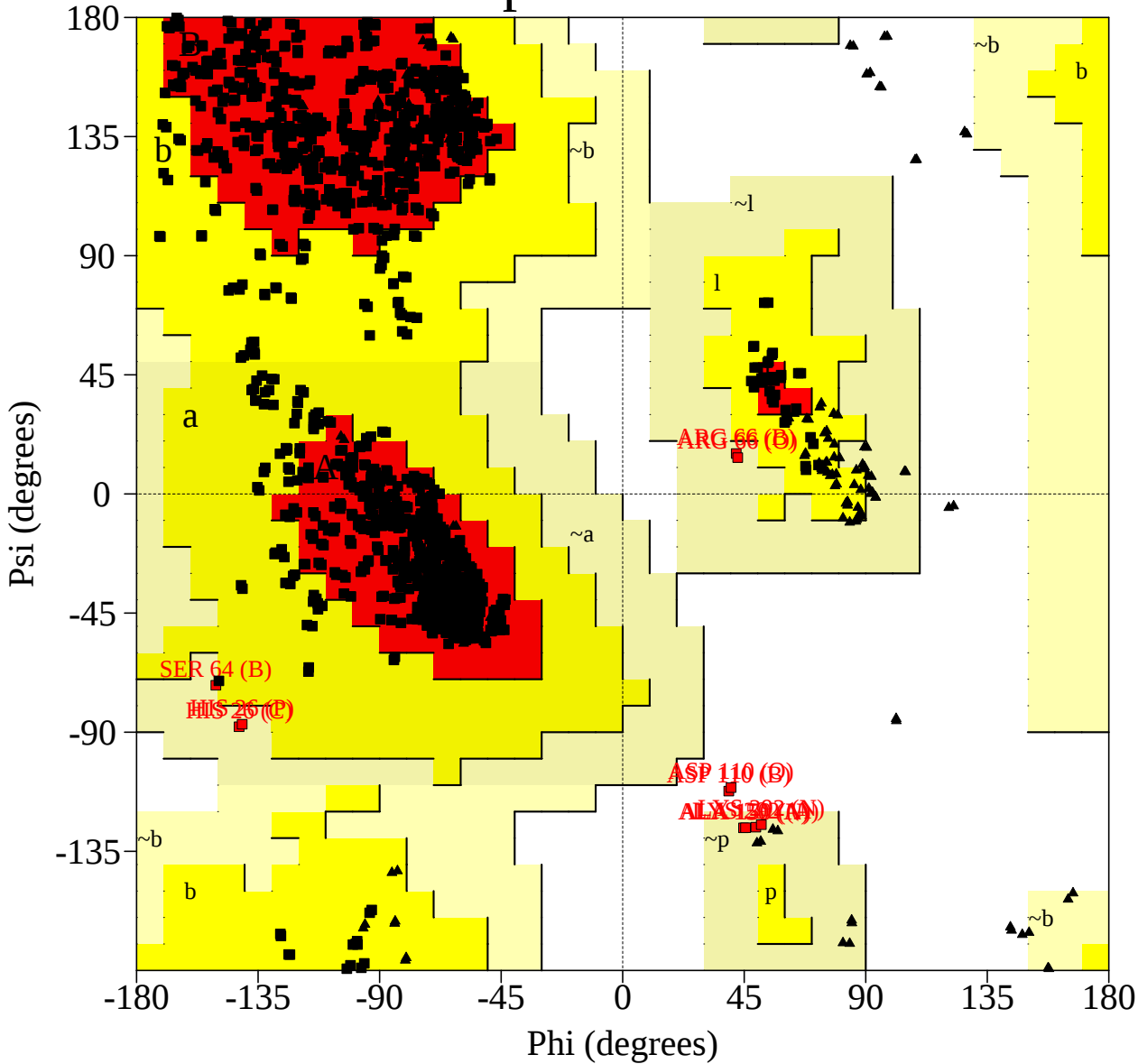


Ramachandran Plot

pdb2h88



Plot statistics

Residues in most favoured regions [A,B,L]	1712	90.7%
Residues in additional allowed regions [a,b,l,p]	165	8.7%
Residues in generously allowed regions [~a,~b,~l,~p]	9	0.5%
Residues in disallowed regions	2	0.1%

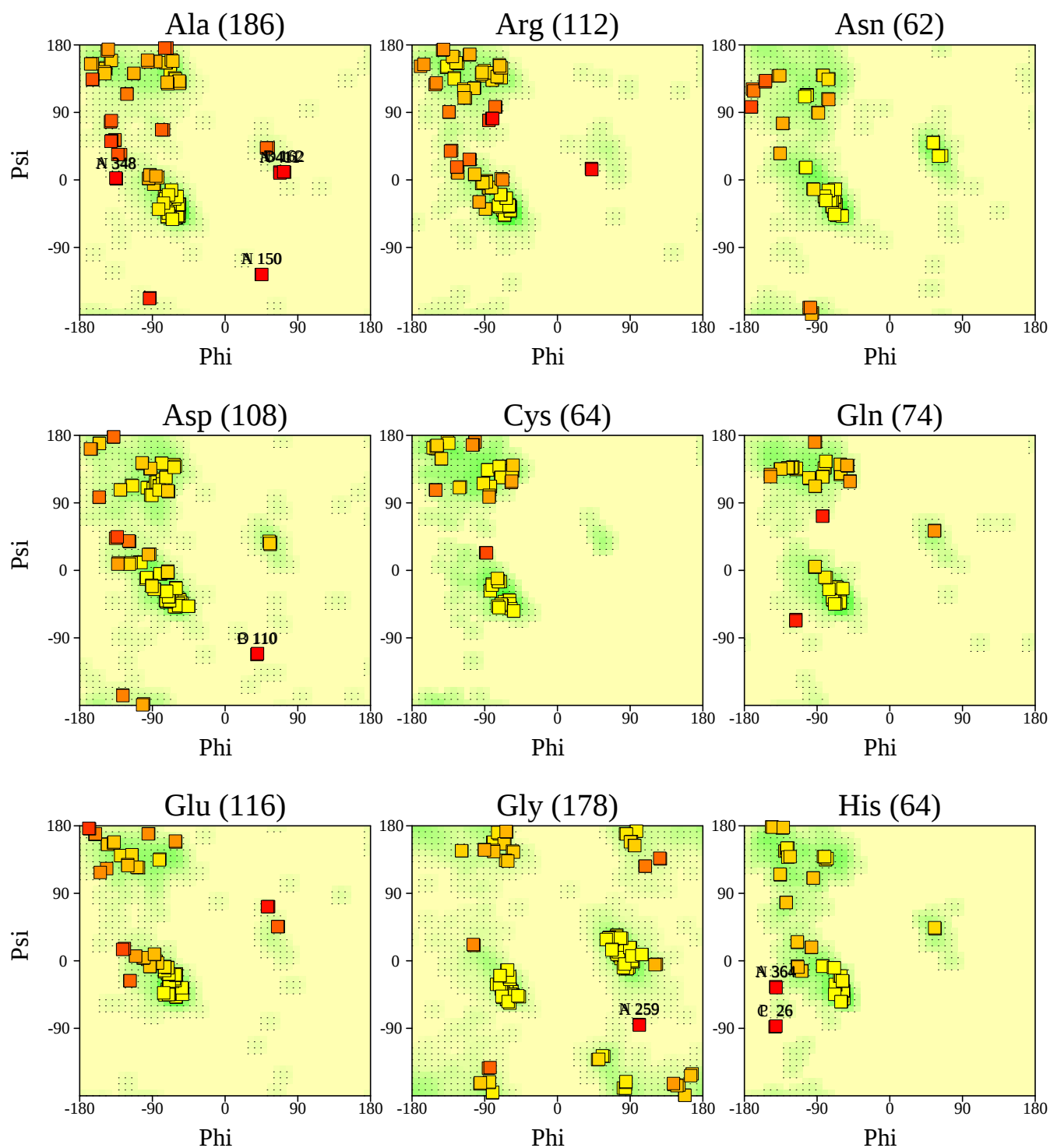
Number of non-glycine and non-proline residues	1888	100.0%
Number of end-residues (excl. Gly and Pro)	16	
Number of glycine residues (shown as triangles)	178	
Number of proline residues	100	

