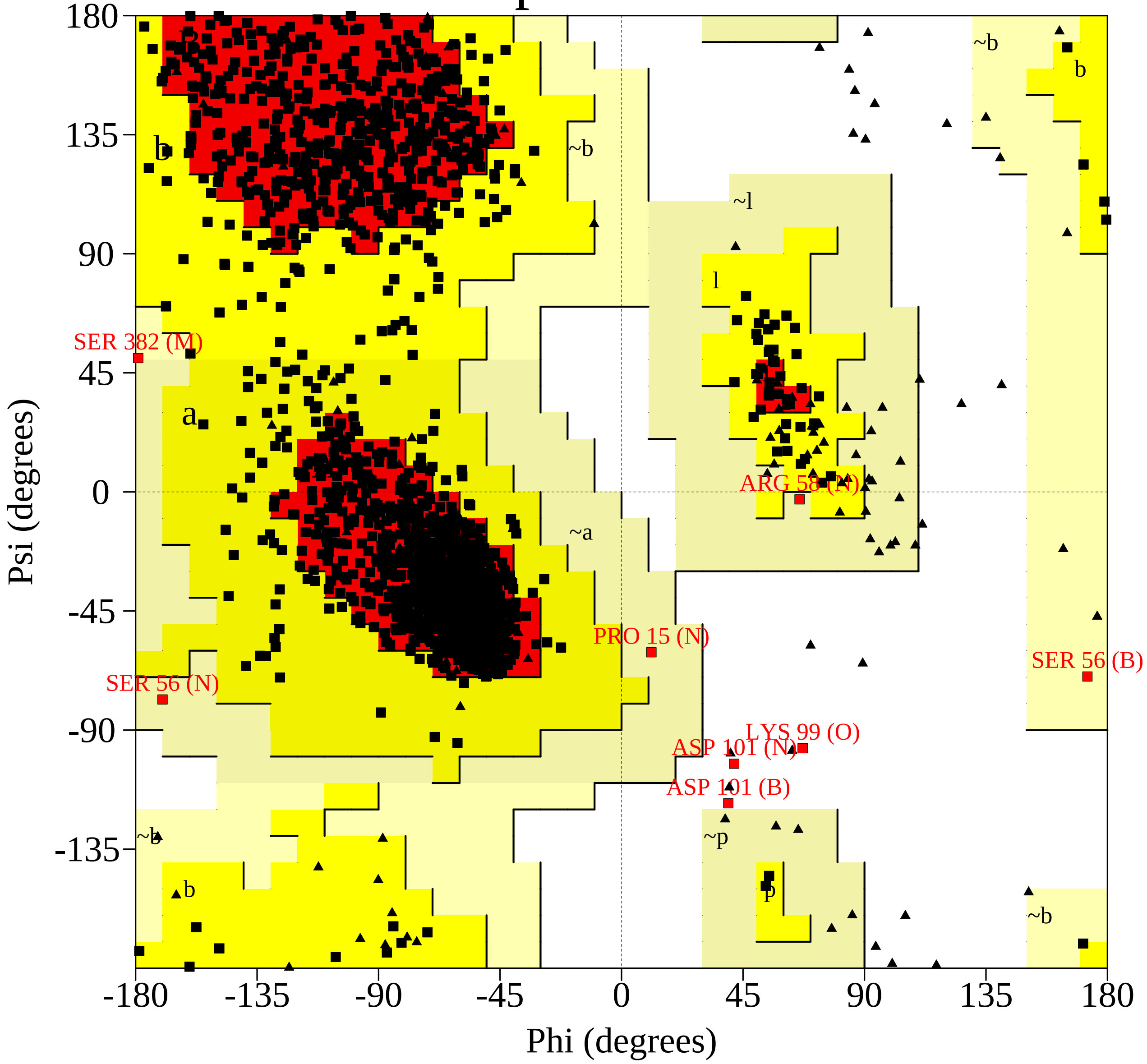
PROCHECK

Ramachandran Plot

pdb3cir



Plot statistics

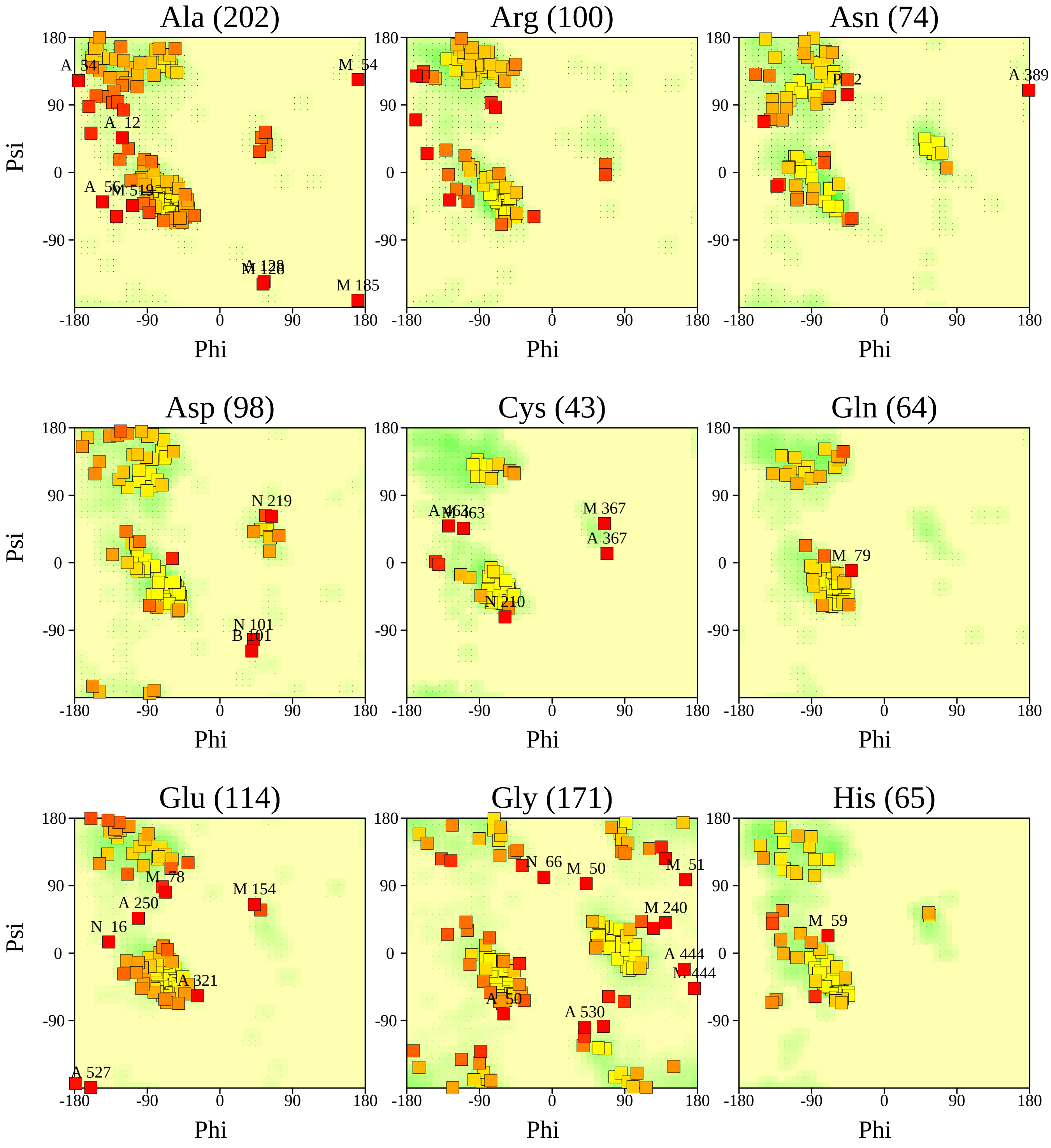
Residues in most favoured regions [A,B,L]	1555	89.4%
Residues in additional allowed regions [a,b,l,p]	177	10.2%
Residues in generously allowed regions [~a,~b,~l,~p]	4	0.2%
Residues in disallowed regions	3	0.2%
	----	------
Number of non-glycine and non-proline residues	1739	100.0%
Number of end-residues (excl. Gly and Pro)	26	
Number of glycine residues (shown as triangles)	172	
Number of proline residues	92	

