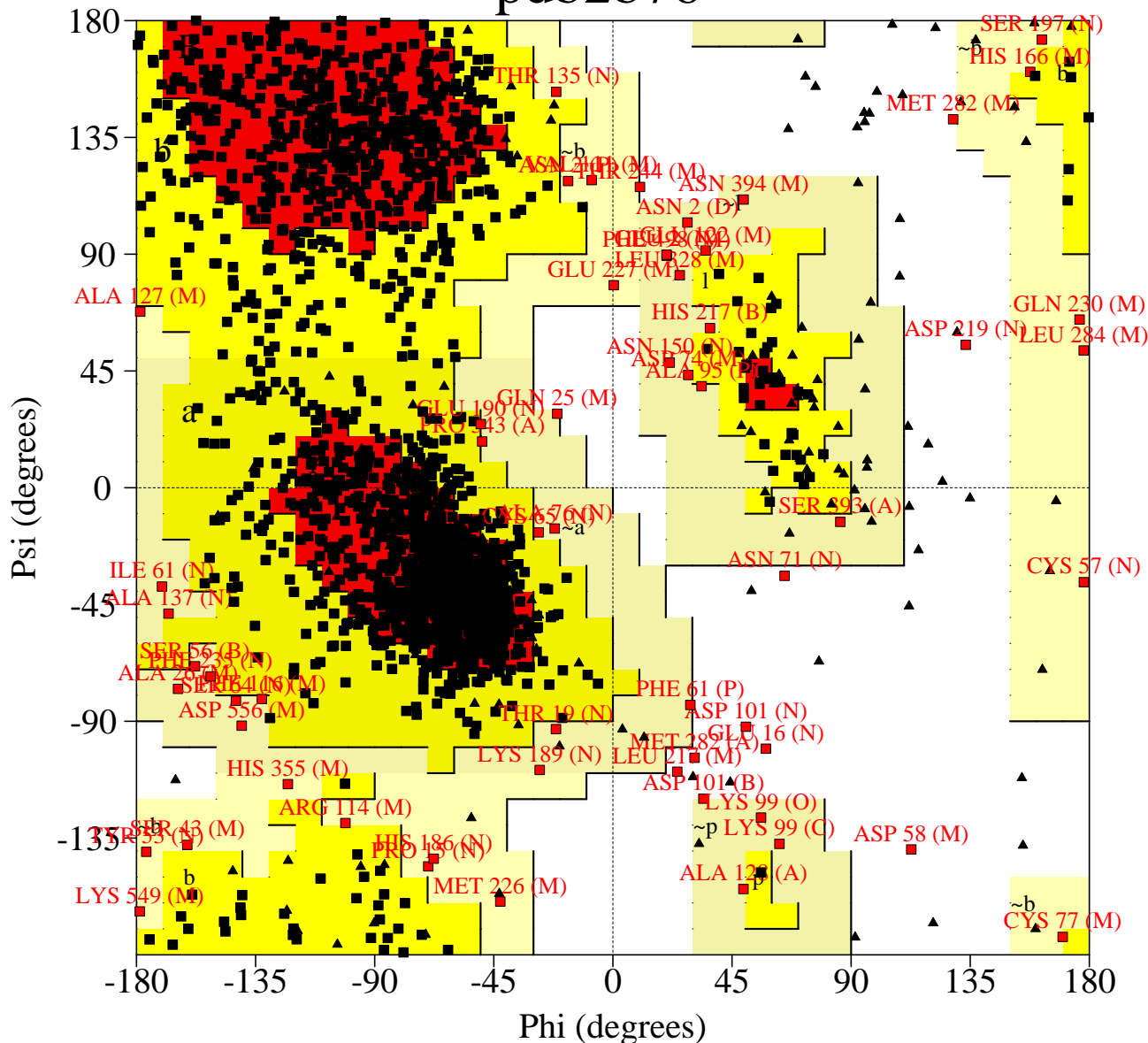


Ramachandran Plot

pdb2b76



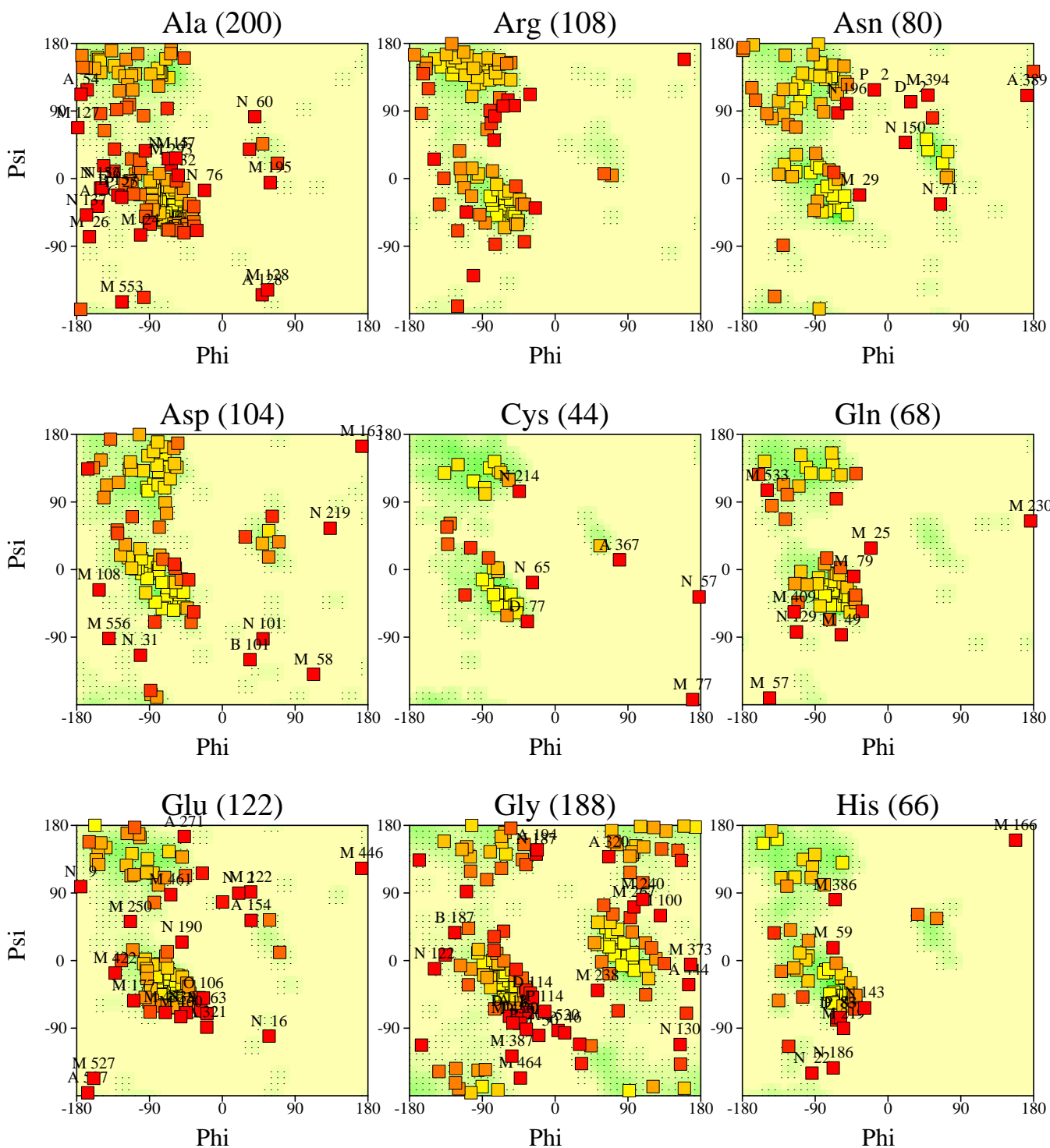
Plot statistics

| | | |
|--|------|--------|
| Residues in most favoured regions [A,B,L] | 1347 | 73.8% |
| Residues in additional allowed regions [a,b,l,p] | 421 | 23.1% |
| Residues in generously allowed regions [-a,-b,-l,-p] | 47 | 2.6% |
| Residues in disallowed regions | 10 | 0.5% |
| | ---- | ----- |
| Number of non-glycine and non-proline residues | 1825 | 100.0% |
| Number of end-residues (excl. Gly and Pro) | 16 | |
| Number of glycine residues (shown as triangles) | 188 | |
| Number of proline residues | 104 | |
| | ---- | ----- |
| Total number of residues | 2133 | |

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

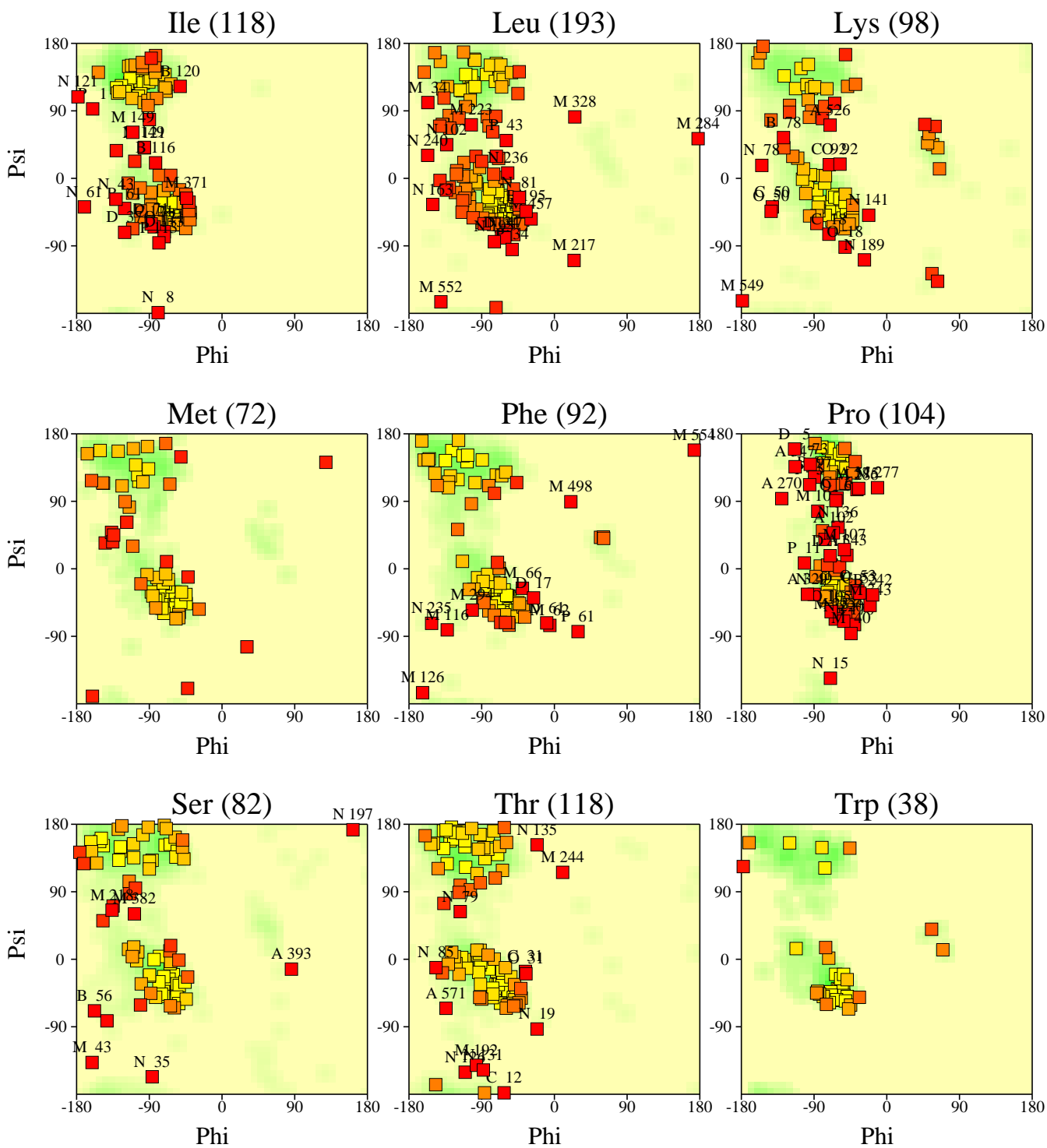
pdb2b76



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

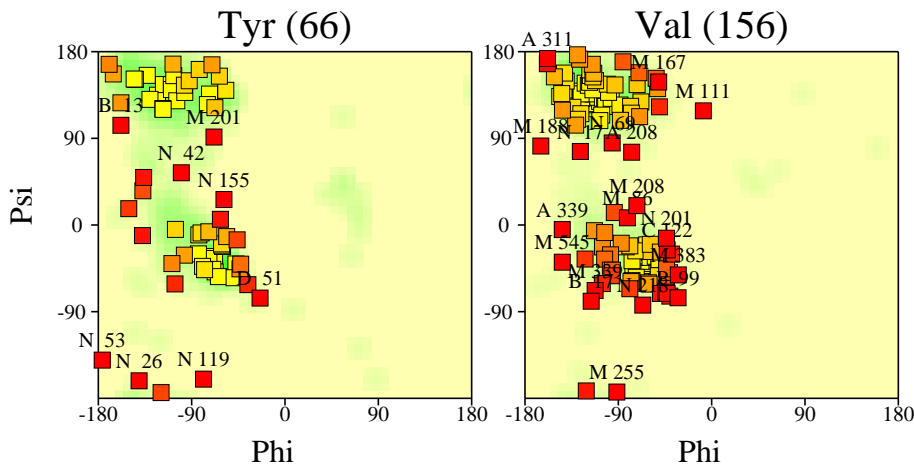
pdb2b76



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

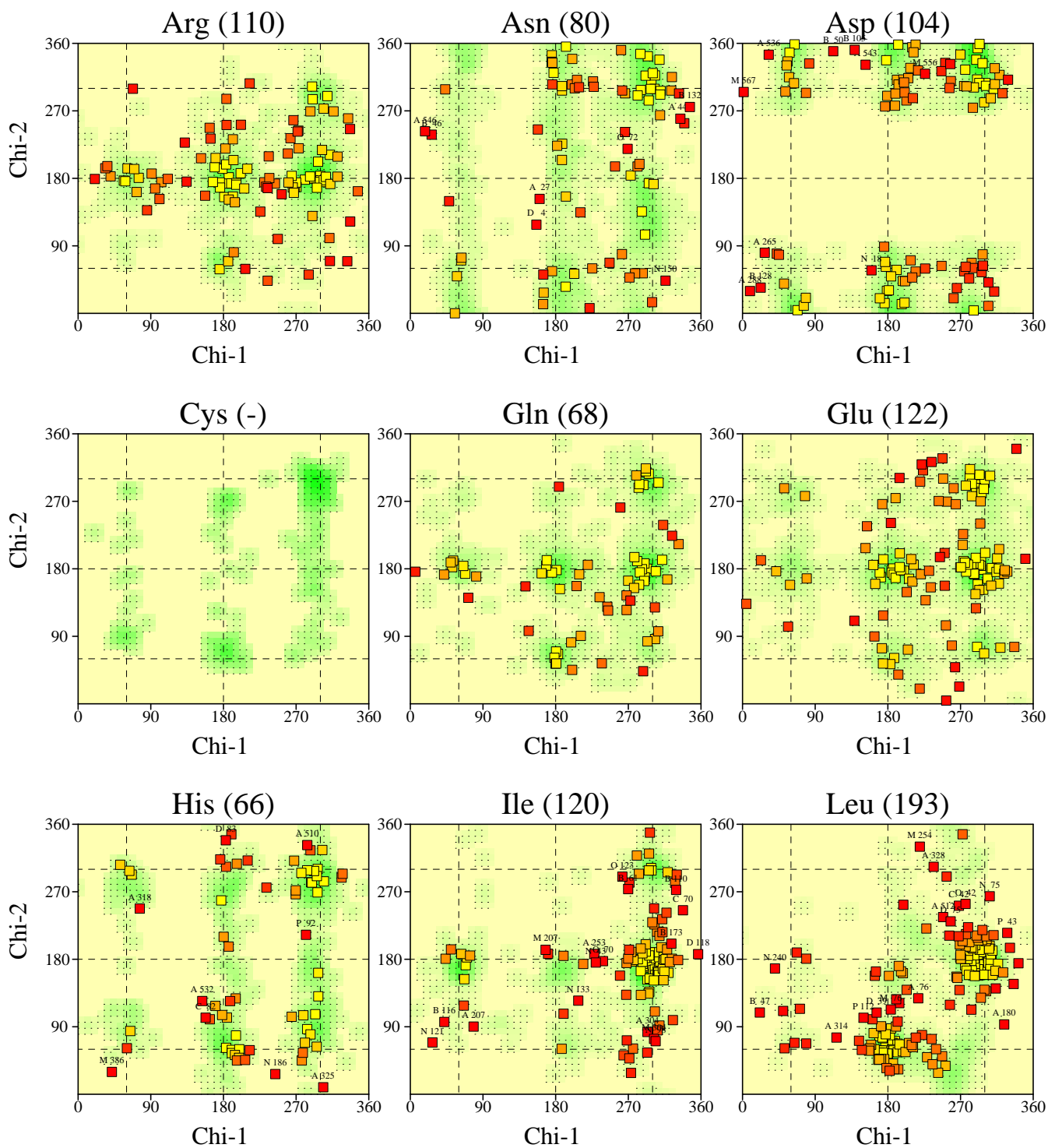
pdb2b76



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

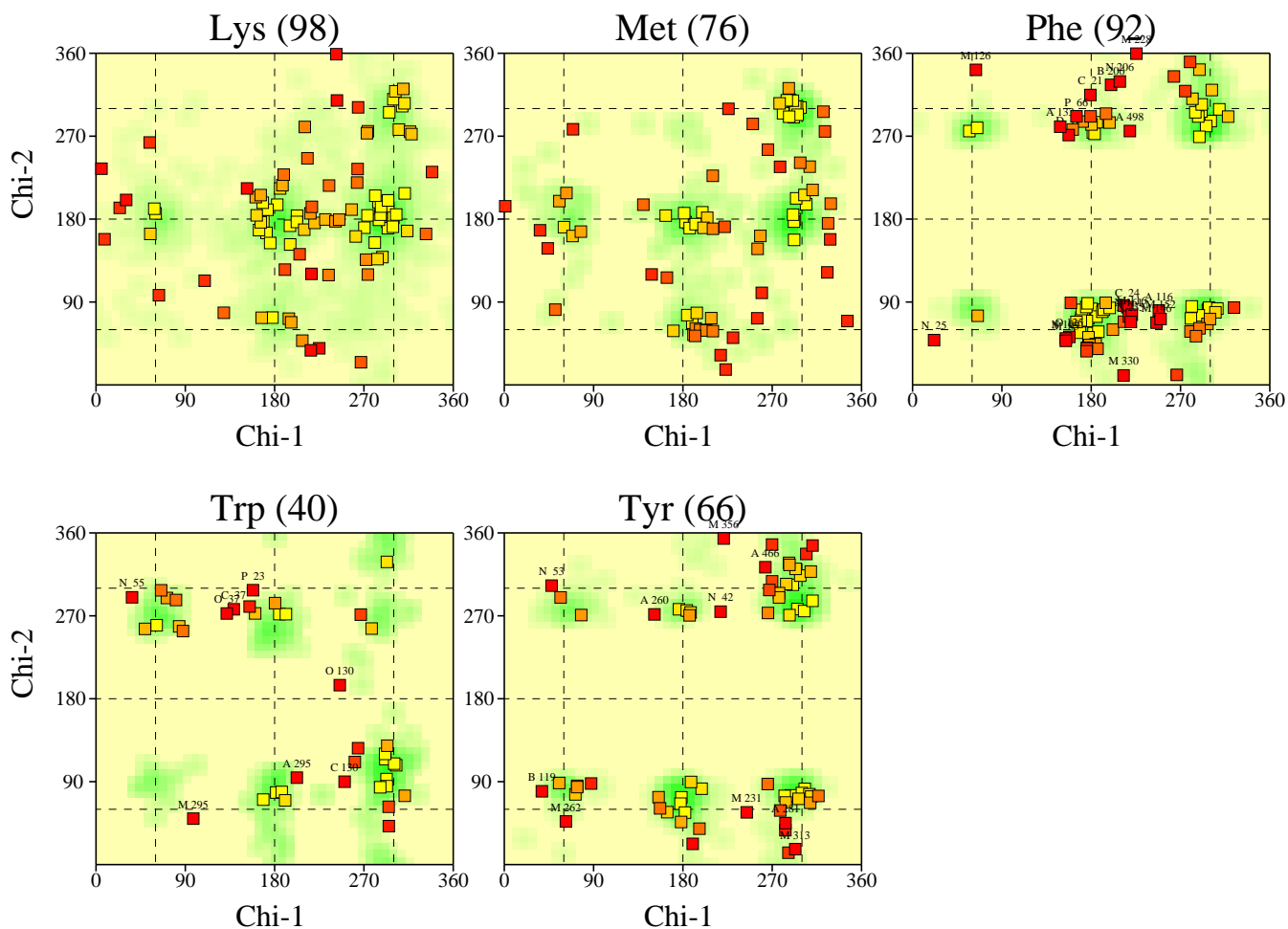
pdb2b76



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 2.0Å or better.

Chi1-Chi2 plots

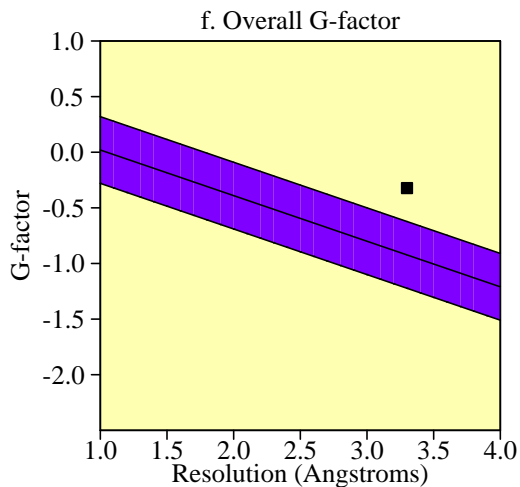
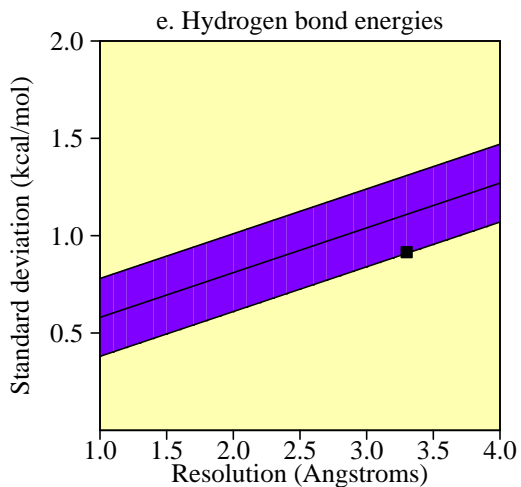
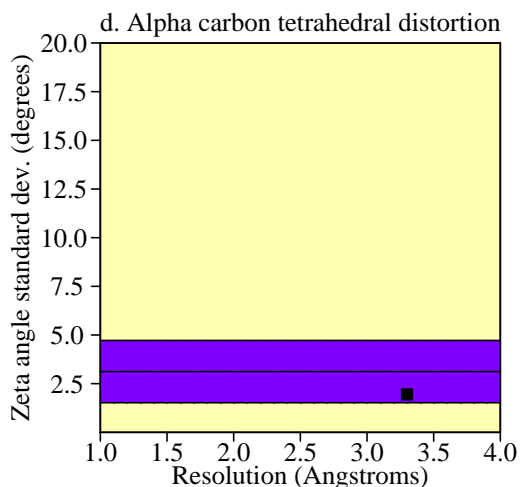
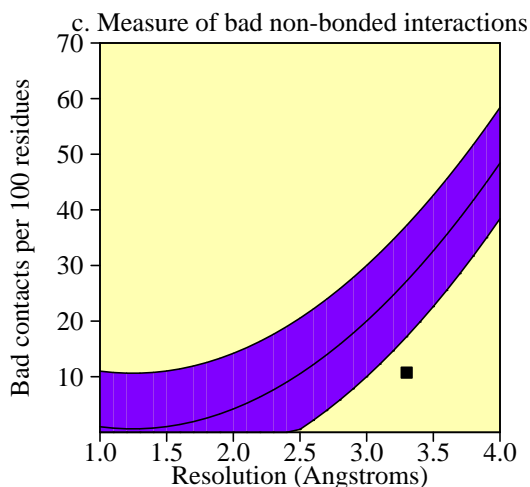
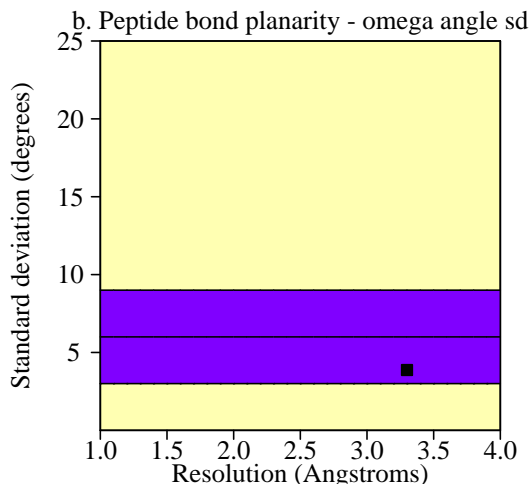
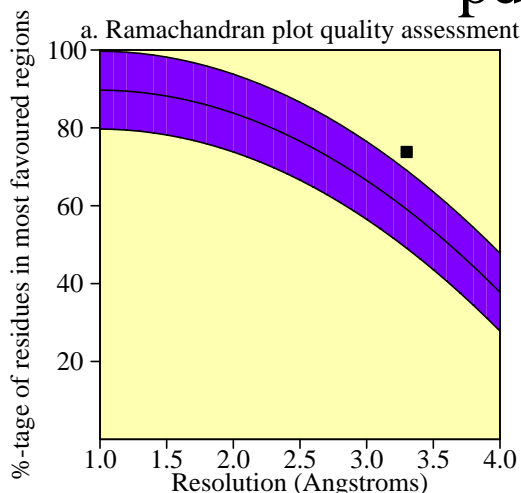
pdb2b76



