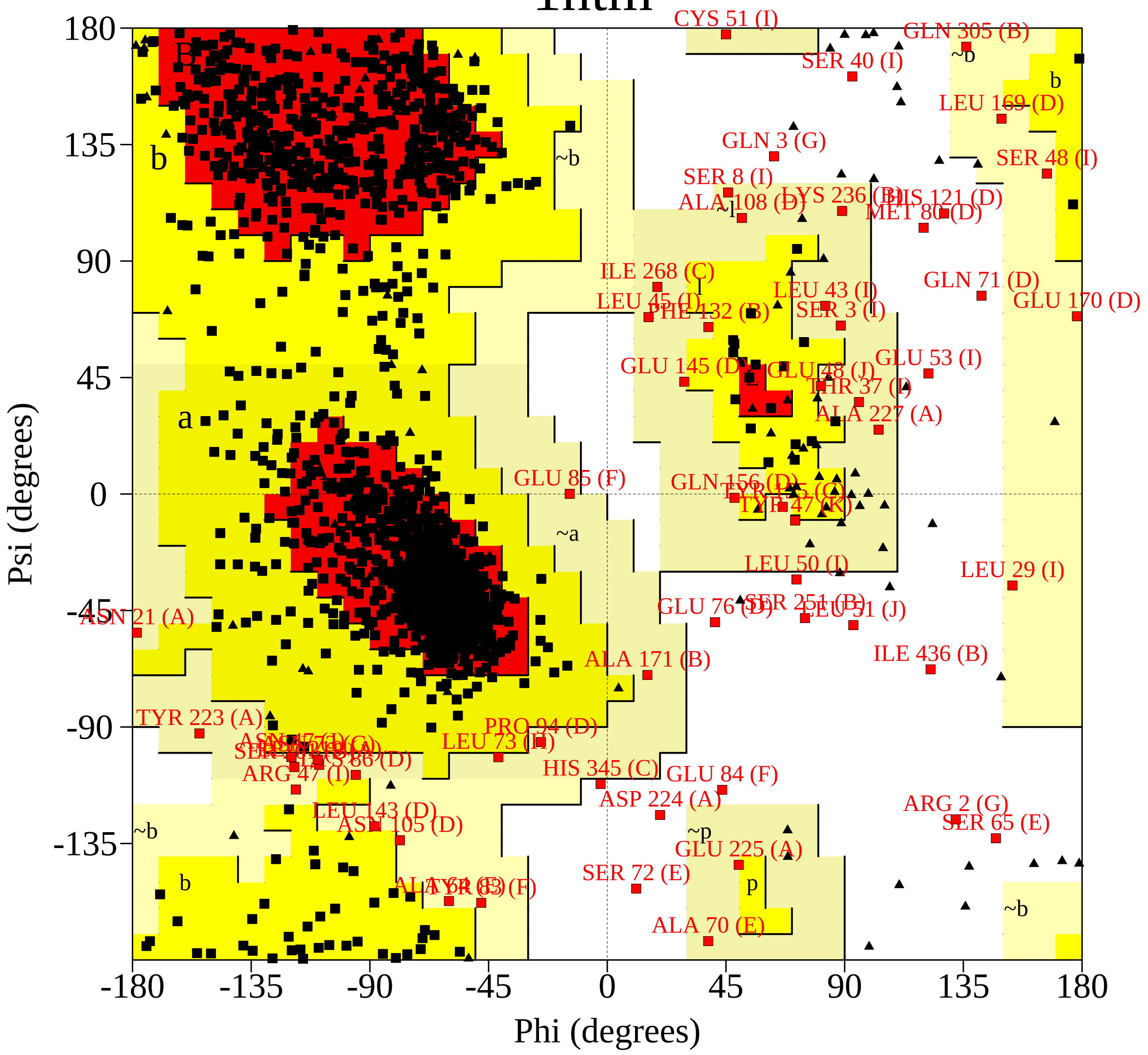
PROCHECK

Ramachandran Plot

1ntm



Plot statistics

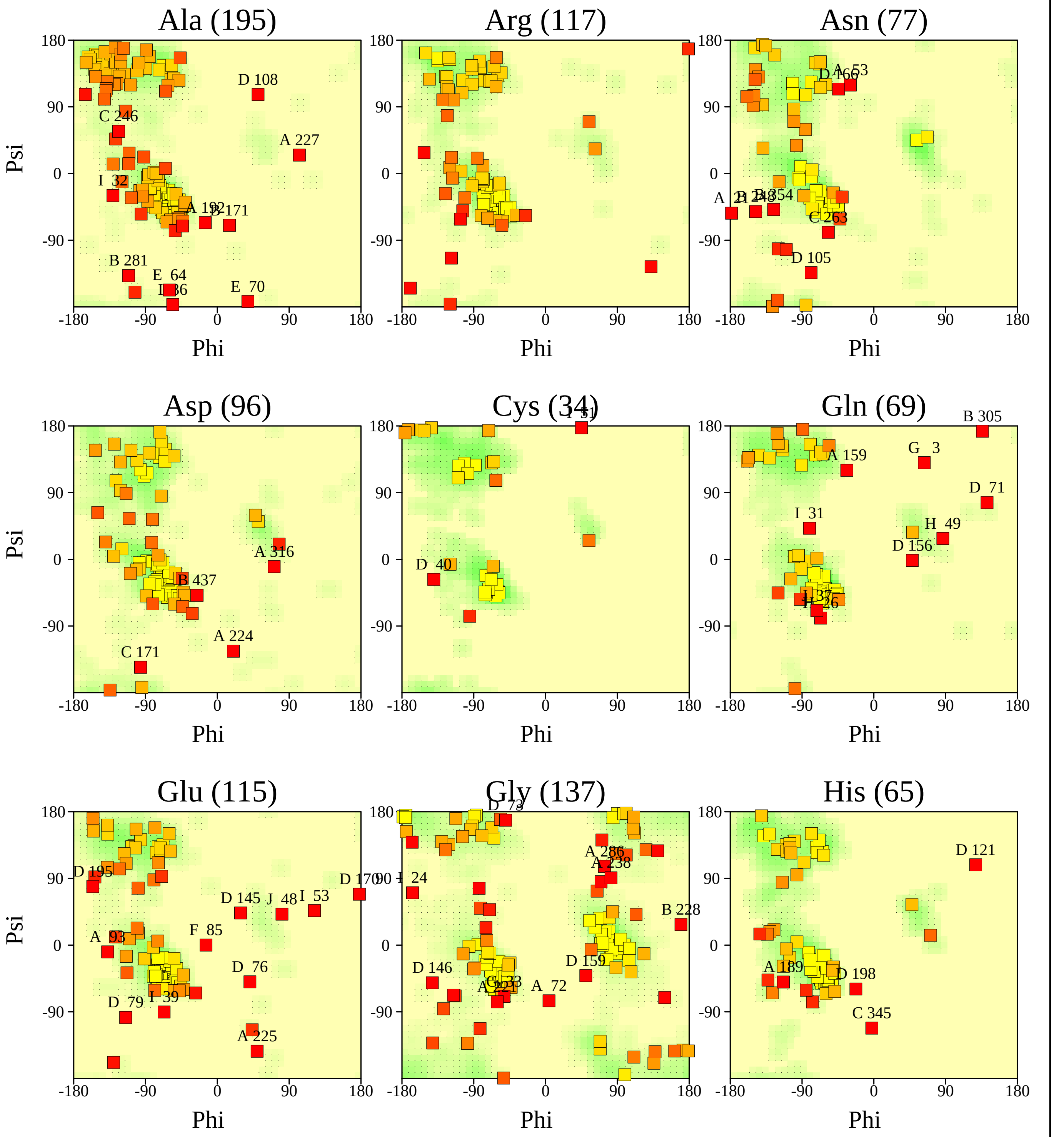
Residues in most favoured regions [A,B,L]	1542	84.2%
Residues in additional allowed regions [a,b,l,p]	234	12.8%
Residues in generously allowed regions [~a,~b,~l,~p]	38	2.1%
Residues in disallowed regions	17	0.9%
	----	------
Number of non-glycine and non-proline residues	1831	100.0%
Number of end-residues (excl. Gly and Pro)	19	
Number of glycine residues (shown as triangles)	140	
Number of proline residues	109	