Total number of residues	2029	

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

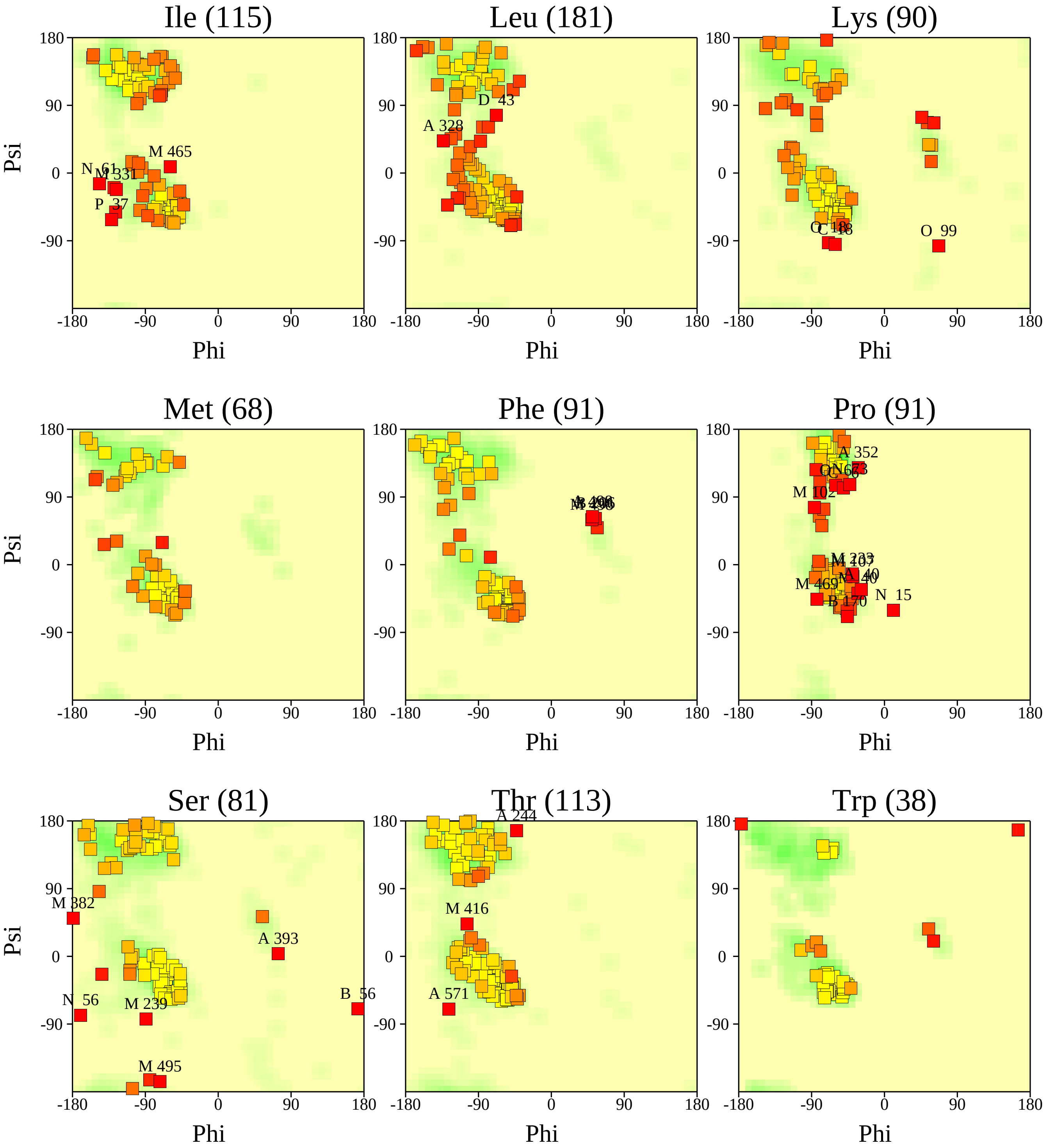
pdb3cir



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

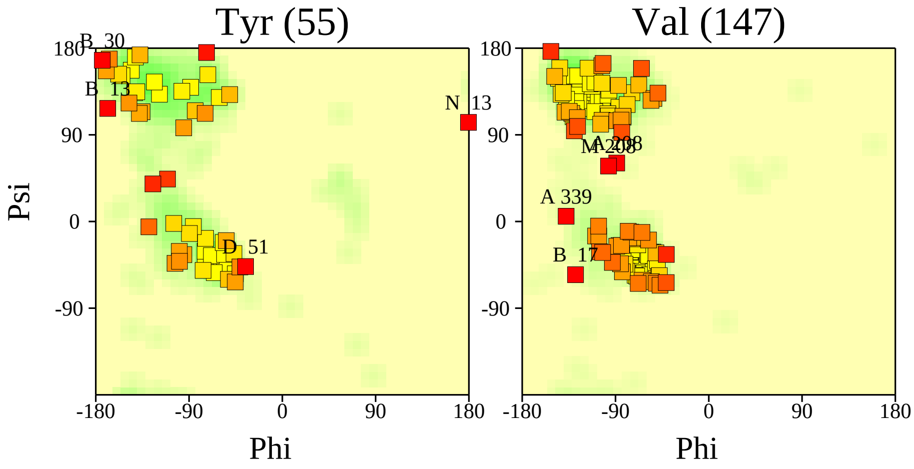
pdb3cir



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

pdb3cir

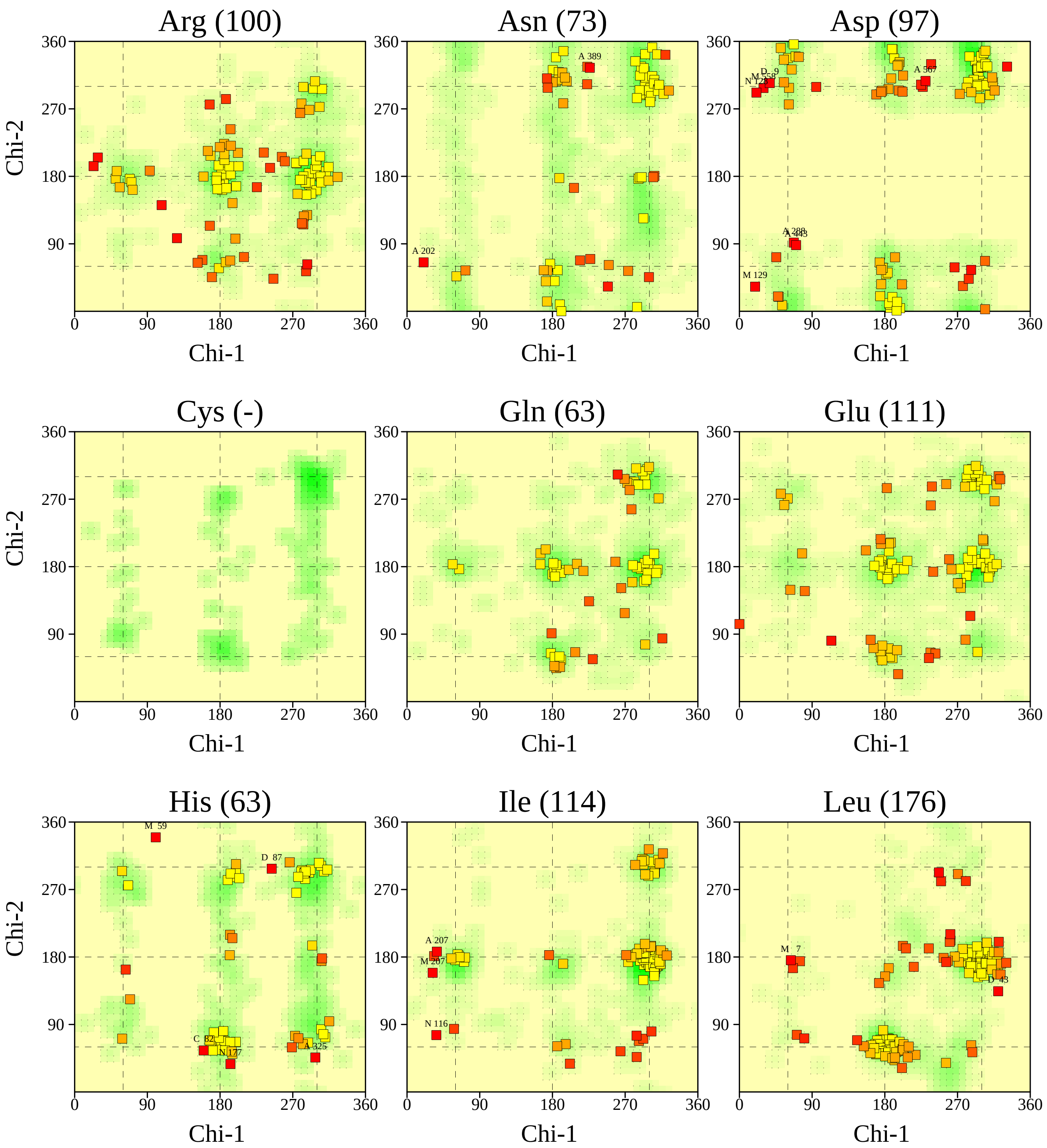


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

Chi1-Chi2 plots

pdb3cir

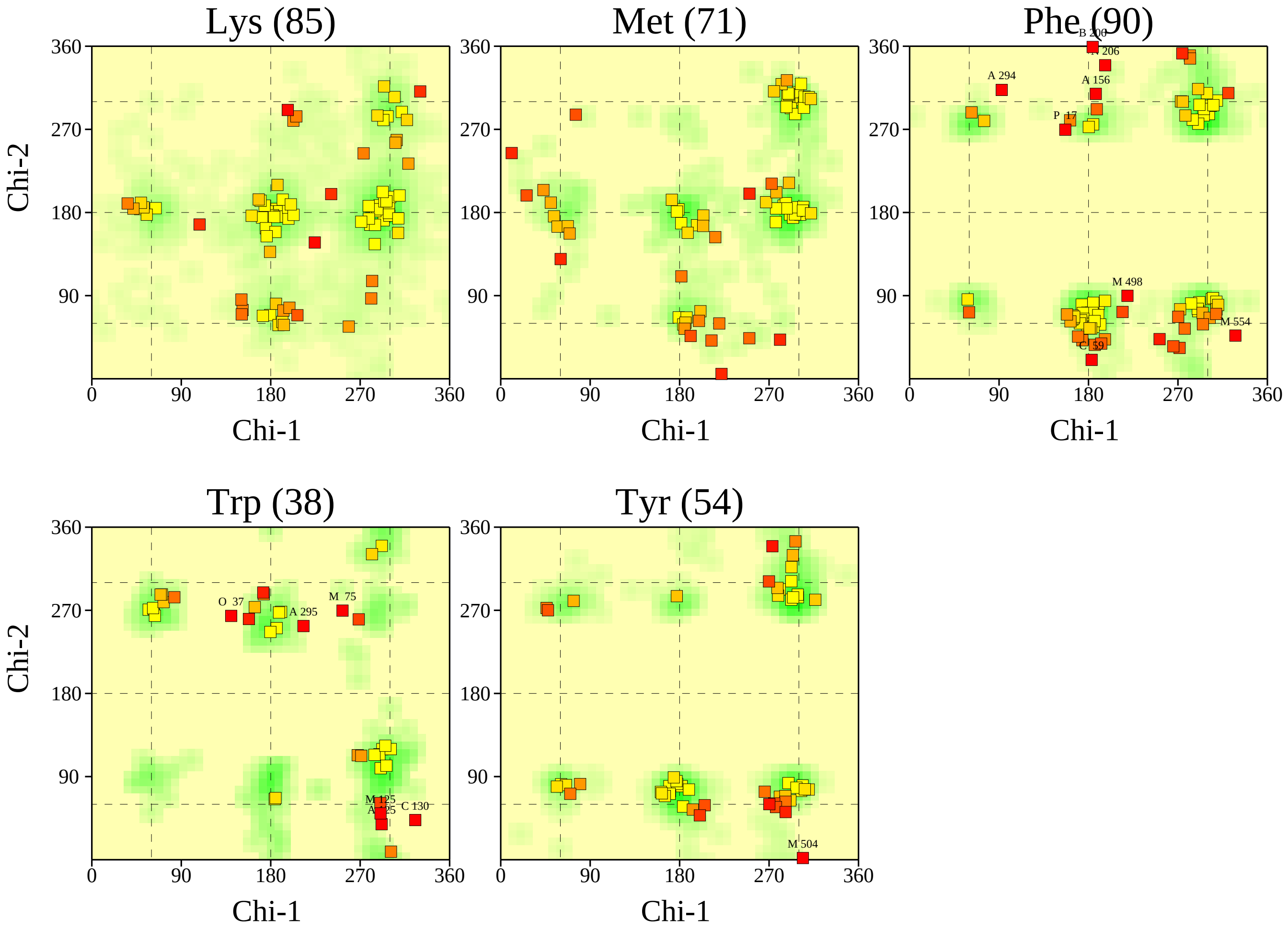


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

Chi1-Chi2 plots

pdb3cir

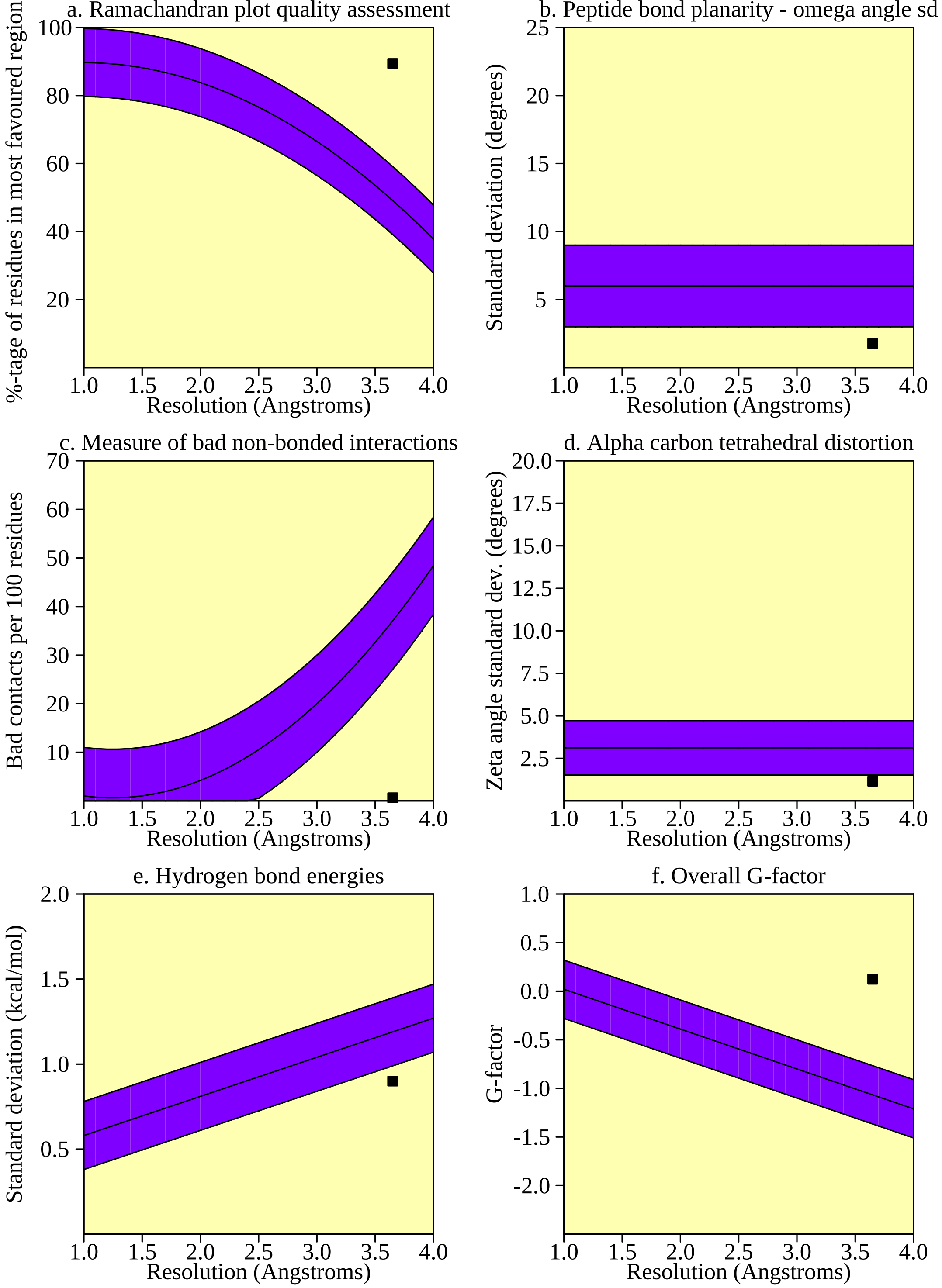


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

Main-chain parameters

pdb3cir



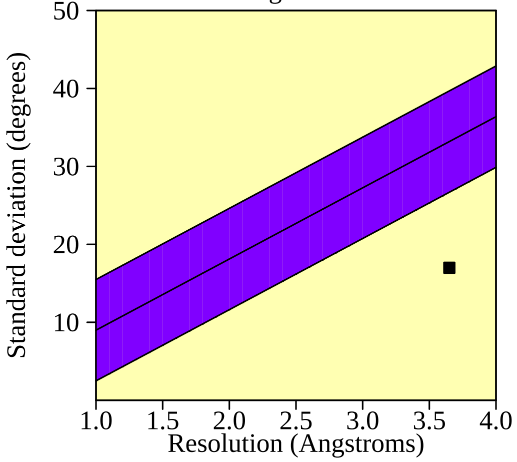
Plot statistics

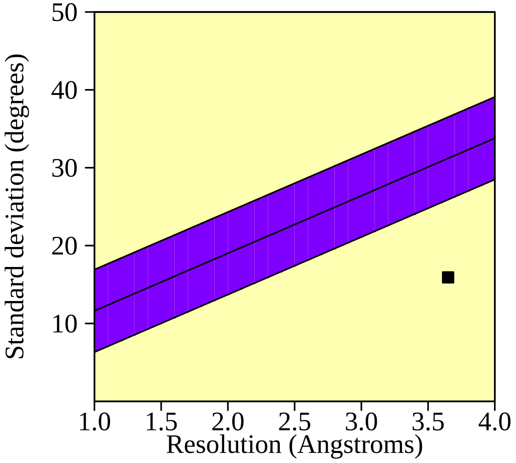
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	1739	89.4	49.1	10.0	4.0	BETTER
b. Omega angle st dev	2015	1.8	6.0	3.0	-1.4	BETTER
c. Bad contacts / 100 residues	13	0.6	37.0	10.0	-3.6	BETTER
d. Zeta angle st dev	1857	1.2	3.1	1.6	-1.2	BETTER
e. H-bond energy st dev	1300	0.9	1.2	0.2	-1.4	BETTER
f. Overall G-factor	2029	0.1	-1.1	0.3	4.0	BETTER

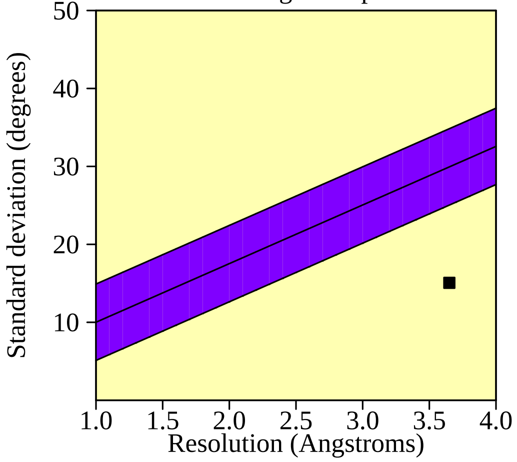
PROCHECK

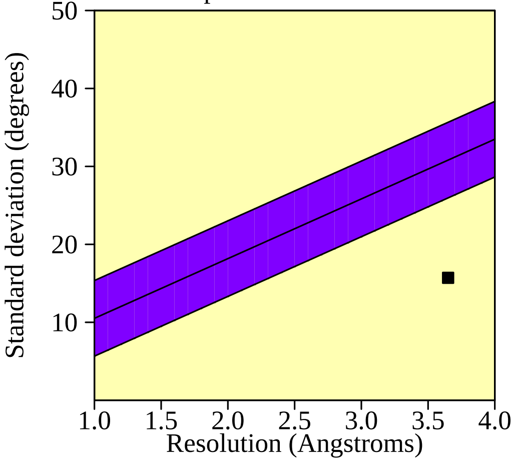
Side-chain parameters

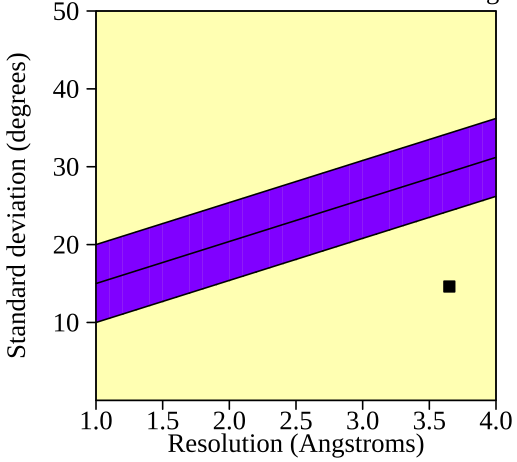
pdb3cir


a. Chi-1 gauche minus


b. Chi-1 trans


c. Chi-1 gauche plus


d. Chi-1 pooled standard deviation


e. Standard deviation of Chi-2 trans angle

pdb3cir

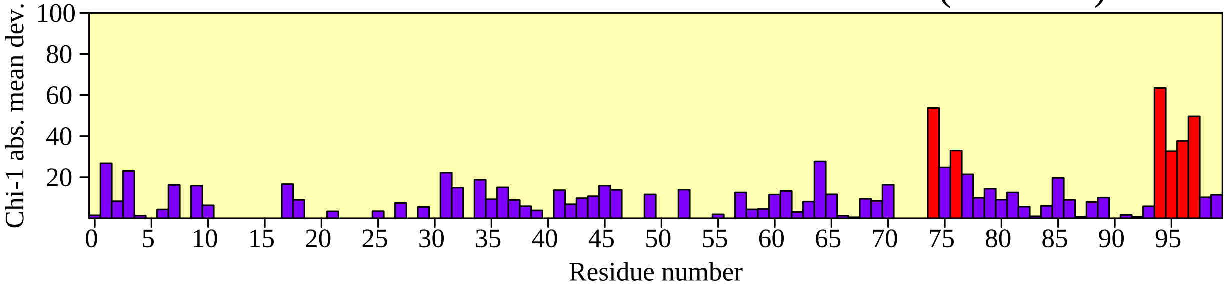
Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	215	17.0	33.2	6.5	-2.5	BETTER
b. Chi-1 trans st dev	554	15.9	31.2	5.3	-2.9	BETTER
c. Chi-1 gauche plus st dev	746	15.1	29.9	4.9	-3.0	BETTER
d. Chi-1 pooled st dev	1515	15.7	30.8	4.8	-3.1	BETTER
e. Chi-2 trans st dev	457	14.6	29.3	5.0	-2.9	BETTER

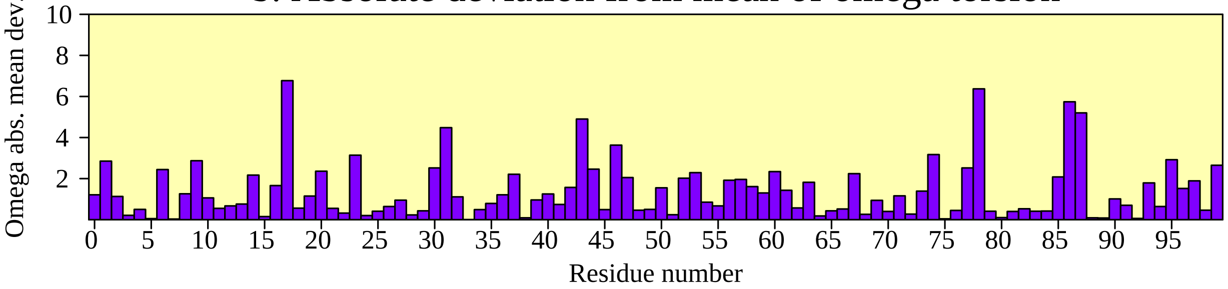
Residue properties

pdb3cir

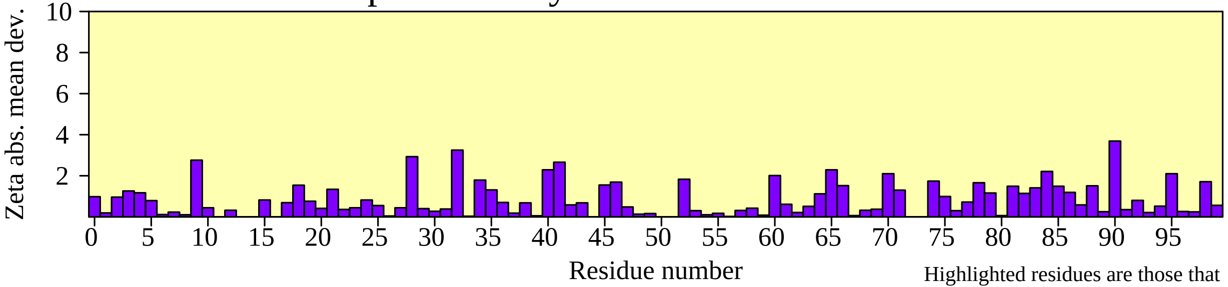
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

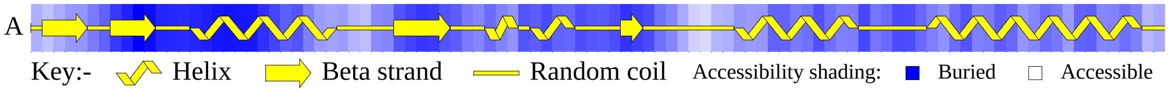


c. C-alpha chirality: abs. deviation of zeta torsion

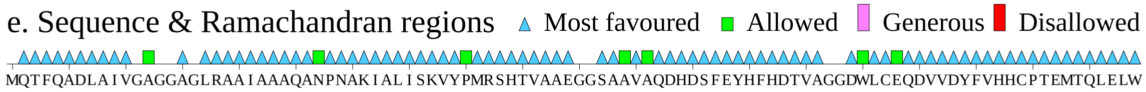


Highlighted residues are those that
deviate by more than 2.0 st. devs. from ideal

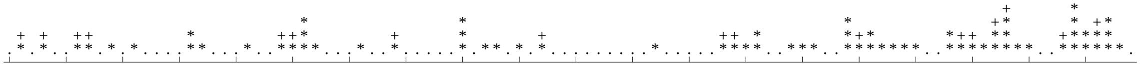
d. Secondary structure & estimated accessibility



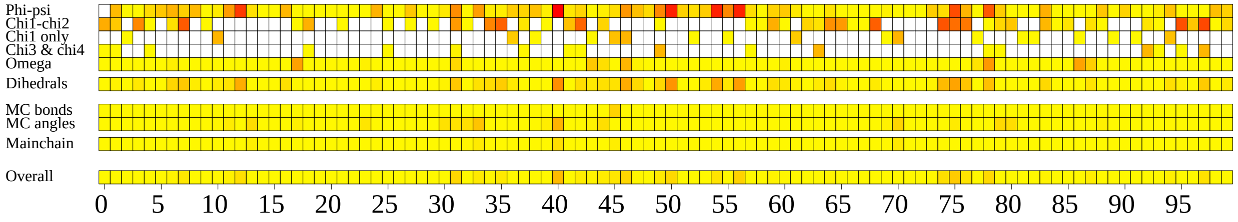
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



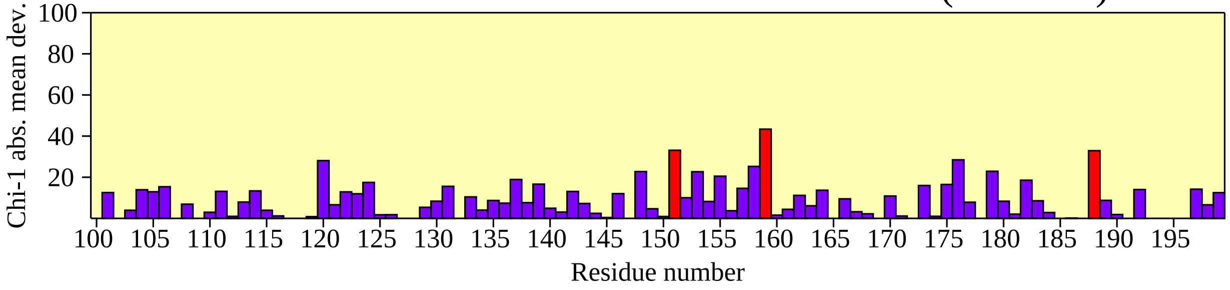
g. G-factors



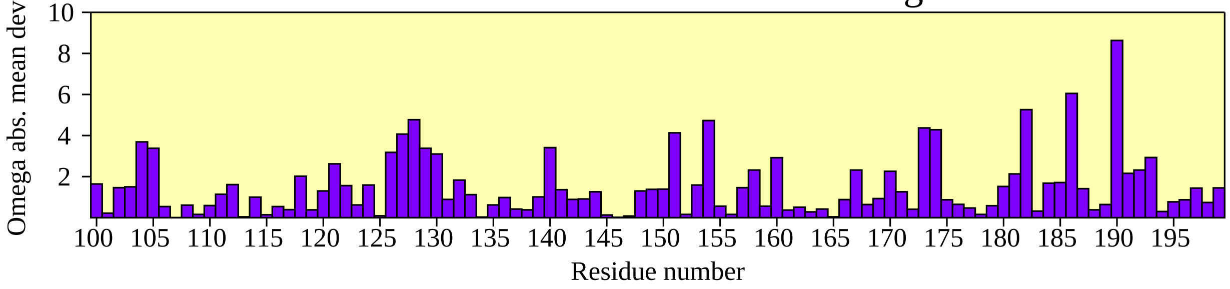
Residue properties

pdb3cir

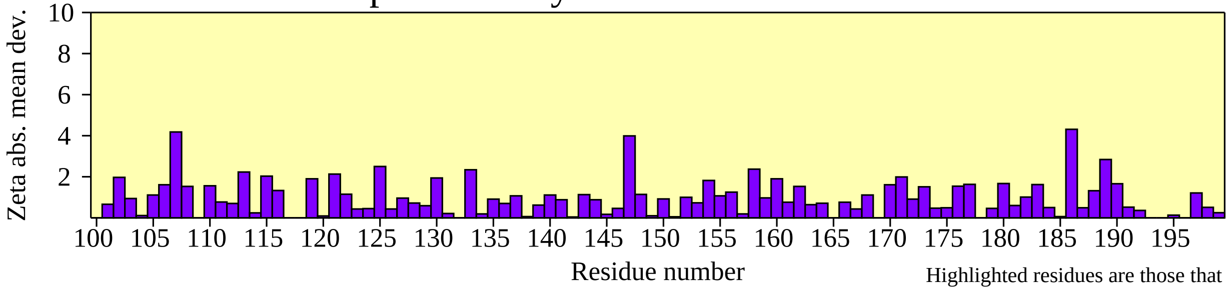
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

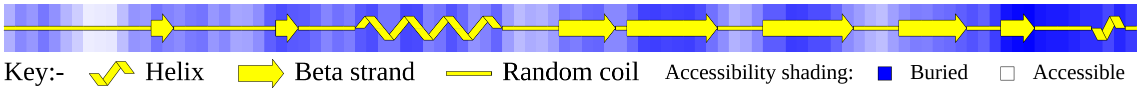


c. C-alpha chirality: abs. deviation of zeta torsion



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

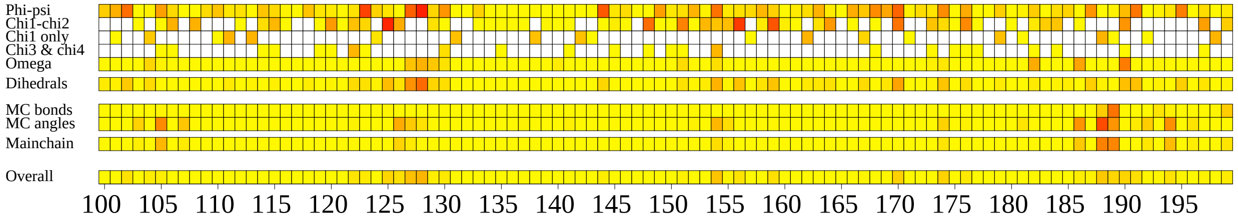
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

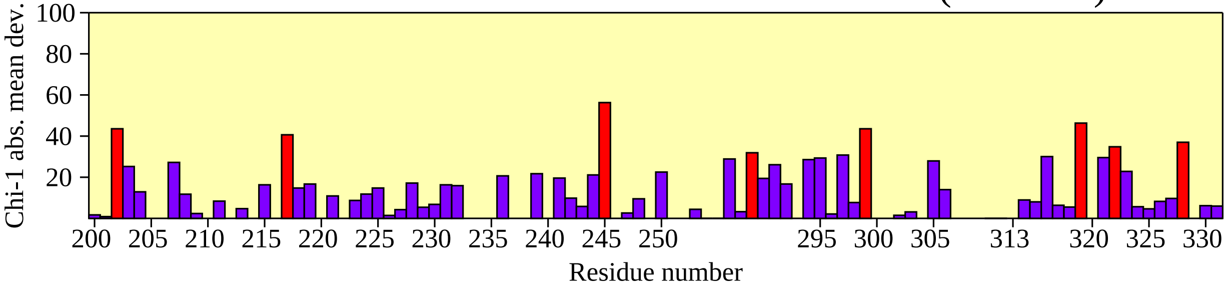
g. G-factors



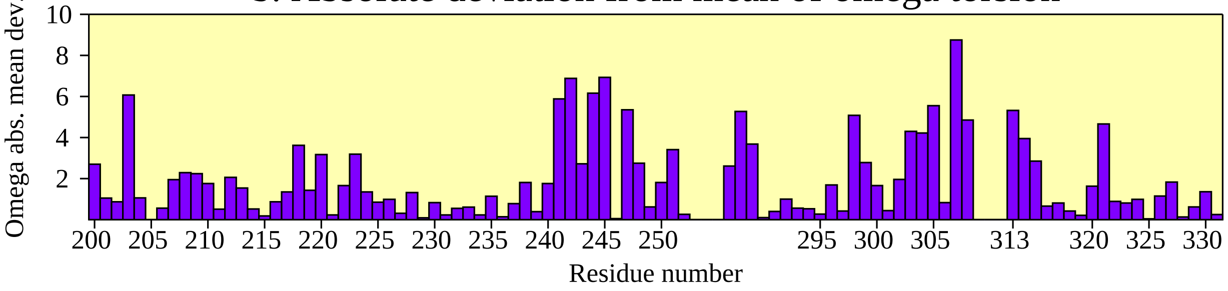
Residue properties

pdb3cir

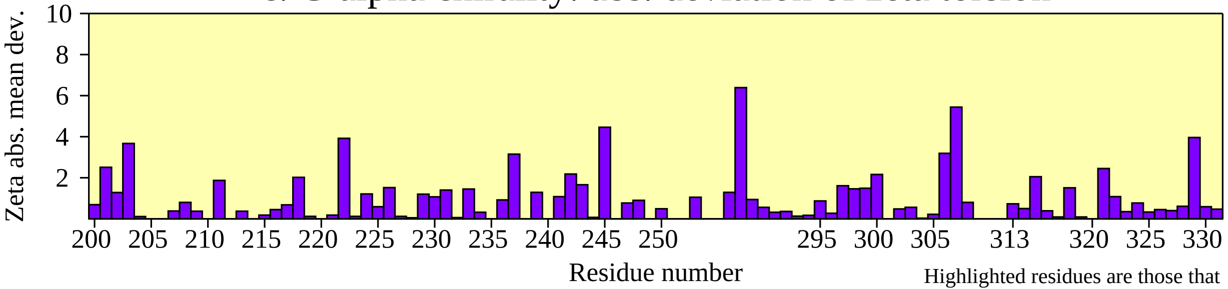
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

