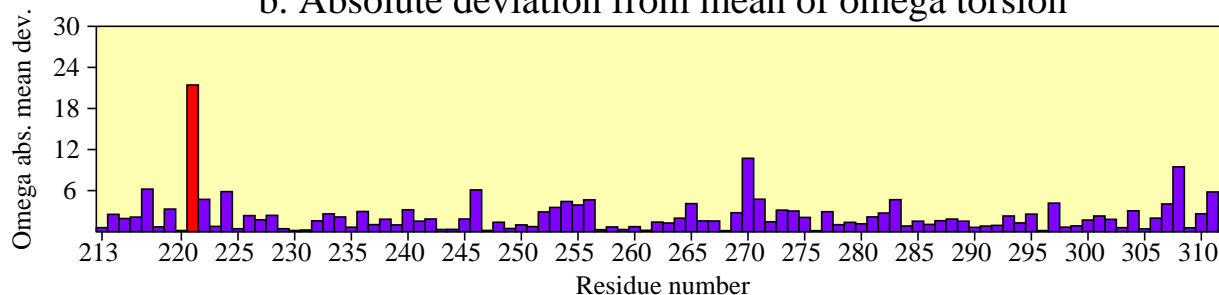


Residue properties 1ntz

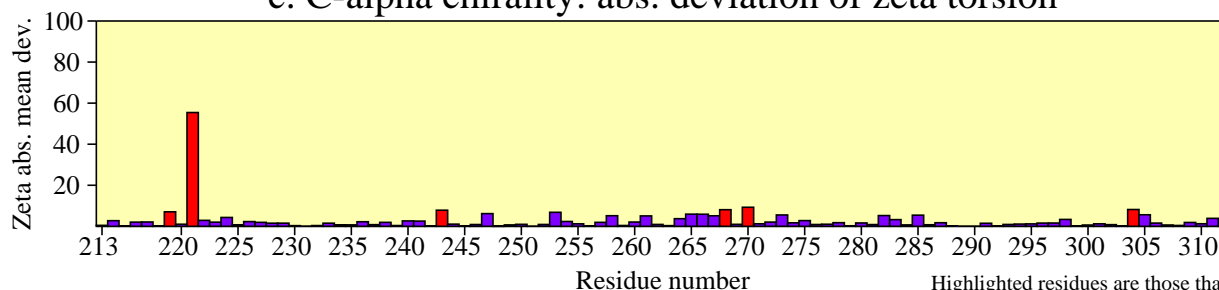
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

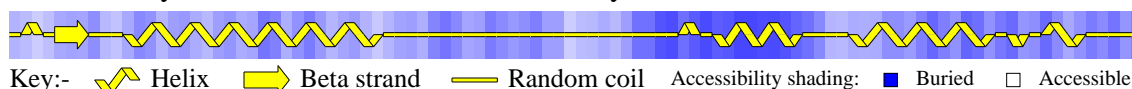


c. C-alpha chirality: abs. deviation of zeta torsion



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

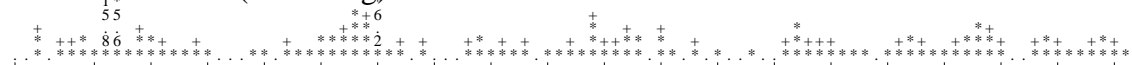
d. Secondary structure & estimated accessibility



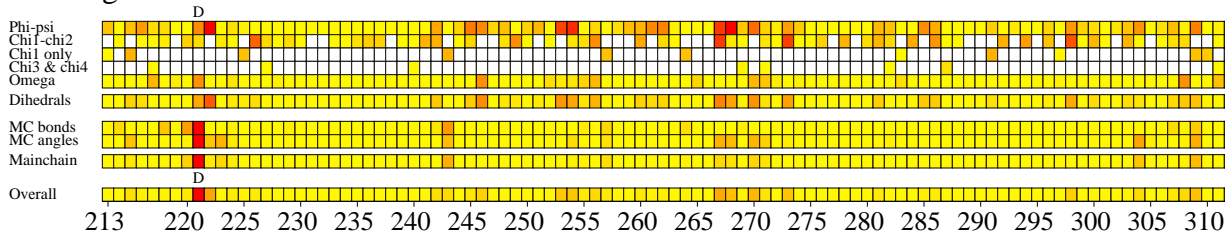
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



g. G-factors

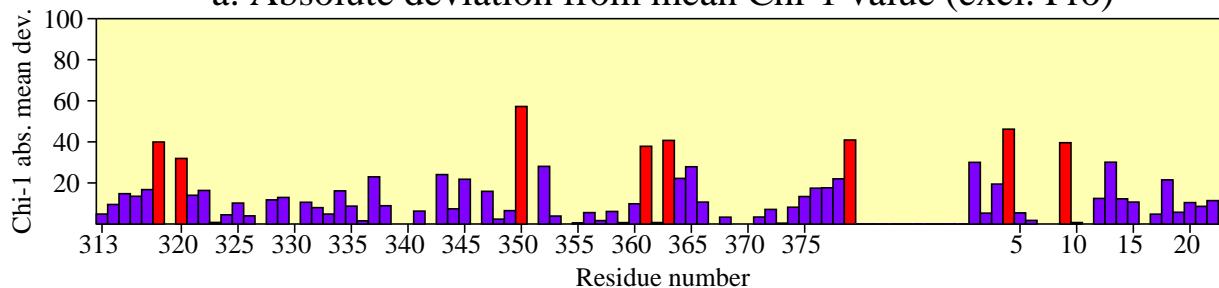


D = D-amino acid

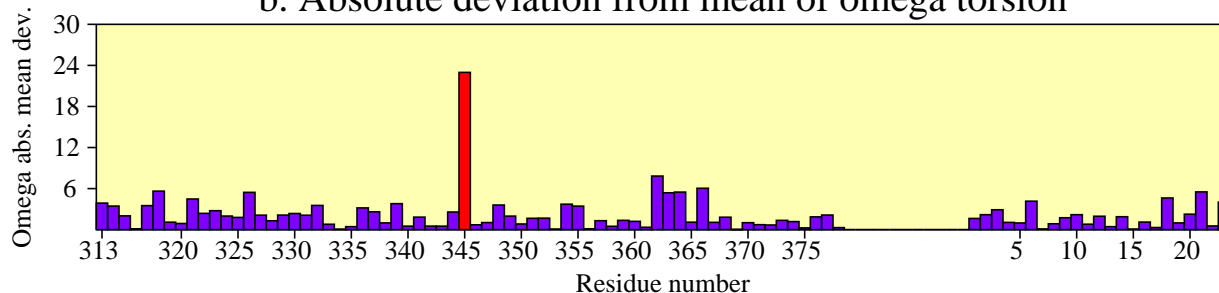
Residue properties

1ntz

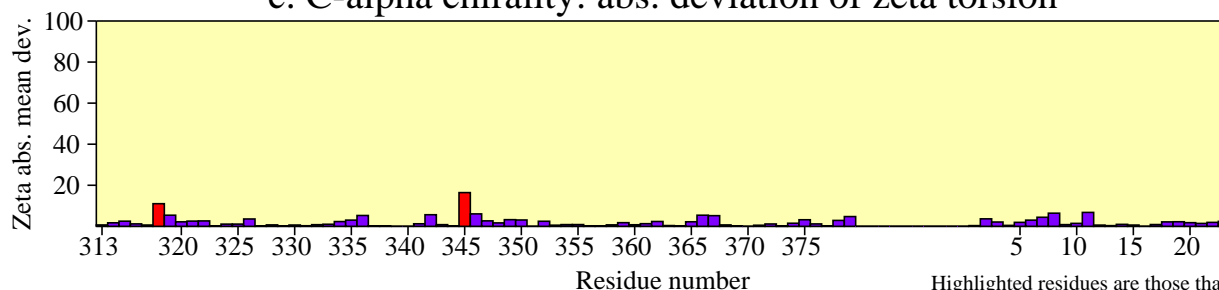
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

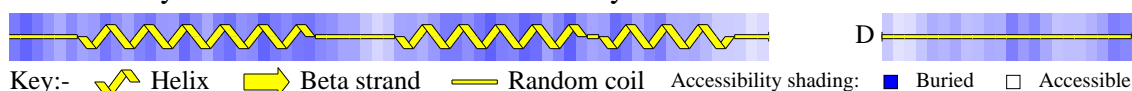


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



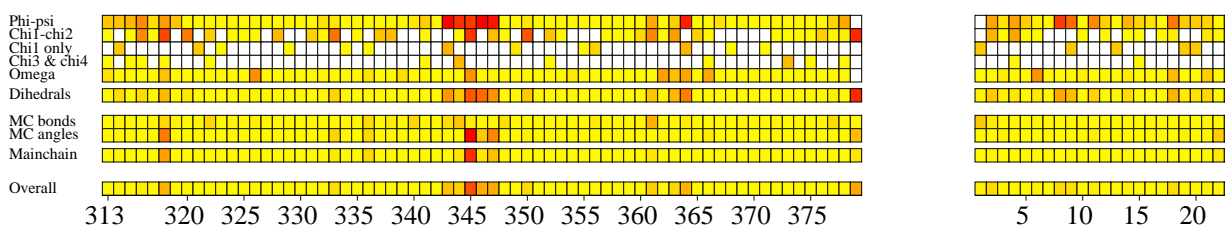
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

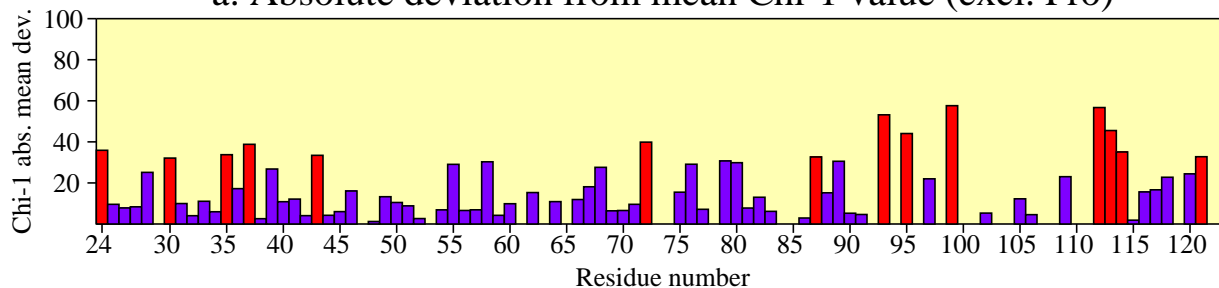


g. G-factors

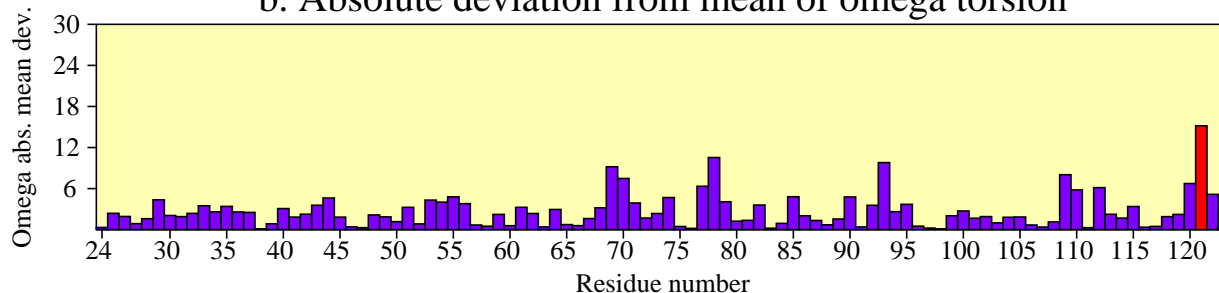


Residue properties 1ntz

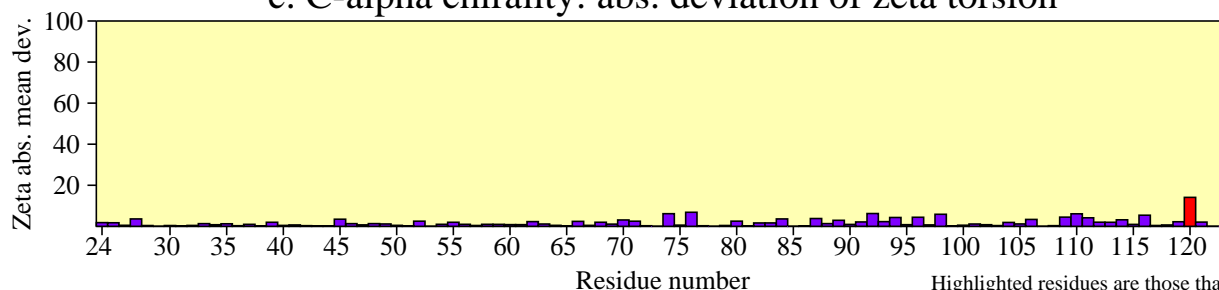
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