Total number of residues	2182	

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

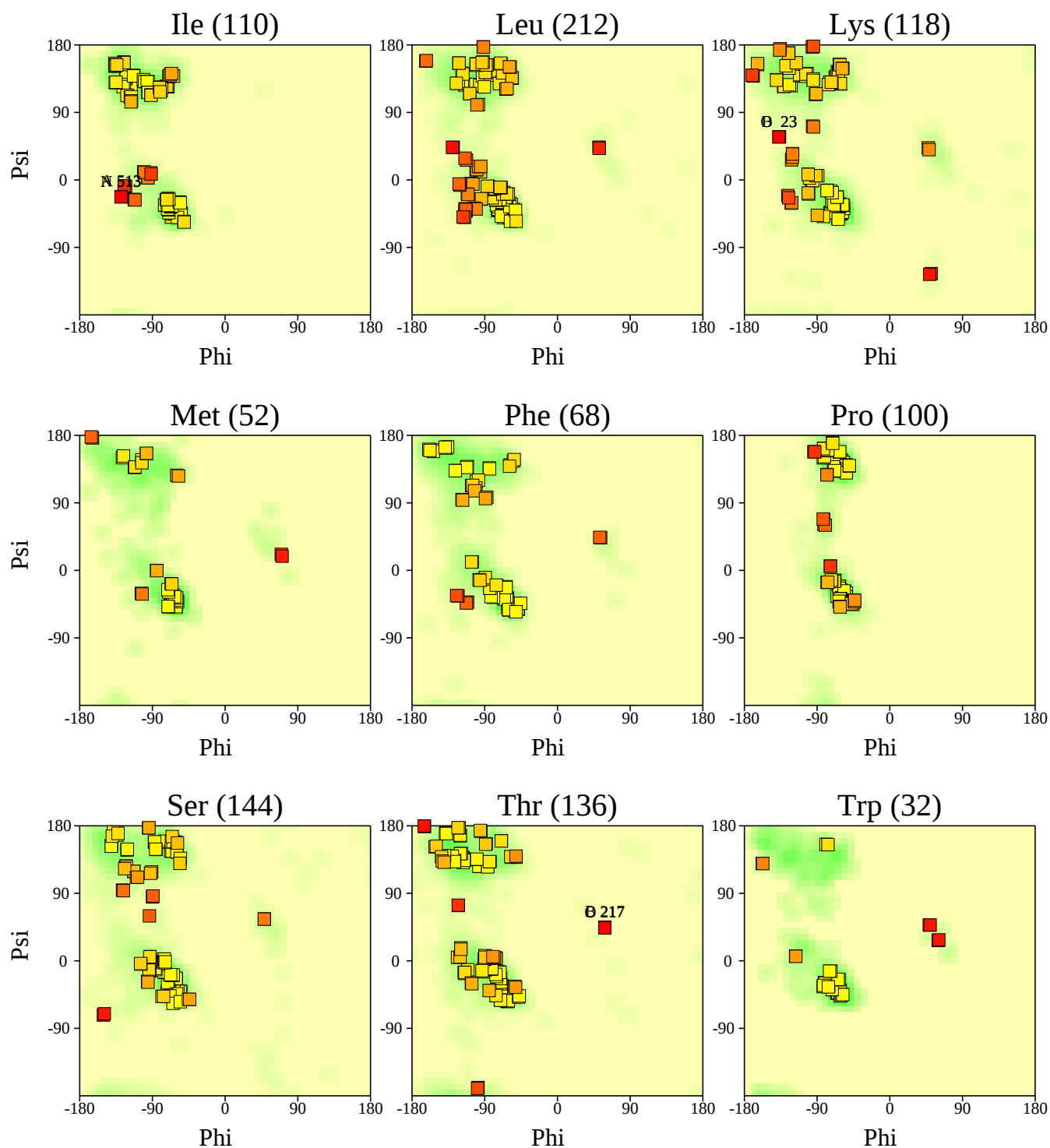
pdb2h88



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

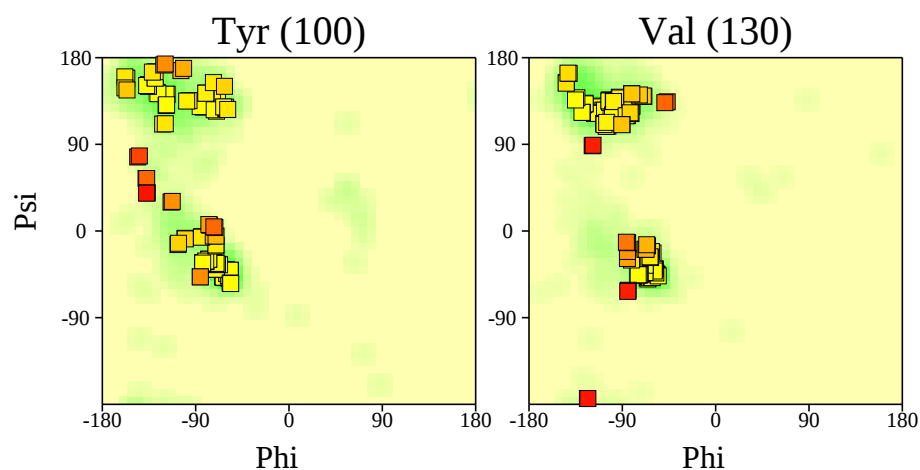
pdb2h88



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

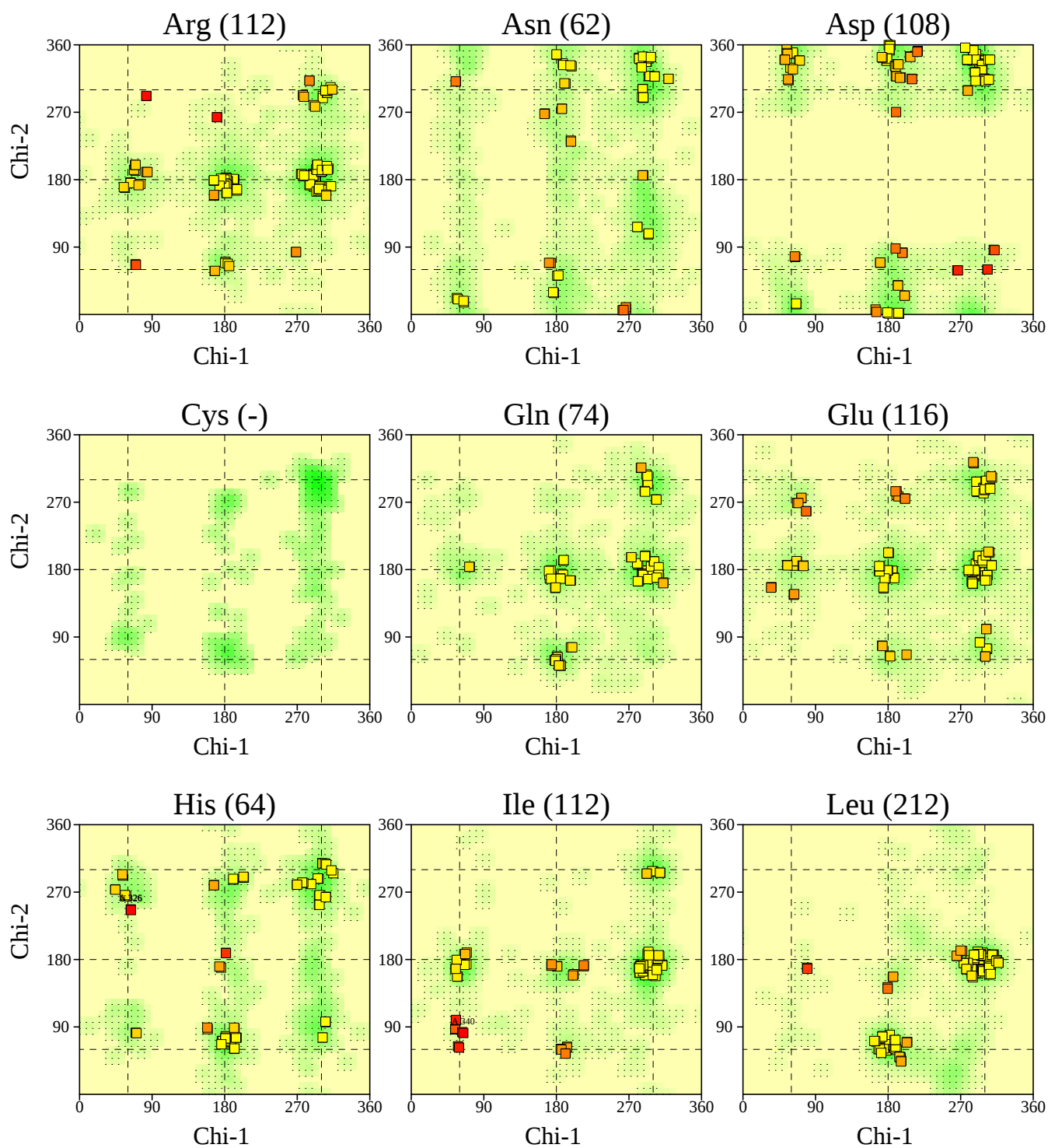
pdb2h88



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

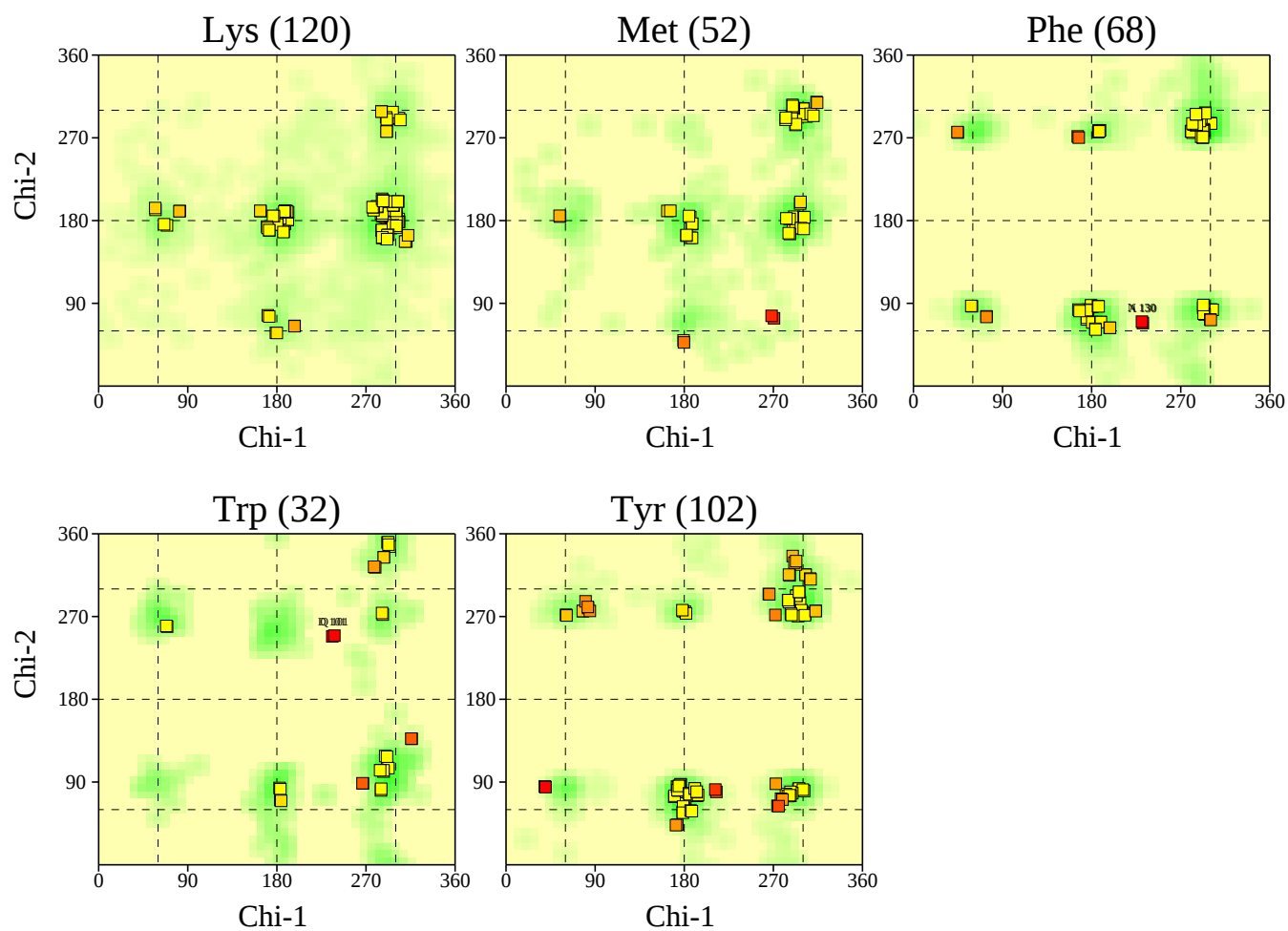
pdb2h88



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

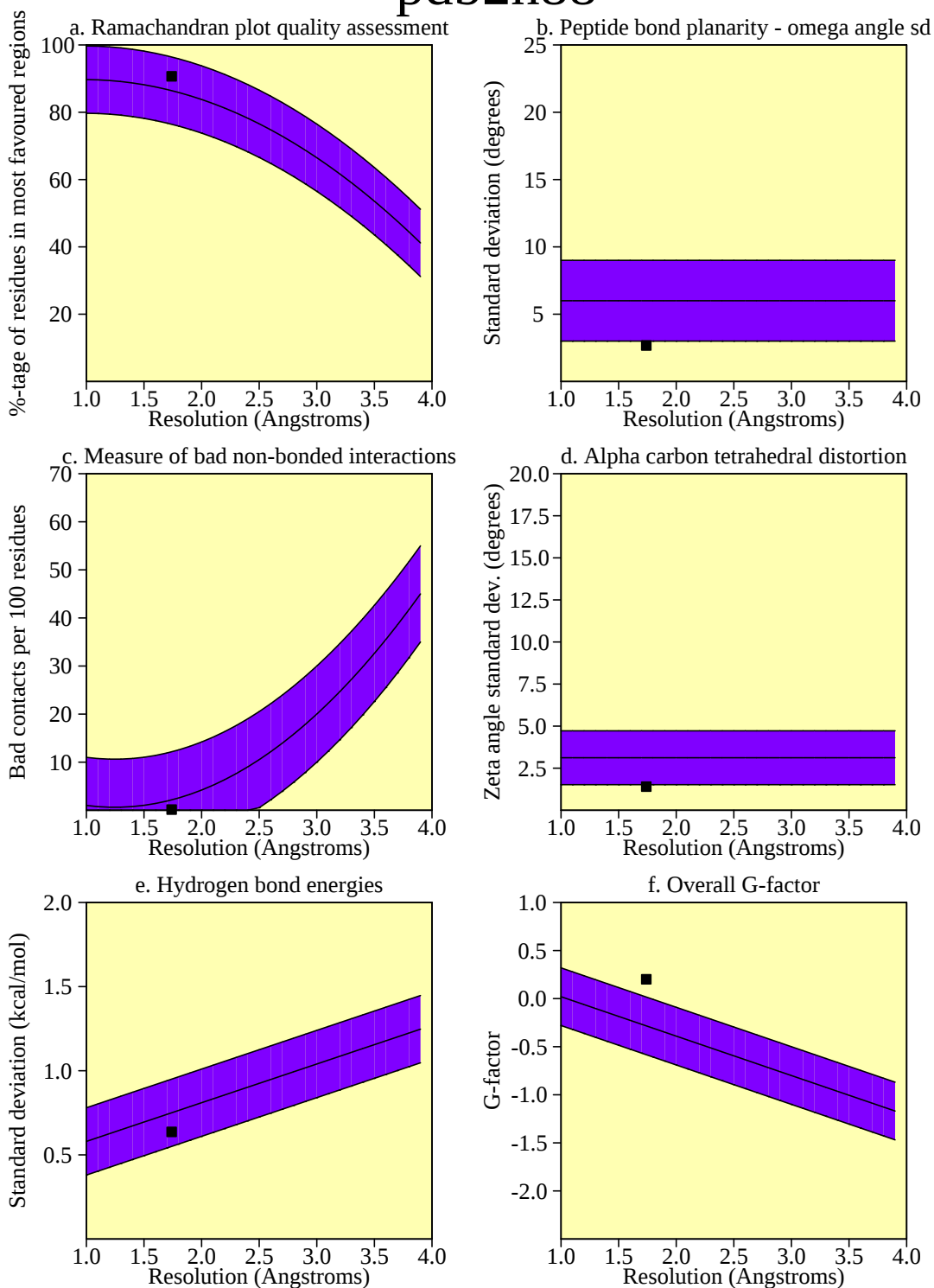
pdb2h88



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

pdb2h88

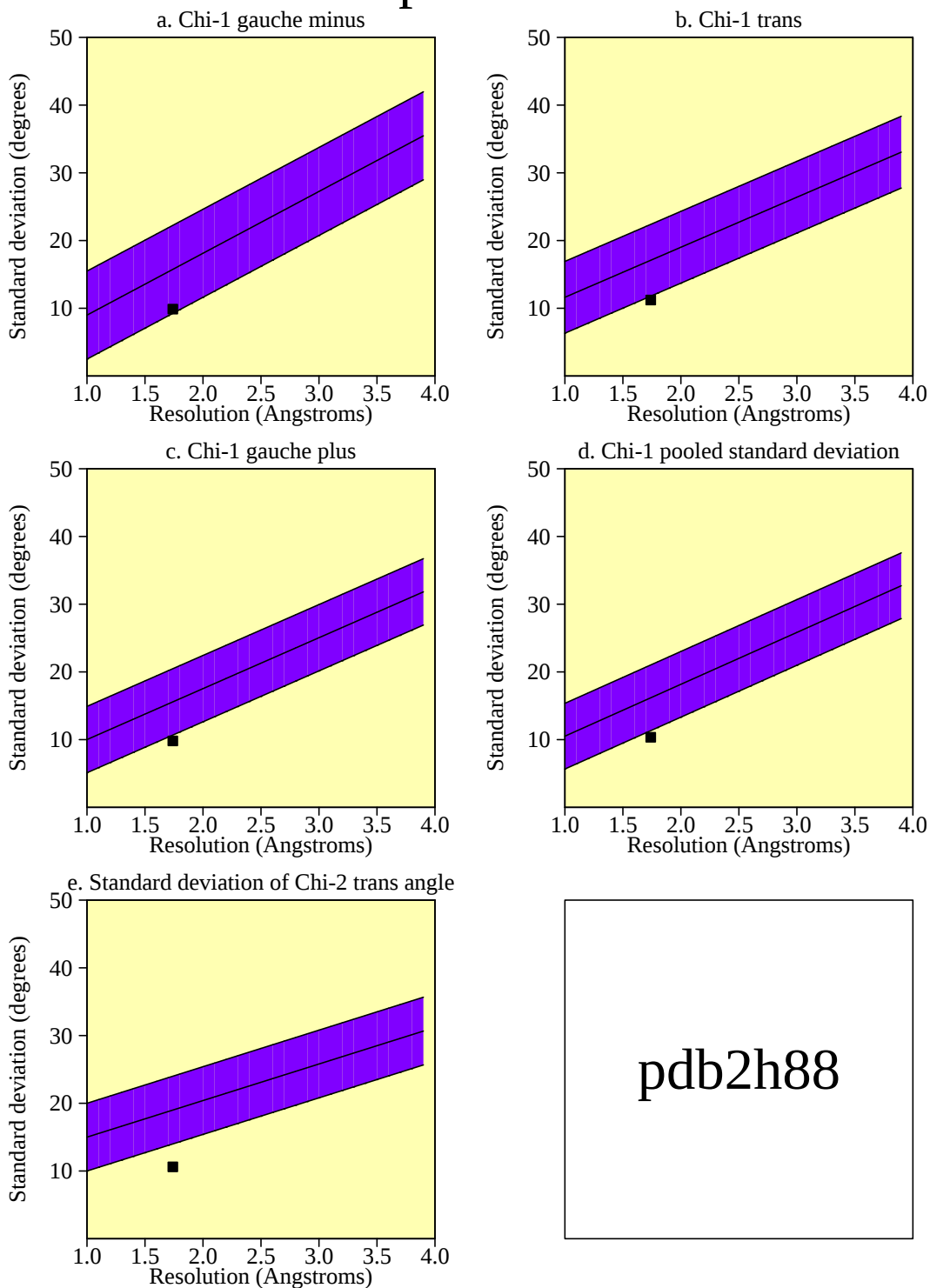


Plot statistics

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	1888	90.7	86.4	10.0	0.4	Inside
b. Omega angle st dev	2172	2.7	6.0	3.0	-1.1	BETTER
c. Bad contacts / 100 residues	3	0.1	2.2	10.0	-0.2	Inside
d. Zeta angle st dev	2004	1.4	3.1	1.6	-1.1	BETTER
e. H-bond energy st dev	1421	0.6	0.8	0.2	-0.6	Inside
f. Overall G-factor	2182	0.2	-0.3	0.3	1.6	BETTER

Side-chain parameters

pdb2h88



pdb2h88

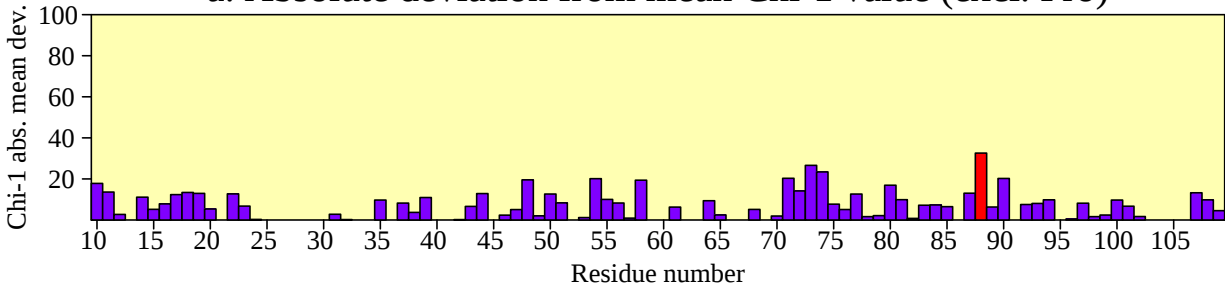
Plot statistics

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	260	9.9	15.7	6.5	-0.9	Inside
b. Chi-1 trans st dev	535	11.2	17.1	5.3	-1.1	BETTER
c. Chi-1 gauche plus st dev	921	9.8	15.6	4.9	-1.2	BETTER
d. Chi-1 pooled st dev	1716	10.3	16.2	4.8	-1.2	BETTER
e. Chi-2 trans st dev	591	10.6	19.0	5.0	-1.7	BETTER

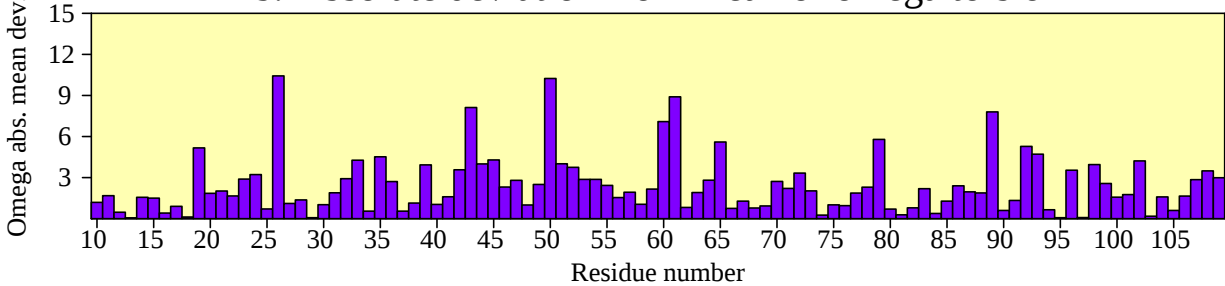
Residue properties

pdb2h88

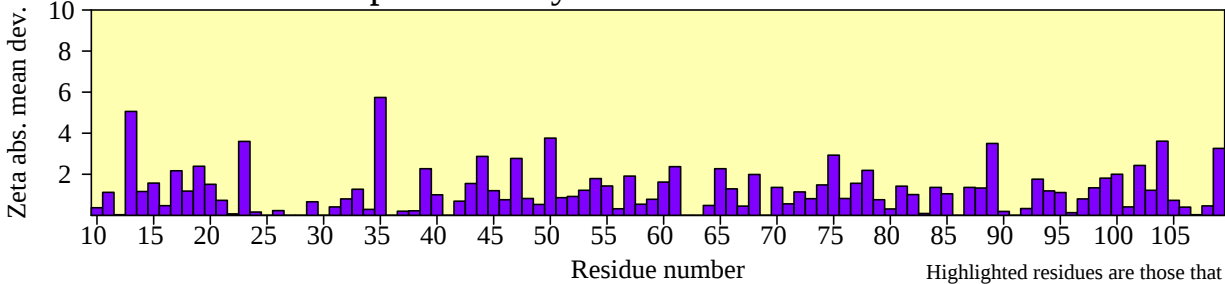
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

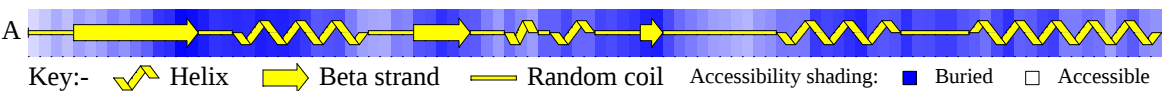


c. C-alpha chirality: abs. deviation of zeta torsion



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

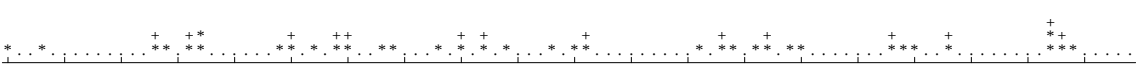
d. Secondary structure & estimated accessibility



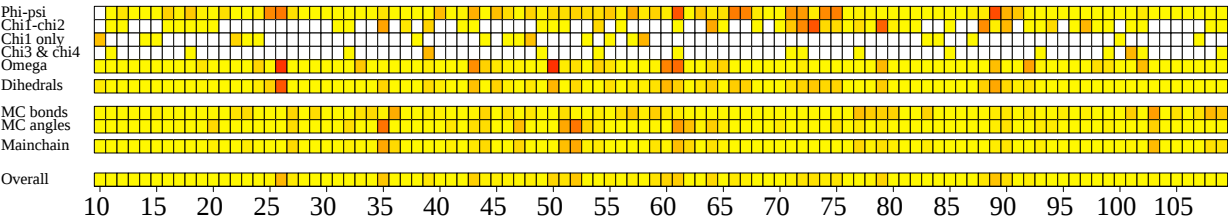
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



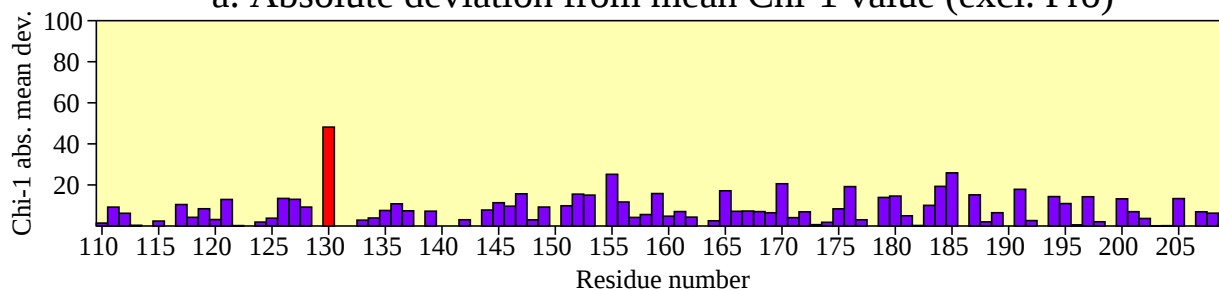
g. G-factors



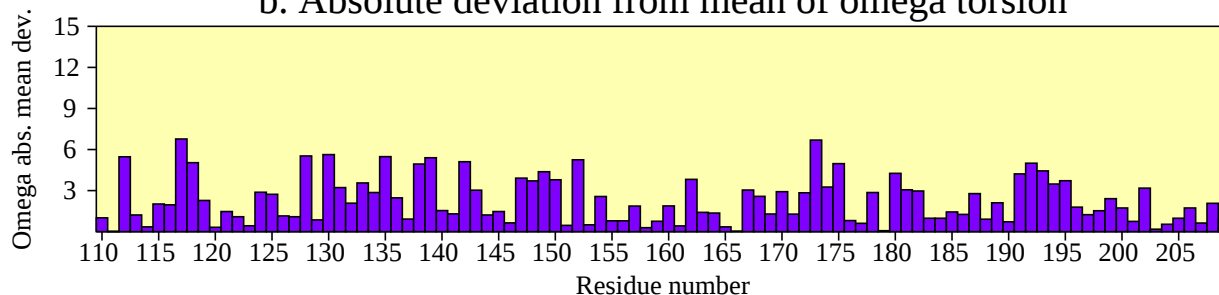
Residue properties

pdb2h88

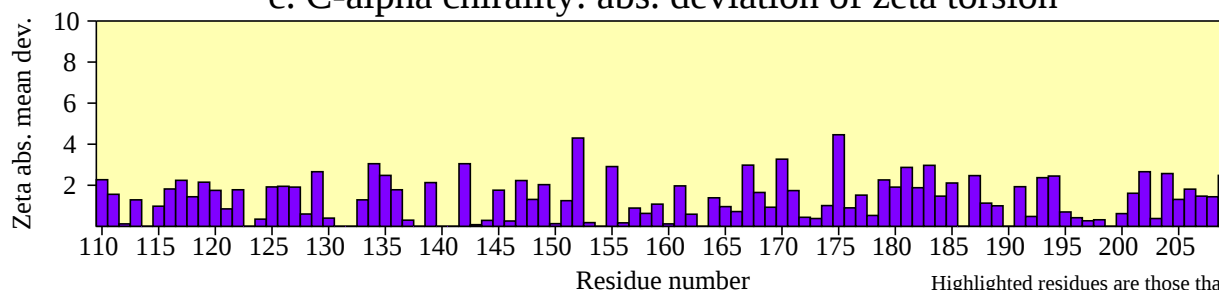
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

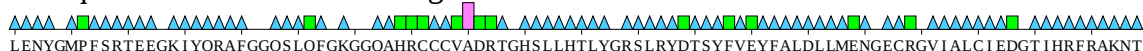


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

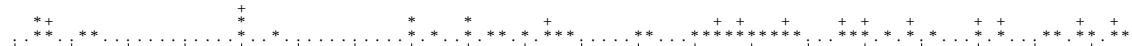
d. Secondary structure & estimated accessibility



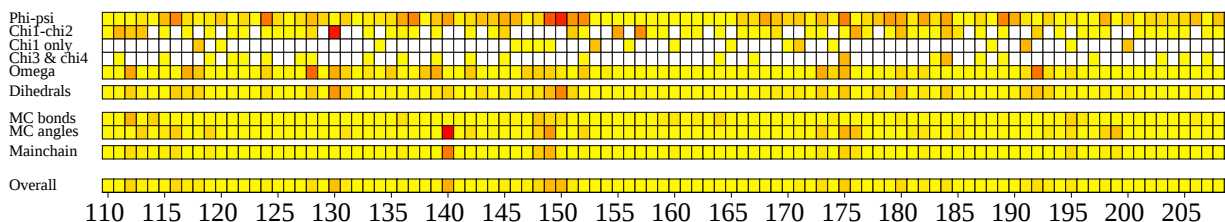
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



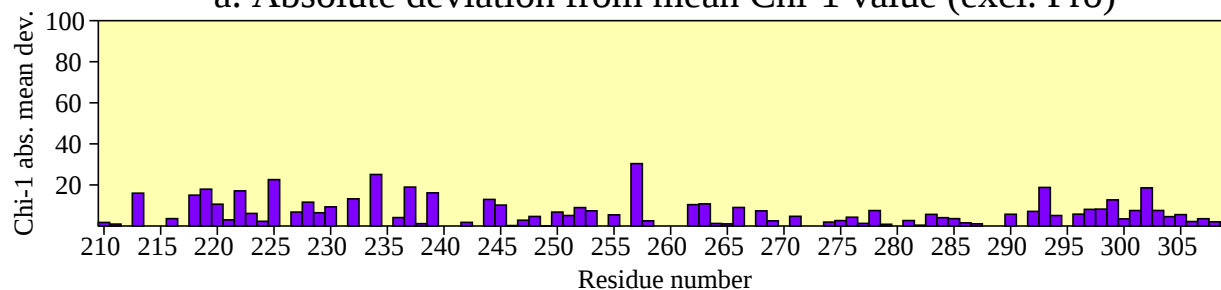
g. G-factors



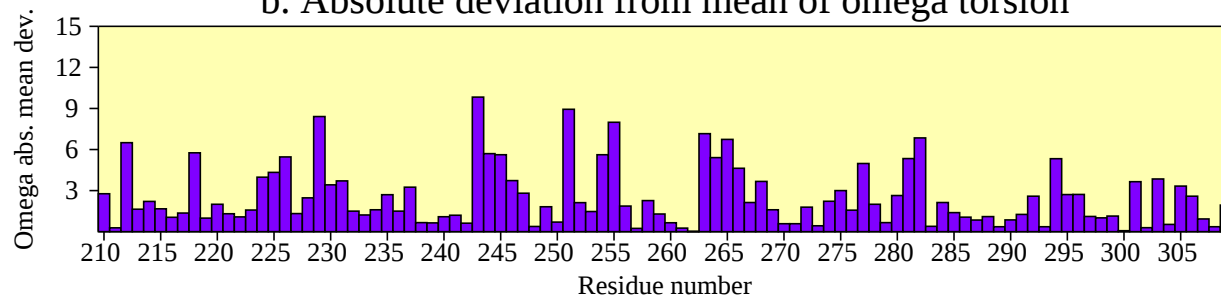
Residue properties

pdb2h88

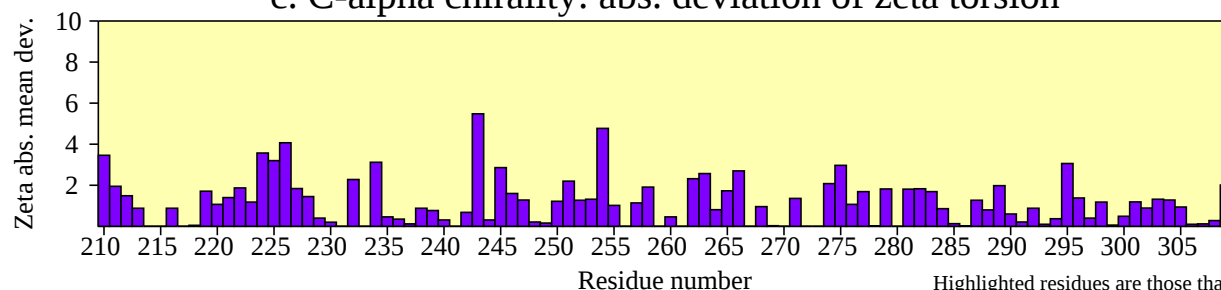
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

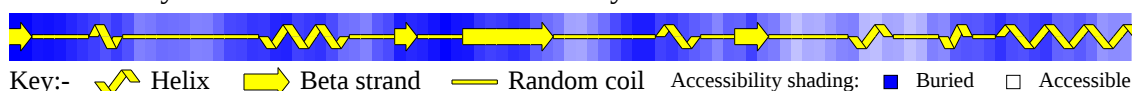


c. C-alpha chirality: abs. deviation of zeta torsion



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

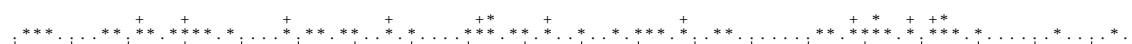
d. Secondary structure & estimated accessibility