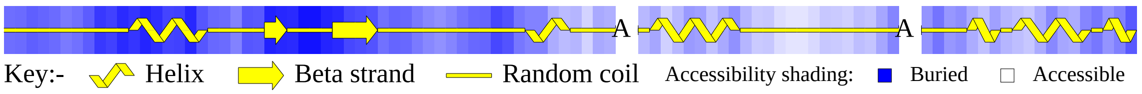


c. C-alpha chirality: abs. deviation of zeta torsion



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

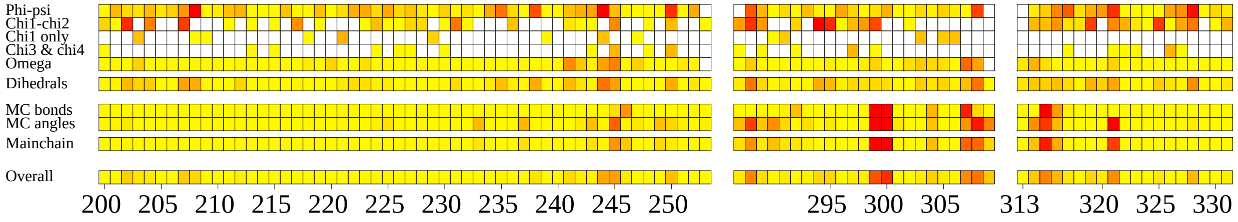
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

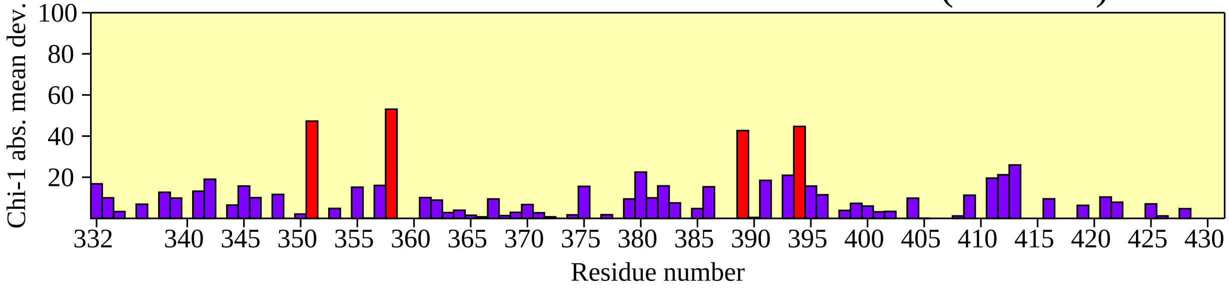
g. G-factors



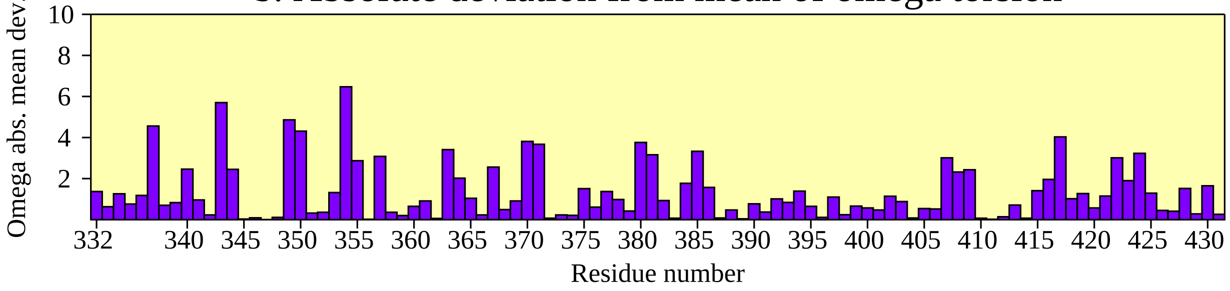
Residue properties

pdb3cir

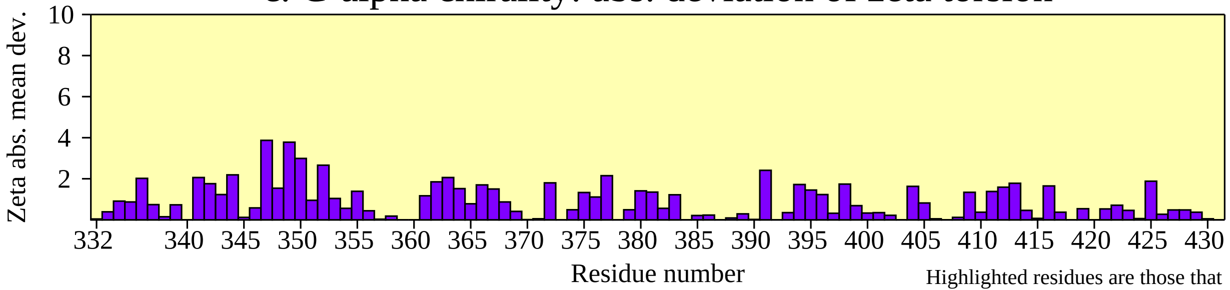
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

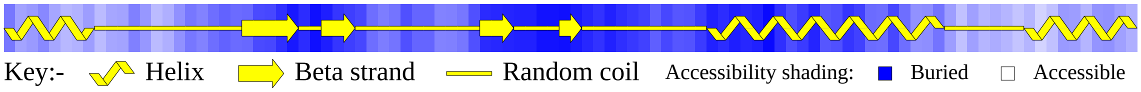


c. C-alpha chirality: abs. deviation of zeta torsion

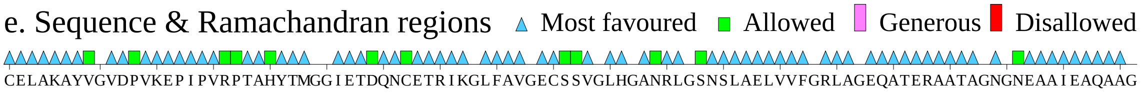


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

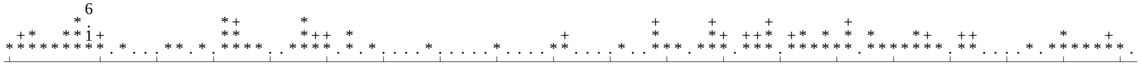
d. Secondary structure & estimated accessibility



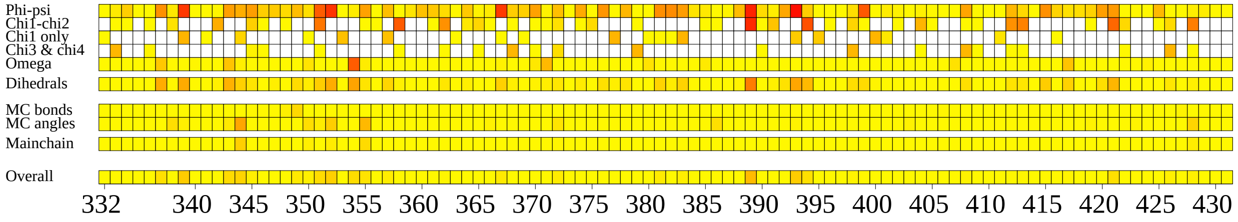
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



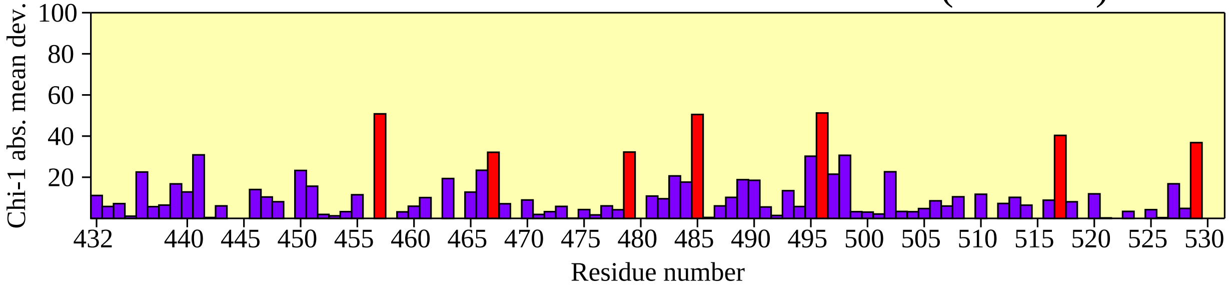
g. G-factors



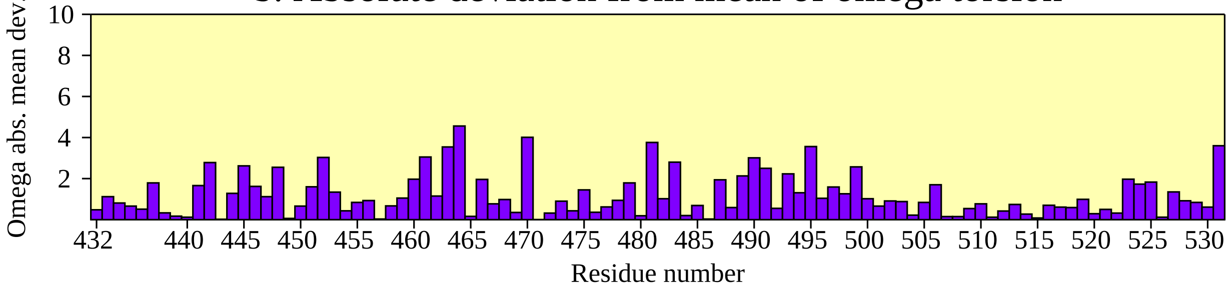
Residue properties

pdb3cir

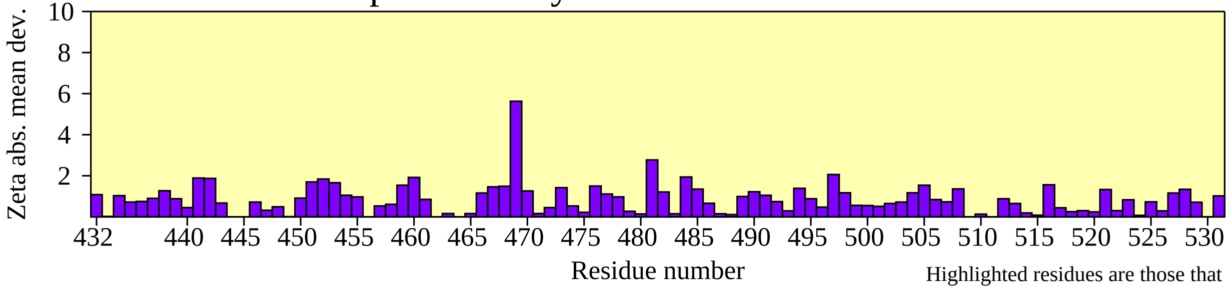
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

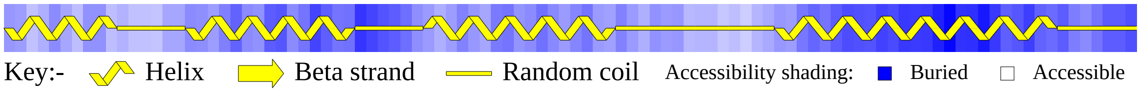


c. C-alpha chirality: abs. deviation of zeta torsion

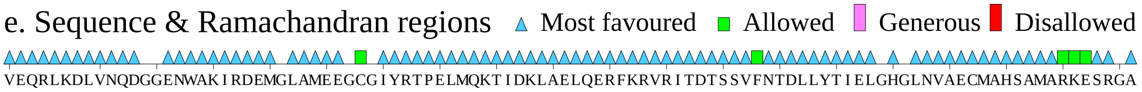


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

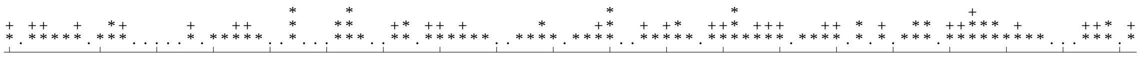
d. Secondary structure & estimated accessibility



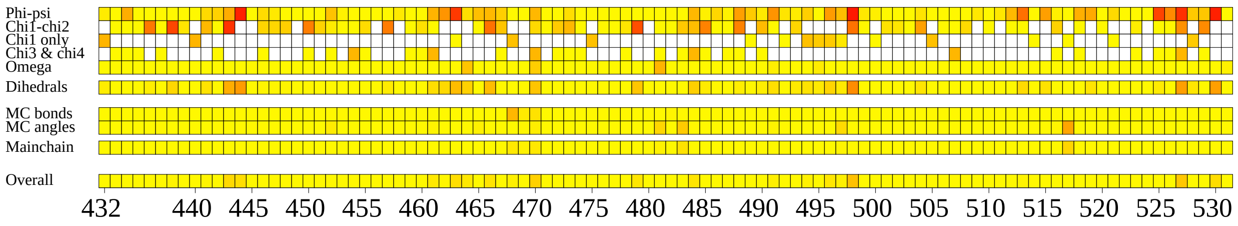
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



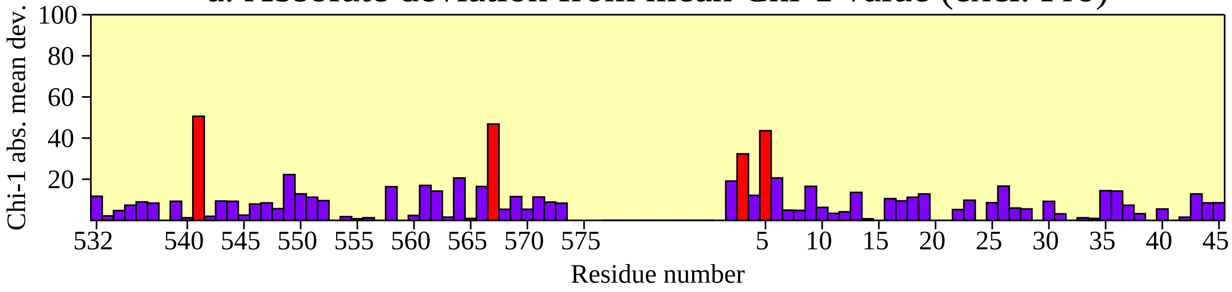
g. G-factors



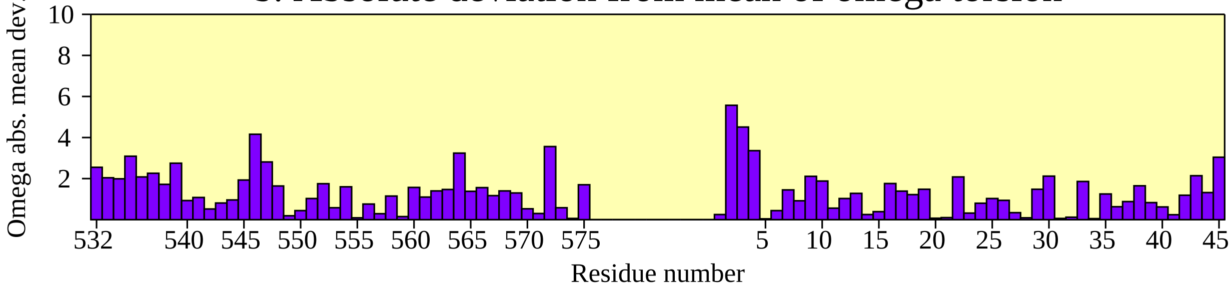
Residue properties

pdb3cir

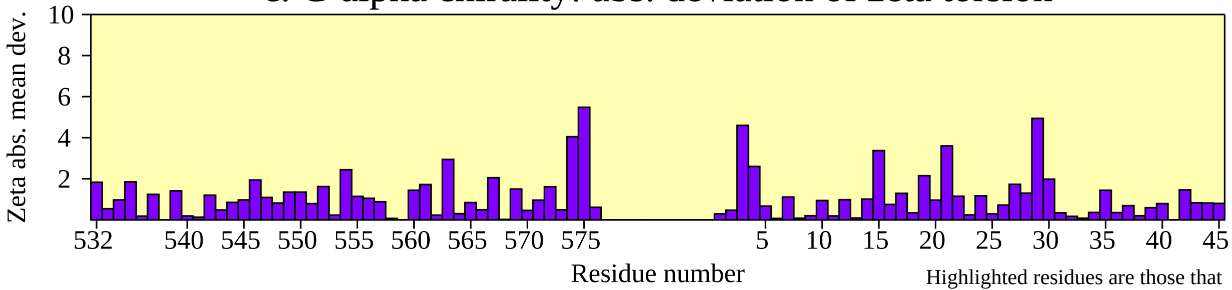
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

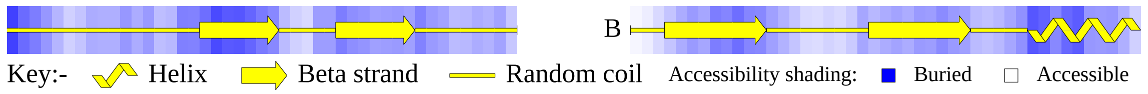


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

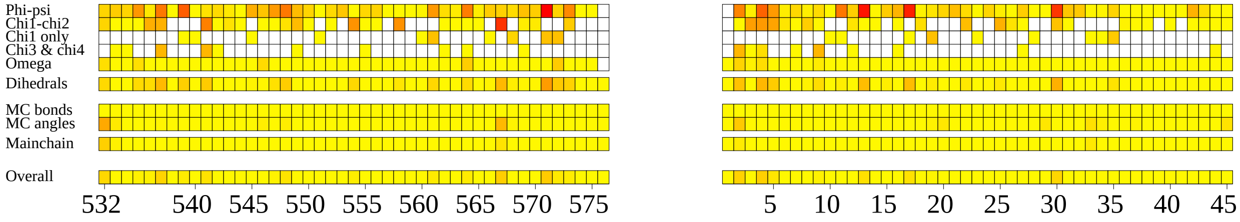


e. Sequence & Ramachandran regions ▲ Most favoured 🟩 Allowed ▯ Generous 🟥 Disallowed

HQRLDEGCTERDDVNFLKHTLAFRDADGTTRLEYSDVKITTLPPA   AEMKNLKIEVVRYNPEVDTAPHSAFYEVPYDATTSLLDALGYIKD

f. Max. deviation (see listing)

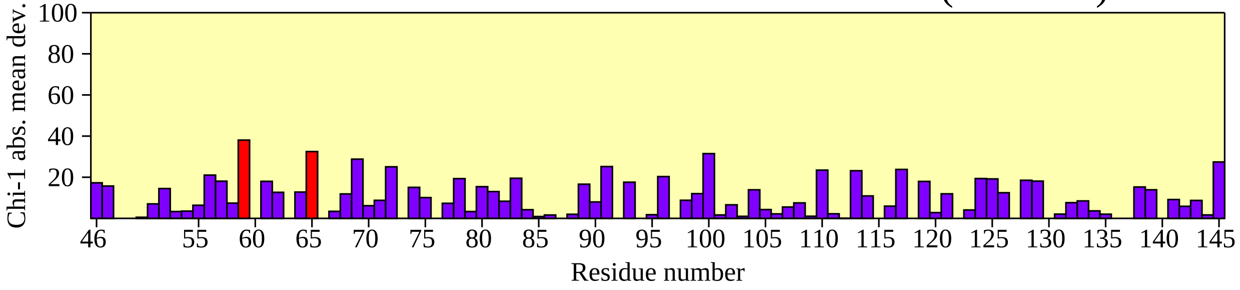
g. G-factors



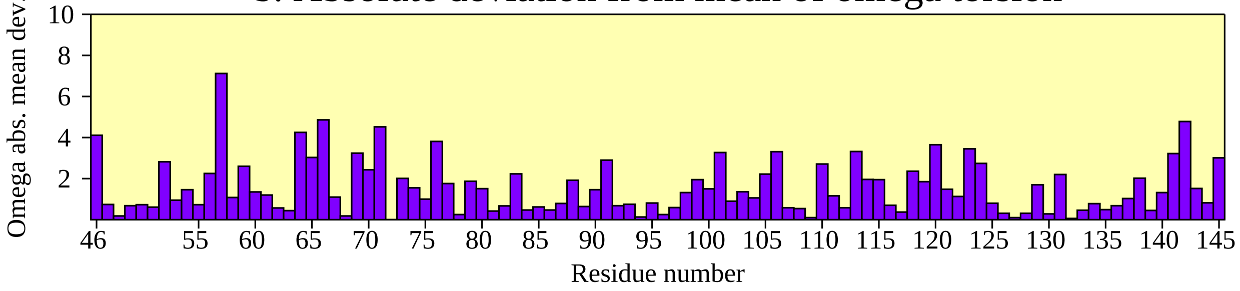
Residue properties

pdb3cir

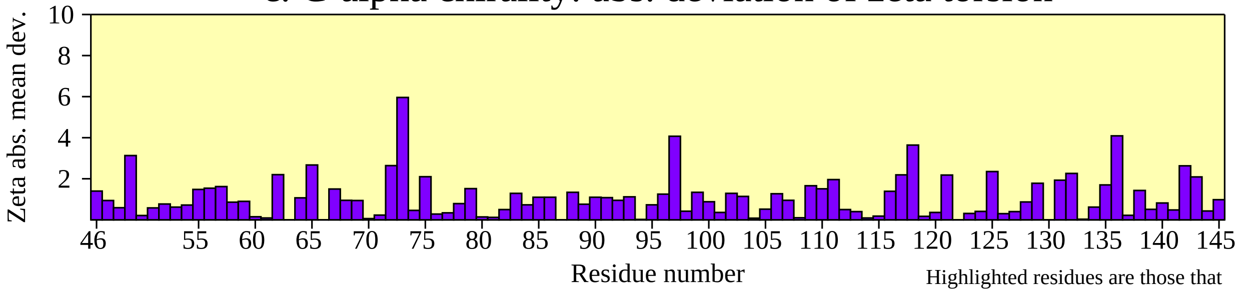
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