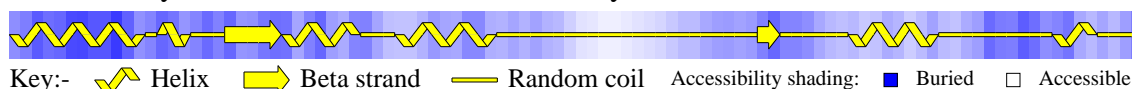


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



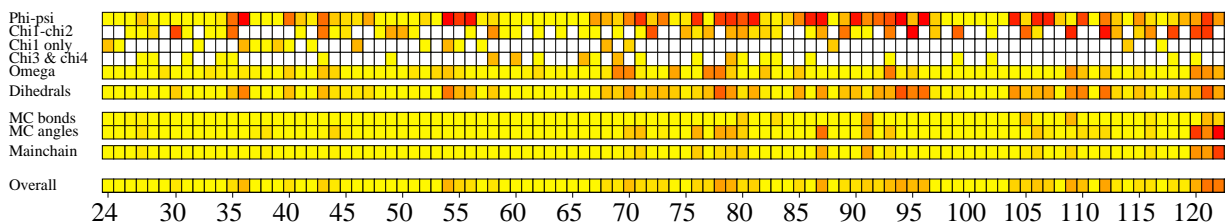
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

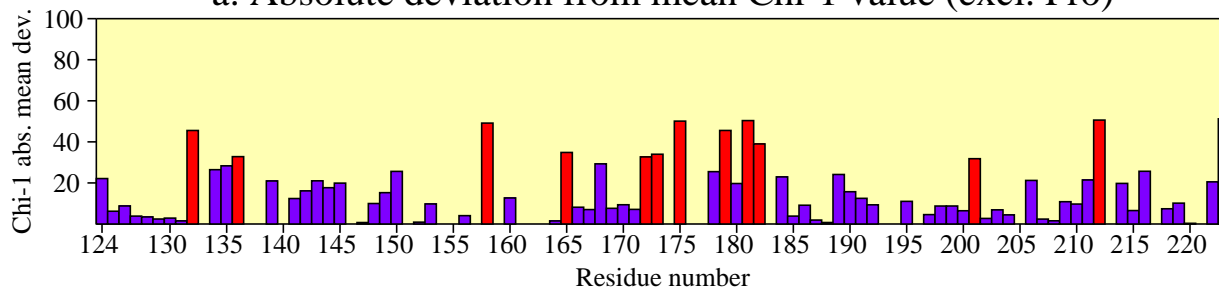


g. G-factors

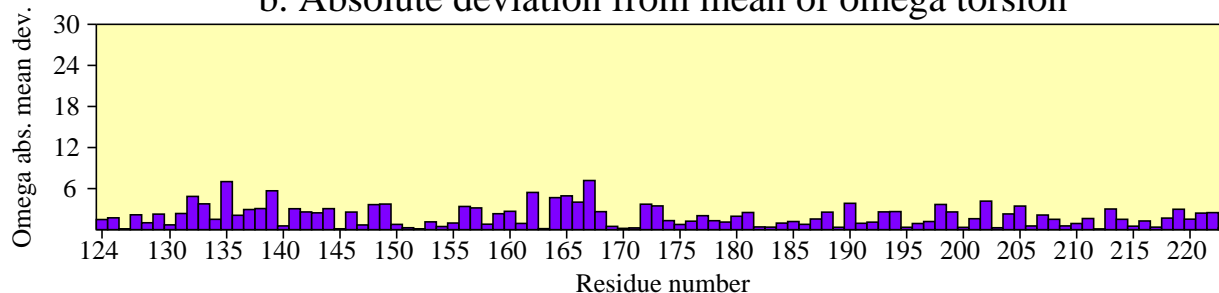


Residue properties 1ntz

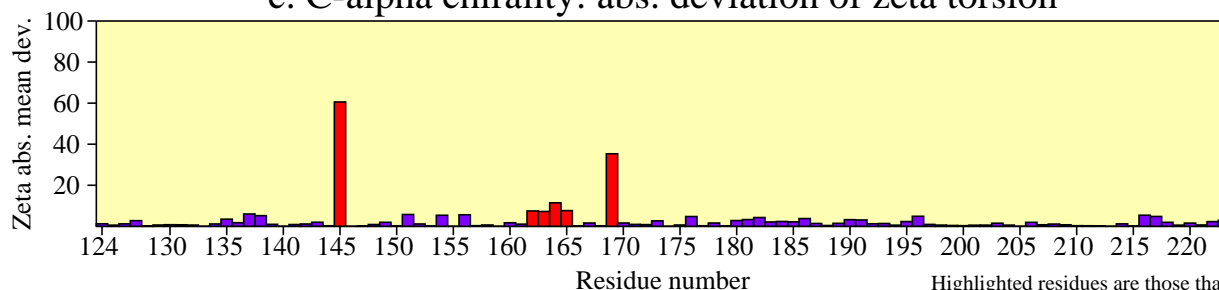
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

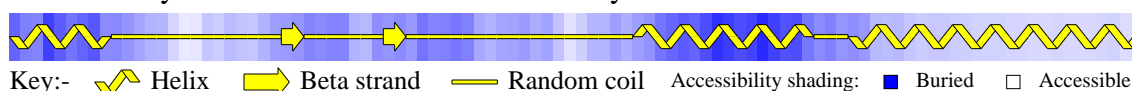


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



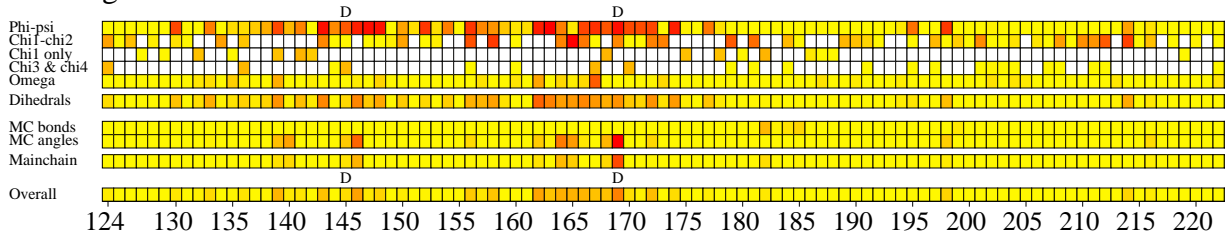
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



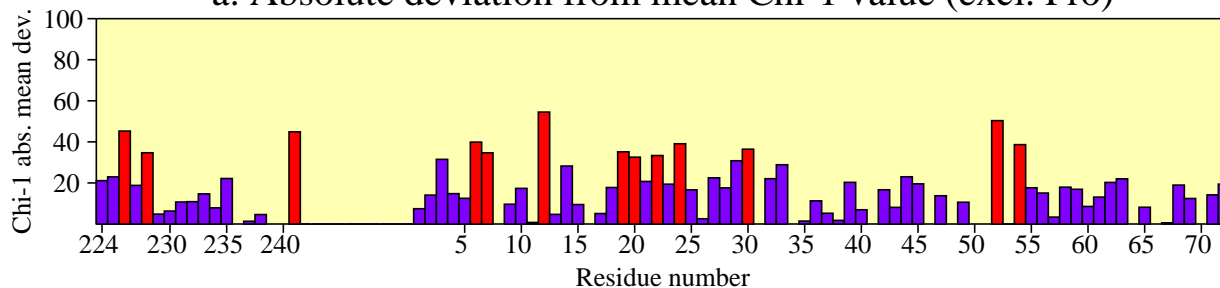
g. G-factors



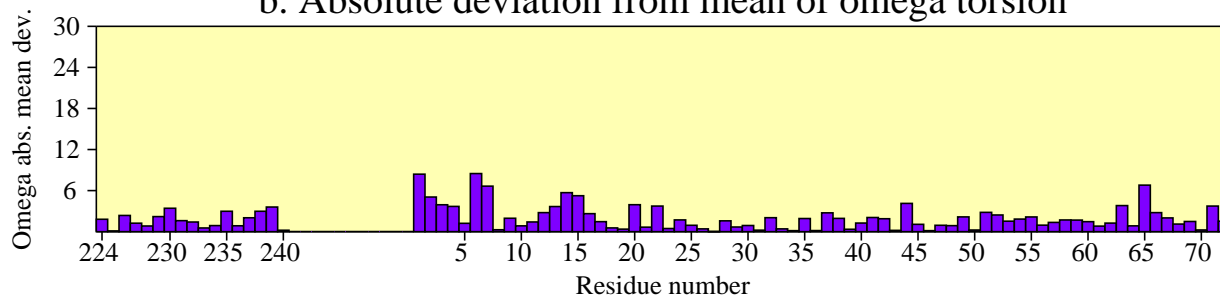
D = D-amino acid

Residue properties 1ntz

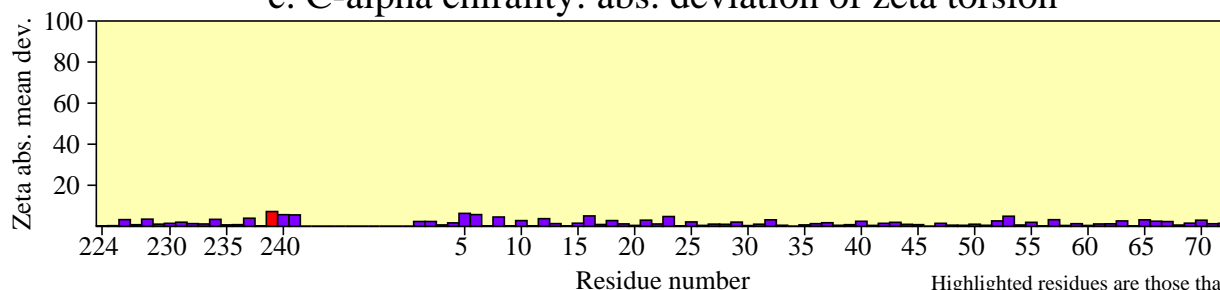
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