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

pdb2b76

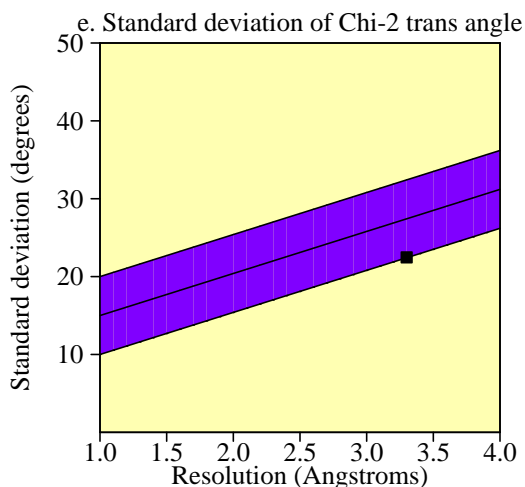
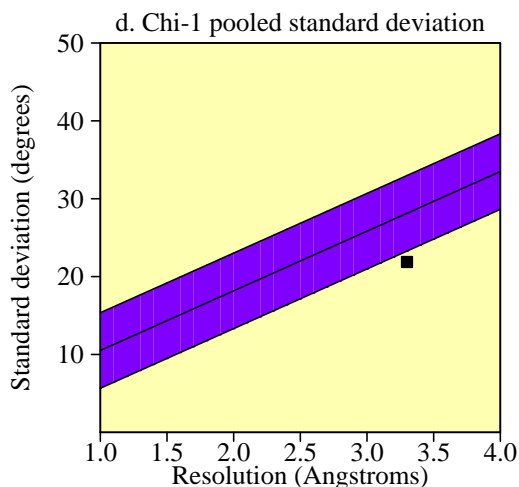
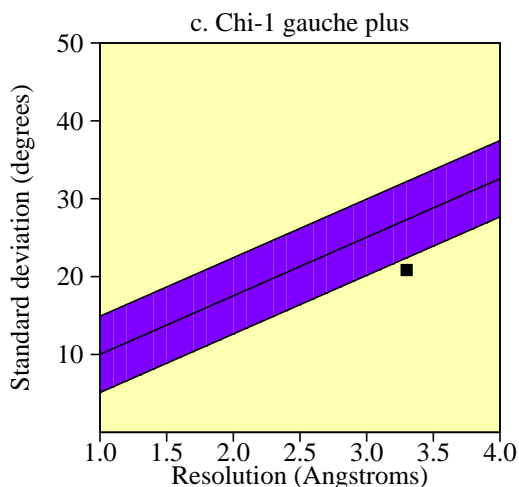
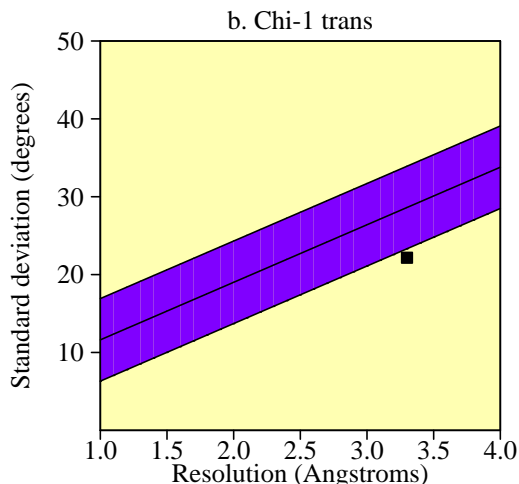
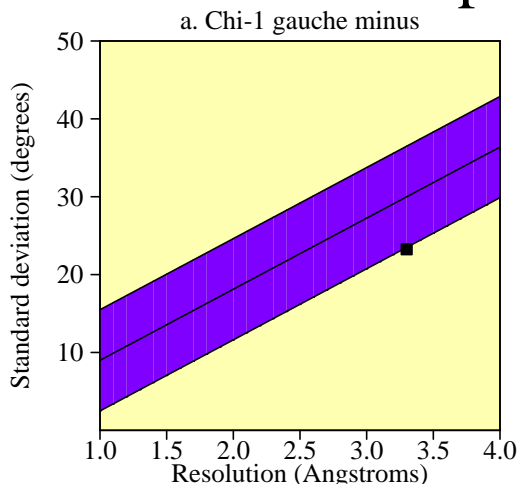


Plot statistics

| 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 | 1825 | 73.8 | 59.1 | 10.0 | 1.5 | BETTER |
| b. Omega angle st dev | 2125 | 3.9 | 6.0 | 3.0 | -0.7 | Inside |
| c. Bad contacts / 100 residues | 229 | 10.7 | 27.2 | 10.0 | -1.6 | BETTER |
| d. Zeta angle st dev | 1945 | 1.9 | 3.1 | 1.6 | -0.7 | Inside |
| e. H-bond energy st dev | 1281 | 0.9 | 1.1 | 0.2 | -1.0 | Inside |
| f. Overall G-factor | 2133 | -0.3 | -0.9 | 0.3 | 2.0 | BETTER |

Side-chain parameters

pdb2b76



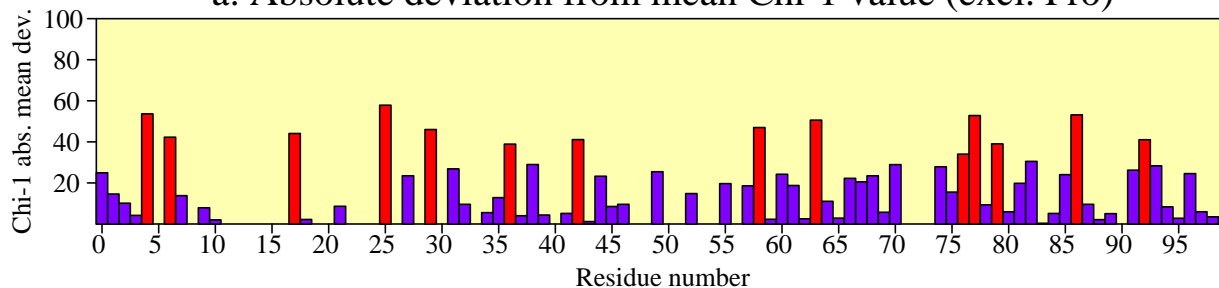
pdb2b76

Plot statistics

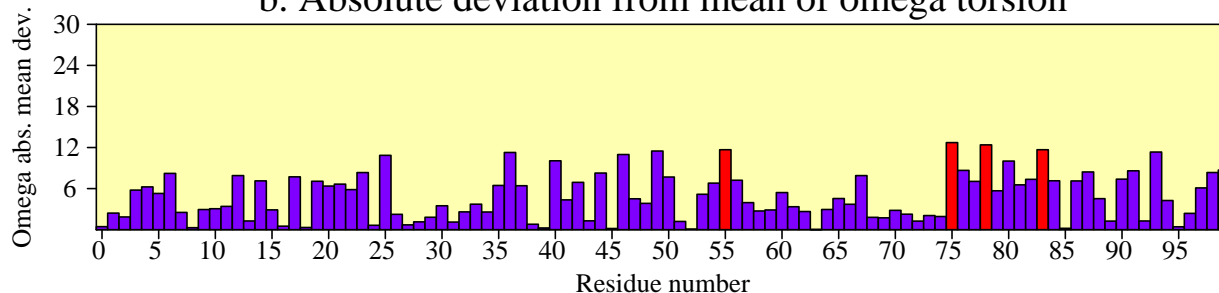
| Stereochemical parameter | No. of data pts | Parameter value | Comparison values | | No. of band widths from mean | |
|------------------------------|-----------------|-----------------|-------------------|------------|------------------------------|--------|
| | | | Typical value | Band width | | |
| a. Chi-1 gauche minus st dev | 251 | 23.3 | 30.0 | 6.5 | -1.0 | BETTER |
| b. Chi-1 trans st dev | 614 | 22.2 | 28.6 | 5.3 | -1.2 | BETTER |
| c. Chi-1 gauche plus st dev | 773 | 20.8 | 27.3 | 4.9 | -1.3 | BETTER |
| d. Chi-1 pooled st dev | 1638 | 21.9 | 28.1 | 4.8 | -1.3 | BETTER |
| e. Chi-2 trans st dev | 496 | 22.5 | 27.4 | 5.0 | -1.0 | Inside |

Residue properties pdb2b76

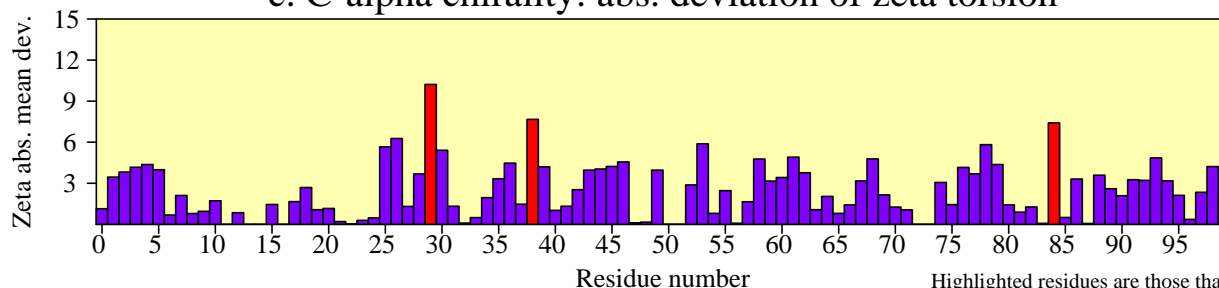
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

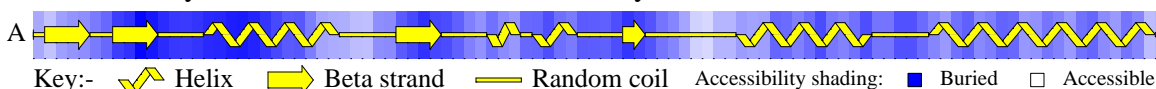


c. C-alpha chirality: abs. deviation of zeta torsion

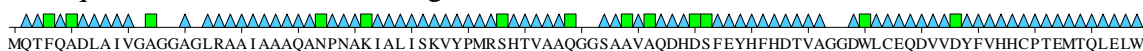


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



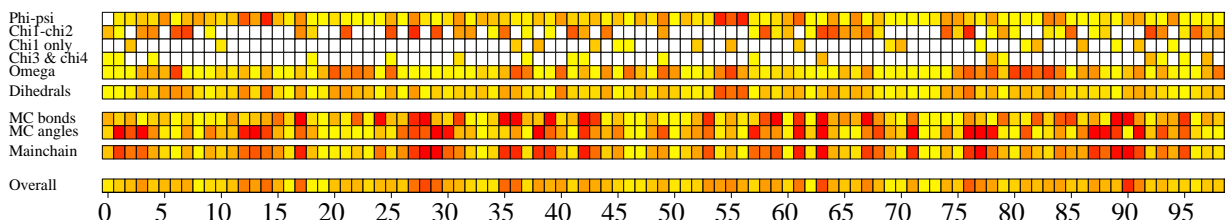
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

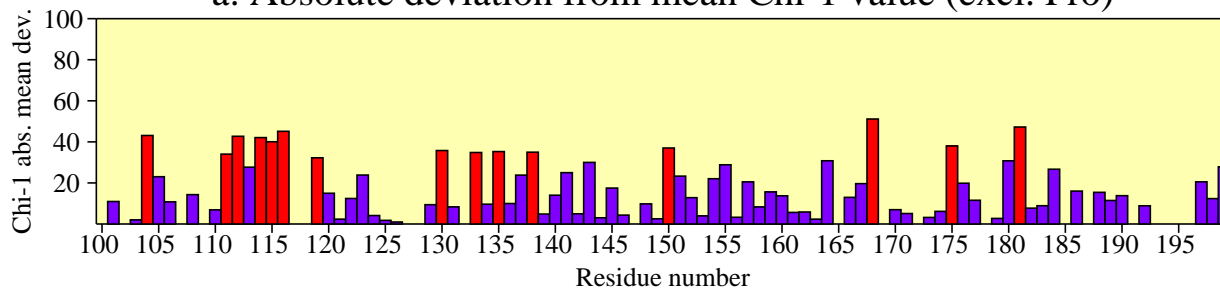


g. G-factors

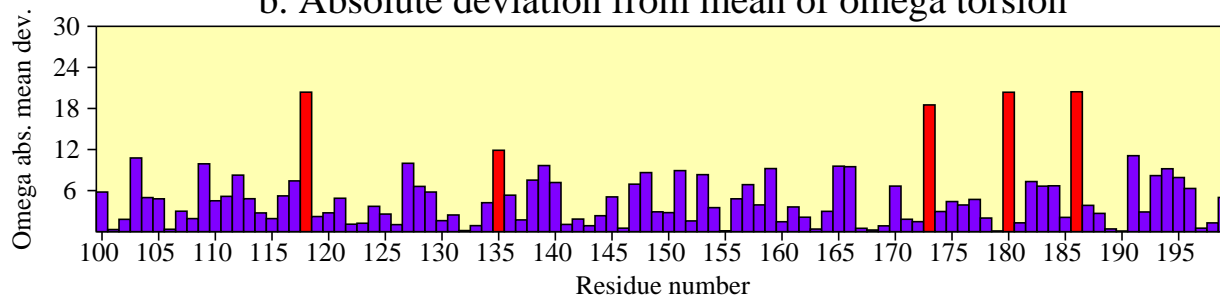


Residue properties pdb2b76

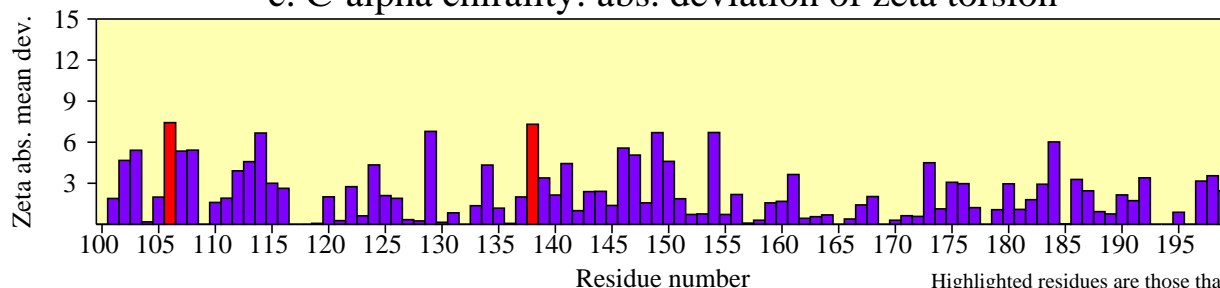
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

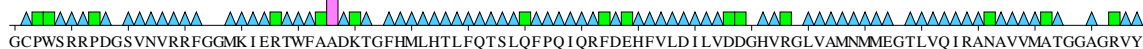


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



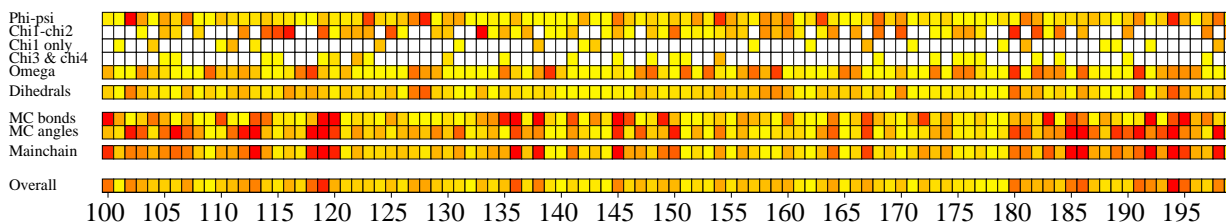
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

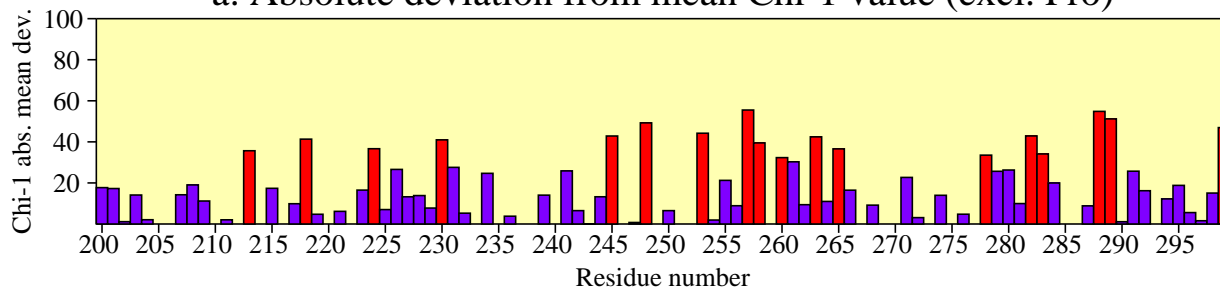


g. G-factors

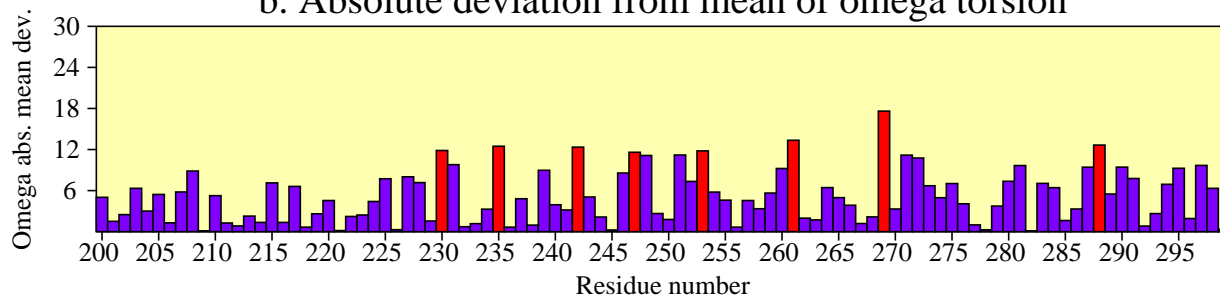


Residue properties pdb2b76

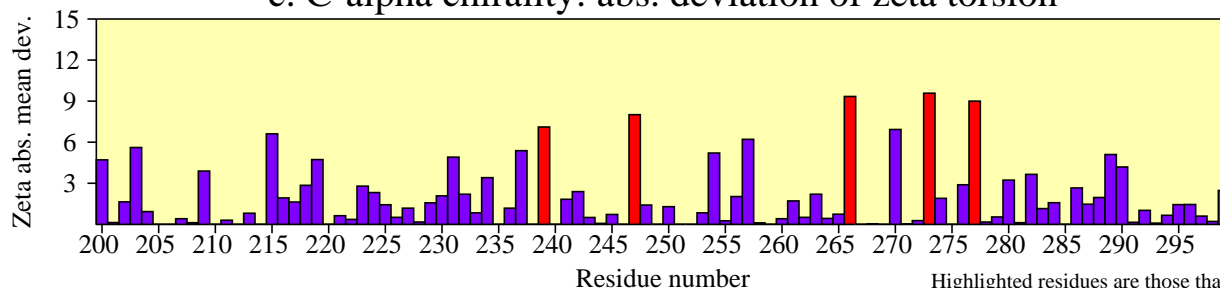
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

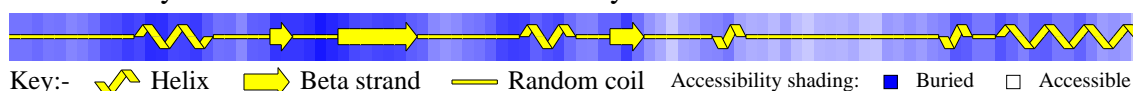


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



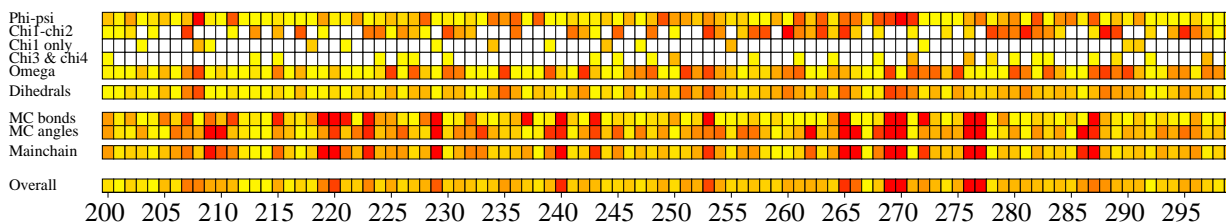
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

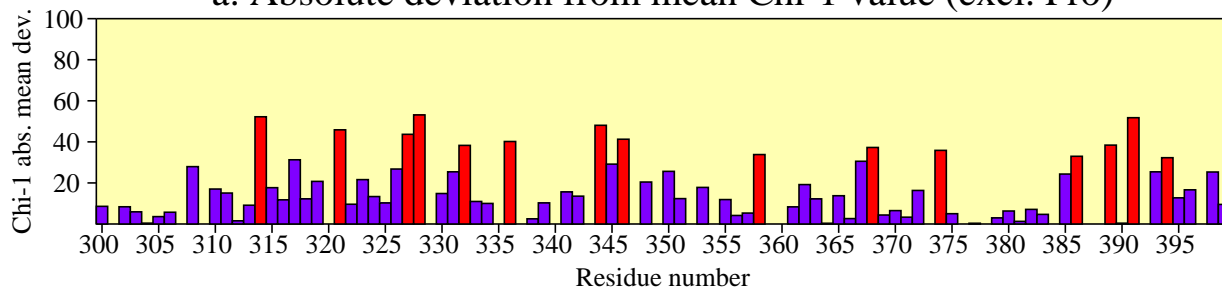


g. G-factors

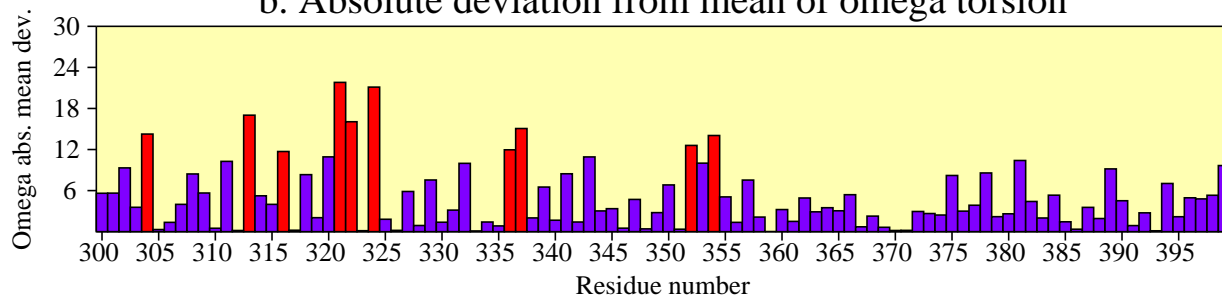


Residue properties pdb2b76

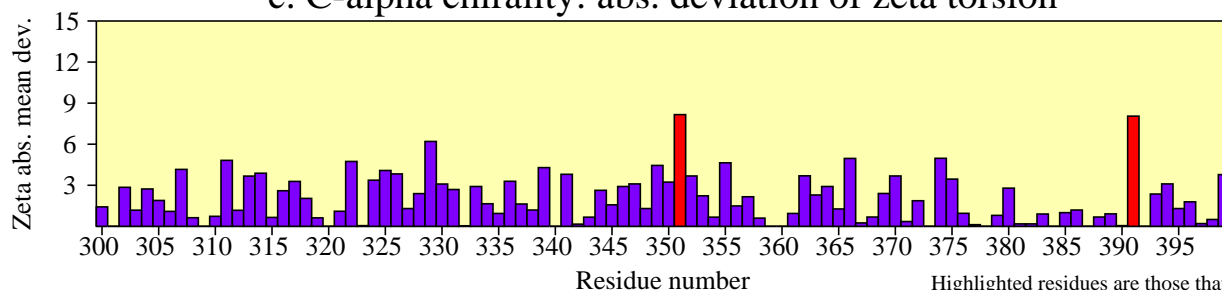
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