Total number of residues	2099	

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

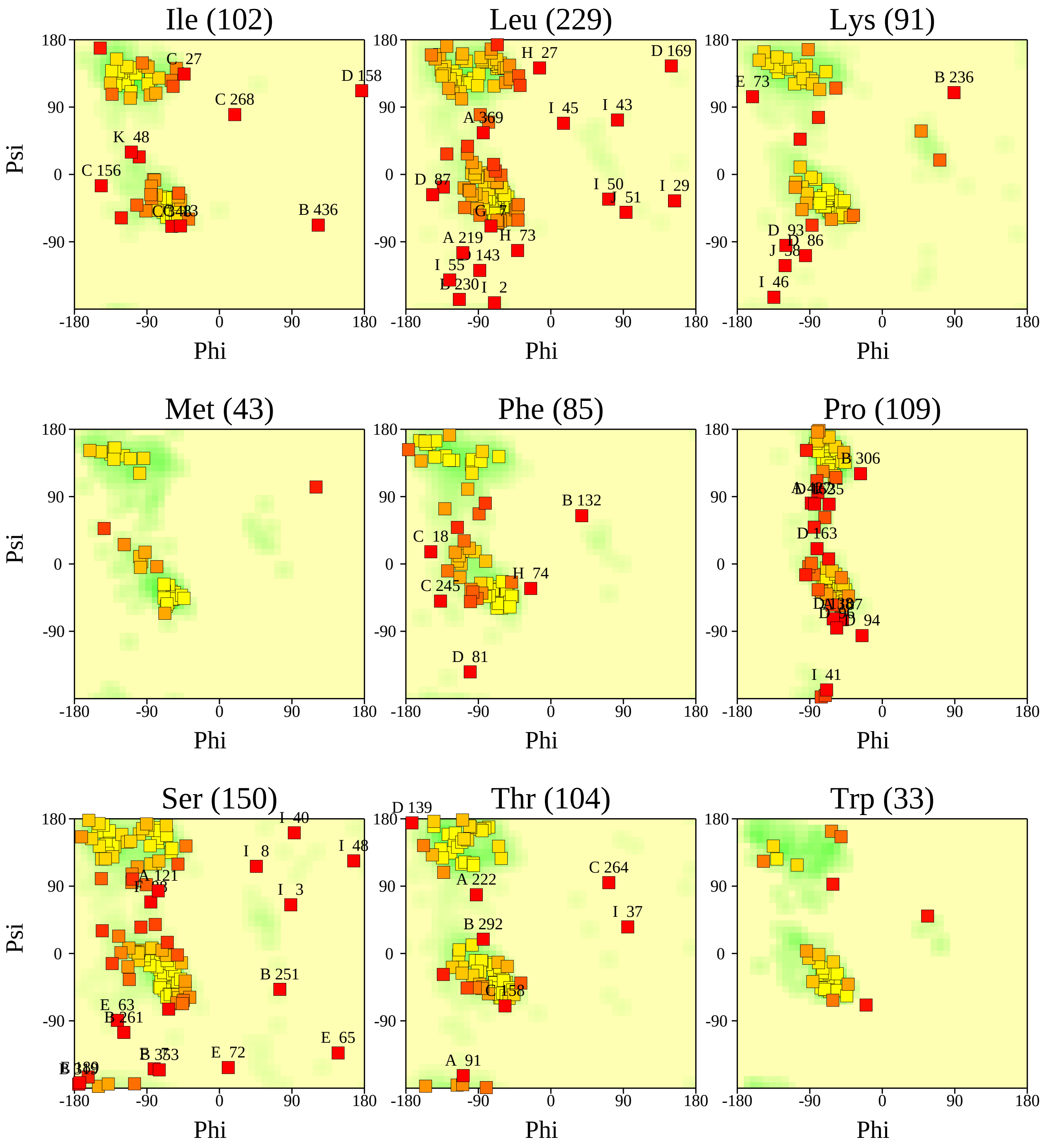
1ntm



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

1ntm

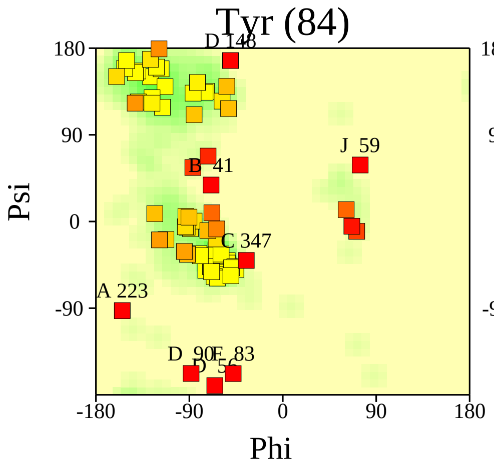


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

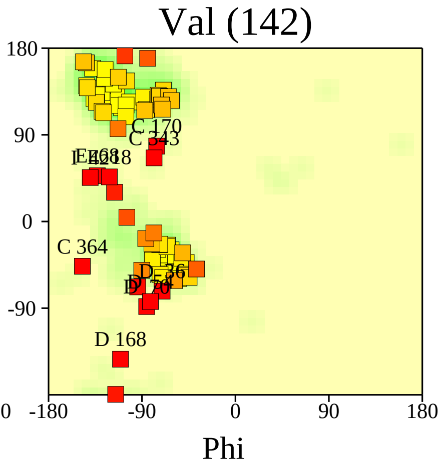
Ramachandran plots for all residue types

1ntm

Tyr (84)



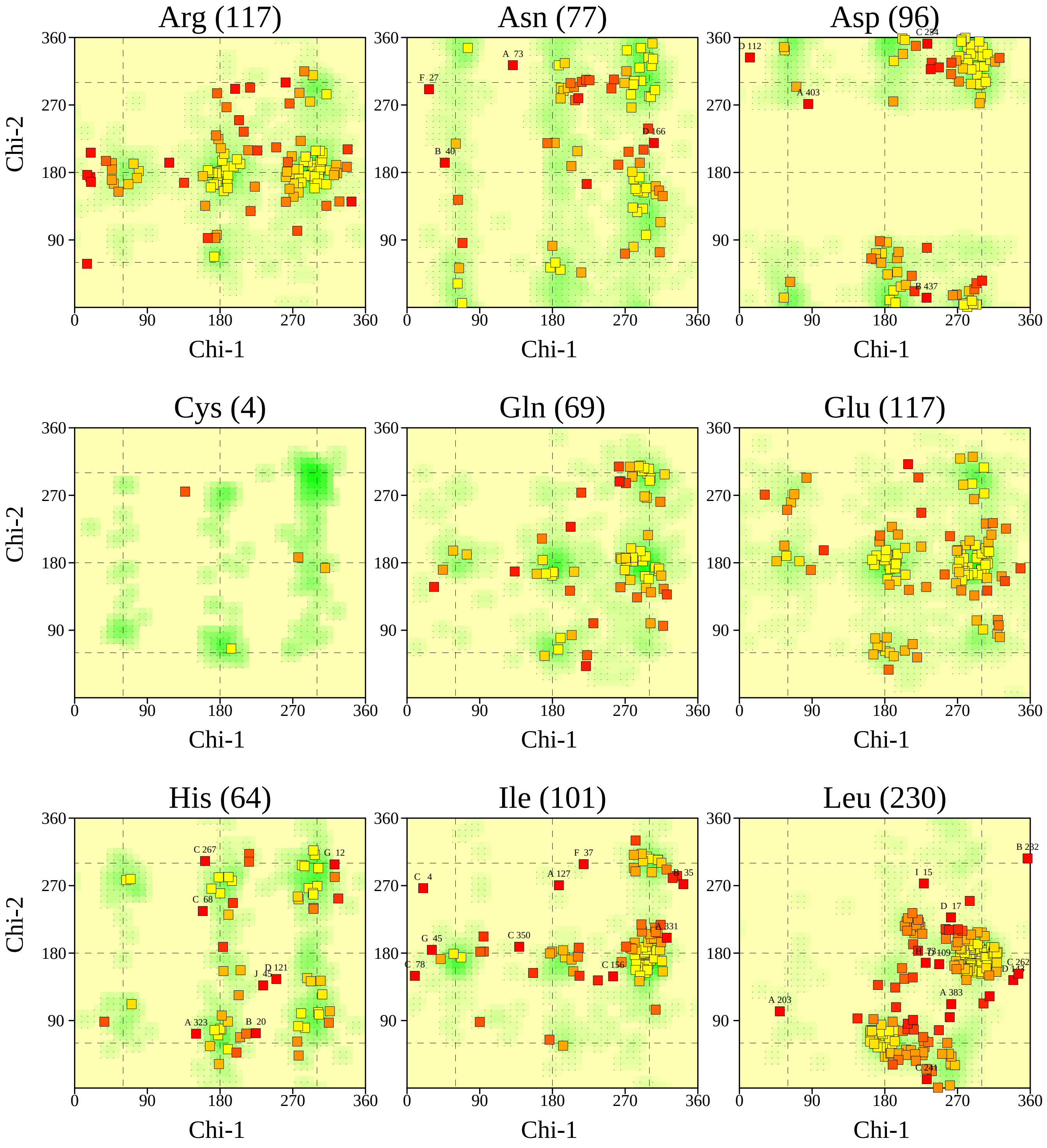
Val (142)