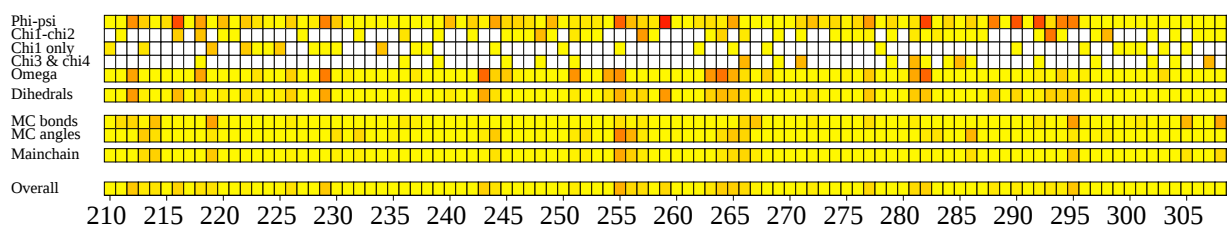
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



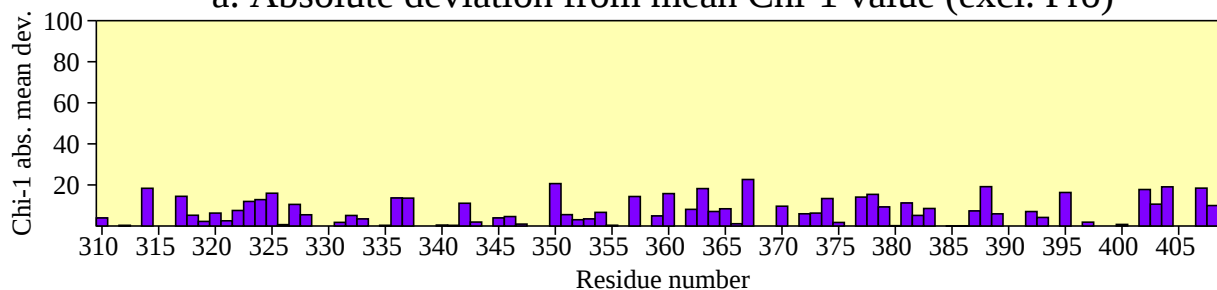
g. G-factors



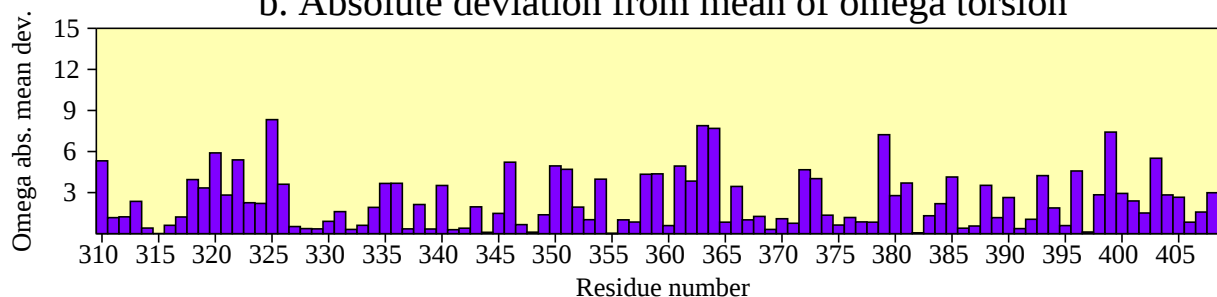
Residue properties

pdb2h88

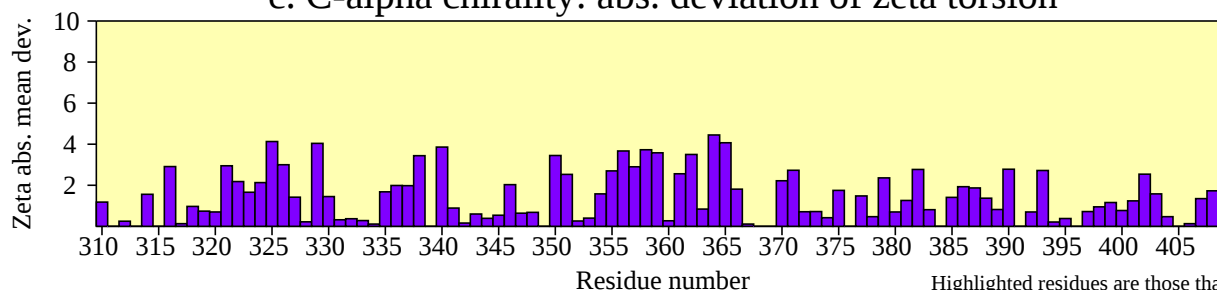
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

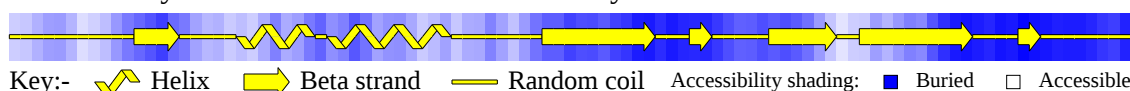


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



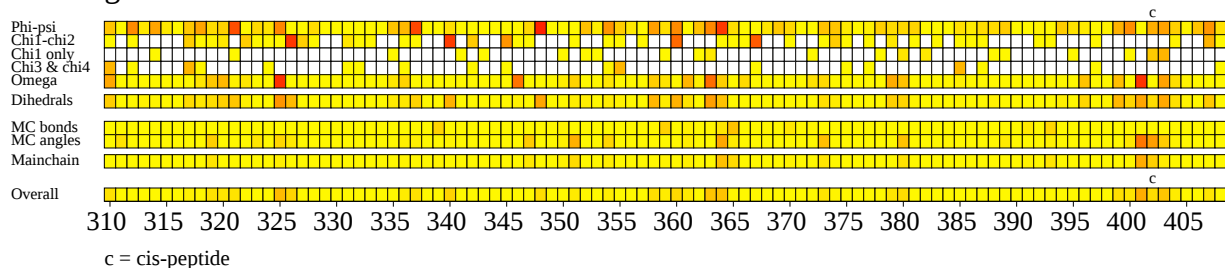
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



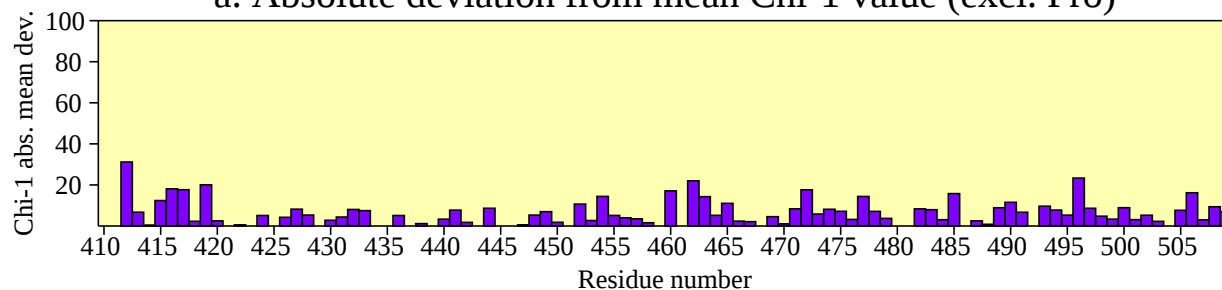
g. G-factors



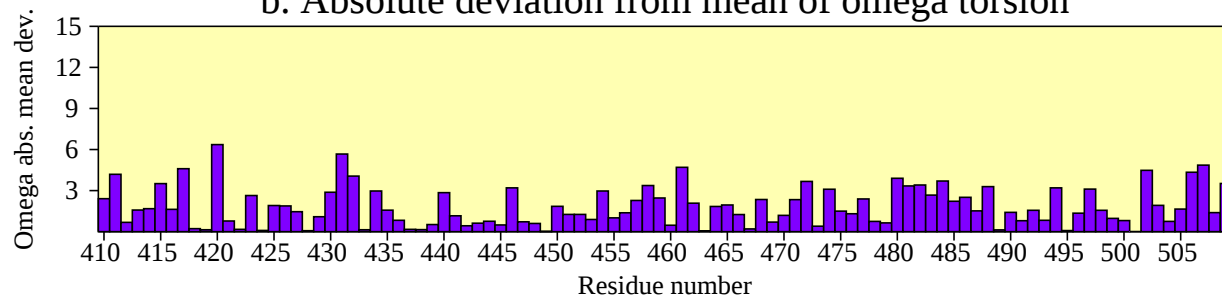
Residue properties

pdb2h88

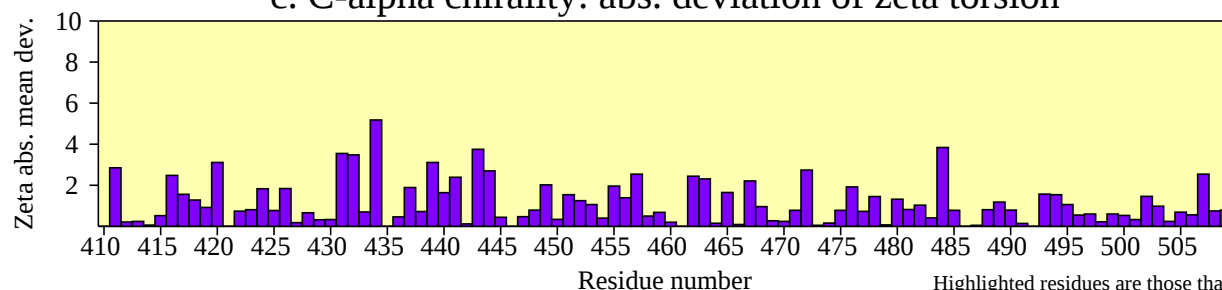
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

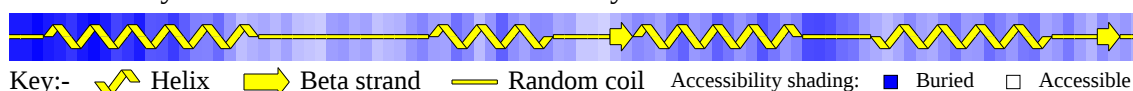


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



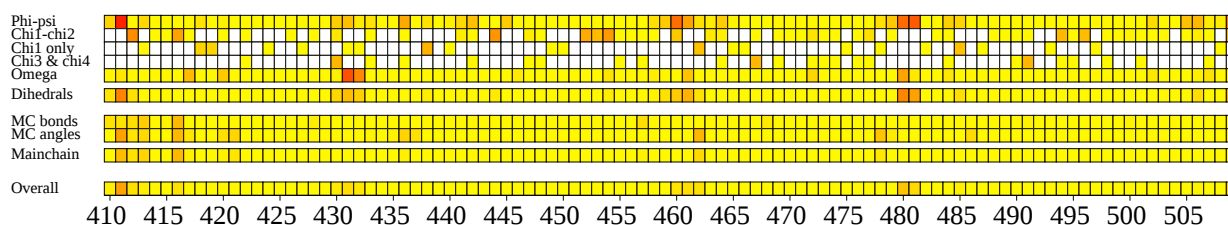
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



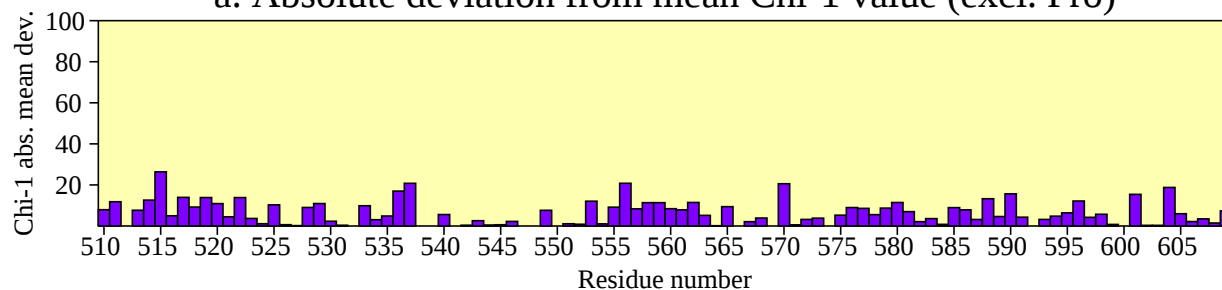
g. G-factors



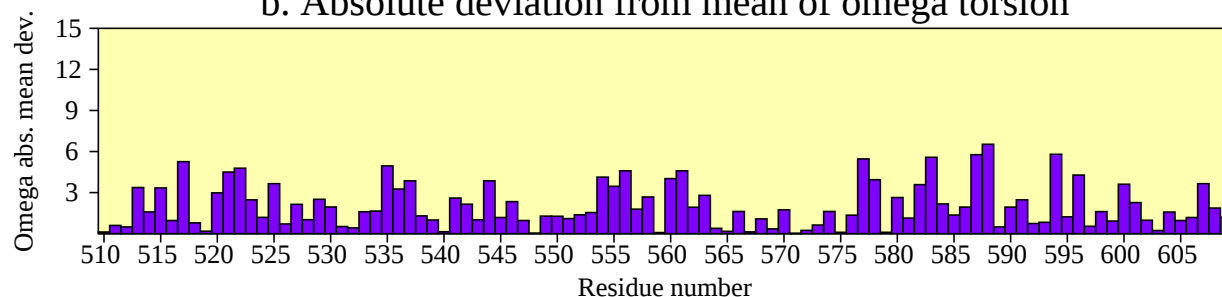
Residue properties

pdb2h88

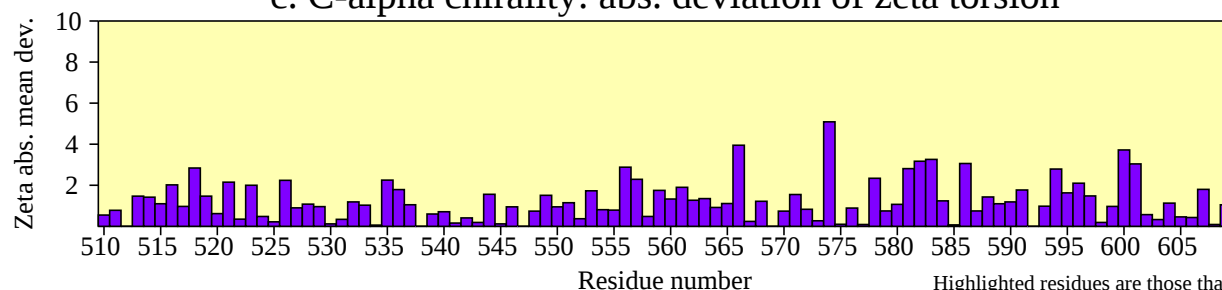
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

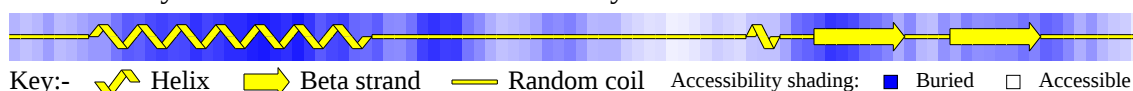


c. C-alpha chirality: abs. deviation of zeta torsion



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

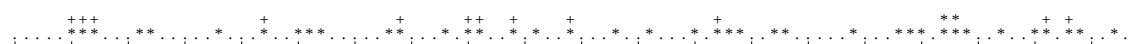
d. Secondary structure & estimated accessibility



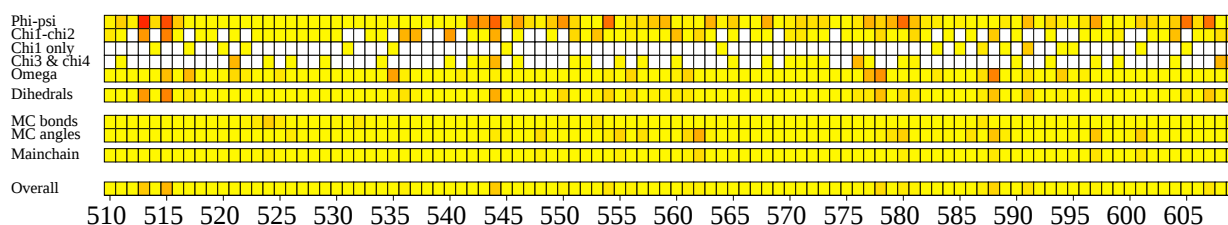
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



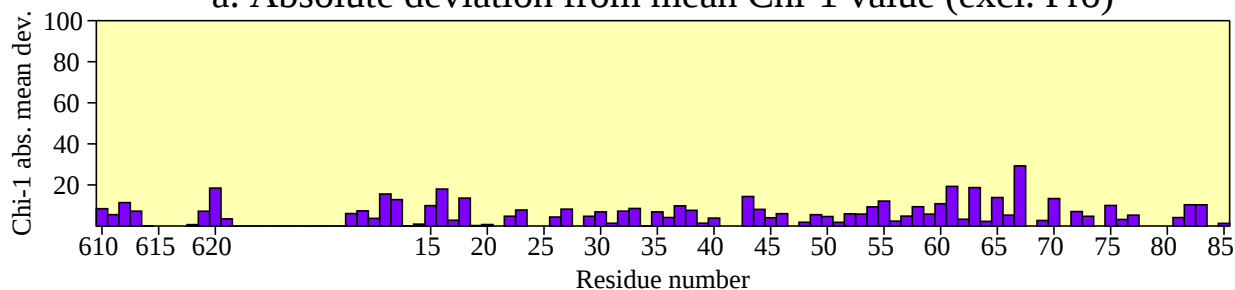
g. G-factors



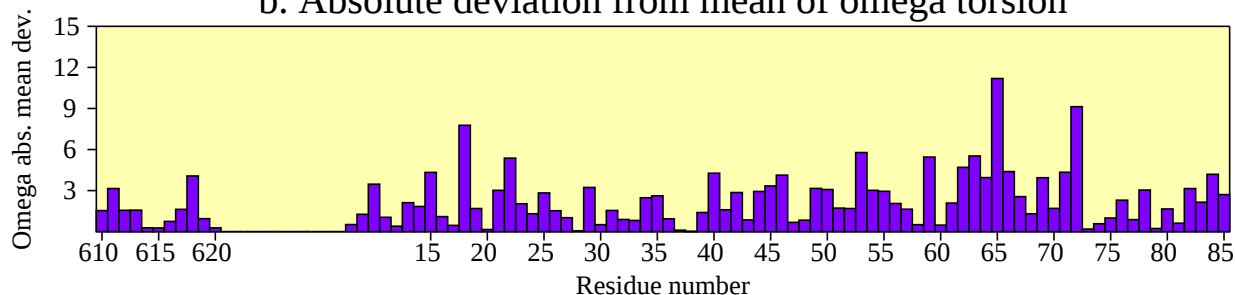
Residue properties

pdb2h88

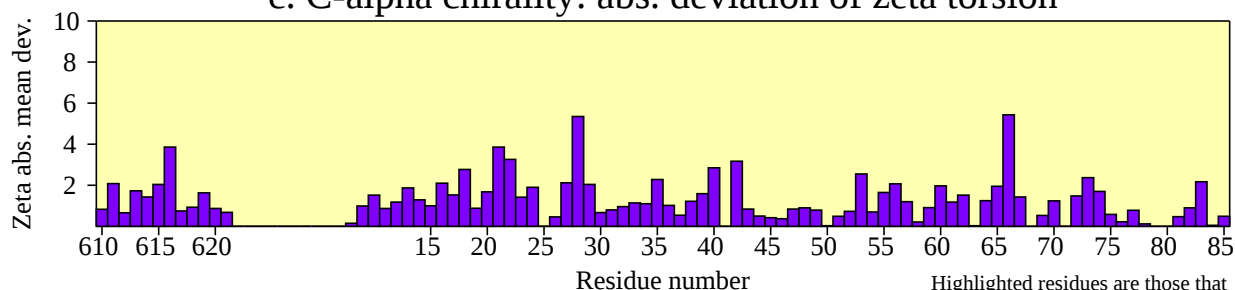
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

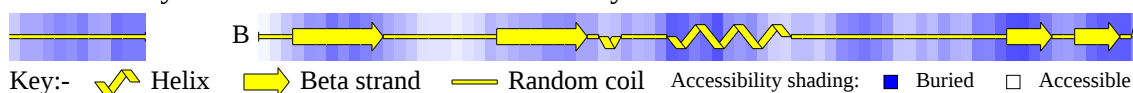


c. C-alpha chirality: abs. deviation of zeta torsion

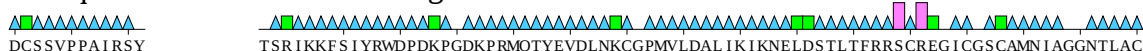


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

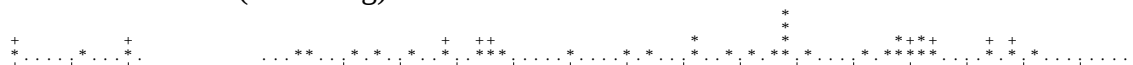
d. Secondary structure & estimated accessibility



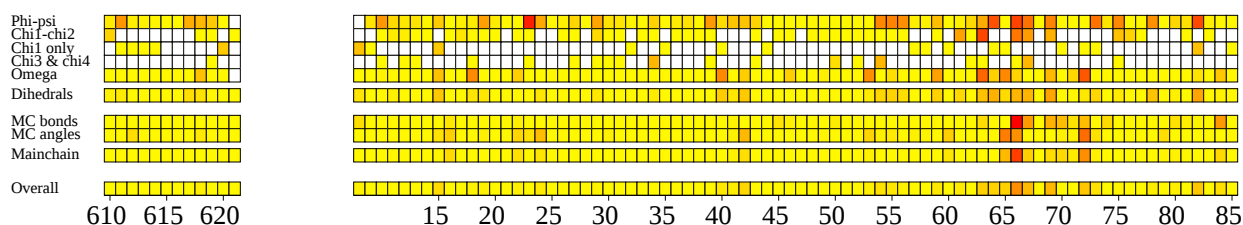
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