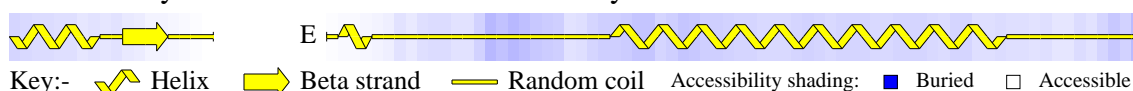


c. C-alpha chirality: abs. deviation of zeta torsion



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

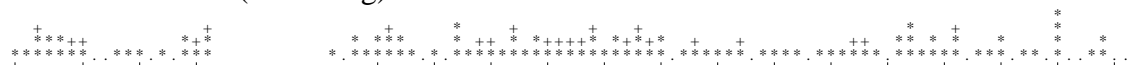
d. Secondary structure & estimated accessibility



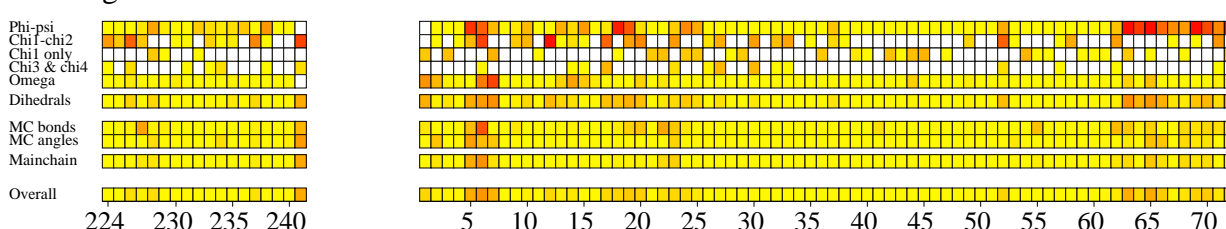
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

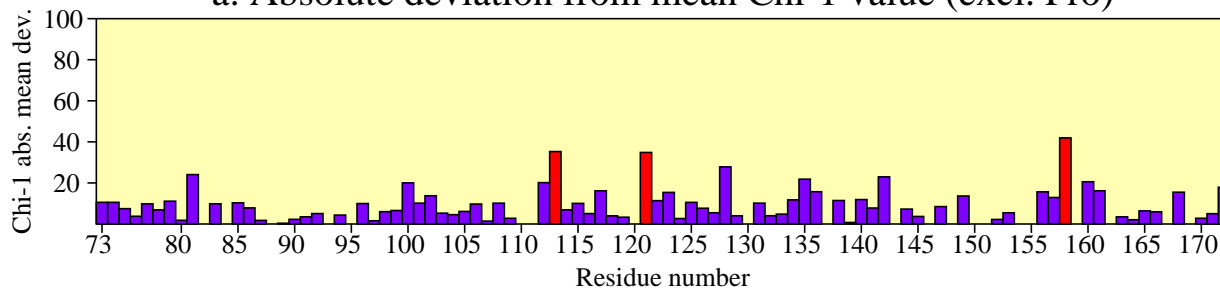


g. G-factors

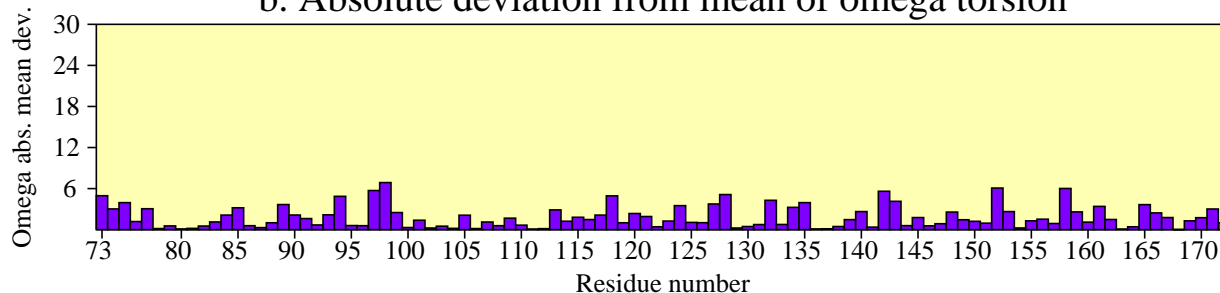


Residue properties 1ntz

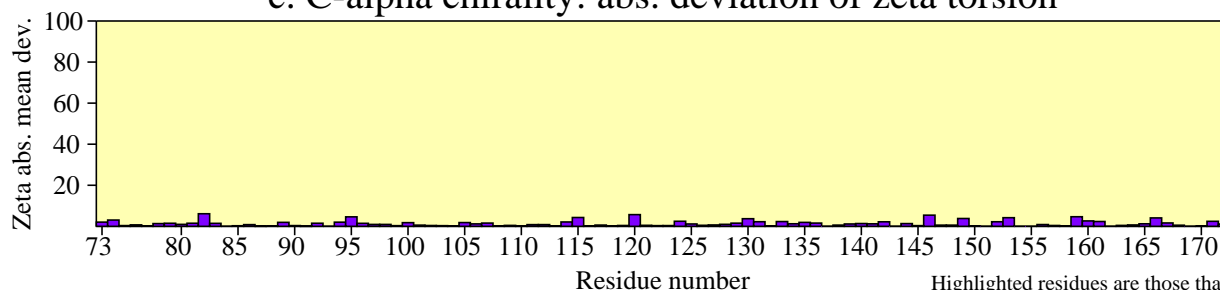
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

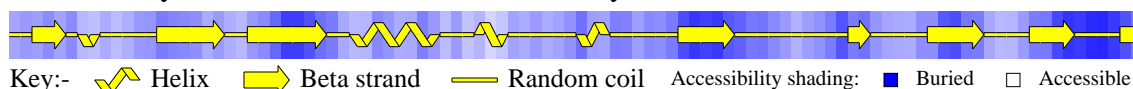


c. C-alpha chirality: abs. deviation of zeta torsion



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

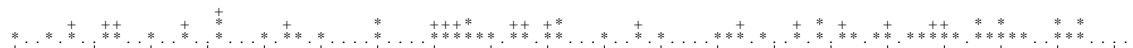
d. Secondary structure & estimated accessibility



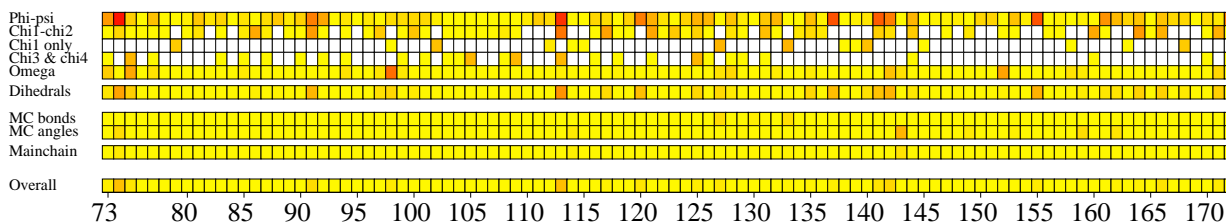
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

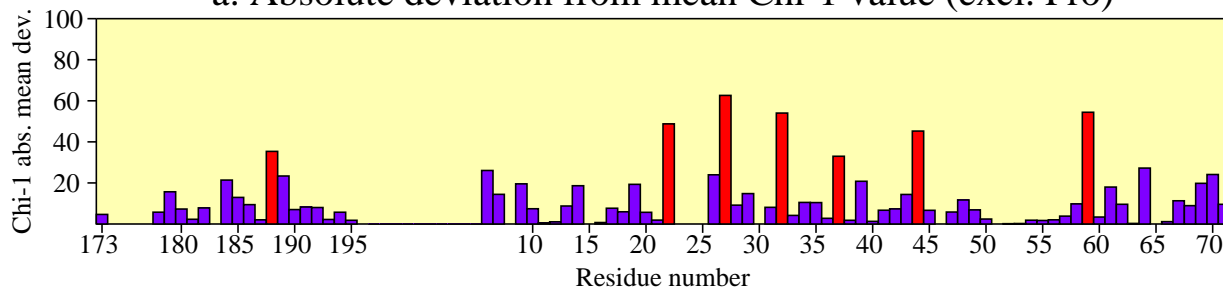


g. G-factors

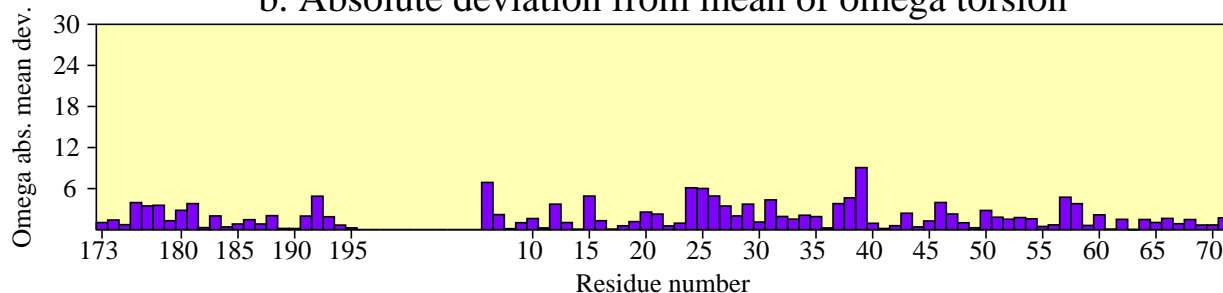


Residue properties 1ntz

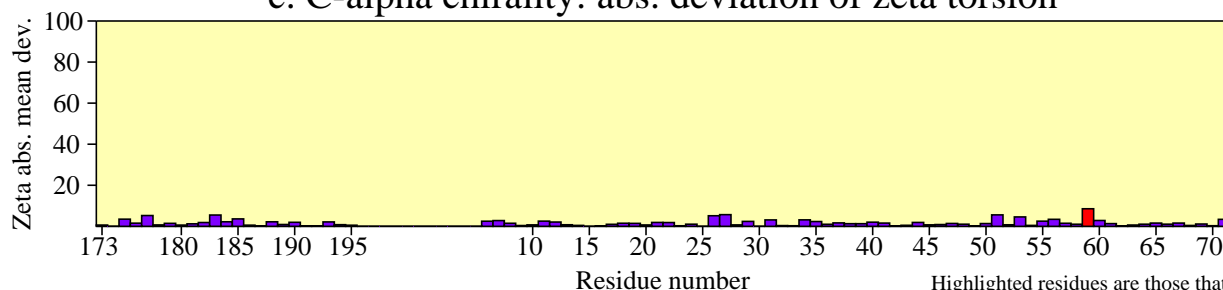
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

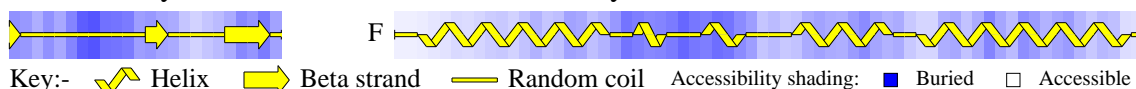


c. C-alpha chirality: abs. deviation of zeta torsion



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

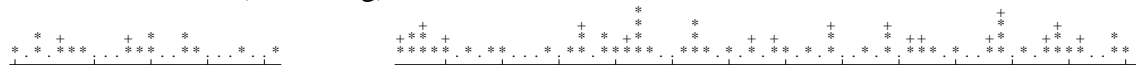
d. Secondary structure & estimated accessibility



