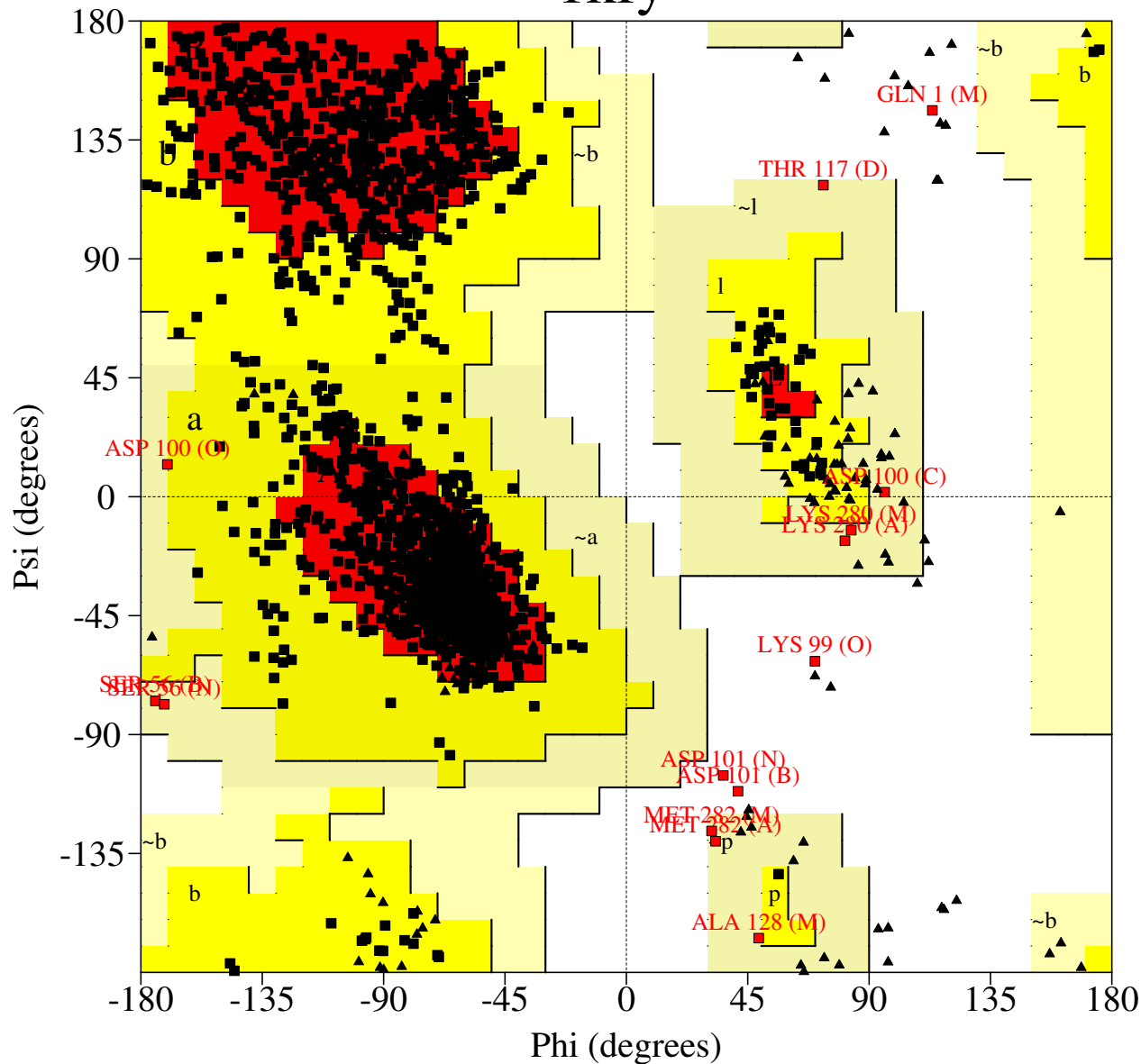


Ramachandran Plot

1kfy



Plot statistics

Residues in most favoured regions [A,B,L]	1545	84.5%
Residues in additional allowed regions [a,b,l,p]	269	14.7%
Residues in generously allowed regions [-a,-b,-l,-p]	10	0.5%
Residues in disallowed regions	4	0.2%

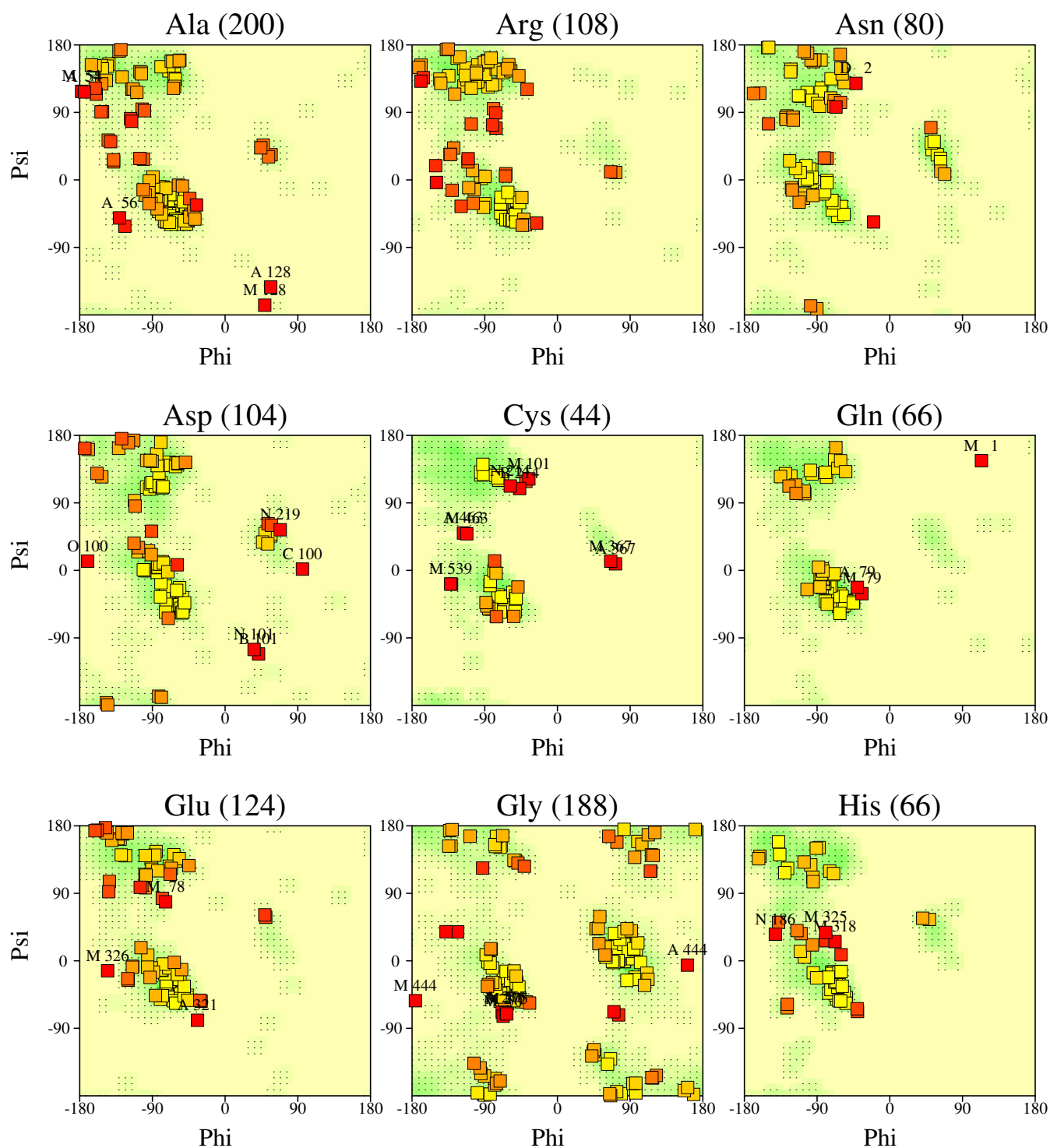
Number of non-glycine and non-proline residues	1828	100.0%
Number of end-residues (excl. Gly and Pro)	16	
Number of glycine residues (shown as triangles)	188	
Number of proline residues	106	

Total number of residues	2138	

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

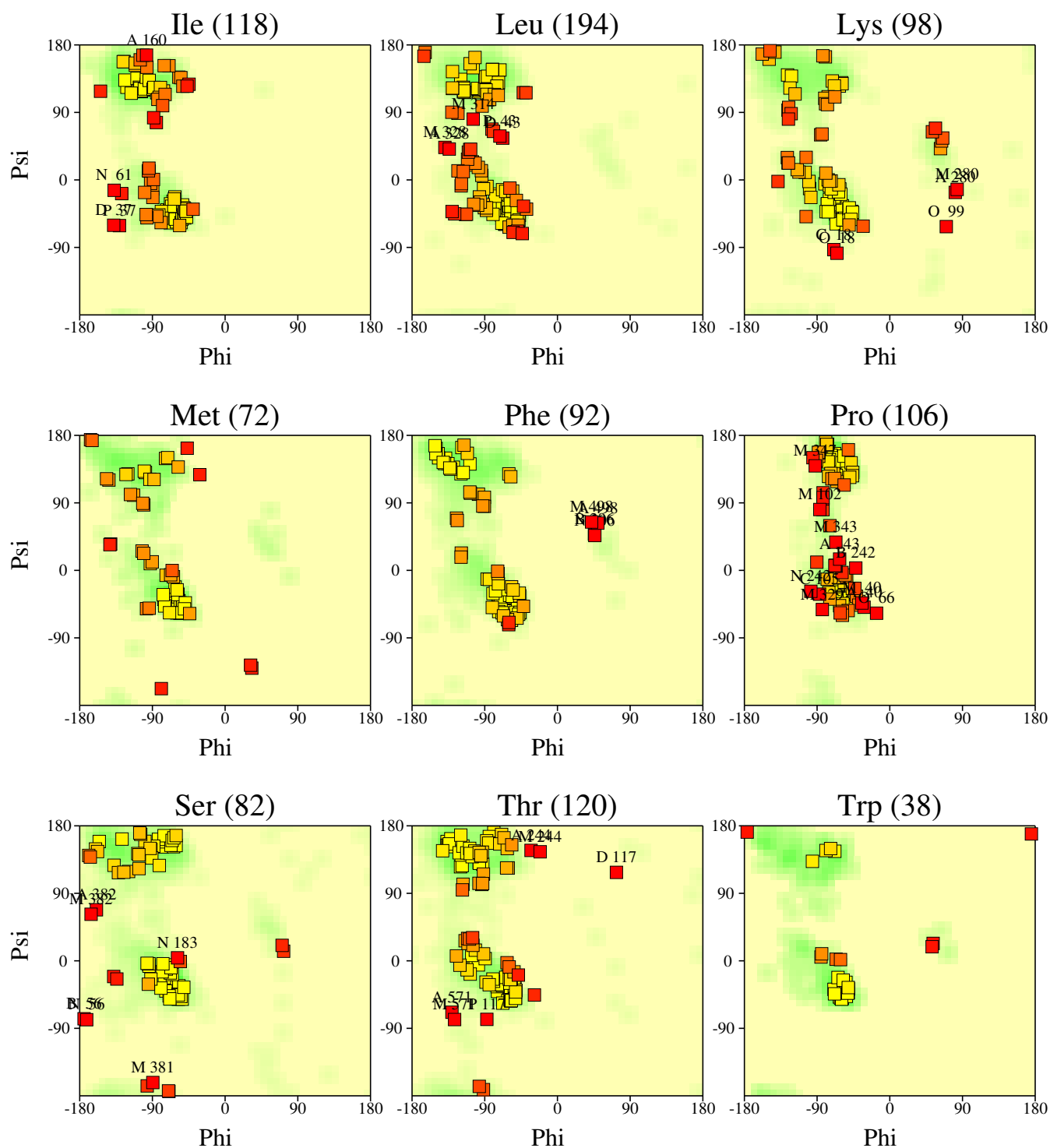
1kfy



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.