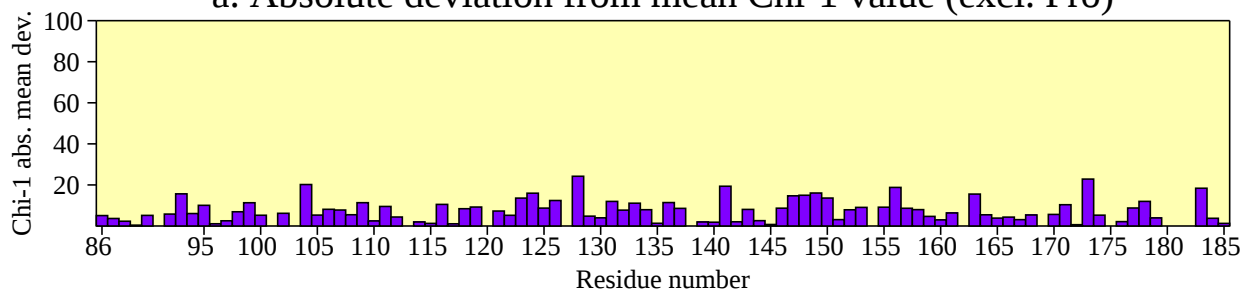
g. G-factors



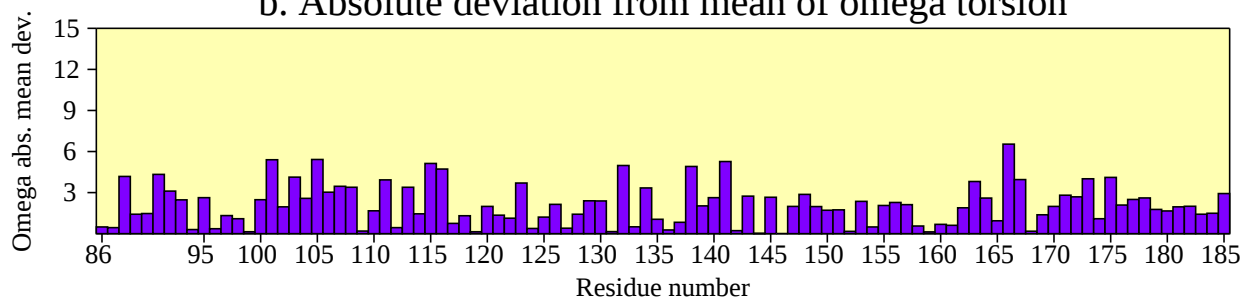
Residue properties

pdb2h88

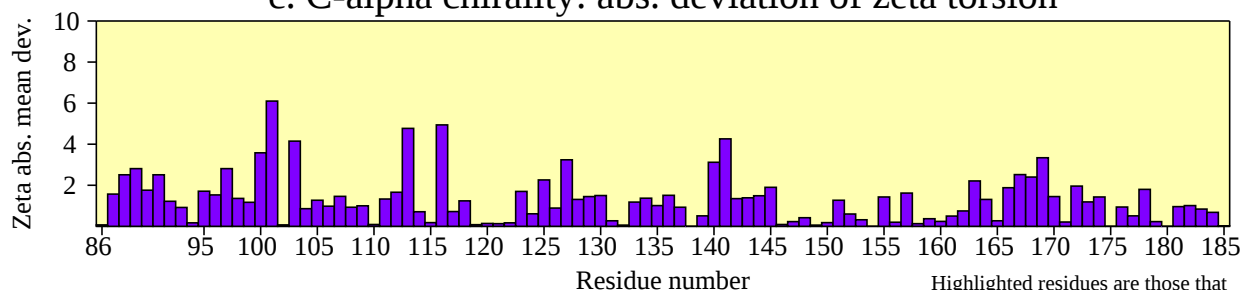
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

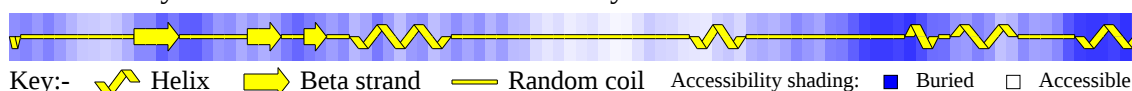


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



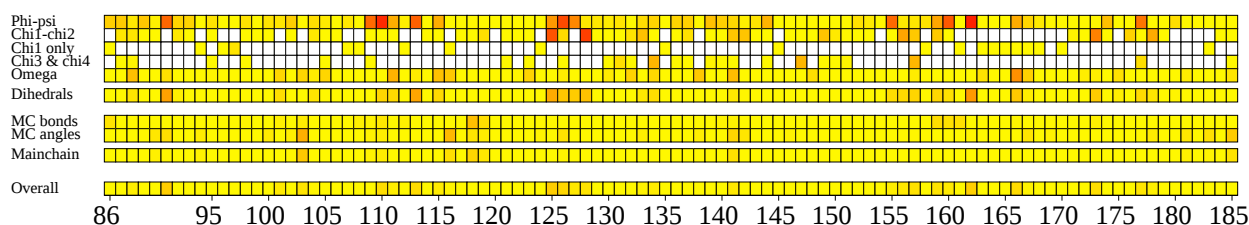
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



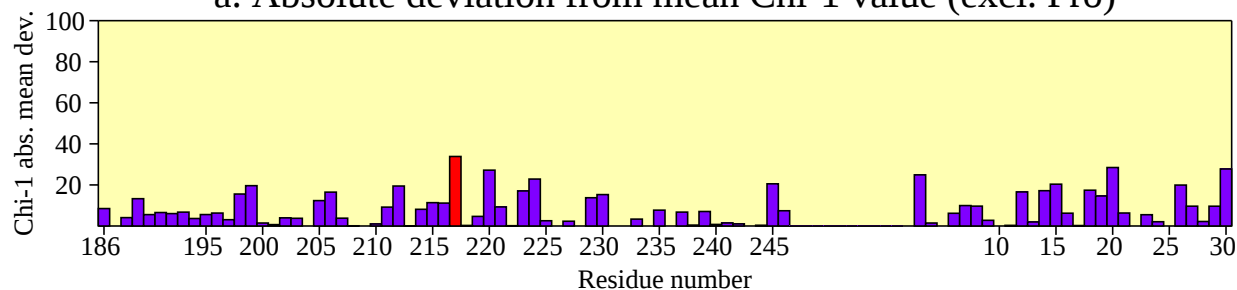
g. G-factors



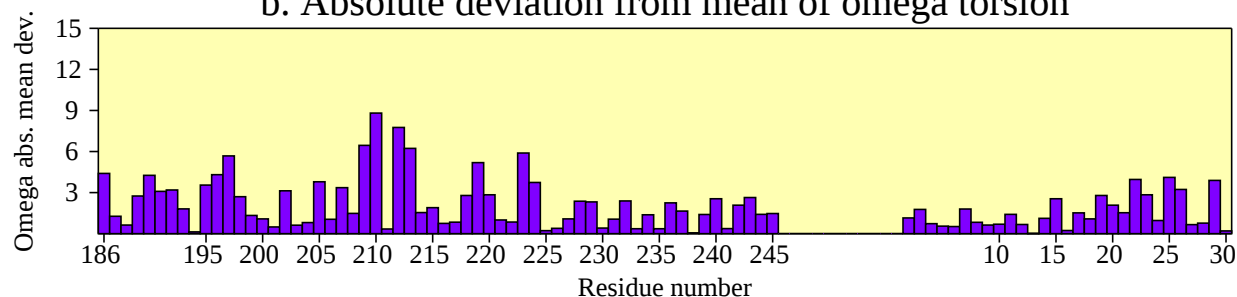
Residue properties

pdb2h88

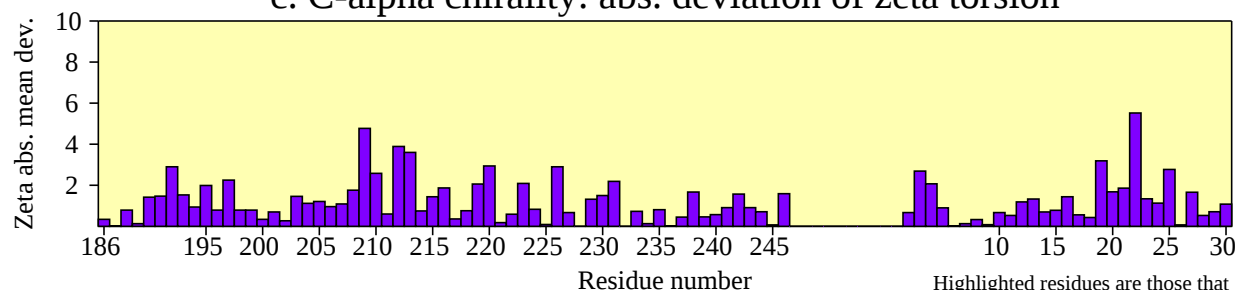
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

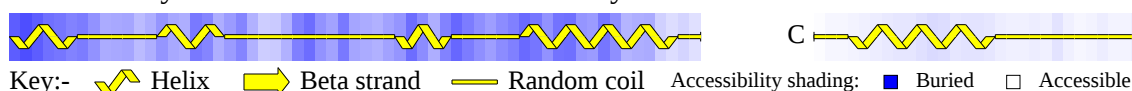


c. C-alpha chirality: abs. deviation of zeta torsion

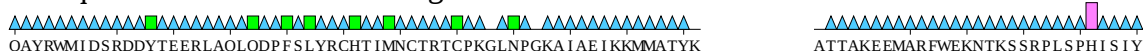


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



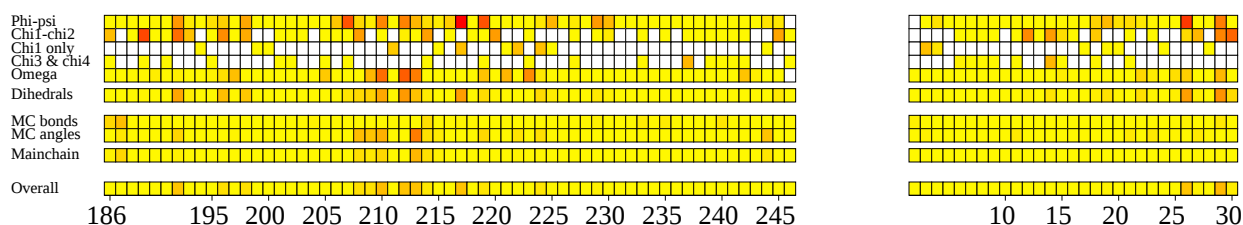
e. Sequence & Ramachandran regions



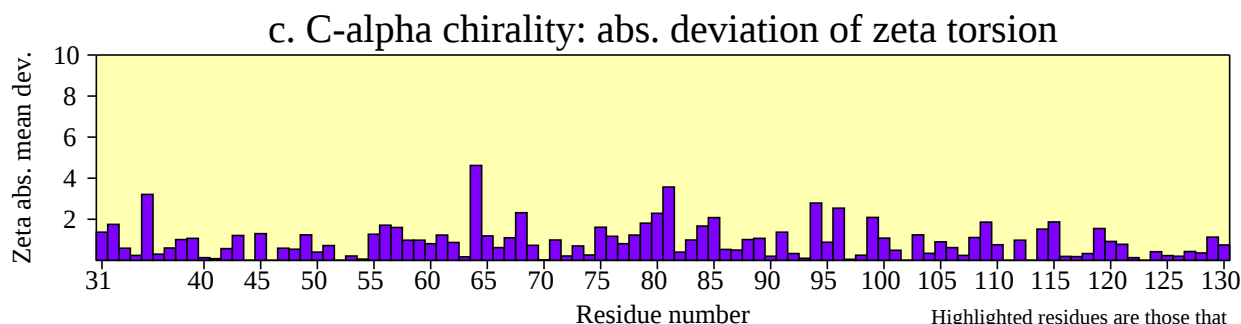
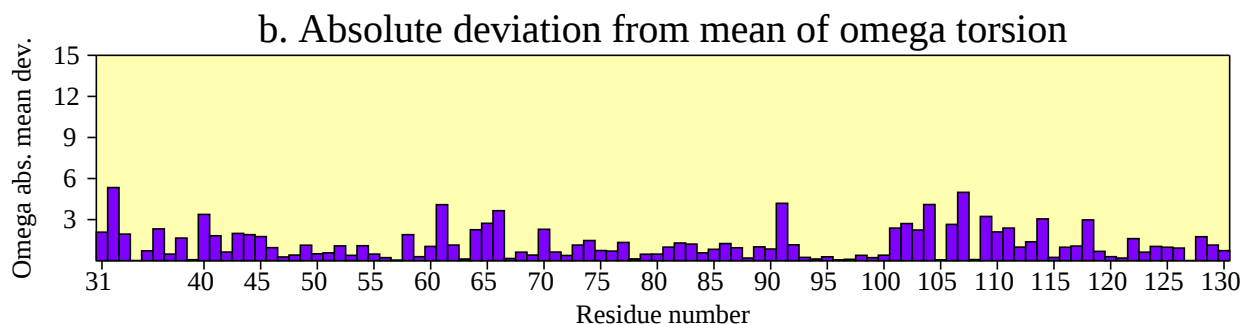
f. Max. deviation (see listing)



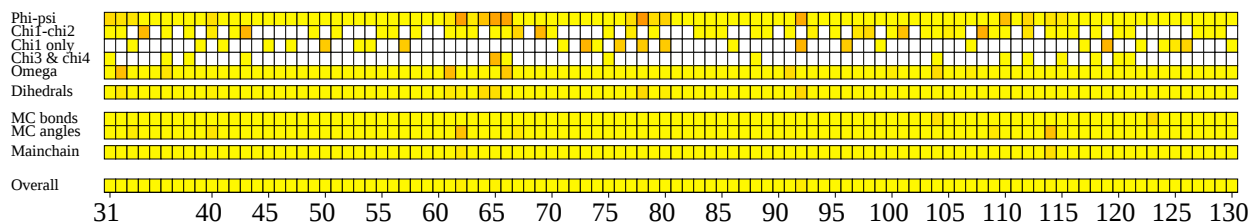
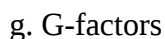
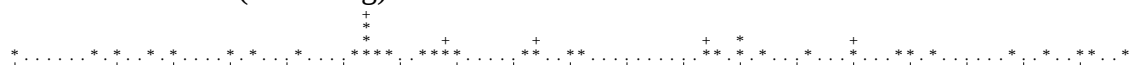
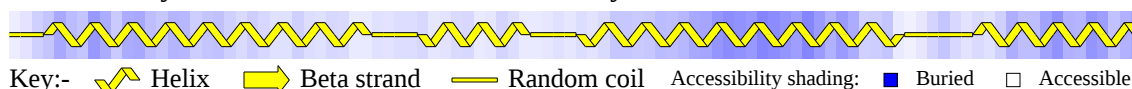
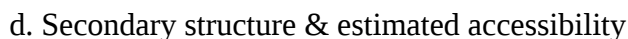
g. G-factors



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



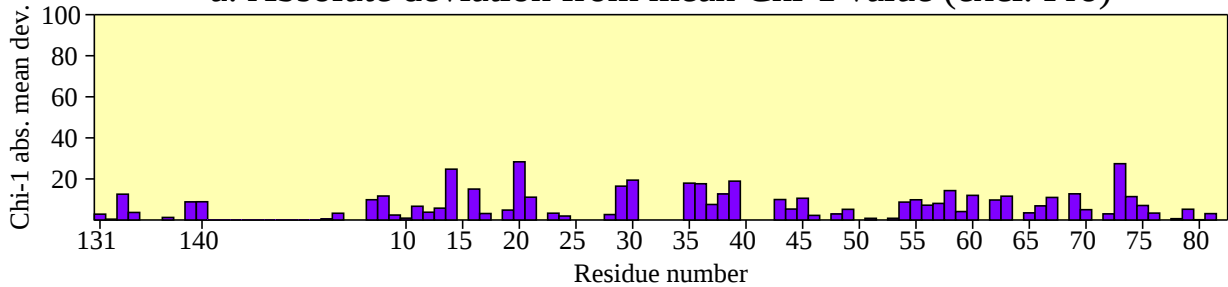
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal



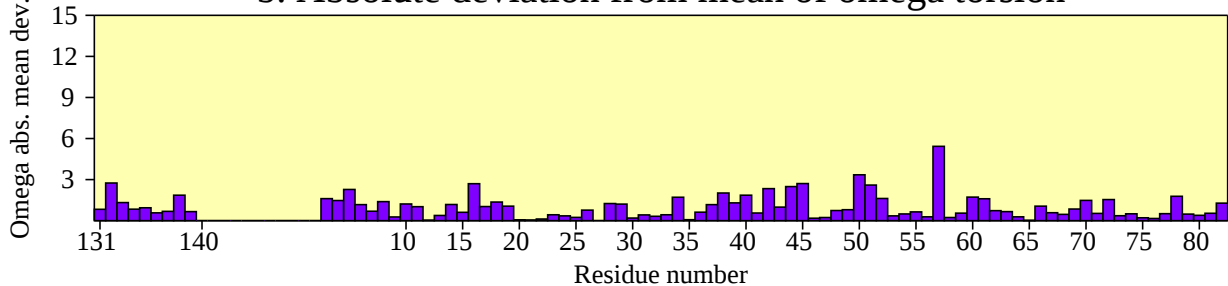
Residue properties

pdb2h88

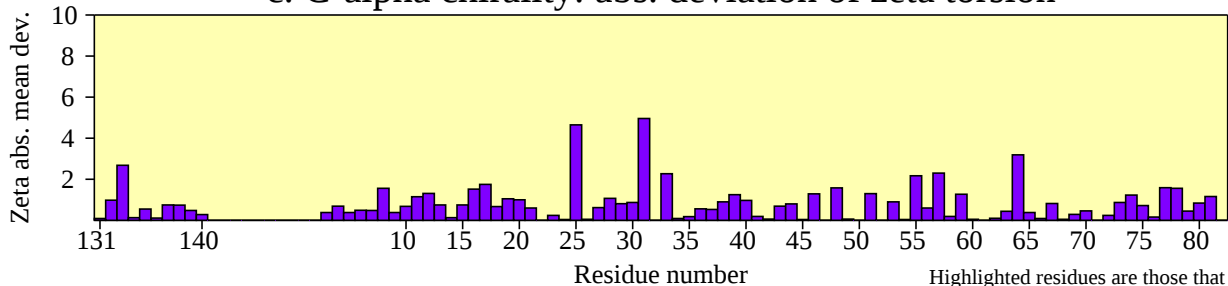
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

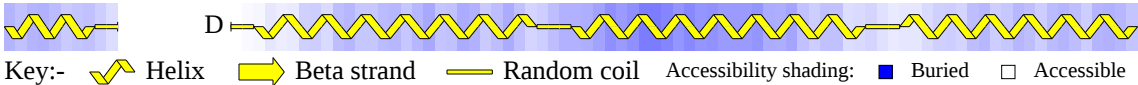


c. C-alpha chirality: abs. deviation of zeta torsion

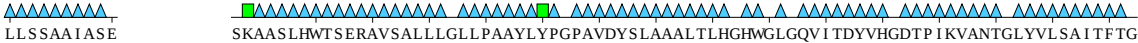


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

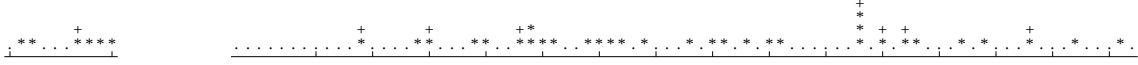
d. Secondary structure & estimated accessibility



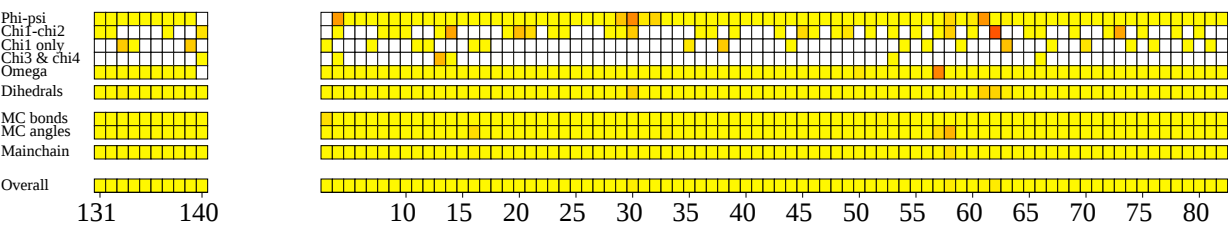
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



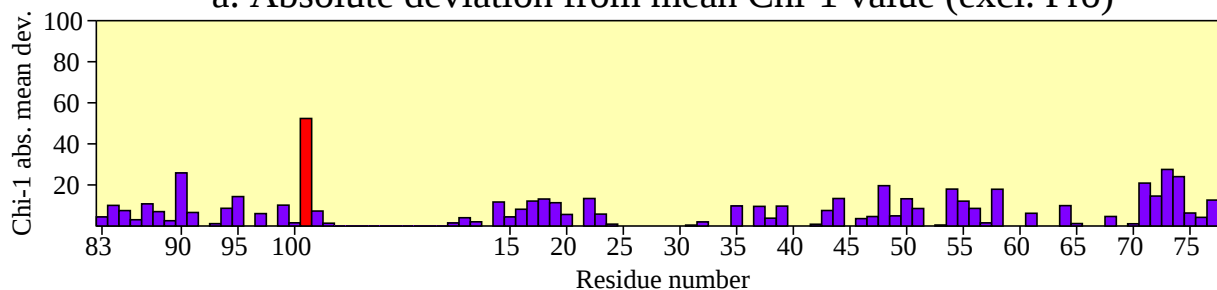
g. G-factors



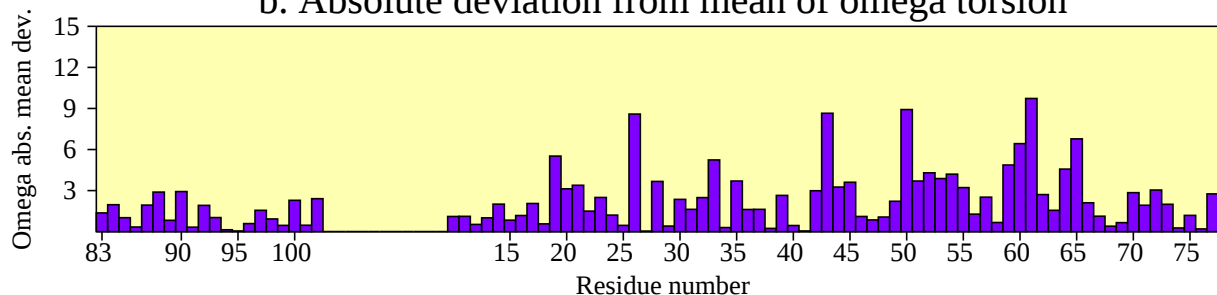
Residue properties

pdb2h88

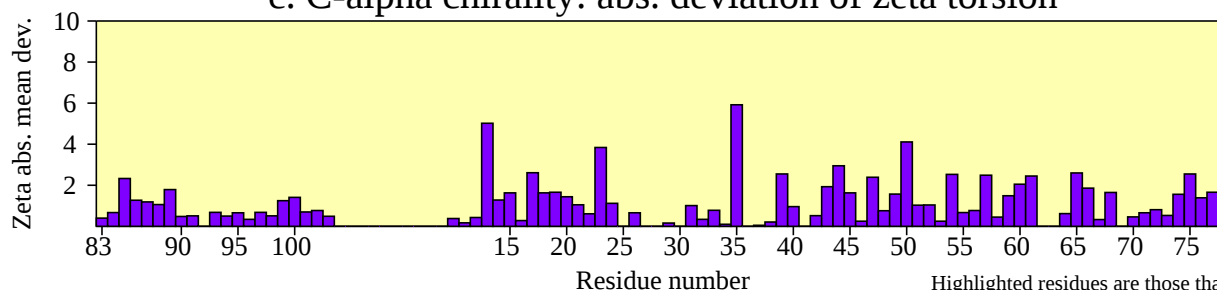
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