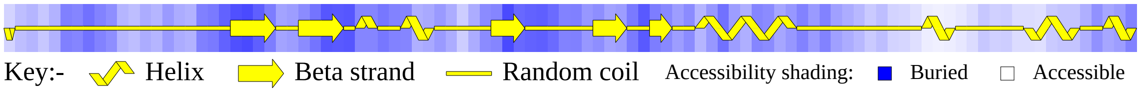


c. C-alpha chirality: abs. deviation of zeta torsion



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

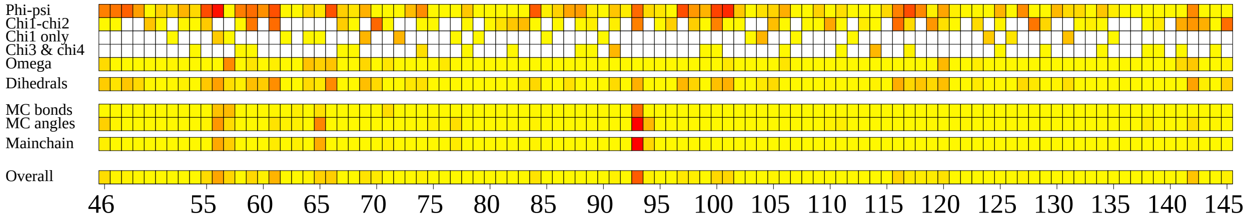
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

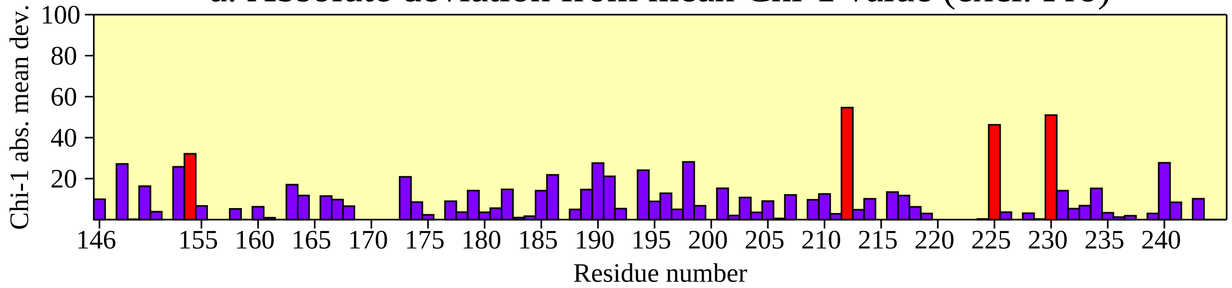
g. G-factors



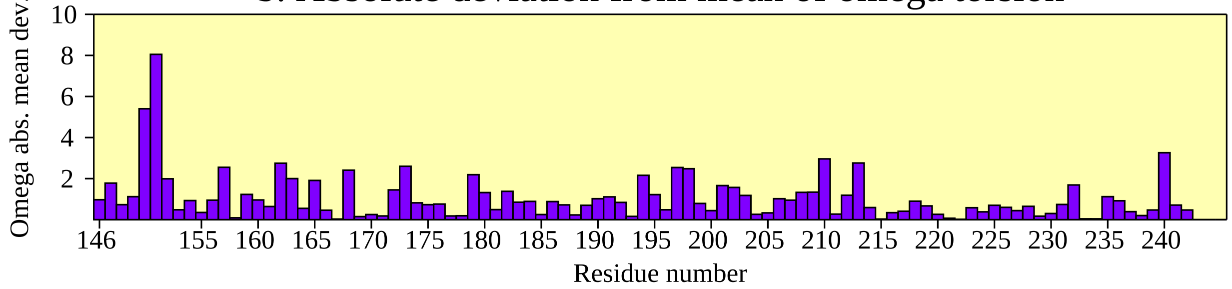
Residue properties

pdb3cir

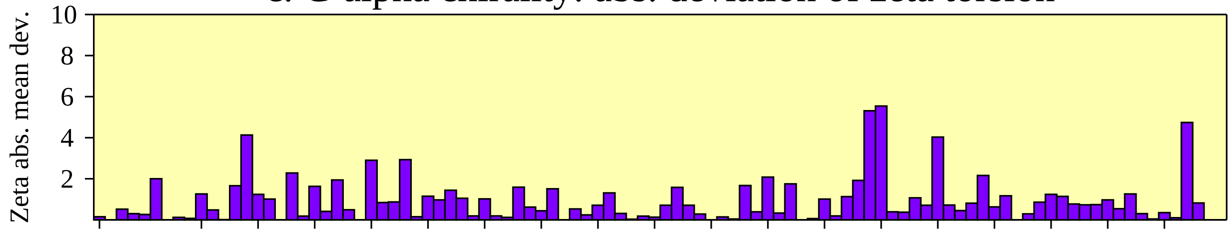
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



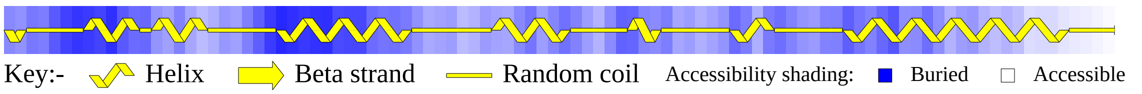
c. C-alpha chirality: abs. deviation of zeta torsion



Residue number

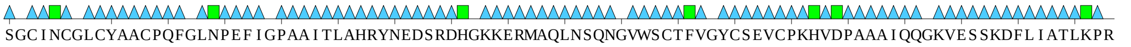
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

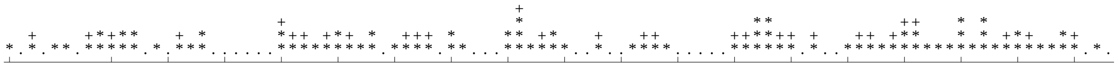


e. Sequence & Ramachandran regions

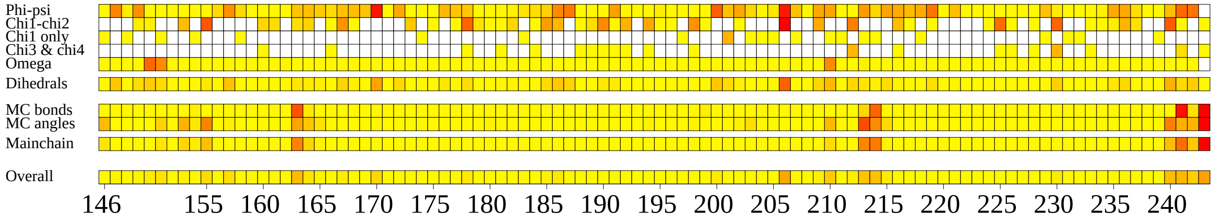
▲ Most favoured 🟩 Allowed ▯ Generous 🟥 Disallowed



f. Max. deviation (see listing)



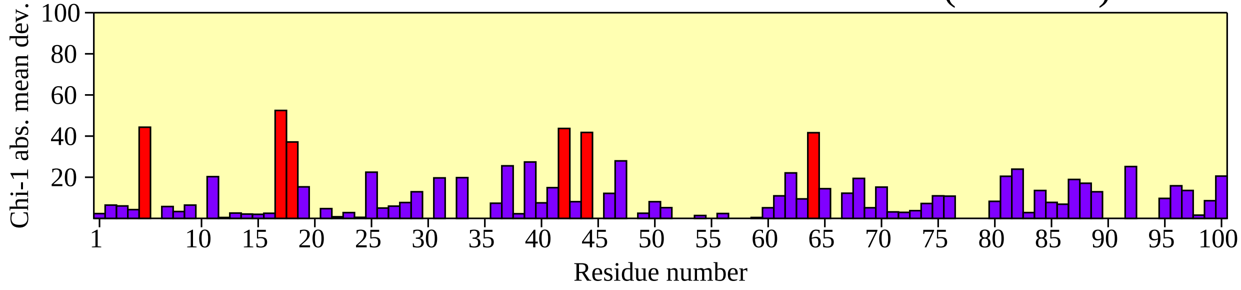
g. G-factors



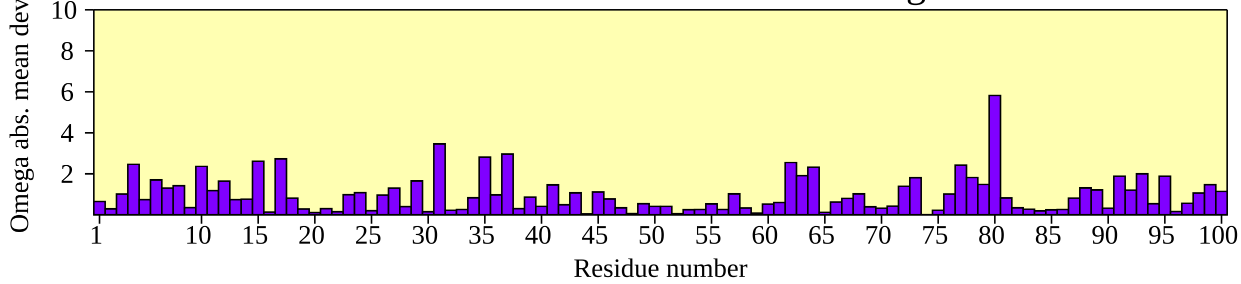
Residue properties

pdb3cir

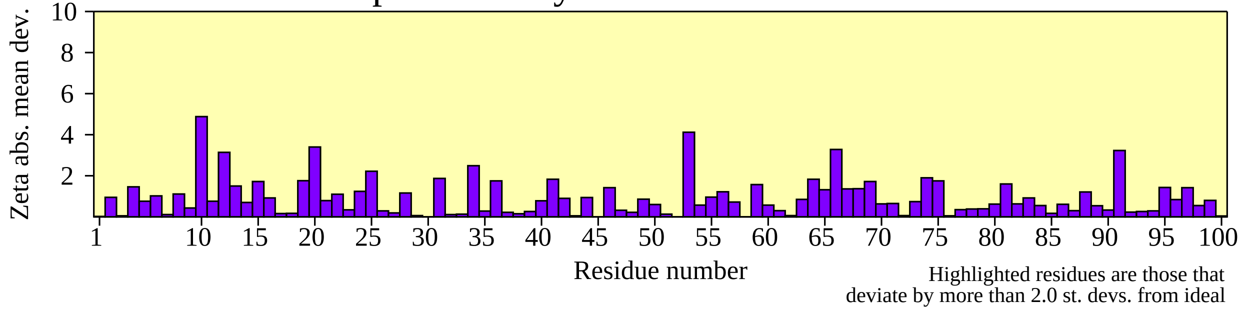
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

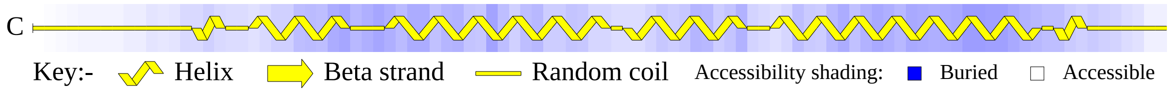


c. C-alpha chirality: abs. deviation of zeta torsion



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

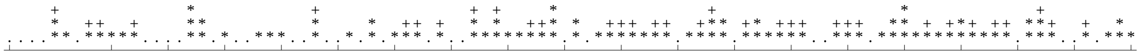
d. Secondary structure & estimated accessibility



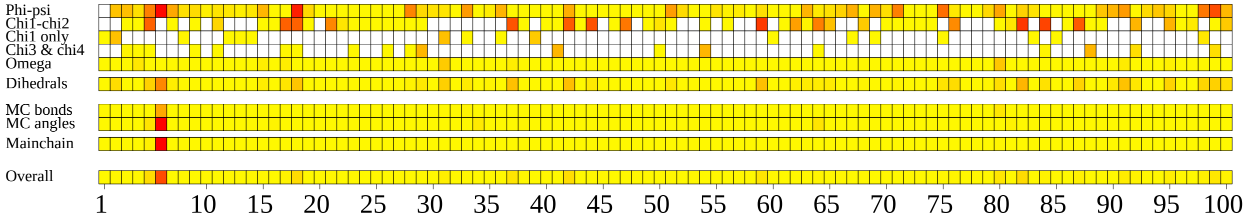
e. Sequence & Ramachandran regions

△ Most favoured 🟩 Allowed ▯ Generous 🟥 Disallowed

f. Max. deviation (see listing)



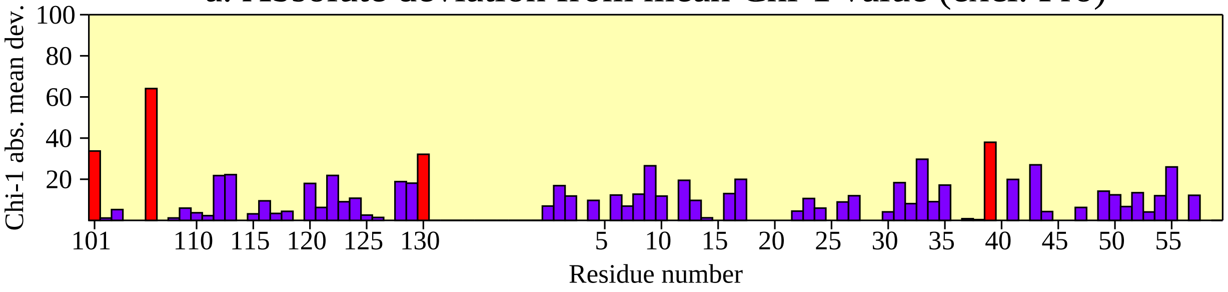
g. G-factors



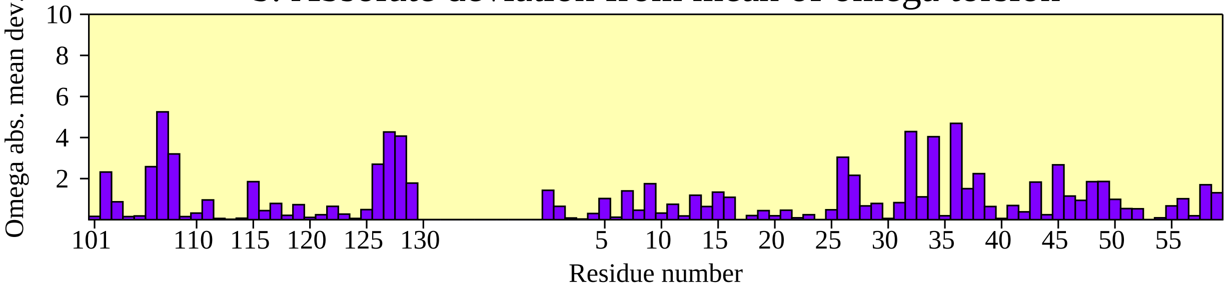
Residue properties

pdb3cir

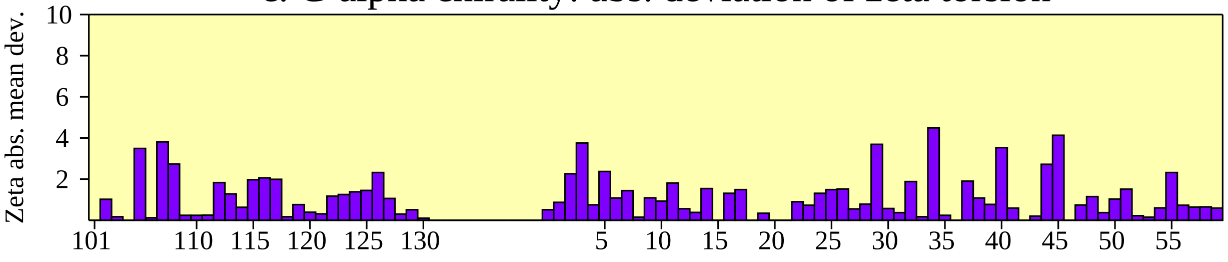
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



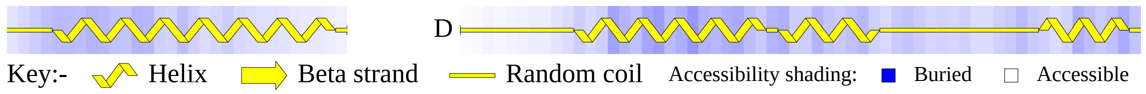
c. C-alpha chirality: abs. deviation of zeta torsion



Residue number

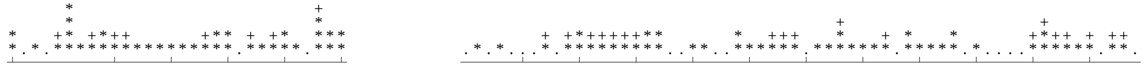
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

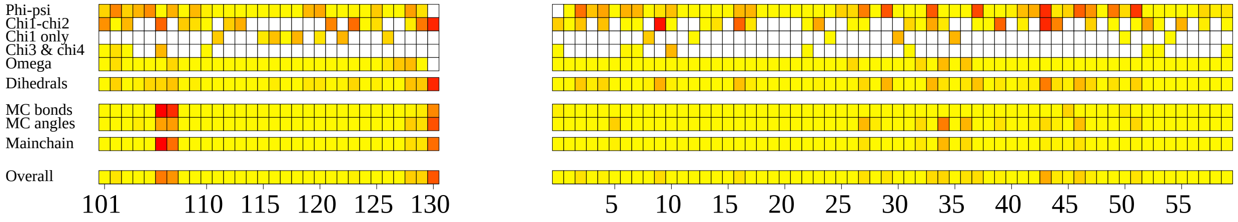


e. Sequence & Ramachandran regions

f. Max. deviation (see listing)



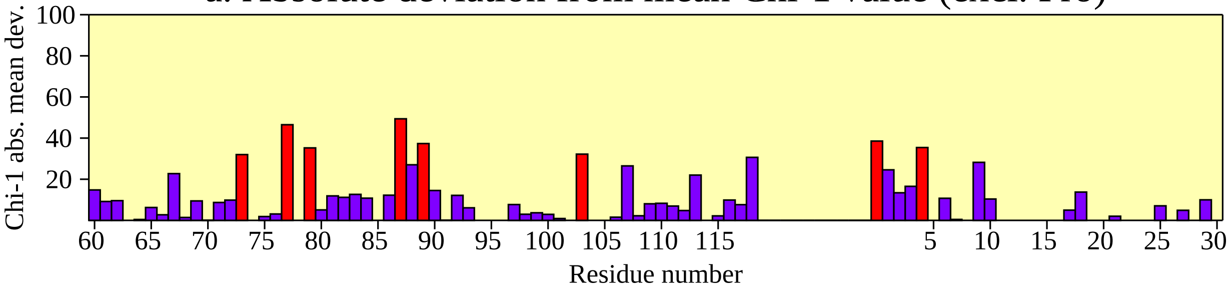
g. G-factors



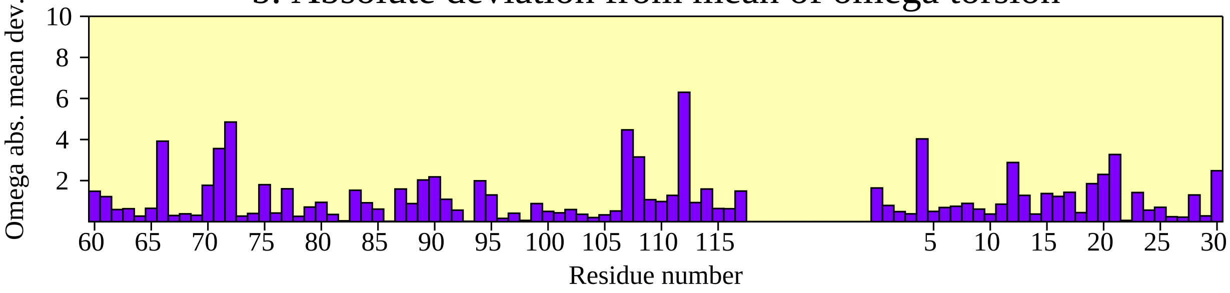
Residue properties

pdb3cir

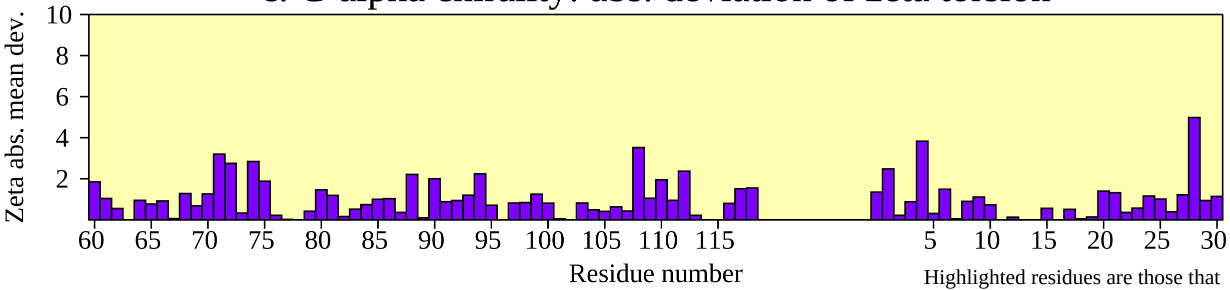
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