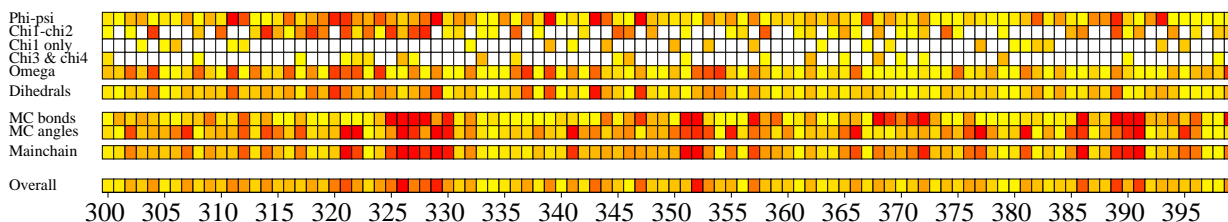
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

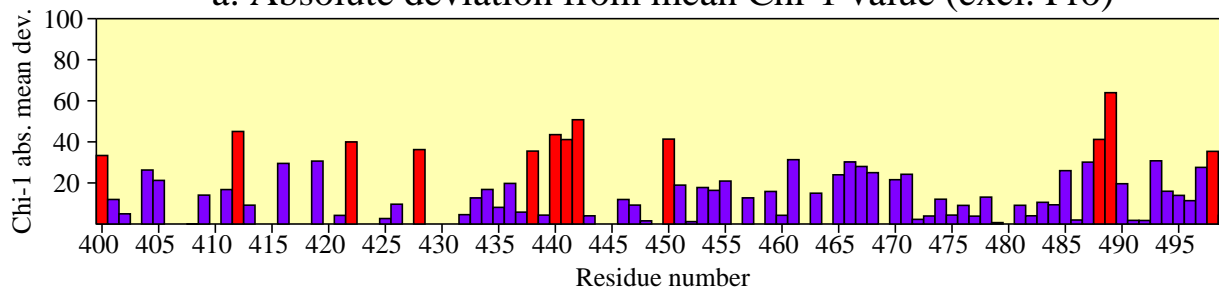


g. G-factors

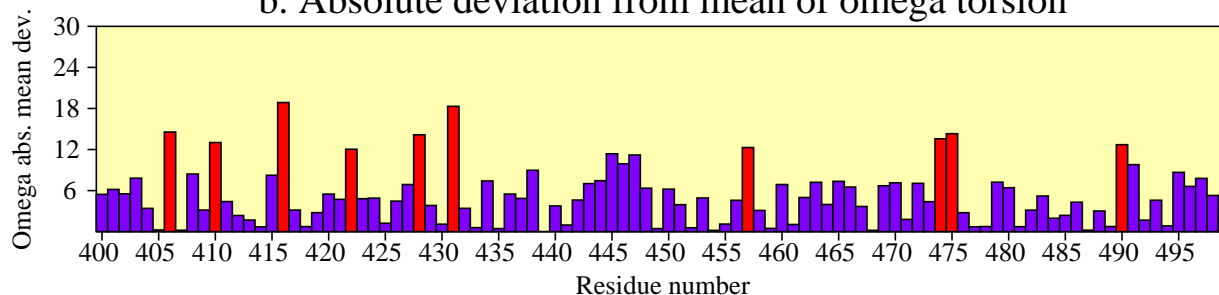


Residue properties pdb2b76

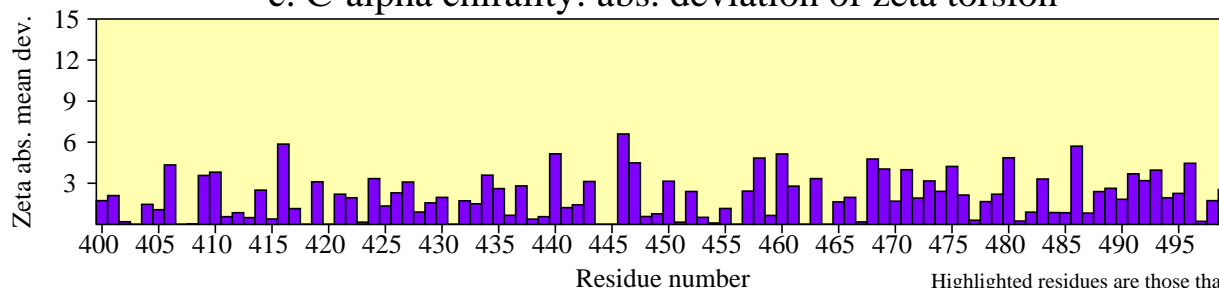
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

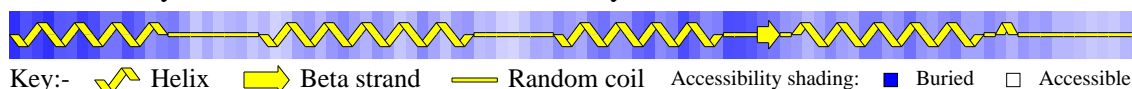


c. C-alpha chirality: abs. deviation of zeta torsion



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

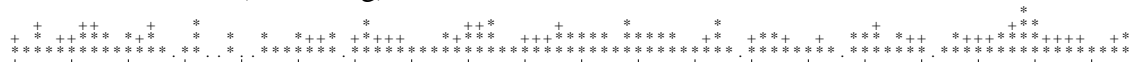
d. Secondary structure & estimated accessibility



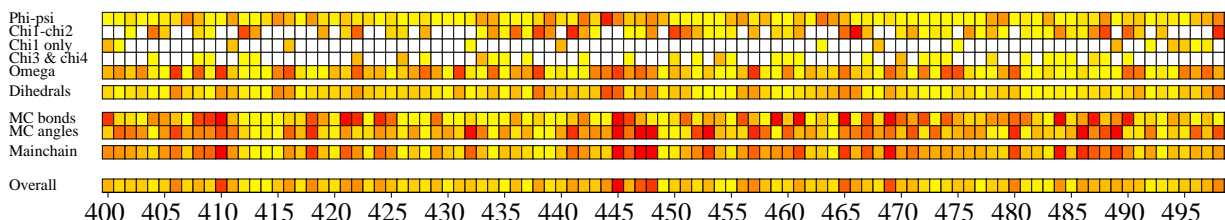
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

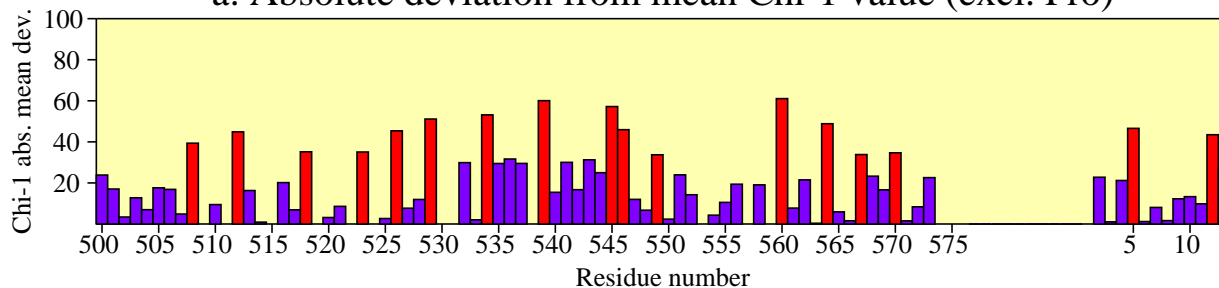


g. G-factors

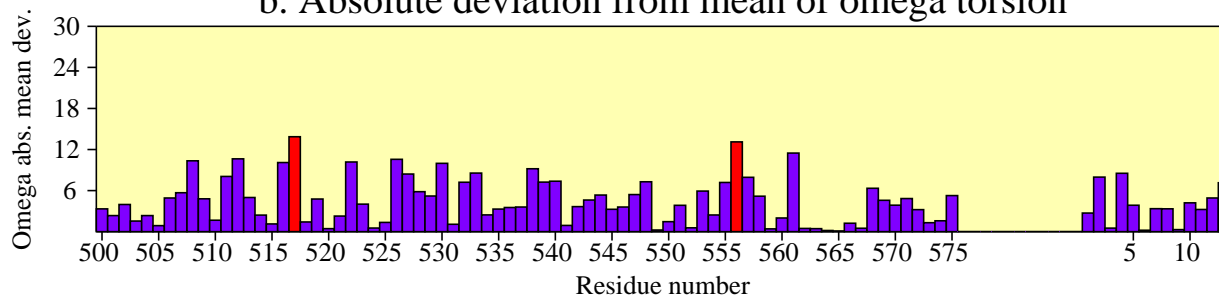


Residue properties pdb2b76

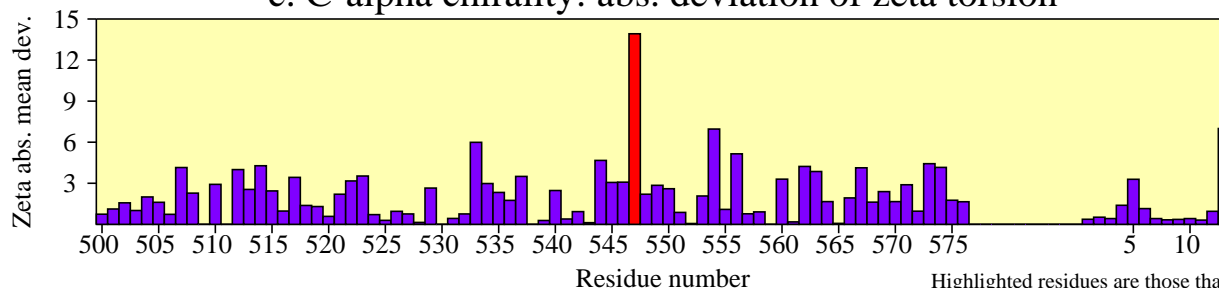
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

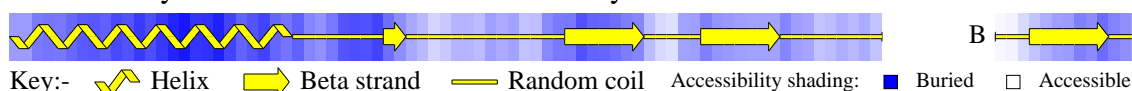


c. C-alpha chirality: abs. deviation of zeta torsion



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

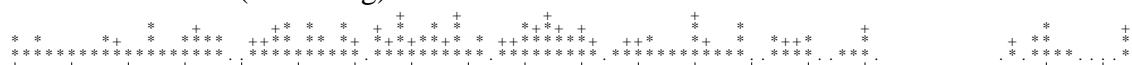
d. Secondary structure & estimated accessibility



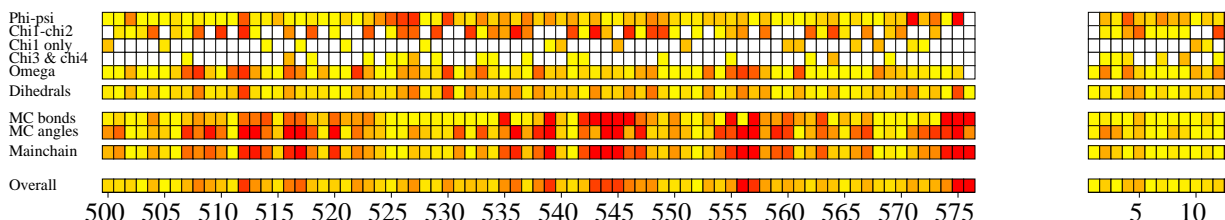
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

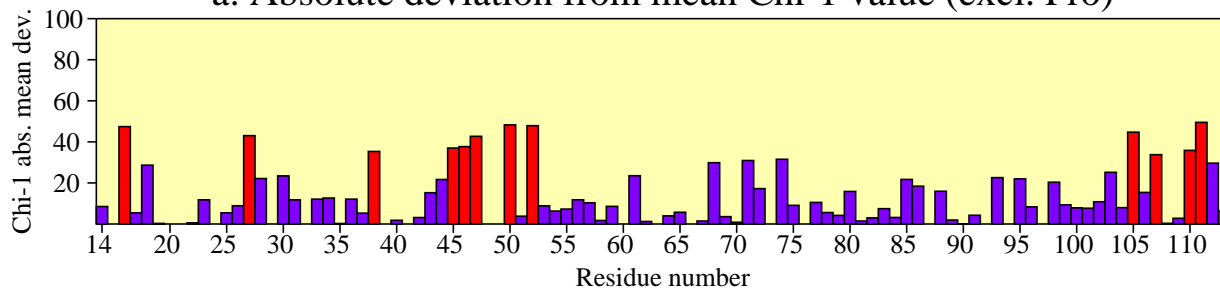


g. G-factors

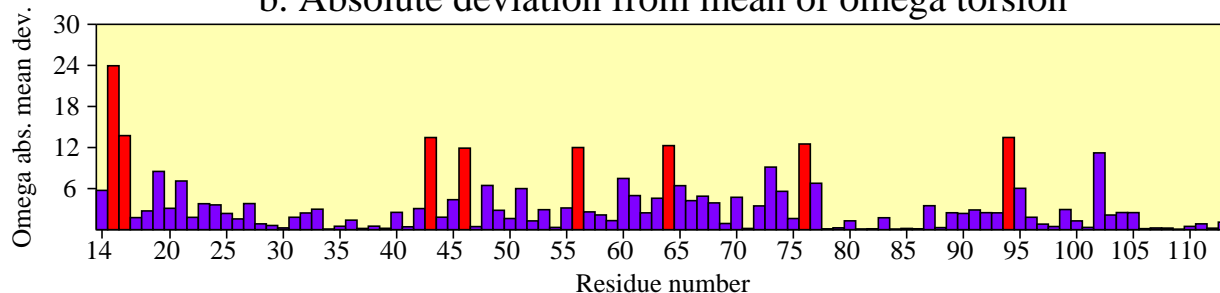


Residue properties pdb2b76

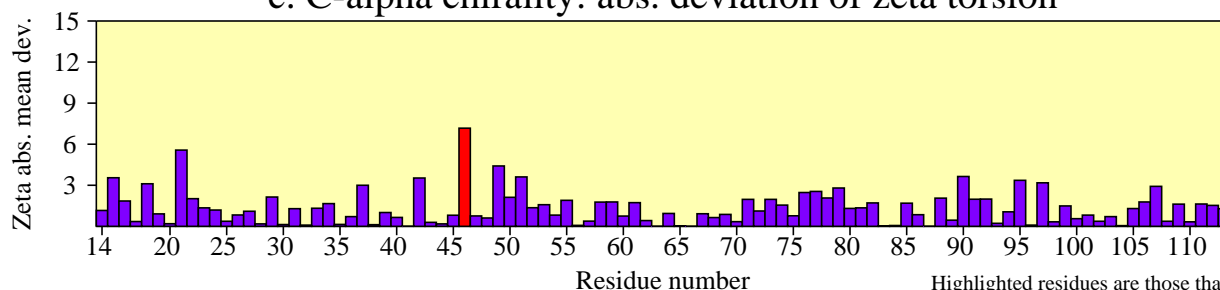
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

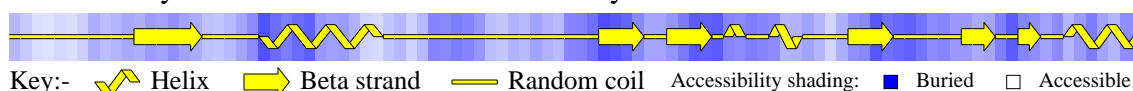


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



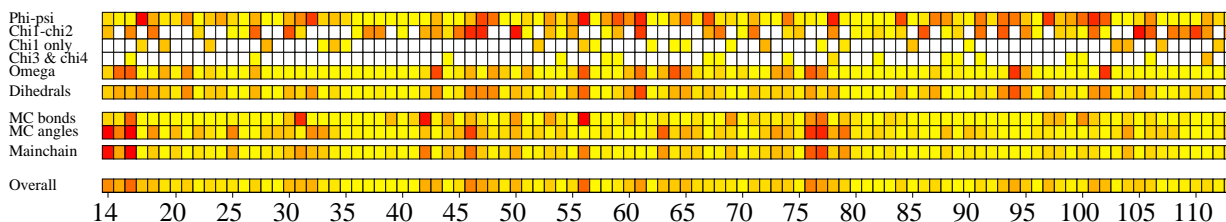
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

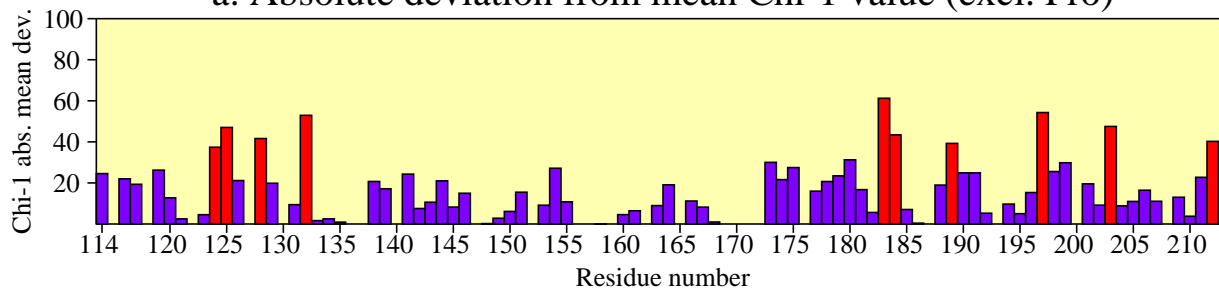


g. G-factors

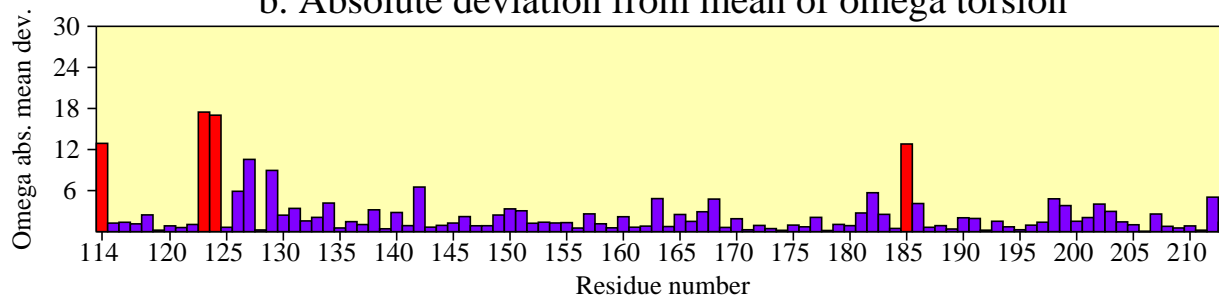


Residue properties pdb2b76

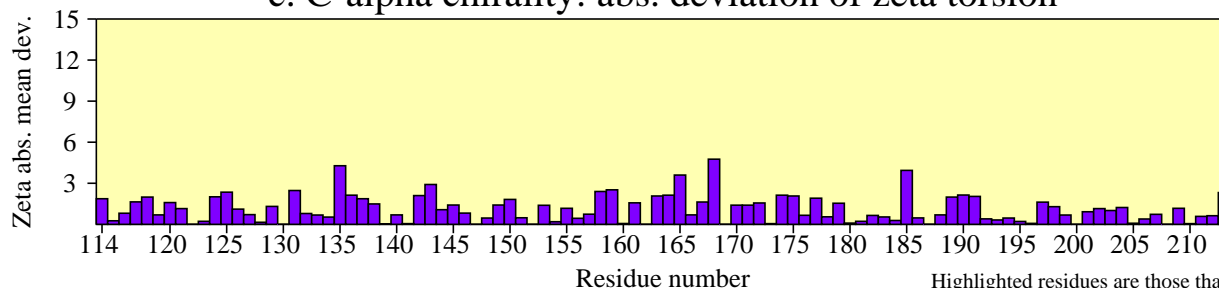
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

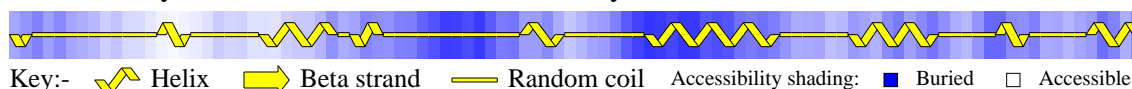


c. C-alpha chirality: abs. deviation of zeta torsion



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

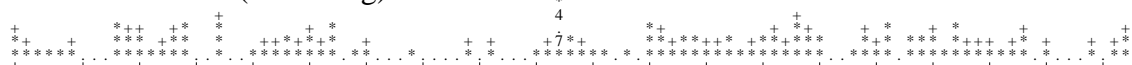
d. Secondary structure & estimated accessibility



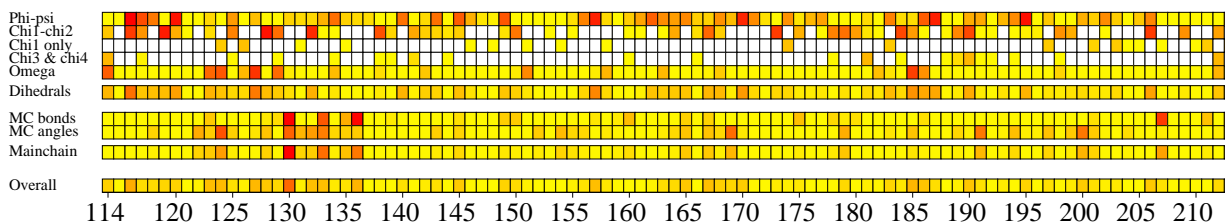
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

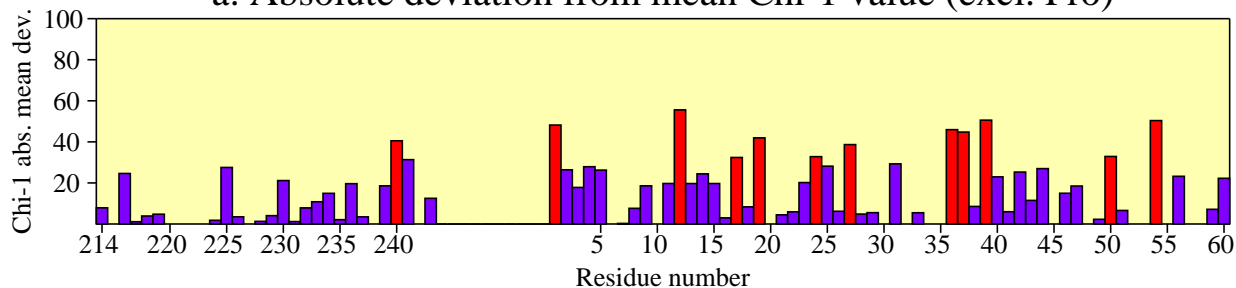


g. G-factors

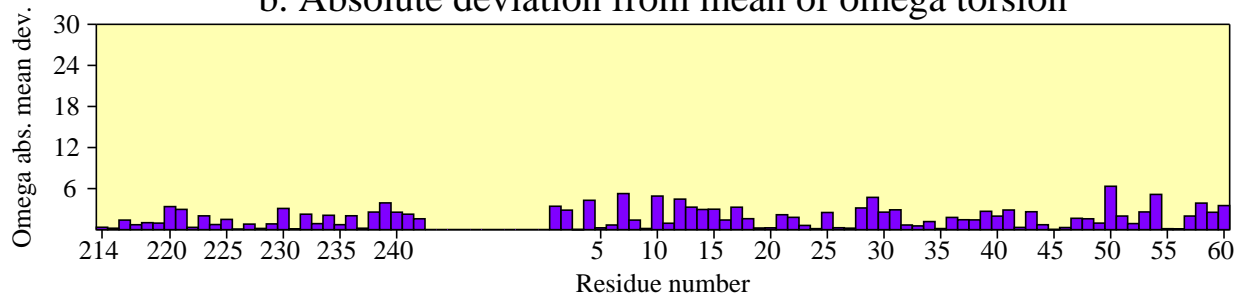


Residue properties pdb2b76

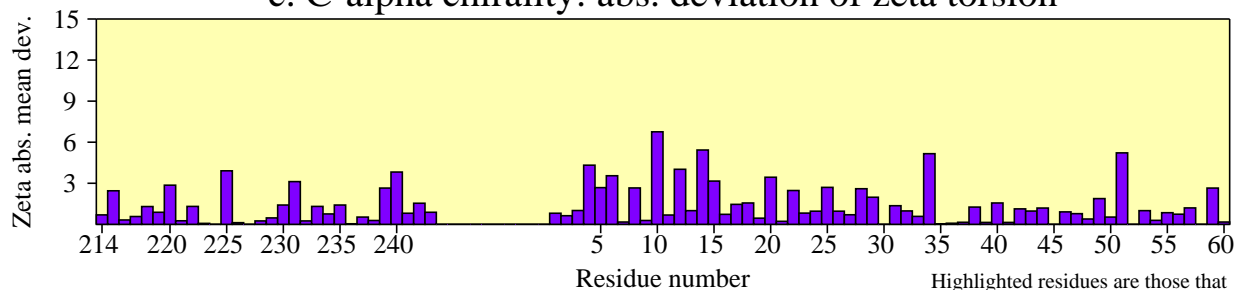
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