Ramachandran plots for all residue types

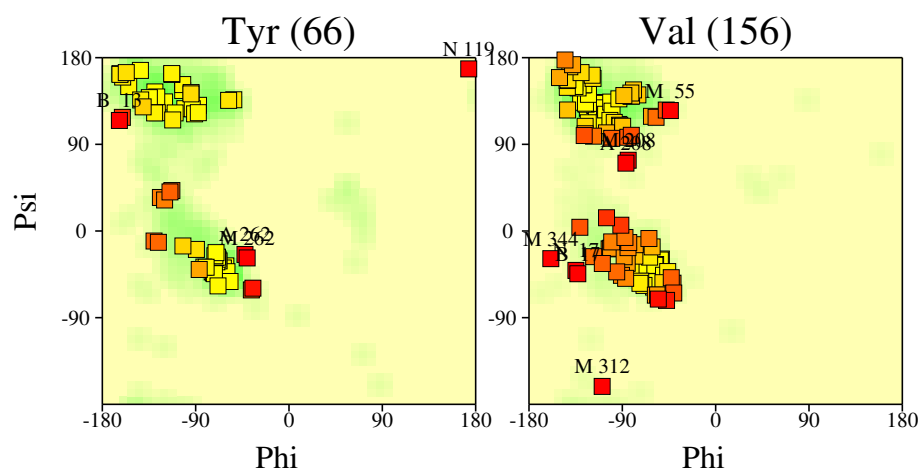
1kfy



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

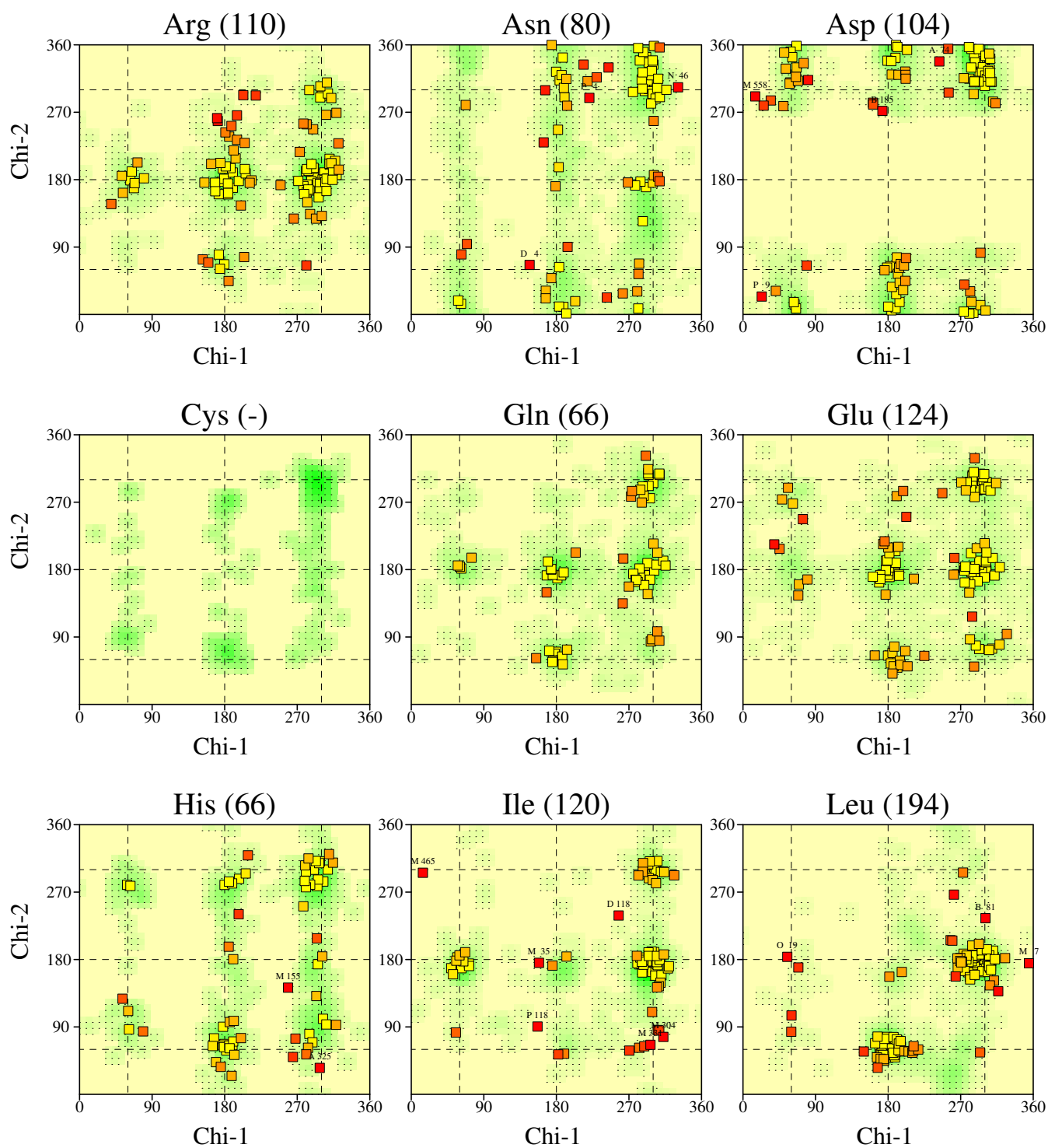
1kfy



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

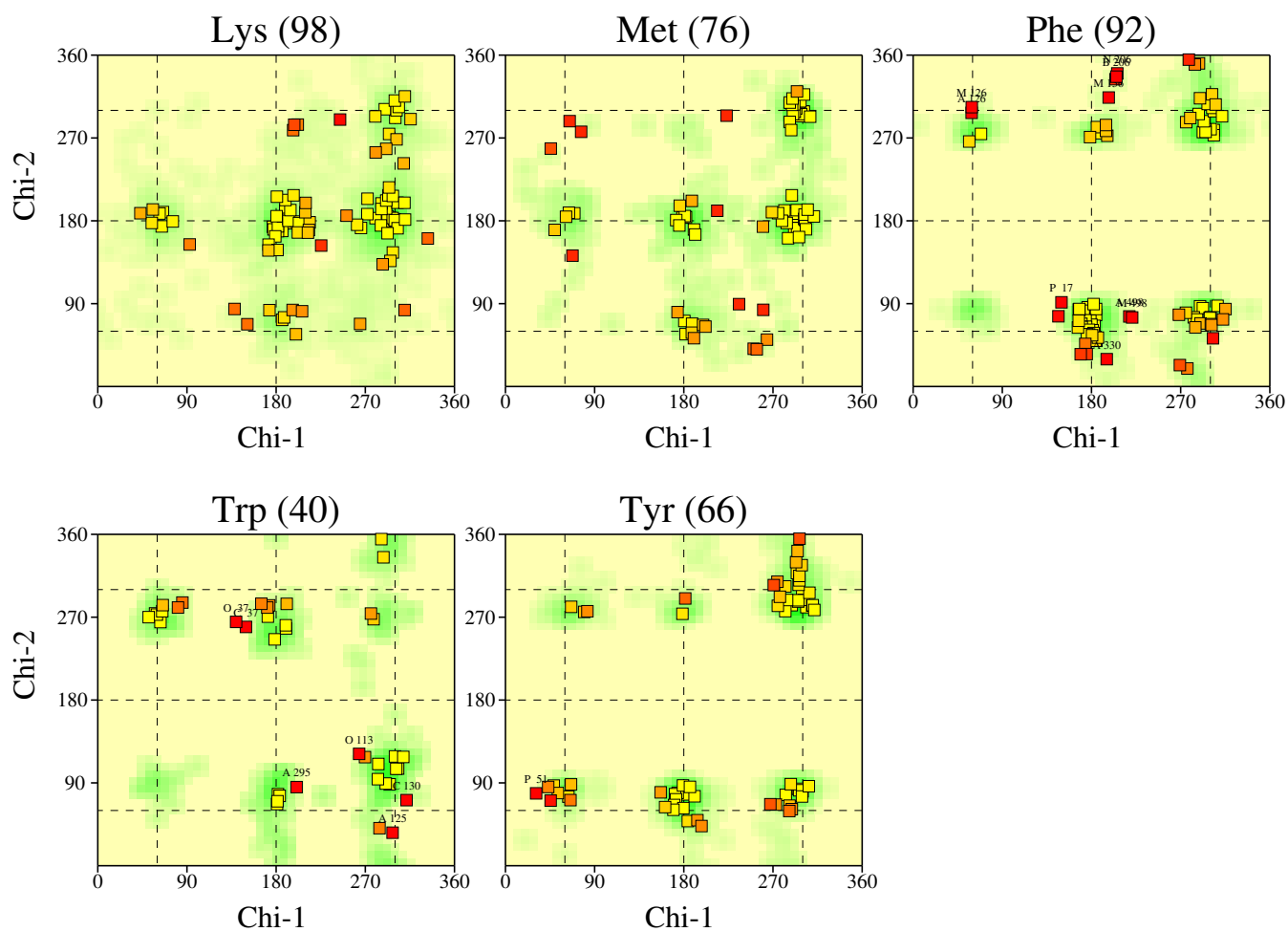
1kfy



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

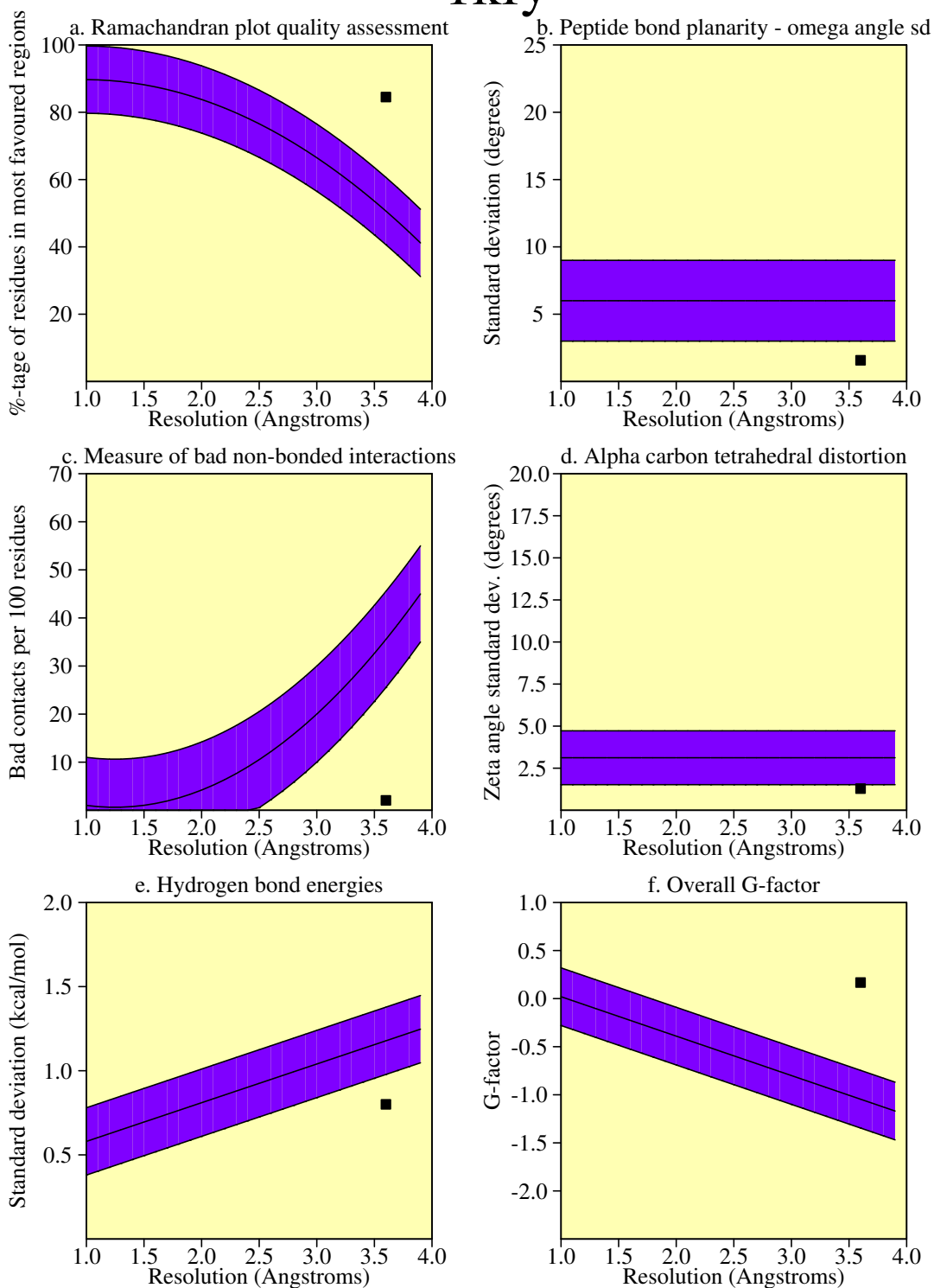
1kfy



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.

Main-chain parameters

1kfy

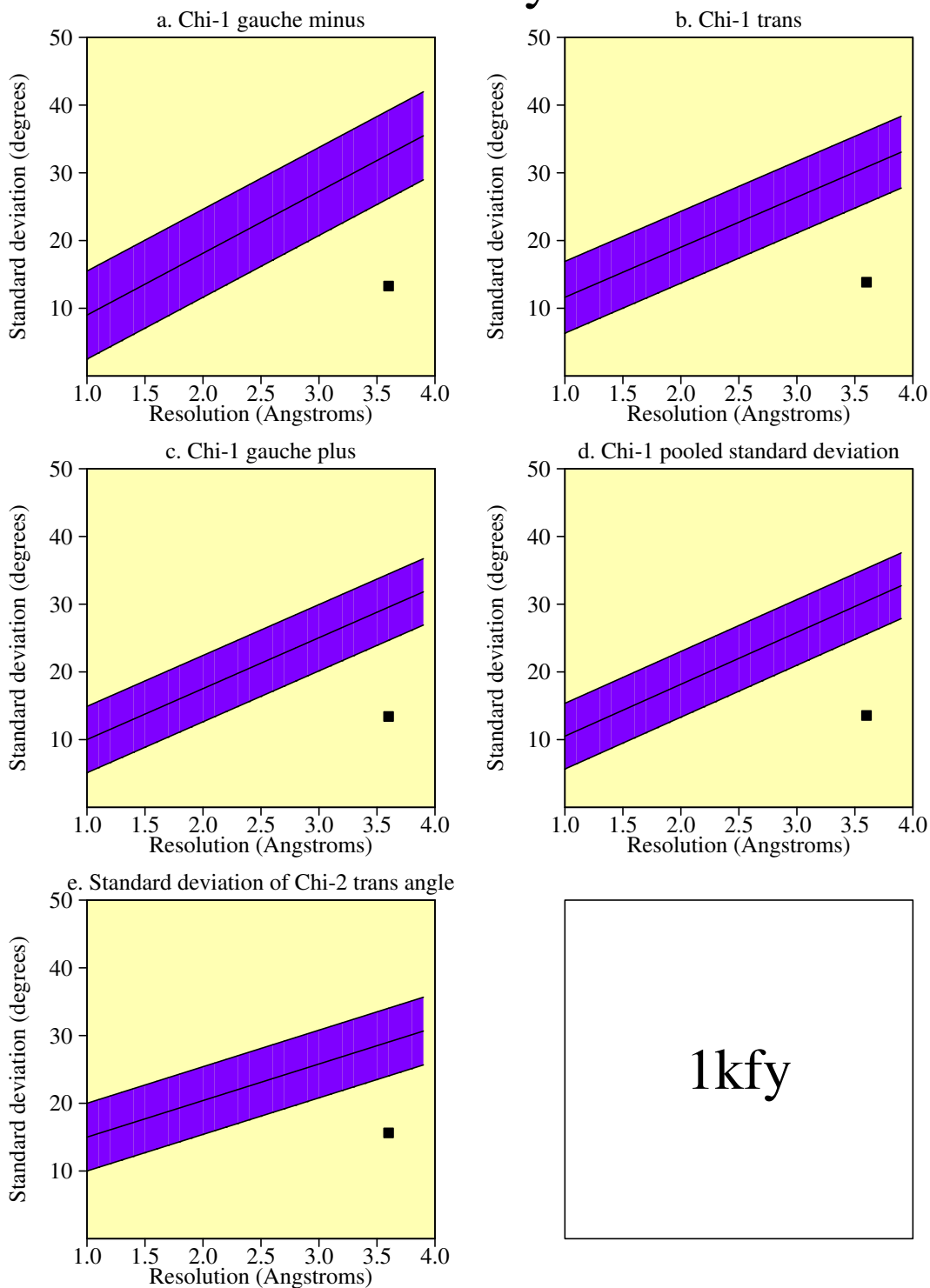


Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	1828	84.5	50.6	10.0	3.4	BETTER
b. Omega angle st dev	2126	1.6	6.0	3.0	-1.5	BETTER
c. Bad contacts / 100 residues	44	2.1	35.5	10.0	-3.3	BETTER
d. Zeta angle st dev	1950	1.3	3.1	1.6	-1.1	BETTER
e. H-bond energy st dev	1412	0.8	1.2	0.2	-1.9	BETTER
f. Overall G-factor	2138	0.2	-1.0	0.3	4.0	BETTER

Side-chain parameters

1kfy



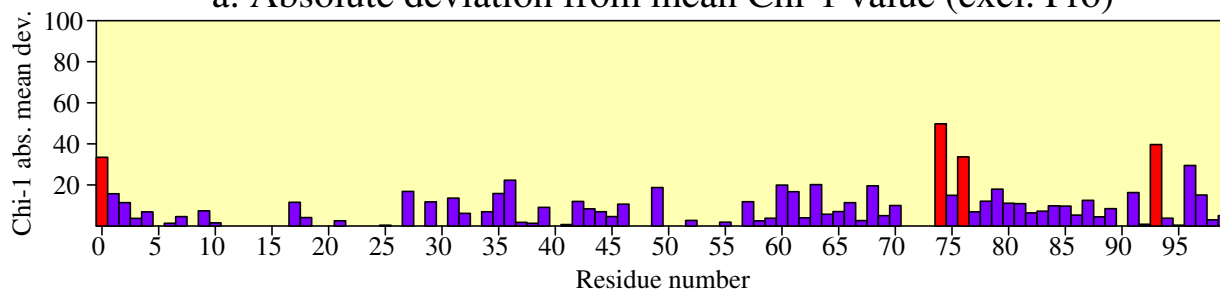
Plot statistics

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	221	13.3	32.7	6.5	-3.0	BETTER
b. Chi-1 trans st dev	561	13.9	30.8	5.3	-3.2	BETTER
c. Chi-1 gauche plus st dev	858	13.4	29.6	4.9	-3.3	BETTER
d. Chi-1 pooled st dev	1640	13.6	30.4	4.8	-3.5	BETTER
e. Chi-2 trans st dev	508	15.6	29.0	5.0	-2.7	BETTER

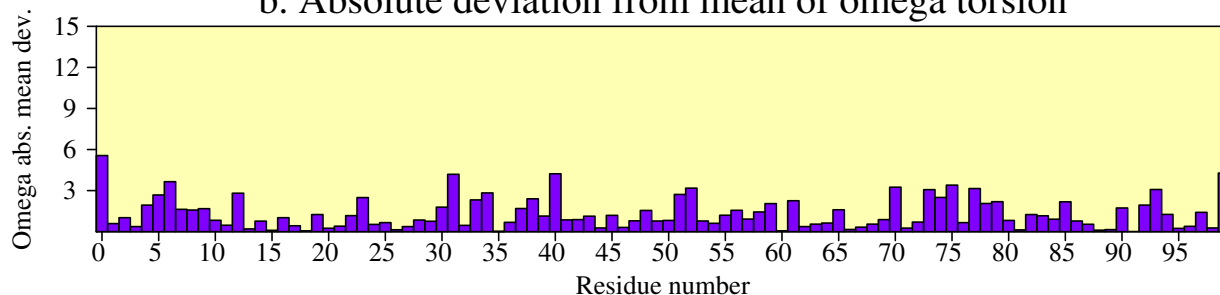
Residue properties

1kfy

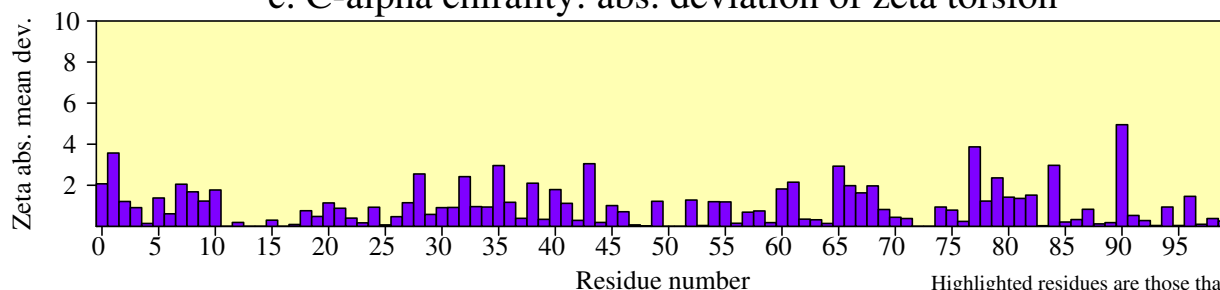
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

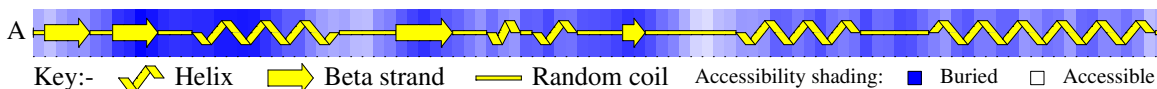


c. C-alpha chirality: abs. deviation of zeta torsion



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

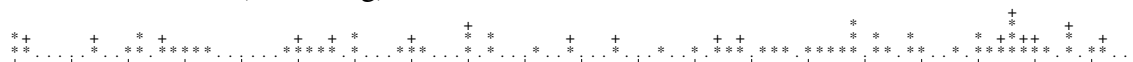
d. Secondary structure & estimated accessibility



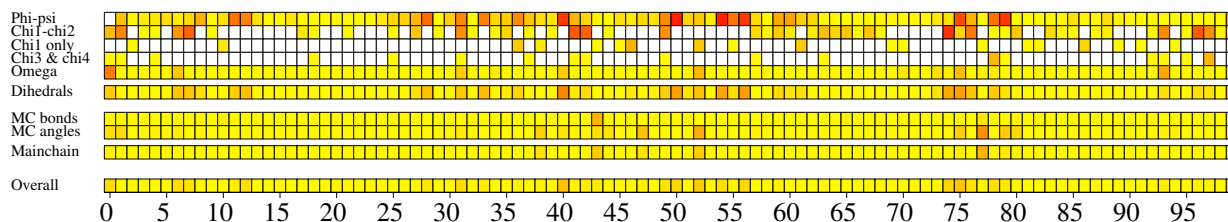
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



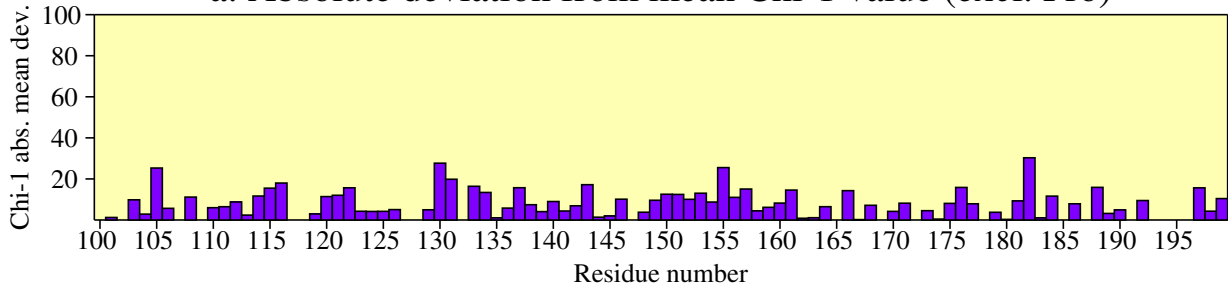
g. G-factors



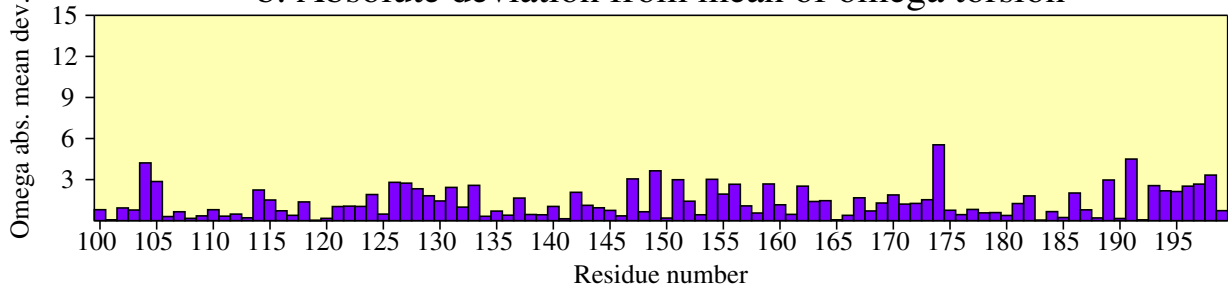
Residue properties

1kfy

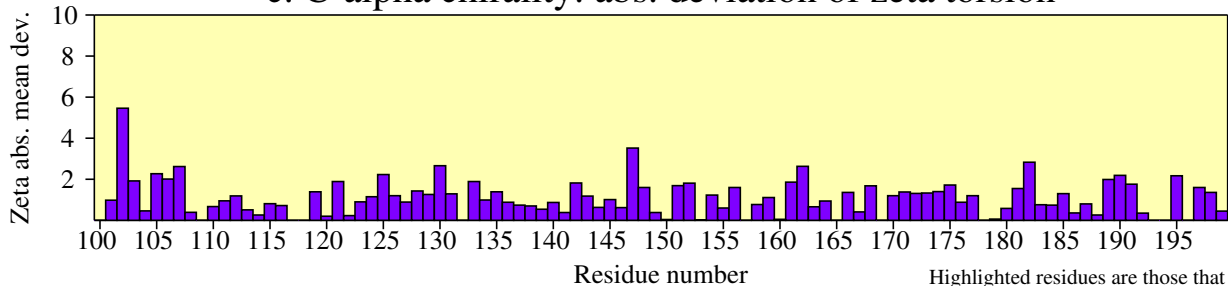
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

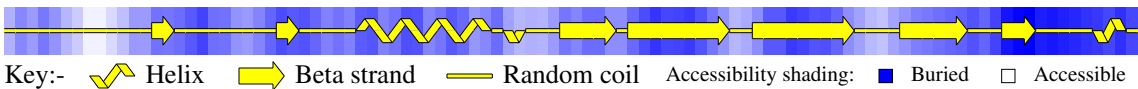


c. C-alpha chirality: abs. deviation of zeta torsion

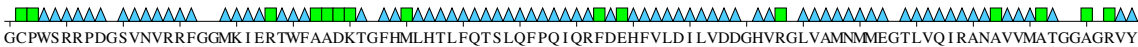


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

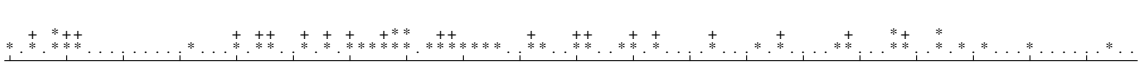
d. Secondary structure & estimated accessibility



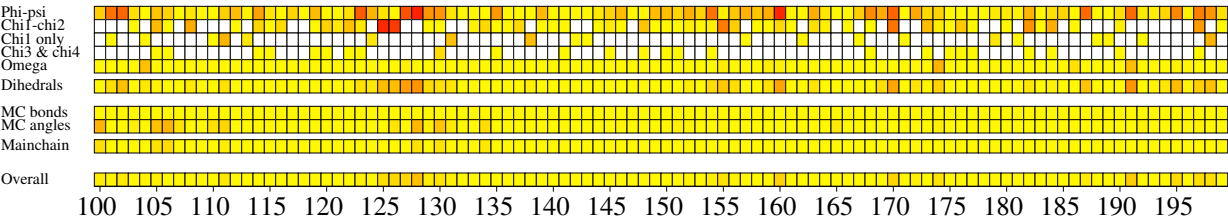
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



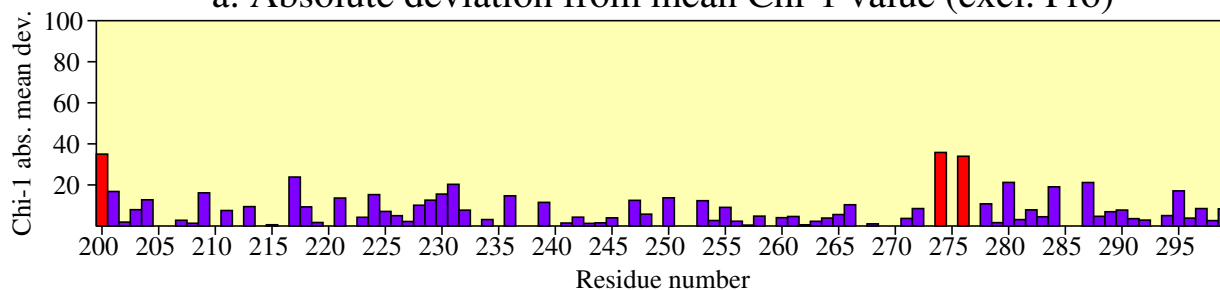
g. G-factors



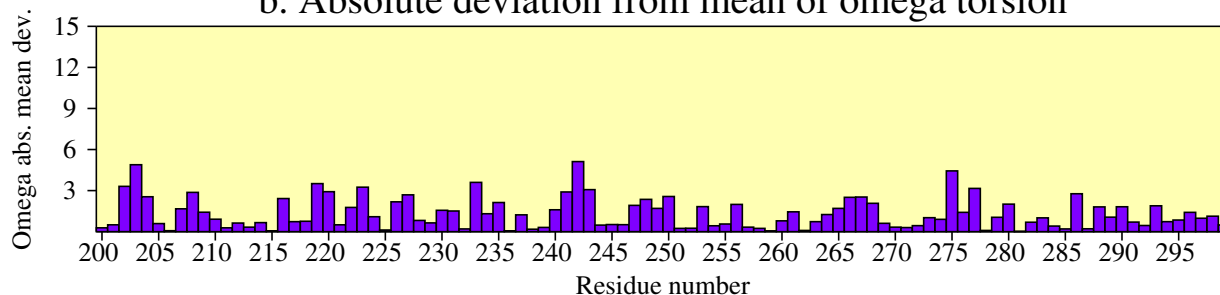
Residue properties

1kfy

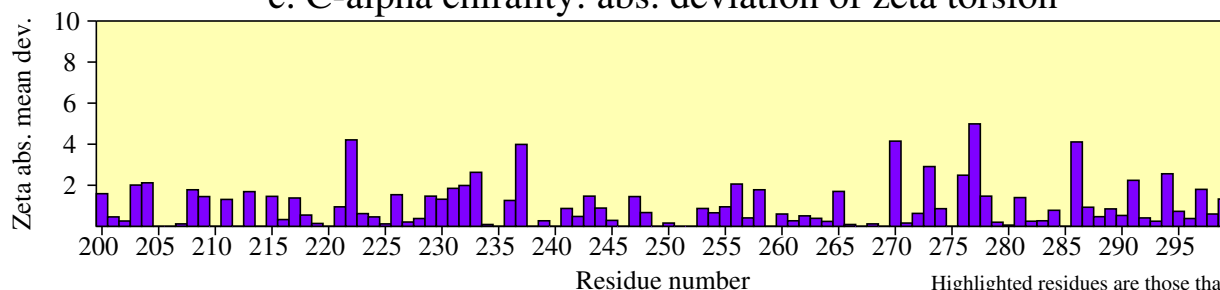
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