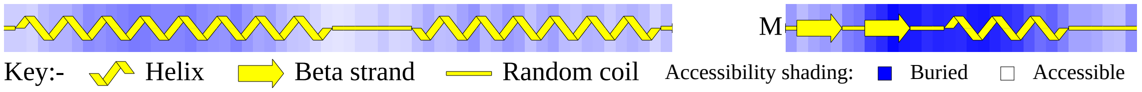


c. C-alpha chirality: abs. deviation of zeta torsion



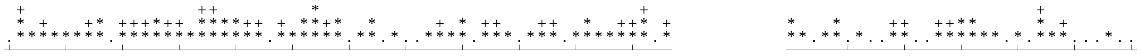
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

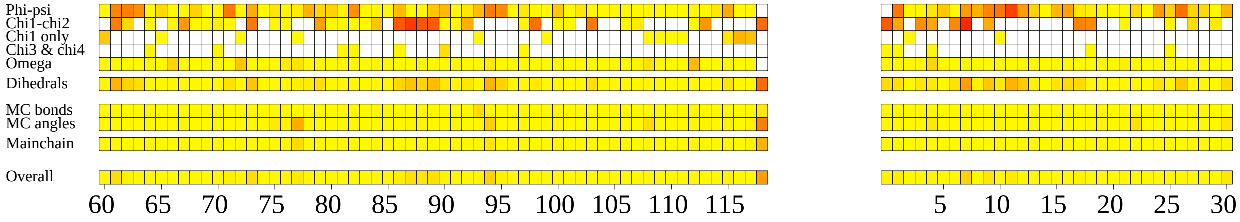


e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

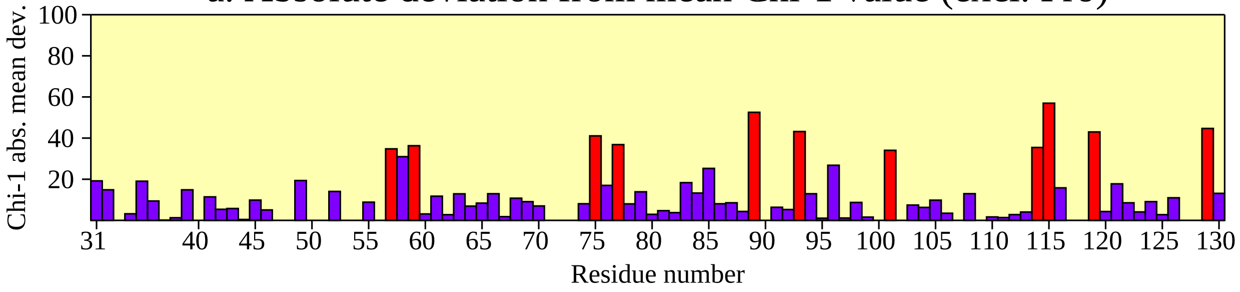


g. G-factors

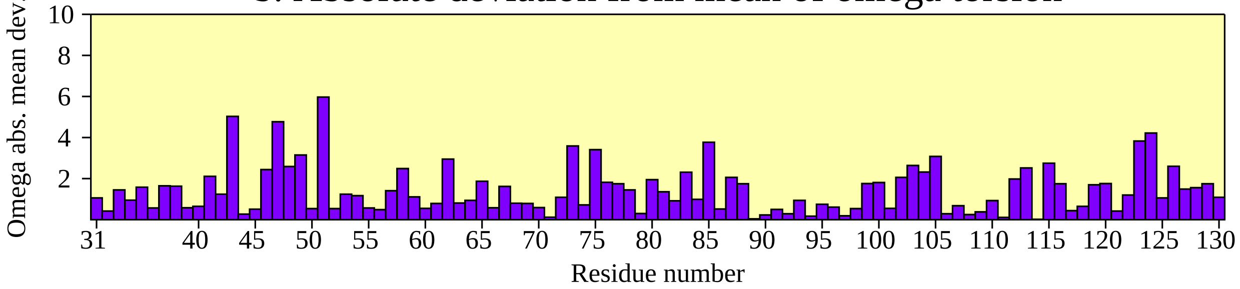


Residue properties
pdb3cir

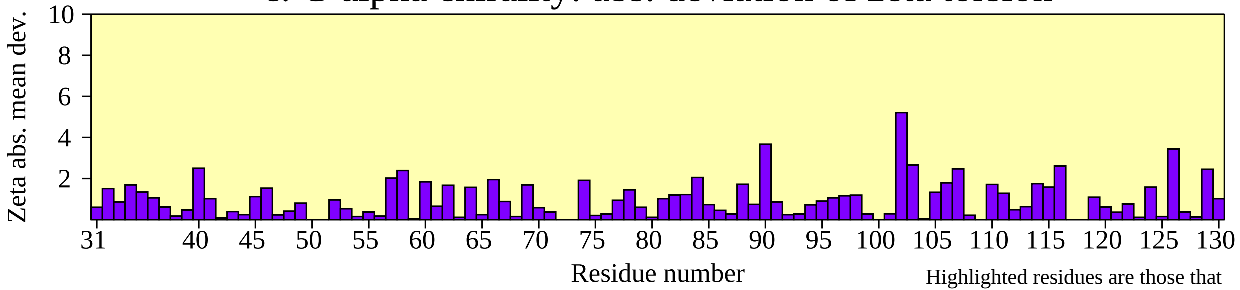
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

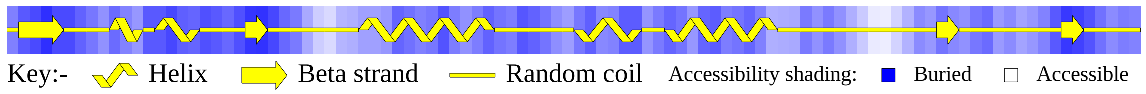


c. C-alpha chirality: abs. deviation of zeta torsion

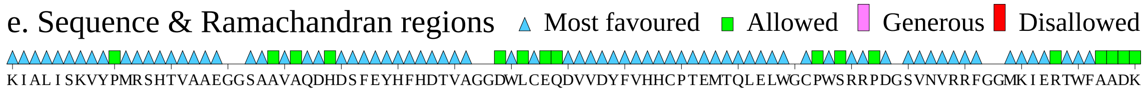


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

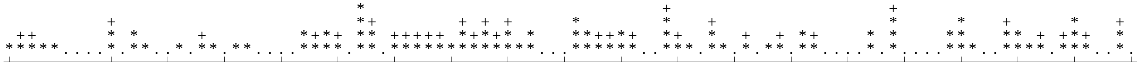
d. Secondary structure & estimated accessibility



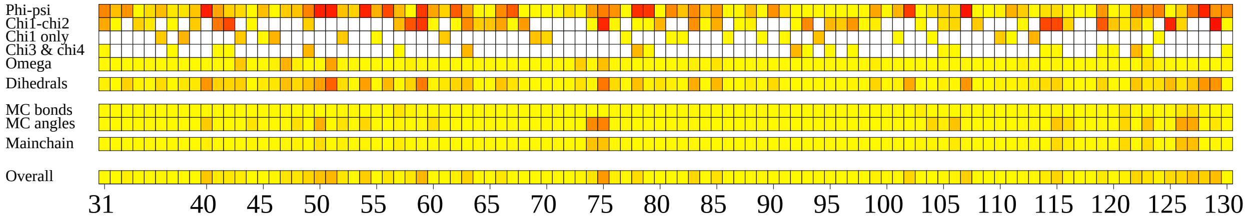
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



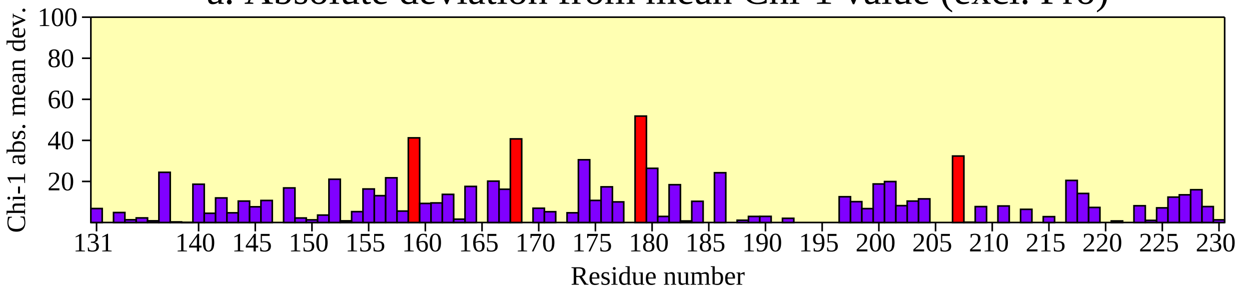
g. G-factors



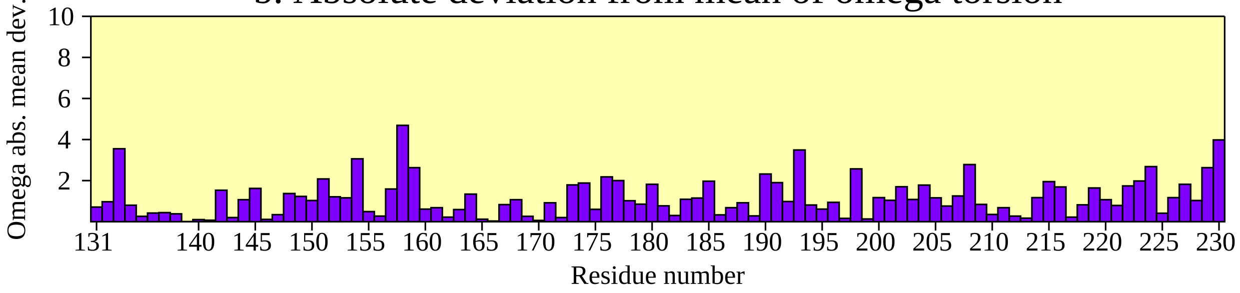
Residue properties

pdb3cir

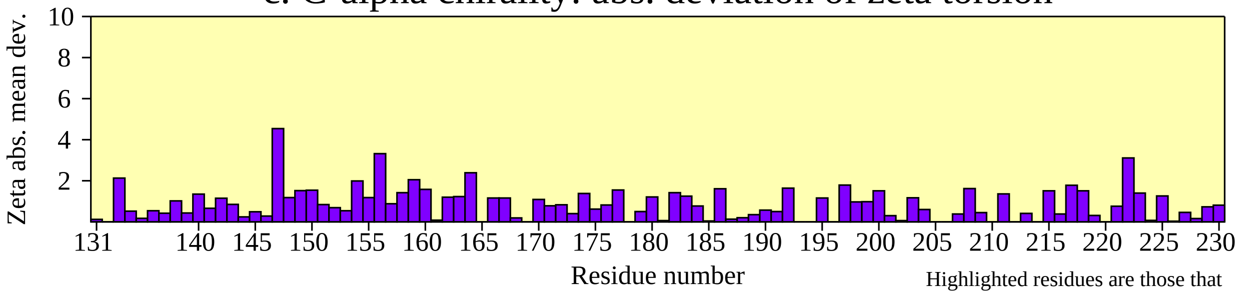
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

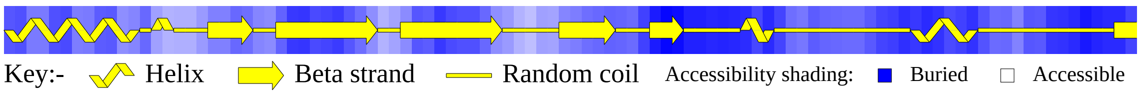


c. C-alpha chirality: abs. deviation of zeta torsion

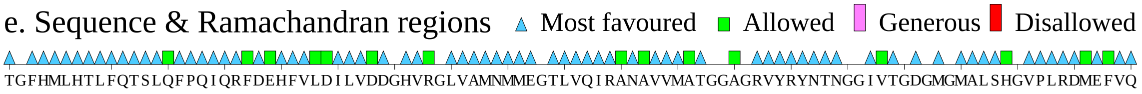


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

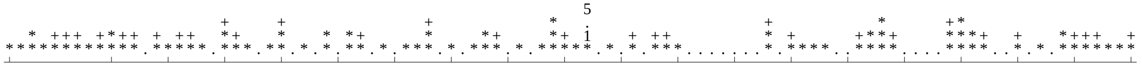
d. Secondary structure & estimated accessibility



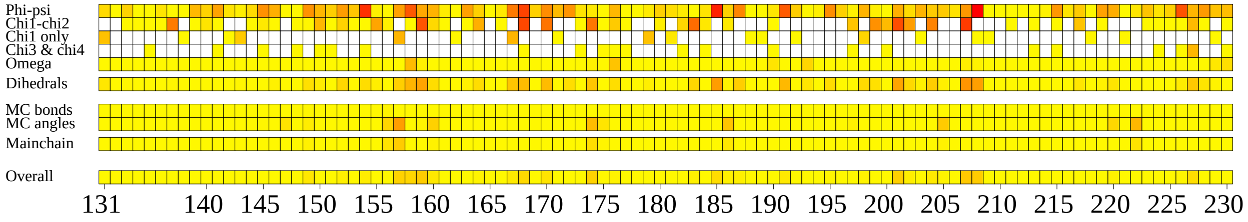
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



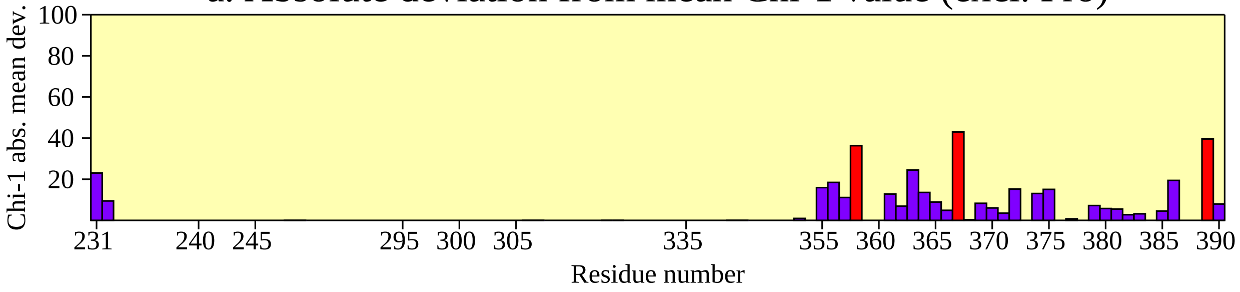
g. G-factors



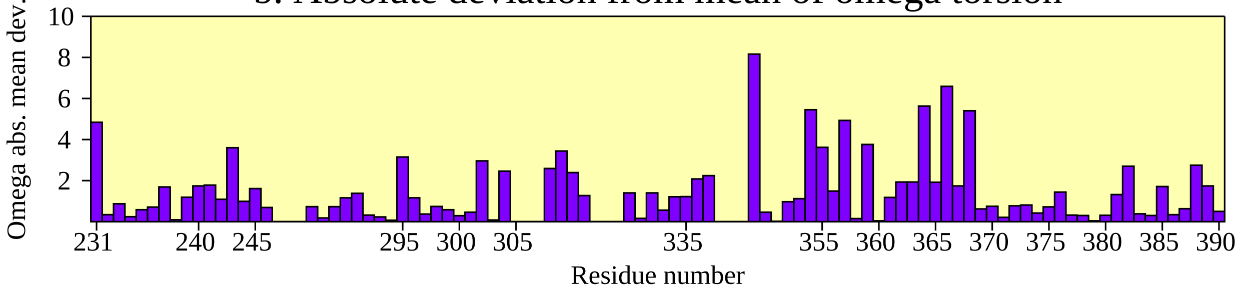
Residue properties

pdb3cir

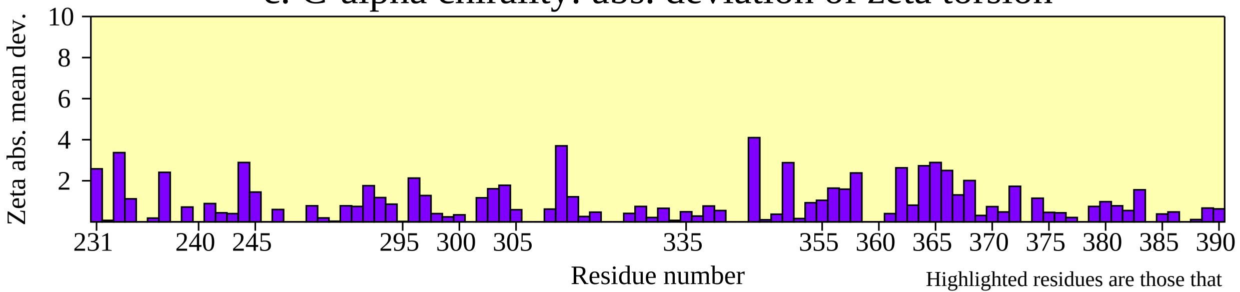
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

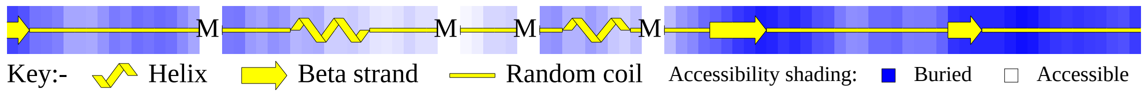


c. C-alpha chirality: abs. deviation of zeta torsion

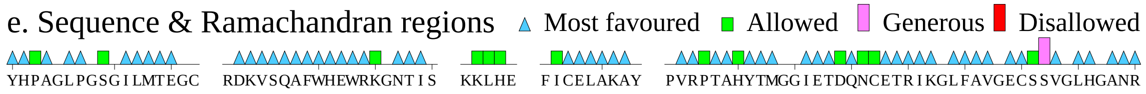


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

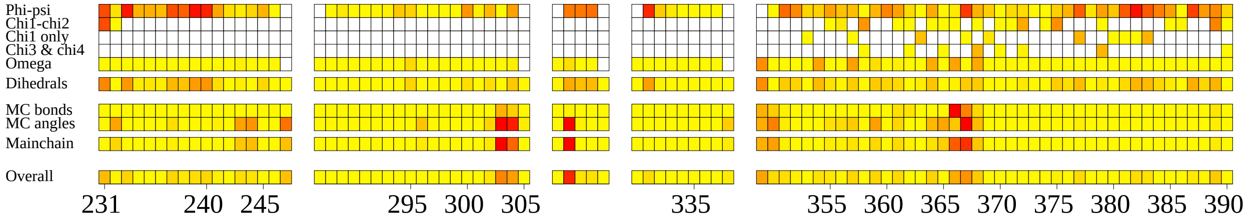


e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

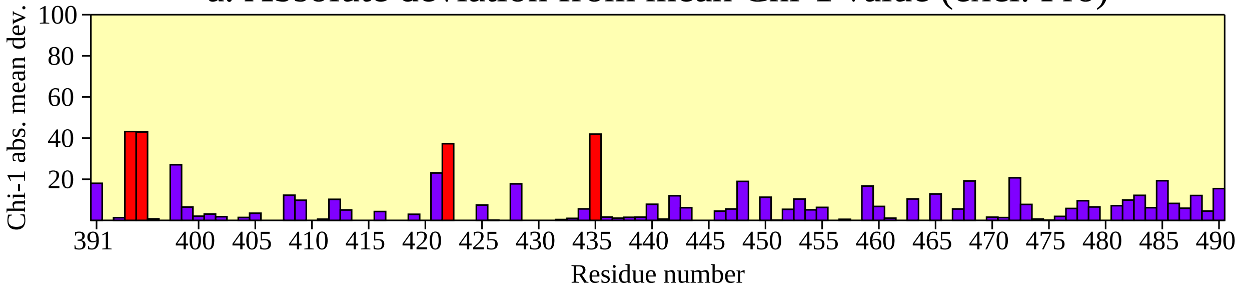
g. G-factors



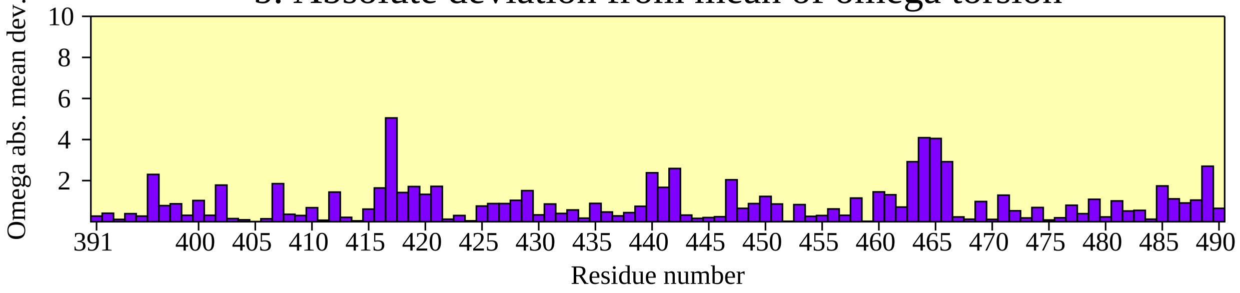
Residue properties

pdb3cir

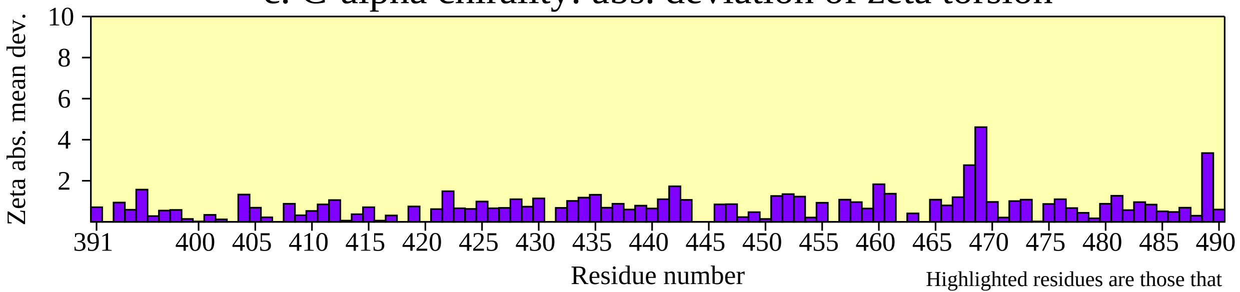
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