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

Chi1-Chi2 plots

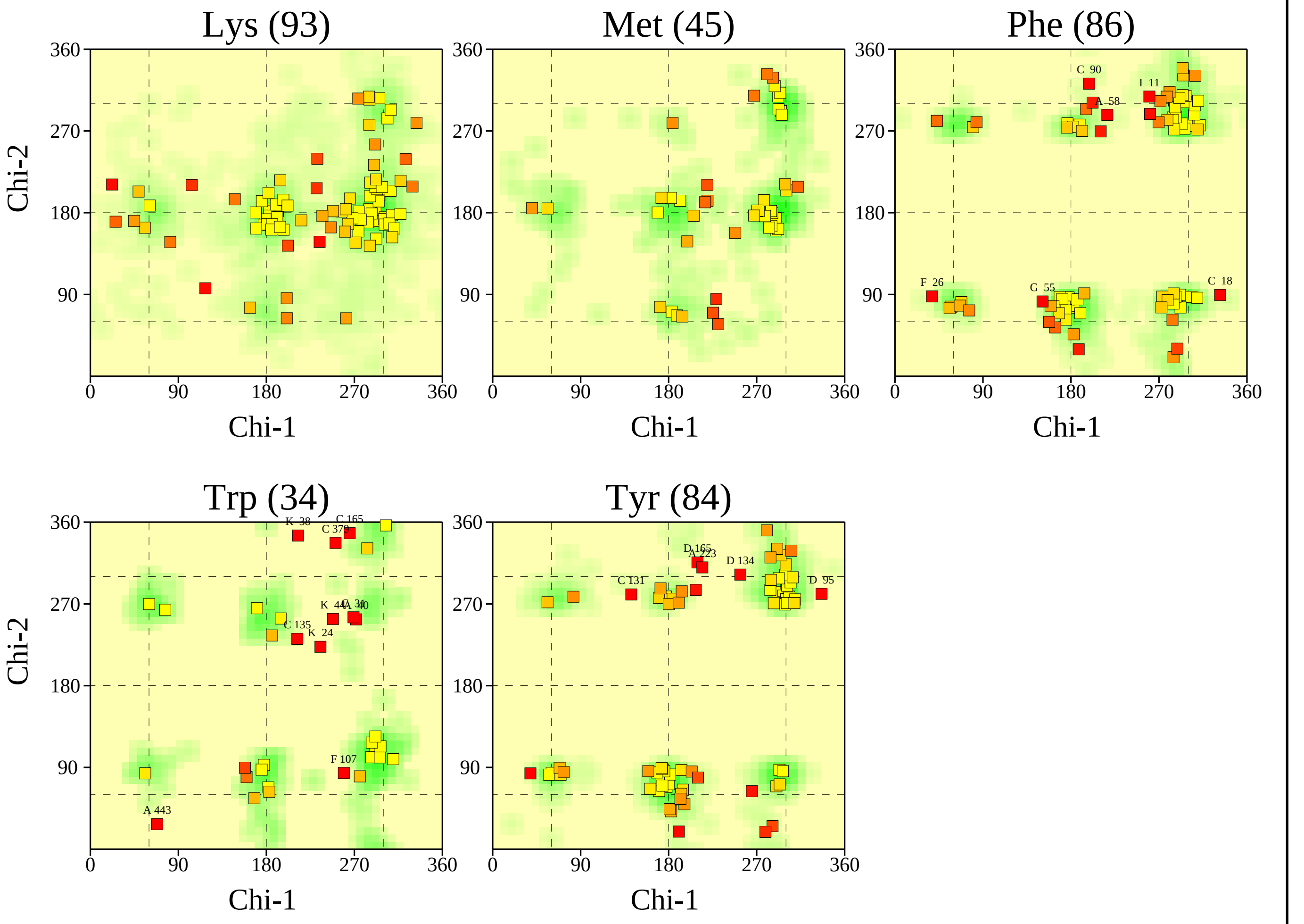
1ntm



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

Chi1-Chi2 plots

1ntm

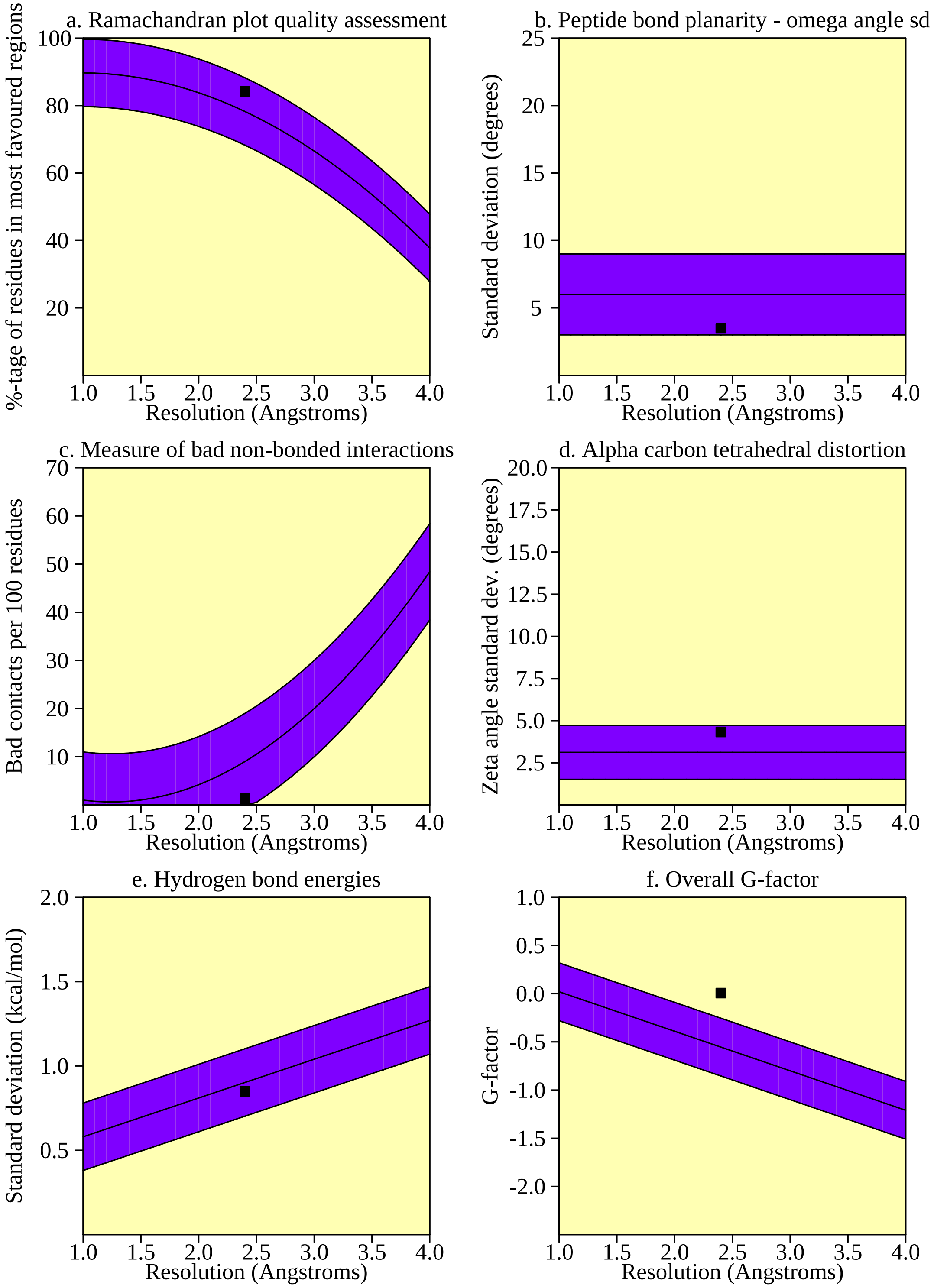


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

Main-chain parameters

1ntm



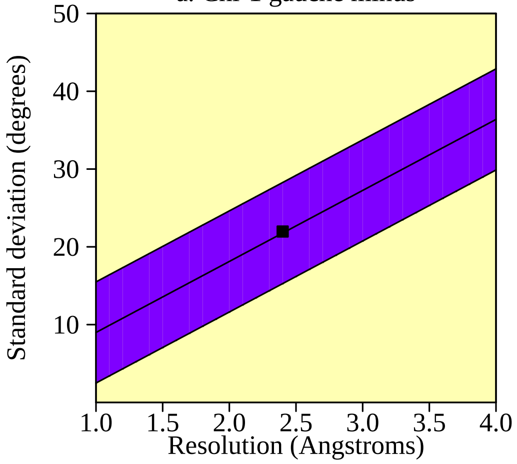
Plot statistics

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	1831	84.2	78.2	10.0	0.6	Inside
b. Omega angle st dev	2087	3.5	6.0	3.0	-0.8	Inside
c. Bad contacts / 100 residues	28	1.3	9.0	10.0	-0.8	Inside
d. Zeta angle st dev	1959	4.3	3.1	1.6	0.8	Inside
e. H-bond energy st dev	1374	0.8	0.9	0.2	-0.3	Inside
f. Overall G-factor	2099	0.0	-0.6	0.3	1.9	BETTER

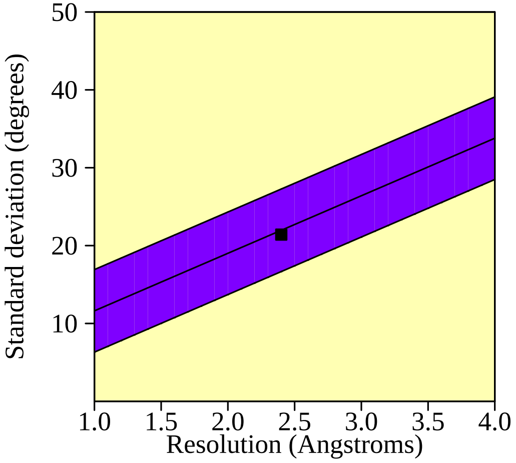
Side-chain parameters

1ntm

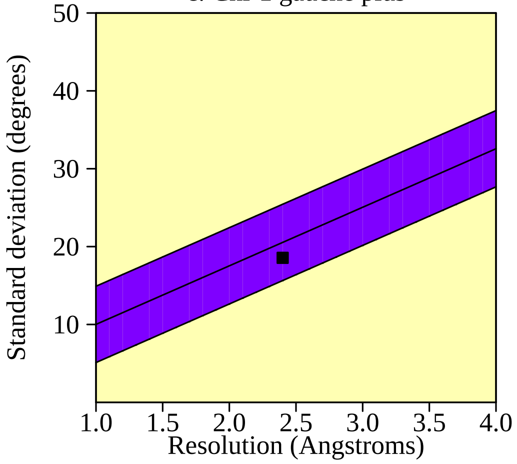
a. Chi-1 gauche minus



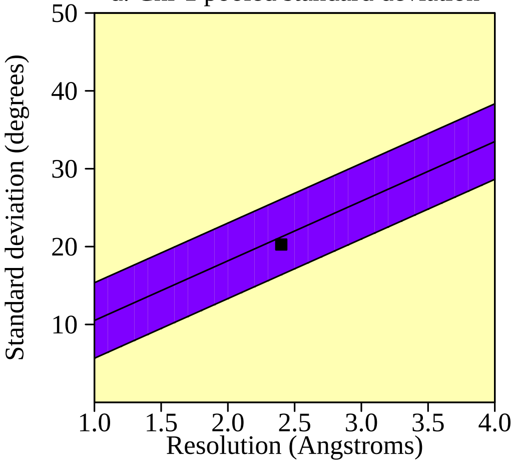
b. Chi-1 trans



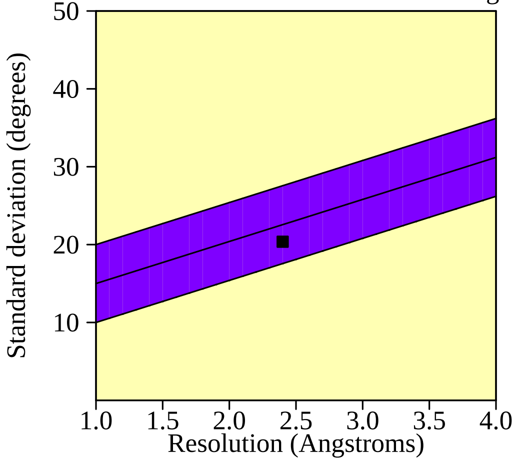
c. Chi-1 gauche plus



d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



1ntm

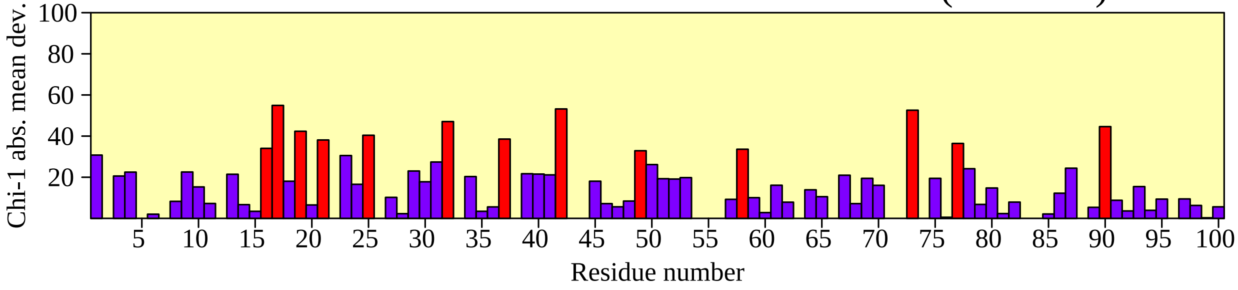
Plot statistics

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	219	22.0	21.8	6.5	0.0	Inside
b. Chi-1 trans st dev	610	21.4	22.0	5.3	-0.1	Inside
c. Chi-1 gauche plus st dev	821	18.6	20.5	4.9	-0.4	Inside
d. Chi-1 pooled st dev	1650	20.3	21.2	4.8	-0.2	Inside
e. Chi-2 trans st dev	555	20.4	22.6	5.0	-0.4	Inside