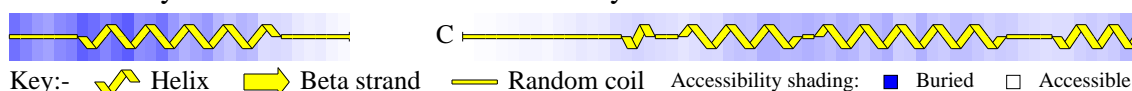


c. C-alpha chirality: abs. deviation of zeta torsion



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

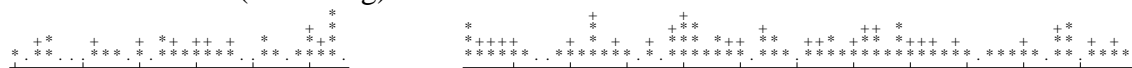
d. Secondary structure & estimated accessibility



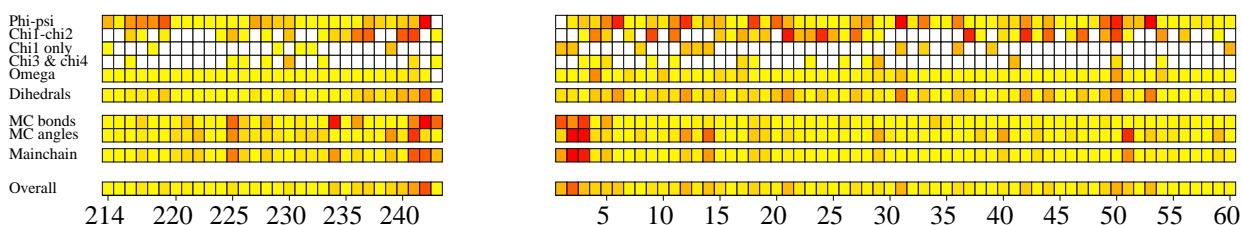
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

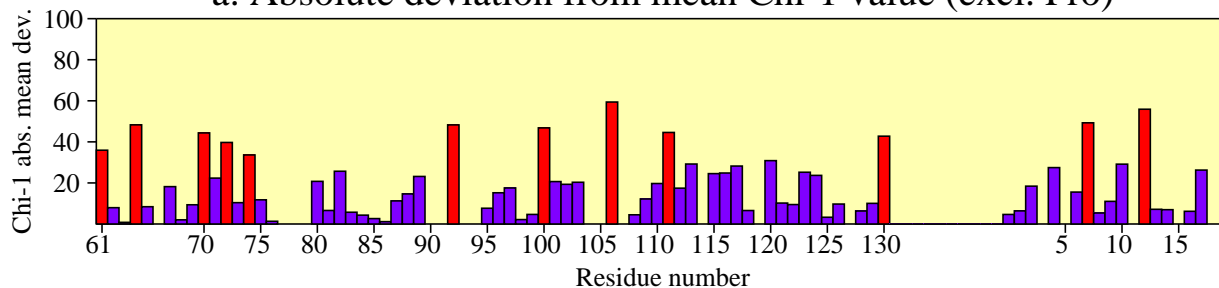


g. G-factors

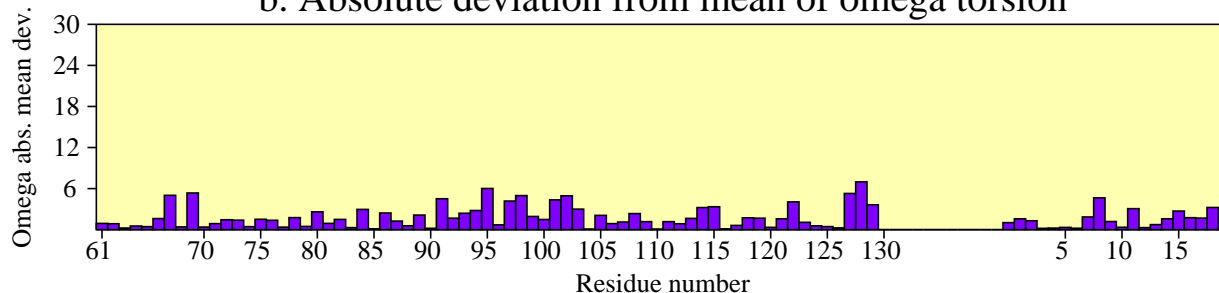


Residue properties pdb2b76

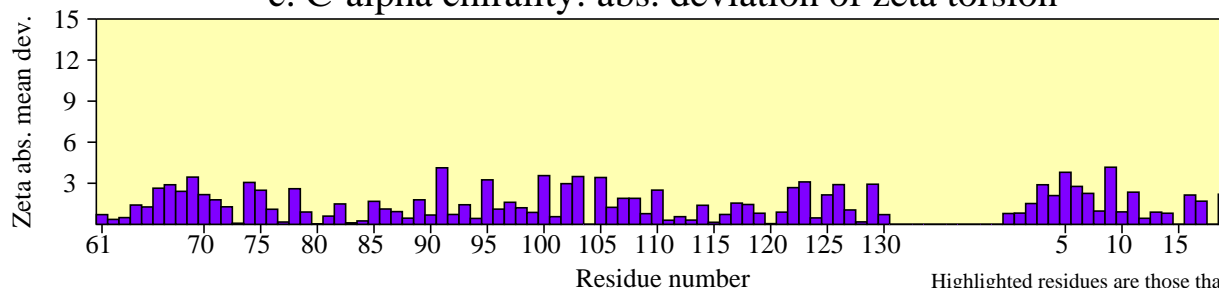
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

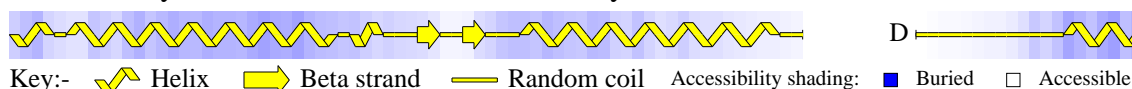


c. C-alpha chirality: abs. deviation of zeta torsion



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

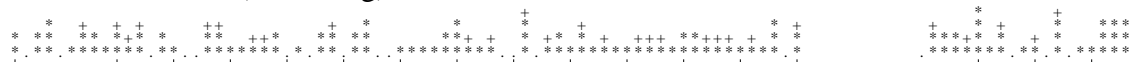
d. Secondary structure & estimated accessibility



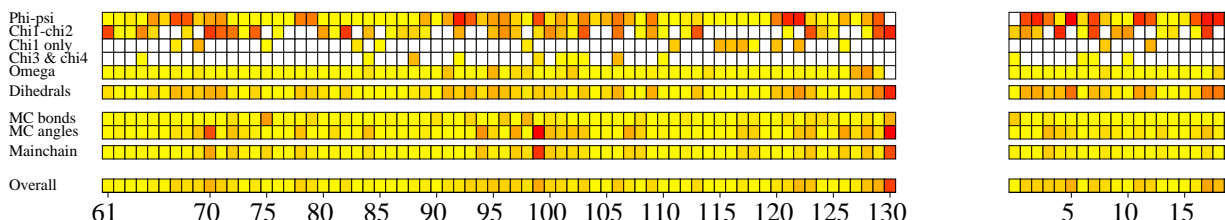
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



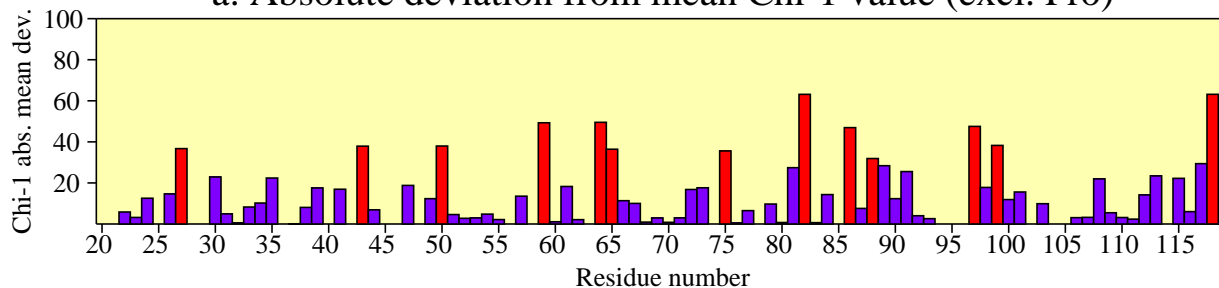
g. G-factors



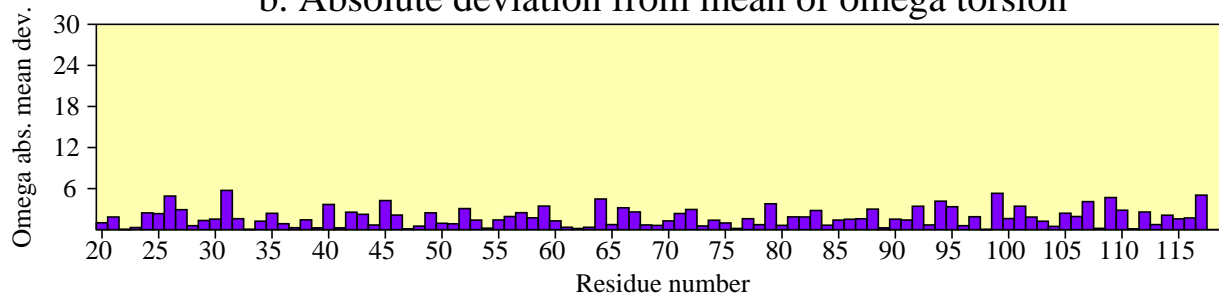
Residue properties

pdb2b76

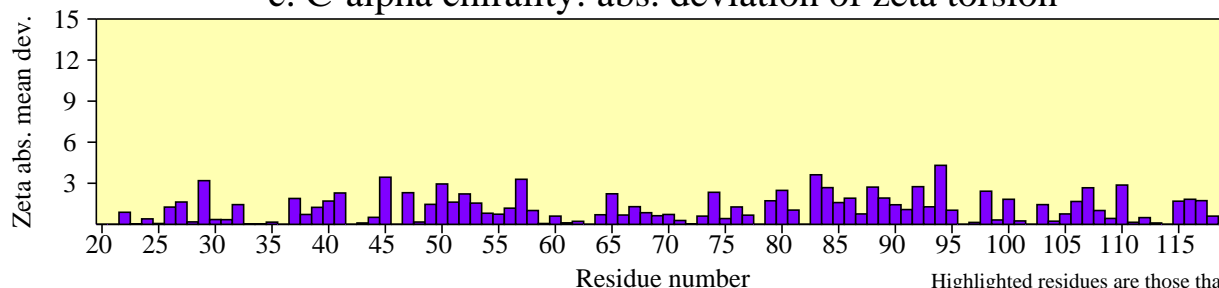
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

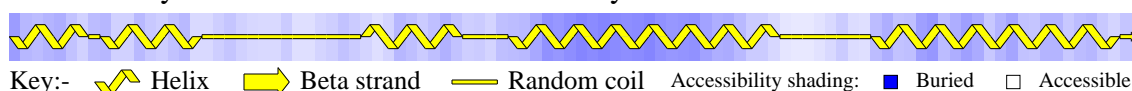


c. C-alpha chirality: abs. deviation of zeta torsion

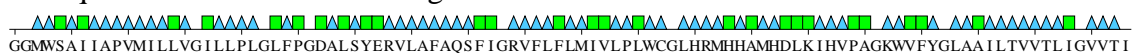


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

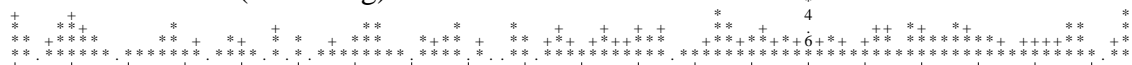
d. Secondary structure & estimated accessibility



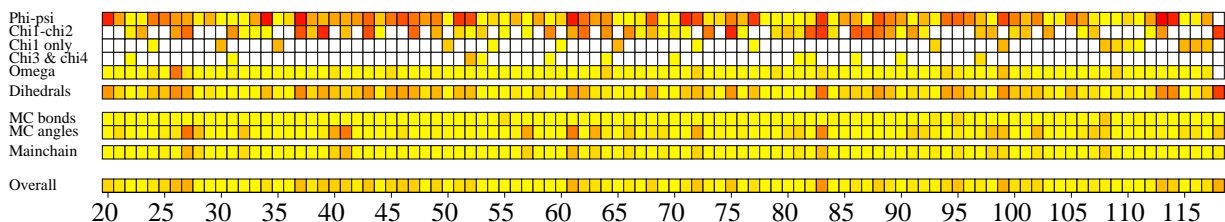
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

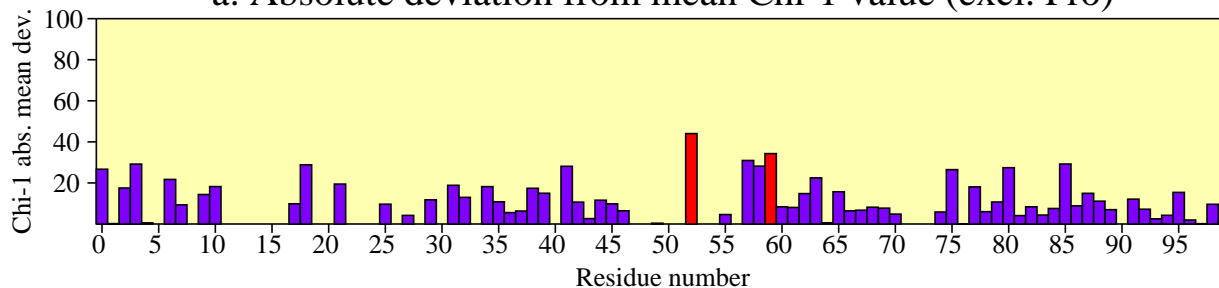


g. G-factors

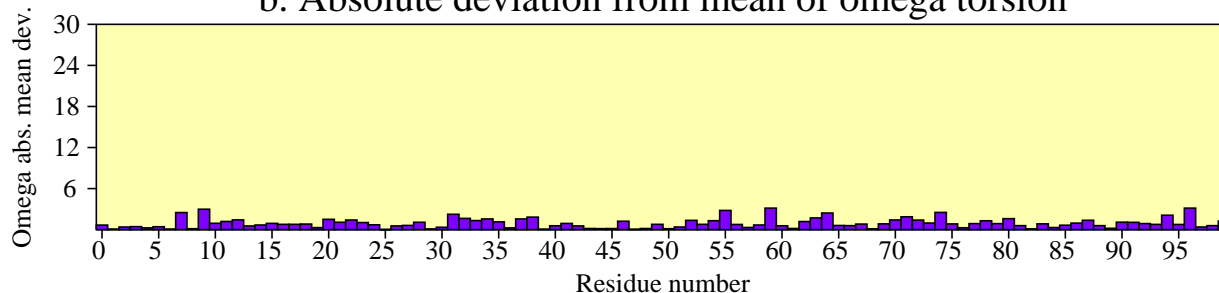


Residue properties pdb2b76

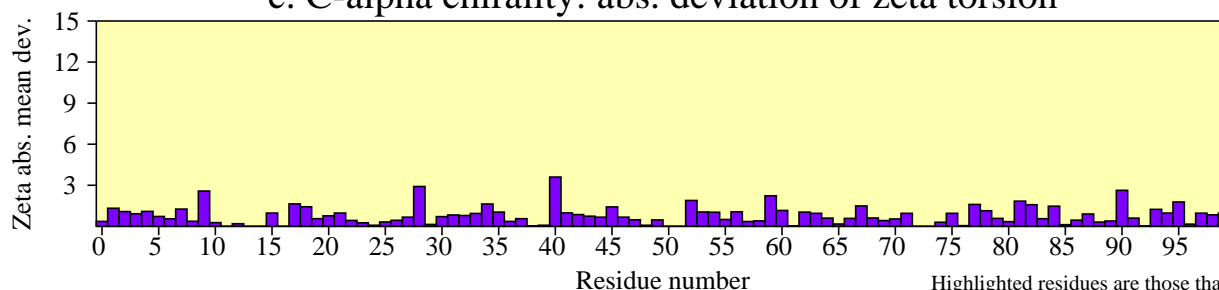
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

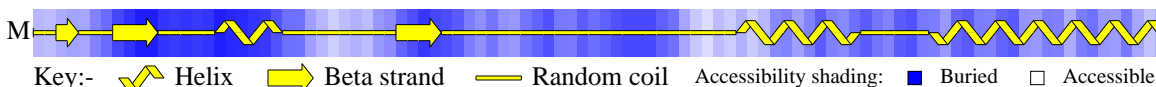


c. C-alpha chirality: abs. deviation of zeta torsion

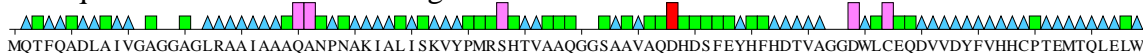


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



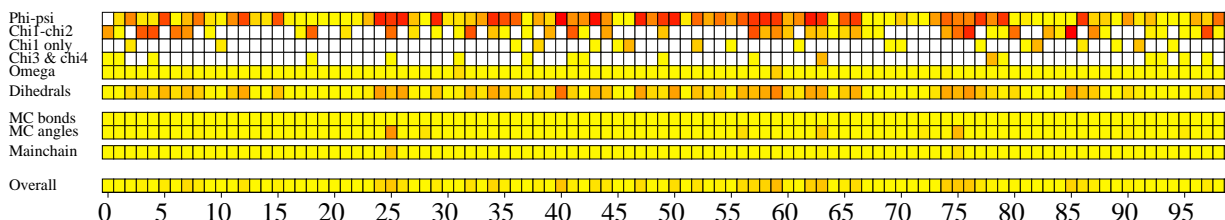
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

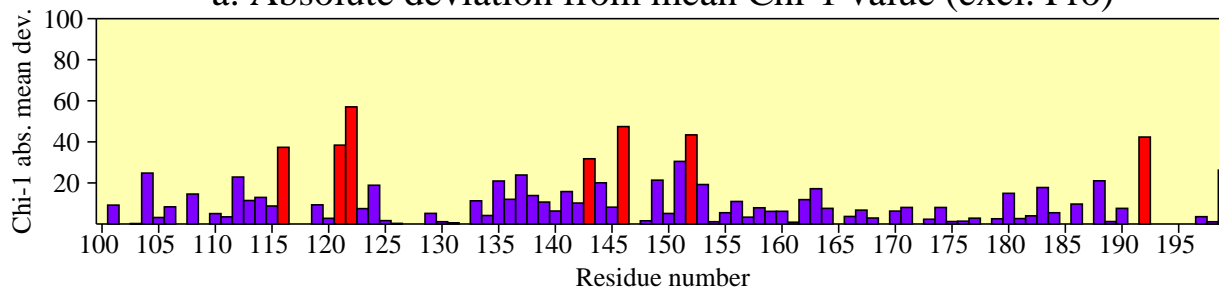


g. G-factors

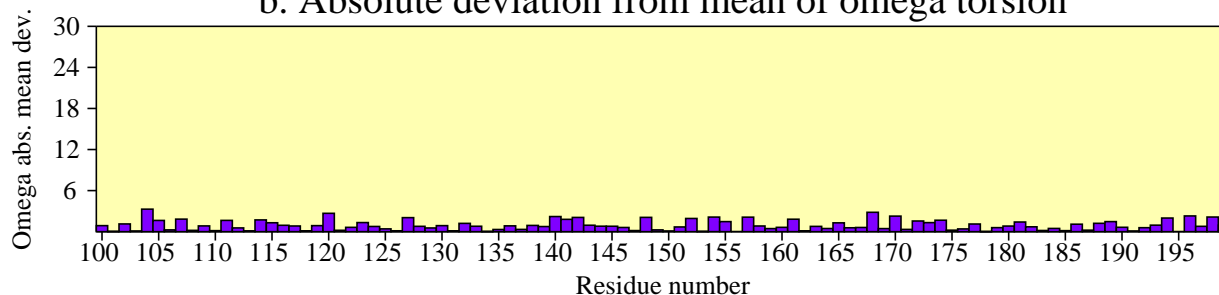


Residue properties pdb2b76

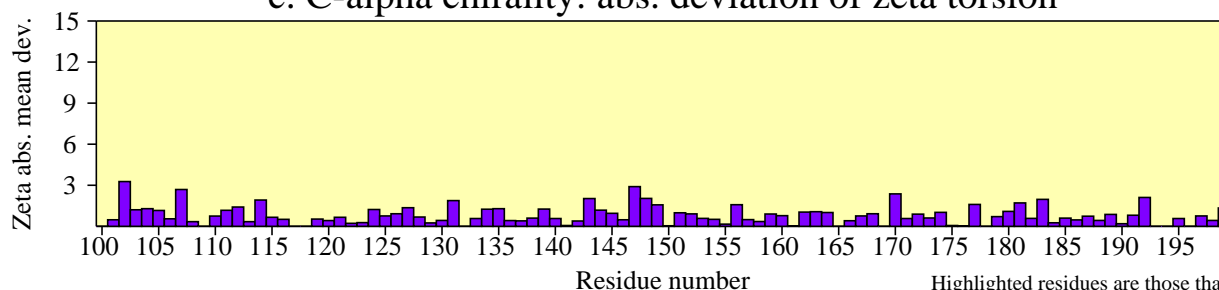
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

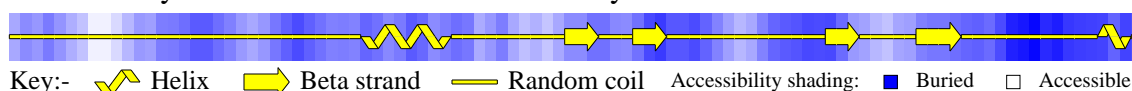


c. C-alpha chirality: abs. deviation of zeta torsion



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

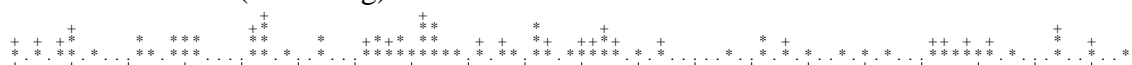
d. Secondary structure & estimated accessibility



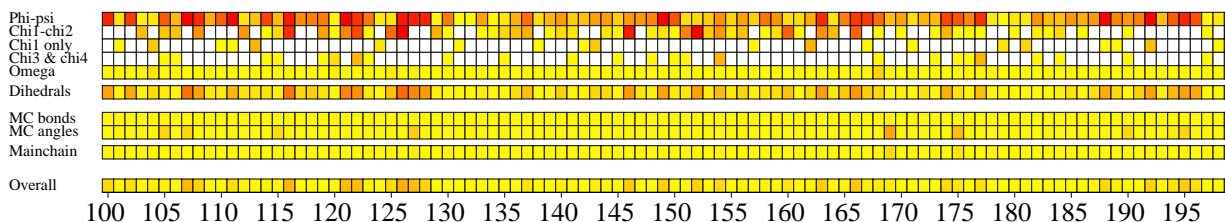
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