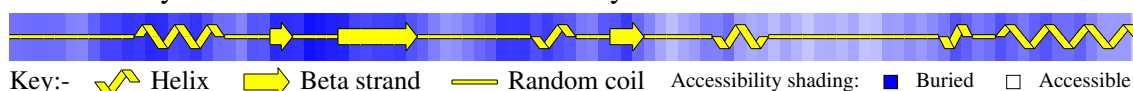


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



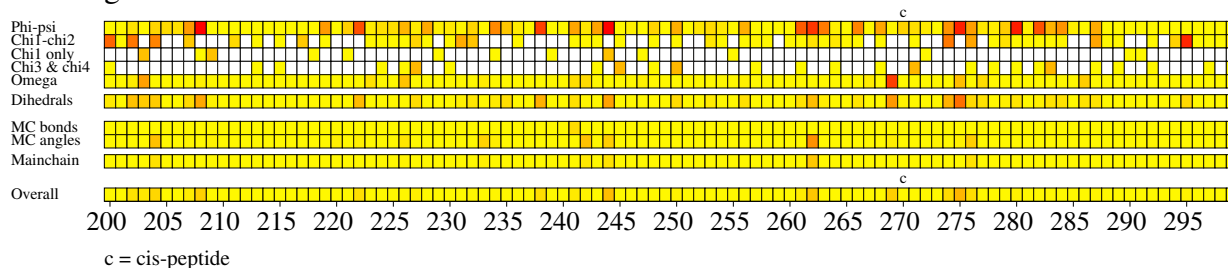
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

RYNTNGG I VTGDGMGMALSHGVP LRDMEFVQYHPTGLPGSG I LMTEGCRGEGG I LVNKNQYRYLQDYGMGPETPLGEPKNKYMELGPRDKVSQAFWHEWR

f. Max. deviation (see listing)



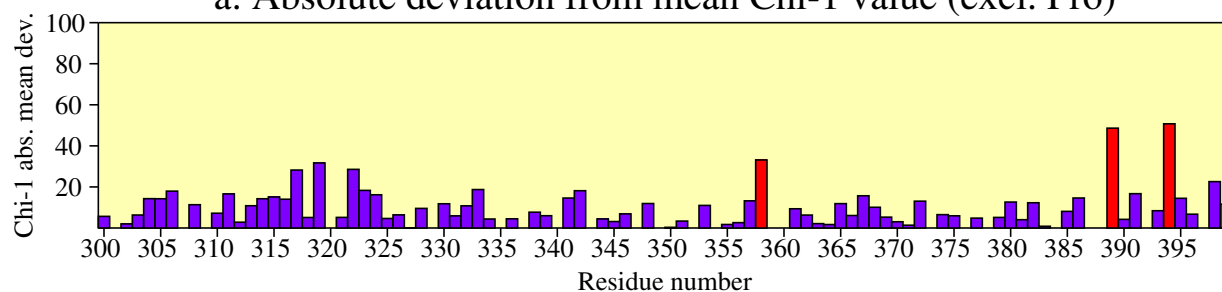
g. G-factors



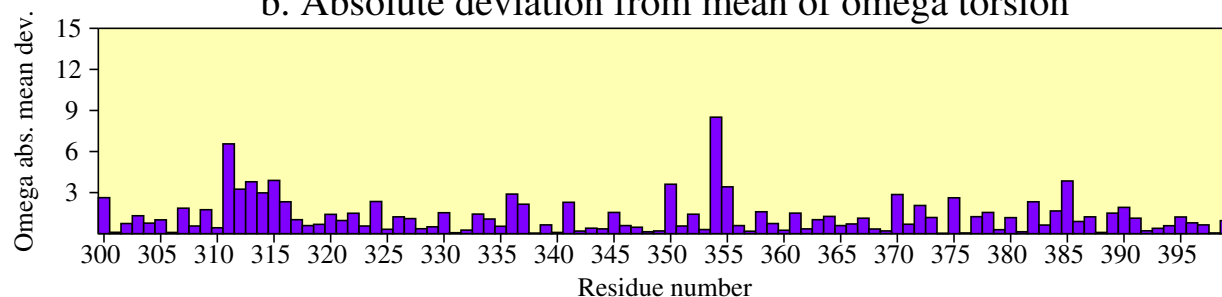
Residue properties

1kfy

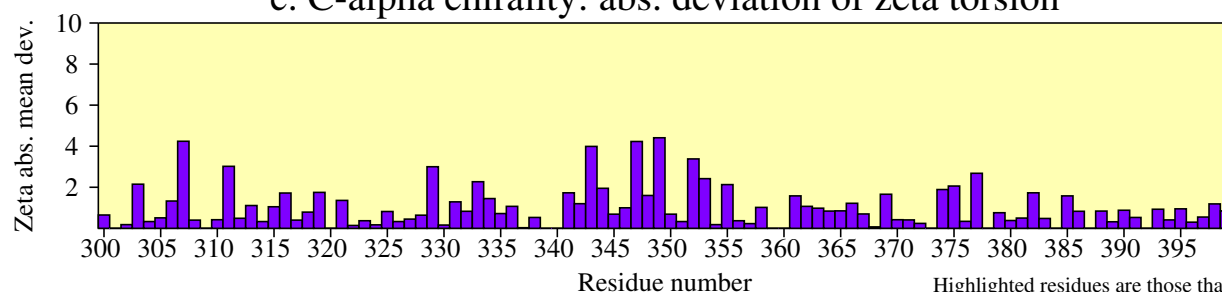
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

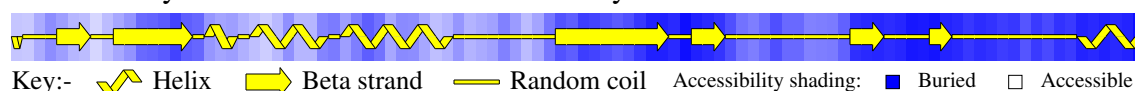


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



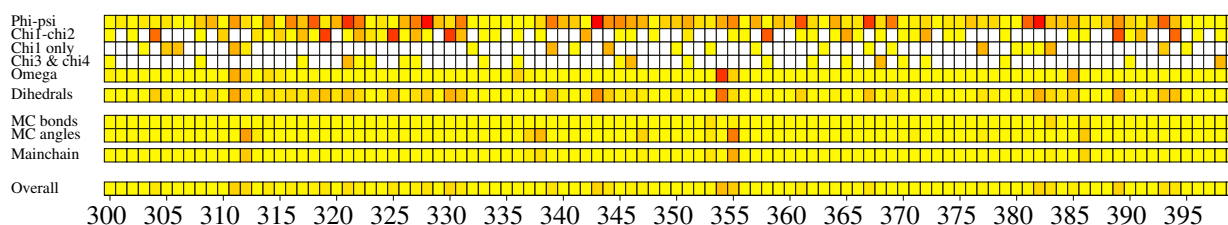
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



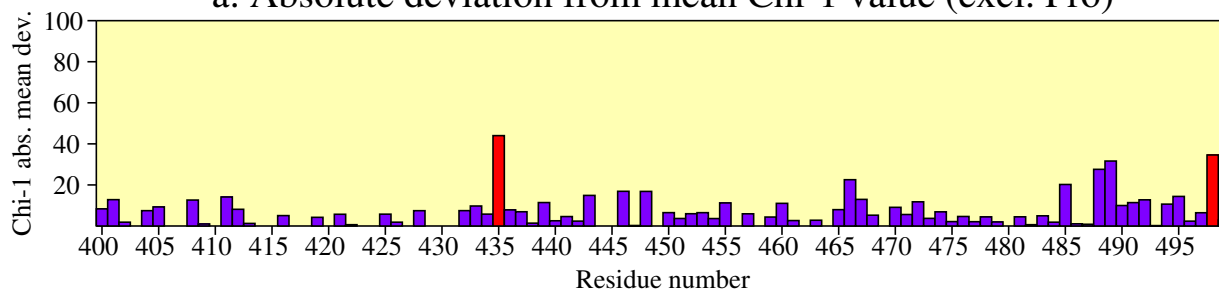
g. G-factors



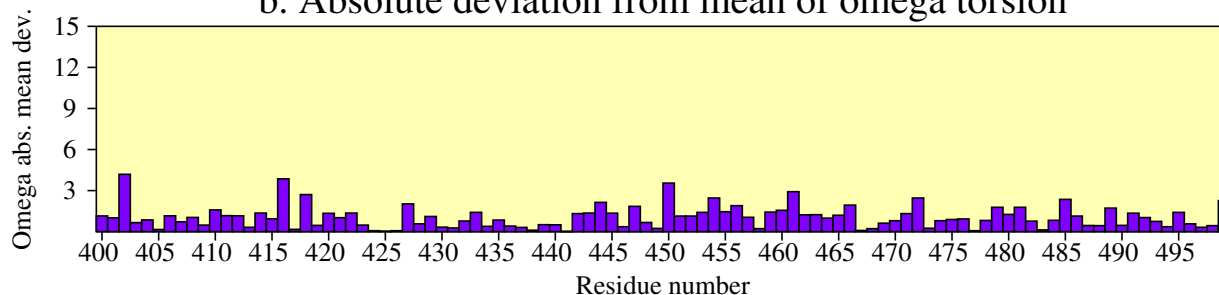
Residue properties

1kfy

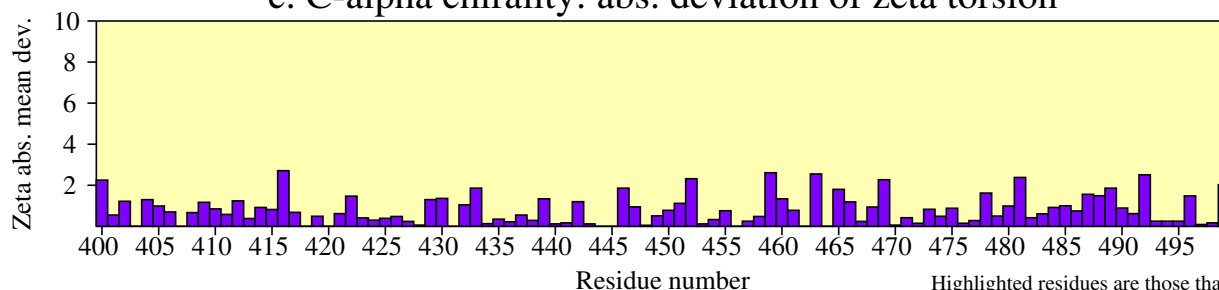
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

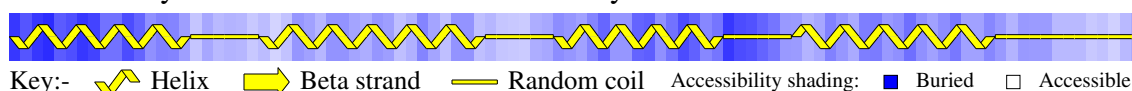


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



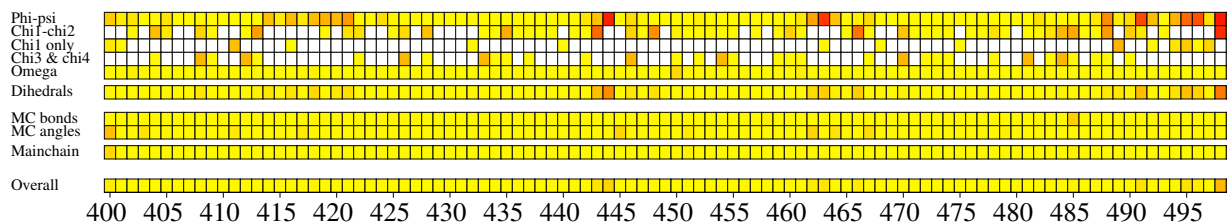
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



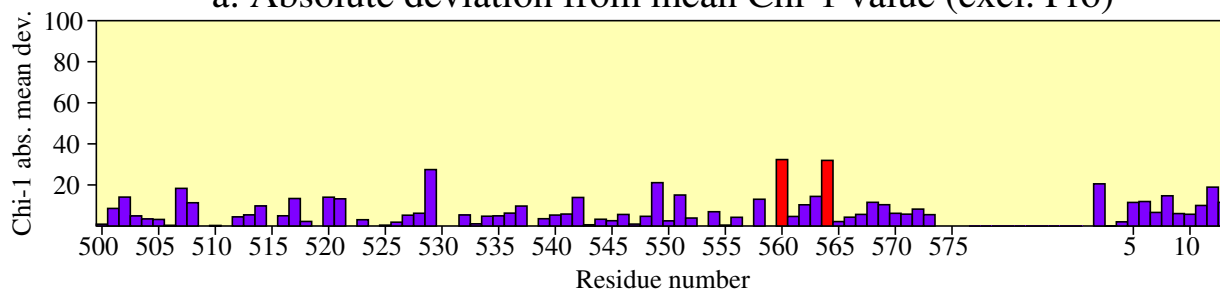
g. G-factors



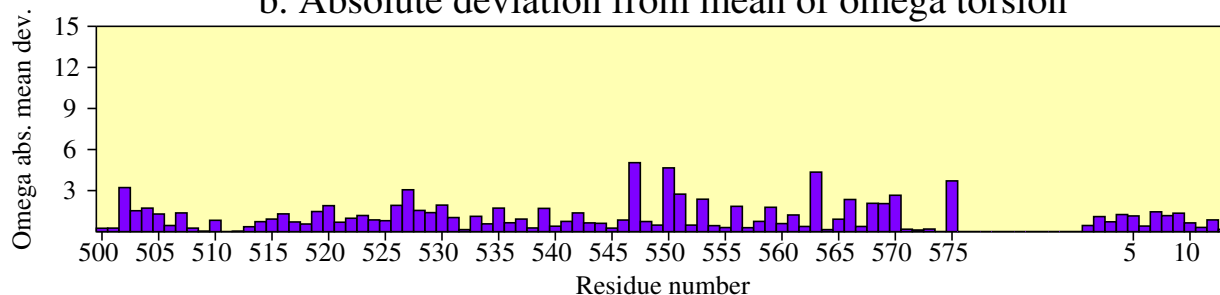
Residue properties

1kfy

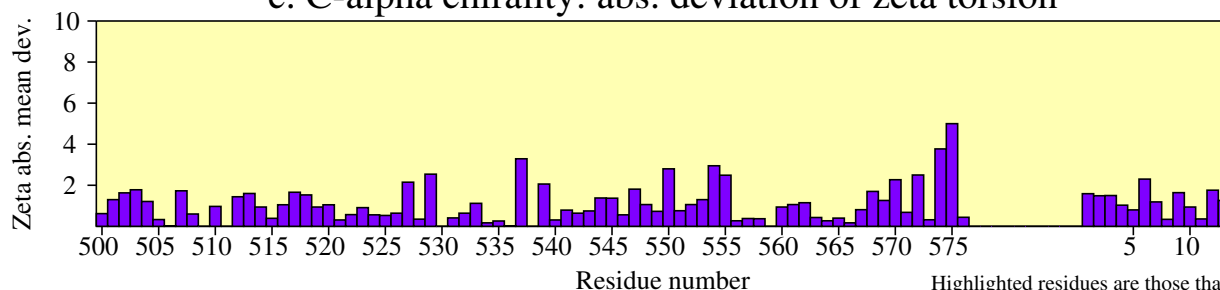
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

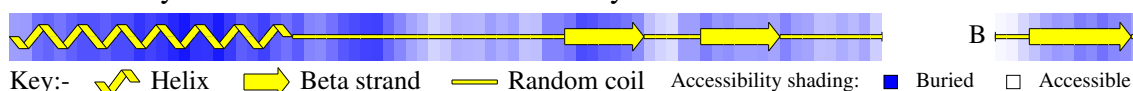


c. C-alpha chirality: abs. deviation of zeta torsion



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

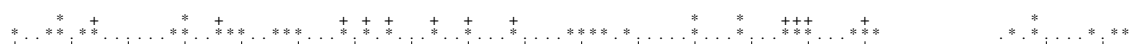
d. Secondary structure & estimated accessibility



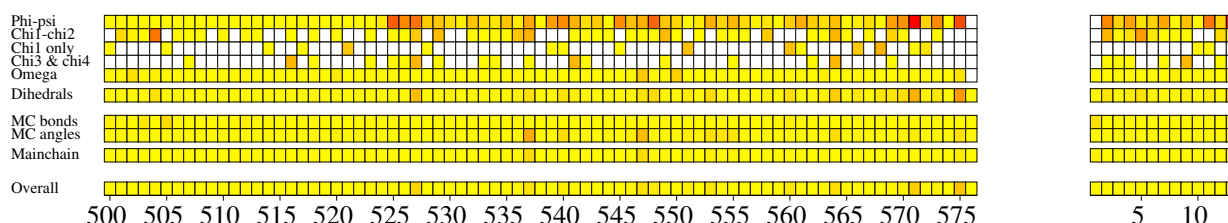
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



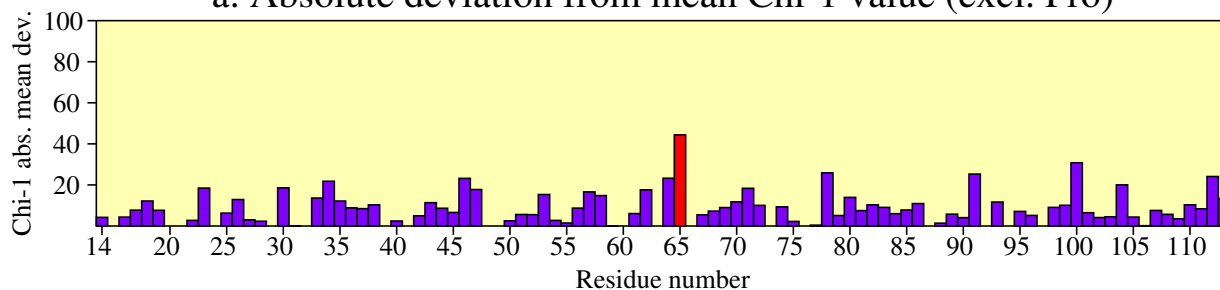
g. G-factors



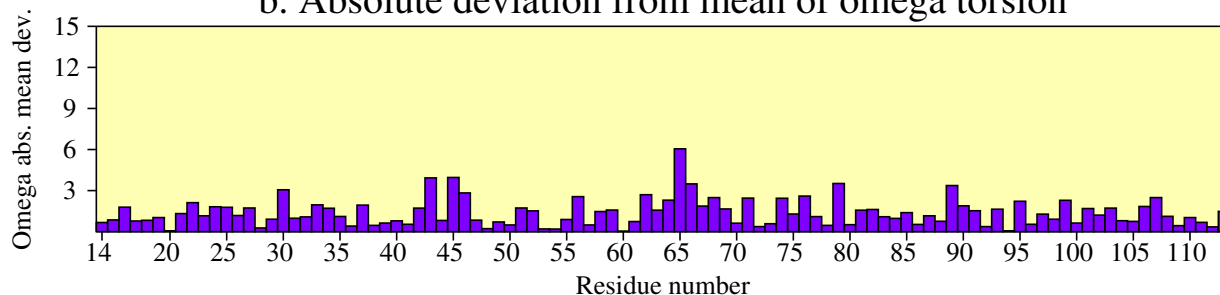
Residue properties

1kfy

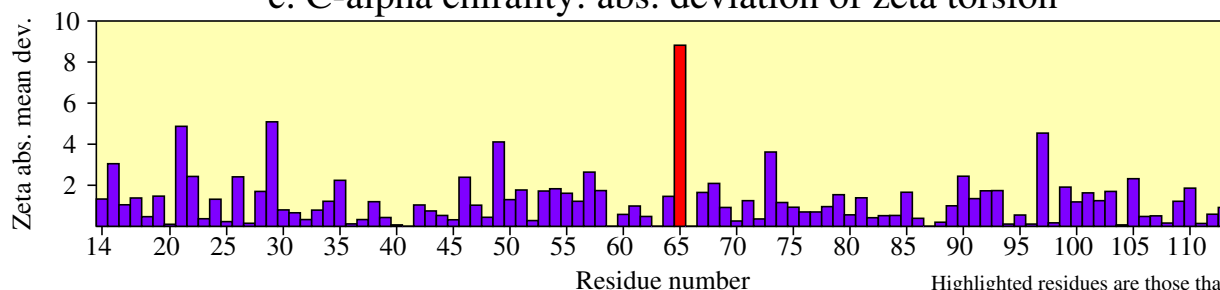
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