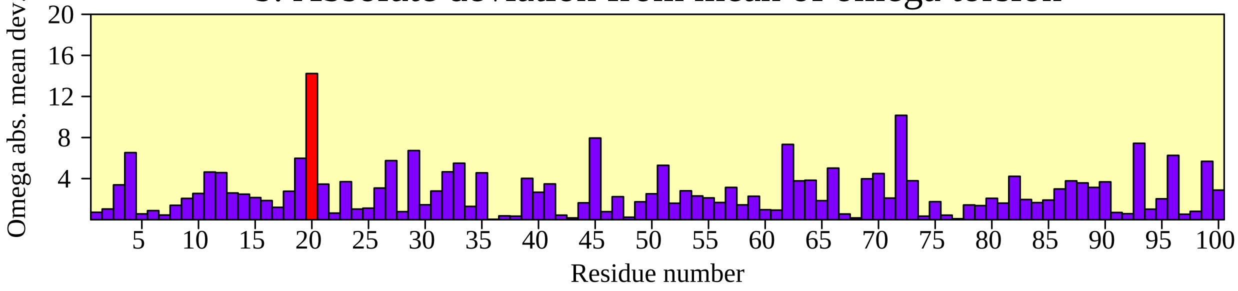
Residue properties

1ntm

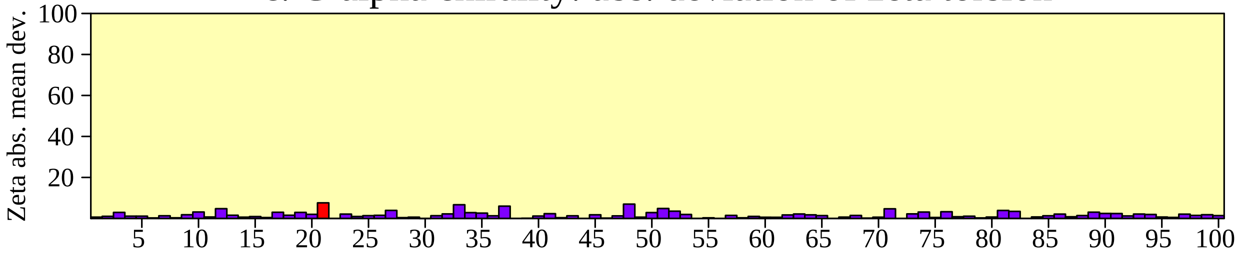
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



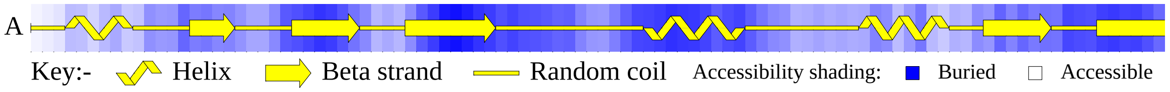
c. C-alpha chirality: abs. deviation of zeta torsion



Residue number

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

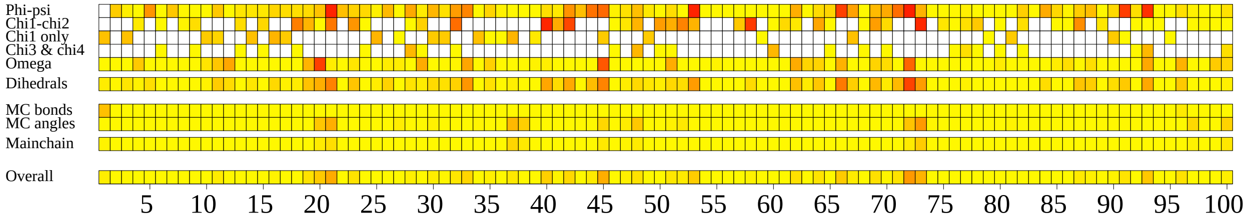
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

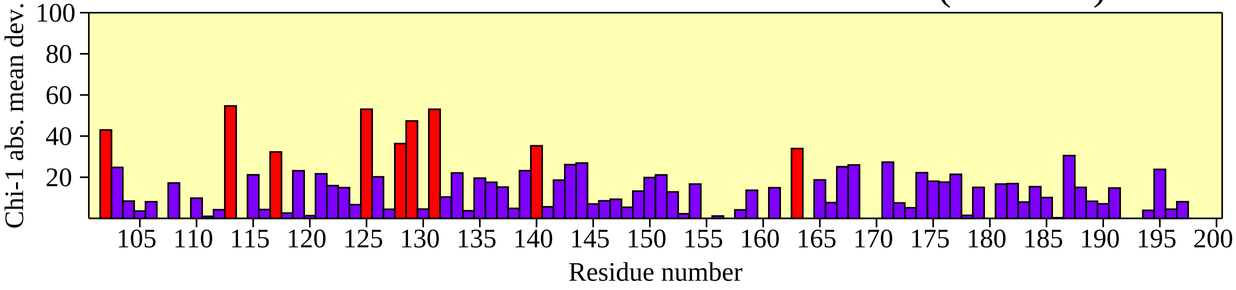
g. G-factors



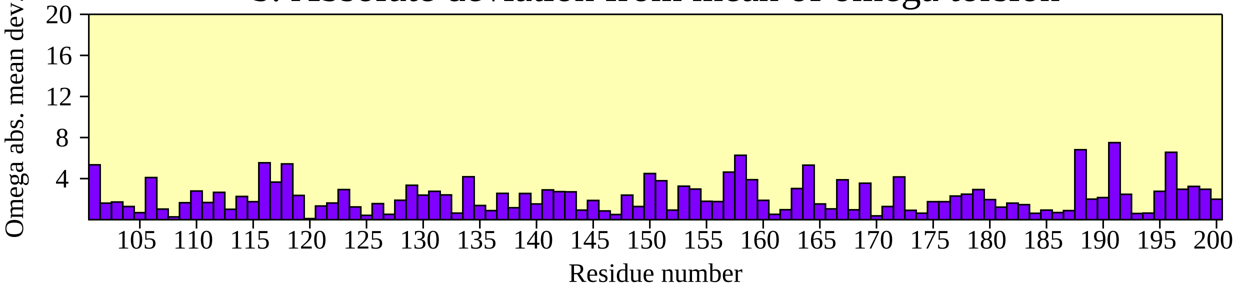
Residue properties

1ntm

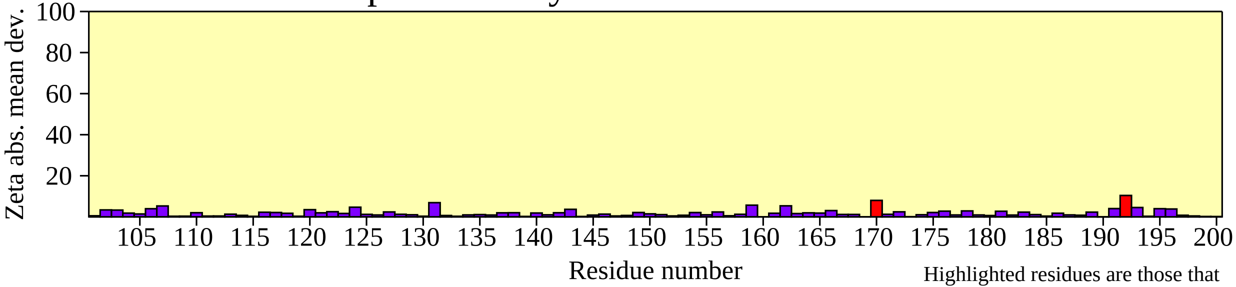
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

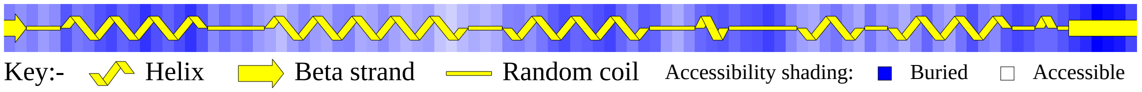


c. C-alpha chirality: abs. deviation of zeta torsion



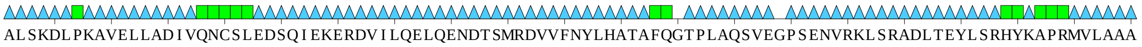
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

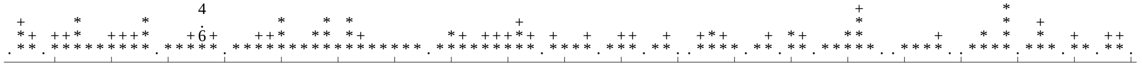


e. Sequence & Ramachandran regions

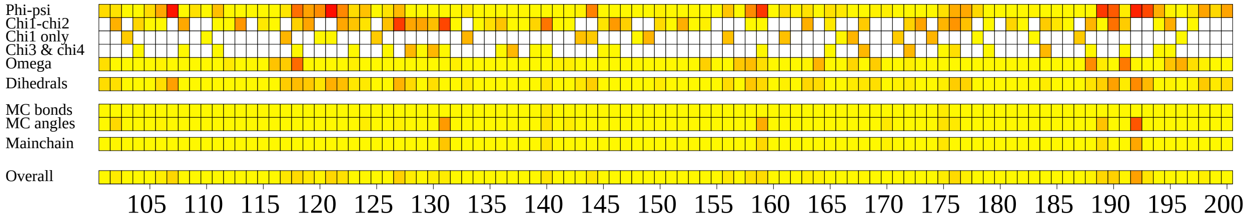
▲ Most favoured 🟩 Allowed ▯ Generous 🟥 Disallowed



f. Max. deviation (see listing)



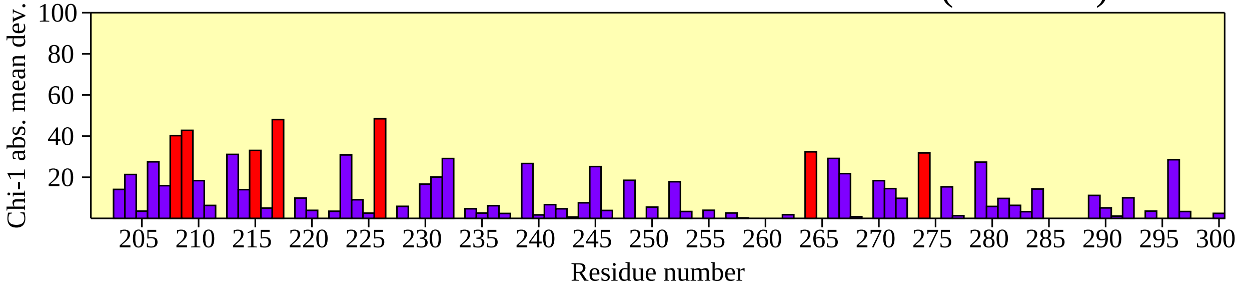
g. G-factors



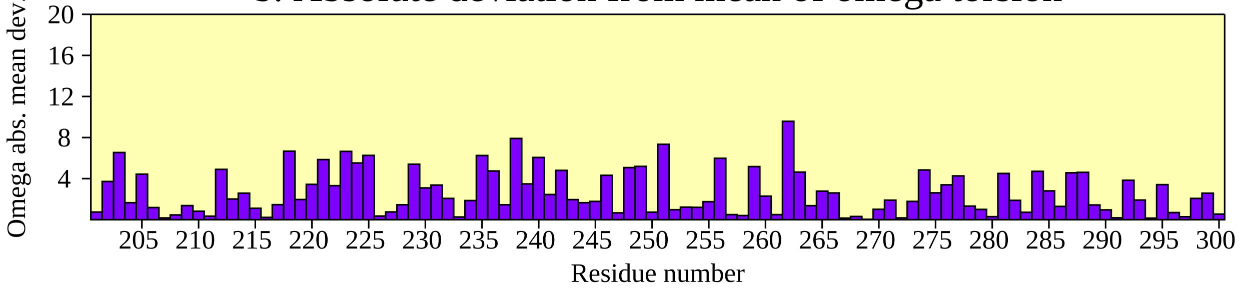
Residue properties

1ntm

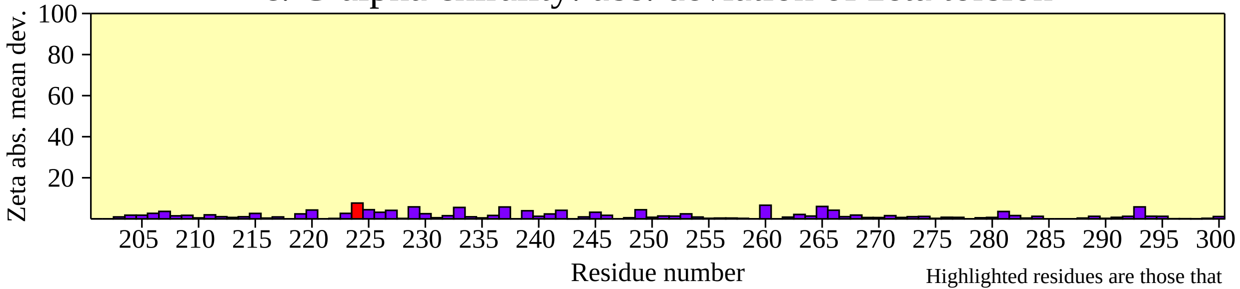
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