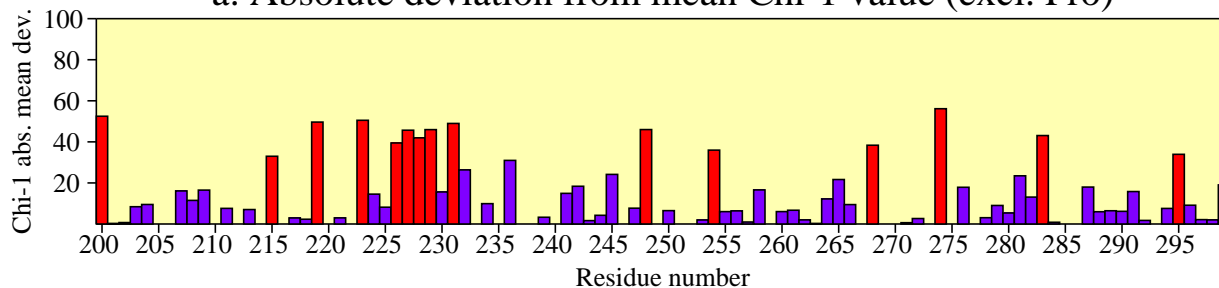


g. G-factors

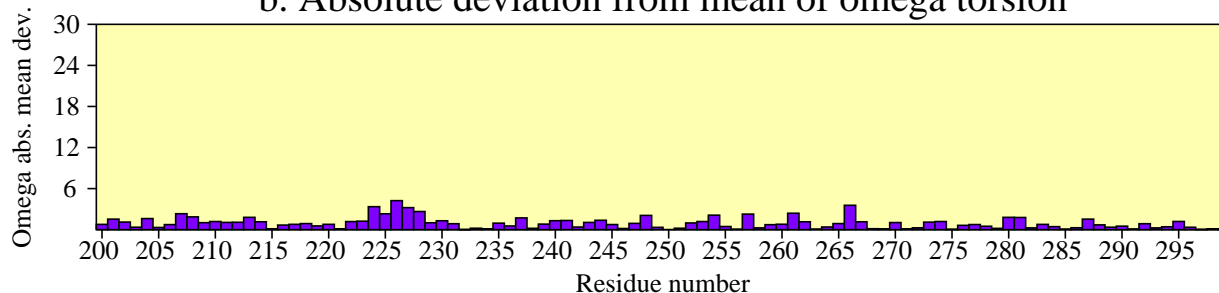


Residue properties pdb2b76

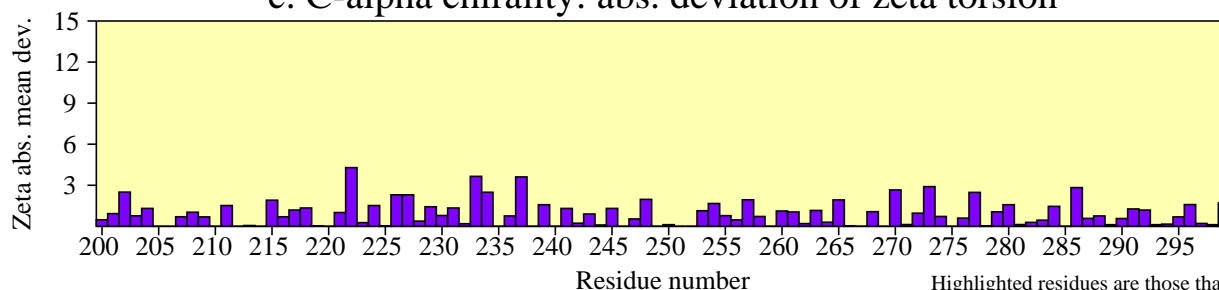
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

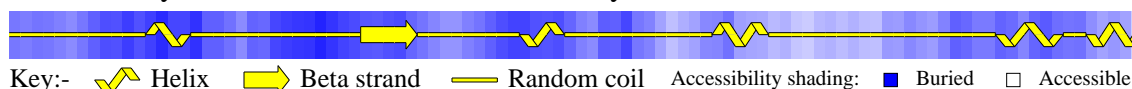


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



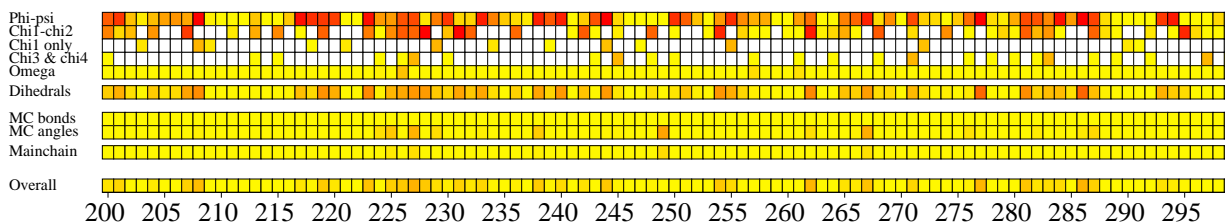
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

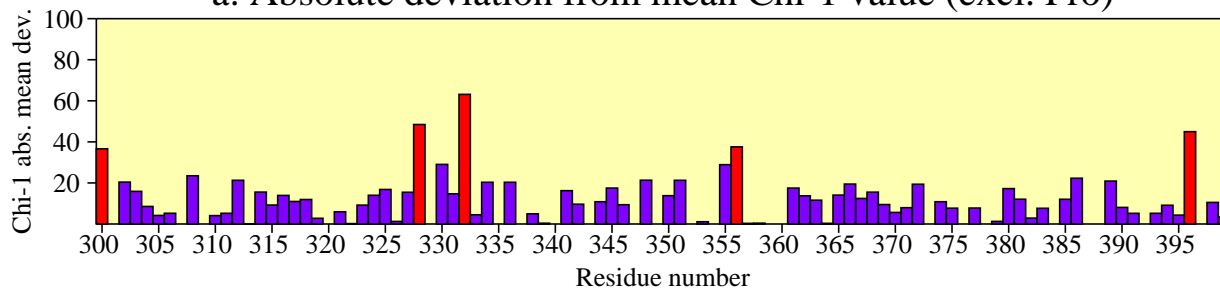


g. G-factors

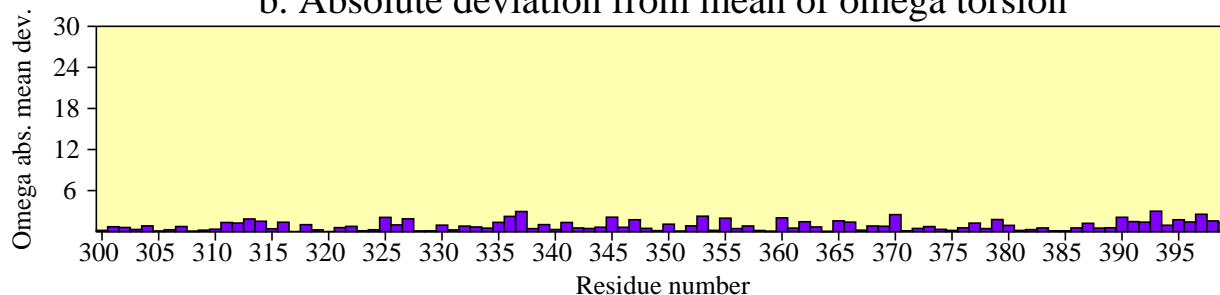


Residue properties pdb2b76

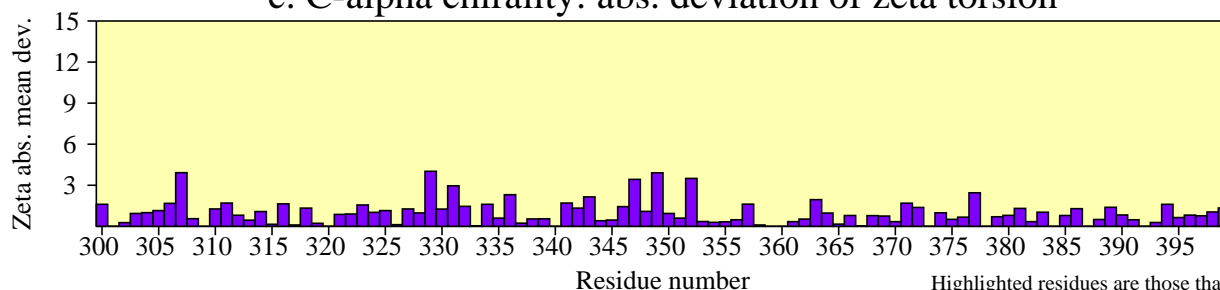
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

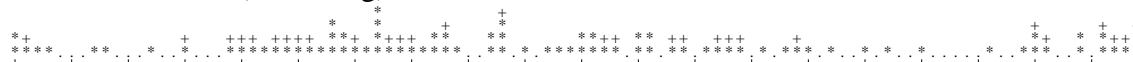
d. Secondary structure & estimated accessibility



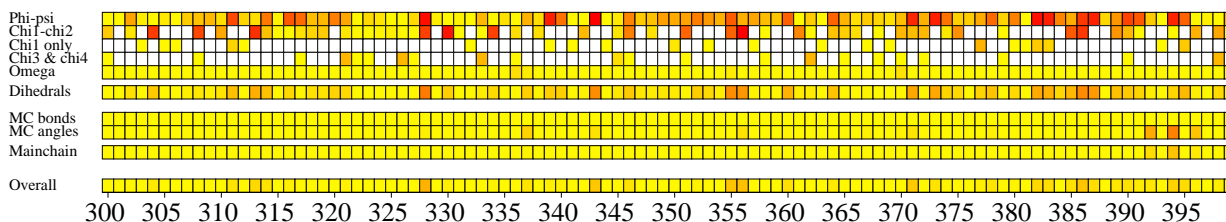
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

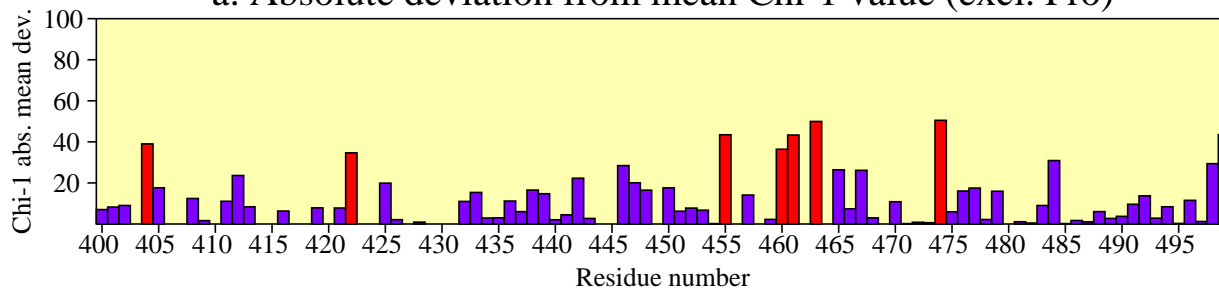


g. G-factors

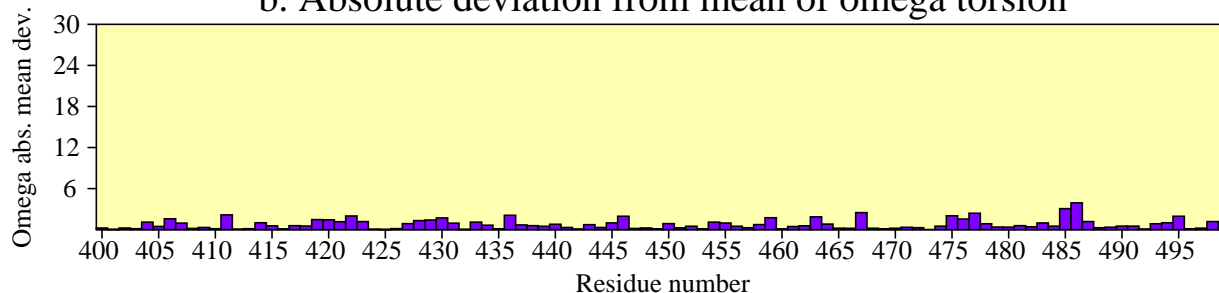


Residue properties pdb2b76

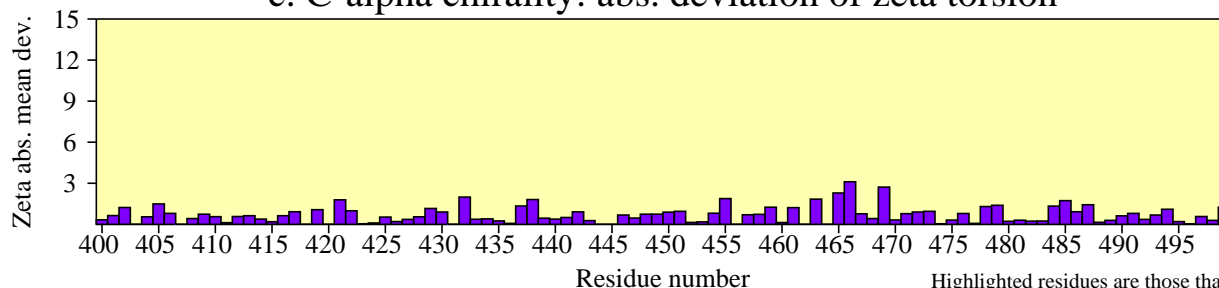
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

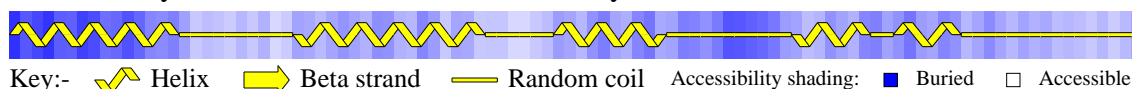


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



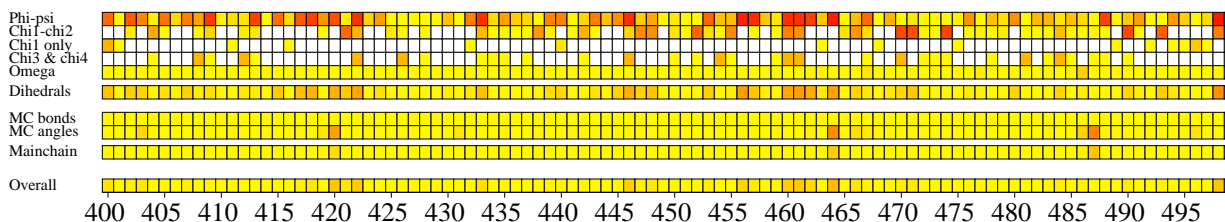
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

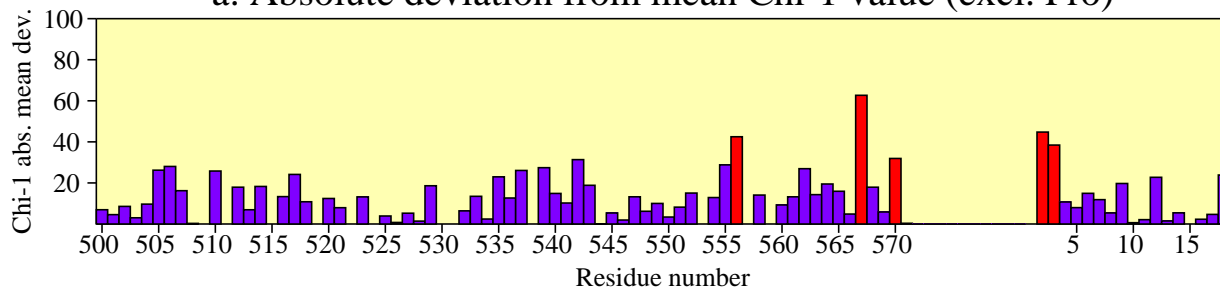


g. G-factors

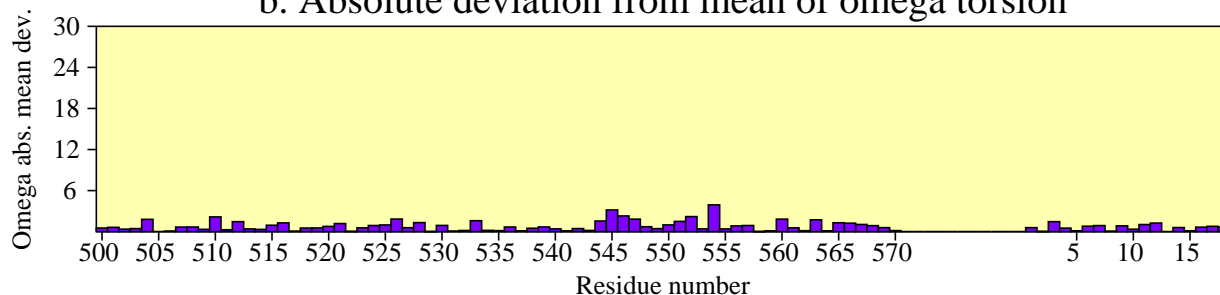


Residue properties pdb2b76

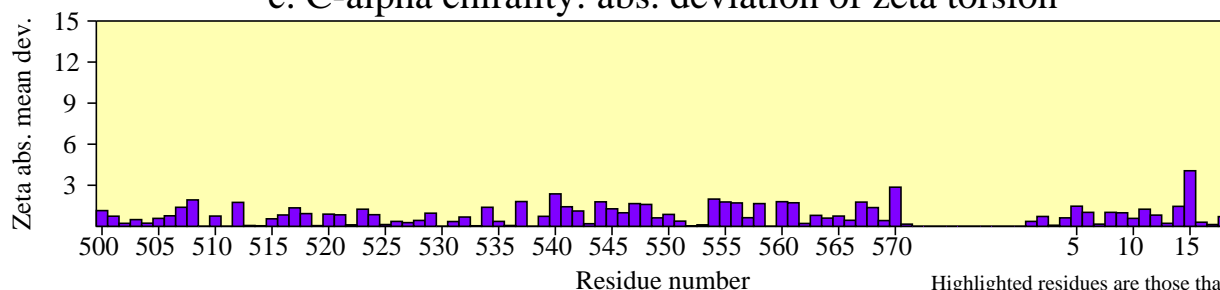
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

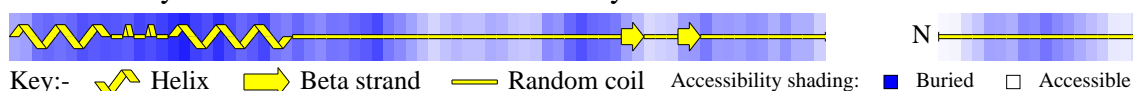


c. C-alpha chirality: abs. deviation of zeta torsion

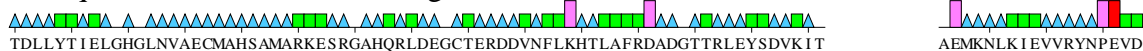


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

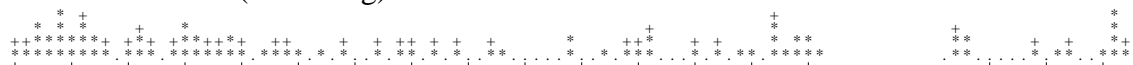
d. Secondary structure & estimated accessibility



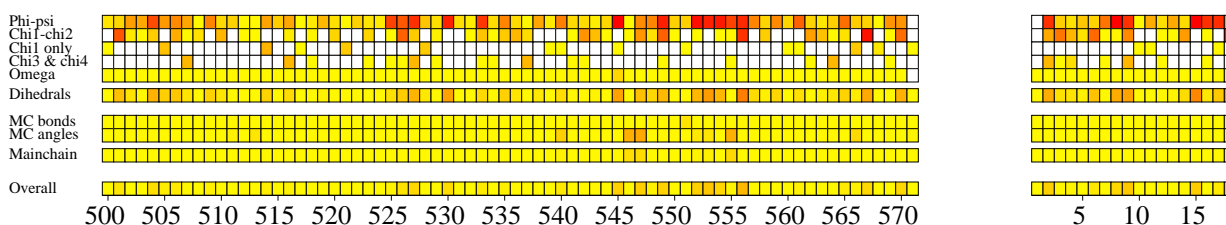
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

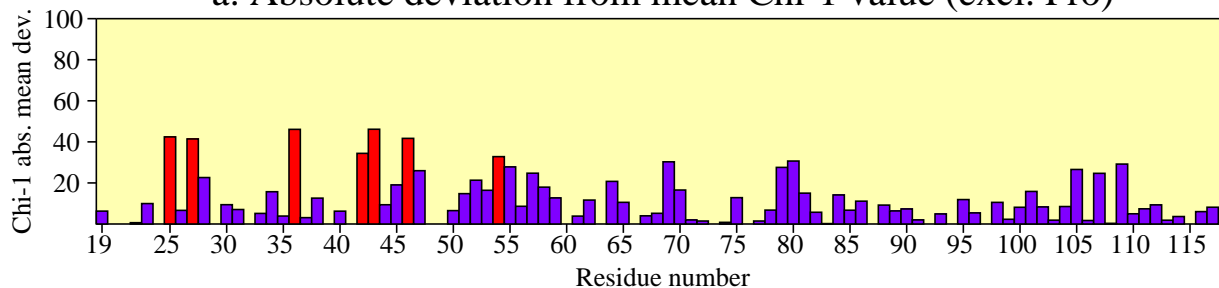


g. G-factors

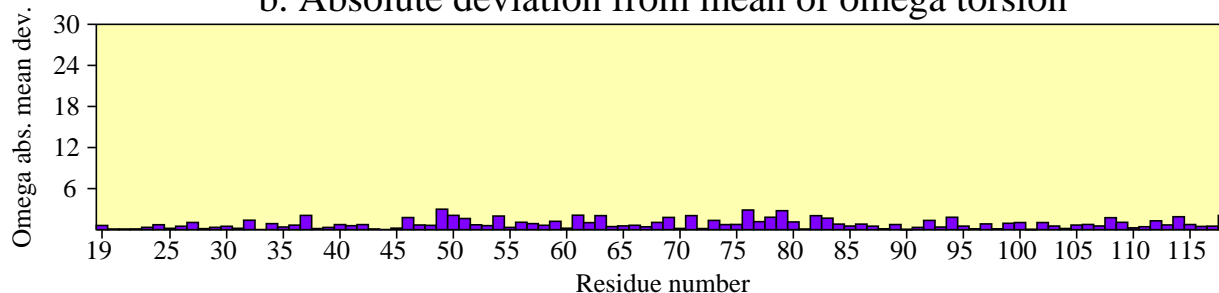


Residue properties pdb2b76

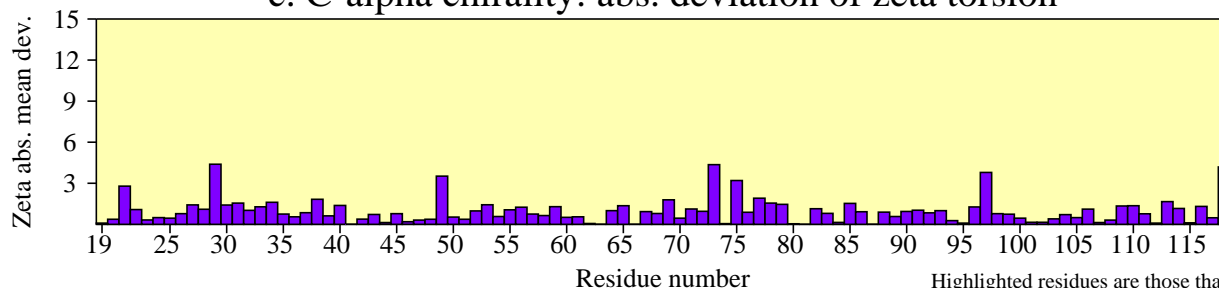
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

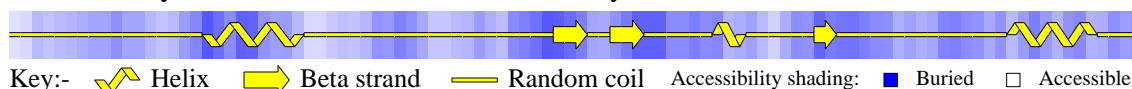


c. C-alpha chirality: abs. deviation of zeta torsion



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

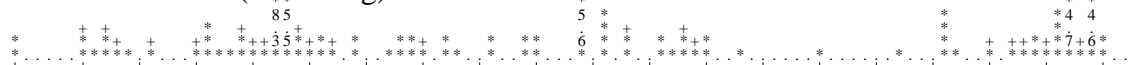
d. Secondary structure & estimated accessibility



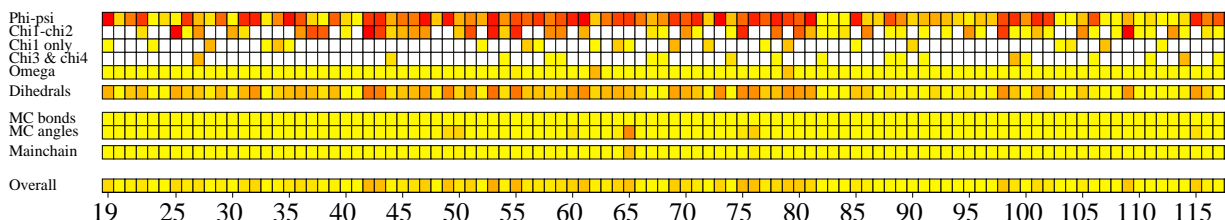
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