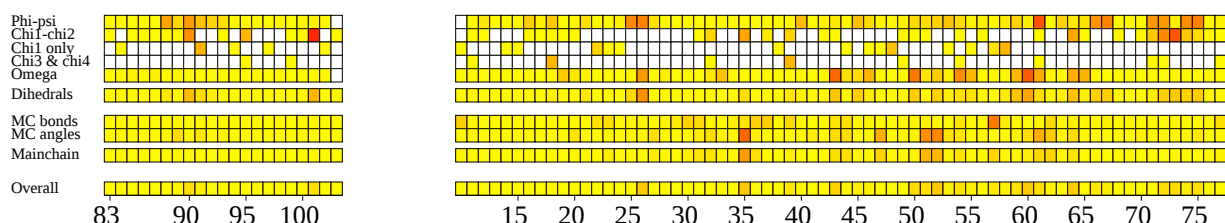
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



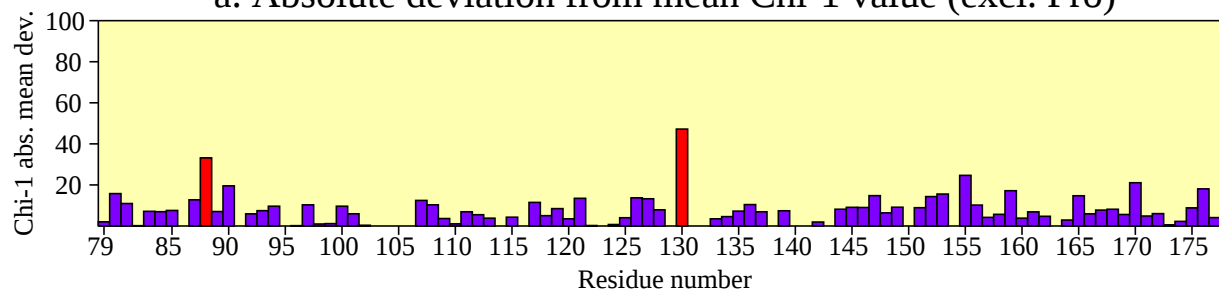
g. G-factors



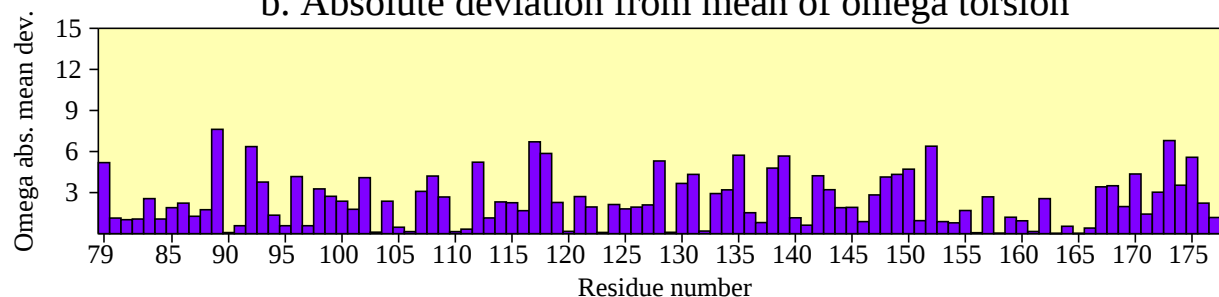
Residue properties

pdb2h88

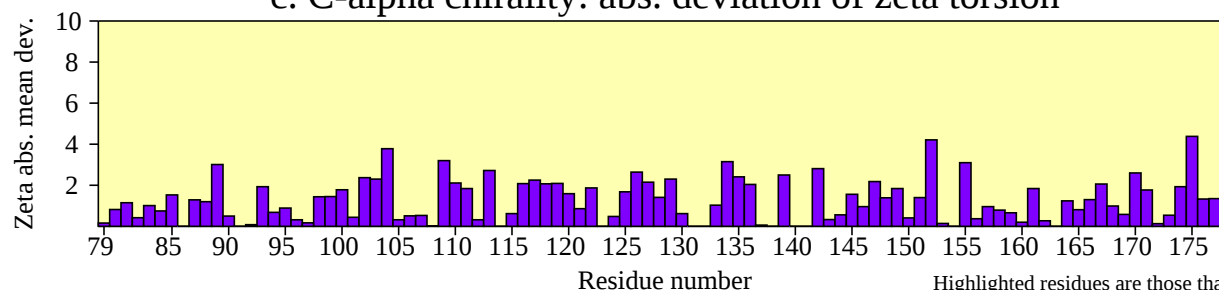
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

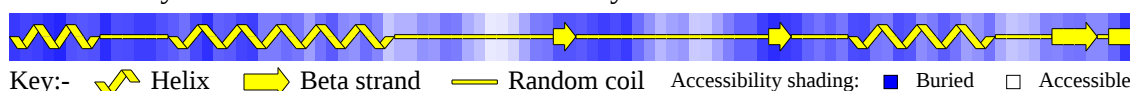


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



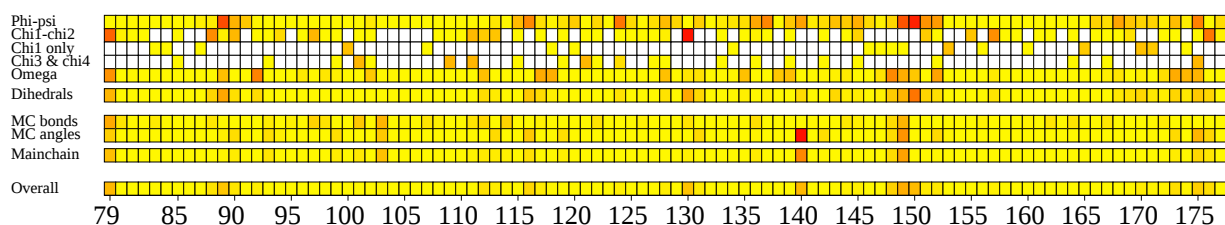
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



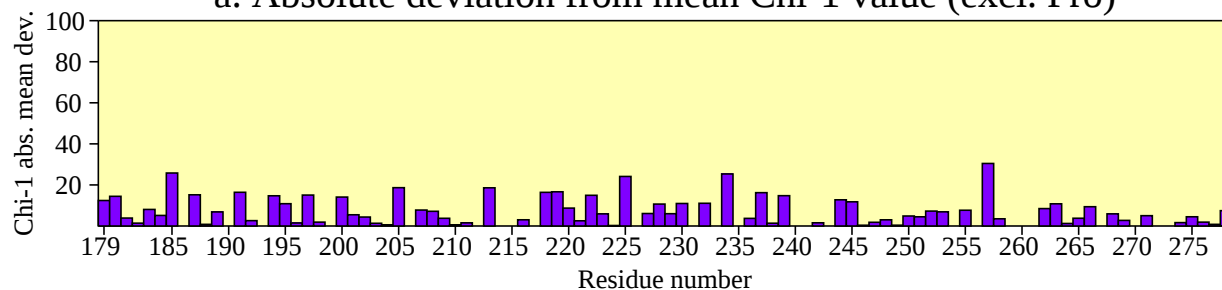
g. G-factors



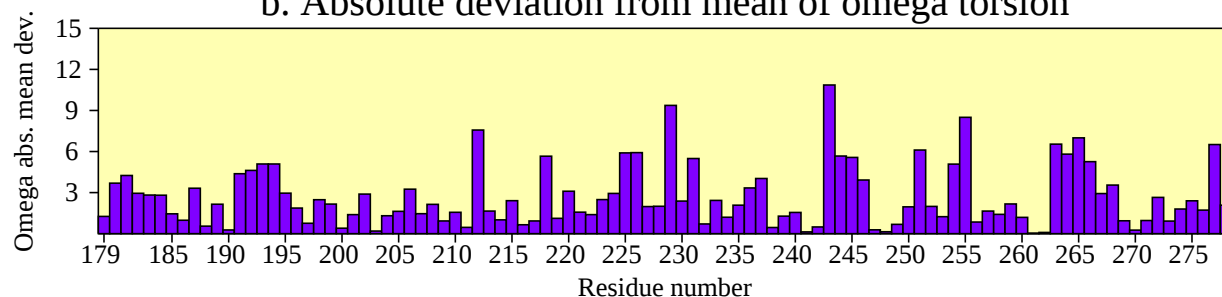
Residue properties

pdb2h88

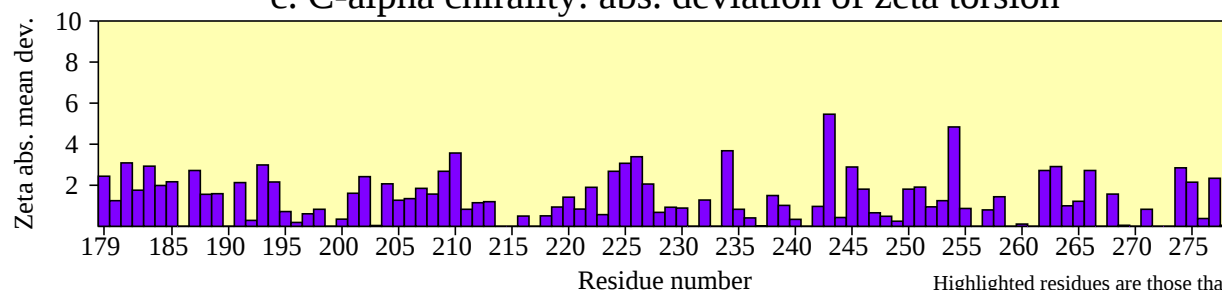
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

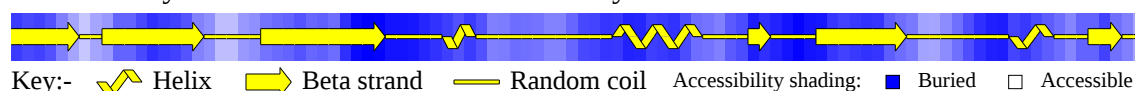


c. C-alpha chirality: abs. deviation of zeta torsion



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

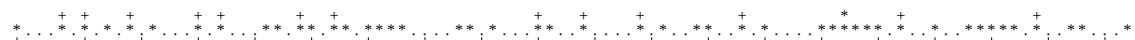
d. Secondary structure & estimated accessibility



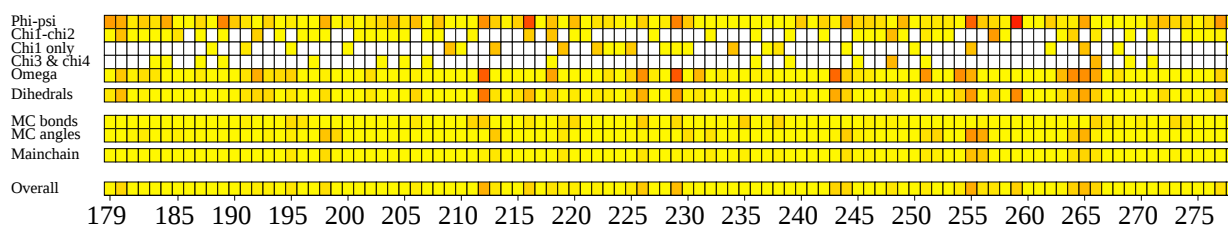
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



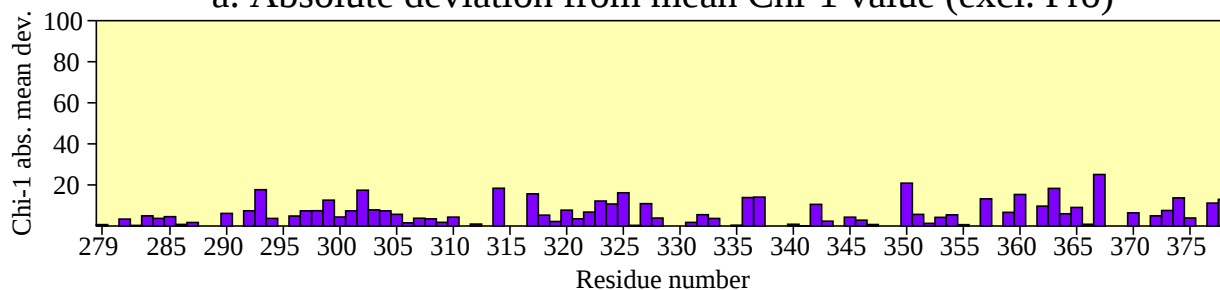
g. G-factors



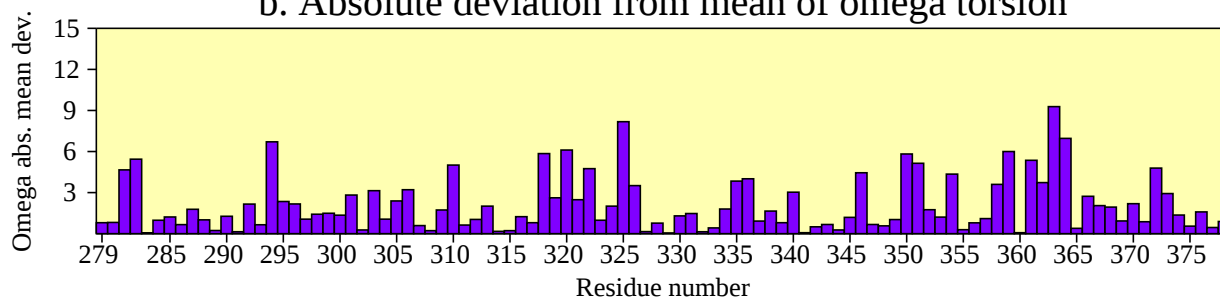
Residue properties

pdb2h88

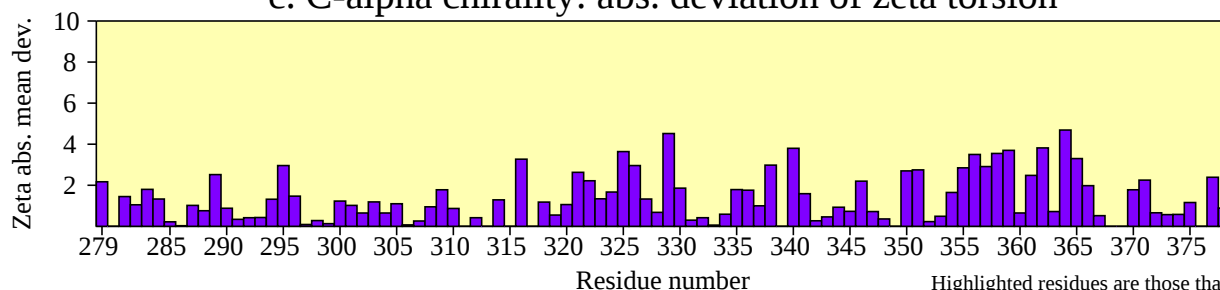
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

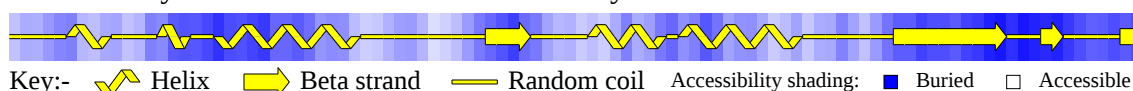


c. C-alpha chirality: abs. deviation of zeta torsion



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

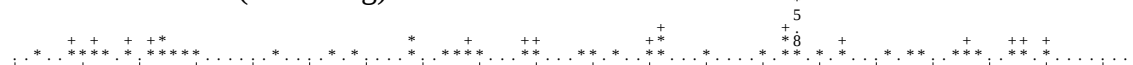
d. Secondary structure & estimated accessibility



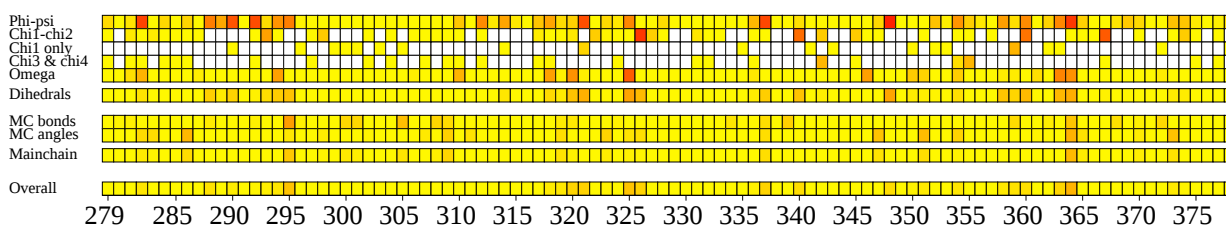
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



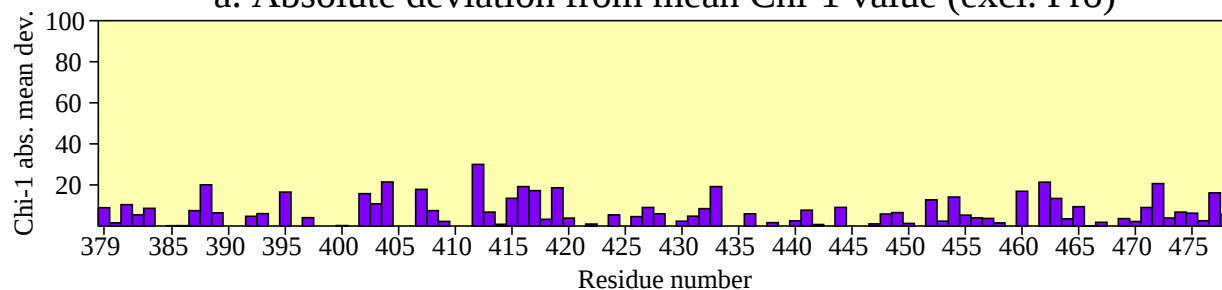
g. G-factors



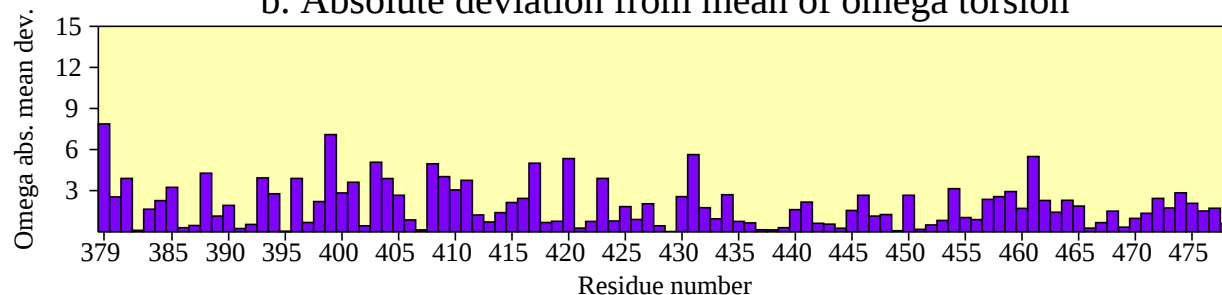
Residue properties

pdb2h88

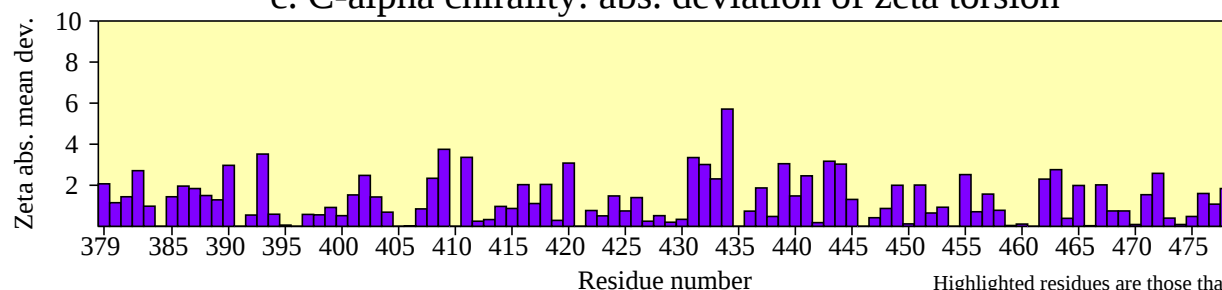
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

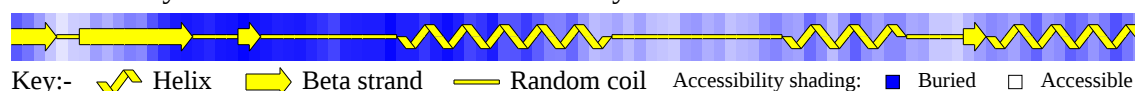


c. C-alpha chirality: abs. deviation of zeta torsion



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

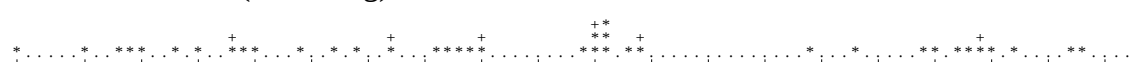
d. Secondary structure & estimated accessibility