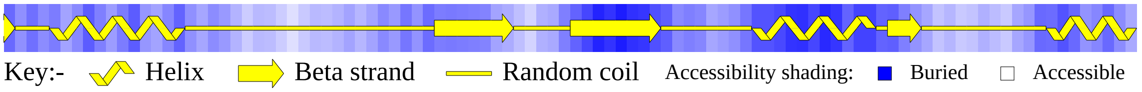


c. C-alpha chirality: abs. deviation of zeta torsion



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

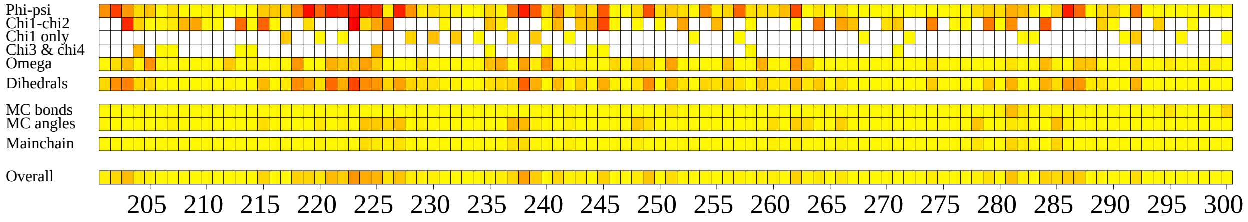
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

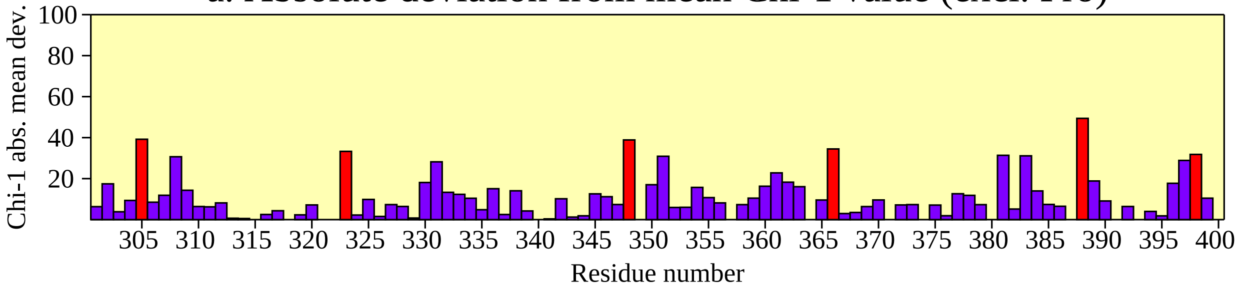
g. G-factors



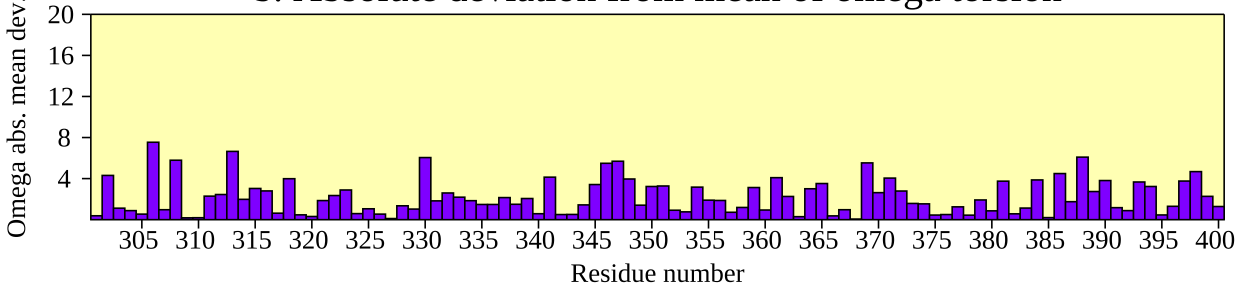
Residue properties

1ntm

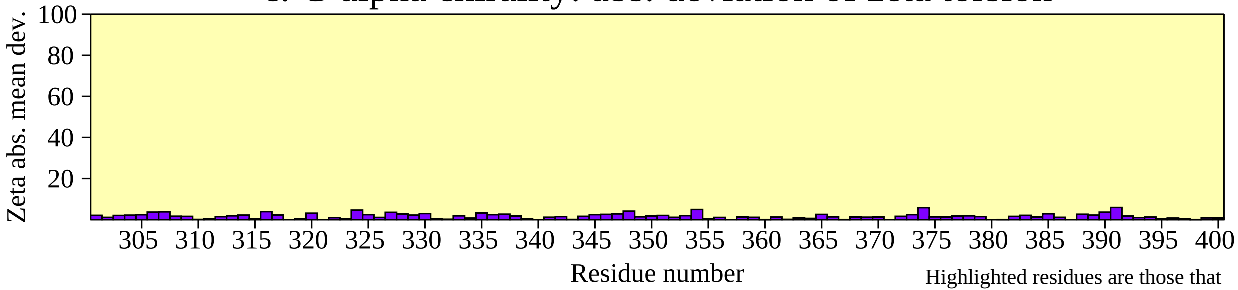
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

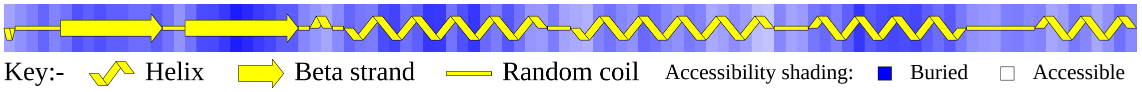


c. C-alpha chirality: abs. deviation of zeta torsion

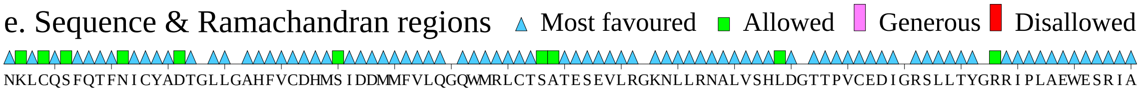


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

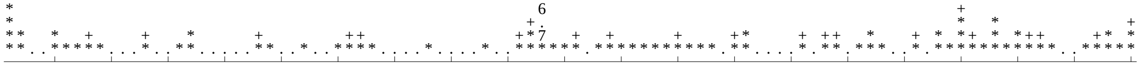
d. Secondary structure & estimated accessibility



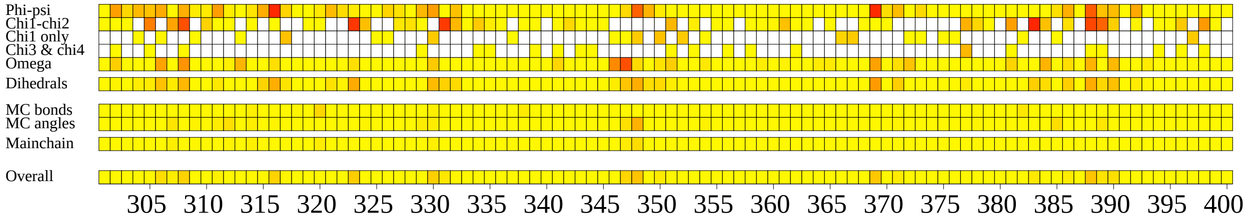
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



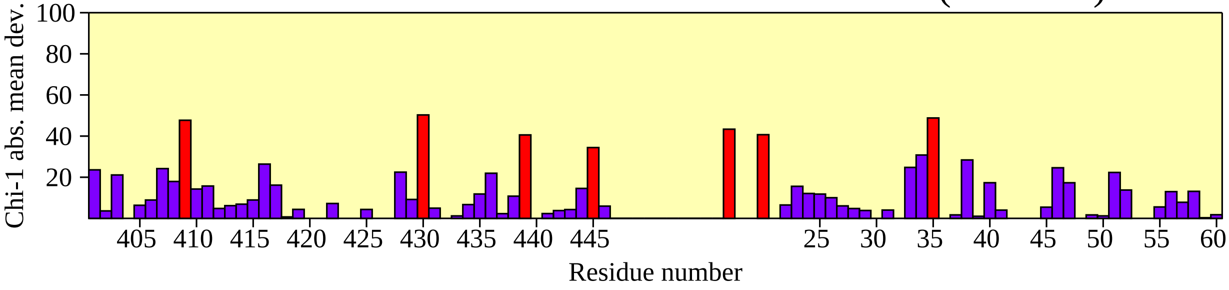
g. G-factors



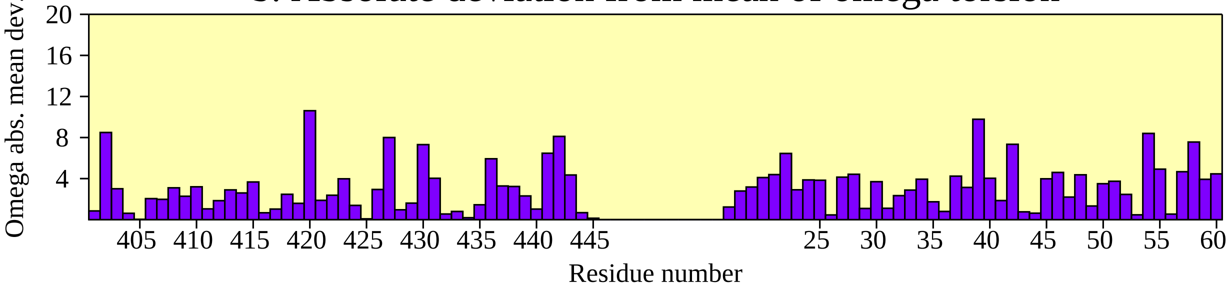
Residue properties

1ntm

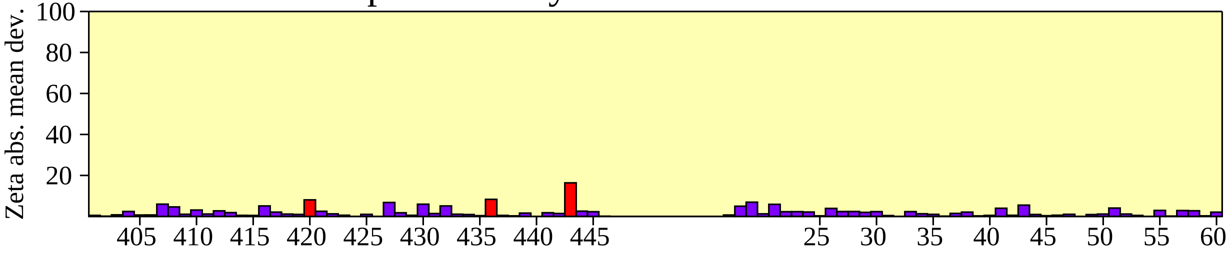
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