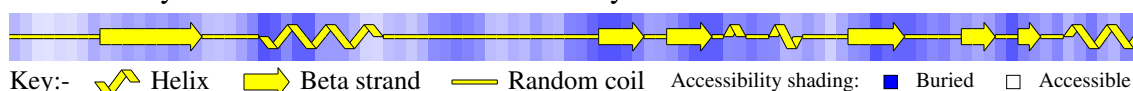


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



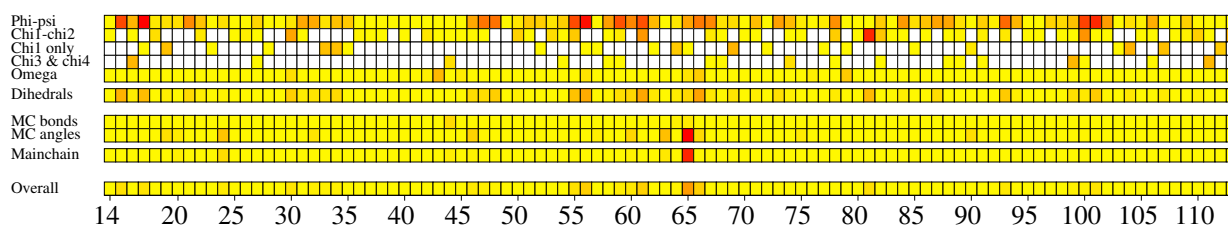
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



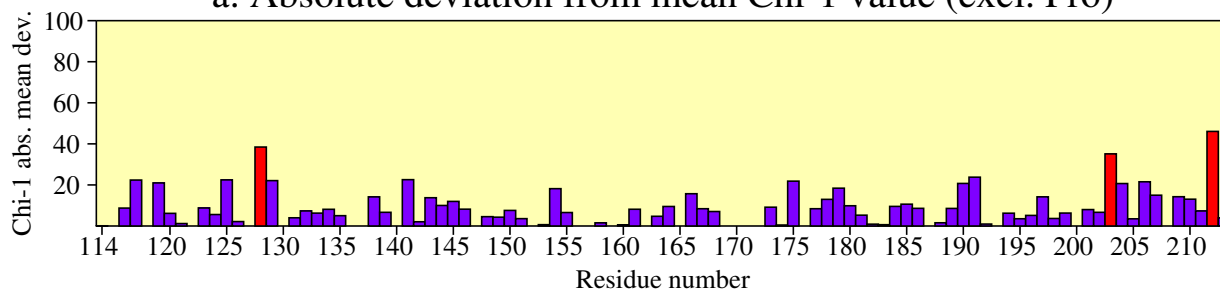
g. G-factors



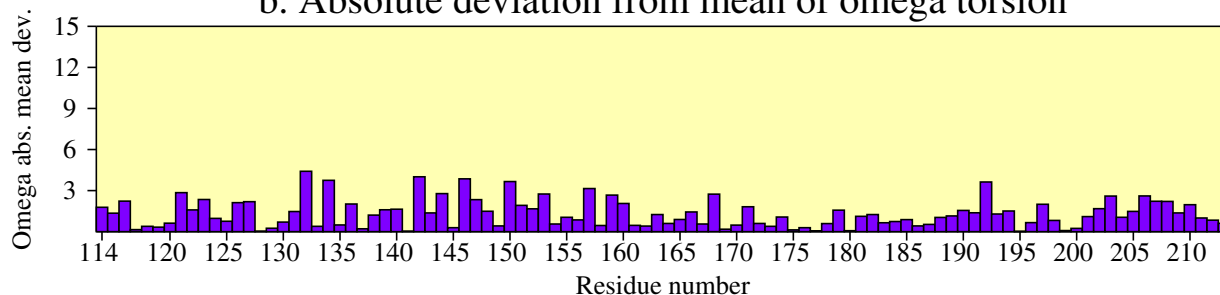
Residue properties

1kfy

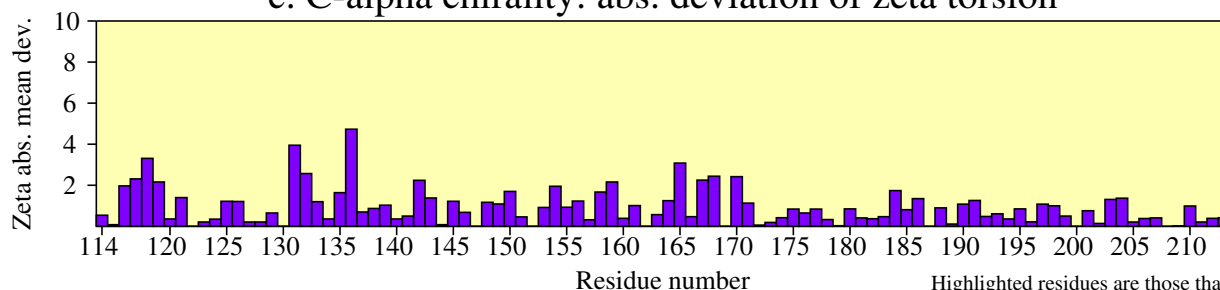
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

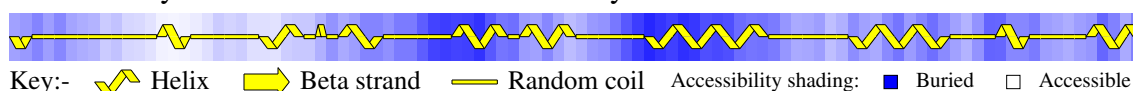


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



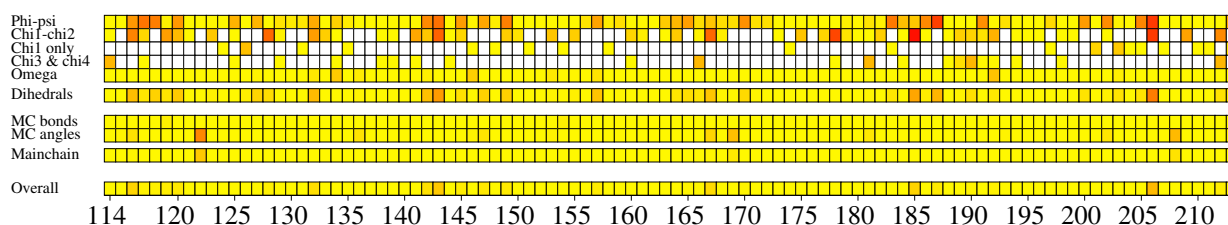
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



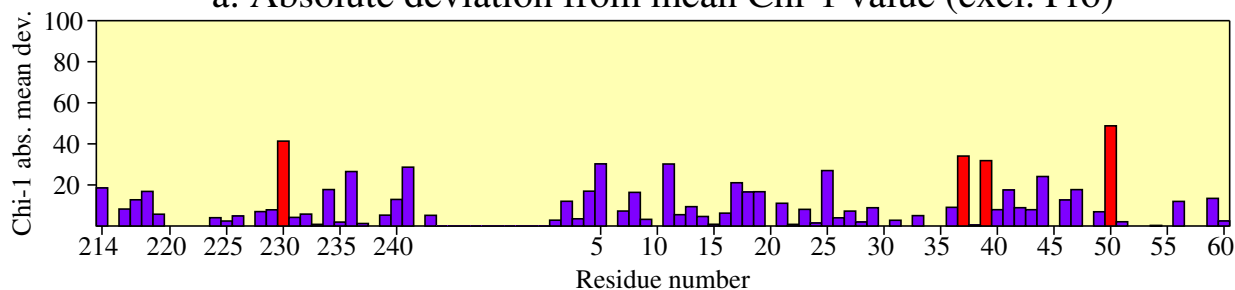
g. G-factors



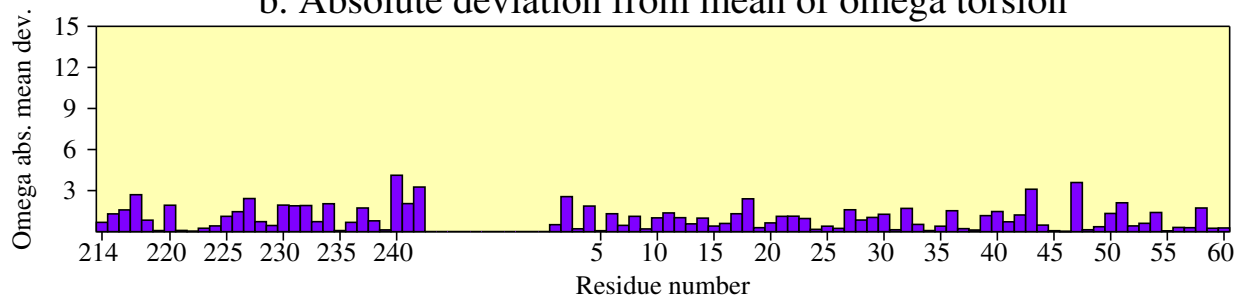
Residue properties

1kfy

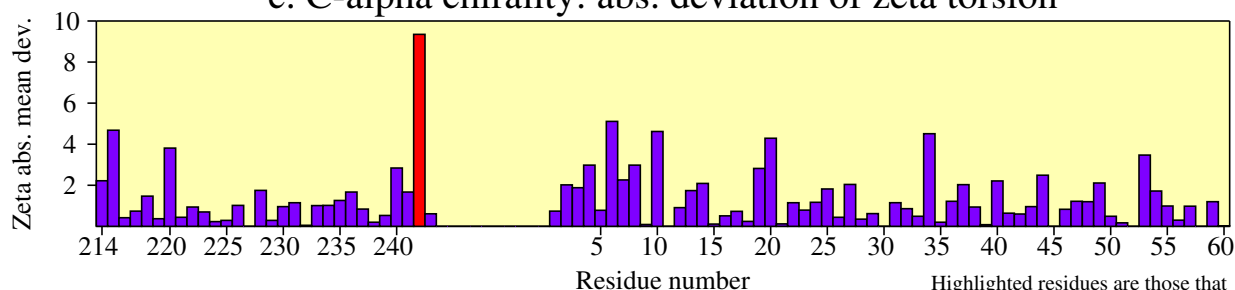
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

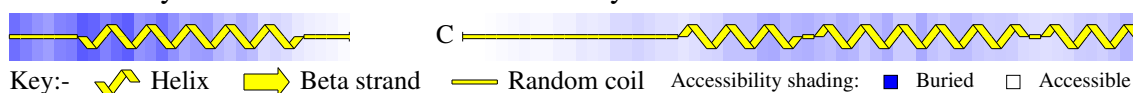


c. C-alpha chirality: abs. deviation of zeta torsion



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

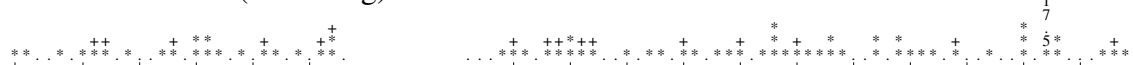
d. Secondary structure & estimated accessibility



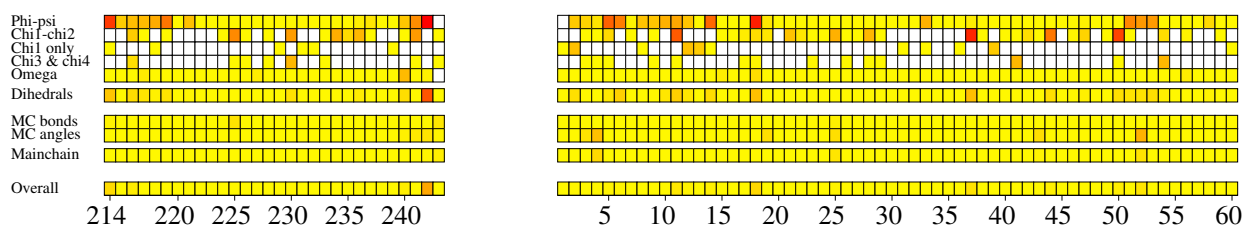
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



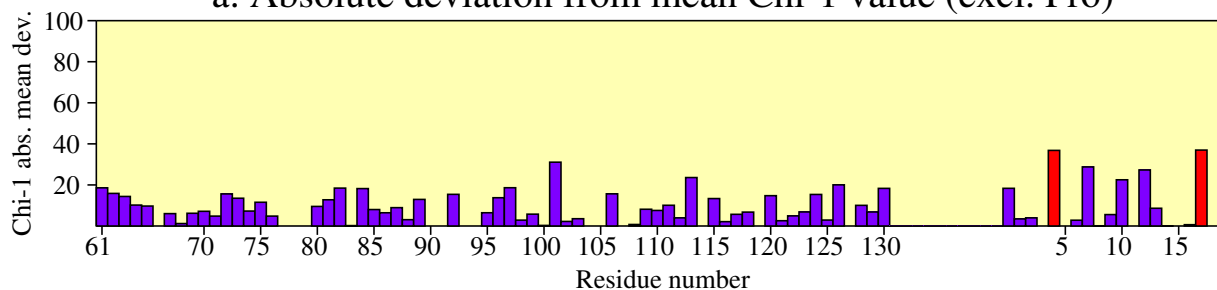
g. G-factors



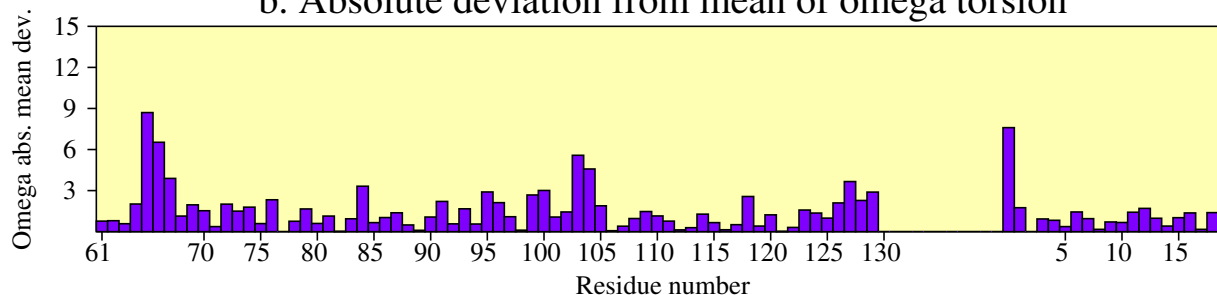
Residue properties

1kfy

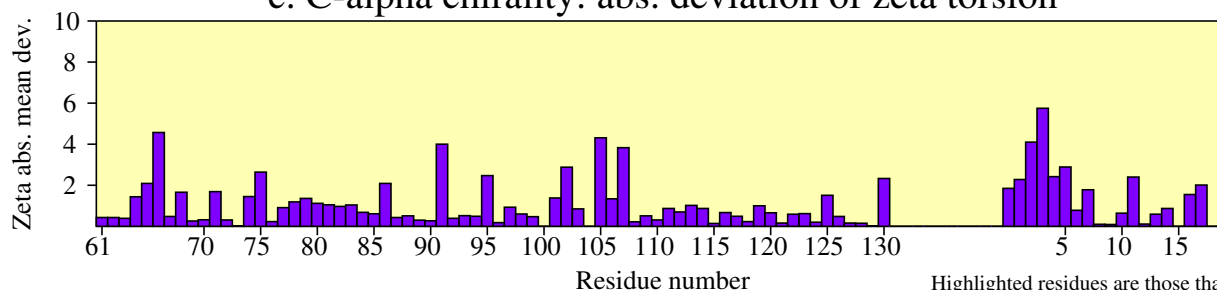
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

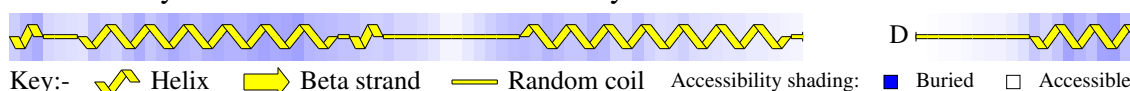


c. C-alpha chirality: abs. deviation of zeta torsion

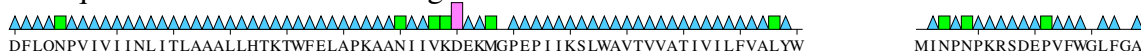


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



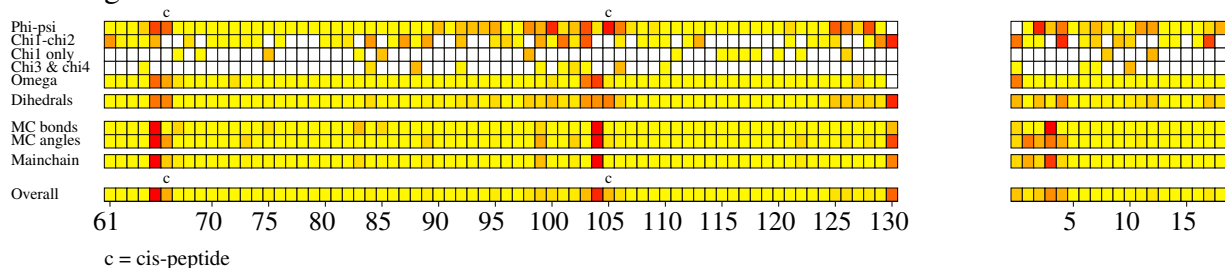
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



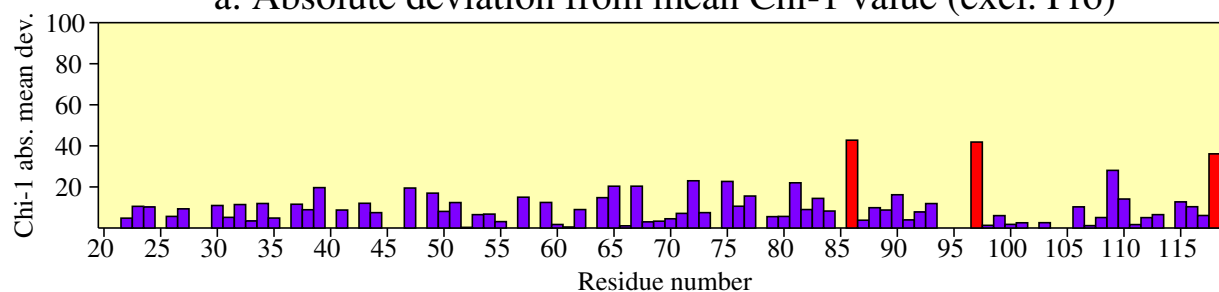
g. G-factors



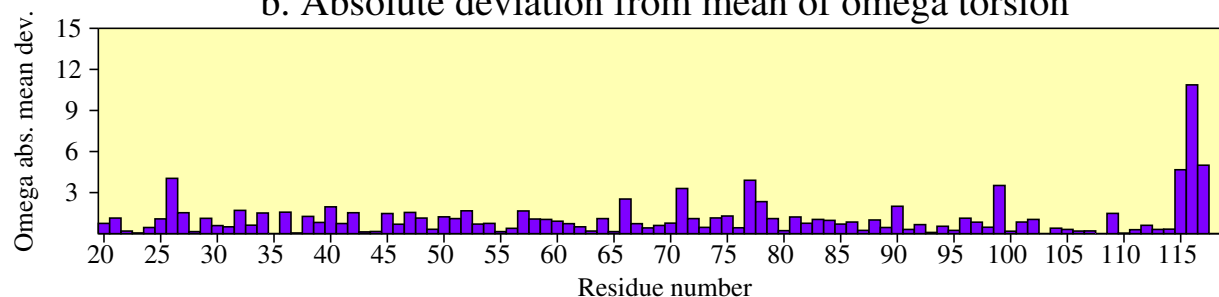
Residue properties

1kfy

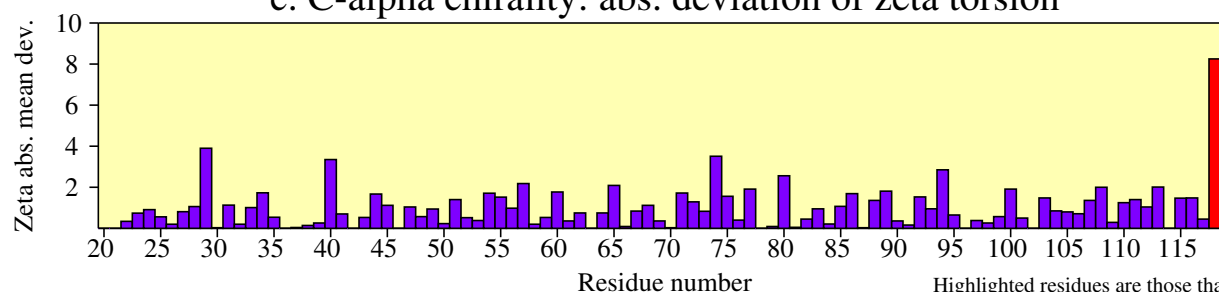
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

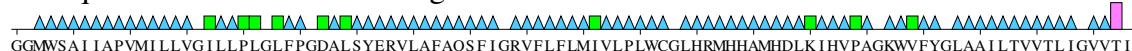


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

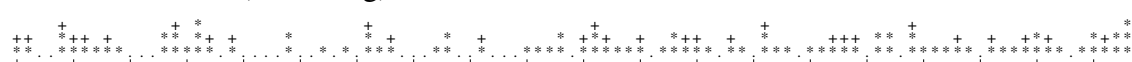
d. Secondary structure & estimated accessibility