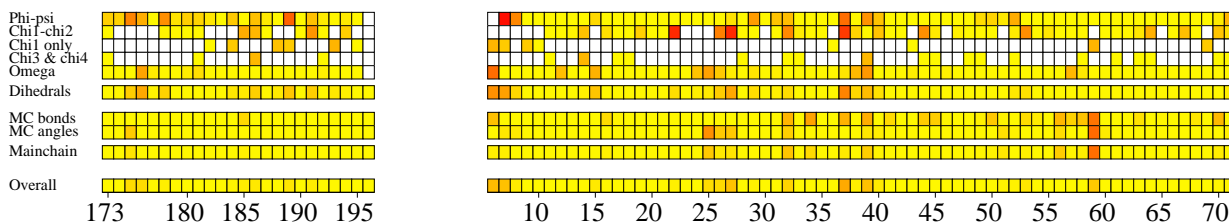
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

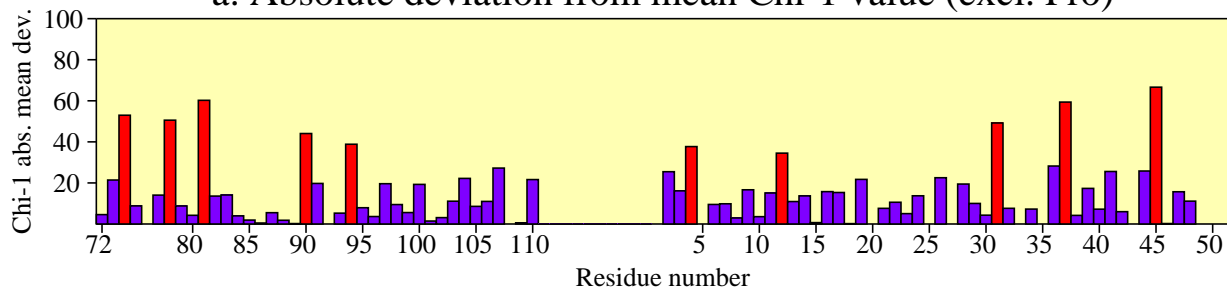


g. G-factors

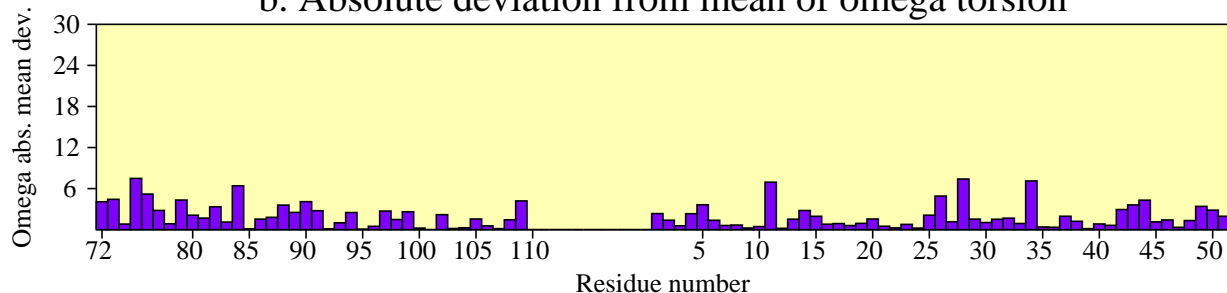


Residue properties 1ntz

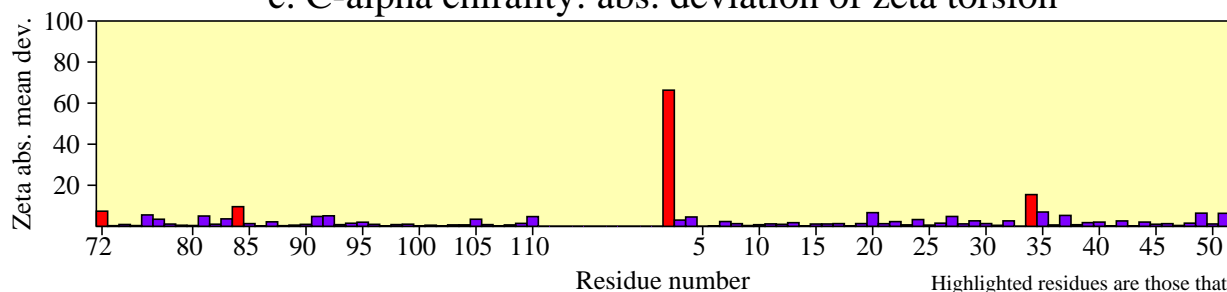
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

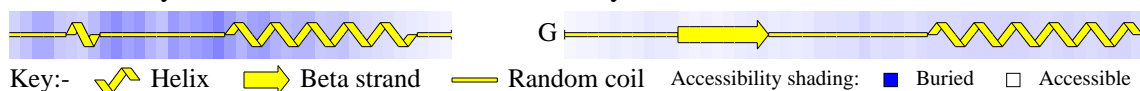


c. C-alpha chirality: abs. deviation of zeta torsion



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

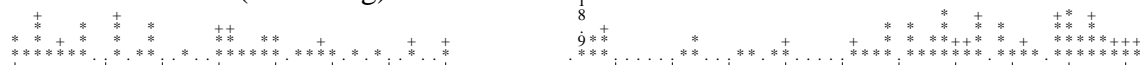
d. Secondary structure & estimated accessibility



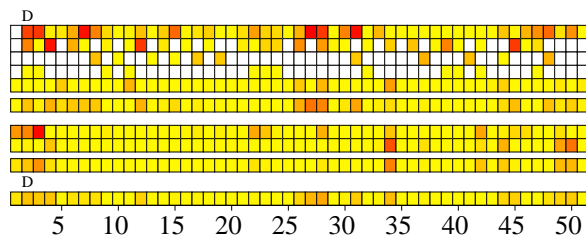
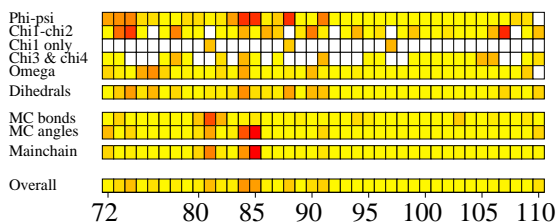
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



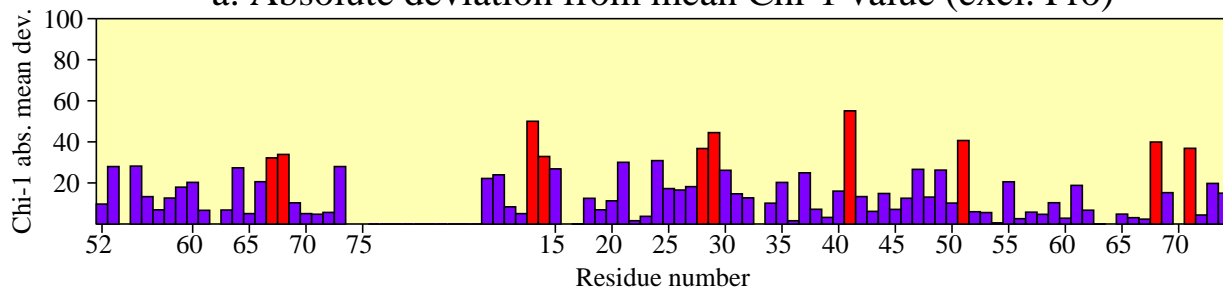
g. G-factors



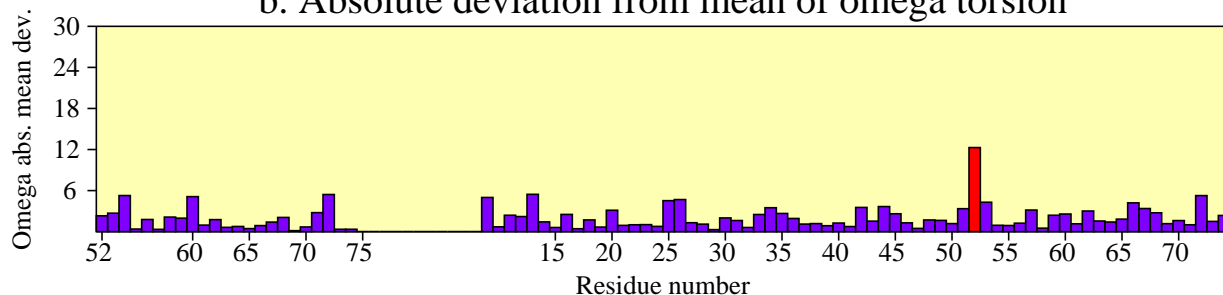
D = D-amino acid

Residue properties 1ntz

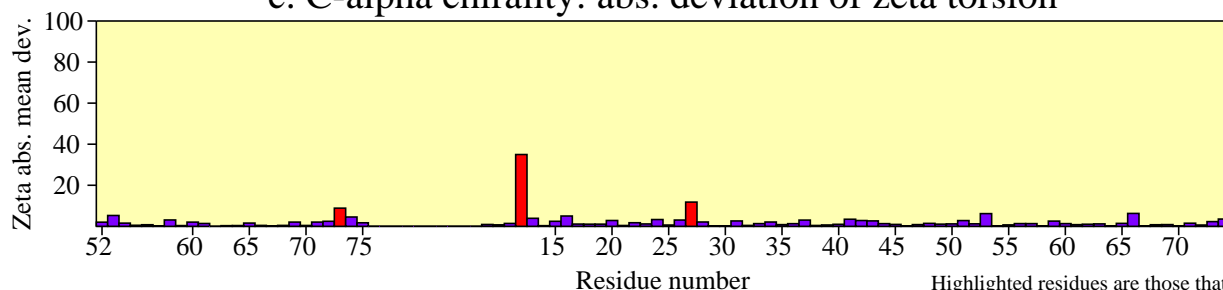
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

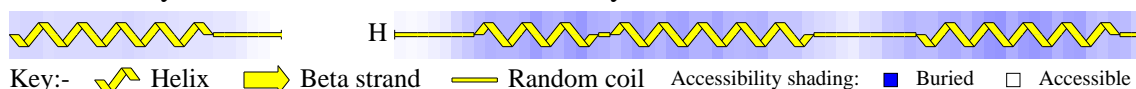


c. C-alpha chirality: abs. deviation of zeta torsion



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

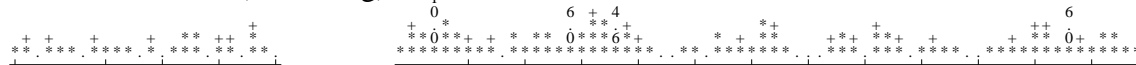
d. Secondary structure & estimated accessibility



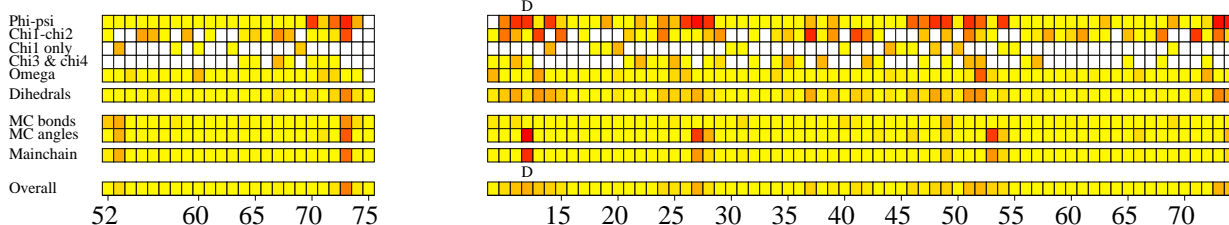
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