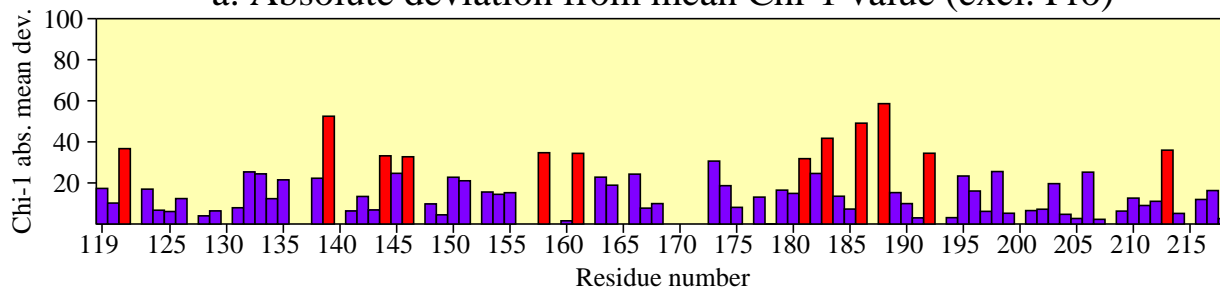


g. G-factors

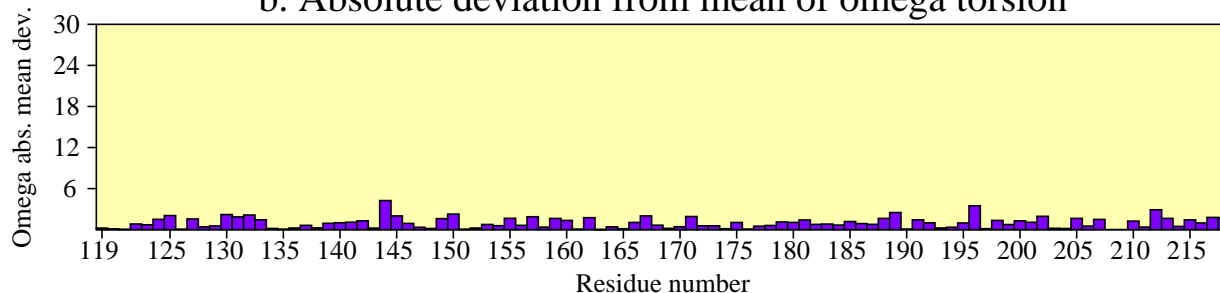


Residue properties pdb2b76

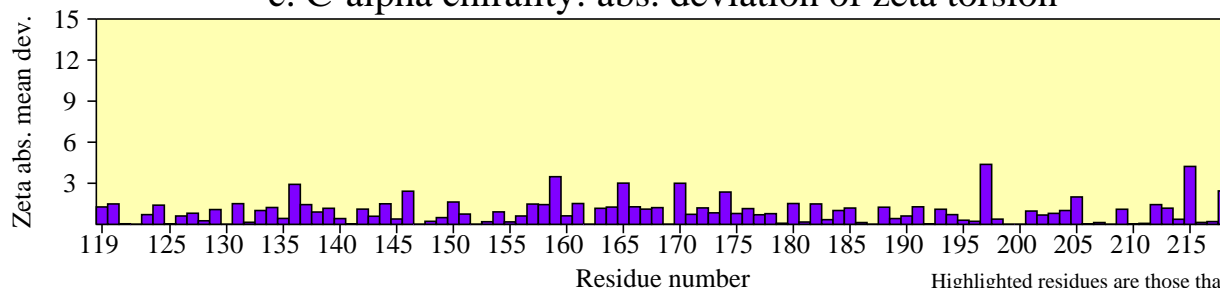
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

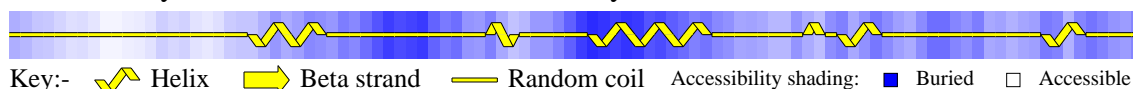


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



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

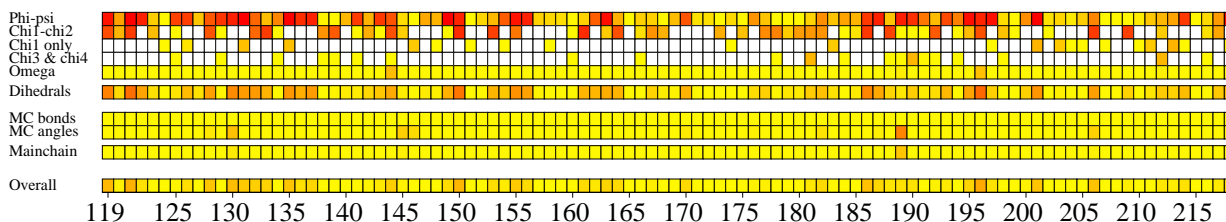
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

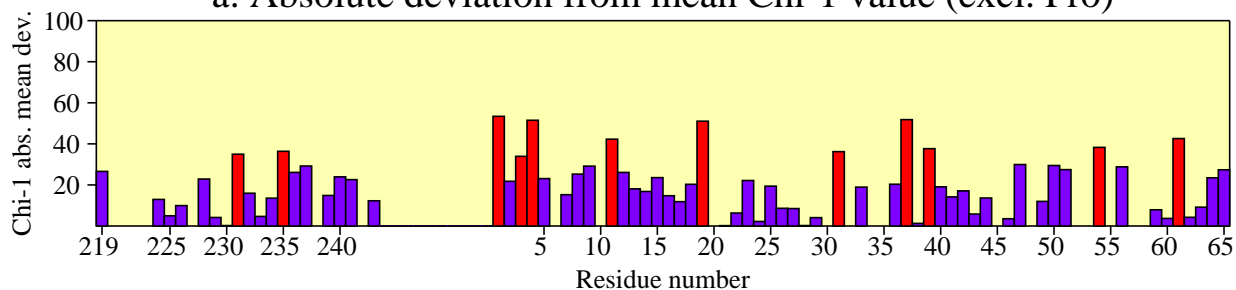


g. G-factors

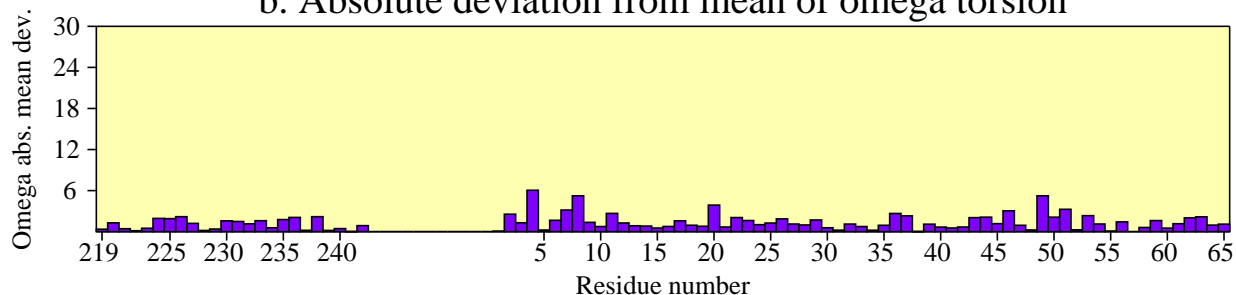


Residue properties pdb2b76

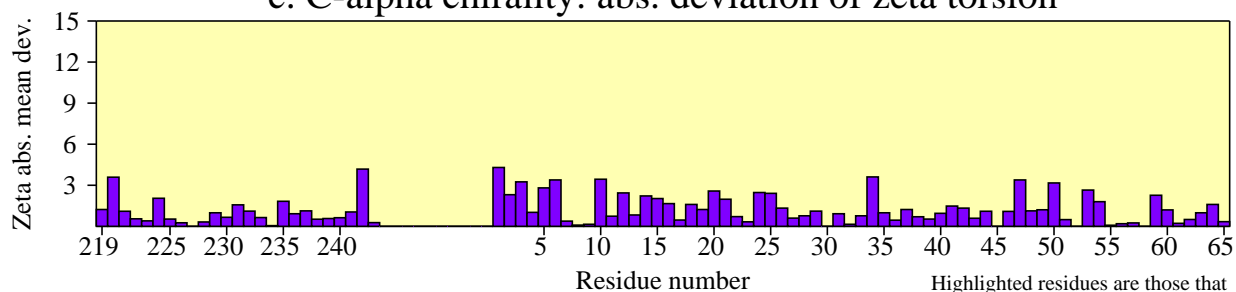
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

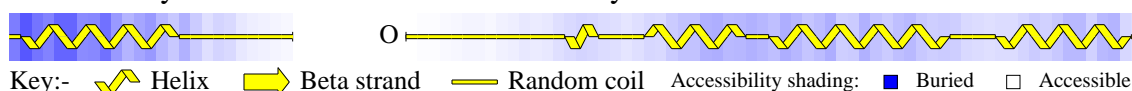


c. C-alpha chirality: abs. deviation of zeta torsion



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

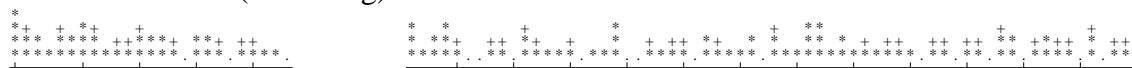
d. Secondary structure & estimated accessibility



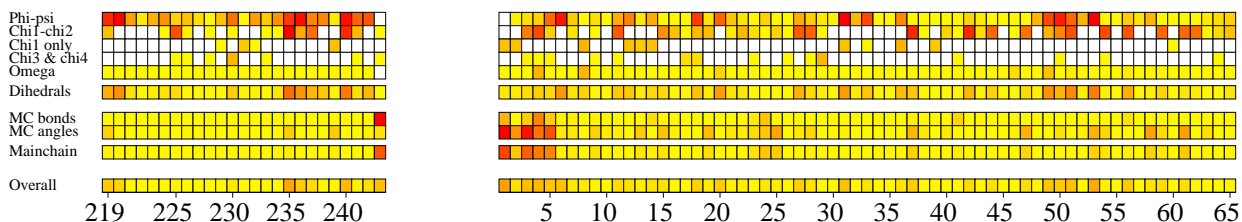
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

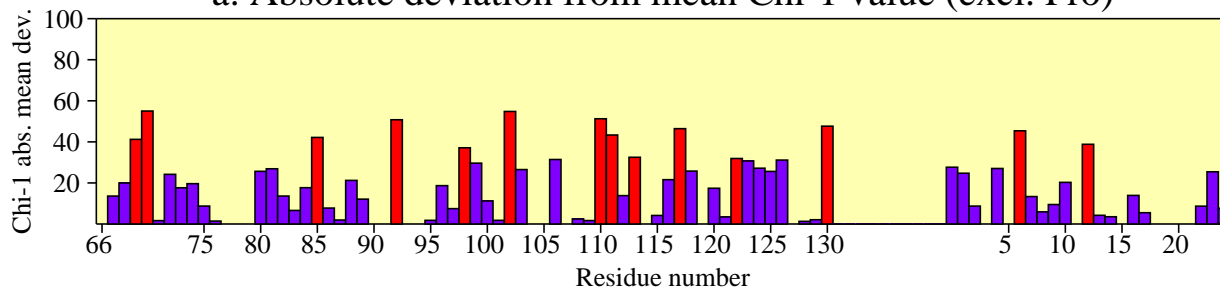


g. G-factors

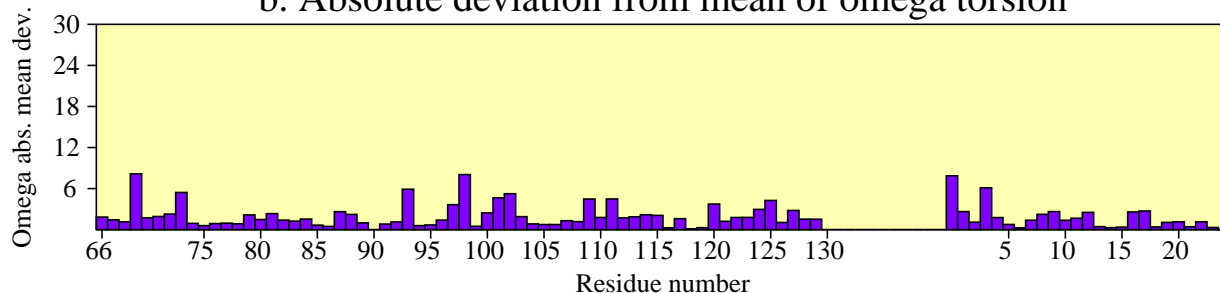


Residue properties pdb2b76

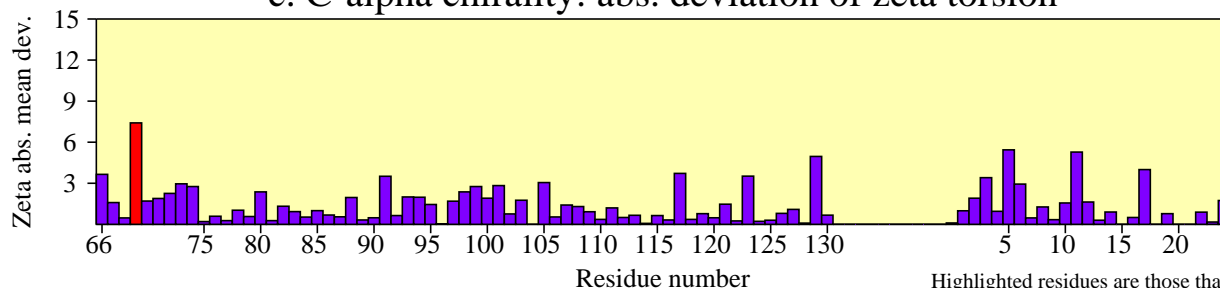
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

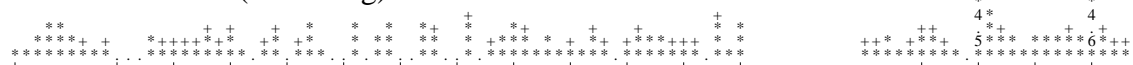
d. Secondary structure & estimated accessibility



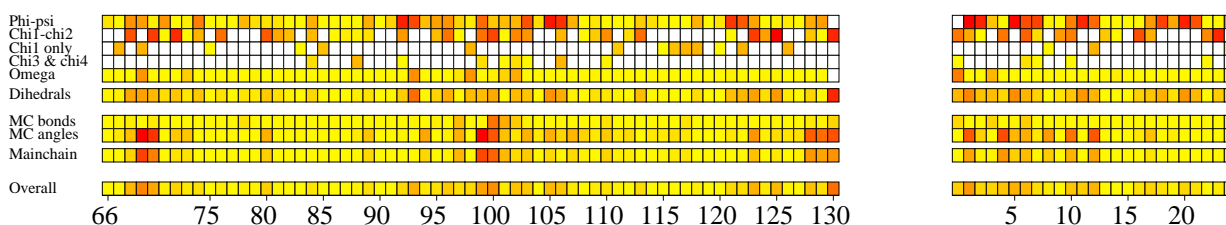
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

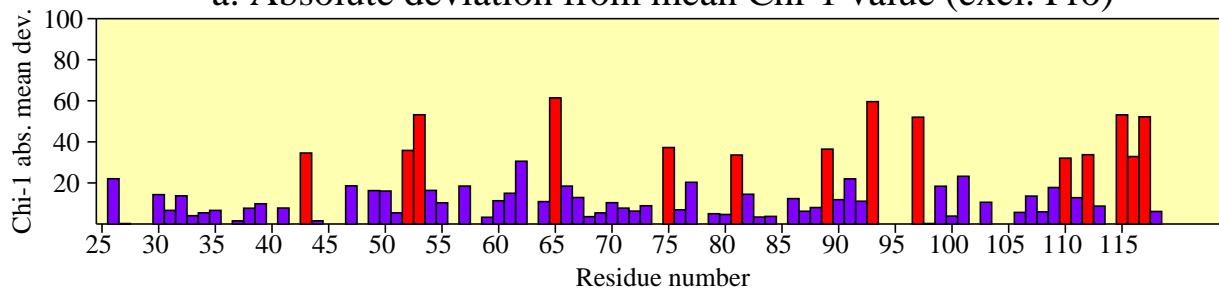


g. G-factors

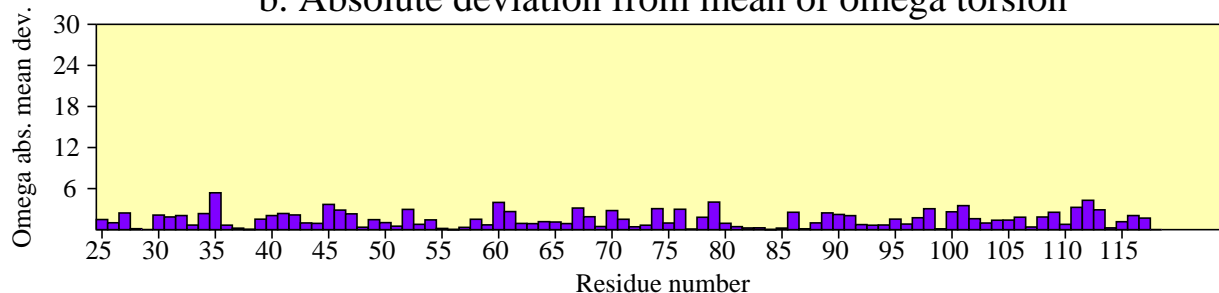


Residue properties pdb2b76

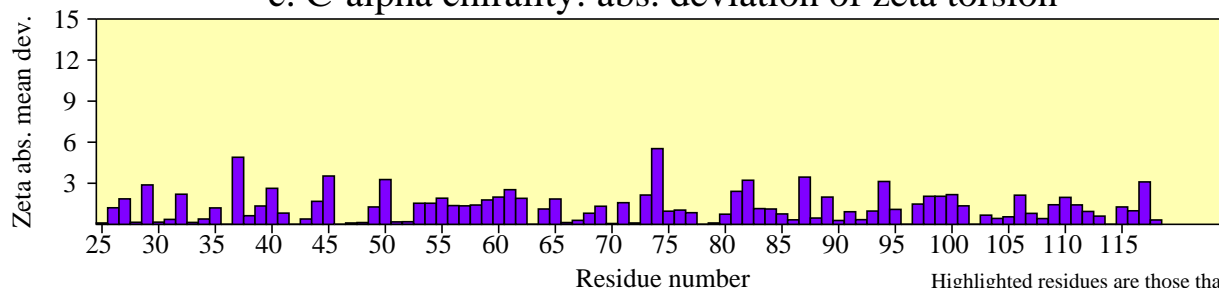
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

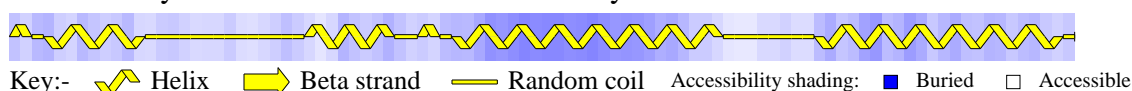


c. C-alpha chirality: abs. deviation of zeta torsion

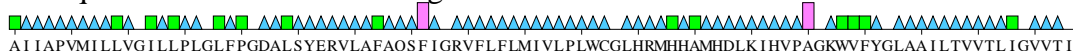


Highlighted residues are those that deviate by more than 2.0 st. dev. from ideal

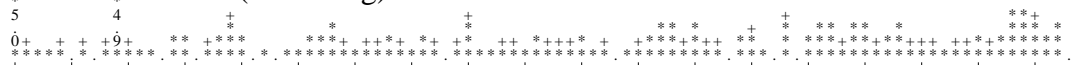
d. Secondary structure & estimated accessibility



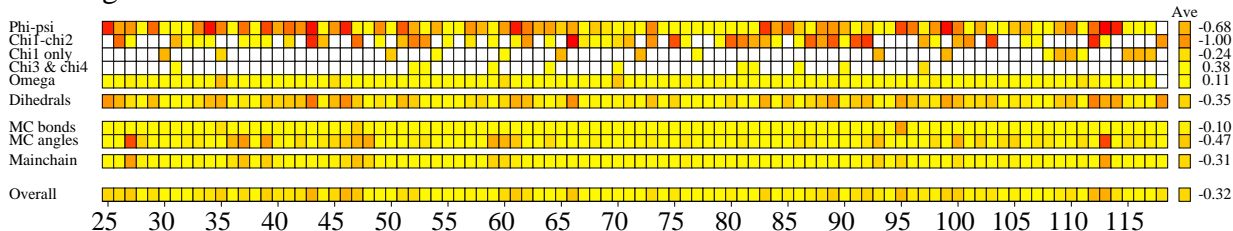
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

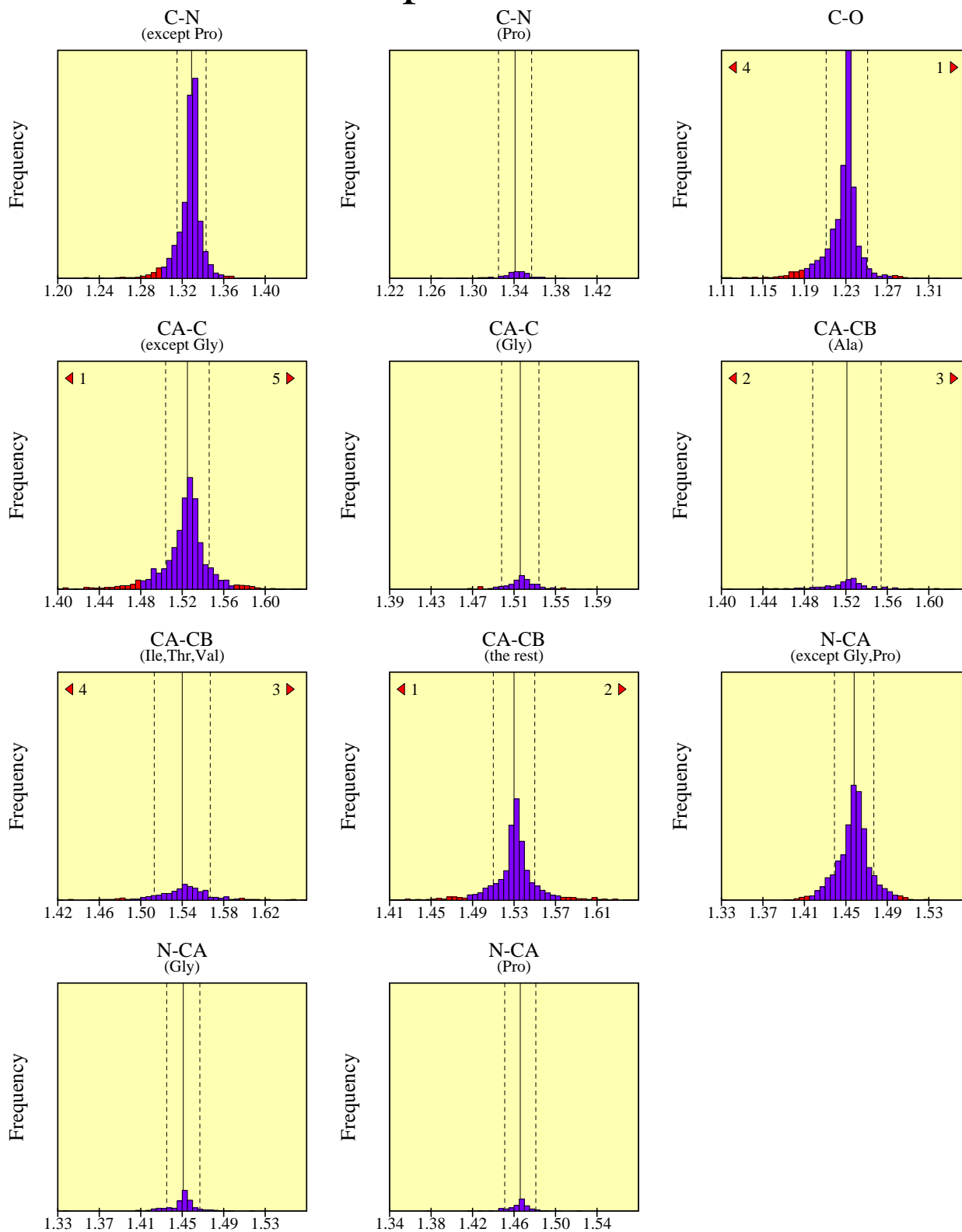


g. G-factors



Main-chain bond lengths

pdb2b76



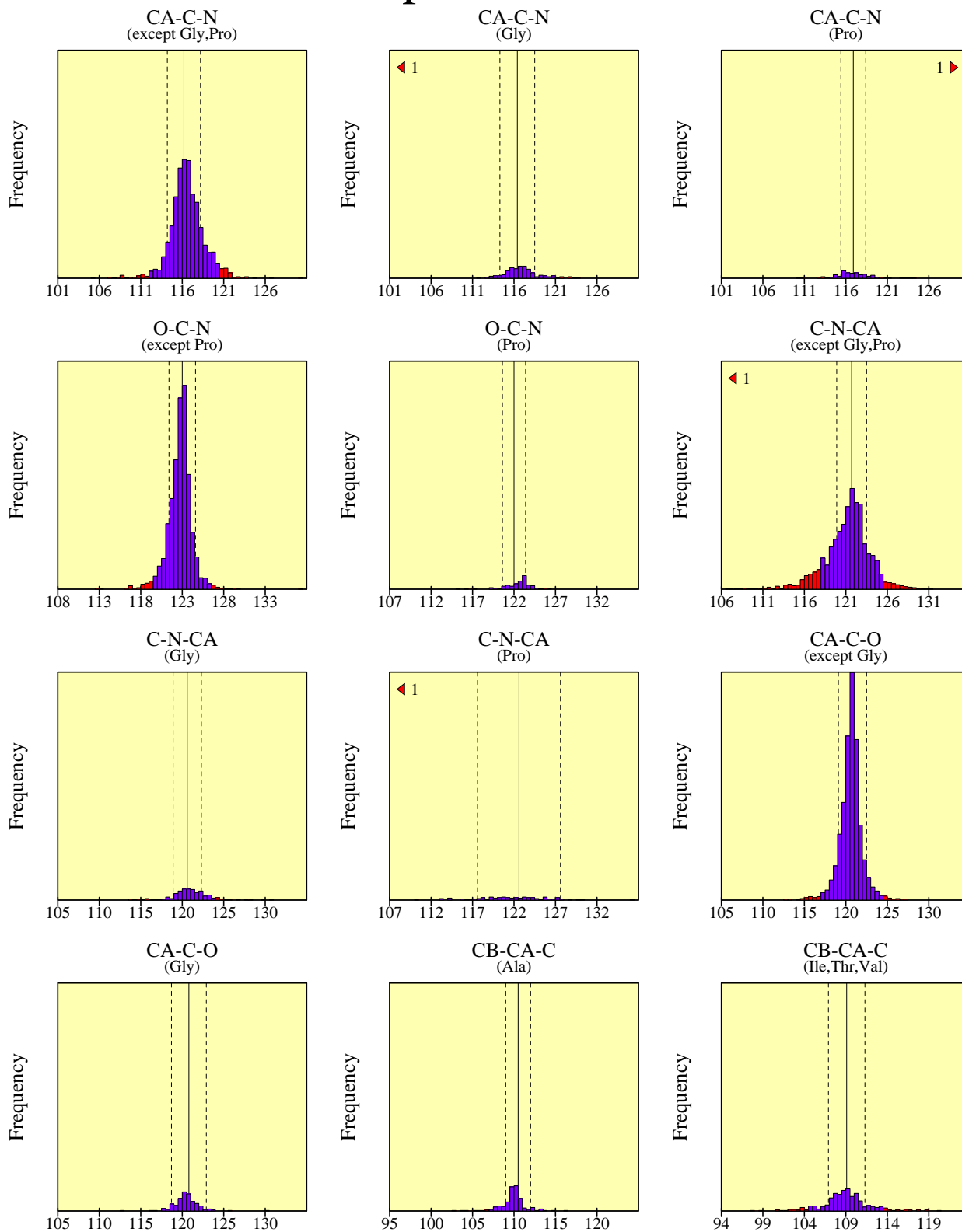
Black bars > 2.0 st. devs. from mean.