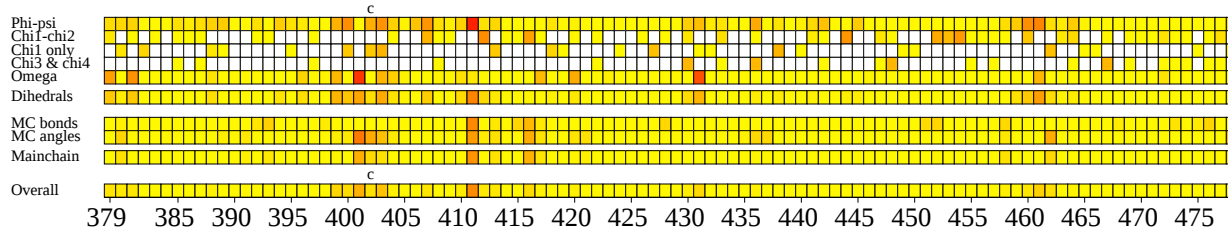
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

I THVNGEDKVPGLYACGEAASVHGANGRLGANSLLDLVVFGRACALTIAETCKPGEVPVPSIKPNAGEESVANLDKLRFDAGTIRTSPEARLNMQKTMQS

f. Max. deviation (see listing)



g. G-factors

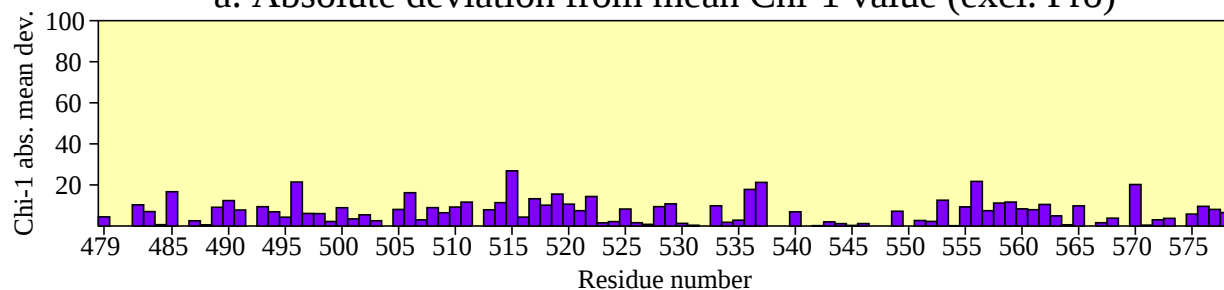


c = cis-peptide

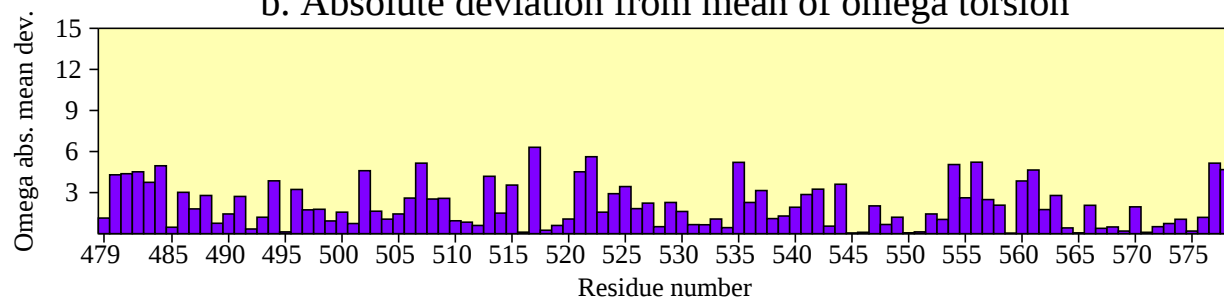
Residue properties

pdb2h88

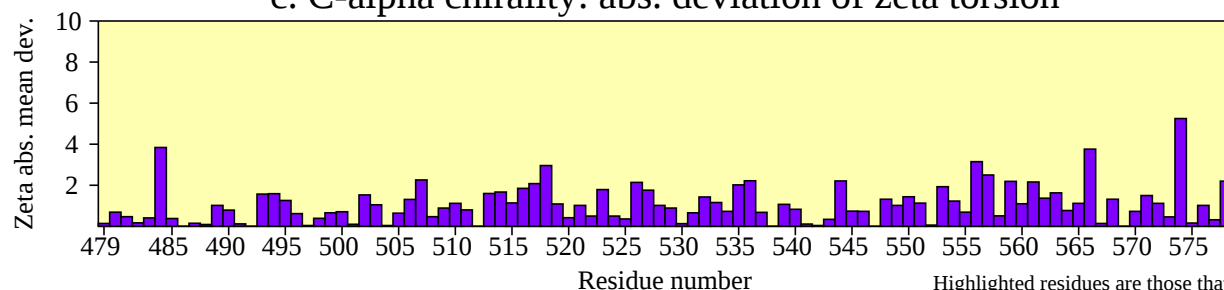
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



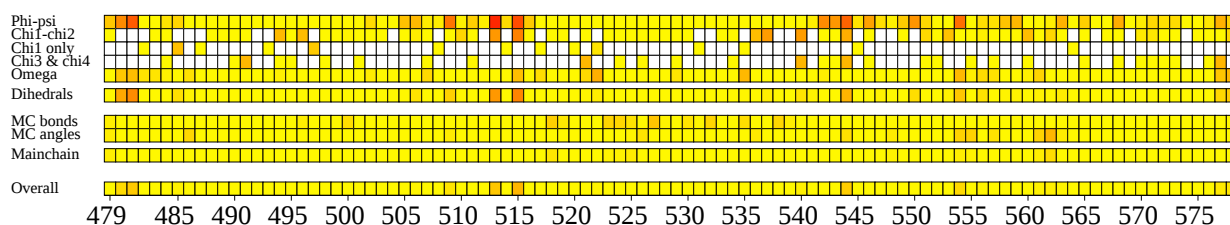
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

HAAVFTGS ILQEGCEKLSQIYRDLAHLKTFDRGI VVNTDLVETLELQNLMLCALQTIYGAEARKE SRGAHAREDYKLRIDEFDYSKPLQGQKRPFEH

f. Max. deviation (see listing)



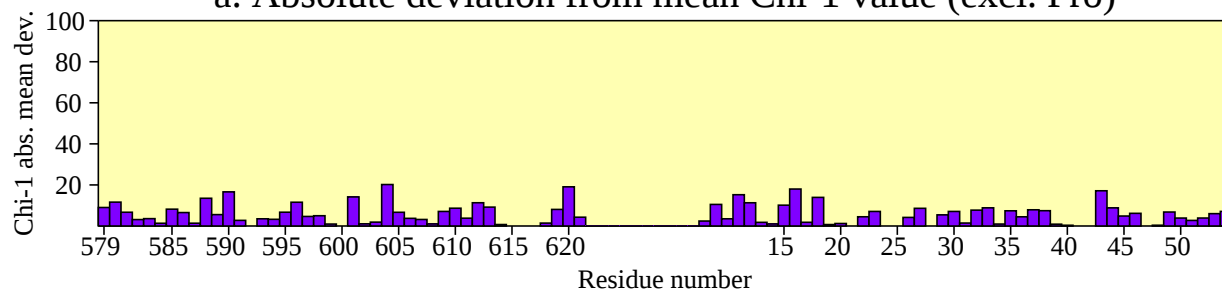
g. G-factors



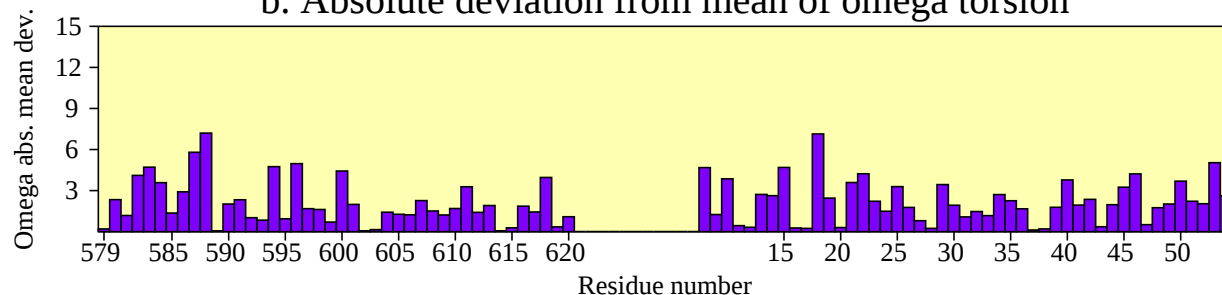
Residue properties

pdb2h88

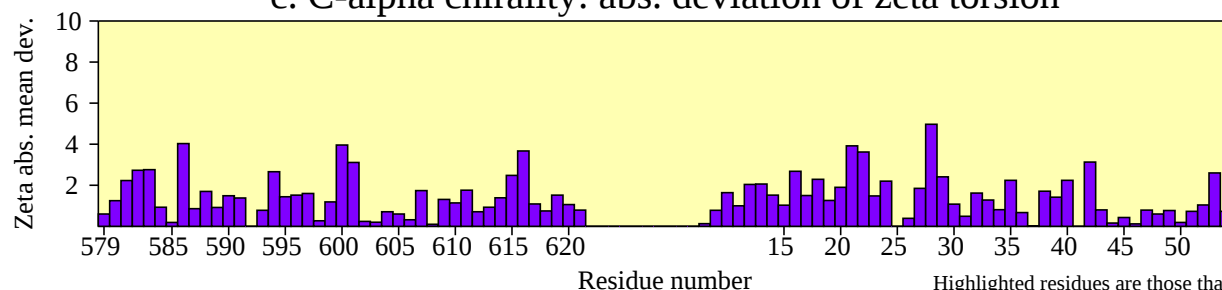
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

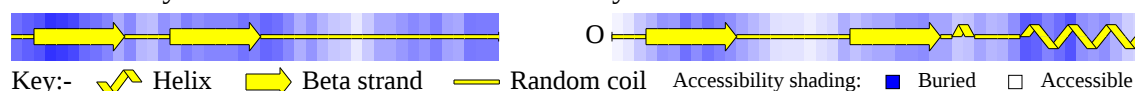


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



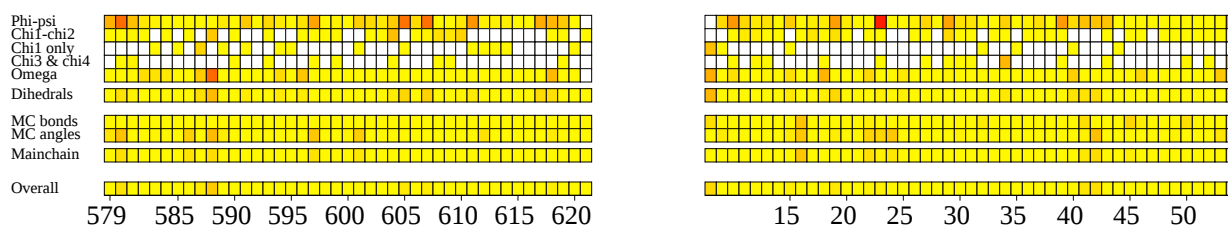
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



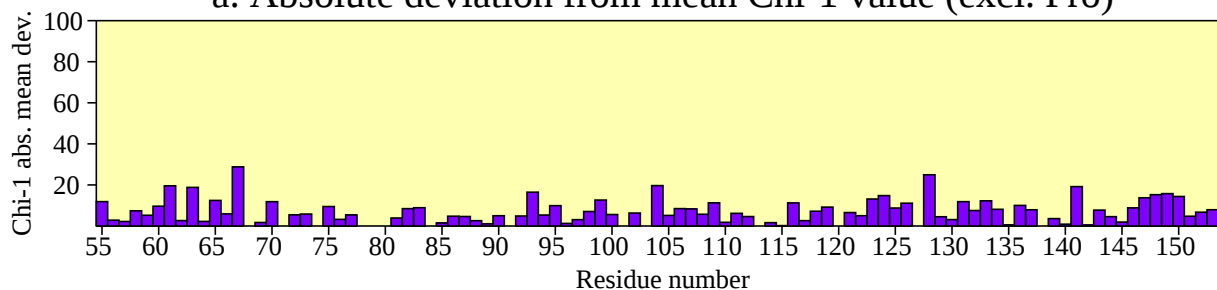
g. G-factors



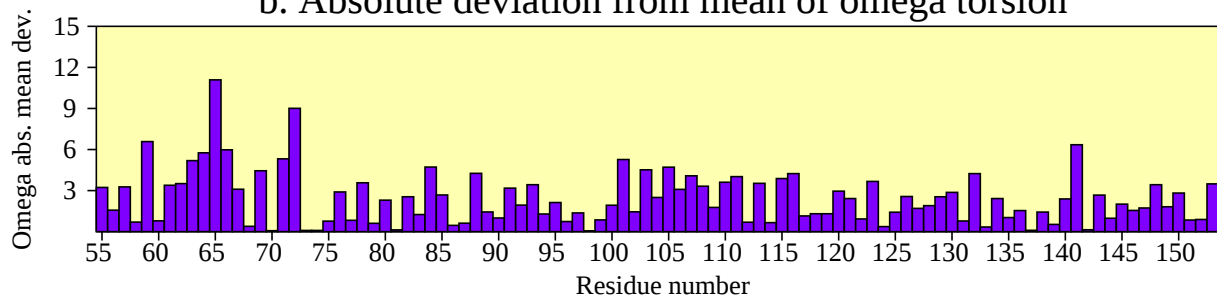
Residue properties

pdb2h88

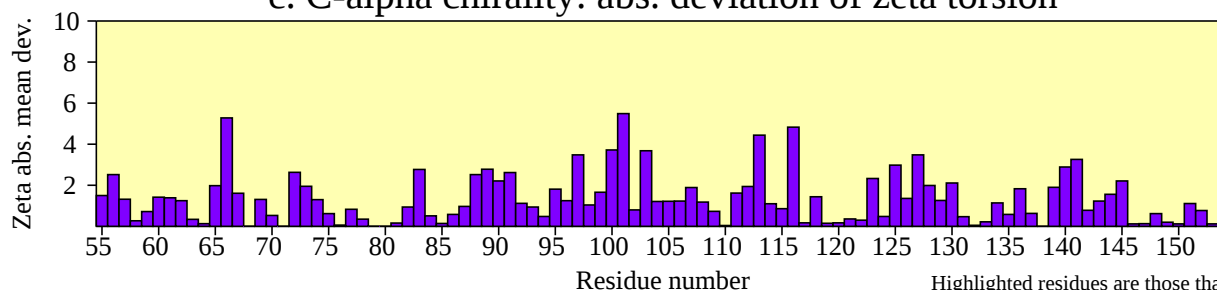
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

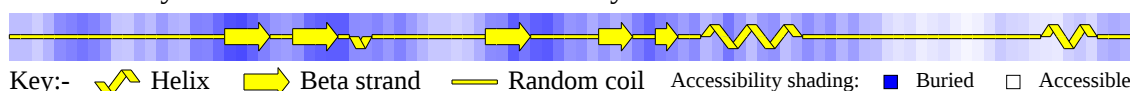


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

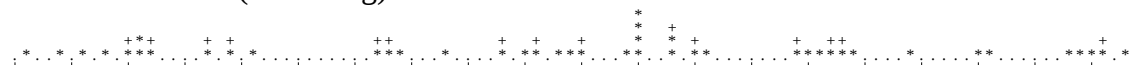


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

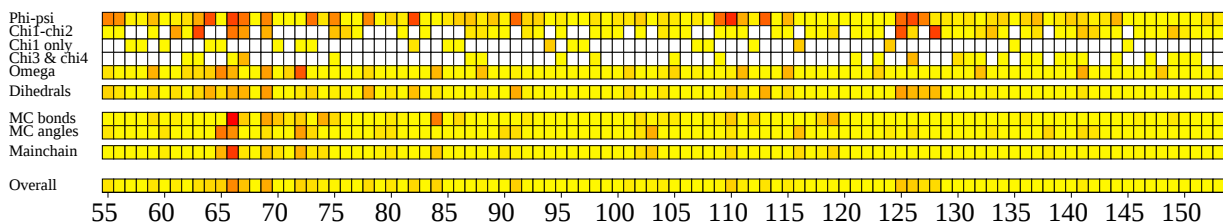
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

LDSTLTFRRSREGICGSCAMNIAGGNTLACTKKIDPDL SKTTKIYPLPHMYVVKDLVPDL SNFYAQYKSIEPYLKKKDESKQGKEQYLSIEDRQKLDG

f. Max. deviation (see listing)



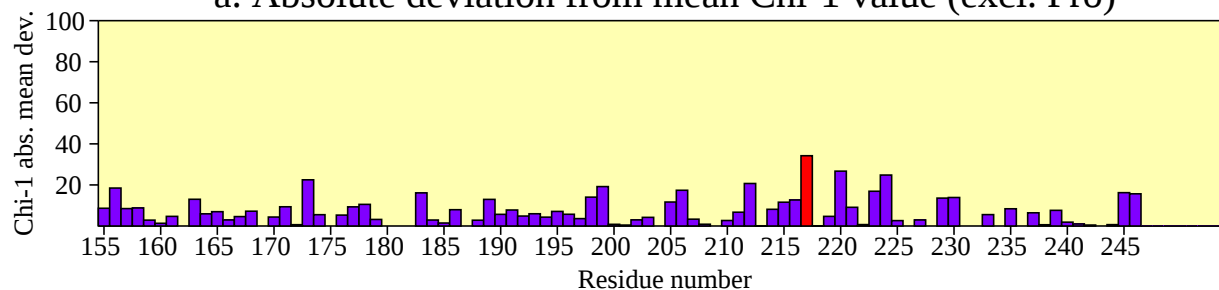
g. G-factors



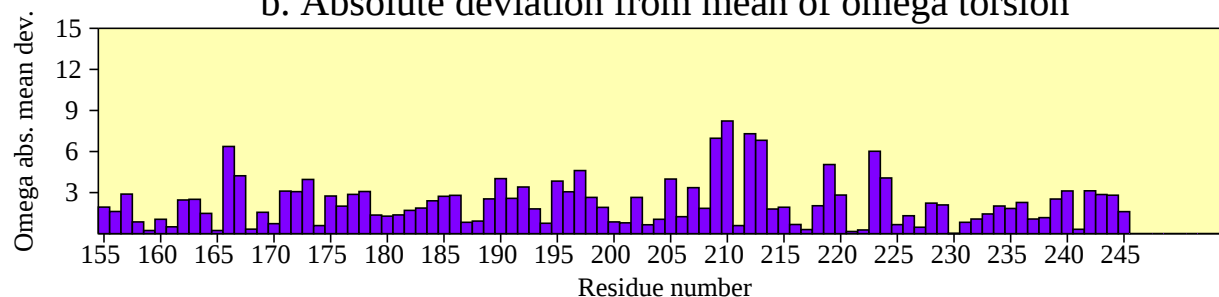
Residue properties

pdb2h88

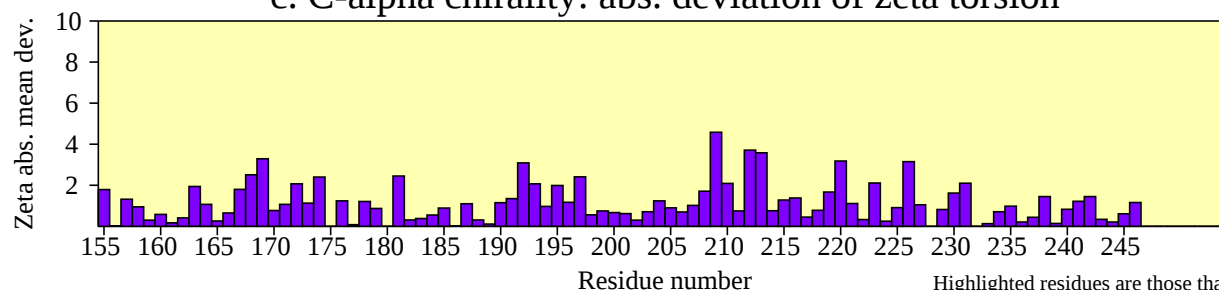
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

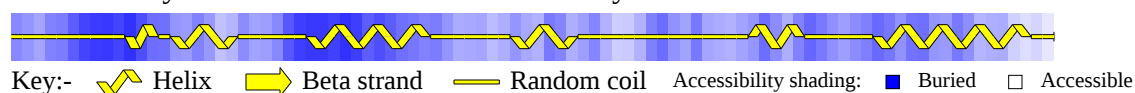


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



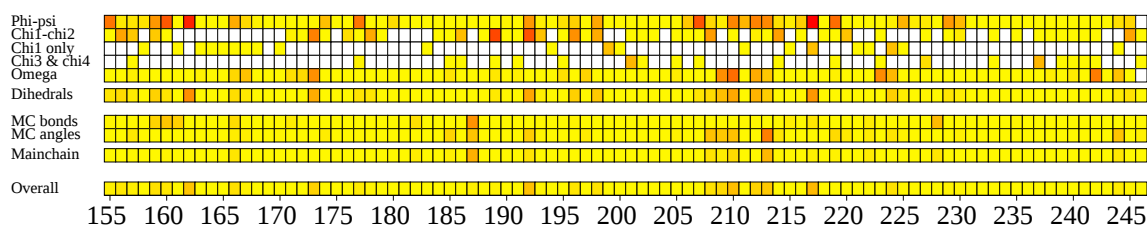
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

LYEC1LCACCTSCPSYWWNGDKYLGPVLMQAYRWIMDSRDDYTEERLAQLQDPFSLYRCHTIMNCTRTPKGLNPGKAI AEIKKMMATYK

f. Max. deviation (see listing)