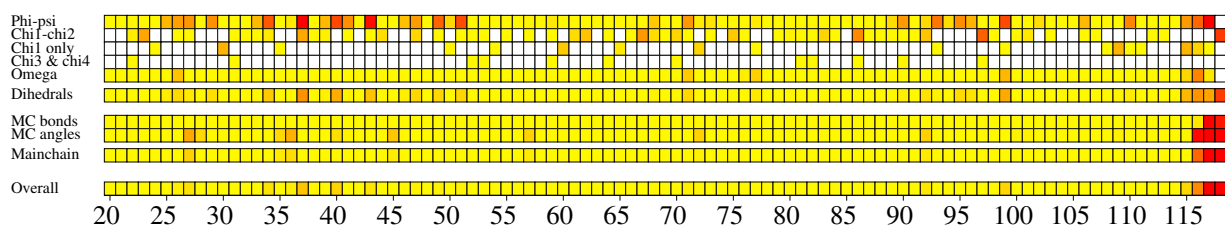
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



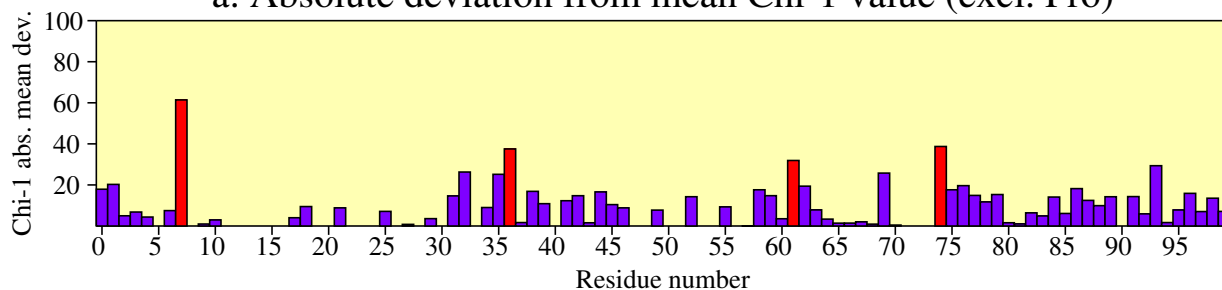
g. G-factors



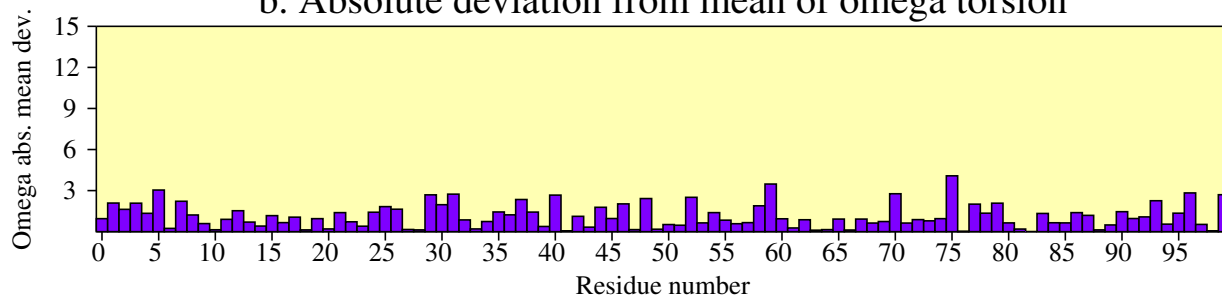
Residue properties

1kfy

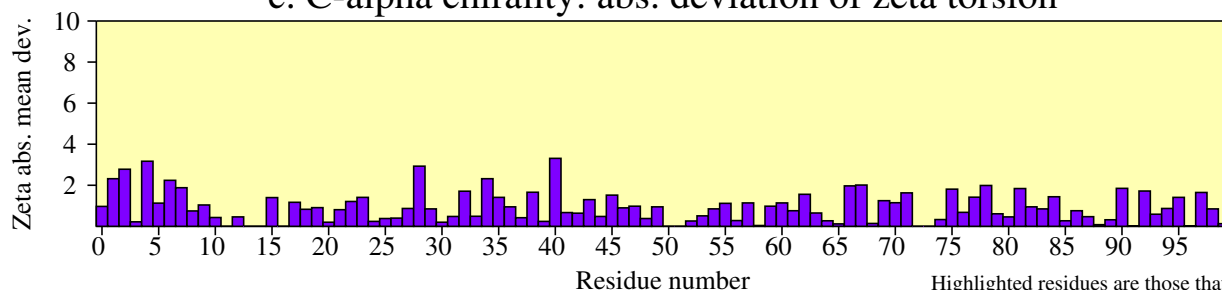
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



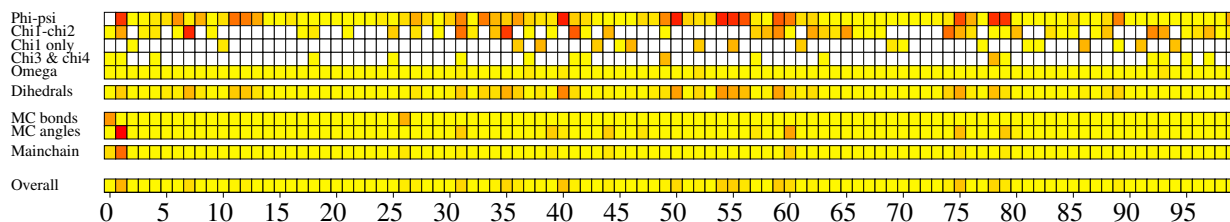
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

MQTFQADLAIVGAGGAGLRAAIAAAQANPNAKIALISKVYPMRSHTVAAEGGSAAVAQDHDSEFYHFDHTVAGGDWLCEDVDYFVHHCPTEMTQLELW

f. Max. deviation (see listing)



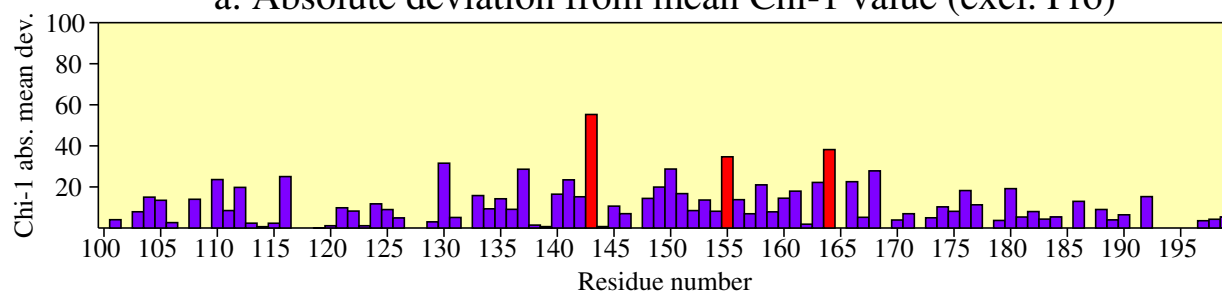
g. G-factors



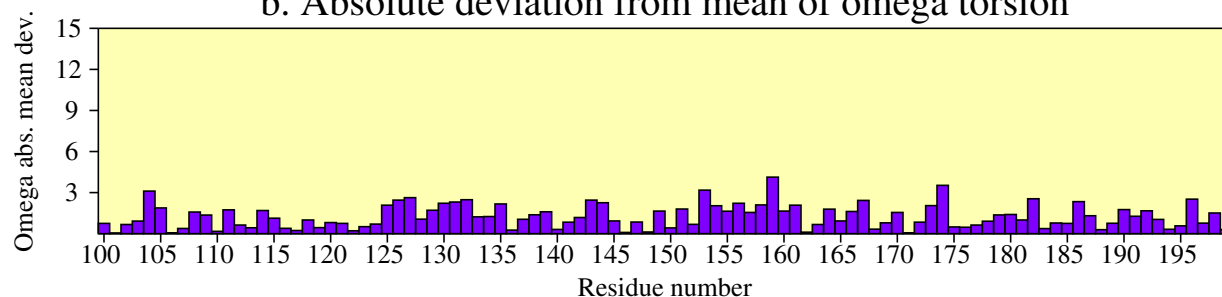
Residue properties

1kfy

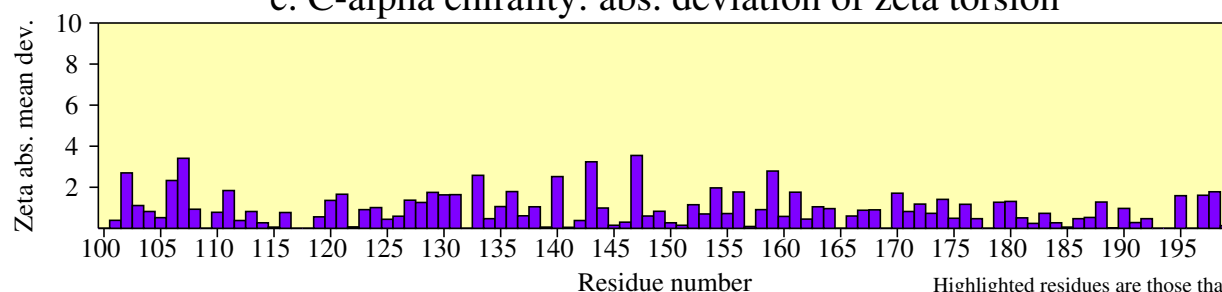
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

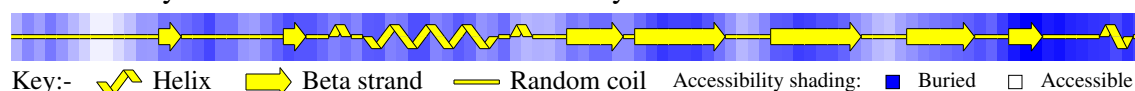


c. C-alpha chirality: abs. deviation of zeta torsion



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

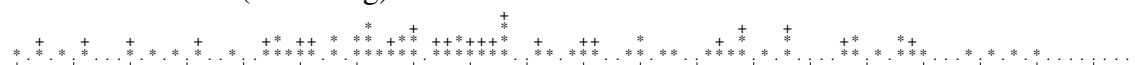
d. Secondary structure & estimated accessibility



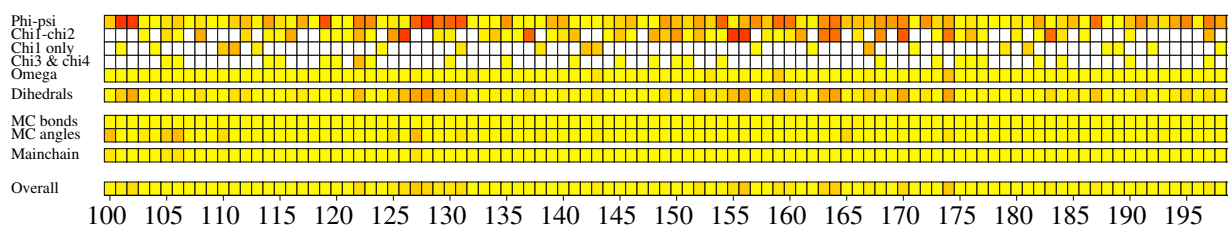
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



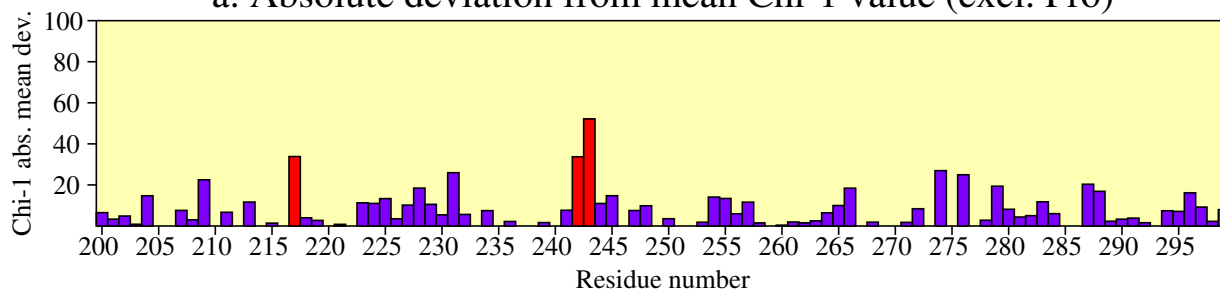
g. G-factors



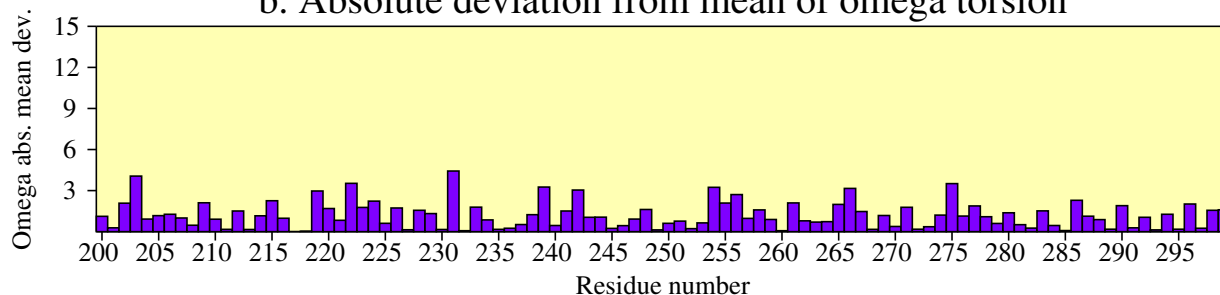
Residue properties

1kfy

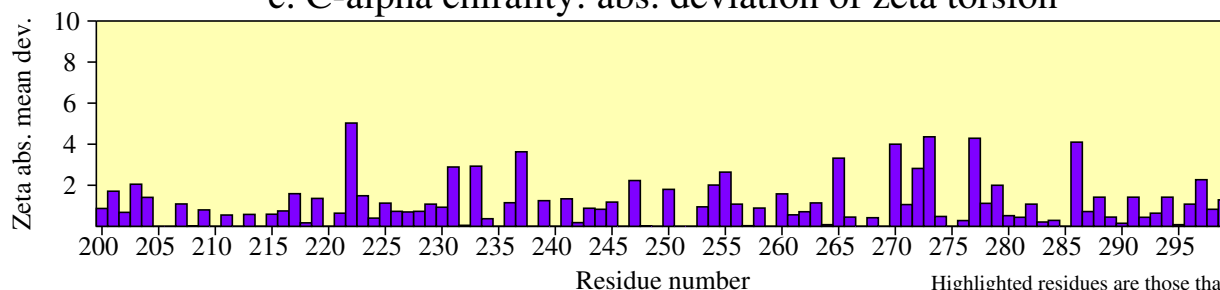
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

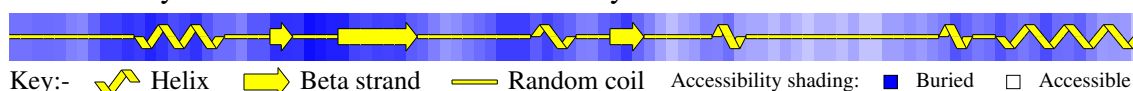


c. C-alpha chirality: abs. deviation of zeta torsion



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

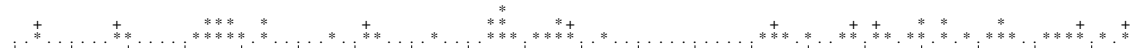
d. Secondary structure & estimated accessibility



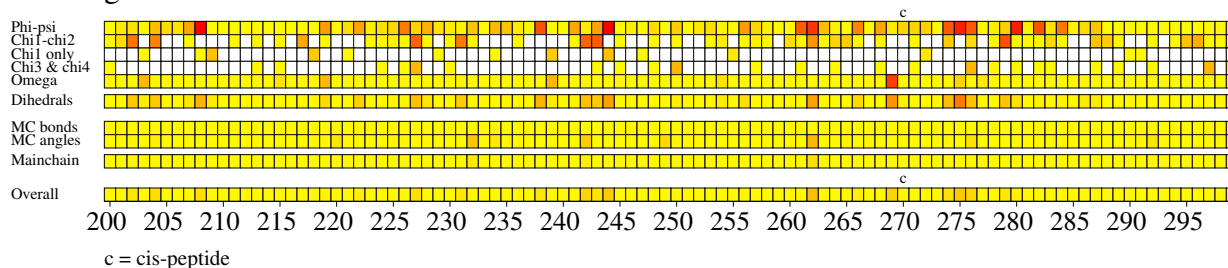
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



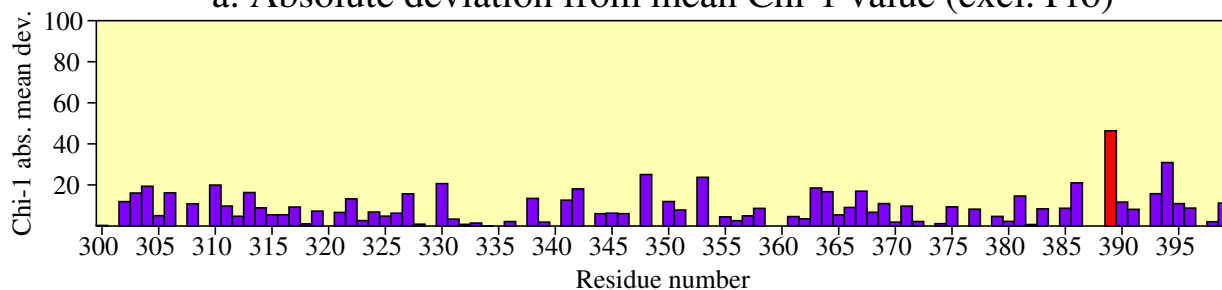
g. G-factors



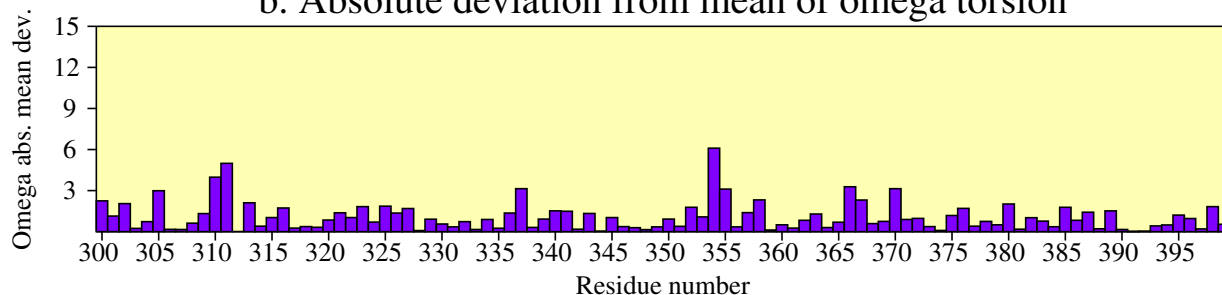
Residue properties

1kfy

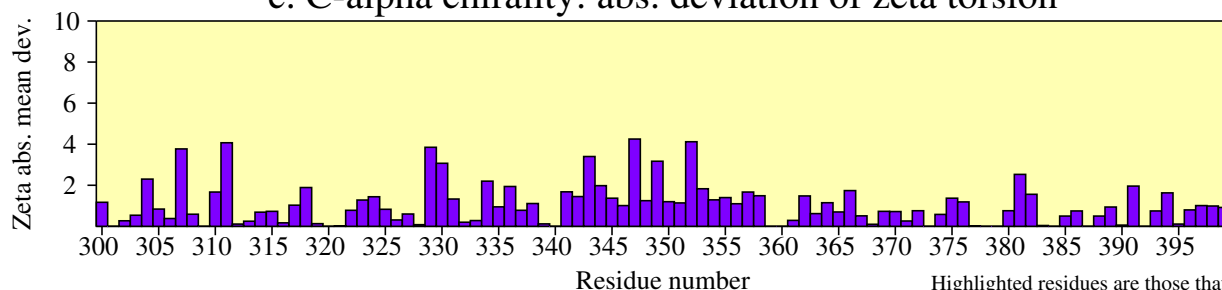
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

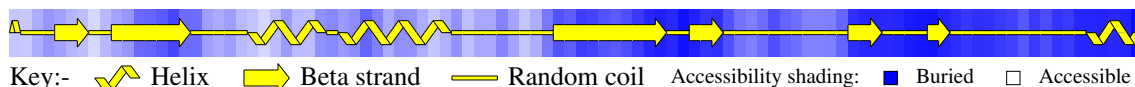


c. C-alpha chirality: abs. deviation of zeta torsion



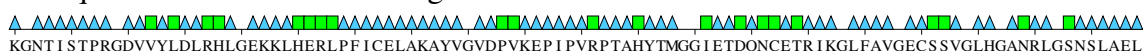
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