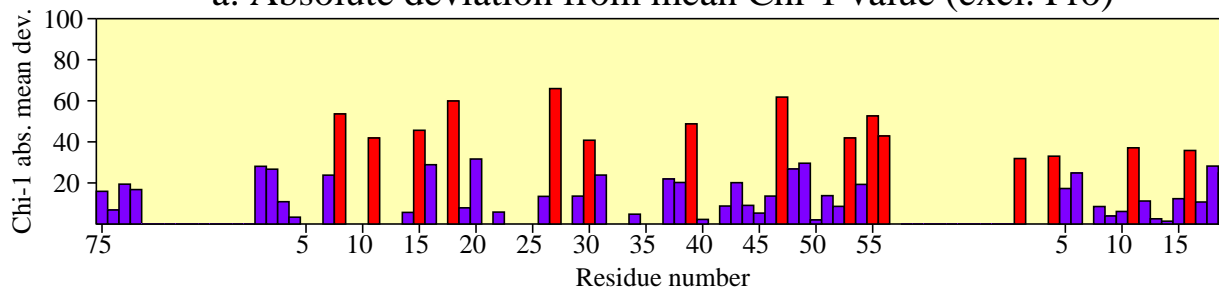
g. G-factors



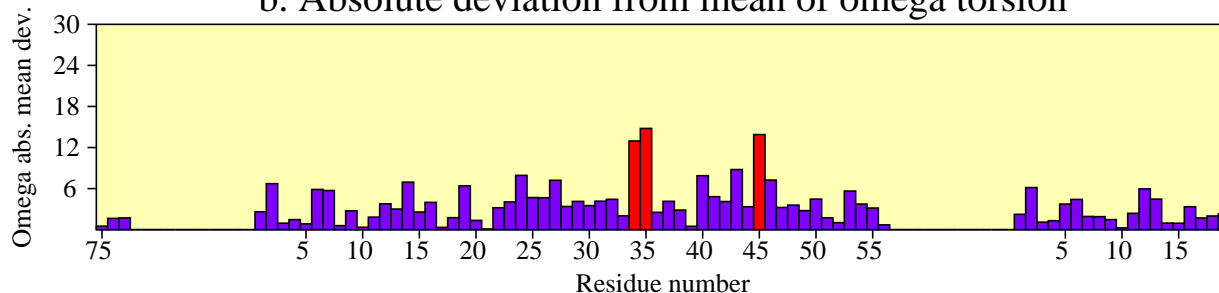
D = D-amino acid

Residue properties 1ntz

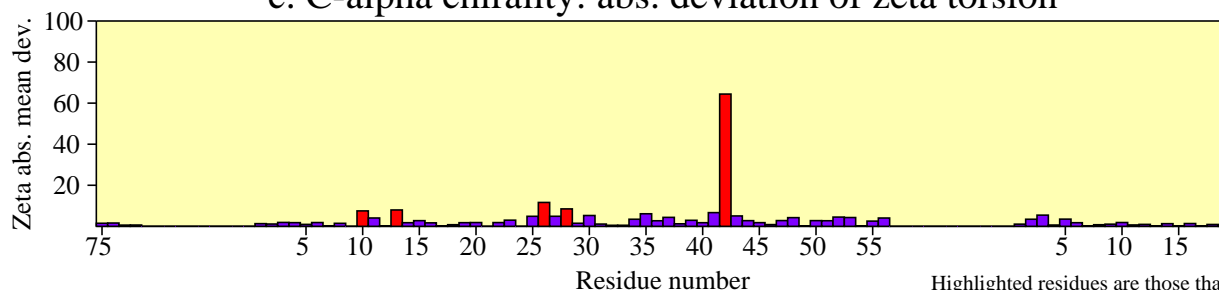
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

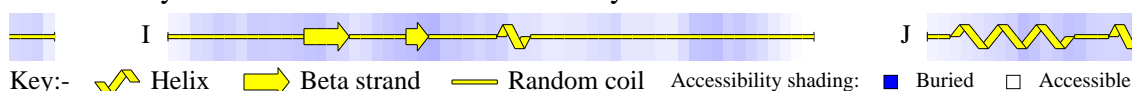


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



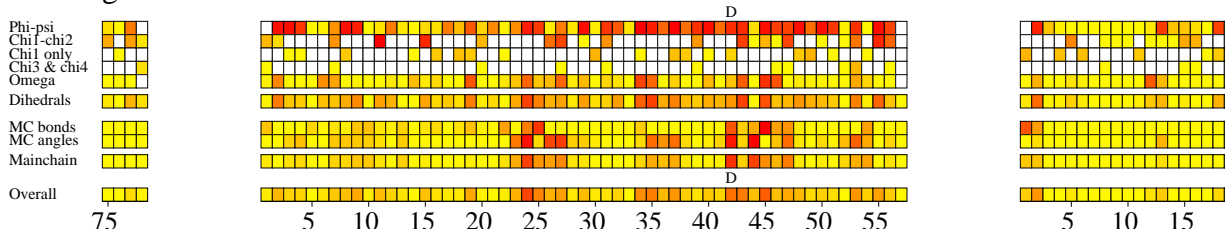
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

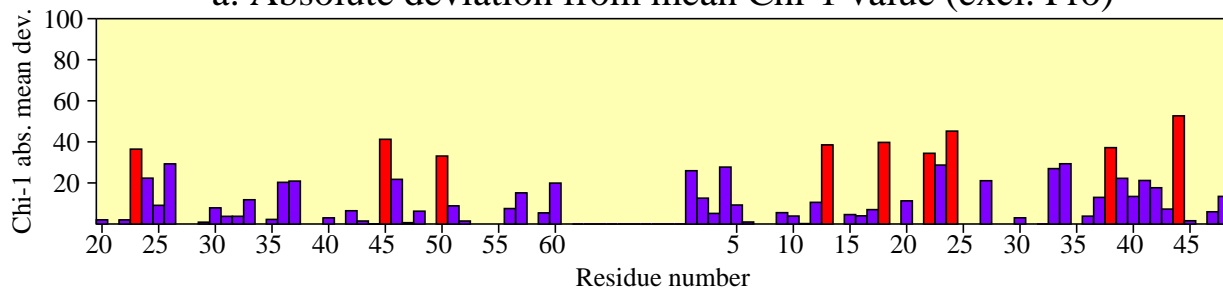


D = D-amino acid

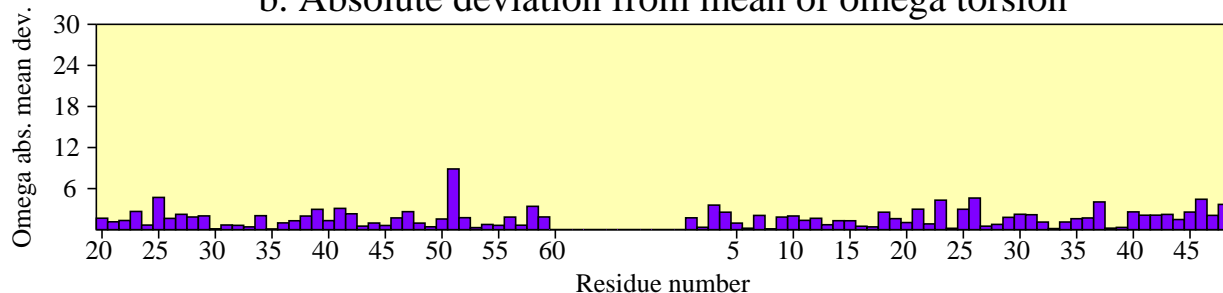
Residue properties

1ntz

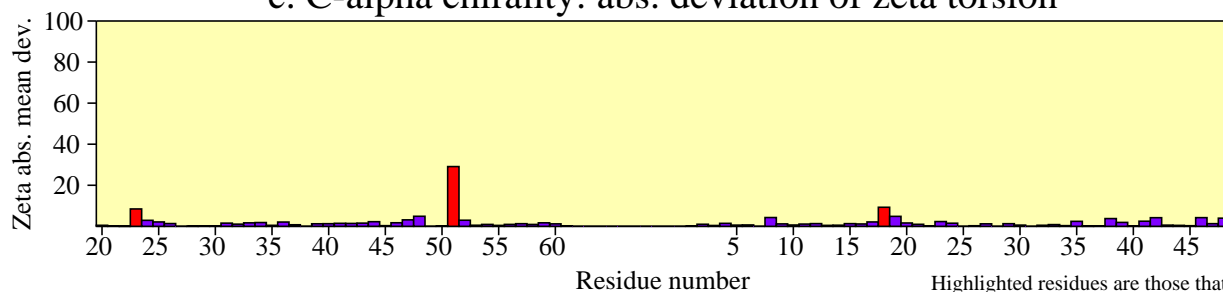
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

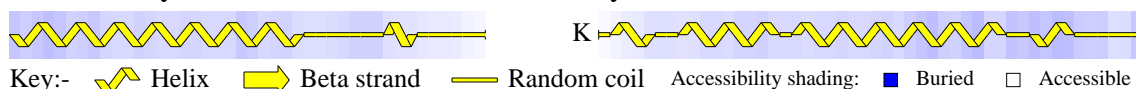


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



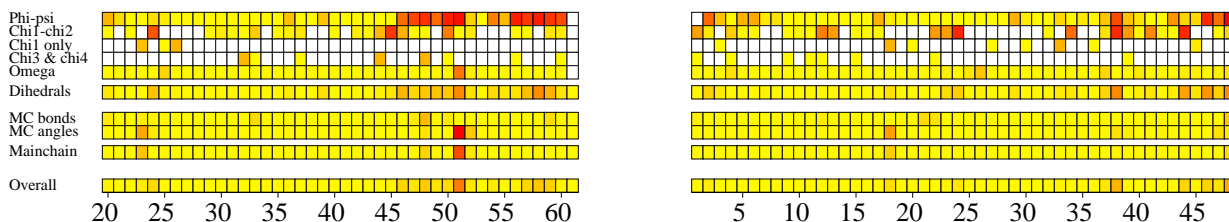
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