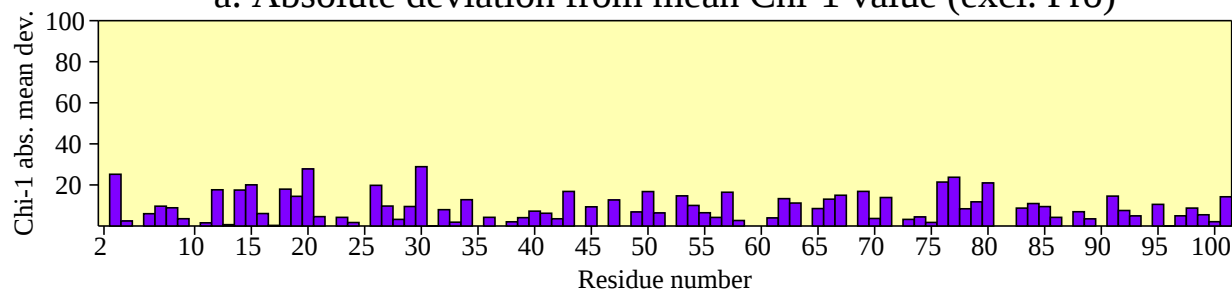
g. G-factors



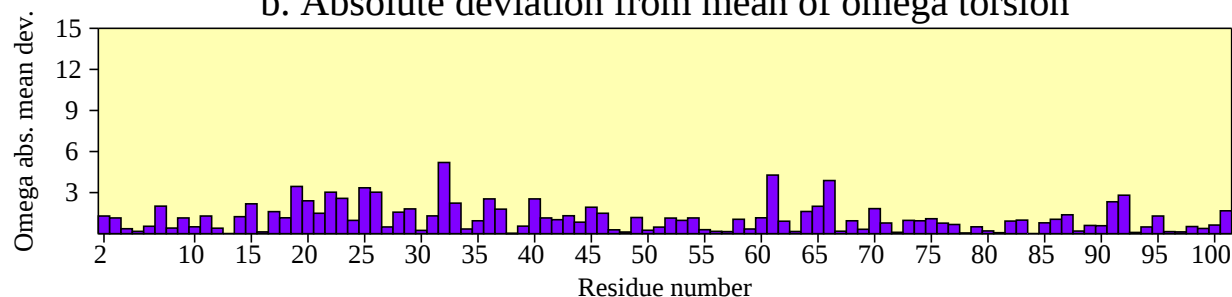
Residue properties

pdb2h88

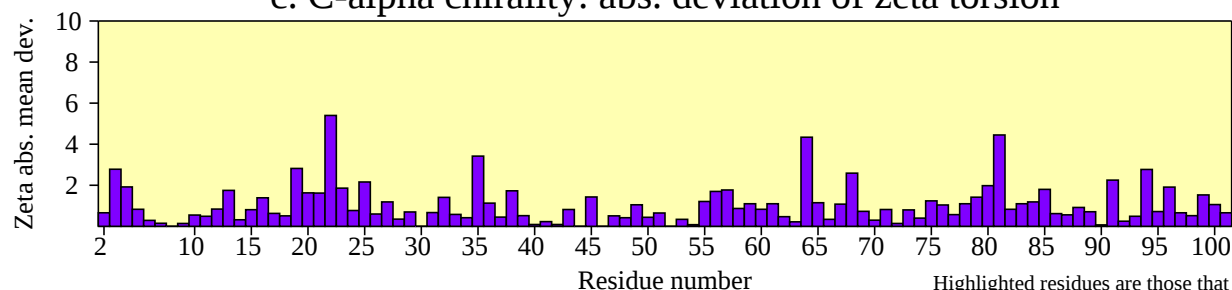
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



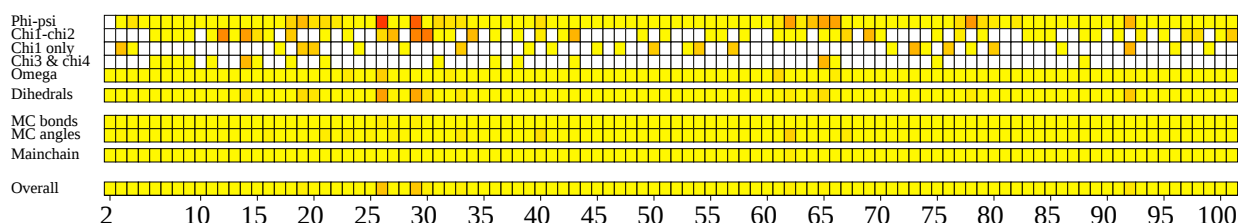
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

ATTAKEEMARFWEKNTKSSRPLSPHIS IYKWSLPMAMS I THRG TGVALSLGVSLFSLAALLLPEQFPHYVAVVKSLSLSPAL IYSAKFALVFPLSYHTWN

f. Max. deviation (see listing)



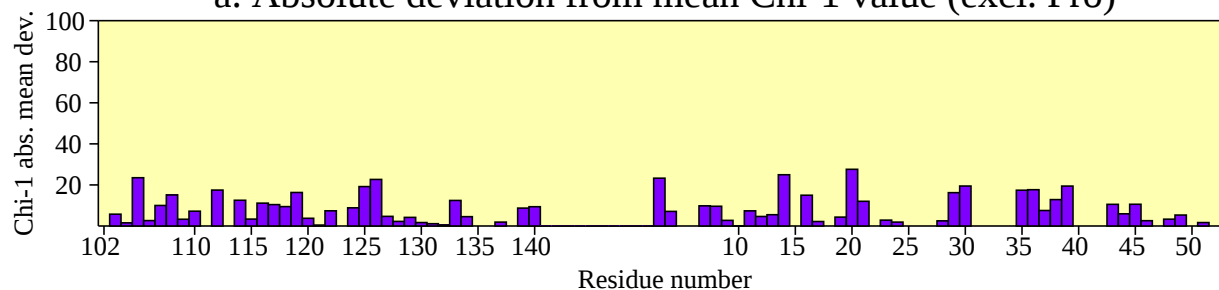
g. G-factors



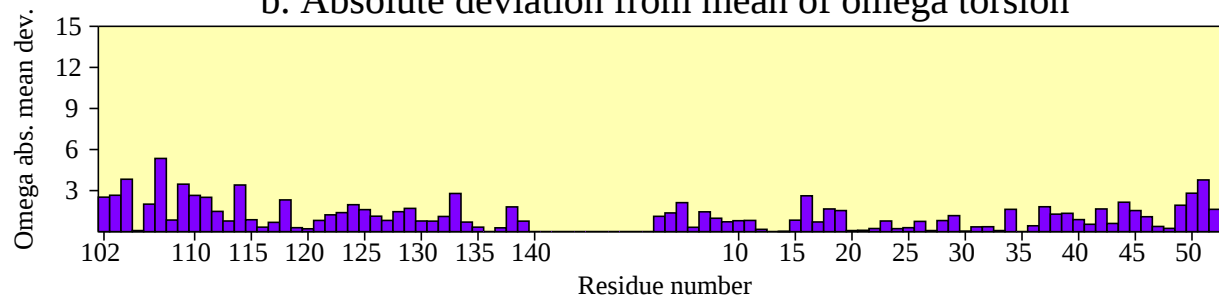
Residue properties

pdb2h88

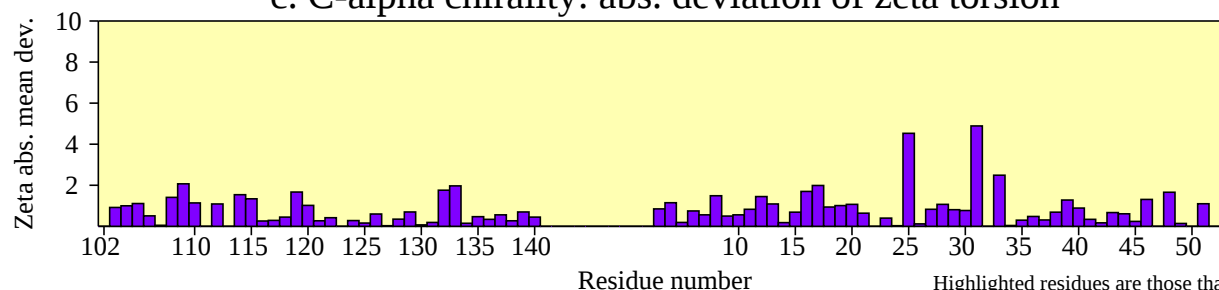
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

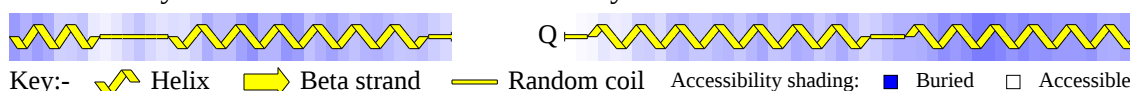


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



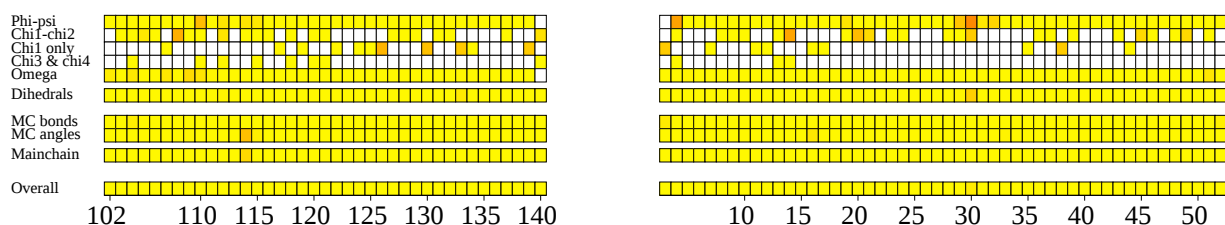
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



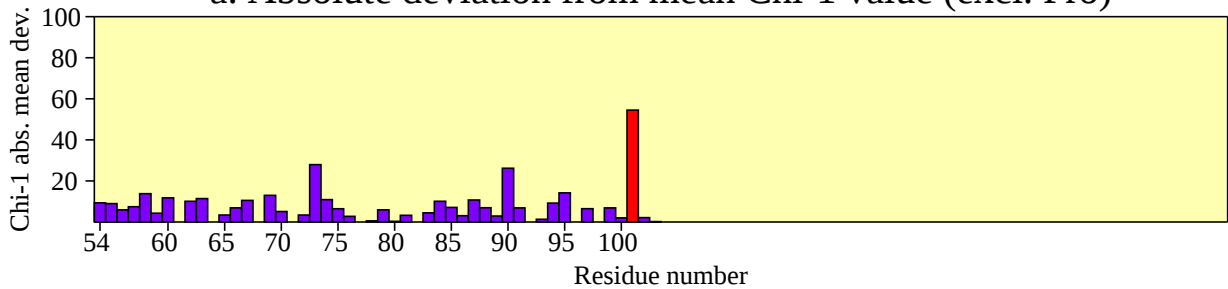
g. G-factors



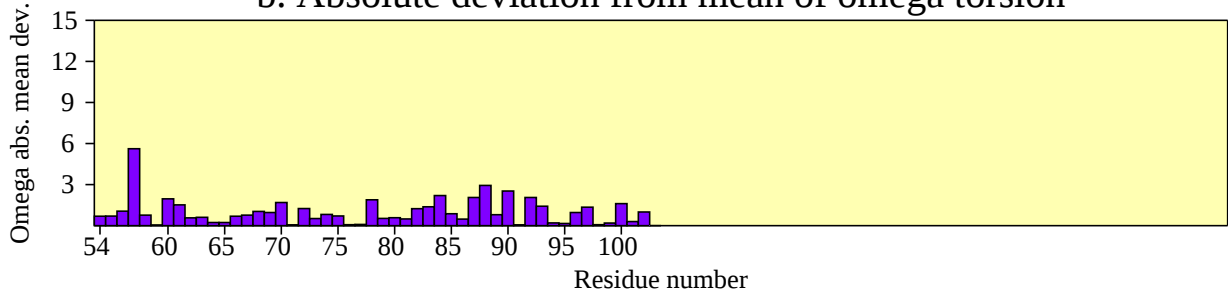
Residue properties

pdb2h88

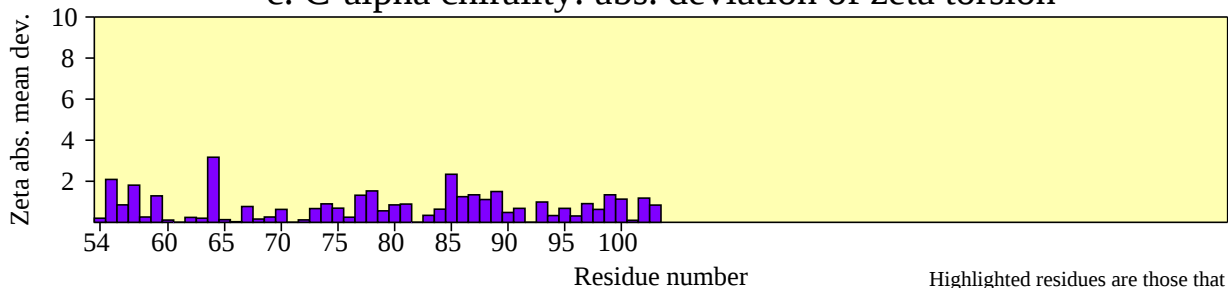
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

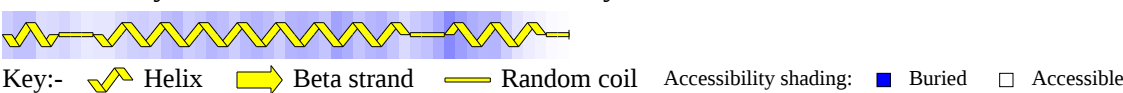


c. C-alpha chirality: abs. deviation of zeta torsion



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

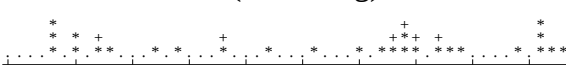
d. Secondary structure & estimated accessibility



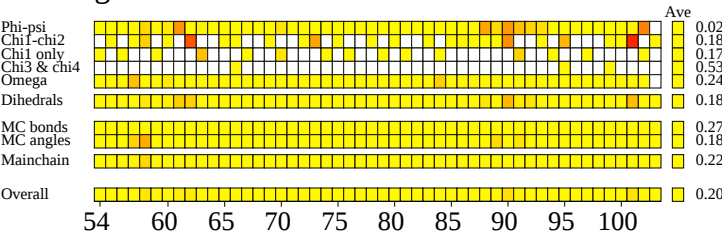
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

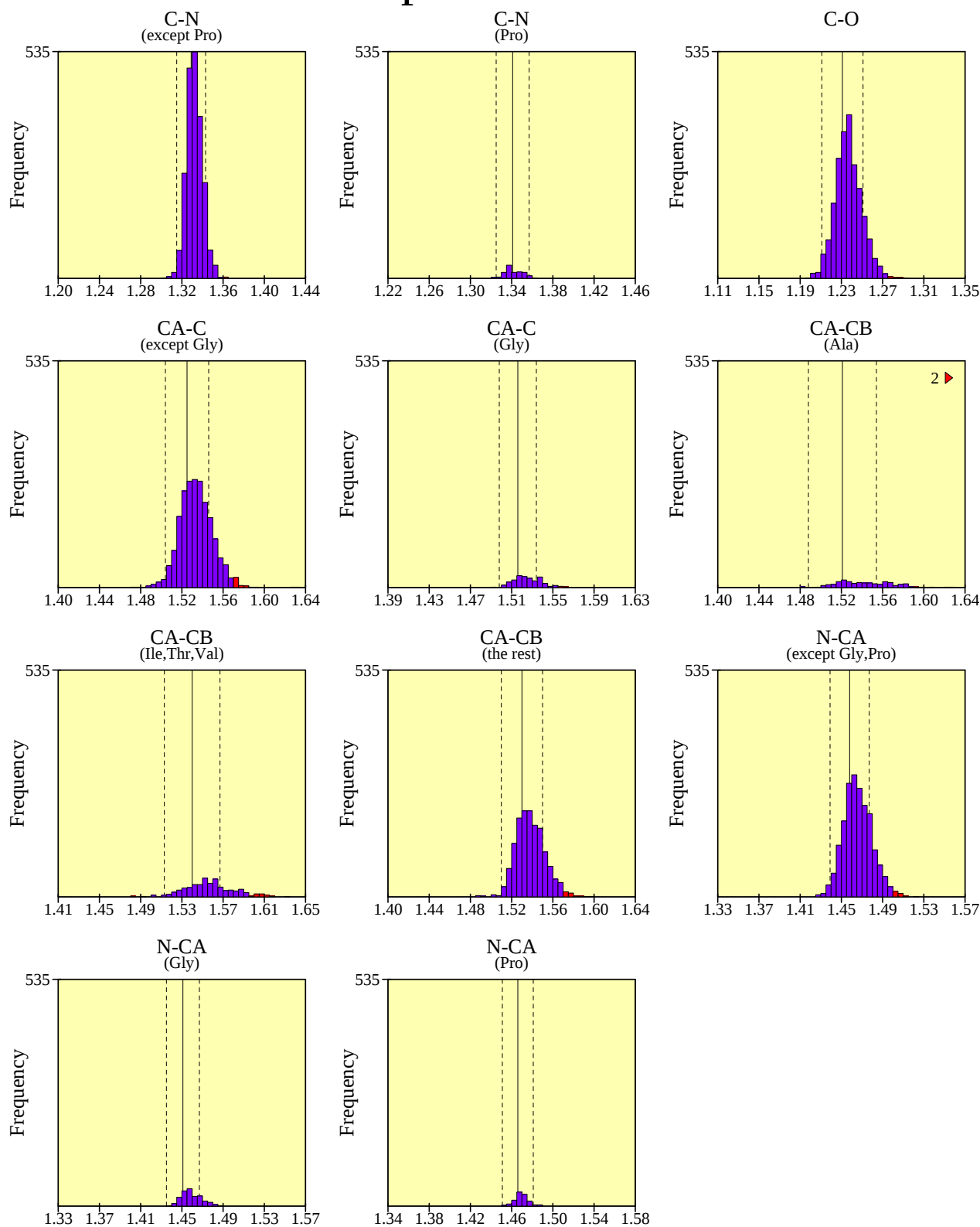


g. G-factors



Main-chain bond lengths

pdb2h88



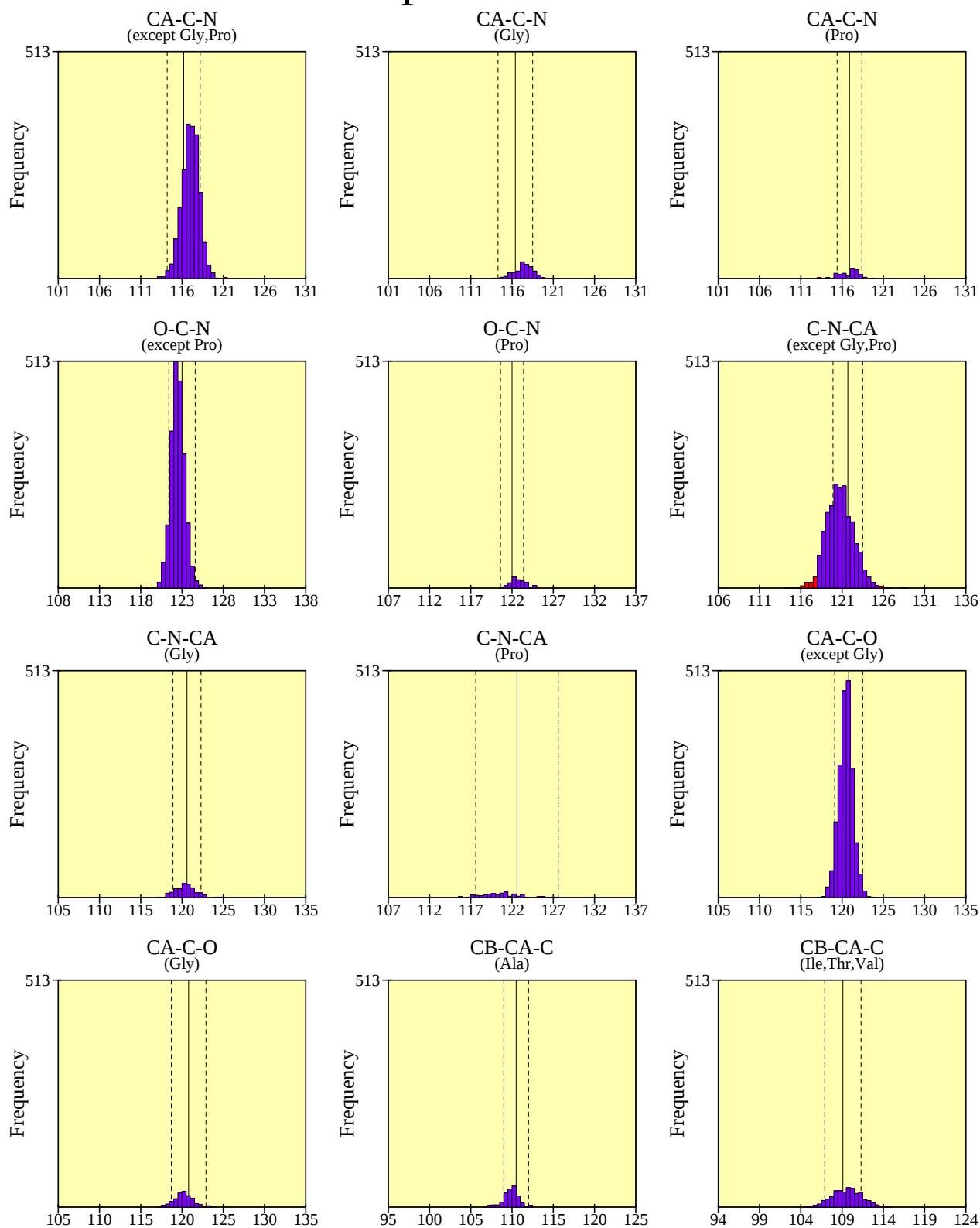
Black bars > 2.0 st. devs. from mean.