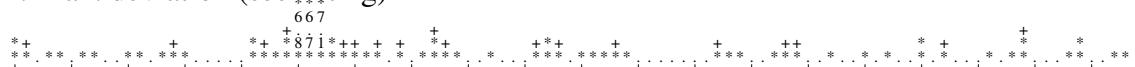


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

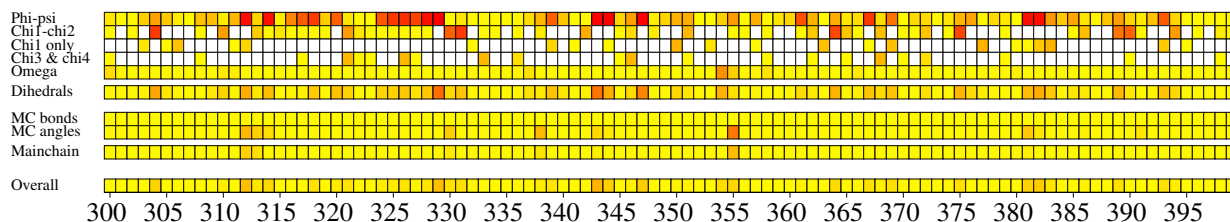
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



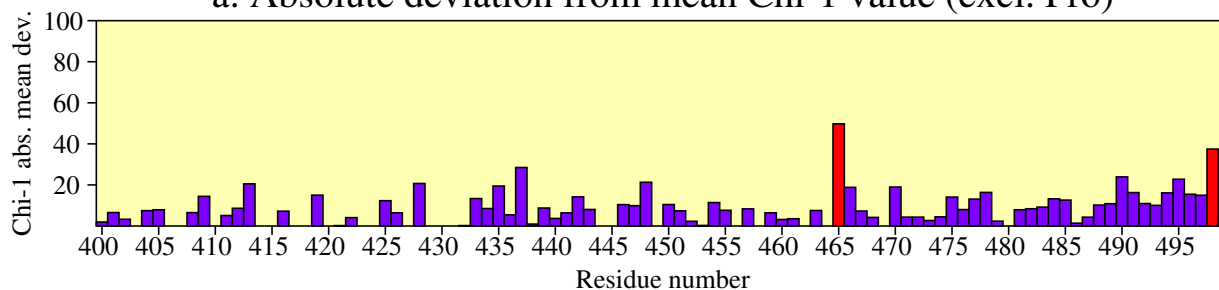
g. G-factors



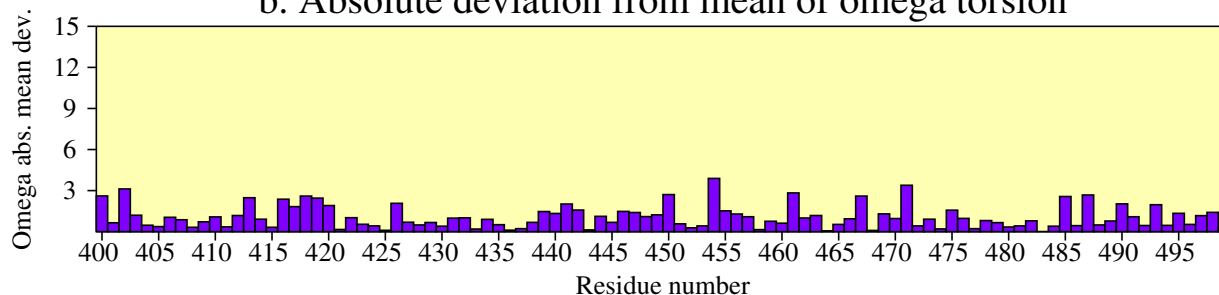
Residue properties

1kfy

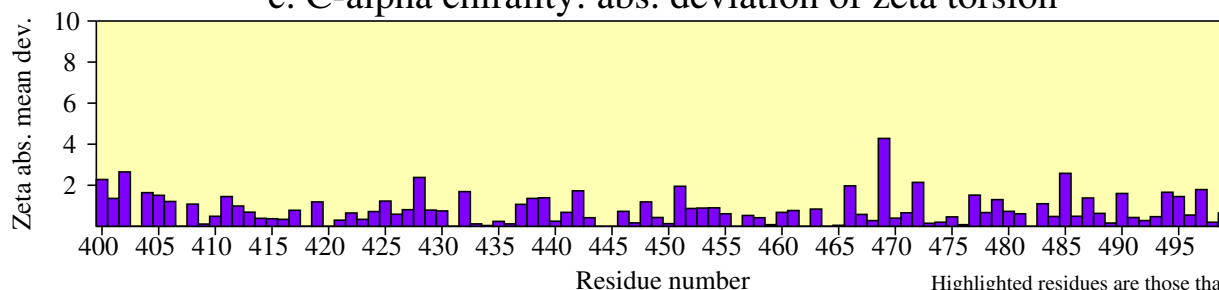
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

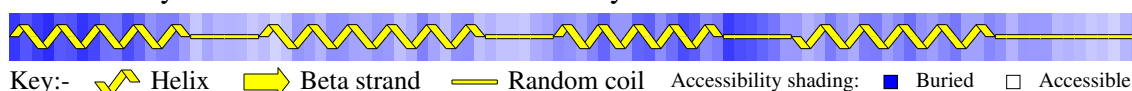


c. C-alpha chirality: abs. deviation of zeta torsion

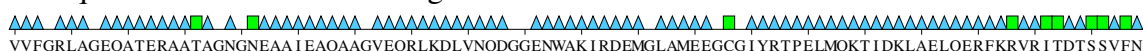


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



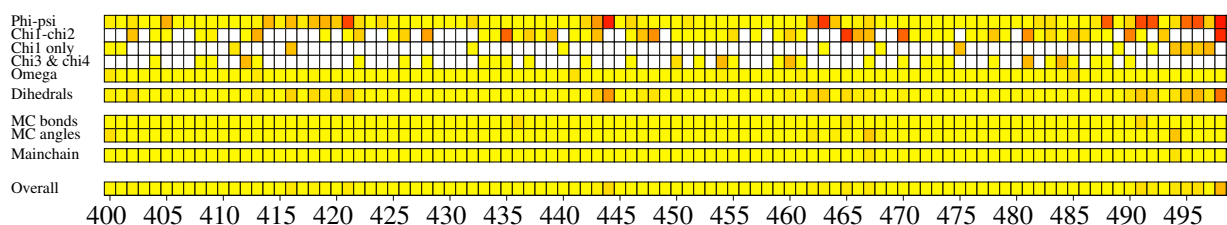
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



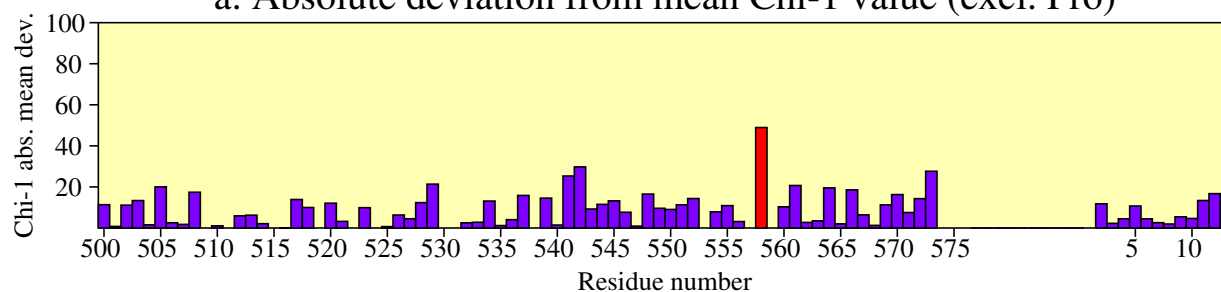
g. G-factors



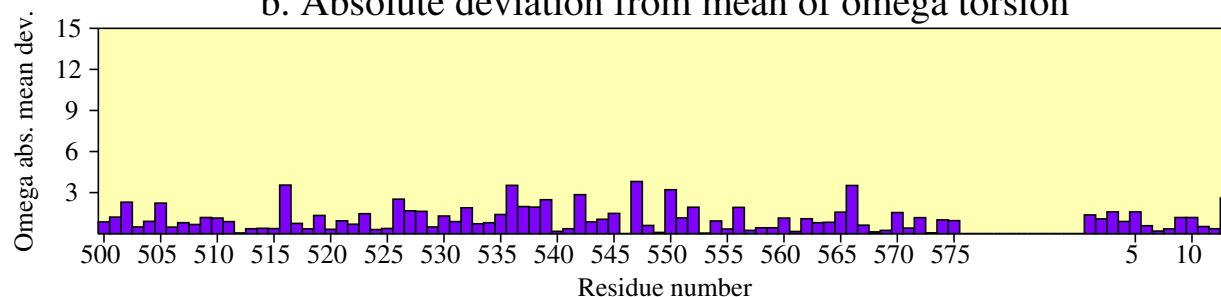
Residue properties

1kfy

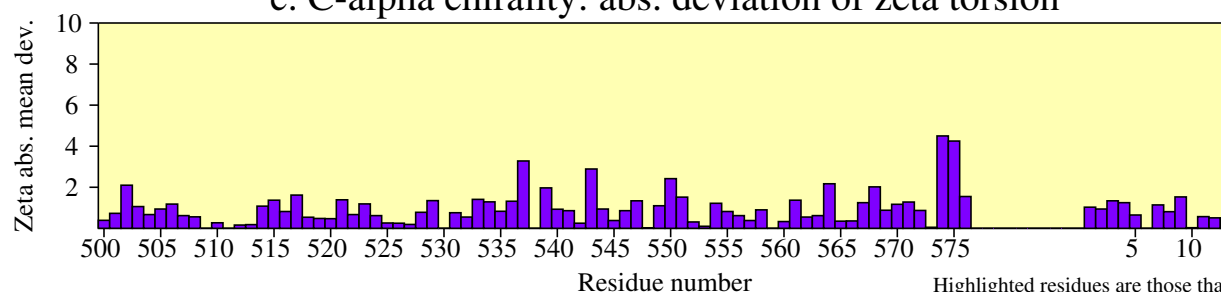
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

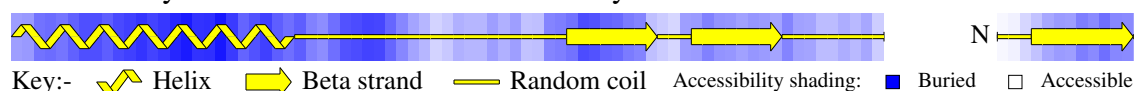


c. C-alpha chirality: abs. deviation of zeta torsion

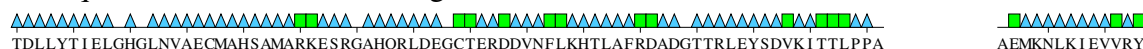


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

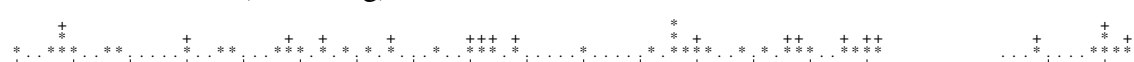
d. Secondary structure & estimated accessibility



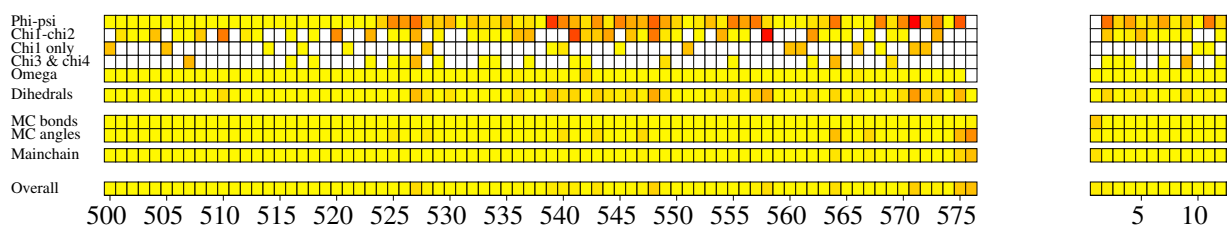
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



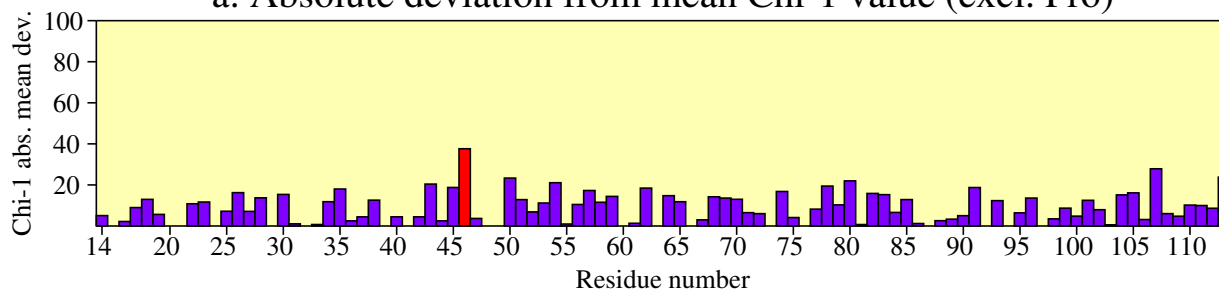
g. G-factors



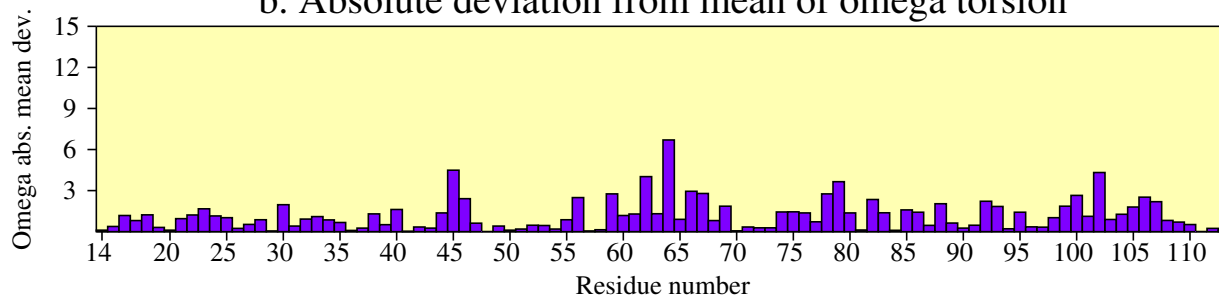
Residue properties

1kfy

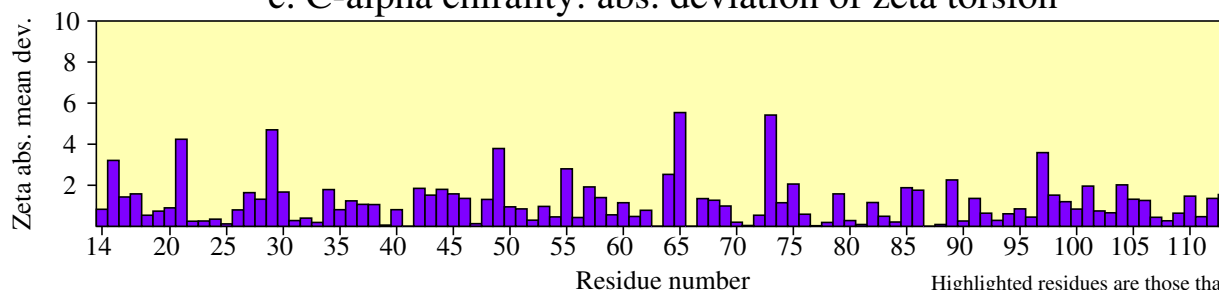
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

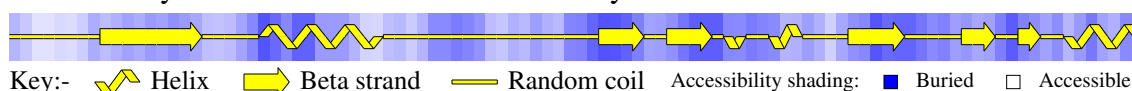


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



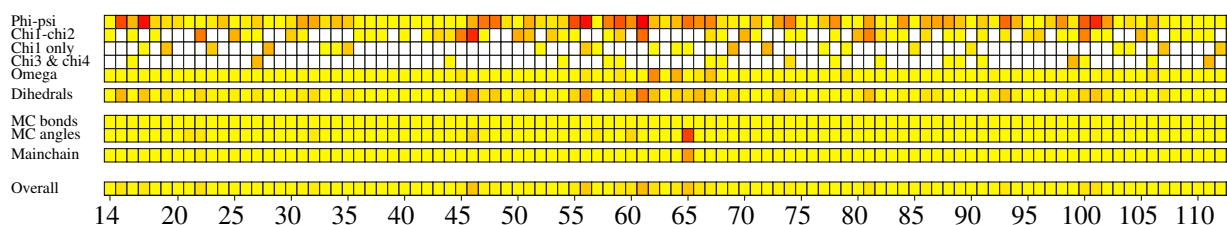
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



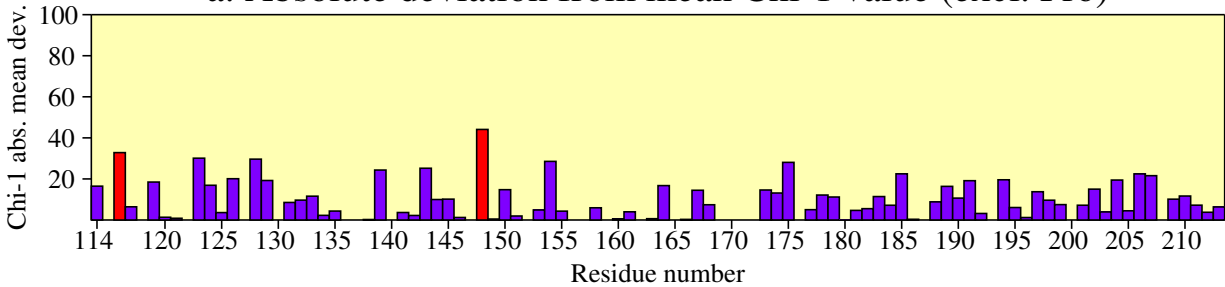
g. G-factors



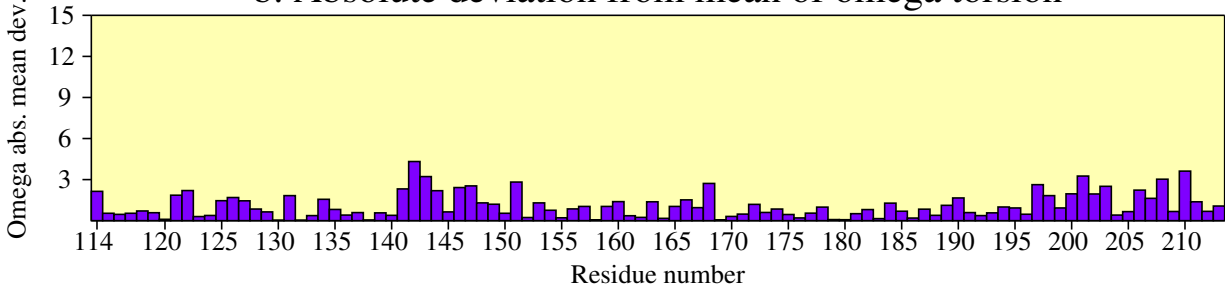
Residue properties

1kfy

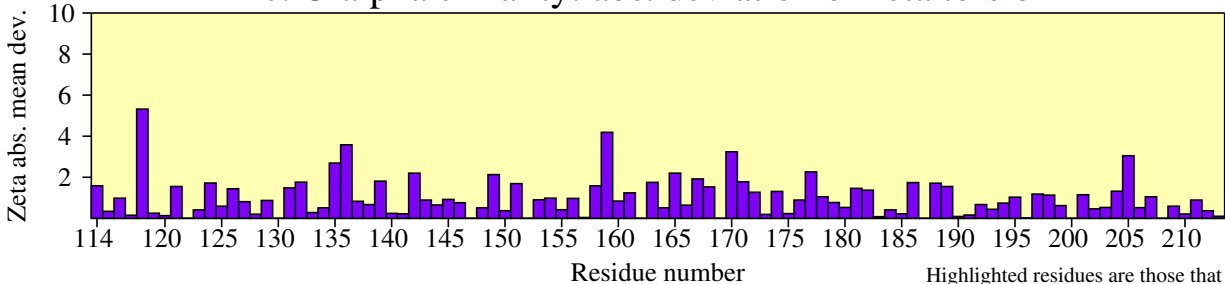
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

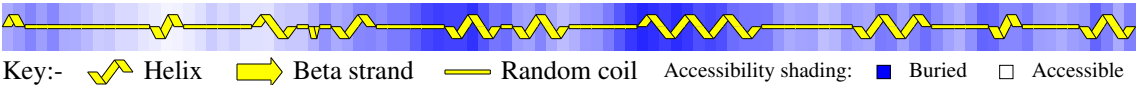


c. C-alpha chirality: abs. deviation of zeta torsion



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

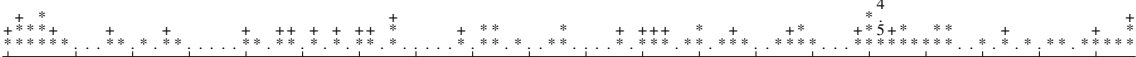
d. Secondary structure & estimated accessibility