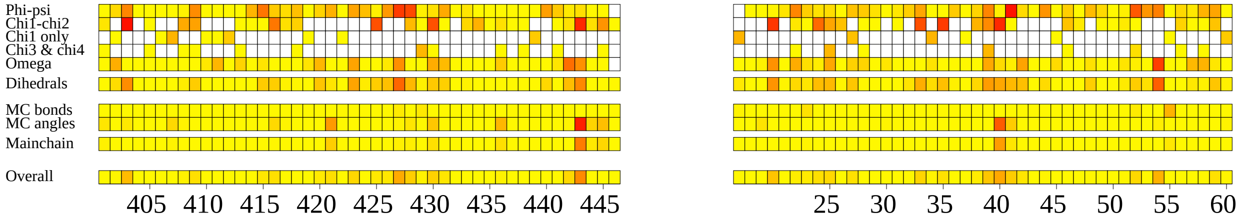
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

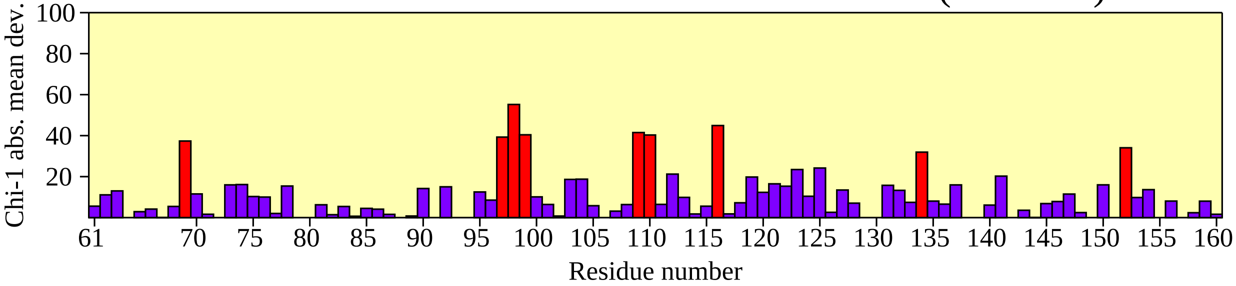
g. G-factors



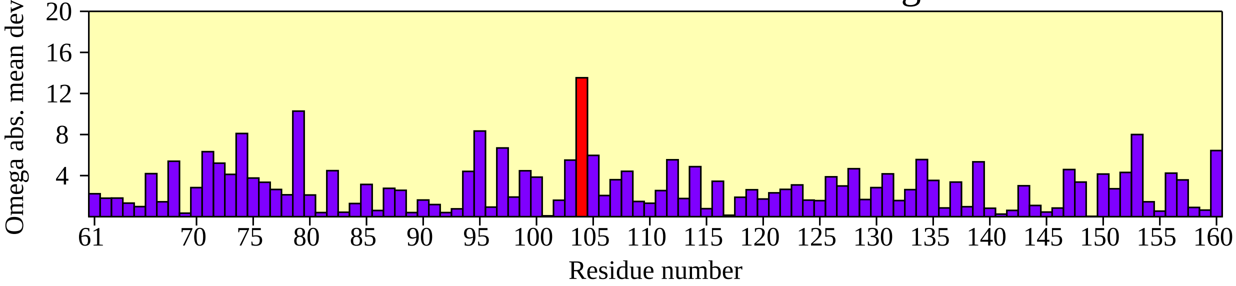
Residue properties

1ntm

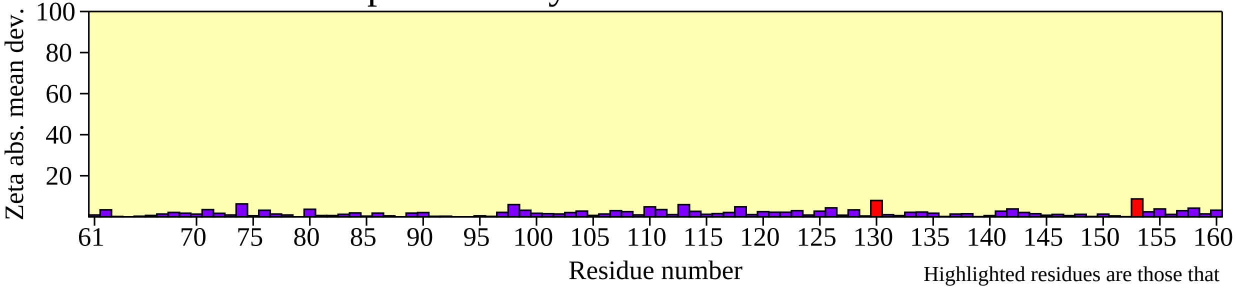
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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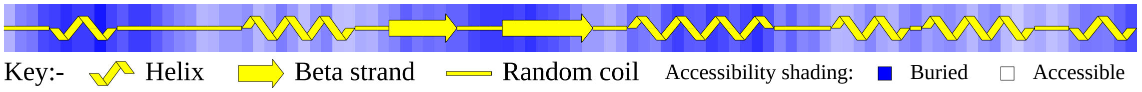
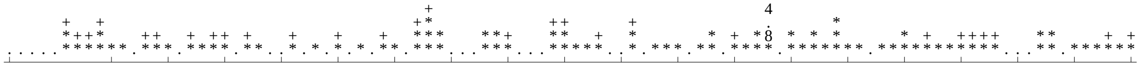
d. Secondary structure & estimated accessibility

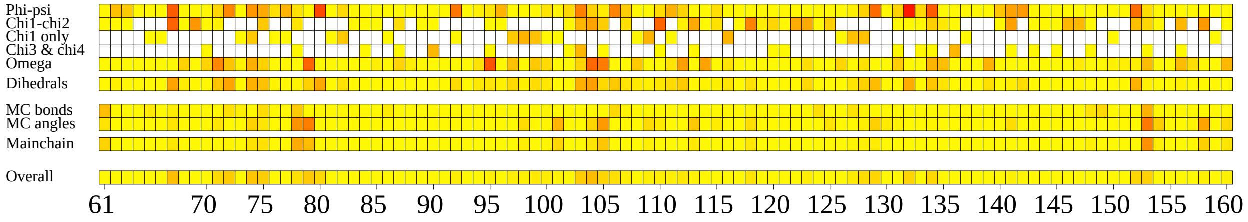


e. Sequence & Ramachandran regions

f. Max. deviation (see listing)



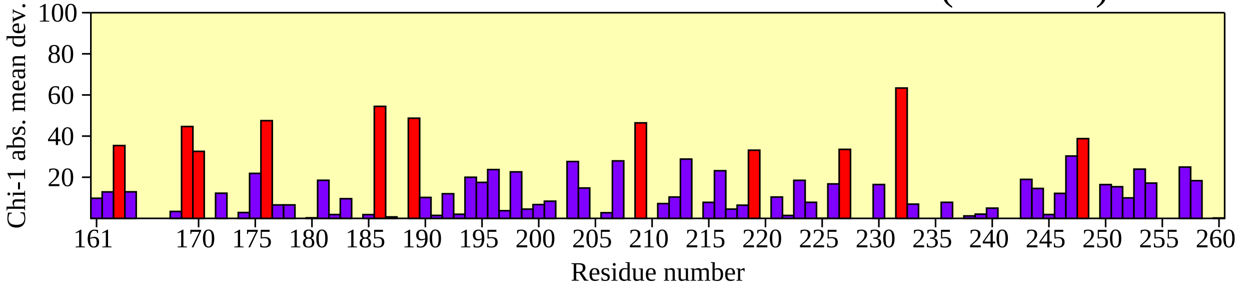
g. G-factors



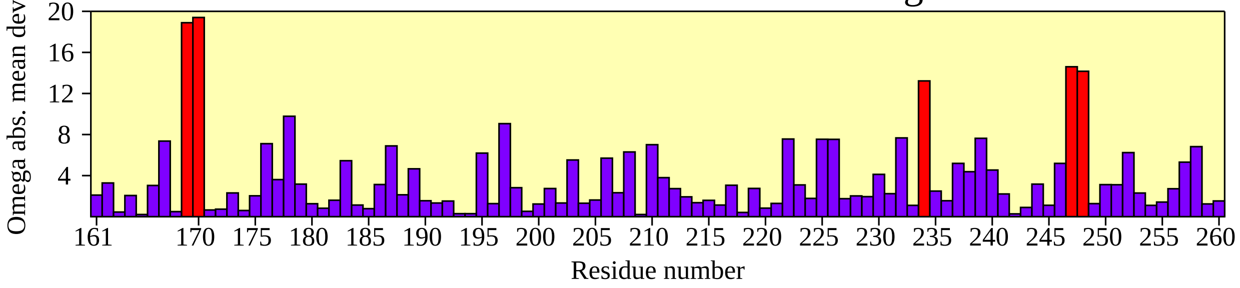
Residue properties

1ntm

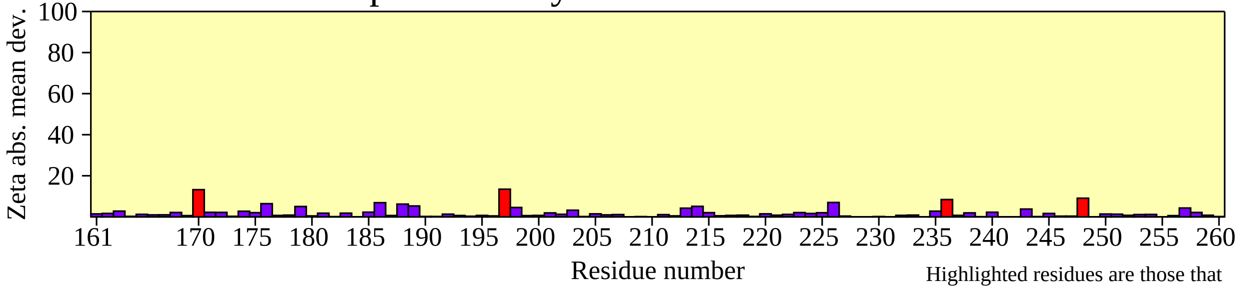
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