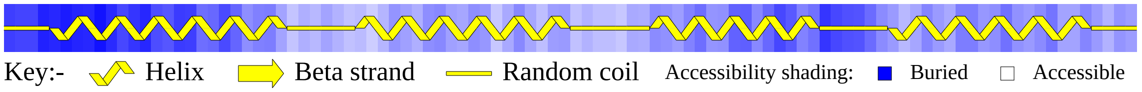


c. C-alpha chirality: abs. deviation of zeta torsion



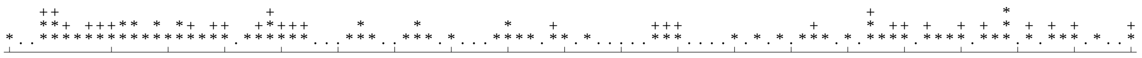
Highlighted residues are those that
deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

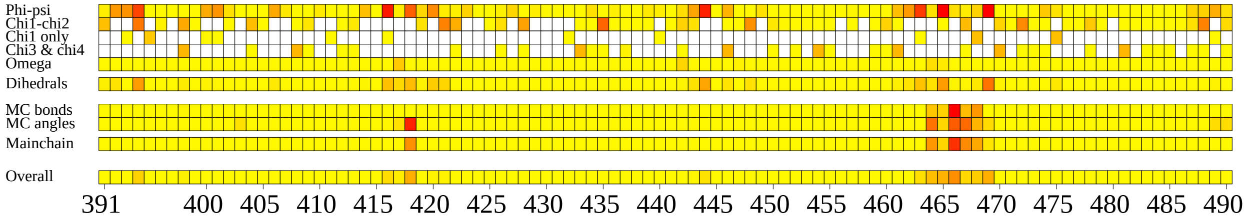


e. Sequence & Ramachandran regions

f. Max. deviation (see listing)



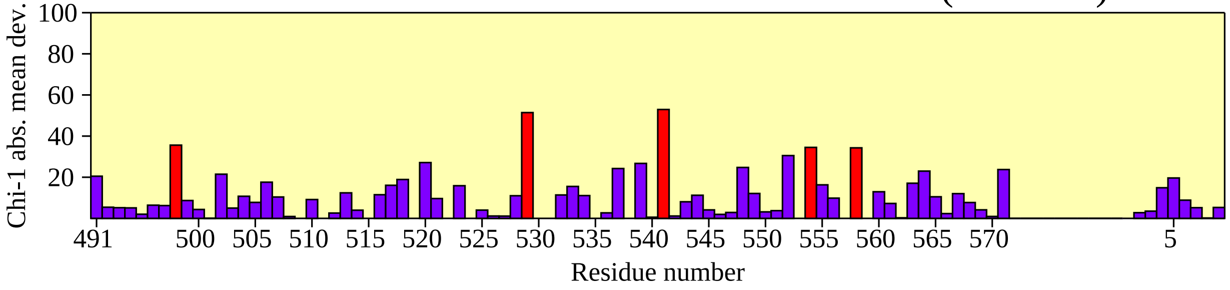
g. G-factors



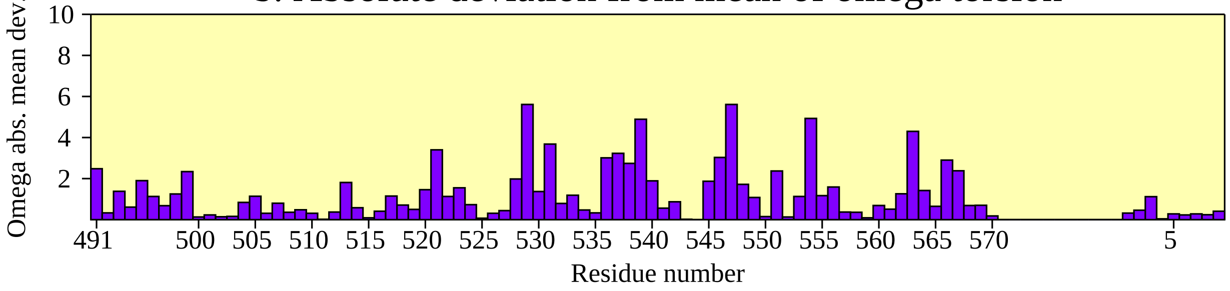
Residue properties

pdb3cir

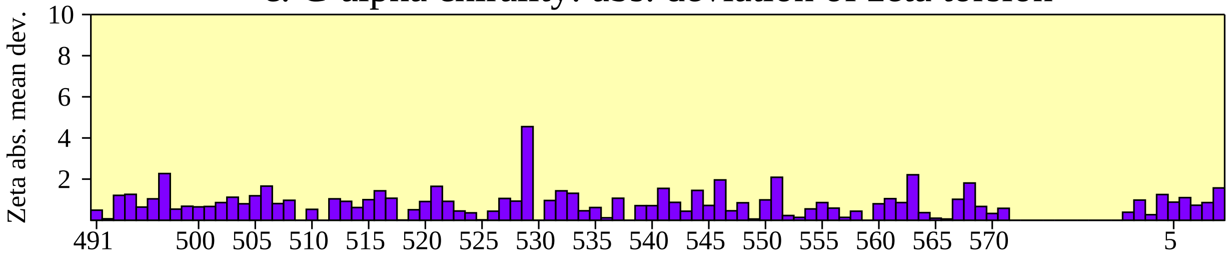
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

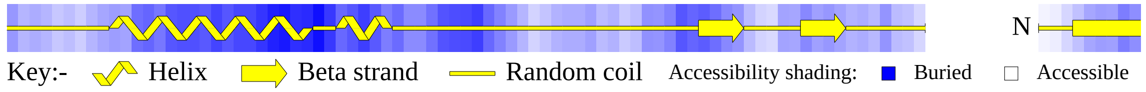


c. C-alpha chirality: abs. deviation of zeta torsion

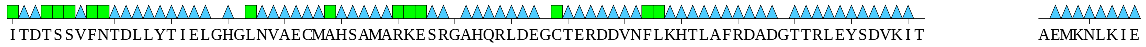


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

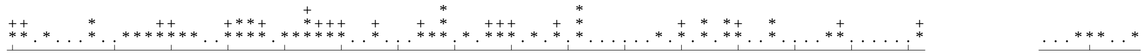
d. Secondary structure & estimated accessibility



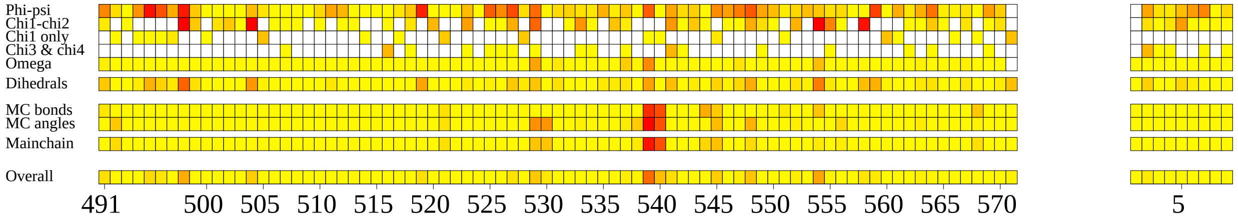
e. Sequence & Ramachandran regions ▲ Most favoured 🟩 Allowed ▯ Generous 🟥 Disallowed



f. Max. deviation (see listing)

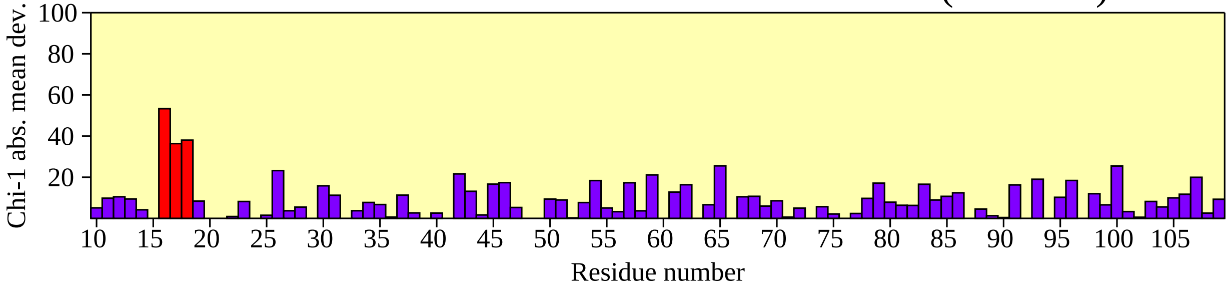


g. G-factors

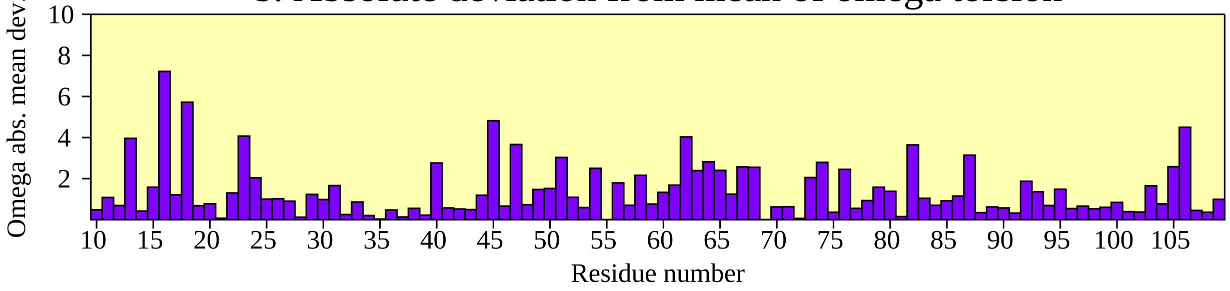


Residue properties
pdb3cir

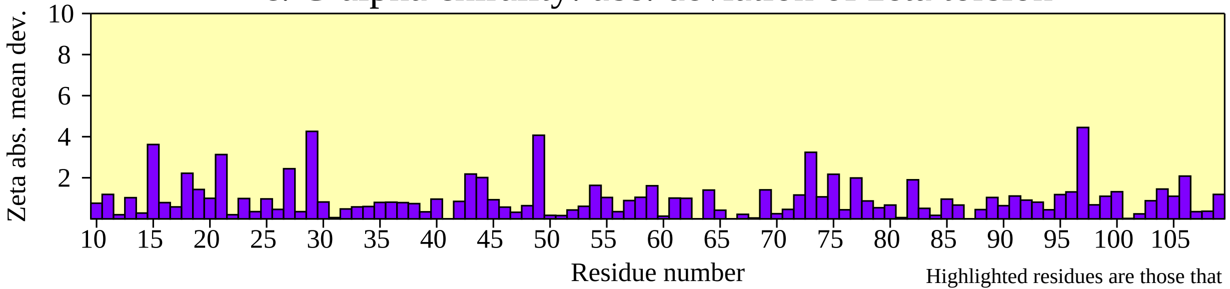
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

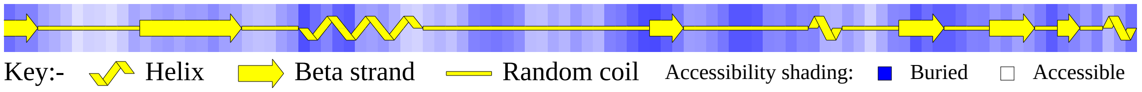


c. C-alpha chirality: abs. deviation of zeta torsion

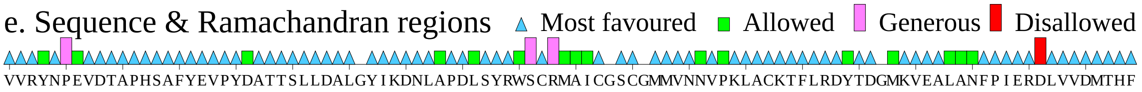


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

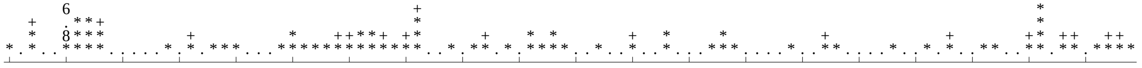
d. Secondary structure & estimated accessibility



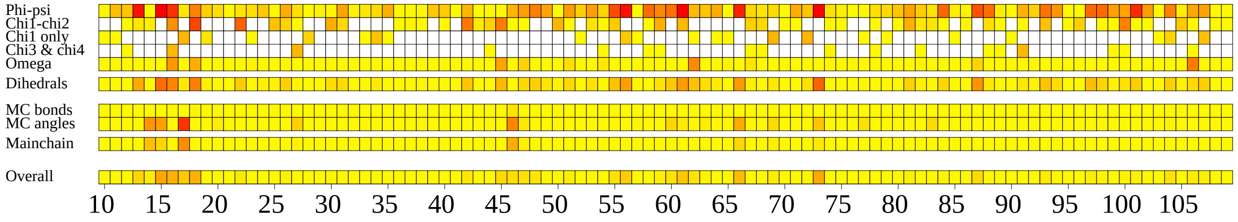
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



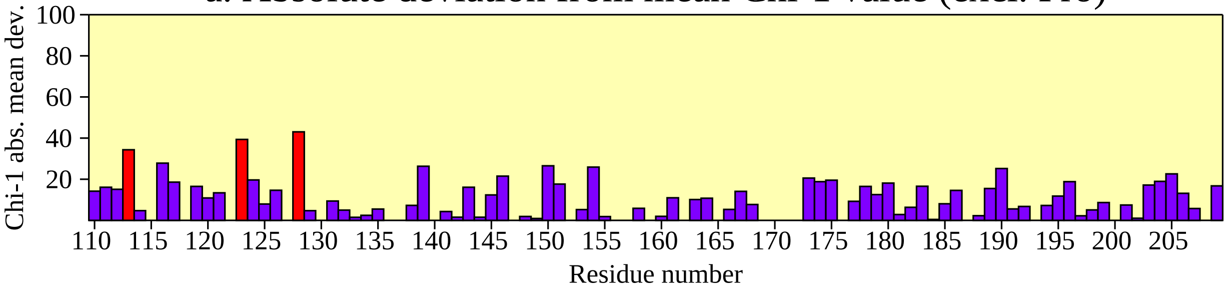
g. G-factors



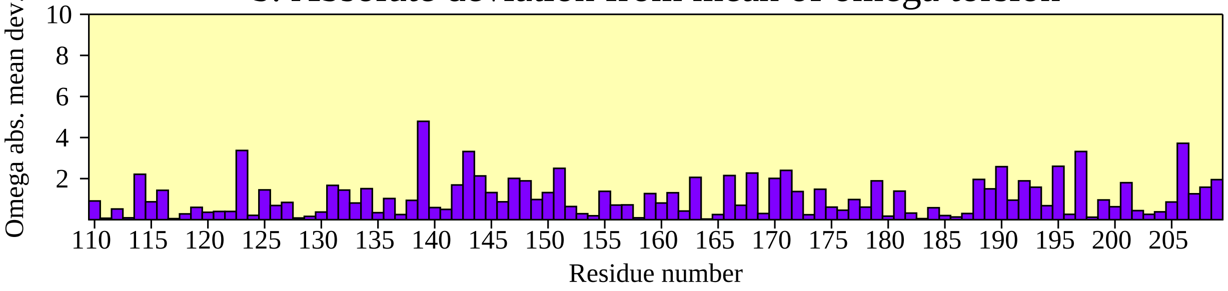
Residue properties

pdb3cir

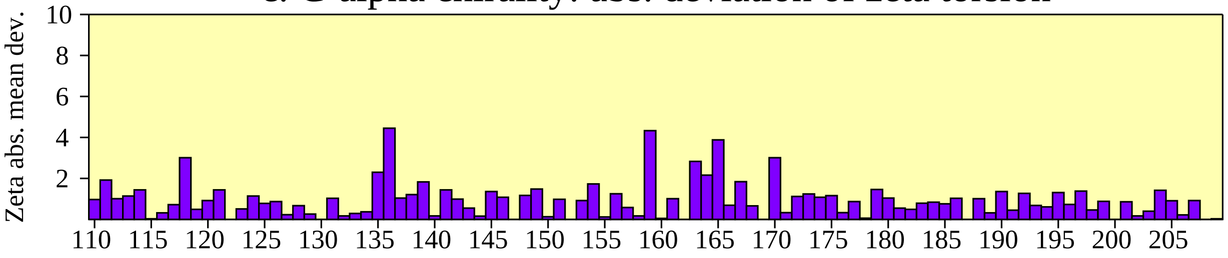
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

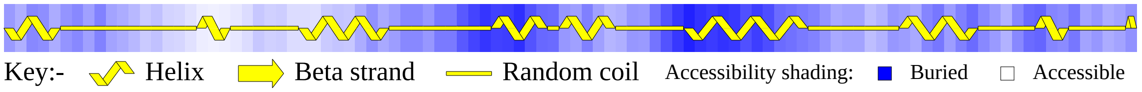


c. C-alpha chirality: abs. deviation of zeta torsion

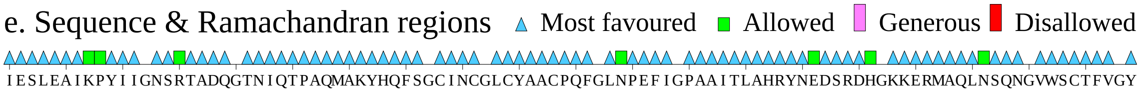


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

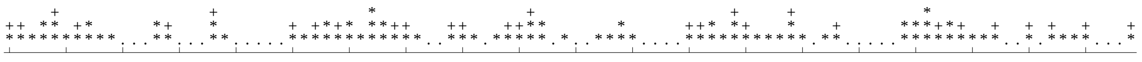
d. Secondary structure & estimated accessibility



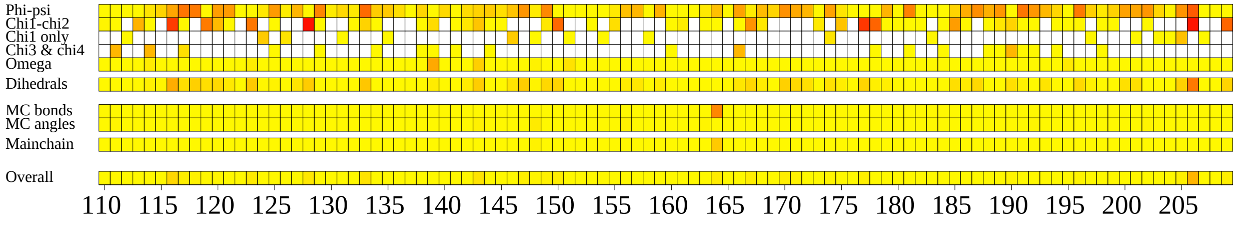
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



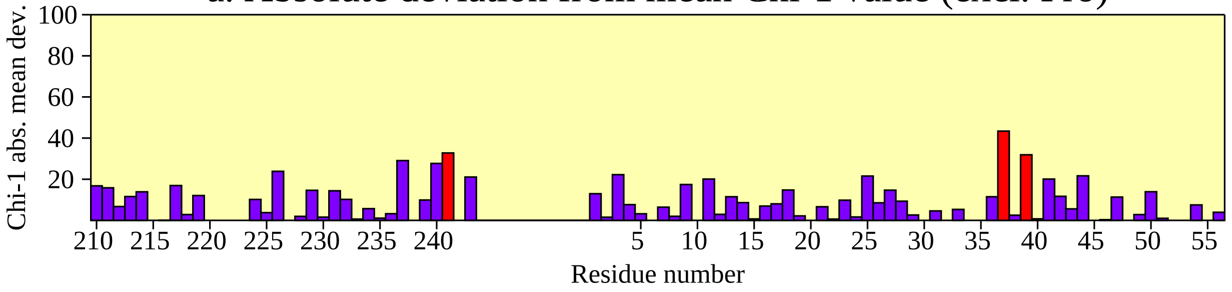
g. G-factors



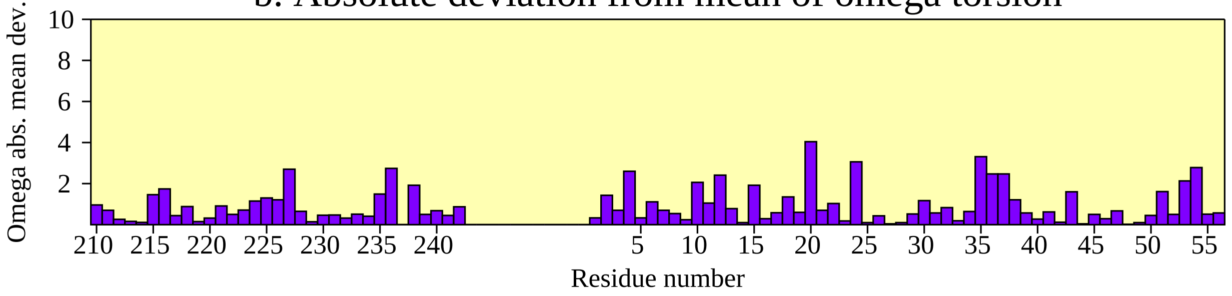
Residue properties

pdb3cir

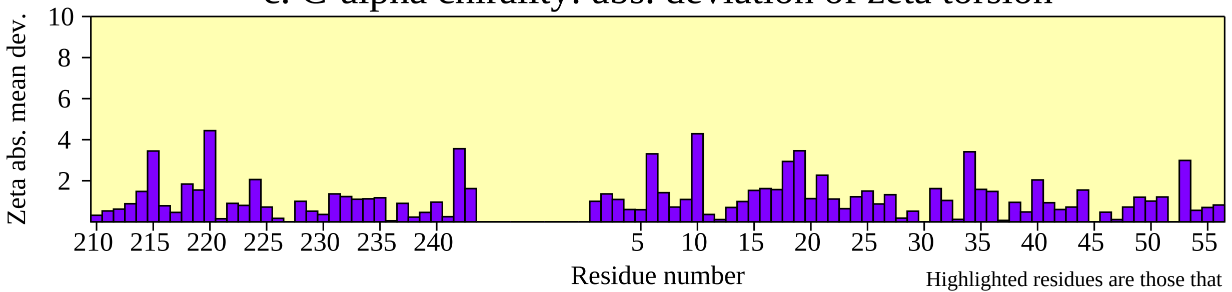
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