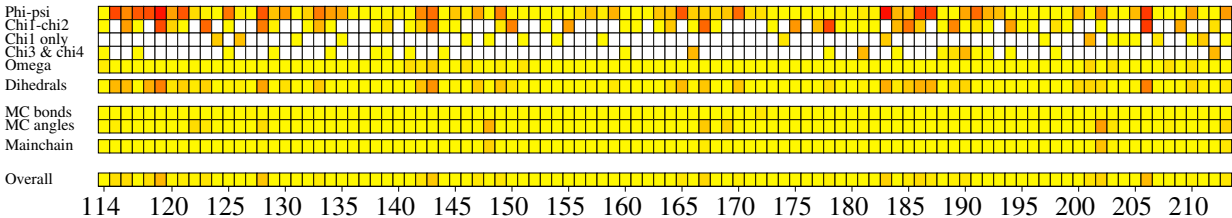
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



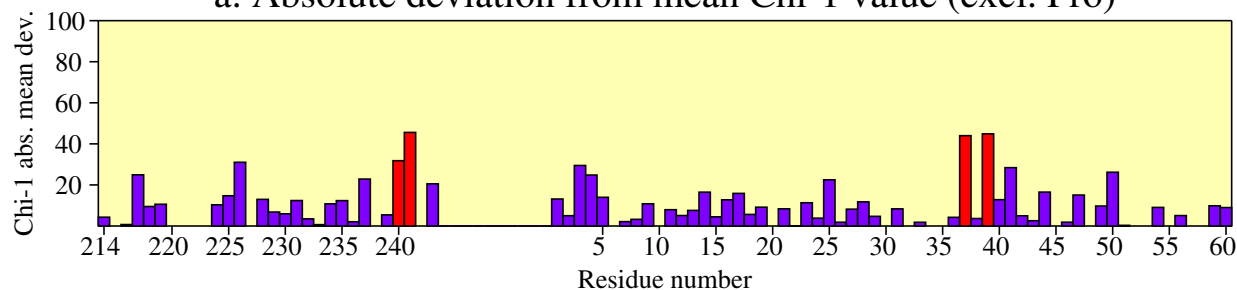
g. G-factors



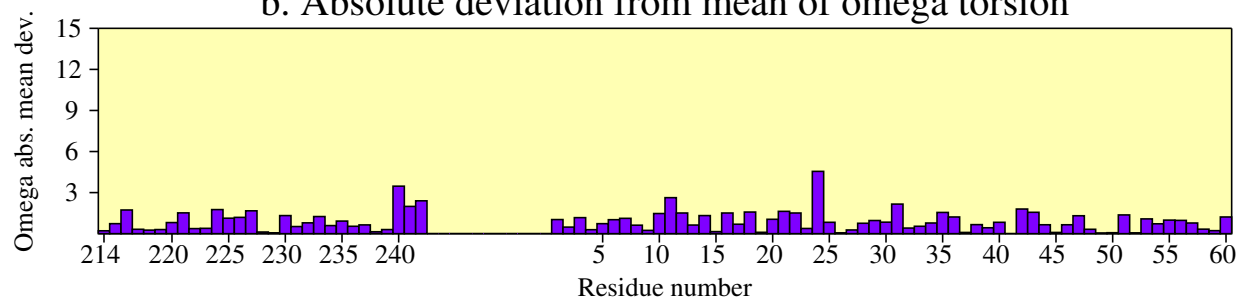
Residue properties

1kfy

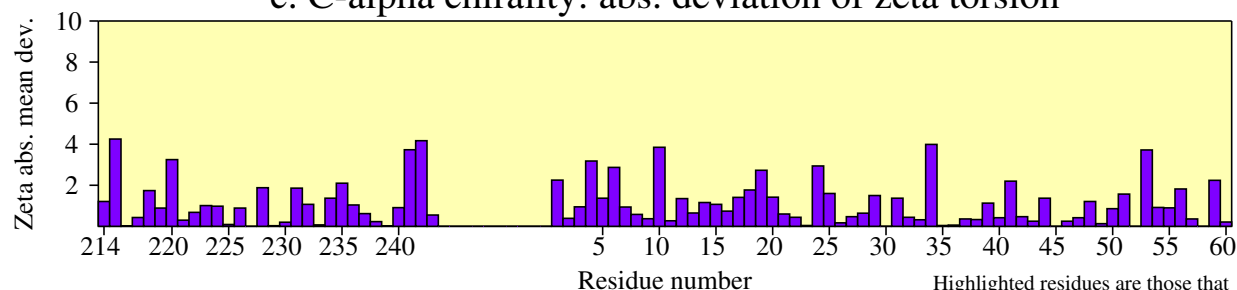
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

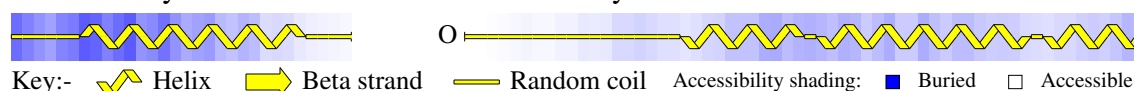


c. C-alpha chirality: abs. deviation of zeta torsion

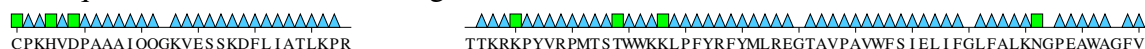


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



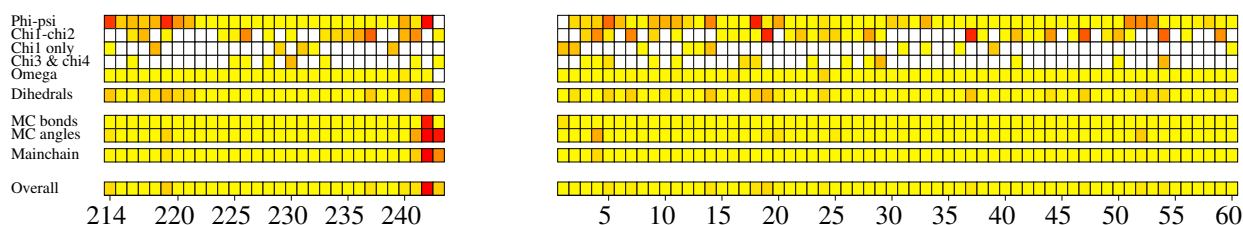
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



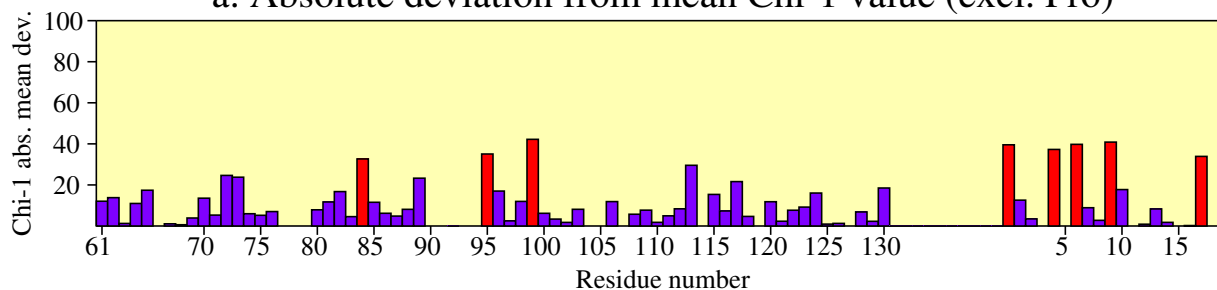
g. G-factors



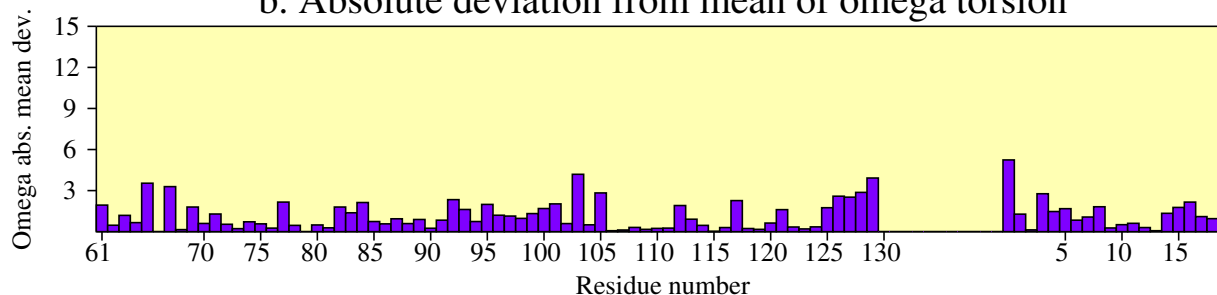
Residue properties

1kfy

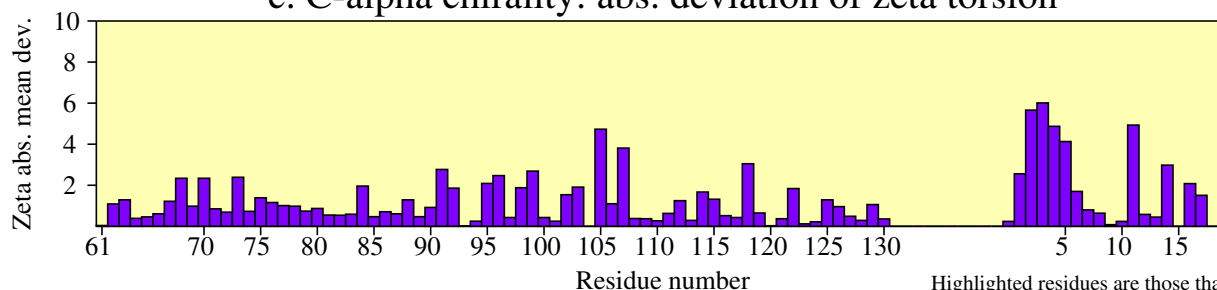
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

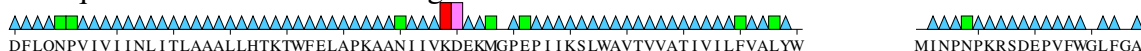


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



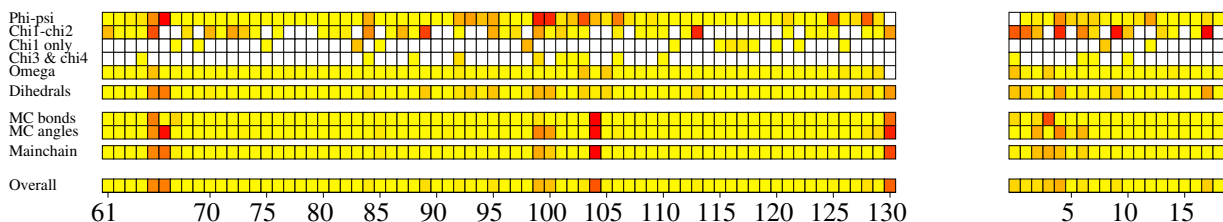
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



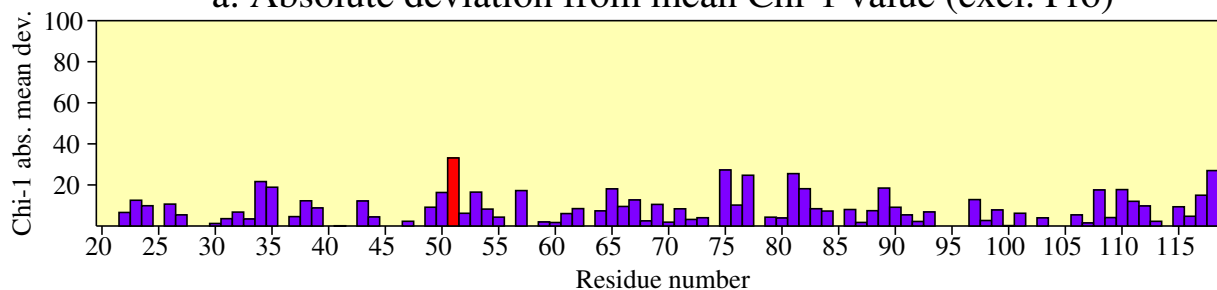
g. G-factors



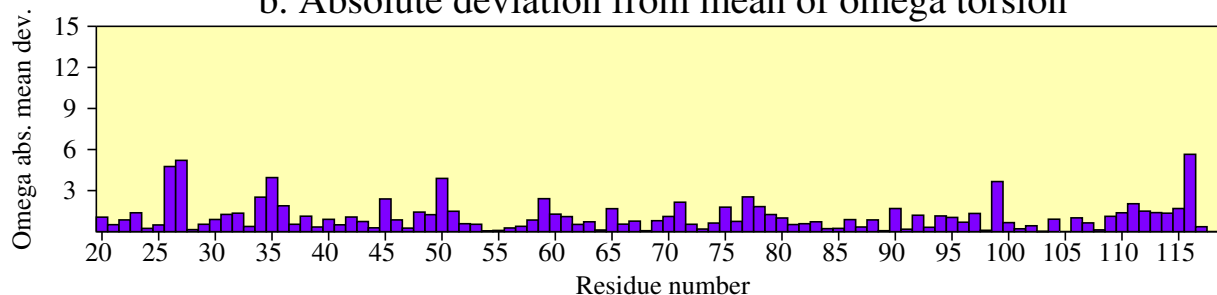
Residue properties

1kfy

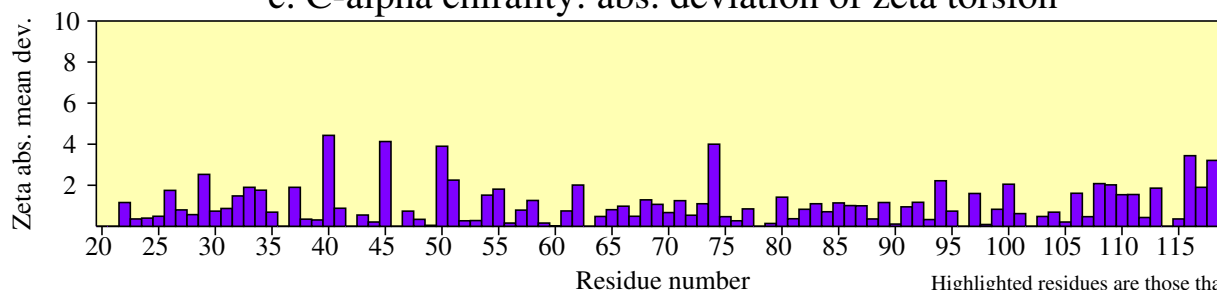
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

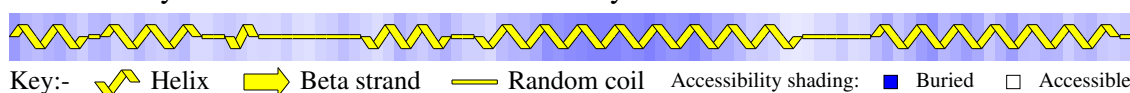


c. C-alpha chirality: abs. deviation of zeta torsion

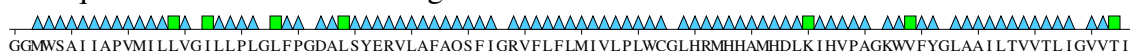


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

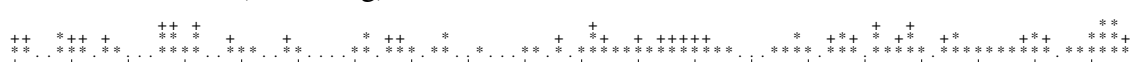
d. Secondary structure & estimated accessibility



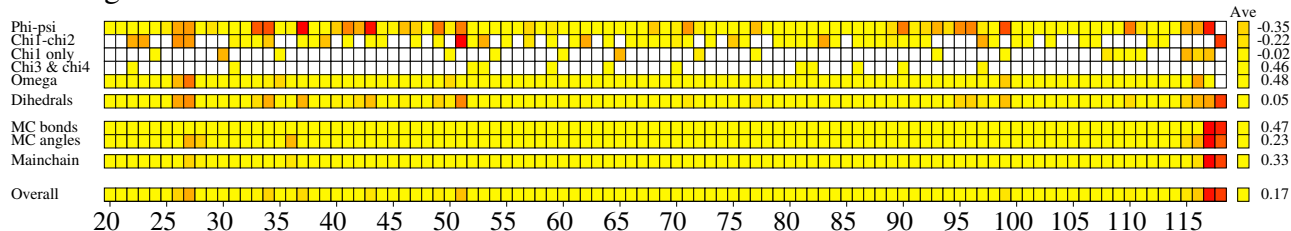
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

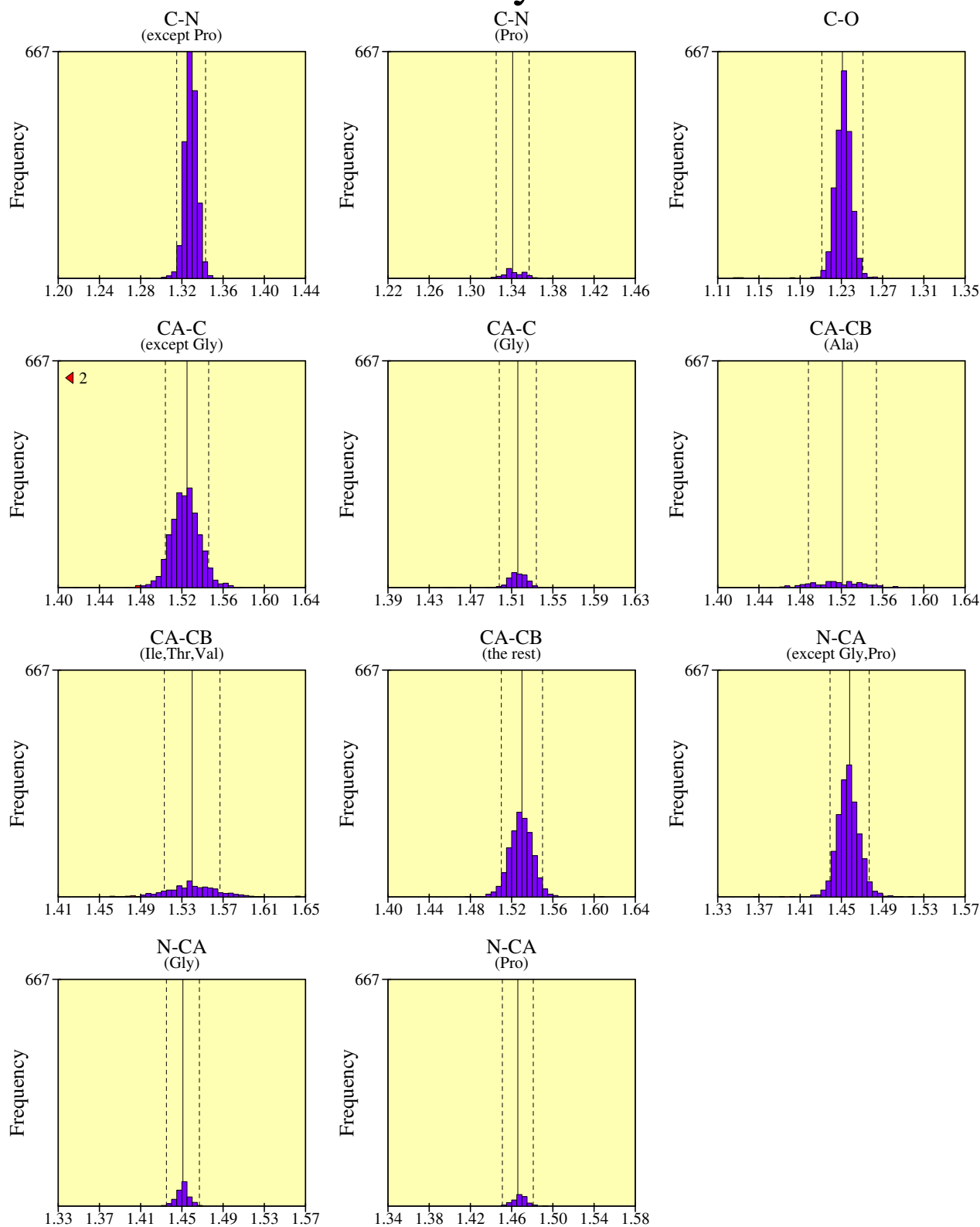


g. G-factors



Main-chain bond lengths

1kfy



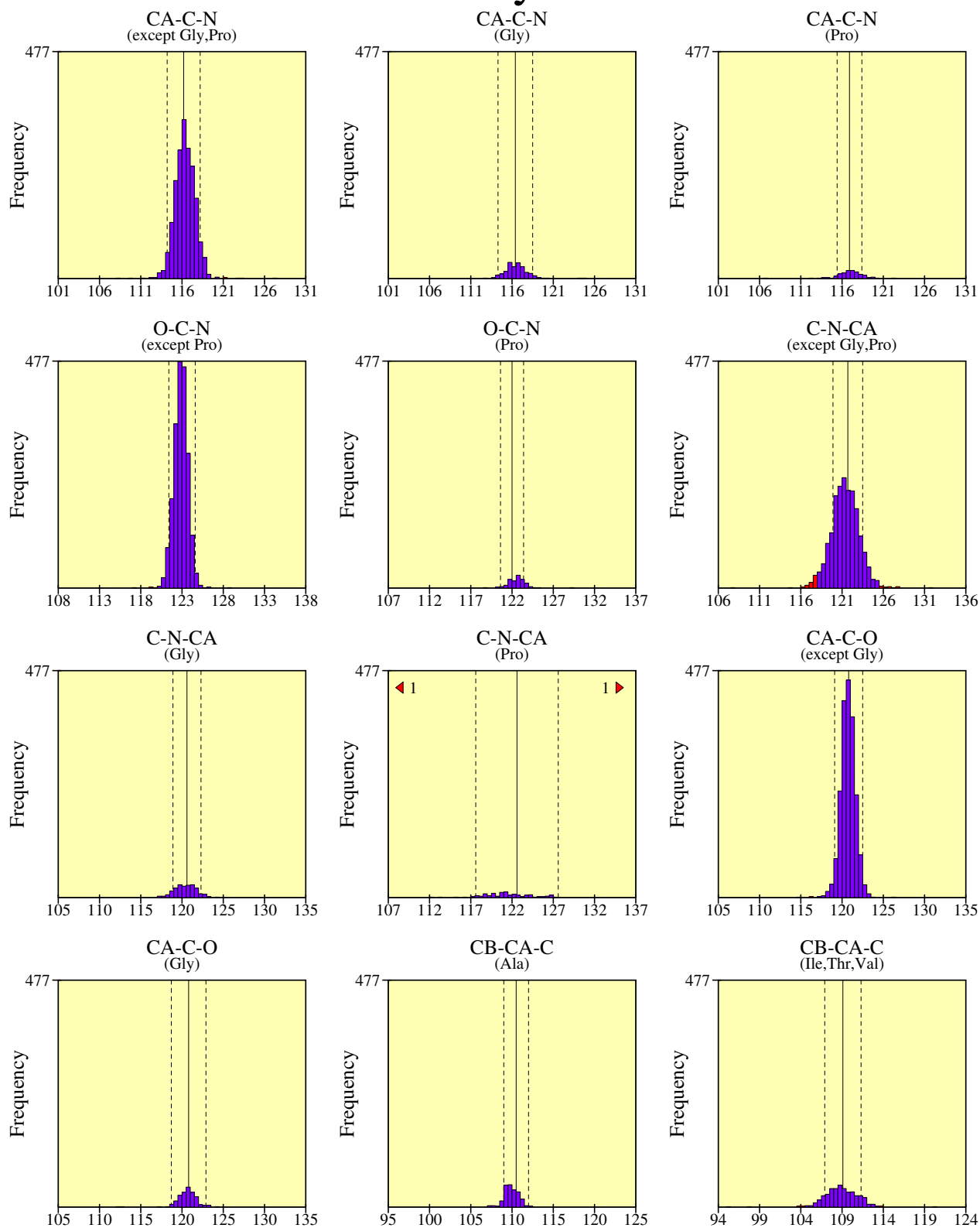
Black bars > 2.0 st. devs. from mean.