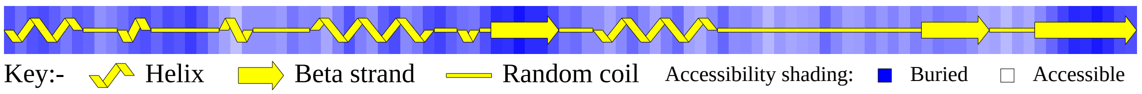


c. C-alpha chirality: abs. deviation of zeta torsion

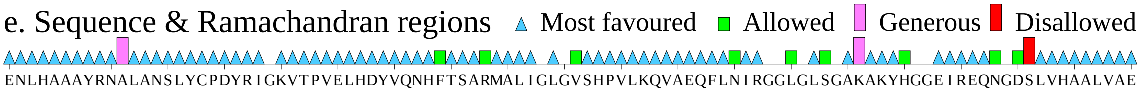


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

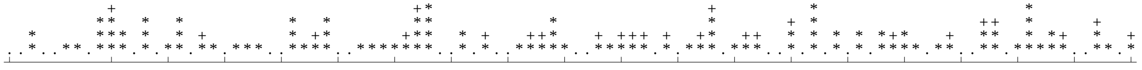
d. Secondary structure & estimated accessibility



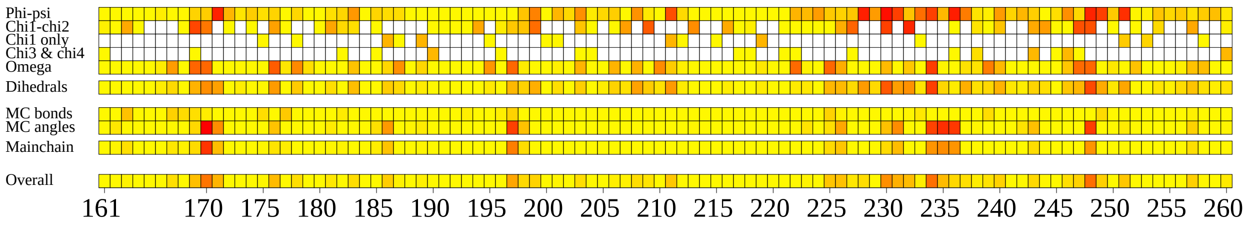
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



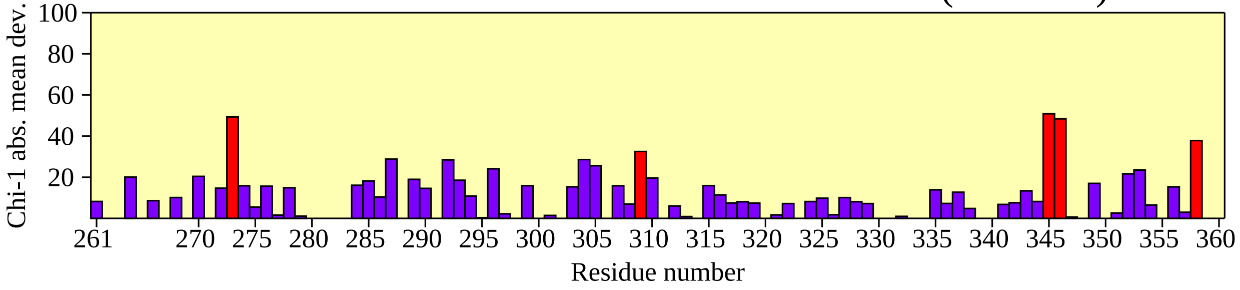
g. G-factors



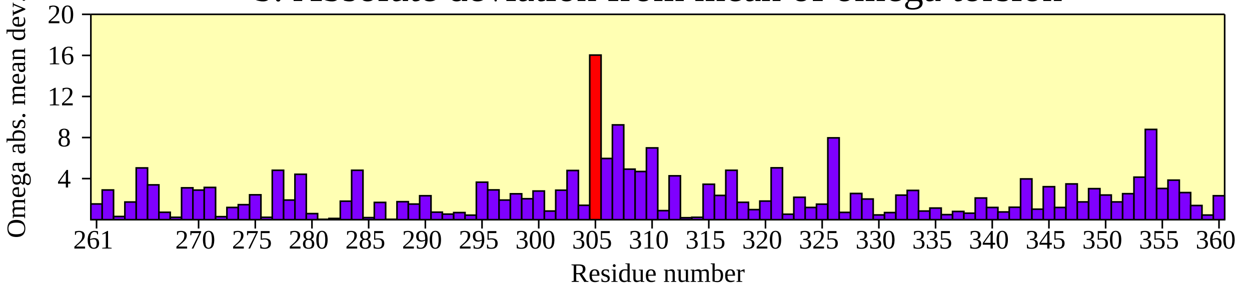
Residue properties

1ntm

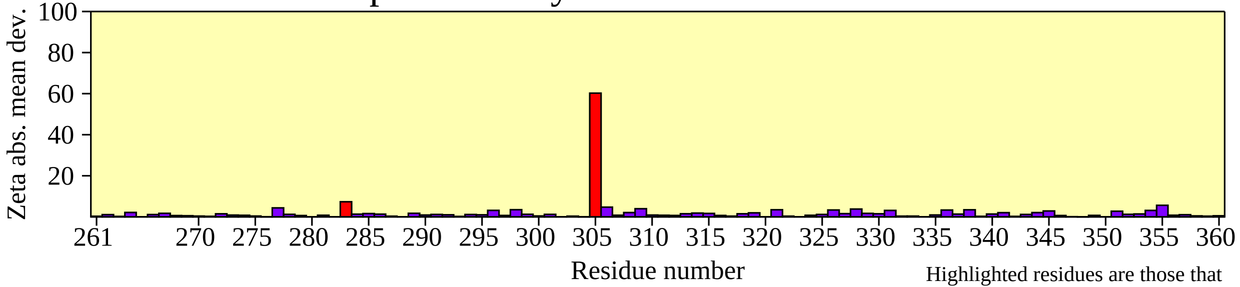
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



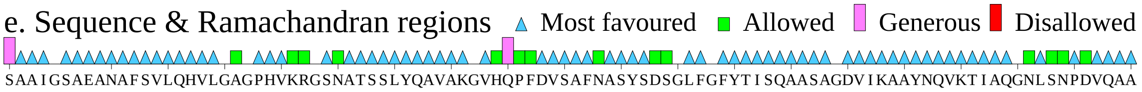
c. C-alpha chirality: abs. deviation of zeta torsion



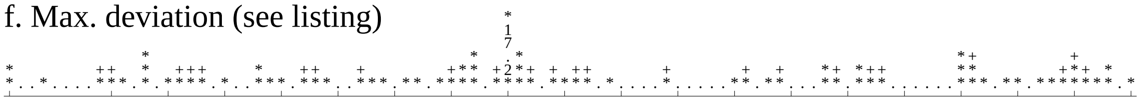
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

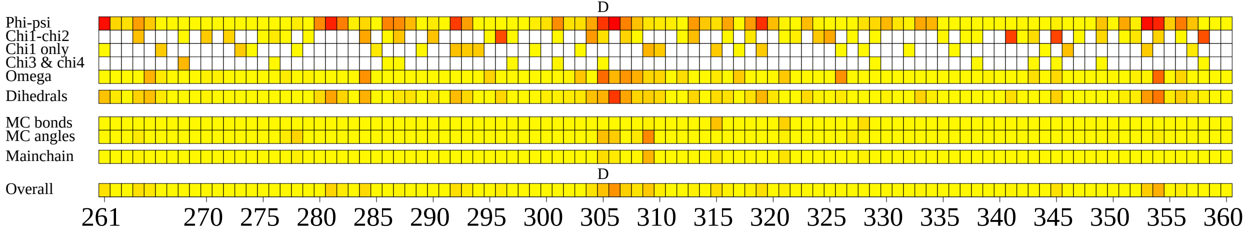
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

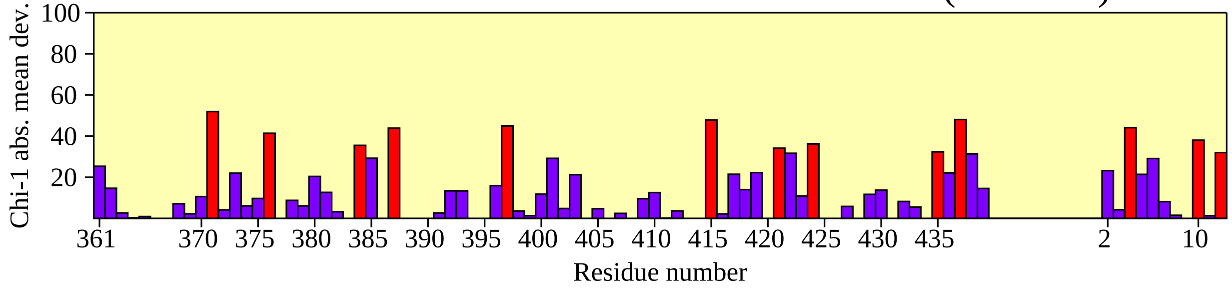


D = D-amino acid

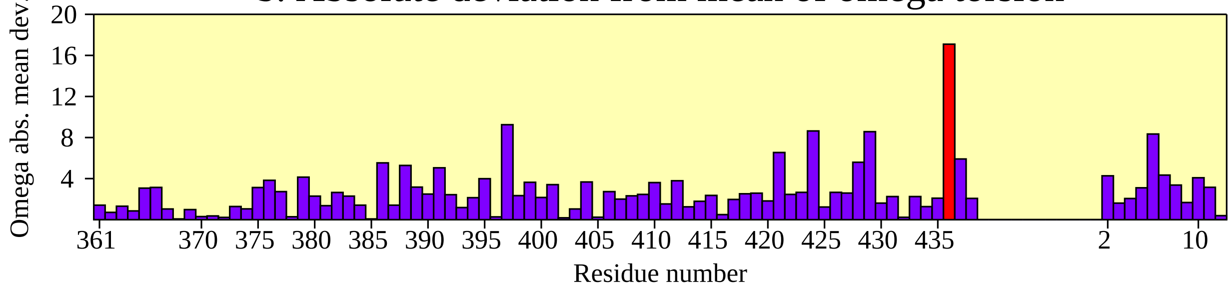
Residue properties

1ntm

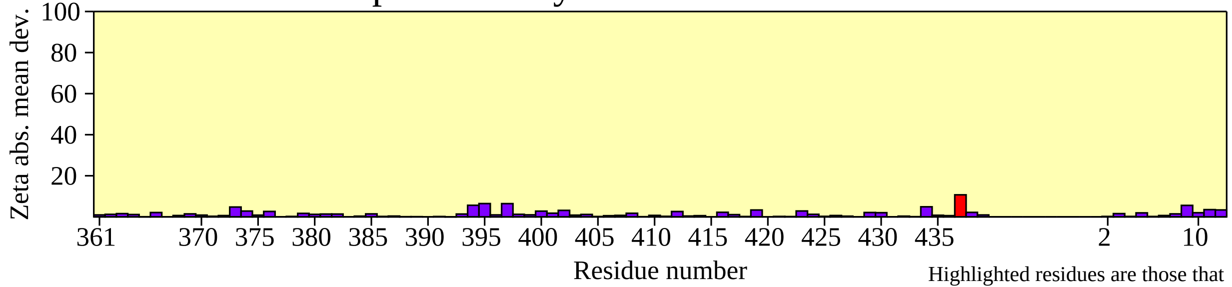
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