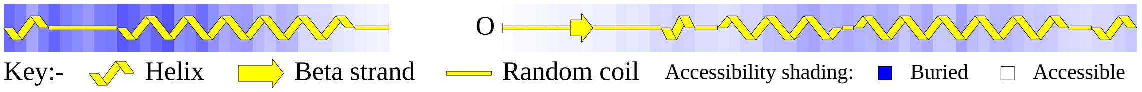


c. C-alpha chirality: abs. deviation of zeta torsion



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

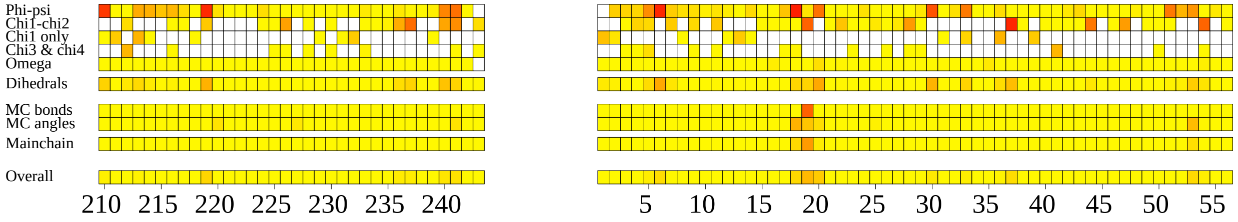
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

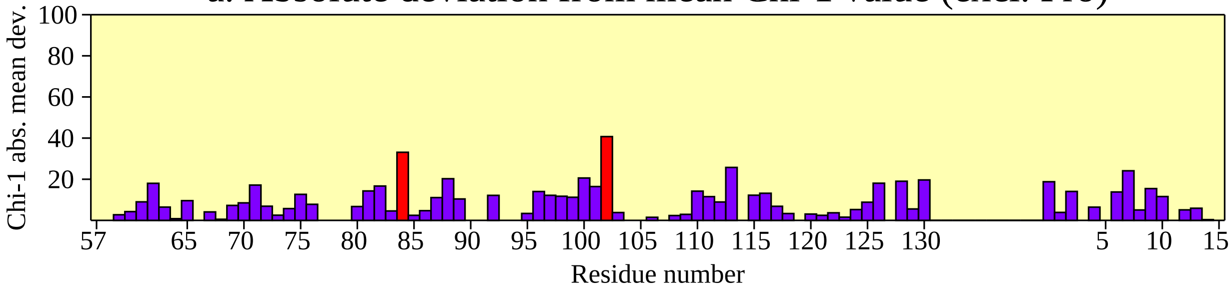
g. G-factors



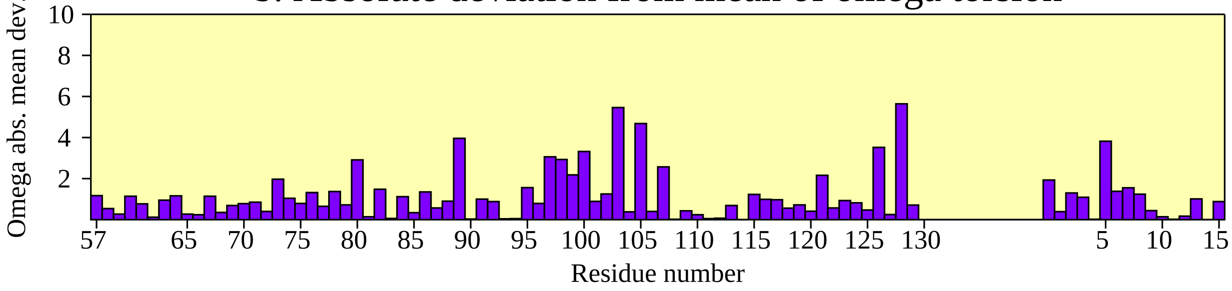
Residue properties

pdb3cir

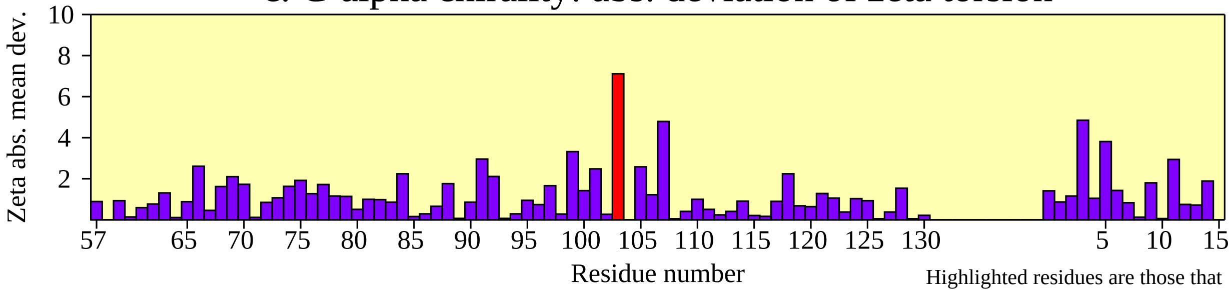
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

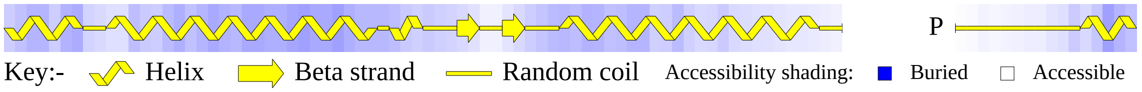


c. C-alpha chirality: abs. deviation of zeta torsion

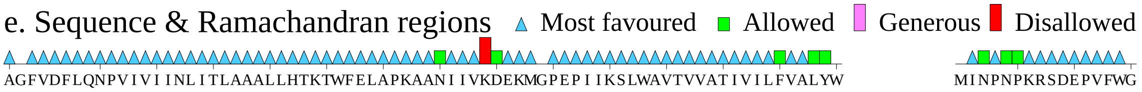


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

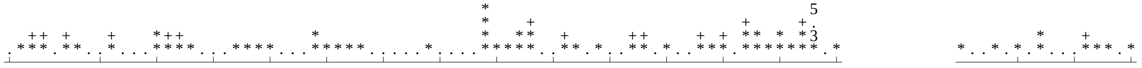
d. Secondary structure & estimated accessibility



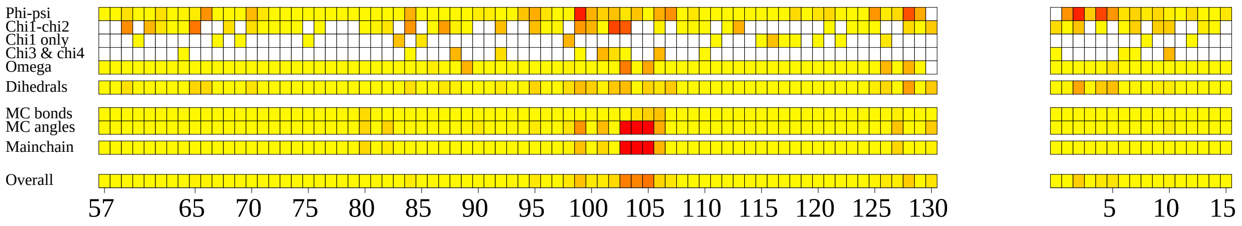
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



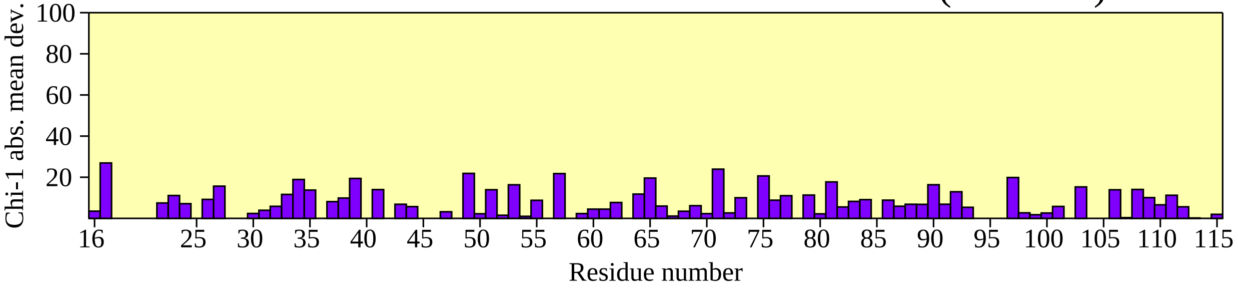
g. G-factors



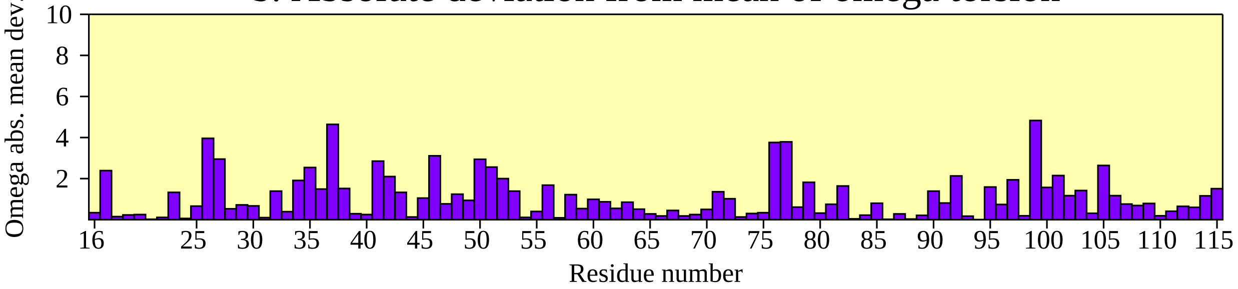
Residue properties

pdb3cir

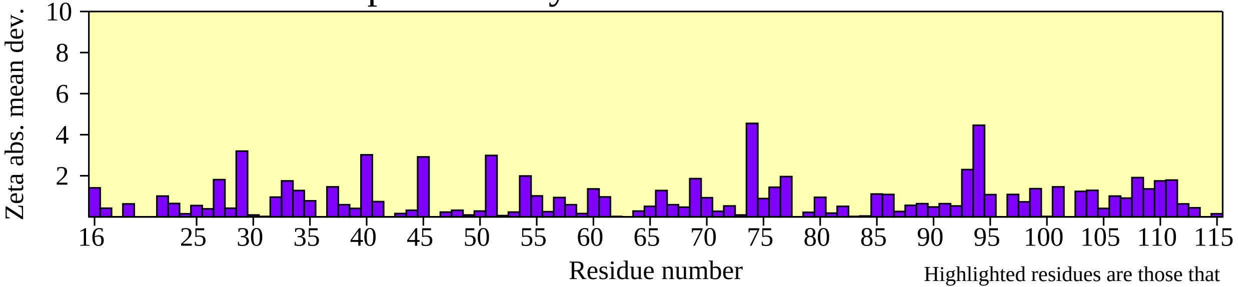
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

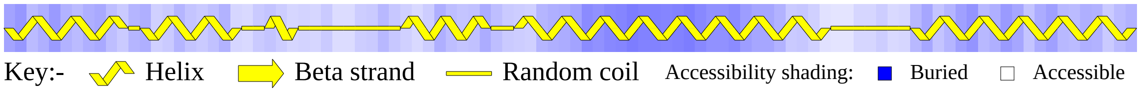


c. C-alpha chirality: abs. deviation of zeta torsion

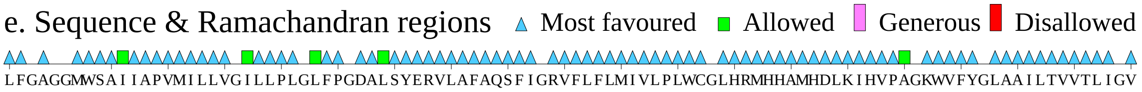


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

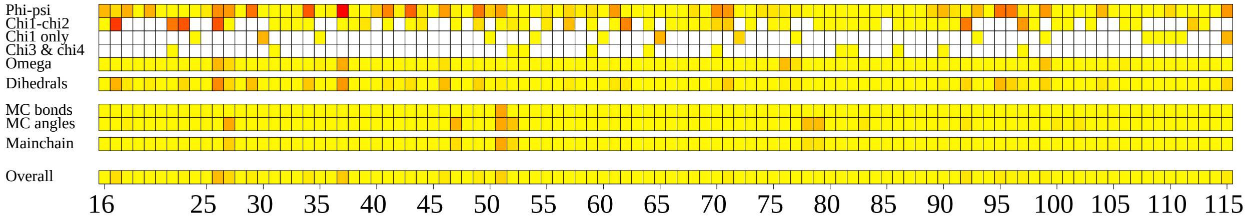


e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

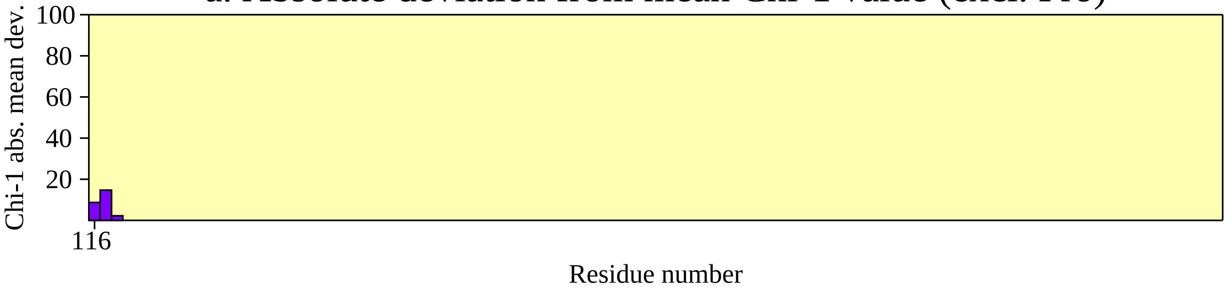
g. G-factors



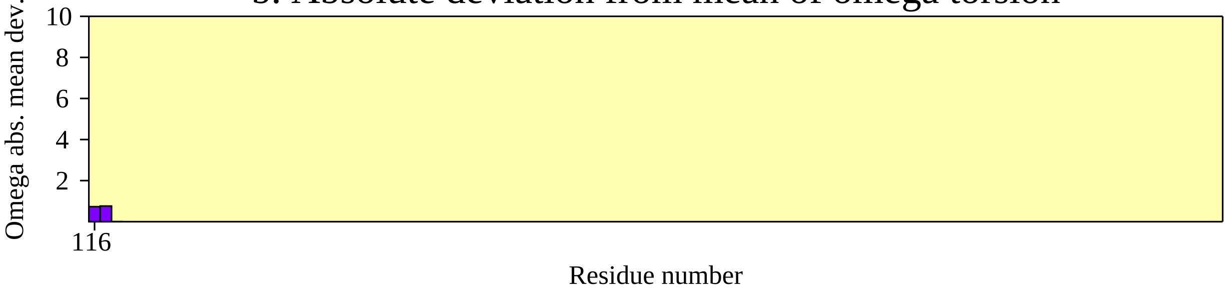
Residue properties

pdb3cir

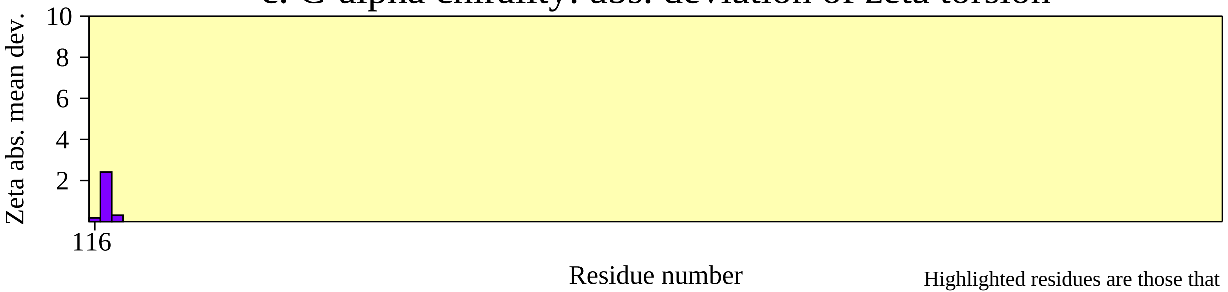
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

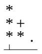
d. Secondary structure & estimated accessibility

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

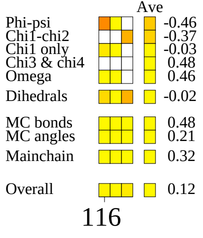
e. Sequence & Ramachandran regions

▲ Most favoured 🟩 Allowed ▯ Generous 🟥 Disallowed

f. Max. deviation (see listing)

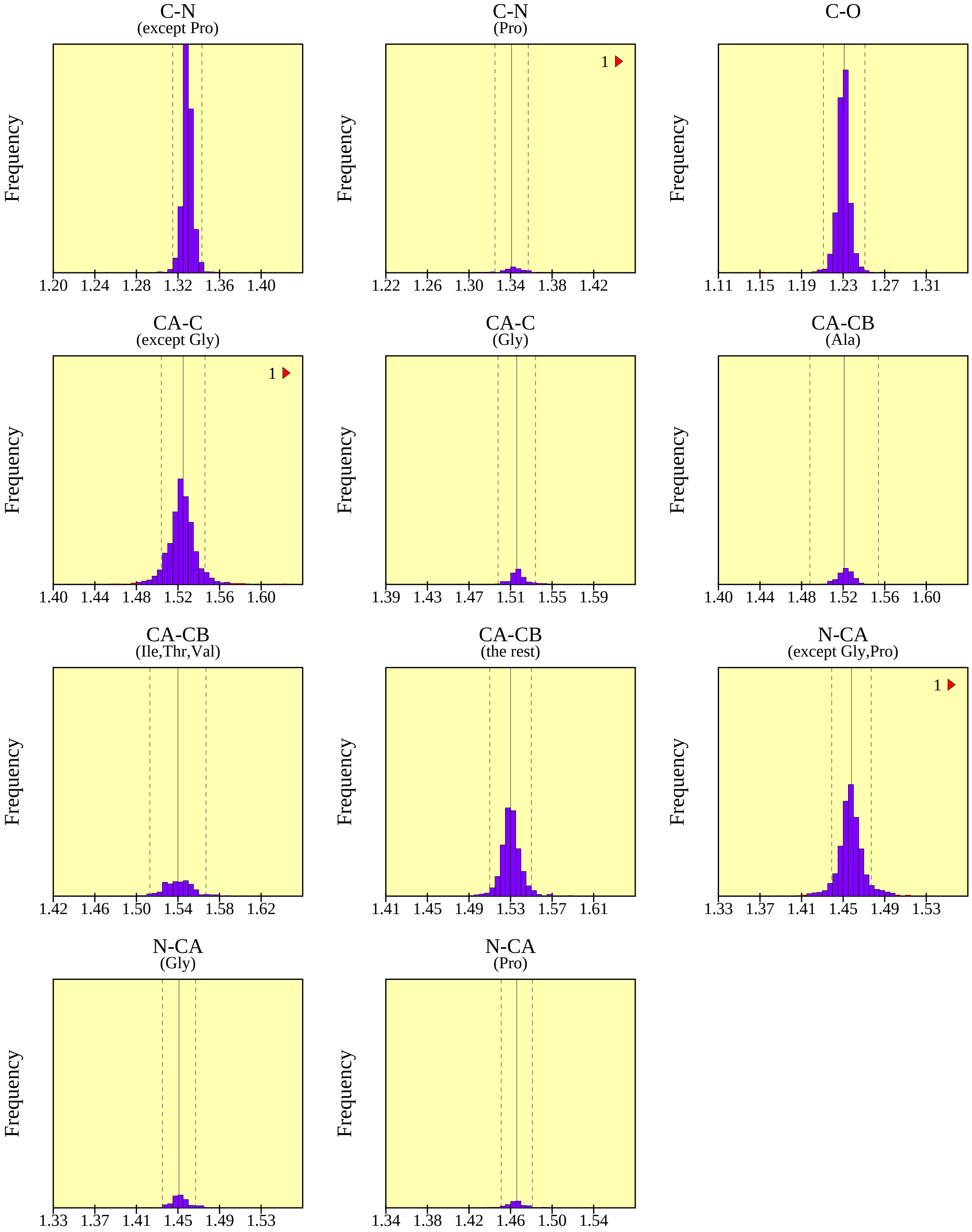


g. G-factors



Main-chain bond lengths

pdb3cir

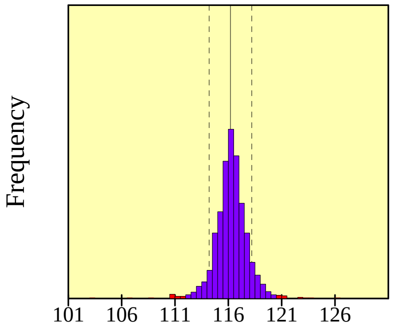


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

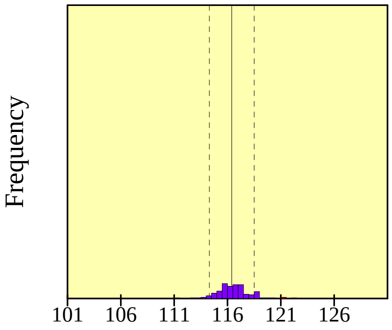
Main-chain bond angles

pdb3cir

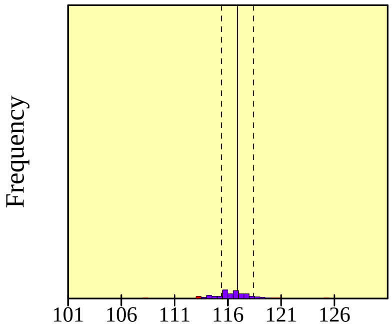
CA-C-N
(except Gly,Pro)