◀ 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

1kfy



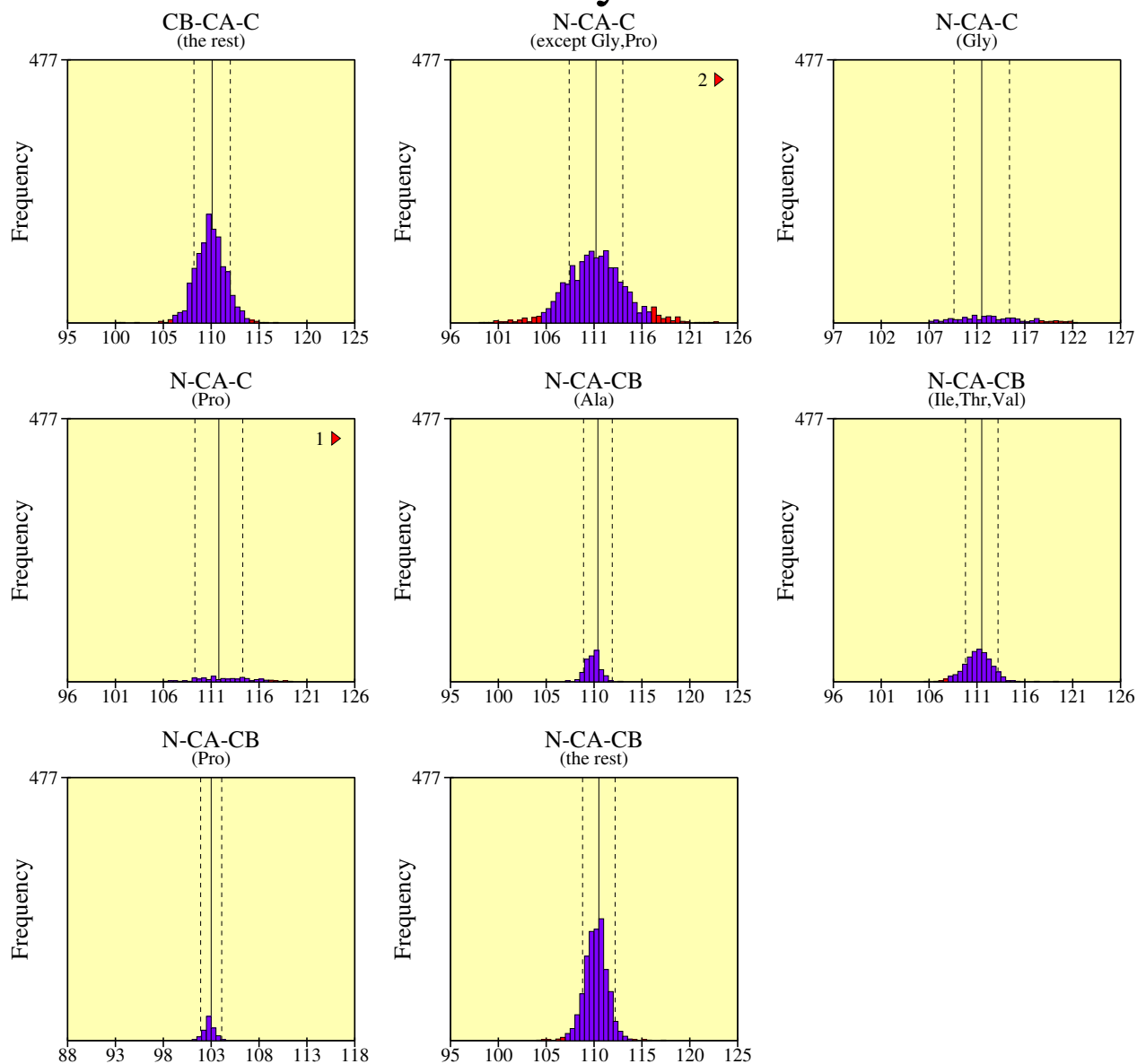
Black bars > 2.0 st. devs. from mean.

◀ 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

1kfy



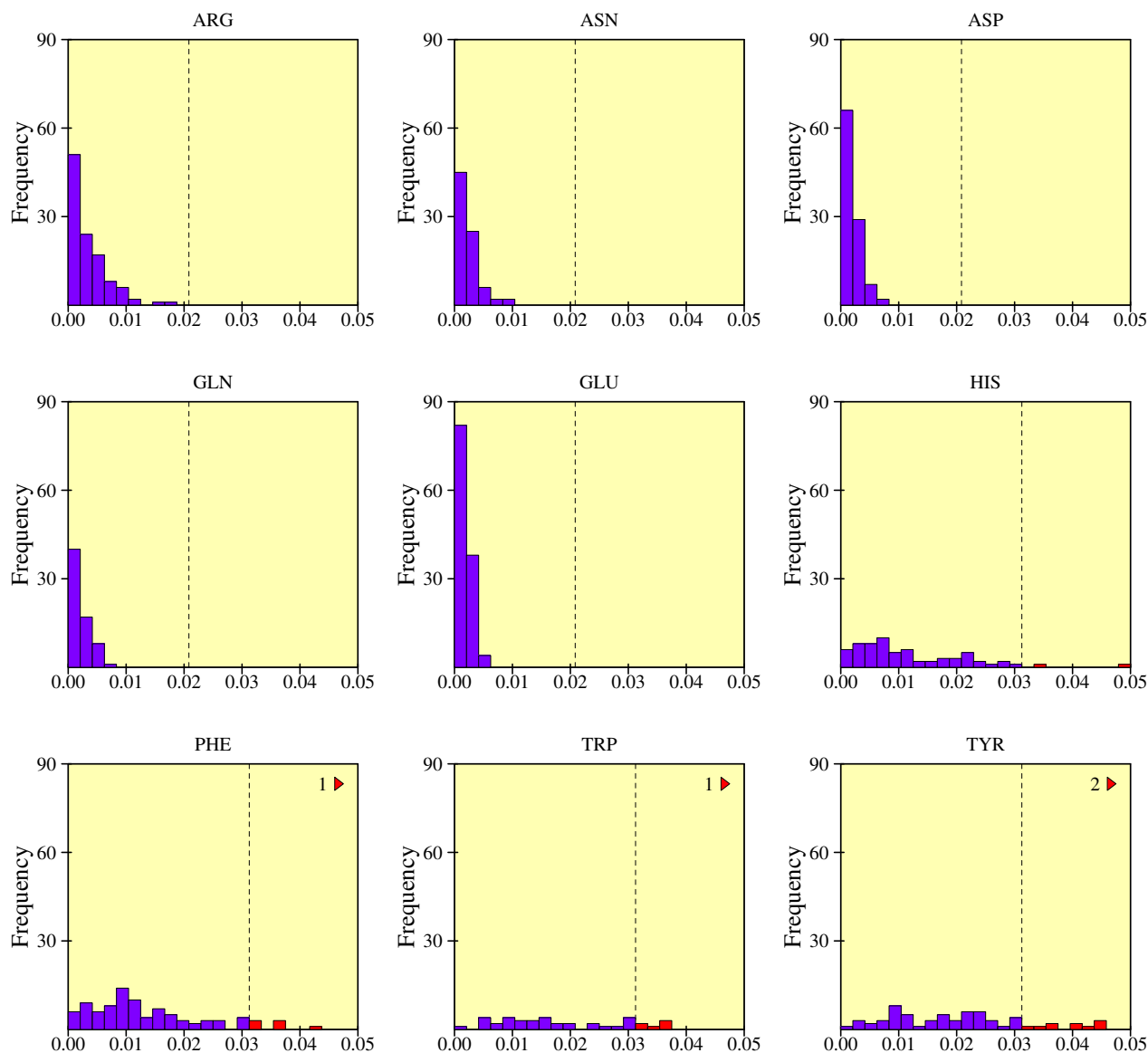
Black bars > 2.0 st. devs. from mean.

◀ 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

1kfy



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

1kfy

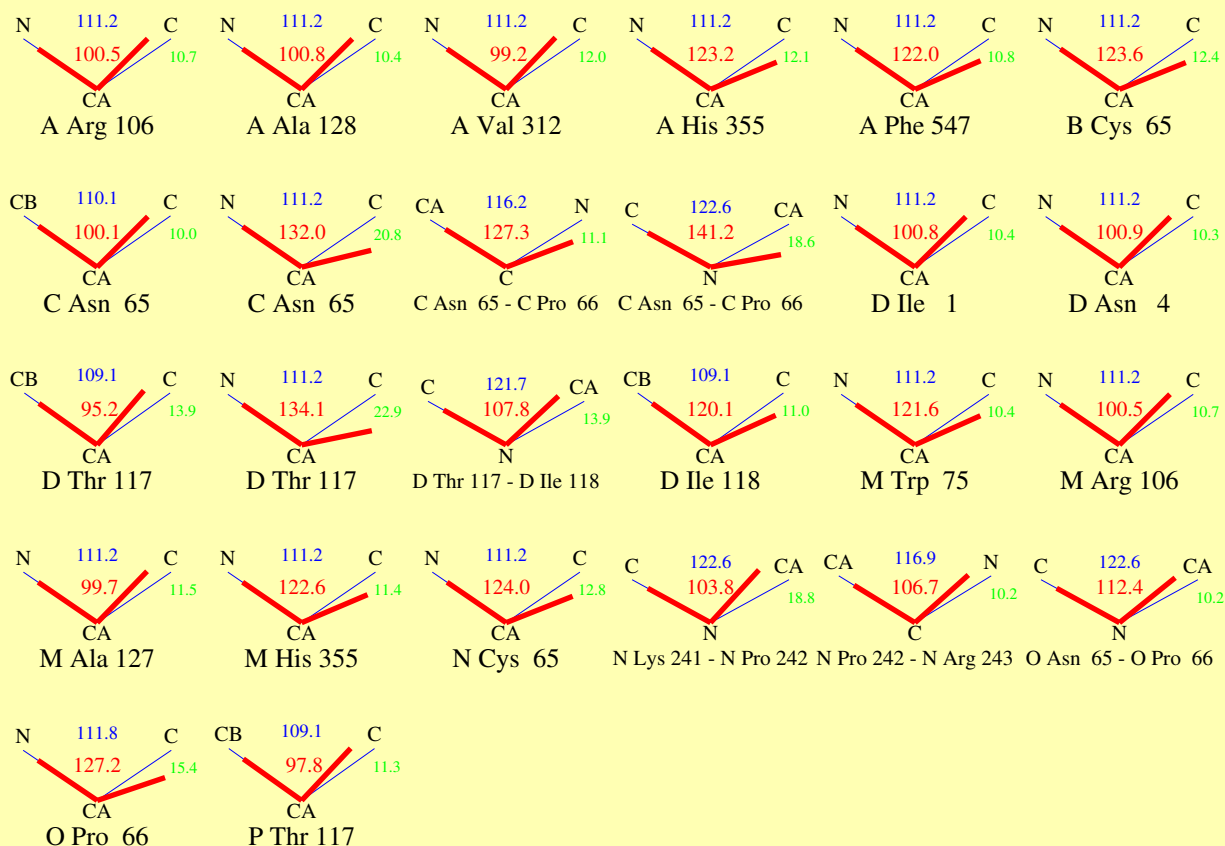
Main-chain bond lengths

CA 1.540 CB 0.061 1.479 A Val 10	CA 1.525 C 0.057 1.468 A Ser 43	CA 1.521 CB 0.055 1.466 A Ala 195	CA 1.540 CB 0.076 1.464 A Ile 241	CA 1.540 CB 0.063 1.477 A Thr 353	CA 1.521 CB 0.056 1.465 A Ala 458
CA 1.540 CB 0.057 1.597 A Thr 500	CA 1.540 CB 0.055 1.485 A Val 514	CA 1.521 CB 0.055 1.466 B Ala 24	CA 1.530 CB 0.050 1.480 B Cys 65	CA 1.540 CB 0.052 1.488 B Thr 131	CA 1.521 CB 0.057 1.464 B Ala 171
CA 1.540 CB 0.053 1.593 B Thr 174	CA 1.521 CB 0.054 1.467 C Ala 55	C 1.231 O 0.099 1.132 C Asn 65	N 1.458 CA 0.065 1.393 C Asn 65	CA 1.525 C 0.052 1.577 C Val 67	CA 1.540 CB 0.066 1.474 C Thr 75
CA 1.540 CB 0.078 1.462 C Thr 83	CA 1.540 CB 0.071 1.469 C Thr 85	C 1.231 O 0.102 1.129 C Gly 104	CA 1.516 C 0.066 1.450 C Gly 104	CA 1.521 CB 0.053 1.469 C Ala 114	C 1.231 O 0.105 1.126 D Pro 3
CA 1.525 C 0.167 1.358 D Thr 117	CA 1.540 CB 0.103 1.643 D Thr 117	N 1.458 CA 0.090 1.368 D Ile 118	N 1.458 CA 0.058 1.515 M Met 0	CA 1.521 CB 0.070 1.591 M Ala 26	CA 1.540 CB 0.057 1.483 M Val 312
CA 1.540 CB 0.067 1.607 M Ile 465	CA 1.540 CB 0.052 1.592 M Ile 491	CA 1.521 CB 0.052 1.573 M Ala 519	CA 1.540 CB 0.052 1.592 M Val 545	CA 1.521 CB 0.052 1.573 M Ala 557	CA 1.521 CB 0.057 1.464 M Ala 576
CA 1.521 CB 0.065 1.586 N Ala 1	CA 1.540 CB 0.058 1.482 N Thr 79	CA 1.521 CB 0.071 1.450 N Ala 172	CA 1.540 CB 0.053 1.593 N Ile 237	CA 1.525 C 0.108 1.417 N Pro 242	CA 1.540 CB 0.061 1.601 O Thr 12
C 1.231 O 0.075 1.156 O Asn 65	C 1.231 O 0.100 1.131 O Gly 104	CA 1.516 C 0.068 1.448 O Gly 104	CA 1.530 CB 0.079 1.609 O Trp 130	C 1.231 O 0.081 1.150 P Pro 3	CA 1.521 CB 0.053 1.574 P Ala 85
CA 1.525 C 0.143 1.382 P Thr 117	CA 1.540 CB 0.058 1.598 P Thr 117	CA 1.540 CB 0.103 1.643 P Ile 118	N 1.458 CA 0.056 1.402 P Ile 118		

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

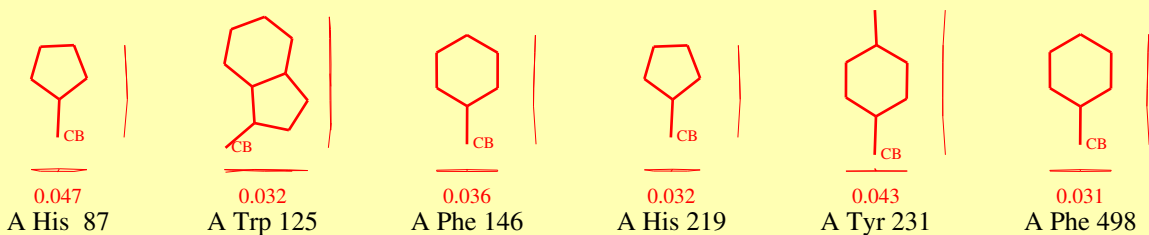
Distorted geometry 1kfy

Main-chain bond angles



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

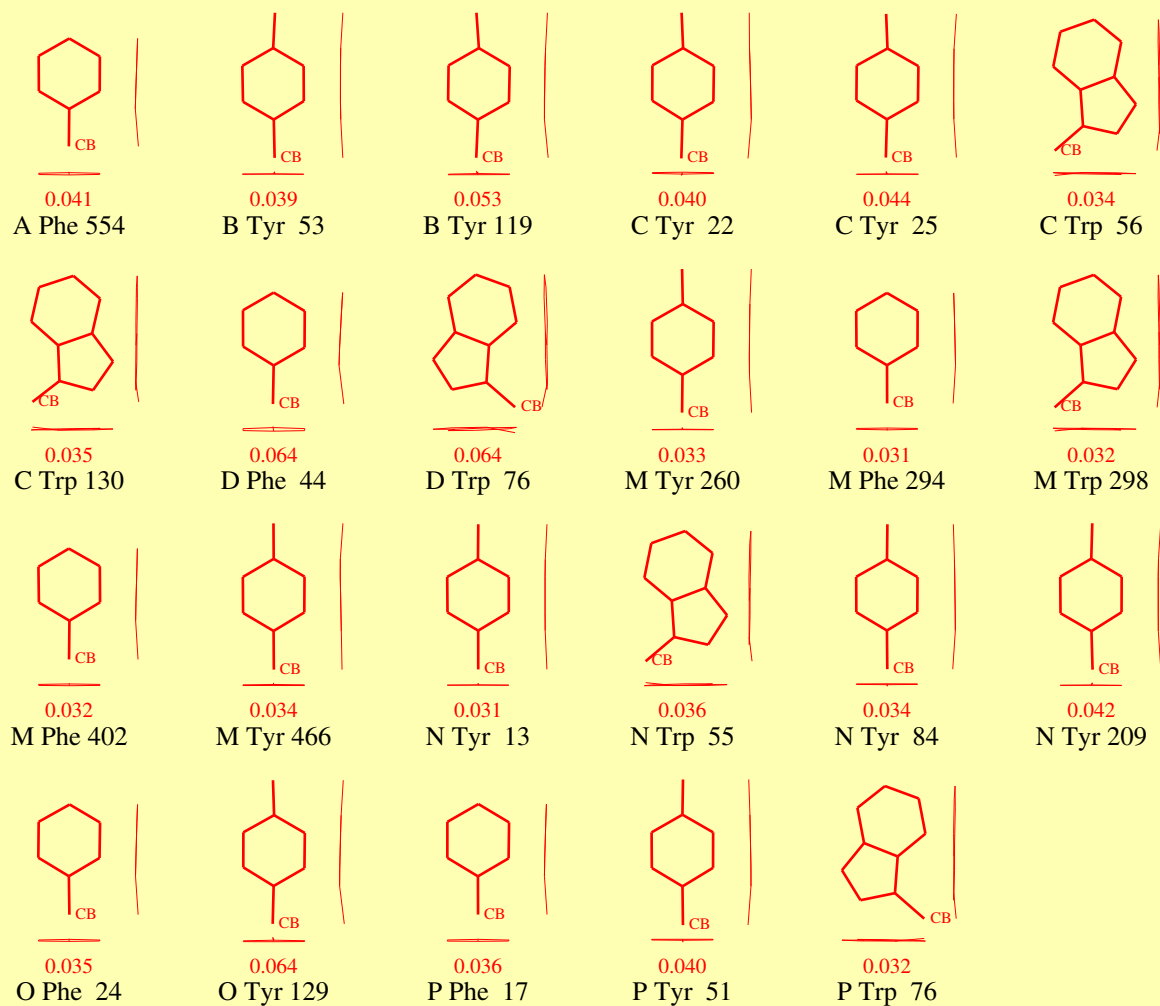
Planar groups



Distorted geometry

1kfy

Planar groups (contd)



Sidechains with RMS dist. from planarity > 0.03A for rings, or > 0.02A otherwise. Value shown is RMS dist.