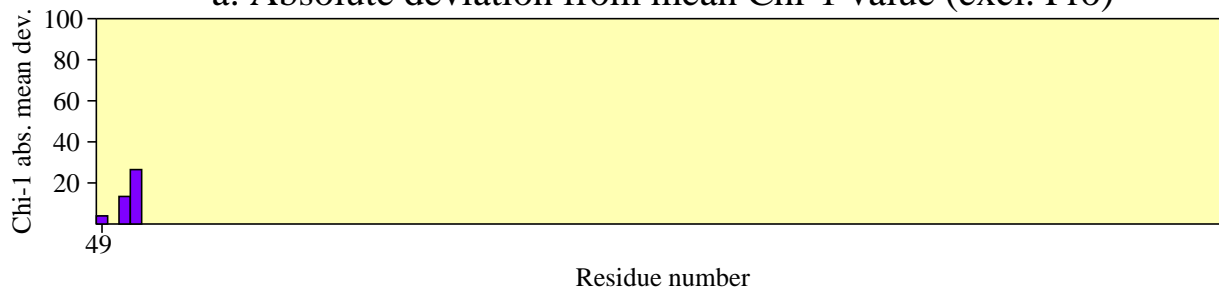
g. G-factors



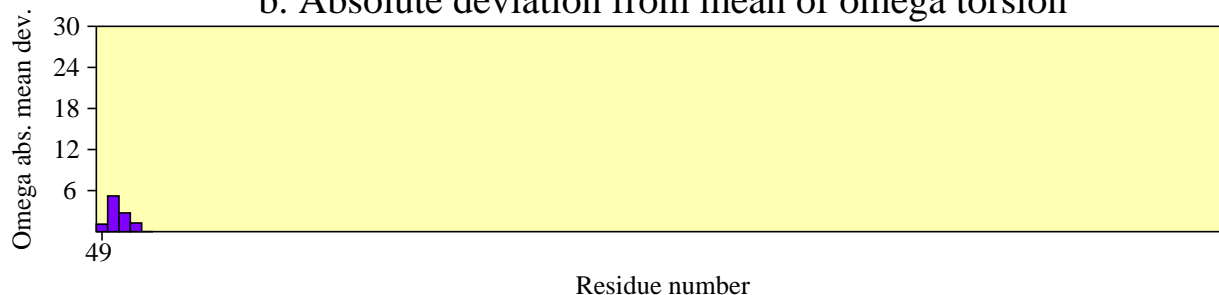
Residue properties

1ntz

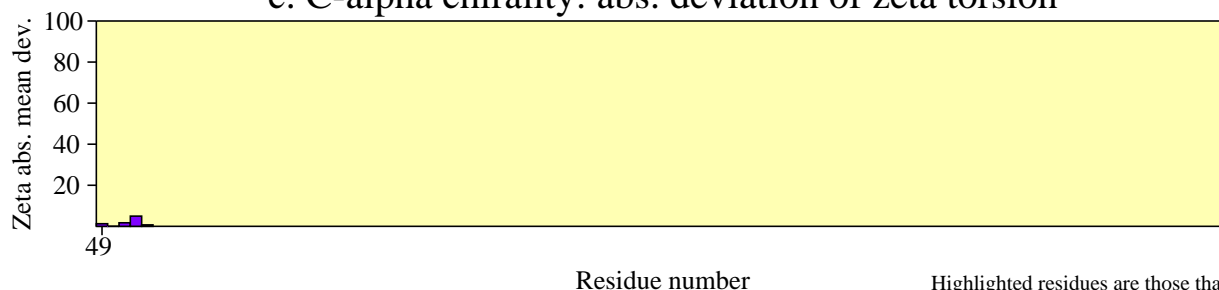
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

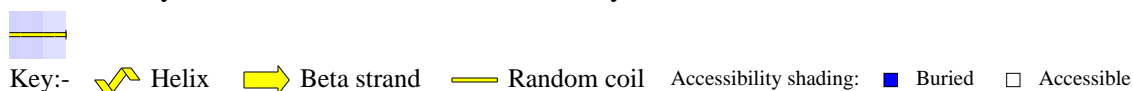


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



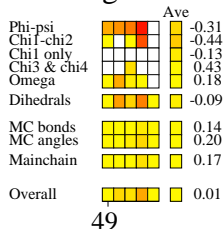
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

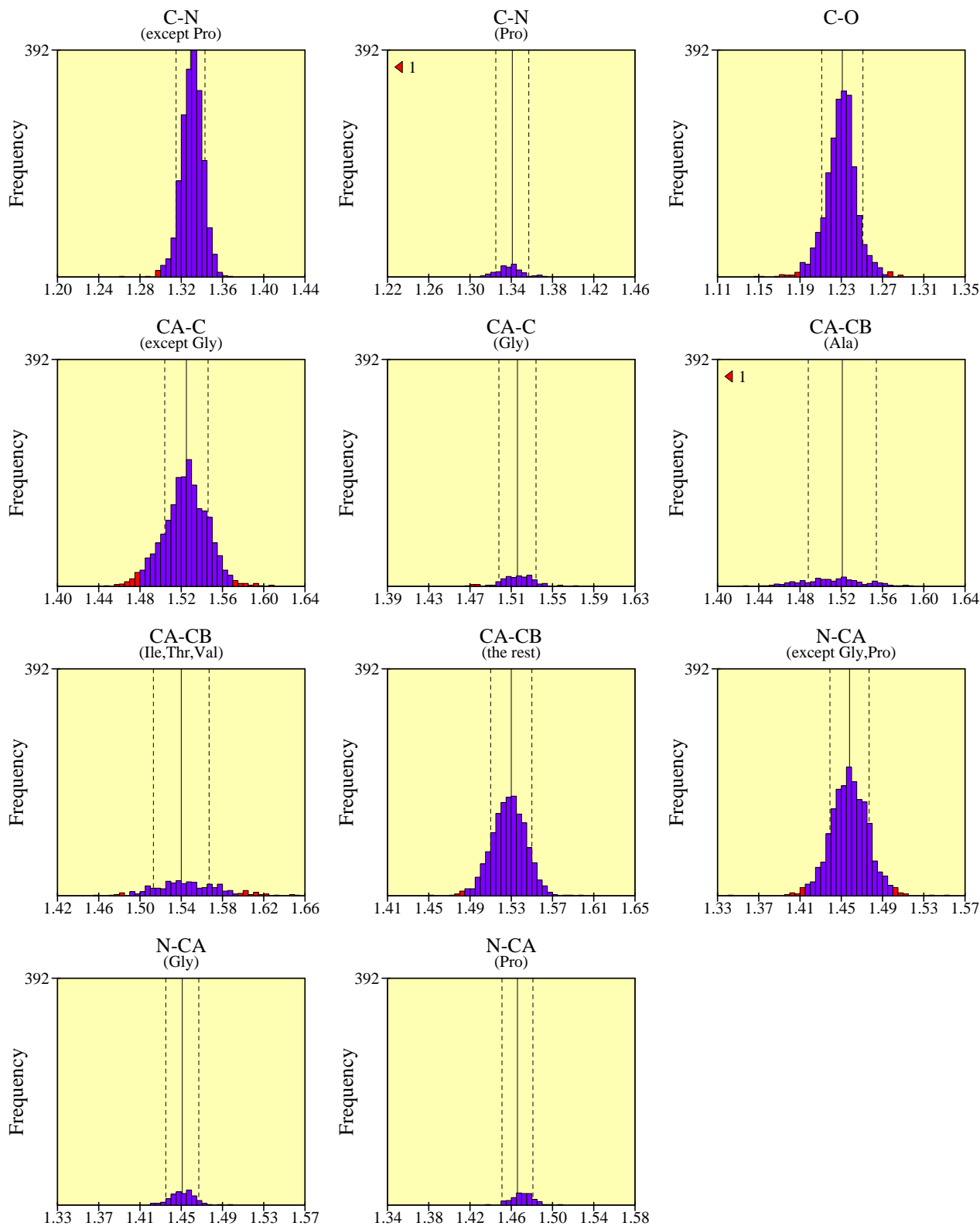


g. G-factors



Main-chain bond lengths

1ntz



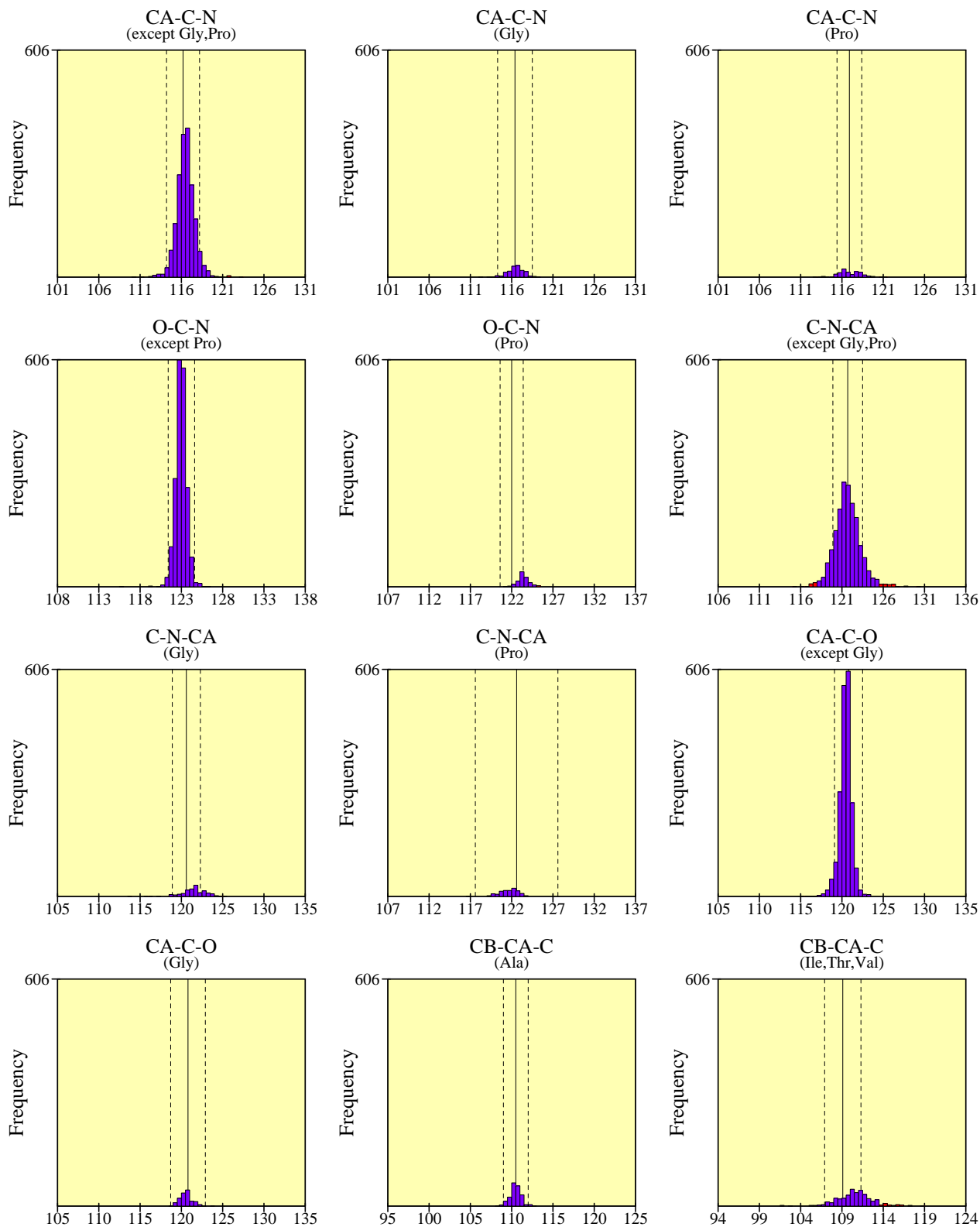
Black bars > 2.0 st. devs. from mean.