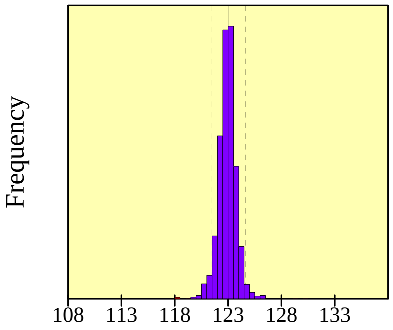
CA-C-N
(Gly)



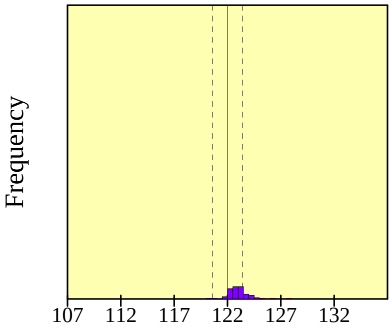
CA-C-N
(Pro)



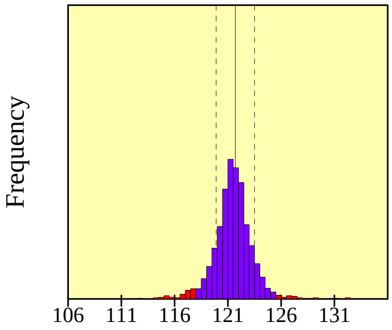
O-C-N
(except Pro)



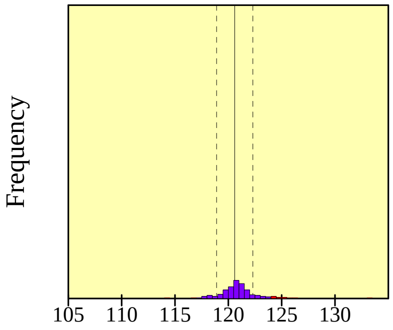
O-C-N
(Pro)



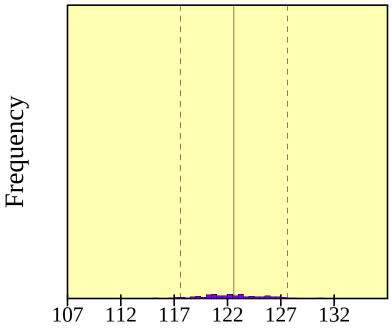
C-N-CA
(except Gly,Pro)



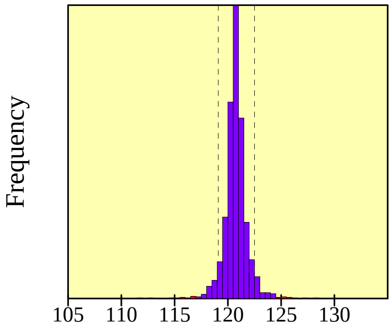
C-N-CA
(Gly)



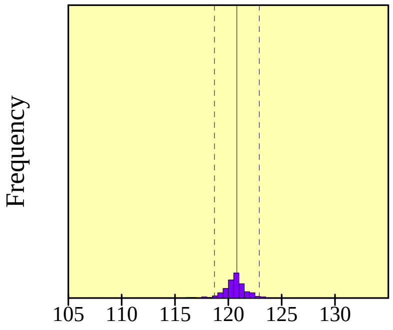
C-N-CA
(Pro)



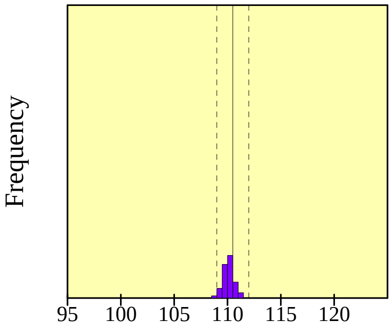
CA-C-O
(except Gly)



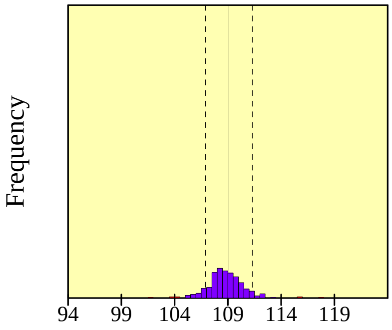
CA-C-O
(Gly)



CB-CA-C
(Ala)



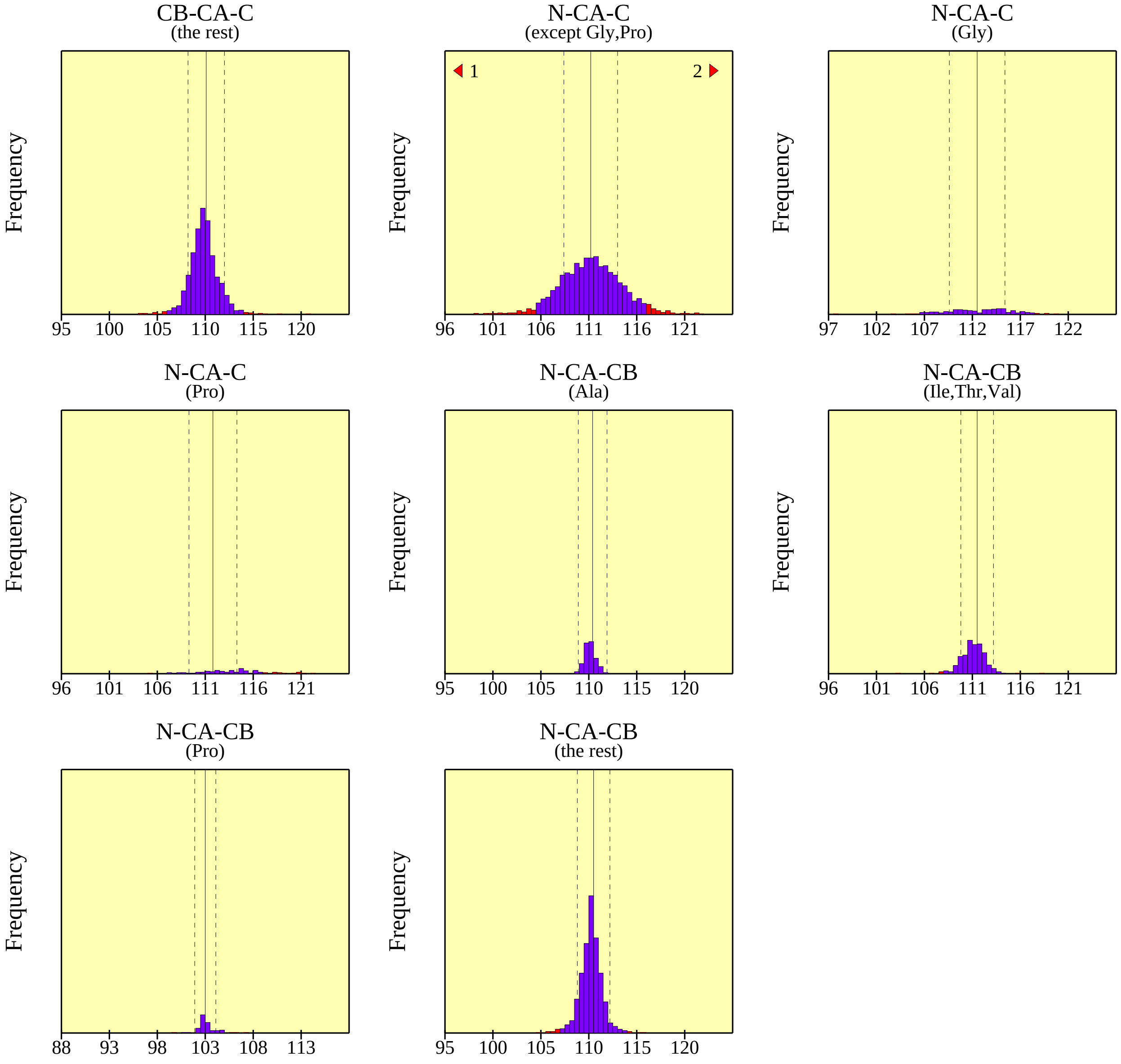
CB-CA-C
(Ile,Thr,Val)



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

pdb3cir

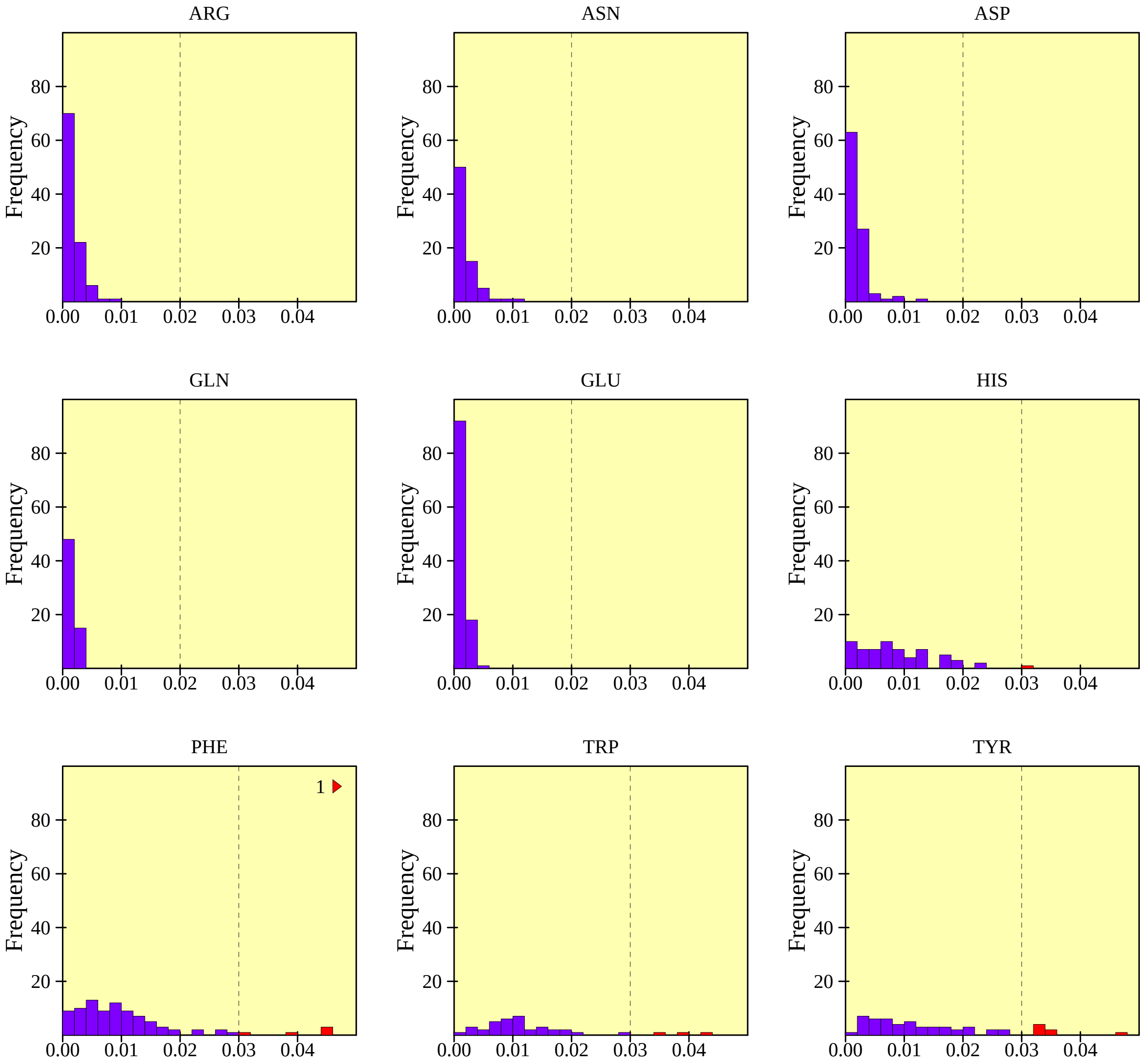


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

RMS distances from planarity

pdb3cir



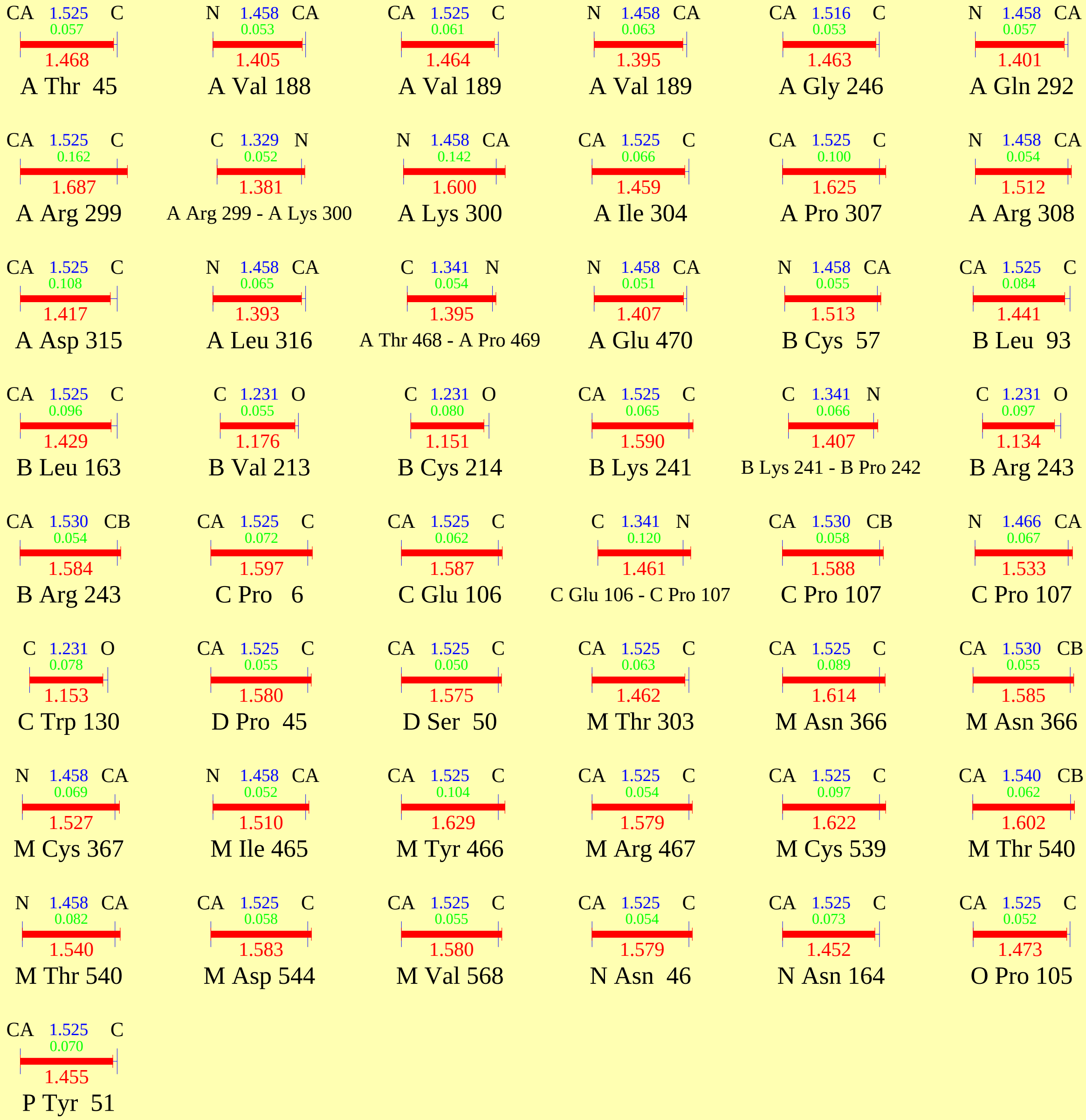
Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

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

Distorted geometry

pdb3cir

Main-chain bond lengths

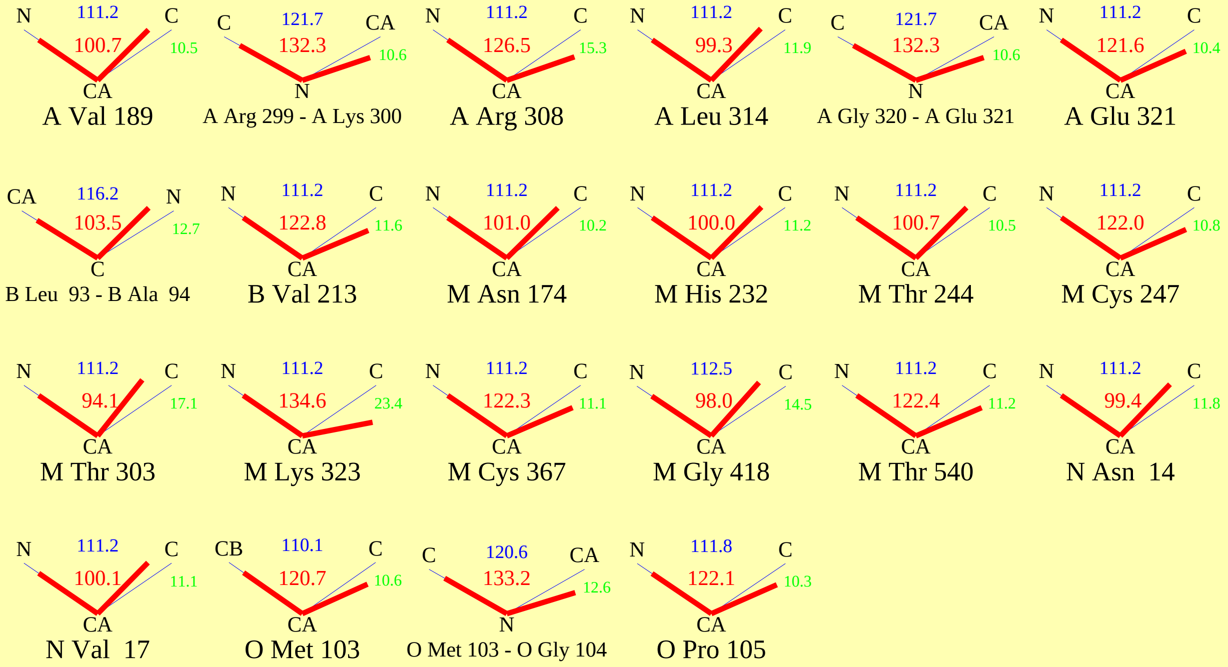


Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

Distorted geometry

pdb3cir

Main-chain bond angles



A Val 189 | A Arg 299 - A Lys 300 | A Arg 308 | A Leu 314 | A Gly 320 - A Glu 321 | A Glu 321

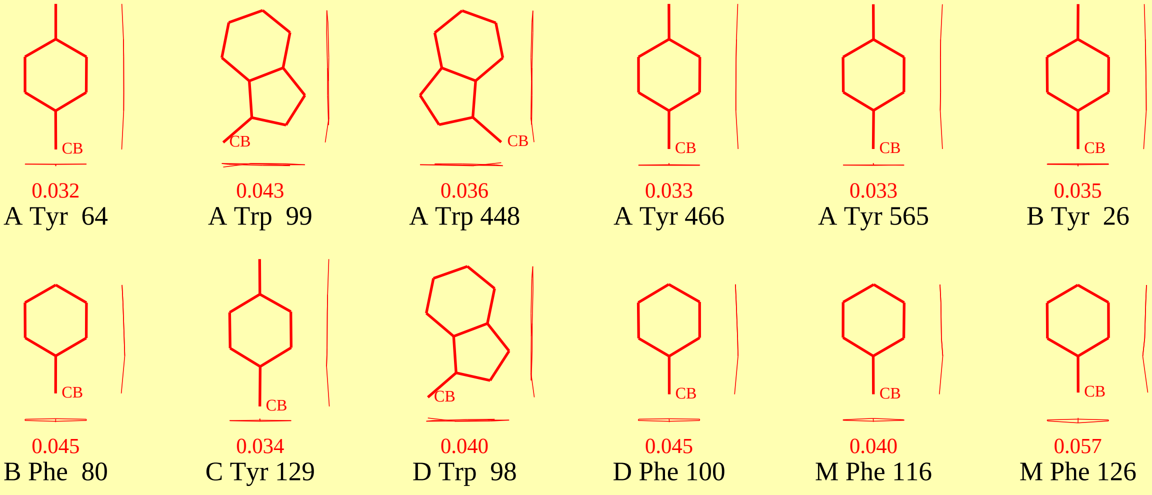
B Leu 93 - B Ala 94 | B Val 213 | M Asn 174 | M His 232 | M Thr 244 | M Cys 247

M Thr 303 | M Lys 323 | M Cys 367 | M Gly 418 | M Thr 540 | N Asn 14

N Val 17 | O Met 103 | O Met 103 - O Gly 104 | O Pro 105

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

Planar groups



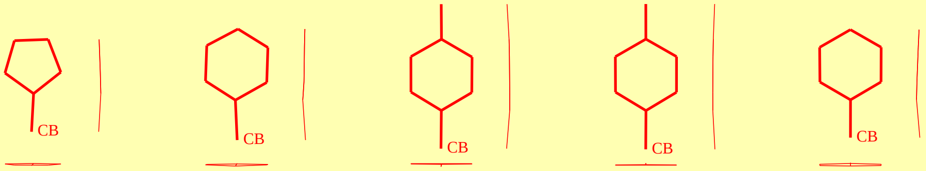
A Tyr 64 | A Trp 99 | A Trp 448 | A Tyr 466 | A Tyr 565 | B Tyr 26

B Phe 80 | C Tyr 129 | D Trp 98 | D Phe 100 | M Phe 116 | M Phe 126

Distorted geometry

pdb3cir

Planar groups (contd)



0.030 M His 232

0.031 M Phe 554

0.047 N Tyr 155

0.032 N Tyr 179

0.045 O Phe 21

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