◀ 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

pdb2b76



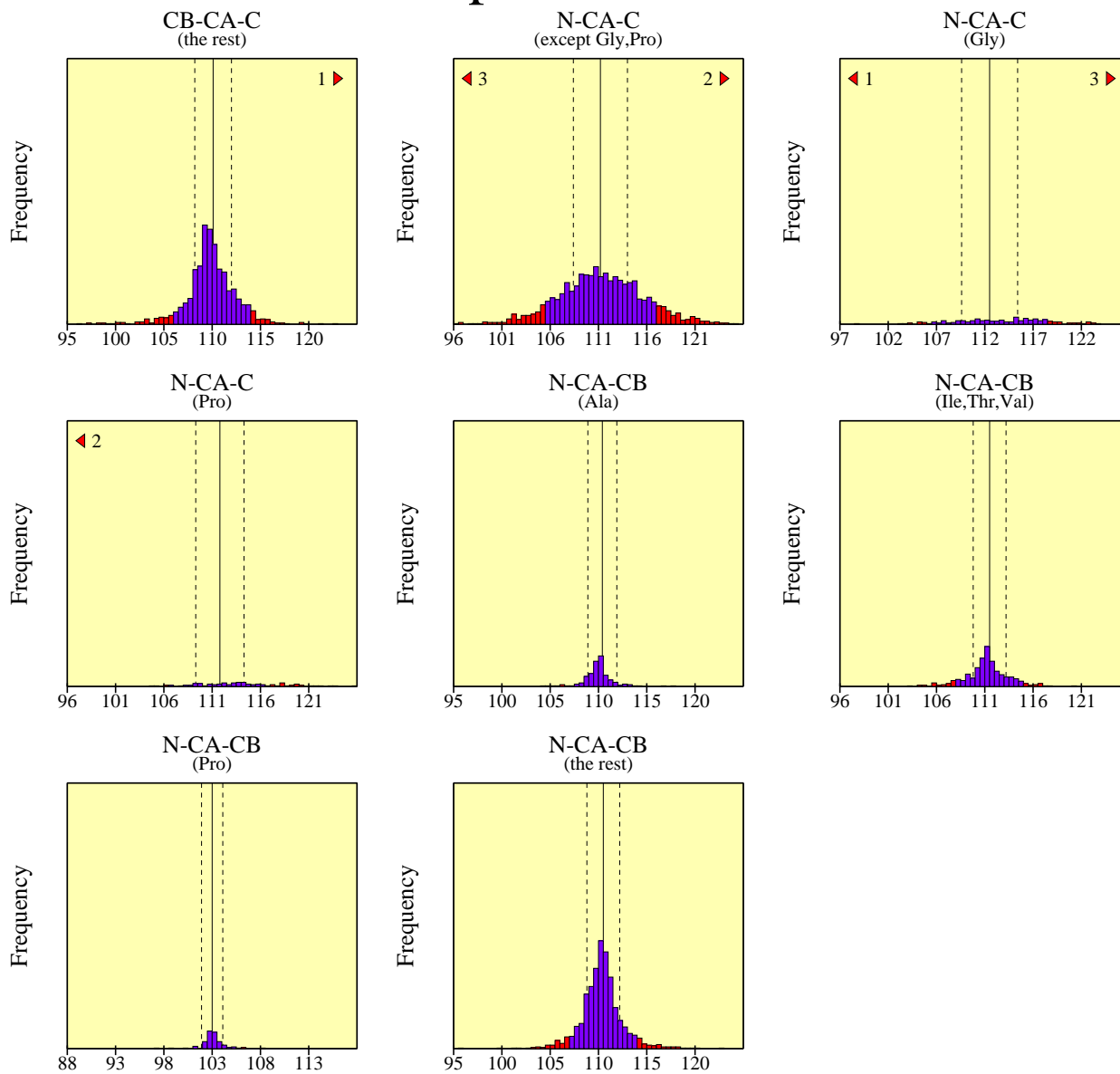
Black bars > 2.0 st. devs. from mean.

◀ 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

pdb2b76



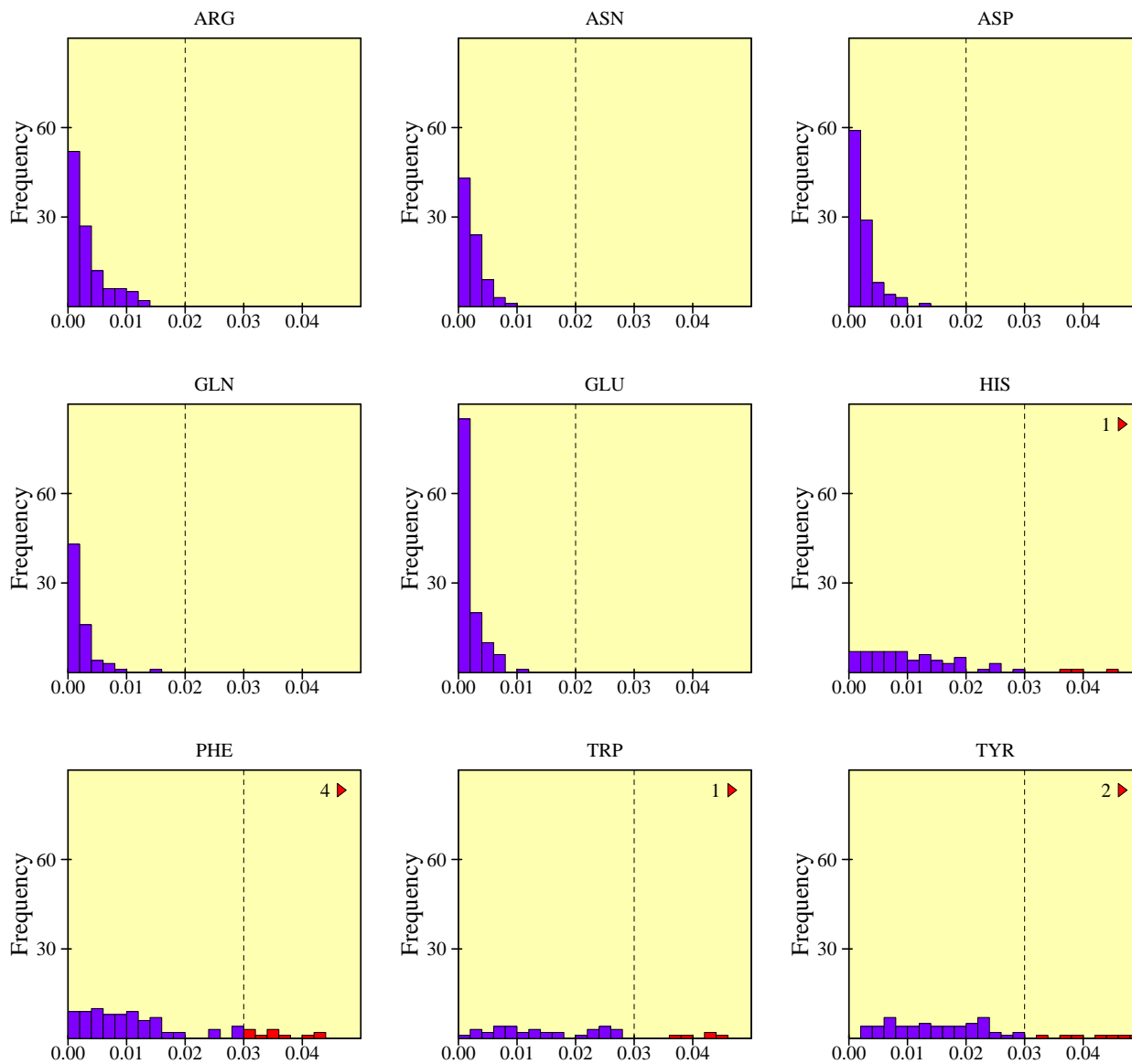
Black bars > 2.0 st. devs. from mean.

◀ 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

pdb2b76



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.

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

Distorted geometry

pdb2b76

Main-chain bond lengths

| | | | | | |
|--|---|---|--|---|---|
| CA 1.530 CB 0.059 1.471 A Met 0 | N 1.458 CA 0.053 1.405 A Ala 5 | CA 1.525 C 0.059 1.584 A Ala 15 | CA 1.521 CB 0.054 1.575 A Ala 15 | CA 1.525 C 0.095 1.430 A Leu 17 | CA 1.530 CB 0.070 1.460 A Leu 17 |
| CA 1.521 CB 0.100 1.621 A Ala 20 | CA 1.521 CB 0.143 1.378 A Ala 22 | CA 1.525 C 0.098 1.427 A Ala 24 | CA 1.521 CB 0.085 1.606 A Ala 24 | CA 1.530 CB 0.063 1.467 A Gln 25 | CA 1.525 C 0.051 1.474 A Asn 27 |
| C 1.341 N 0.072 1.269 A Asn 27 - A Pro 28 | CA 1.525 C 0.116 1.409 A Pro 28 | N 1.466 CA 0.087 1.378 A Pro 28 | CA 1.530 CB 0.067 1.597 A Asn 29 | CA 1.521 CB 0.059 1.581 A Ala 30 | CA 1.525 C 0.054 1.579 A Lys 31 |
| CA 1.530 CB 0.079 1.609 A Lys 31 | CA 1.530 CB 0.059 1.589 A Leu 34 | C 1.231 O 0.099 1.132 A Ile 35 | C 1.329 N 0.069 1.260 A Ile 35 - A Ser 36 | CA 1.525 C 0.068 1.593 A Ser 36 | CA 1.530 CB 0.104 1.426 A Ser 36 |
| CA 1.525 C 0.062 1.463 A Lys 37 | CA 1.540 CB 0.055 1.485 A Val 38 | CA 1.525 C 0.099 1.426 A Tyr 39 | CA 1.525 C 0.056 1.469 A Met 41 | C 1.231 O 0.053 1.178 A Arg 42 | CA 1.525 C 0.063 1.588 A Arg 42 |
| N 1.458 CA 0.053 1.405 A Arg 42 | C 1.231 O 0.053 1.178 A Ser 43 | CA 1.525 C 0.064 1.589 A Ser 43 | CA 1.540 CB 0.060 1.600 A Thr 45 | CA 1.525 C 0.053 1.472 A Ala 48 | CA 1.525 C 0.088 1.437 A Ala 53 |
| CA 1.521 CB 0.072 1.449 A Ala 53 | CA 1.521 CB 0.072 1.593 A Ala 54 | CA 1.525 C 0.063 1.462 A Val 55 | CA 1.525 C 0.058 1.467 A Asp 58 | CA 1.530 CB 0.068 1.462 A Asp 58 | CA 1.525 C 0.063 1.462 A His 59 |
| C 1.329 N 0.060 1.269 A His 59 - A Asp 60 | CA 1.530 CB 0.091 1.439 A Ser 61 | C 1.231 O 0.145 1.086 A Glu 63 | CA 1.530 CB 0.062 1.468 A Glu 63 | CA 1.530 CB 0.055 1.585 A Tyr 64 | C 1.231 O 0.059 1.172 A His 65 |
| CA 1.525 C 0.057 1.468 A His 65 | CA 1.525 C 0.052 1.473 A Phe 66 | CA 1.525 C 0.055 1.470 A His 67 | CA 1.530 CB 0.083 1.447 A His 67 | N 1.458 CA 0.054 1.404 A His 67 | N 1.458 CA 0.052 1.510 A Asp 68 |
| C 1.231 O 0.064 1.167 A Ala 71 | CA 1.525 C 0.077 1.448 A Leu 76 | CA 1.525 C 0.054 1.471 A Gln 79 | C 1.231 O 0.052 1.179 A Val 82 | CA 1.525 C 0.066 1.459 A Val 82 | CA 1.530 CB 0.089 1.619 A Tyr 84 |
| C 1.231 O 0.056 1.175 A Phe 85 | CA 1.525 C 0.057 1.468 A Phe 85 | CA 1.530 CB 0.053 1.477 A His 87 | CA 1.525 C 0.053 1.578 A Cys 89 | CA 1.530 CB 0.099 1.629 A Cys 89 | CA 1.525 C 0.117 1.408 A Pro 90 |

Distorted geometry

pdb2b76

Main-chain bond lengths (contd)

| | | | | | |
|--|--|--|--|--|--|
| CA 1.530 CB 0.135 1.395 A Pro 90 | CA 1.540 CB 0.103 1.643 A Thr 91 | CA 1.525 C 0.064 1.589 A Thr 94 | C 1.231 O 0.051 1.180 A Gln 95 | CA 1.525 C 0.063 1.462 A Gln 95 | C 1.231 O 0.052 1.179 A Glu 97 |
| CA 1.525 C 0.057 1.582 A Leu 98 | C 1.231 O 0.072 1.158 A Gly 100 | C 1.329 N 0.063 1.266 A Gly 100 - A Cys 101 | CA 1.525 C 0.053 1.472 A Trp 103 | CA 1.530 CB 0.058 1.588 A Arg 105 | CA 1.525 C 0.056 1.581 A Pro 107 |
| CA 1.530 CB 0.075 1.455 A Ser 110 | CA 1.525 C 0.082 1.607 A Val 113 | CA 1.540 CB 0.069 1.471 A Val 113 | C 1.231 O 0.067 1.164 A Arg 114 | CA 1.525 C 0.155 1.680 A Met 119 | N 1.458 CA 0.067 1.525 A Met 119 |
| C 1.329 N 0.064 1.393 A Met 119 - A Lys 120 | CA 1.530 CB 0.085 1.615 A Lys 120 | N 1.458 CA 0.073 1.531 A Lys 120 | N 1.458 CA 0.054 1.404 A Trp 125 | CA 1.530 CB 0.058 1.472 A Phe 133 | CA 1.530 CB 0.066 1.596 A His 134 |
| C 1.231 O 0.054 1.177 A Met 135 | CA 1.525 C 0.081 1.444 A Met 135 | C 1.231 O 0.098 1.133 A Leu 136 | CA 1.525 C 0.080 1.445 A Leu 136 | CA 1.530 CB 0.078 1.452 A Leu 136 | C 1.231 O 0.083 1.148 A Thr 138 |
| CA 1.540 CB 0.141 1.681 A Thr 138 | CA 1.525 C 0.058 1.583 A Gln 141 | CA 1.530 CB 0.079 1.609 A Gln 141 | CA 1.530 CB 0.066 1.464 A Ser 143 | C 1.231 O 0.122 1.109 A Gln 145 | CA 1.525 C 0.066 1.459 A Phe 146 |
| CA 1.525 C 0.061 1.464 A Ile 149 | CA 1.540 CB 0.064 1.476 A Ile 149 | C 1.231 O 0.050 1.181 A Phe 156 | N 1.458 CA 0.050 1.508 A Val 157 | CA 1.525 C 0.070 1.595 A Ile 160 | CA 1.540 CB 0.054 1.594 A Ile 160 |
| CA 1.525 C 0.056 1.581 A Asp 164 | N 1.458 CA 0.060 1.398 A Asp 164 | CA 1.525 C 0.085 1.440 A Val 167 | CA 1.540 CB 0.079 1.461 A Val 171 | CA 1.521 CB 0.132 1.389 A Ala 172 | CA 1.525 C 0.066 1.591 A Asn 174 |
| CA 1.530 CB 0.050 1.580 A Glu 177 | CA 1.525 C 0.064 1.589 A Val 181 | CA 1.525 C 0.066 1.459 A Ile 183 | CA 1.540 CB 0.117 1.657 A Ile 183 | CA 1.525 C 0.076 1.449 A Ala 185 | N 1.458 CA 0.053 1.511 A Ala 185 |
| CA 1.525 C 0.082 1.443 A Asn 186 | CA 1.540 CB 0.080 1.620 A Val 188 | CA 1.540 CB 0.064 1.604 A Val 189 | C 1.231 O 0.080 1.151 A Thr 192 | CA 1.525 C 0.118 1.407 A Thr 192 | CA 1.525 C 0.092 1.617 A Ala 195 |
| N 1.458 CA 0.071 1.529 A Ala 195 | CA 1.525 C 0.079 1.446 A Arg 197 | N 1.458 CA 0.051 1.407 A Val 198 | CA 1.530 CB 0.059 1.471 A Arg 200 | CA 1.525 C 0.053 1.578 A Tyr 201 | CA 1.530 CB 0.072 1.458 A Asn 202 |

Distorted geometry

pdb2b76

Main-chain bond lengths (contd)

| | | | | | |
|--|--|--|--|--|--|
| C 1.231 O 0.051 1.180 A Gly 205 | C 1.231 O 0.063 1.168 A Ile 207 | CA 1.525 C 0.064 1.461 A Ile 207 | C 1.329 N 0.053 1.382 A Thr 209 - A Gly 210 | C 1.329 N 0.064 1.265 A Asp 211 - A Gly 212 | CA 1.530 CB 0.079 1.609 A Met 215 |
| CA 1.521 CB 0.095 1.616 A Ala 216 | CA 1.525 C 0.109 1.416 A His 219 | CA 1.530 CB 0.102 1.428 A His 219 | C 1.231 O 0.112 1.119 A Gly 220 | C 1.329 N 0.052 1.277 A Gly 220 - A Val 221 | CA 1.540 CB 0.136 1.404 A Val 221 |
| CA 1.525 C 0.073 1.452 A Leu 223 | CA 1.530 CB 0.053 1.583 A Leu 223 | CA 1.525 C 0.052 1.473 A Arg 224 | CA 1.530 CB 0.061 1.469 A Asp 225 | CA 1.525 C 0.060 1.585 A Phe 228 | CA 1.530 CB 0.064 1.594 A Phe 228 |
| C 1.231 O 0.120 1.111 A Val 229 | CA 1.525 C 0.051 1.576 A Val 229 | CA 1.540 CB 0.074 1.614 A Val 229 | C 1.329 N 0.057 1.272 A Val 229 - A Gln 230 | CA 1.530 CB 0.060 1.470 A His 232 | C 1.231 O 0.066 1.165 A Pro 237 |
| CA 1.525 C 0.059 1.466 A Pro 237 | CA 1.530 CB 0.061 1.469 A Pro 237 | C 1.231 O 0.134 1.097 A Gly 240 | C 1.329 N 0.052 1.277 A Gly 240 - A Ile 241 | C 1.231 O 0.090 1.141 A Met 243 | CA 1.525 C 0.051 1.576 A Arg 248 |
| CA 1.525 C 0.069 1.594 A Ile 253 | CA 1.540 CB 0.124 1.664 A Ile 253 | CA 1.530 CB 0.053 1.477 A Asp 265 | C 1.329 N 0.066 1.263 A Asp 265 - A Tyr 266 | N 1.451 CA 0.113 1.338 A Gly 269 | C 1.341 N 0.051 1.290 A Gly 269 - A Pro 270 |
| CA 1.525 C 0.155 1.680 A Pro 270 | C 1.329 N 0.061 1.390 A Pro 270 - A Glu 271 | CA 1.525 C 0.126 1.651 A Thr 272 | CA 1.530 CB 0.141 1.671 A Glu 276 | N 1.458 CA 0.126 1.332 A Glu 276 | CA 1.525 C 0.183 1.708 A Pro 277 |
| N 1.466 CA 0.058 1.524 A Pro 277 | CA 1.530 CB 0.064 1.594 A Asn 279 | C 1.231 O 0.127 1.104 A Arg 287 | CA 1.525 C 0.056 1.469 A Asp 288 | CA 1.525 C 0.051 1.576 A Lys 289 | CA 1.525 C 0.051 1.474 A Ser 291 |
| C 1.231 O 0.055 1.176 A His 296 | CA 1.530 CB 0.099 1.629 A Arg 299 | CA 1.525 C 0.060 1.585 A Asn 302 | CA 1.525 C 0.056 1.581 A Thr 303 | CA 1.530 CB 0.050 1.480 A Pro 307 | N 1.458 CA 0.052 1.406 A Arg 308 |
| CA 1.516 C 0.053 1.569 A Gly 309 | CA 1.540 CB 0.118 1.422 A Val 312 | CA 1.525 C 0.054 1.579 A Leu 314 | CA 1.530 CB 0.055 1.585 A Leu 324 | CA 1.525 C 0.116 1.409 A His 325 | CA 1.530 CB 0.057 1.473 A Glu 326 |
| N 1.458 CA 0.077 1.535 A Glu 326 | CA 1.525 C 0.101 1.626 A Arg 327 | CA 1.530 CB 0.059 1.589 A Arg 327 | CA 1.525 C 0.057 1.582 A Leu 328 | N 1.458 CA 0.111 1.569 A Leu 328 | CA 1.525 C 0.060 1.465 A Pro 329 |