◀ 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

pdb2h88

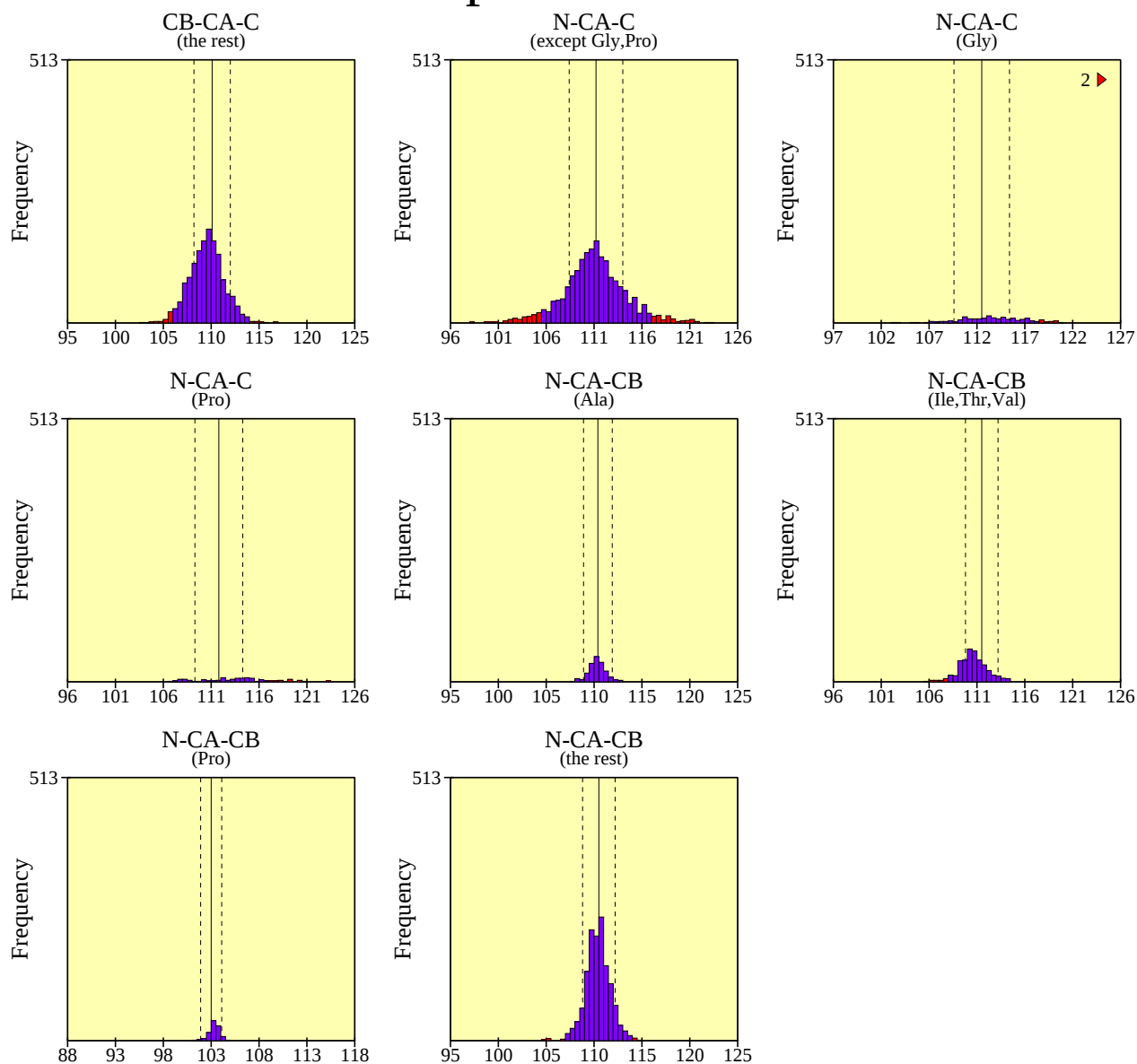


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

pdb2h88



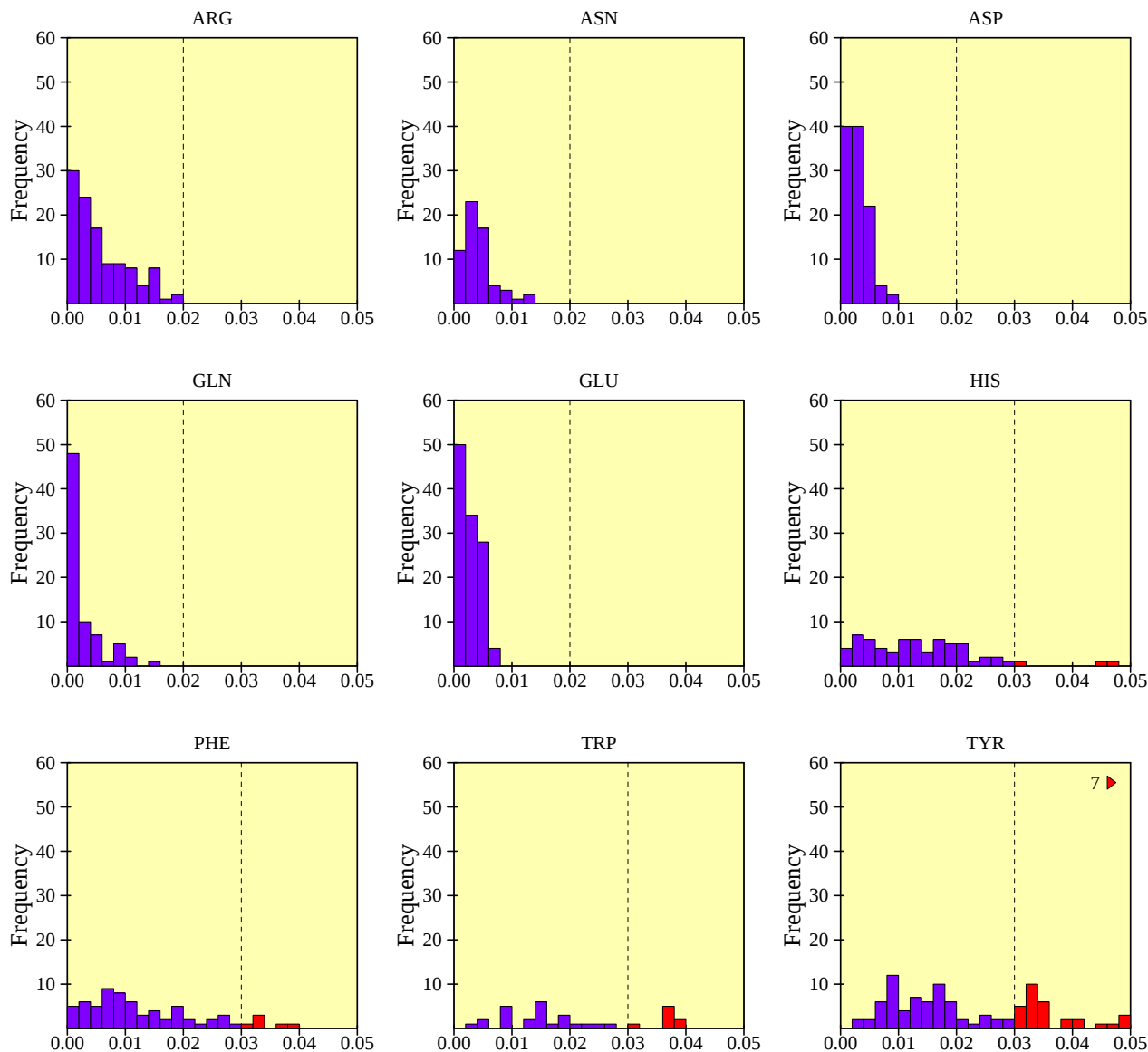
Black bars > 2.0 st. devs. from mean.

◀ 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

pdb2h88



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

pdb2h88

Main-chain bond lengths

CA 1.521 CB 0.055 1.576 A Ala 33	CA 1.540 CB 0.054 1.594 A Thr 48	CA 1.540 CB 0.063 1.603 A Thr 57	CA 1.540 CB 0.051 1.591 A Ile 64	CA 1.525 C 0.051 1.576 A Arg 77	CA 1.525 C 0.060 1.585 A Trp 78
CA 1.540 CB 0.073 1.613 A Thr 83	CA 1.521 CB 0.124 1.645 A Ala 103	CA 1.521 CB 0.053 1.574 A Ala 105	CA 1.540 CB 0.054 1.594 A Val 107	CA 1.525 C 0.050 1.475 A Cys 148	CA 1.540 CB 0.056 1.596 A Val 174
CA 1.540 CB 0.065 1.605 A Ile 196	CA 1.521 CB 0.056 1.577 A Ala 206	CA 1.540 CB 0.055 1.485 A Ile 211	CA 1.525 C 0.053 1.578 A Thr 219	CA 1.540 CB 0.067 1.607 A Thr 219	CA 1.521 CB 0.055 1.576 A Ala 226
CA 1.540 CB 0.065 1.605 A Thr 255	CA 1.525 C 0.051 1.576 A Glu 266	CA 1.525 C 0.058 1.582 A Ala 295	CA 1.521 CB 0.077 1.598 A Ala 295	CA 1.525 C 0.064 1.589 A Thr 305	C 1.231 O 0.056 1.287 A Ile 308
CA 1.540 CB 0.054 1.594 A Val 352	CA 1.540 CB 0.070 1.610 A Val 359	CA 1.540 CB 0.054 1.594 A Thr 372	CA 1.521 CB 0.055 1.576 A Ala 411	CA 1.540 CB 0.054 1.594 A Val 587	CA 1.540 CB 0.053 1.592 B Ile 16
CA 1.530 CB 0.052 1.582 B Arg 63	CA 1.525 C 0.104 1.629 B Arg 66	N 1.458 CA 0.052 1.510 B Arg 66	CA 1.540 CB 0.079 1.619 B Ile 69	CA 1.530 CB 0.067 1.597 B Ser 72	CA 1.521 CB 0.062 1.583 B Ala 74
CA 1.521 CB 0.109 1.630 B Ala 84	CA 1.540 CB 0.061 1.601 B Val 112	CA 1.521 CB 0.066 1.587 B Ala 204	CA 1.521 CB 0.059 1.580 C Ala 10	CA 1.540 CB 0.064 1.604 C Ile 29	CA 1.525 C 0.052 1.577 C Arg 104
CA 1.521 CB 0.055 1.576 D Ala 6	CA 1.521 CB 0.060 1.581 N Ala 21	CA 1.525 C 0.054 1.579 N Val 22	CA 1.521 CB 0.060 1.581 N Ala 26	CA 1.530 CB 0.050 1.580 N Phe 35	CA 1.530 CB 0.056 1.586 N Glu 39
CA 1.540 CB 0.065 1.605 N Thr 44	CA 1.540 CB 0.093 1.633 N Thr 57	N 1.458 CA 0.055 1.513 N His 79	CA 1.540 CB 0.065 1.605 N Thr 83	N 1.458 CA 0.050 1.508 N Glu 101	CA 1.521 CB 0.100 1.621 N Ala 103
CA 1.521 CB 0.063 1.584 N Ala 105	CA 1.540 CB 0.069 1.609 N Ile 196	CA 1.521 CB 0.060 1.581 N Ala 206	CA 1.540 CB 0.058 1.482 N Ile 211	CA 1.540 CB 0.051 1.591 N Thr 219	CA 1.521 CB 0.061 1.582 N Ala 235
CA 1.525 C 0.058 1.583 N Glu 266	CA 1.521 CB 0.059 1.580 N Ala 288	CA 1.525 C 0.069 1.594 N Ala 295	CA 1.521 CB 0.063 1.584 N Ala 295	N 1.458 CA 0.050 1.508 N Ser 301	CA 1.521 CB 0.072 1.593 N Ala 334

Distorted geometry

pdb2h88

Main-chain bond lengths (contd)

CA 1.540 CB 0.075 1.615 N Val 359	CA 1.540 CB 0.053 1.593 N Thr 362	CA 1.530 CB 0.060 1.590 N His 364	CA 1.540 CB 0.070 1.610 N Thr 372	C 1.231 O 0.062 1.293 N Ala 411	CA 1.521 CB 0.070 1.591 N Ala 411
CA 1.521 CB 0.087 1.608 N Ala 451	CA 1.540 CB 0.057 1.597 N Thr 535	CA 1.521 CB 0.062 1.583 N Ala 539	CA 1.521 CB 0.054 1.575 N Ala 548	CA 1.540 CB 0.051 1.591 N Val 587	CA 1.540 CB 0.079 1.619 O Ile 16
CA 1.525 C 0.057 1.582 O Leu 45	CA 1.525 C 0.108 1.633 O Arg 66	CA 1.540 CB 0.069 1.609 O Ile 69	CA 1.530 CB 0.059 1.589 O Ser 72	C 1.231 O 0.056 1.287 O Met 75	CA 1.521 CB 0.133 1.654 O Ala 84
CA 1.540 CB 0.062 1.602 O Thr 86	CA 1.540 CB 0.074 1.614 O Val 112	CA 1.521 CB 0.065 1.586 O Ala 162	N 1.458 CA 0.063 1.521 O Ala 187	CA 1.521 CB 0.055 1.576 O Ala 204	CA 1.540 CB 0.062 1.602 O Thr 217
C 1.231 O 0.051 1.282 O Gly 228	CA 1.521 CB 0.057 1.578 P Ala 10	CA 1.540 CB 0.064 1.604 P Ile 29			

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

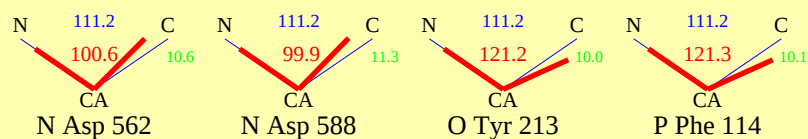
Main-chain bond angles

N 111.2 C 100.8 10.4 CA A Phe 51	N 111.8 C 123.0 11.2 CA A Pro 52	N 112.5 C 128.1 15.6 CA A Gly 140	N 111.2 C 98.2 13.0 CA A Val 149	N 111.2 C 122.8 11.6 CA A Thr 255	N 111.2 C 121.9 10.7 CA A Ala 401
N 111.2 C 100.1 11.1 CA A Asp 562	N 111.2 C 100.5 10.7 CA A Asp 588	N 111.2 C 121.3 10.1 CA B Cys 65	N 111.2 C 121.3 10.1 CA B Tyr 213	N 111.2 C 121.4 10.2 CA C Phe 114	N 111.2 C 99.8 11.4 CA N Phe 51
N 111.8 C 123.2 11.4 CA N Pro 52	N 112.5 C 127.9 15.4 CA N Gly 140	N 111.2 C 98.3 12.9 CA N Val 149	N 111.2 C 123.2 12.0 CA N Thr 255	N 111.2 C 121.5 10.3 CA N Thr 265	N 111.2 C 121.9 10.7 CA N Ala 401

Distorted geometry

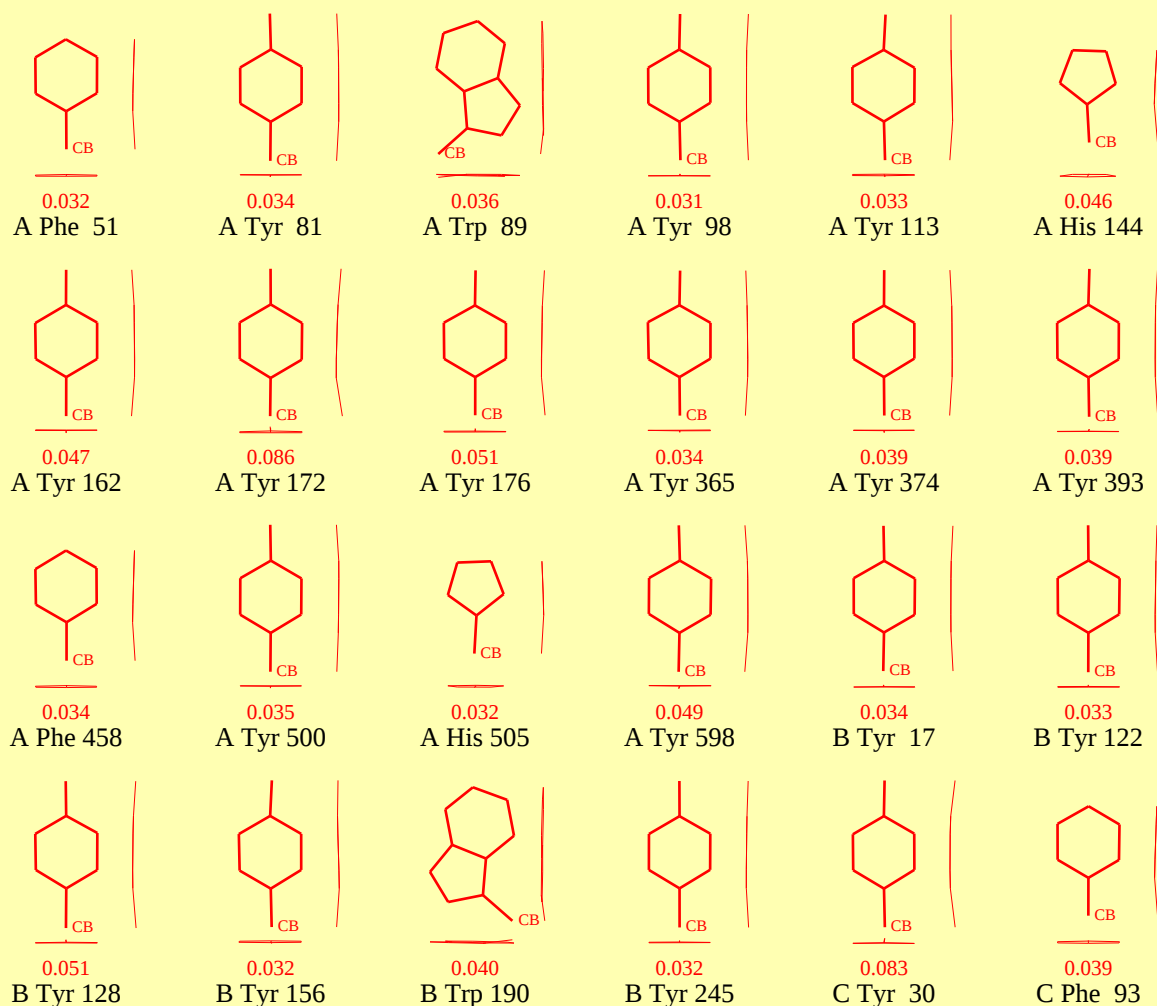
pdb2h88

Main-chain bond angles (contd)



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

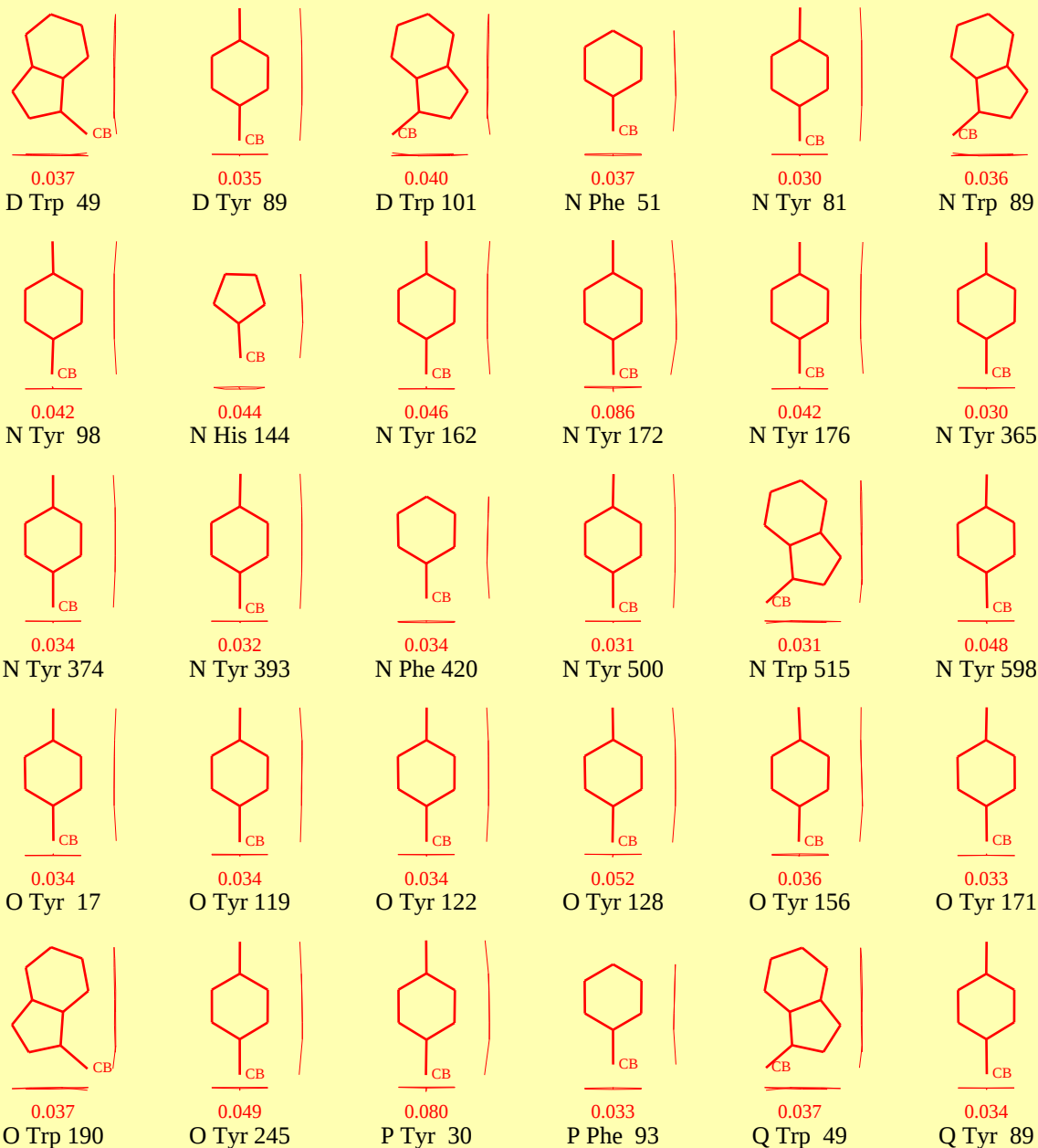
Planar groups



Distorted geometry

pdb2h88

Planar groups (contd)



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