◀ 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

1ntz

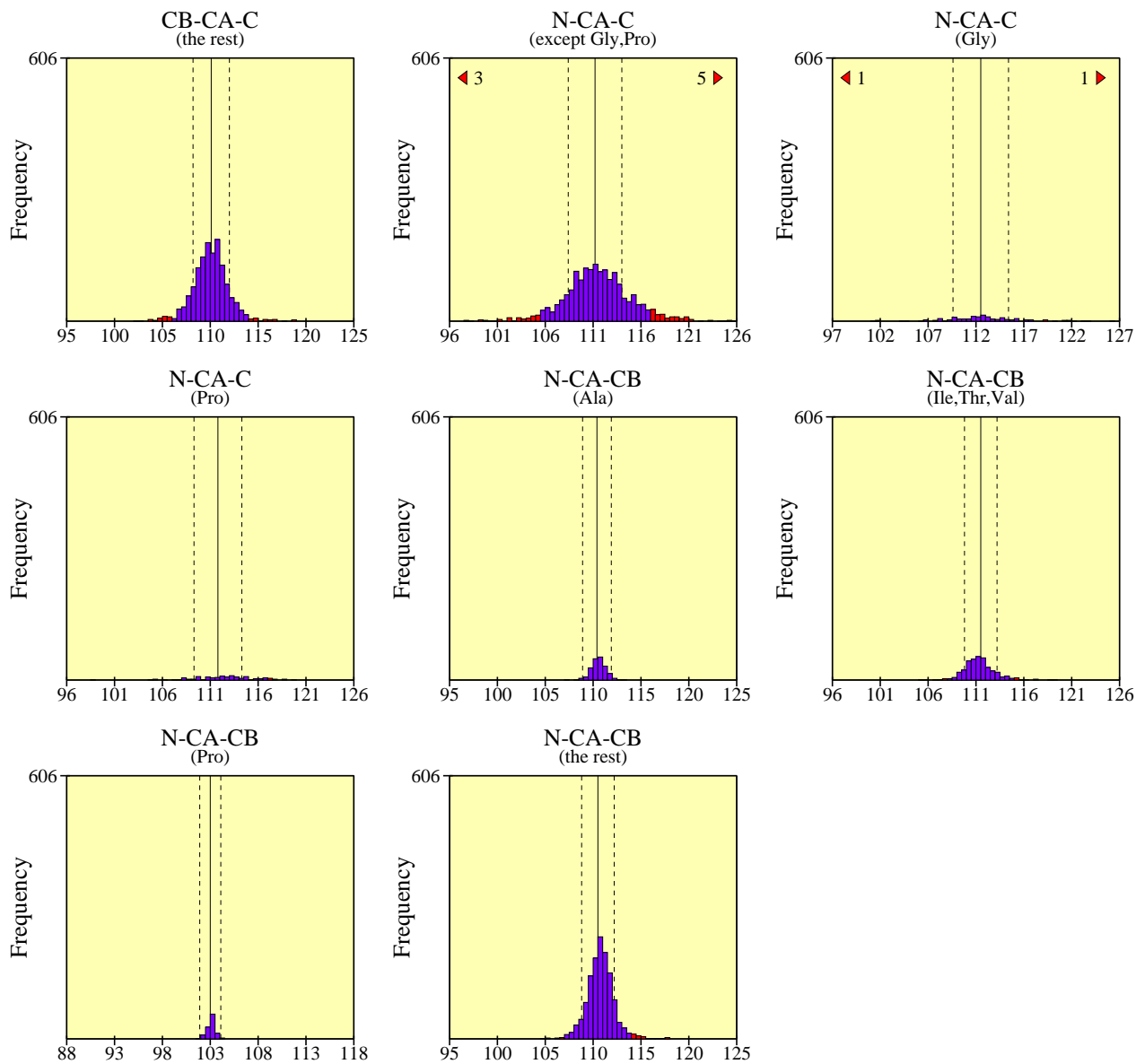


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

1ntz



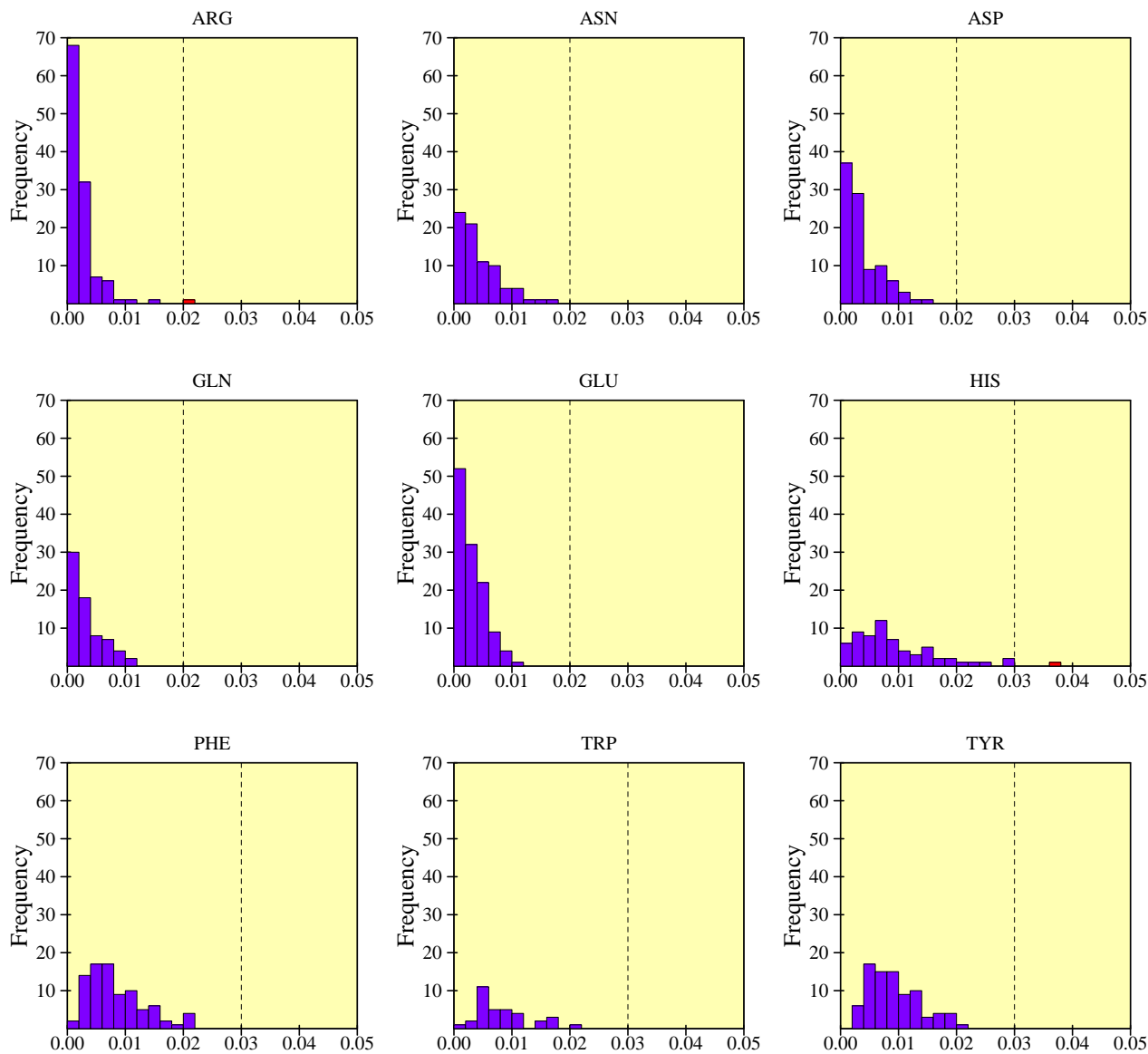
Black bars > 2.0 st. devs. from mean.

◀ 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

1ntz



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

1ntz

Main-chain bond lengths

CA 1.540 CB 0.061 1.601 A Thr 1	CA 1.521 CB 0.062 1.459 A Ala 84	CA 1.525 C 0.068 1.593 A Leu 106	CA 1.540 CB 0.079 1.619 A Ile 127	CA 1.525 C 0.051 1.576 A Asn 141	N 1.458 CA 0.059 1.399 A Arg 175
C 1.231 O 0.055 1.286 A His 252	CA 1.540 CB 0.052 1.592 A Val 253	CA 1.521 CB 0.054 1.467 A Ala 254	CA 1.525 C 0.058 1.467 A Glu 258	CA 1.525 C 0.054 1.471 A Tyr 280	N 1.458 CA 0.053 1.405 A Asp 281
CA 1.521 CB 0.052 1.469 A Ala 298	CA 1.525 C 0.058 1.467 A Thr 300	CA 1.525 C 0.062 1.463 A Gln 308	CA 1.521 CB 0.050 1.471 A Ala 315	CA 1.525 C 0.050 1.475 A Leu 320	CA 1.540 CB 0.057 1.483 A Val 337
CA 1.525 C 0.063 1.588 A Leu 338	CA 1.521 CB 0.052 1.469 A Ala 364	CA 1.530 CB 0.050 1.480 A Asp 378	C 1.231 O 0.052 1.179 A Val 402	CA 1.521 CB 0.093 1.428 A Ala 423	CA 1.540 CB 0.064 1.476 B Thr 27
CA 1.521 CB 0.068 1.453 B Ala 36	CA 1.525 C 0.057 1.582 B Tyr 41	CA 1.530 CB 0.051 1.479 B Ser 60	C 1.231 O 0.050 1.181 B Asn 61	CA 1.525 C 0.061 1.464 B Asn 61	CA 1.530 CB 0.080 1.450 B Asn 61
C 1.231 O 0.058 1.173 B Leu 69	CA 1.525 C 0.051 1.474 B Ser 73	C 1.329 N 0.069 1.260 B Lys 78 - B Gly 79	CA 1.540 CB 0.084 1.456 B Thr 86	CA 1.525 C 0.051 1.474 B Ala 106	CA 1.521 CB 0.057 1.464 B Ala 106
CA 1.540 CB 0.064 1.476 B Thr 108	CA 1.540 CB 0.107 1.647 B Ile 118	CA 1.525 C 0.067 1.592 B Asn 125	C 1.231 O 0.057 1.288 B Ile 146	CA 1.525 C 0.066 1.591 B Ile 146	CA 1.525 C 0.074 1.599 B Lys 148
CA 1.521 CB 0.068 1.589 B Ala 149	CA 1.525 C 0.066 1.459 B Tyr 168	CA 1.525 C 0.062 1.463 B Arg 169	CA 1.525 C 0.069 1.456 B Asn 170	N 1.458 CA 0.115 1.343 B Asn 170	C 1.231 O 0.060 1.171 B Ala 171
CA 1.525 C 0.051 1.474 B Asn 174	CA 1.525 C 0.055 1.470 B Tyr 177	CA 1.525 C 0.052 1.473 B Gln 196	N 1.458 CA 0.062 1.396 B Asn 197	CA 1.521 CB 0.066 1.455 B Ala 220	CA 1.525 C 0.079 1.446 B Ile 226
CA 1.525 C 0.055 1.470 B Arg 227	CA 1.521 CB 0.075 1.446 B Ala 237	CA 1.540 CB 0.059 1.481 B Ile 244	CA 1.530 CB 0.052 1.478 B Arg 245	N 1.458 CA 0.050 1.508 B Gln 247	CA 1.516 C 0.055 1.571 B Gly 249
CA 1.525 C 0.064 1.461 B Leu 257	CA 1.521 CB 0.063 1.458 B Ala 262	CA 1.521 CB 0.054 1.467 B Ala 281	CA 1.521 CB 0.059 1.462 B Ala 298	CA 1.525 C 0.069 1.456 B Val 309	N 1.458 CA 0.057 1.401 B Asn 313