Distorted geometry

pdb2b76

Main-chain bond lengths (contd)

| | | | | | |
|--|--|--|--|--|--|
| CA 1.530 CB 0.054 1.584 A Pro 329 | CA 1.530 CB 0.106 1.636 A Phe 330 | CA 1.540 CB 0.066 1.606 A Ile 331 | CA 1.525 C 0.062 1.587 A Cys 332 | CA 1.521 CB 0.057 1.464 A Ala 335 | CA 1.525 C 0.072 1.597 A Val 344 |
| CA 1.530 CB 0.066 1.595 A Glu 346 | CA 1.525 C 0.083 1.608 A Pro 347 | C 1.231 O 0.051 1.281 A Ile 348 | CA 1.525 C 0.089 1.614 A Arg 351 | CA 1.530 CB 0.096 1.626 A Arg 351 | CA 1.525 C 0.159 1.684 A Pro 352 |
| CA 1.525 C 0.055 1.470 A Thr 353 | CA 1.525 C 0.052 1.577 A Thr 357 | CA 1.540 CB 0.127 1.413 A Thr 357 | CA 1.525 C 0.062 1.463 A Met 358 | C 1.231 O 0.050 1.281 A Gly 359 | CA 1.540 CB 0.060 1.480 A Ile 361 |
| CA 1.530 CB 0.053 1.582 A Glu 362 | CA 1.525 C 0.071 1.596 A Gln 365 | CA 1.525 C 0.063 1.462 A Asn 366 | CA 1.530 CB 0.108 1.422 A Glu 368 | CA 1.540 CB 0.110 1.650 A Thr 369 | CA 1.525 C 0.074 1.451 A Arg 370 |
| CA 1.540 CB 0.134 1.674 A Ile 371 | C 1.231 O 0.076 1.155 A Lys 372 | CA 1.525 C 0.062 1.587 A Lys 372 | CA 1.530 CB 0.079 1.609 A Lys 372 | CA 1.521 CB 0.077 1.444 A Ala 376 | C 1.231 O 0.114 1.117 A His 386 |
| CA 1.530 CB 0.083 1.447 A His 386 | C 1.329 N 0.056 1.273 A His 386 - A Gly 387 | CA 1.521 CB 0.074 1.595 A Ala 388 | C 1.231 O 0.064 1.167 A Asn 389 | CA 1.530 CB 0.099 1.431 A Asn 389 | C 1.231 O 0.061 1.170 A Arg 390 |
| CA 1.525 C 0.094 1.431 A Arg 390 | C 1.231 O 0.093 1.138 A Leu 391 | CA 1.530 CB 0.113 1.417 A Leu 391 | C 1.231 O 0.057 1.174 A Ser 393 | CA 1.525 C 0.052 1.473 A Ser 395 | CA 1.530 CB 0.093 1.623 A Leu 396 |
| CA 1.525 C 0.081 1.444 A Leu 399 | CA 1.540 CB 0.107 1.433 A Val 400 | N 1.458 CA 0.052 1.406 A Val 400 | C 1.231 O 0.050 1.181 A Val 401 | CA 1.530 CB 0.077 1.453 A Arg 404 | CA 1.530 CB 0.061 1.469 A Glu 408 |
| CA 1.525 C 0.091 1.434 A Gln 409 | C 1.231 O 0.109 1.122 A Ala 410 | CA 1.525 C 0.066 1.459 A Ala 410 | CA 1.525 C 0.062 1.463 A Thr 411 | C 1.231 O 0.053 1.178 A Asn 419 | CA 1.525 C 0.077 1.448 A Asn 421 |
| CA 1.530 CB 0.067 1.597 A Asn 421 | C 1.231 O 0.095 1.136 A Glu 422 | CA 1.521 CB 0.137 1.658 A Ala 424 | CA 1.540 CB 0.107 1.647 A Ile 425 | CA 1.525 C 0.080 1.605 A Ala 429 | CA 1.521 CB 0.060 1.581 A Ala 429 |
| CA 1.525 C 0.056 1.581 A Val 432 | N 1.458 CA 0.066 1.392 A Leu 436 | CA 1.525 C 0.054 1.579 A Asn 441 | CA 1.525 C 0.057 1.582 A Gln 442 | C 1.329 N 0.101 1.228 A Gly 445 - A Glu 446 | C 1.329 N 0.053 1.276 A Glu 446 - A Asn 447 |

Distorted geometry

pdb2b76

Main-chain bond lengths (contd)

| | | | | | |
|--|--|--|--|--|--|
| CA 1.525 C 0.055 1.580 A Asn 447 | CA 1.525 C 0.066 1.459 A Ile 451 | CA 1.540 CB 0.072 1.467 A Ile 451 | C 1.231 O 0.058 1.173 A Asp 453 | CA 1.530 CB 0.056 1.474 A Glu 454 | C 1.231 O 0.056 1.175 A Gly 456 |
| CA 1.530 CB 0.090 1.440 A Met 459 | C 1.231 O 0.059 1.172 A Glu 461 | CA 1.530 CB 0.118 1.648 A Glu 461 | C 1.231 O 0.056 1.175 A Ile 465 | CA 1.540 CB 0.146 1.394 A Ile 465 | CA 1.525 C 0.094 1.431 A Arg 467 |
| CA 1.525 C 0.132 1.393 A Pro 469 | CA 1.530 CB 0.057 1.587 A Leu 471 | CA 1.525 C 0.066 1.459 A Met 472 | CA 1.530 CB 0.061 1.469 A Met 472 | CA 1.530 CB 0.085 1.615 A Lys 474 | CA 1.525 C 0.073 1.452 A Thr 475 |
| C 1.231 O 0.052 1.179 A Lys 478 | CA 1.530 CB 0.051 1.479 A Leu 479 | CA 1.525 C 0.090 1.435 A Ala 480 | CA 1.530 CB 0.075 1.605 A Glu 481 | C 1.231 O 0.069 1.162 A Glu 484 | CA 1.525 C 0.121 1.404 A Glu 484 |
| CA 1.530 CB 0.074 1.604 A Glu 484 | C 1.231 O 0.054 1.285 A Phe 486 | CA 1.530 CB 0.086 1.616 A Lys 487 | CA 1.525 C 0.072 1.453 A Val 489 | CA 1.540 CB 0.059 1.599 A Val 489 | CA 1.530 CB 0.102 1.428 A Arg 490 |
| C 1.231 O 0.072 1.159 A Thr 494 | CA 1.530 CB 0.064 1.594 A Asn 499 | CA 1.540 CB 0.052 1.592 A Thr 500 | C 1.231 O 0.060 1.171 A Tyr 504 | C 1.231 O 0.056 1.175 A Glu 507 | CA 1.530 CB 0.060 1.590 A Leu 508 |
| C 1.231 O 0.057 1.174 A His 510 | C 1.231 O 0.071 1.160 A Leu 512 | CA 1.530 CB 0.051 1.581 A Leu 512 | C 1.231 O 0.058 1.173 A Asn 513 | CA 1.540 CB 0.110 1.430 A Val 514 | CA 1.530 CB 0.078 1.608 A Glu 516 |
| CA 1.530 CB 0.053 1.477 A Cys 517 | CA 1.525 C 0.055 1.580 A Met 518 | CA 1.521 CB 0.053 1.574 A Ala 519 | CA 1.530 CB 0.072 1.458 A His 520 | CA 1.525 C 0.055 1.470 A Ser 521 | CA 1.521 CB 0.119 1.640 A Ala 522 |
| CA 1.530 CB 0.072 1.602 A Met 523 | C 1.231 O 0.053 1.178 A Leu 535 | CA 1.525 C 0.088 1.437 A Leu 535 | CA 1.525 C 0.099 1.426 A Cys 539 | C 1.329 N 0.069 1.260 A Cys 539 - A Thr 540 | CA 1.525 C 0.075 1.450 A Arg 542 |
| CA 1.530 CB 0.062 1.468 A Arg 542 | CA 1.530 CB 0.159 1.689 A Asp 543 | C 1.231 O 0.096 1.135 A Asp 544 | C 1.231 O 0.087 1.144 A Val 545 | CA 1.525 C 0.066 1.459 A Val 545 | CA 1.540 CB 0.069 1.609 A Val 545 |
| CA 1.530 CB 0.113 1.643 A Asn 546 | CA 1.530 CB 0.089 1.619 A Phe 547 | CA 1.530 CB 0.066 1.464 A Leu 548 | CA 1.530 CB 0.053 1.477 A His 550 | CA 1.521 CB 0.078 1.443 A Ala 553 | C 1.329 N 0.072 1.257 A Arg 555 - A Asp 556 |

Distorted geometry

pdb2b76

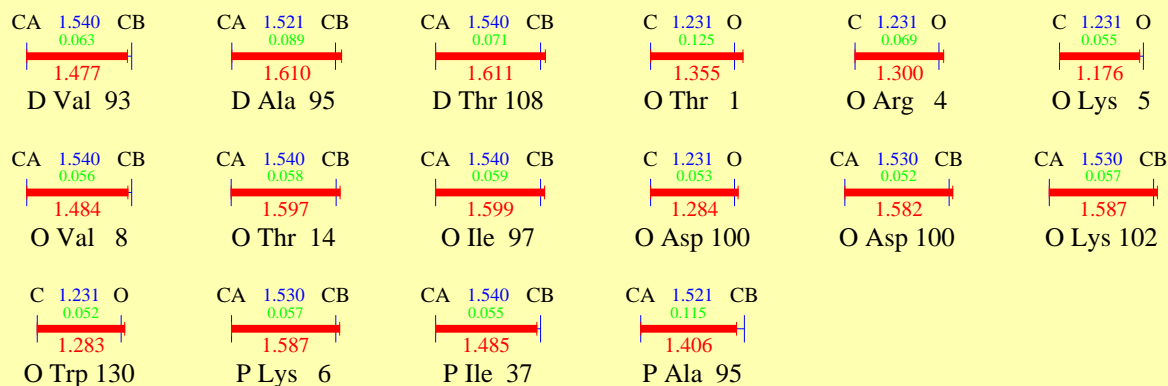
Main-chain bond lengths (contd)

| | | | | | |
|--|--|--|--|--|--|
| CA 1.525 C 0.109 1.633 A Ala 557 | N 1.458 CA 0.063 1.521 A Ala 557 | N 1.458 CA 0.053 1.511 A Asp 558 | CA 1.540 CB 0.082 1.457 A Thr 560 | CA 1.540 CB 0.059 1.481 A Thr 561 | CA 1.530 CB 0.055 1.585 A Arg 562 |
| CA 1.530 CB 0.093 1.437 A Leu 563 | C 1.231 O 0.051 1.180 A Tyr 565 | CA 1.530 CB 0.074 1.456 A Asp 567 | CA 1.530 CB 0.117 1.413 A Pro 574 | CA 1.525 C 0.100 1.425 A Pro 575 | C 1.329 N 0.100 1.229 A Pro 575 - A Ala 576 |
| C 1.231 O 0.063 1.168 A Ala 576 | CA 1.521 CB 0.174 1.695 A Ala 576 | N 1.458 CA 0.054 1.404 A Ala 576 | CA 1.525 C 0.059 1.584 B Asn 5 | CA 1.540 CB 0.054 1.486 B Val 11 | CA 1.525 C 0.070 1.455 B Glu 16 |
| N 1.458 CA 0.051 1.509 B Glu 16 | CA 1.530 CB 0.061 1.469 B Tyr 30 | C 1.231 O 0.080 1.151 B Asp 31 | CA 1.521 CB 0.085 1.436 B Ala 39 | C 1.231 O 0.055 1.176 B Tyr 42 | CA 1.530 CB 0.079 1.451 B Tyr 42 |
| CA 1.530 CB 0.057 1.473 B Asn 46 | CA 1.530 CB 0.057 1.473 B Asp 50 | CA 1.530 CB 0.056 1.474 B Tyr 53 | C 1.231 O 0.119 1.112 B Ser 56 | CA 1.540 CB 0.090 1.450 B Val 69 | CA 1.525 C 0.051 1.474 B Asn 71 |
| CA 1.525 C 0.058 1.467 B Cys 77 | C 1.231 O 0.051 1.180 B Thr 79 | CA 1.521 CB 0.057 1.464 B Ala 92 | CA 1.540 CB 0.080 1.460 B Ile 98 | CA 1.540 CB 0.066 1.474 B Val 104 | CA 1.516 C 0.069 1.585 B Gly 130 |
| N 1.451 CA 0.064 1.515 B Gly 130 | CA 1.525 C 0.063 1.462 B Ile 133 | CA 1.540 CB 0.061 1.479 B Ile 133 | CA 1.525 C 0.052 1.473 B Thr 135 | CA 1.540 CB 0.071 1.469 B Thr 135 | C 1.231 O 0.063 1.168 B Pro 136 |
| CA 1.530 CB 0.059 1.471 B Pro 136 | CA 1.525 C 0.060 1.465 B Leu 175 | CA 1.540 CB 0.121 1.419 B Val 207 | CA 1.540 CB 0.060 1.480 B Val 213 | CA 1.521 CB 0.068 1.453 B Ala 221 | C 1.231 O 0.089 1.142 B Asp 234 |
| C 1.231 O 0.056 1.175 B Leu 236 | CA 1.540 CB 0.051 1.591 B Ile 237 | CA 1.530 CB 0.080 1.610 B Lys 241 | C 1.329 N 0.085 1.244 B Pro 242 - B Arg 243 | C 1.231 O 0.087 1.318 C Thr 1 | CA 1.540 CB 0.081 1.621 C Thr 1 |
| N 1.458 CA 0.058 1.516 C Thr 1 | C 1.231 O 0.055 1.286 C Thr 2 | C 1.231 O 0.057 1.288 C Lys 3 | CA 1.525 C 0.058 1.467 C Thr 75 | CA 1.540 CB 0.065 1.475 C Thr 75 | CA 1.521 CB 0.068 1.453 C Ala 93 |
| CA 1.540 CB 0.055 1.595 C Ile 96 | CA 1.540 CB 0.057 1.597 C Val 98 | CA 1.521 CB 0.054 1.467 C Ala 114 | CA 1.540 CB 0.053 1.487 C Val 118 | CA 1.530 CB 0.053 1.477 C Trp 130 | CA 1.525 C 0.052 1.473 D Pro 3 |

Distorted geometry

pdb2b76

Main-chain bond lengths (contd)



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

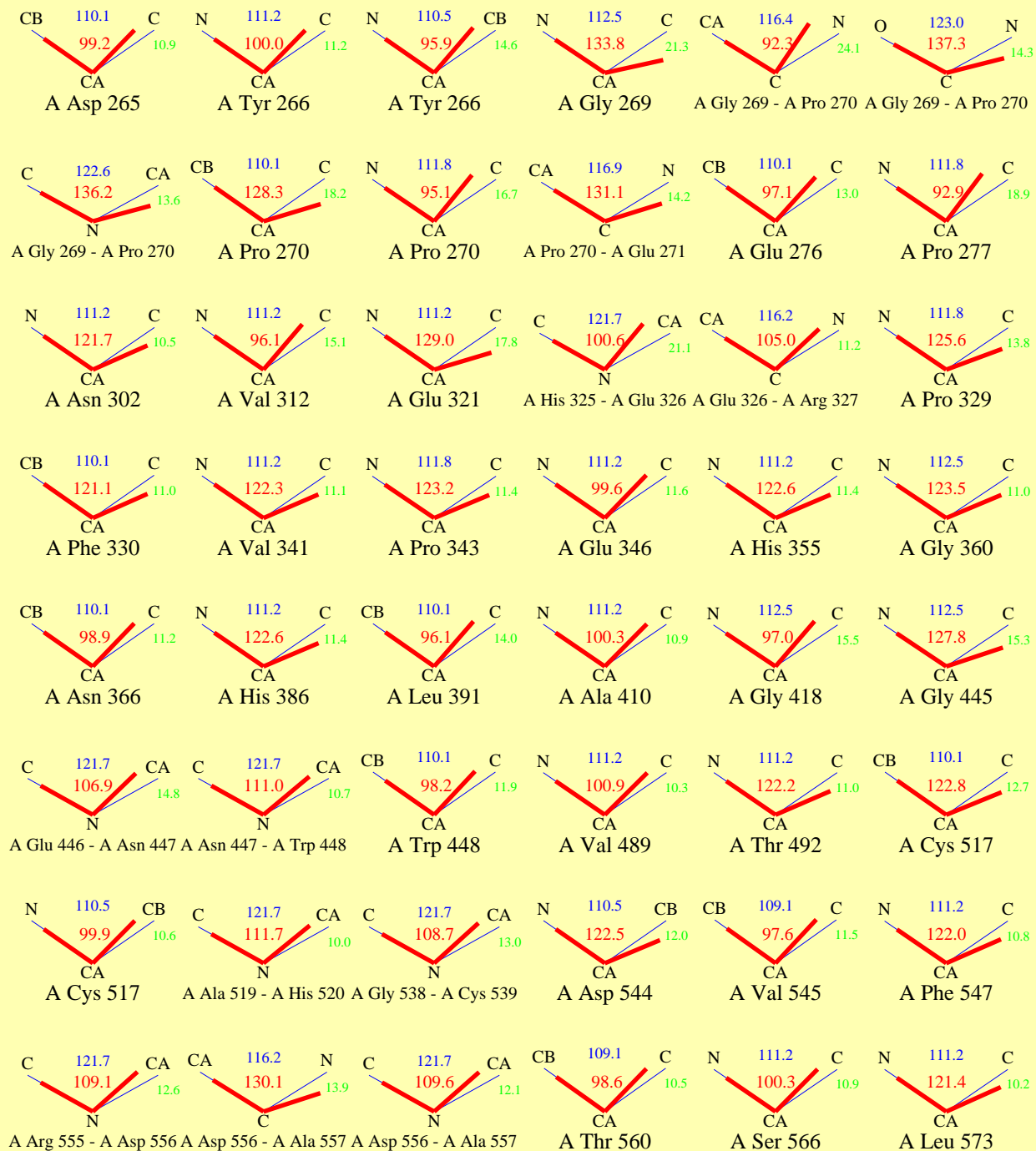
Main-chain bond angles



Distorted geometry

pdb2b76

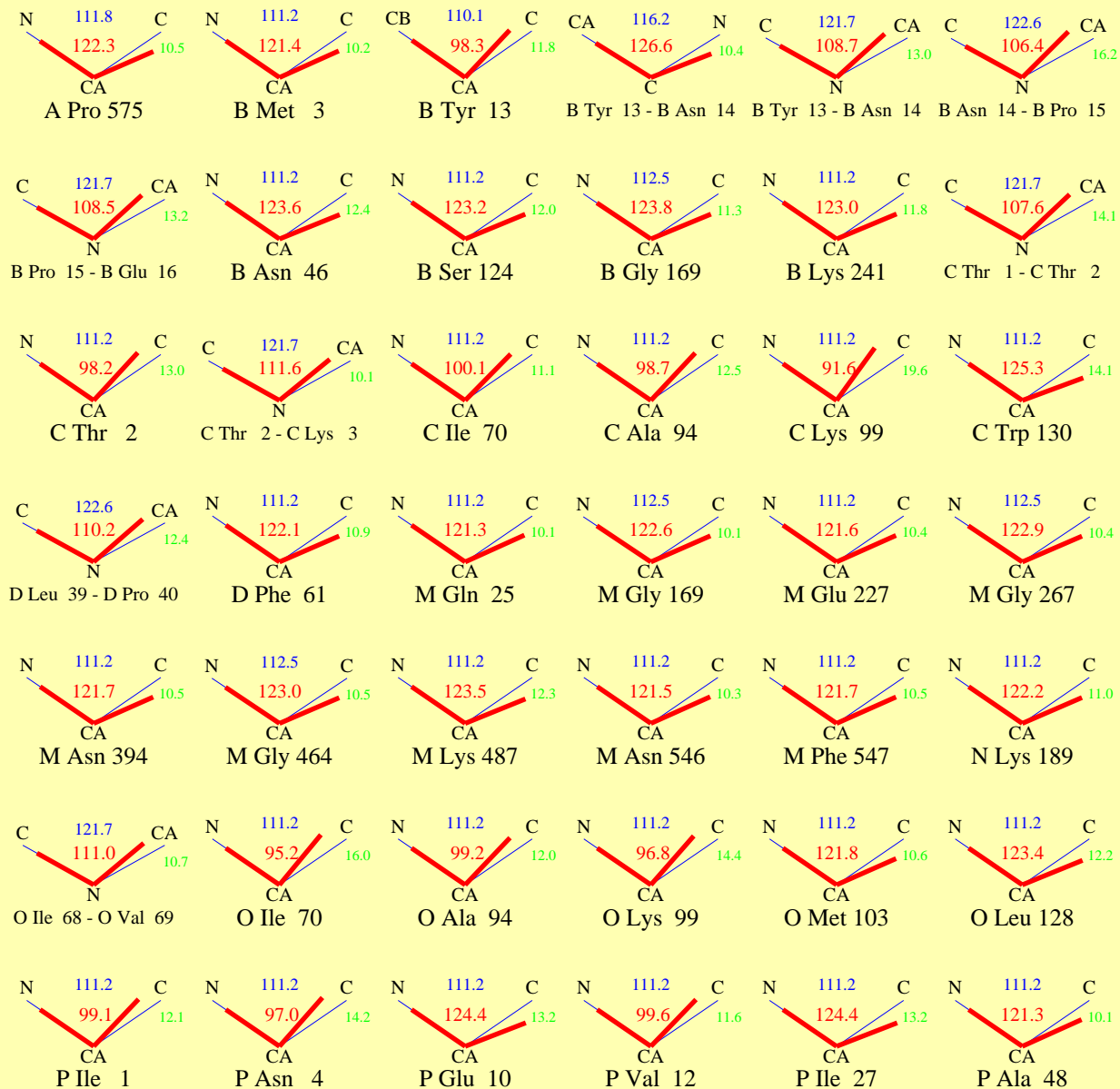
Main-chain bond angles (contd)



Distorted geometry

pdb2b76

Main-chain bond angles (contd)

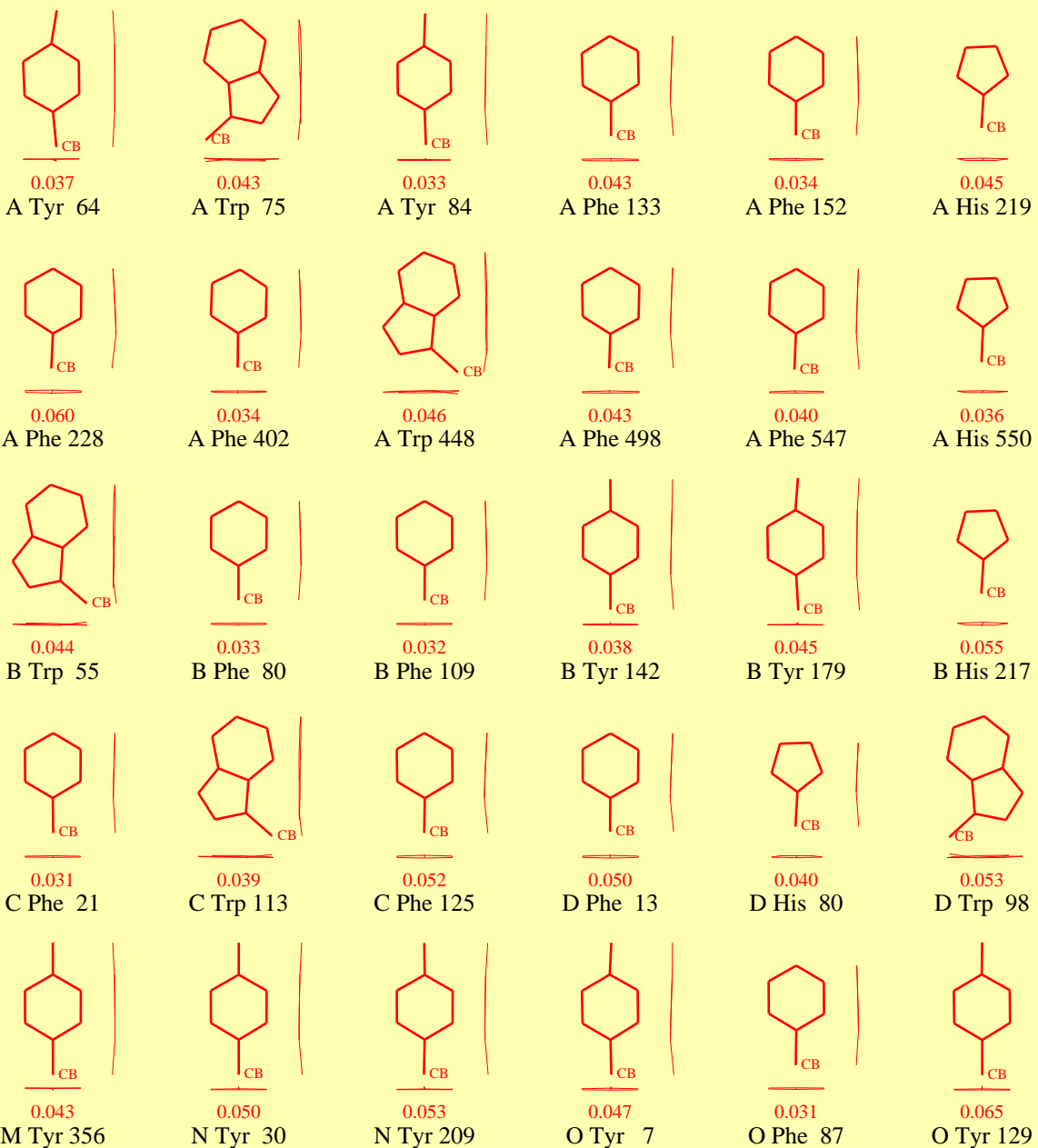


Bond angles differing by > 10.0 degrees from small-molec values. Values shown: "ideal", actual, diff.

Distorted geometry

pdb2b76

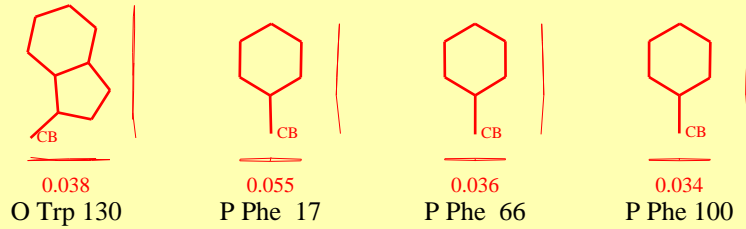
Planar groups



Distorted geometry

pdb2b76

Planar groups (contd)



Sidechains with RMS dist. from planarity $> 0.03\text{\AA}$ for rings, or $> 0.02\text{\AA}$ otherwise. Value shown is RMS dist.