Distorted geometry

1ntz

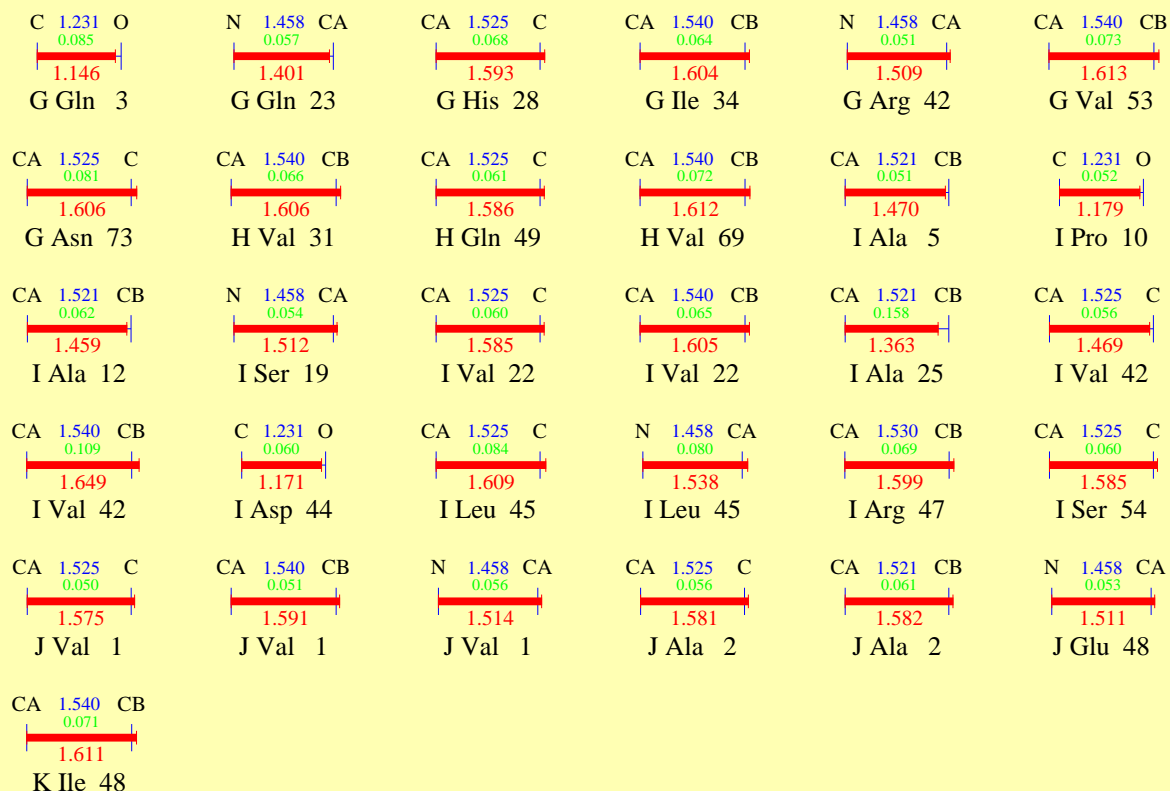
Main-chain bond lengths (contd)

CA 1.521 CB 0.054 1.575 B Ala 330	CA 1.521 CB 0.061 1.582 B Ala 331	CA 1.521 CB 0.050 1.471 B Ala 339	CA 1.521 CB 0.052 1.573 B Ala 340	CA 1.521 CB 0.055 1.466 B Ala 386	CA 1.521 CB 0.056 1.465 B Ala 388
CA 1.525 C 0.057 1.468 B Thr 397	CA 1.525 C 0.055 1.580 B Val 405	CA 1.521 CB 0.060 1.461 B Ala 414	CA 1.530 CB 0.055 1.585 B Met 424	CA 1.521 CB 0.077 1.444 B Ala 425	C 1.231 O 0.077 1.154 B Gly 431
N 1.458 CA 0.095 1.553 B Ile 436	CA 1.540 CB 0.083 1.623 C Thr 2	CA 1.540 CB 0.056 1.484 C Ile 19	CA 1.525 C 0.051 1.474 C Pro 24	CA 1.540 CB 0.057 1.597 C Ile 39	CA 1.525 C 0.060 1.465 C Leu 41
CA 1.540 CB 0.085 1.625 C Ile 42	CA 1.540 CB 0.056 1.484 C Thr 108	CA 1.540 CB 0.063 1.603 C Val 123	CA 1.521 CB 0.050 1.471 C Ala 127	CA 1.525 C 0.053 1.472 C Ile 146	CA 1.540 CB 0.055 1.485 C Thr 147
CA 1.540 CB 0.066 1.606 C Ile 156	CA 1.540 CB 0.068 1.472 C Ile 218	CA 1.525 C 0.052 1.577 C Phe 220	C 1.231 O 0.060 1.171 C His 221	C 1.341 N 0.123 1.218 C His 221 - C Pro 222	CA 1.540 CB 0.075 1.615 C Val 243
CA 1.540 CB 0.075 1.615 C Thr 257	N 1.458 CA 0.055 1.403 C Thr 309	CA 1.525 C 0.056 1.581 C Arg 318	CA 1.540 CB 0.072 1.612 C Thr 336	CA 1.540 CB 0.058 1.598 C Ile 348	CA 1.540 CB 0.061 1.601 C Val 364
CA 1.525 C 0.067 1.592 D Phe 91	CA 1.525 C 0.059 1.466 D Leu 109	CA 1.540 CB 0.054 1.594 D Ile 116	CA 1.516 C 0.051 1.465 D Gly 123	CA 1.540 CB 0.082 1.622 D Val 182	CA 1.525 C 0.051 1.474 D Asp 199
N 1.458 CA 0.052 1.510 D Lys 241	C 1.231 O 0.053 1.178 E Lys 6	CA 1.530 CB 0.051 1.581 E Lys 6	CA 1.540 CB 0.093 1.633 E Thr 22	CA 1.540 CB 0.056 1.596 E Val 39	CA 1.540 CB 0.073 1.613 E Val 55
CA 1.525 C 0.052 1.577 E Met 62	CA 1.540 CB 0.061 1.601 E Val 68	CA 1.540 CB 0.055 1.595 E Ile 74	CA 1.540 CB 0.064 1.604 E Val 133	CA 1.540 CB 0.063 1.603 F Ile 16	N 1.458 CA 0.054 1.404 F Met 32
C 1.231 O 0.056 1.287 F Ile 37	C 1.231 O 0.063 1.168 F Glu 39	CA 1.525 C 0.058 1.467 F Glu 45	CA 1.521 CB 0.070 1.451 F Ala 46	CA 1.540 CB 0.113 1.653 F Val 59	CA 1.525 C 0.051 1.474 F Lys 63
N 1.458 CA 0.050 1.408 F Gln 73	CA 1.525 C 0.051 1.474 F Thr 81	CA 1.540 CB 0.064 1.604 F Thr 81	N 1.458 CA 0.053 1.405 F Thr 81	CA 1.525 C 0.051 1.474 G Arg 2	CA 1.530 CB 0.057 1.473 G Arg 2

Distorted geometry

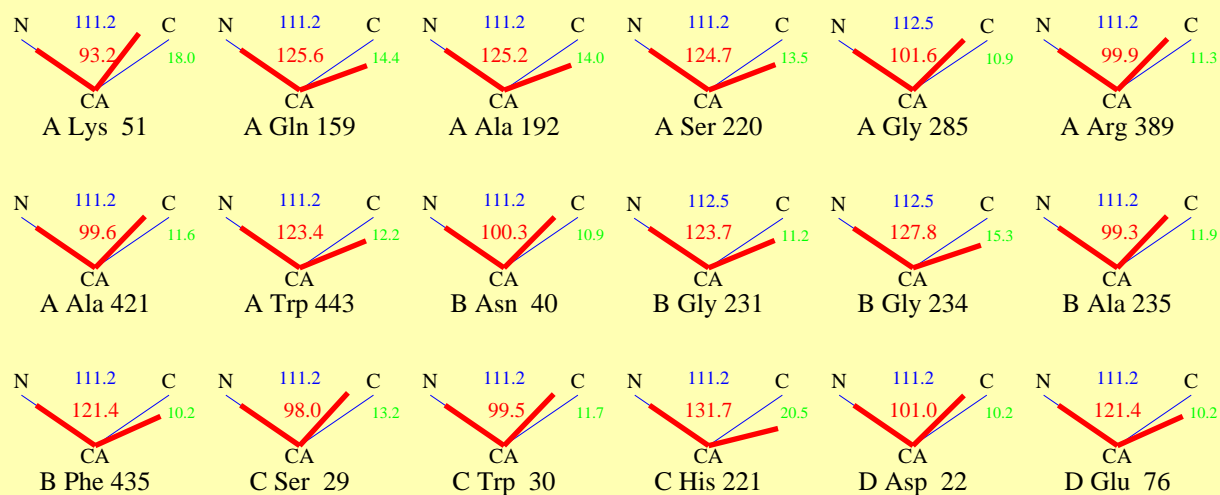
1ntz

Main-chain bond lengths (contd)



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

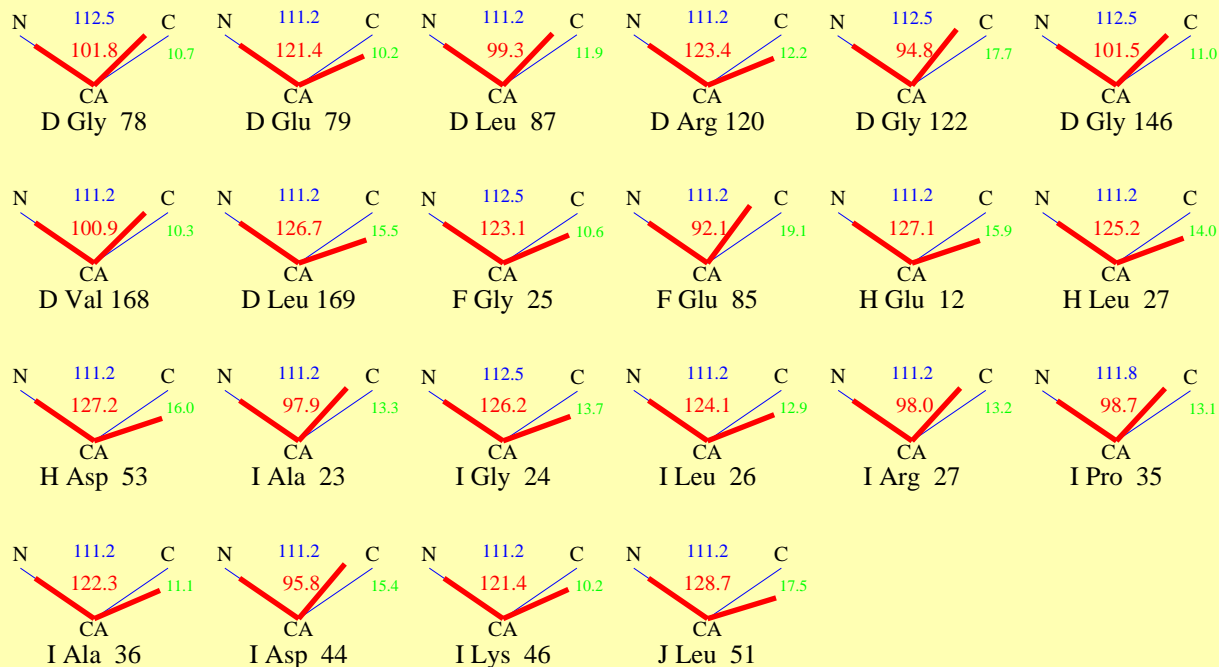
Main-chain bond angles



Distorted geometry

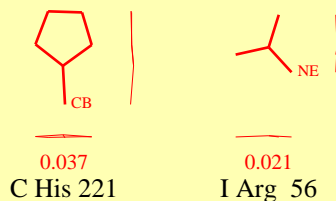
Intz

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.