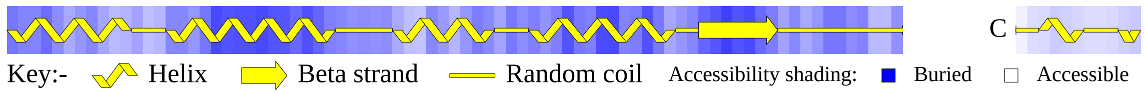


c. C-alpha chirality: abs. deviation of zeta torsion



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

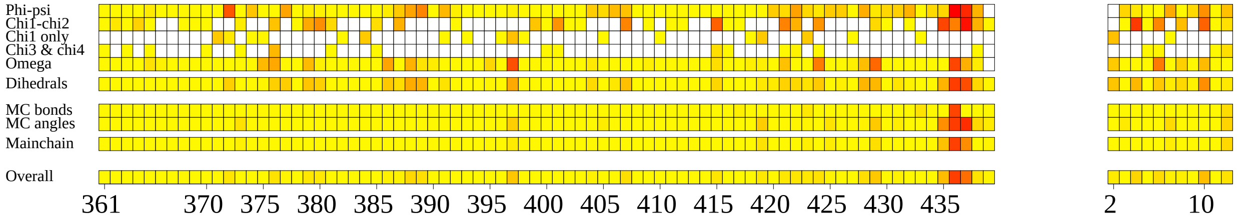
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

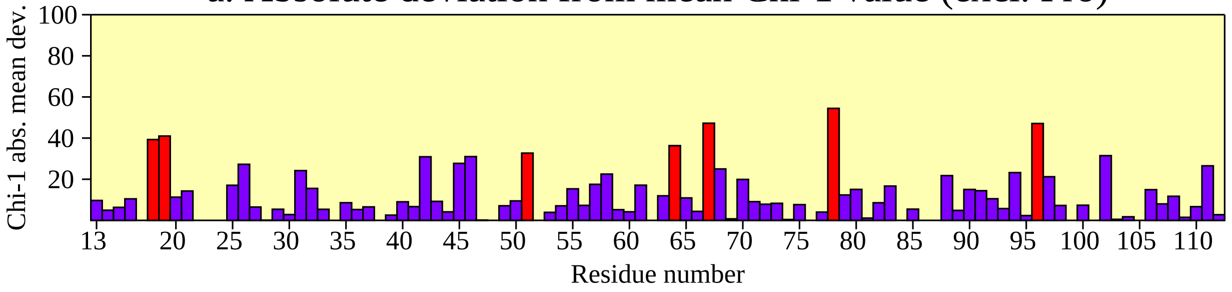
g. G-factors



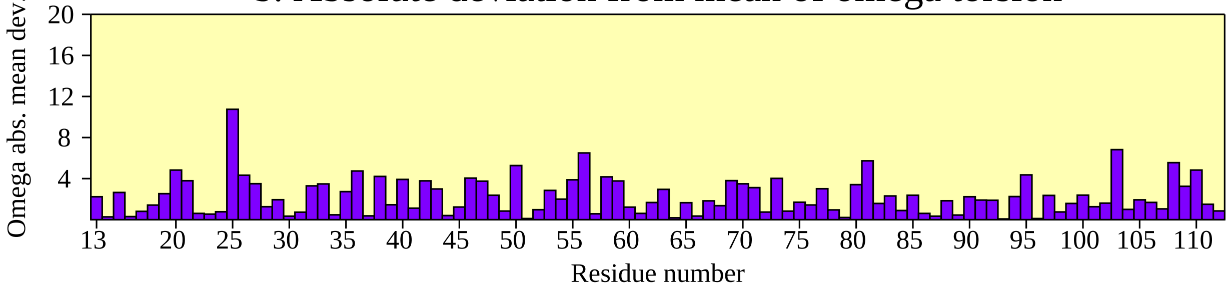
Residue properties

1ntm

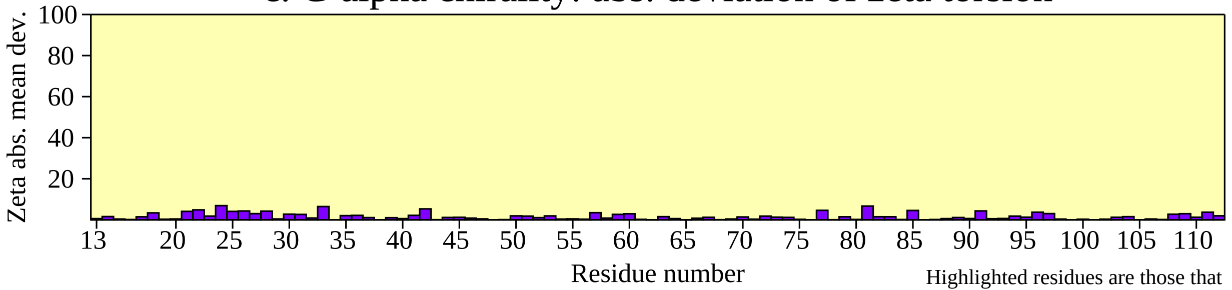
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

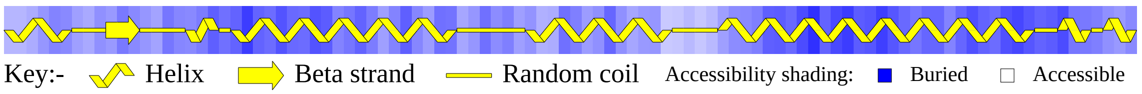


c. C-alpha chirality: abs. deviation of zeta torsion



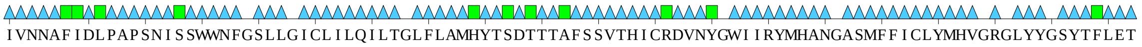
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

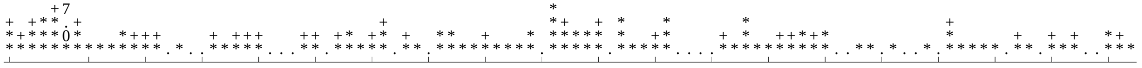


e. Sequence & Ramachandran regions

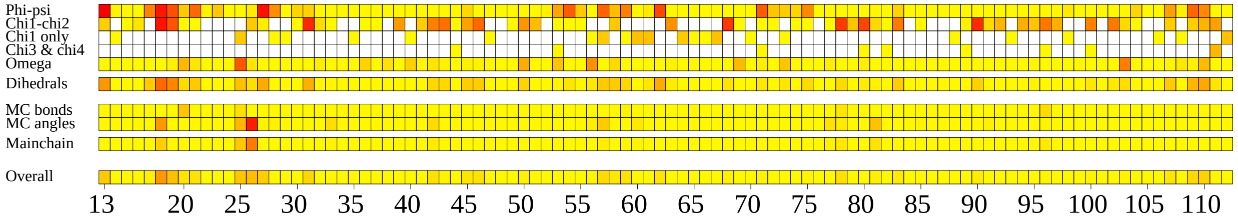
▲ Most favoured 🟩 Allowed ▯ Generous 🟥 Disallowed



f. Max. deviation (see listing)



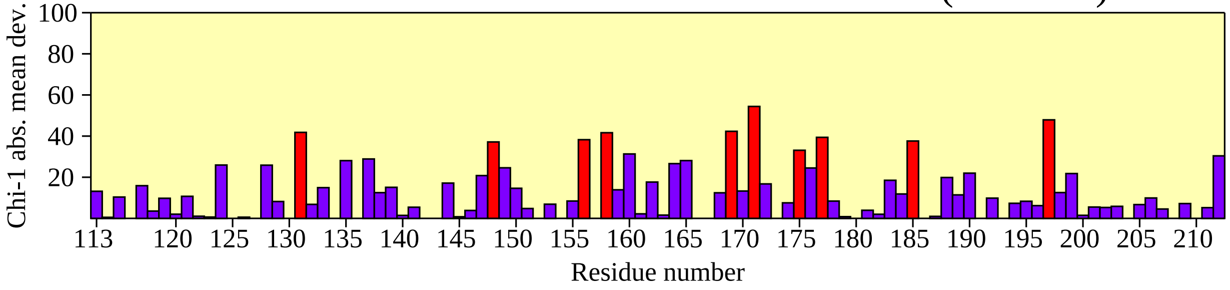
g. G-factors



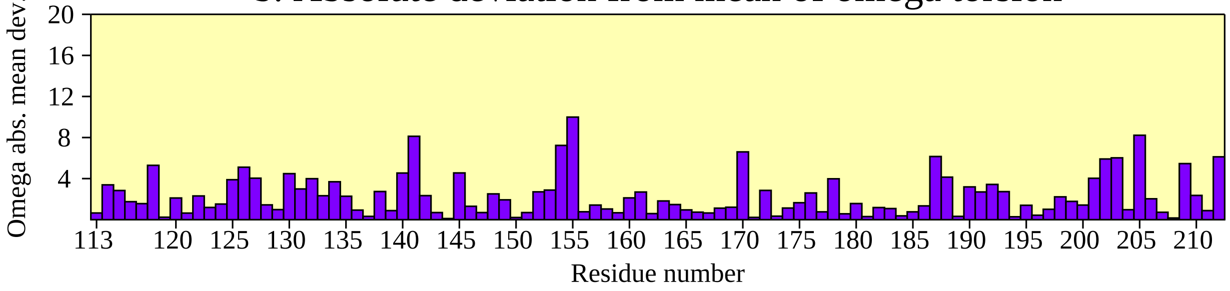
Residue properties

1ntm

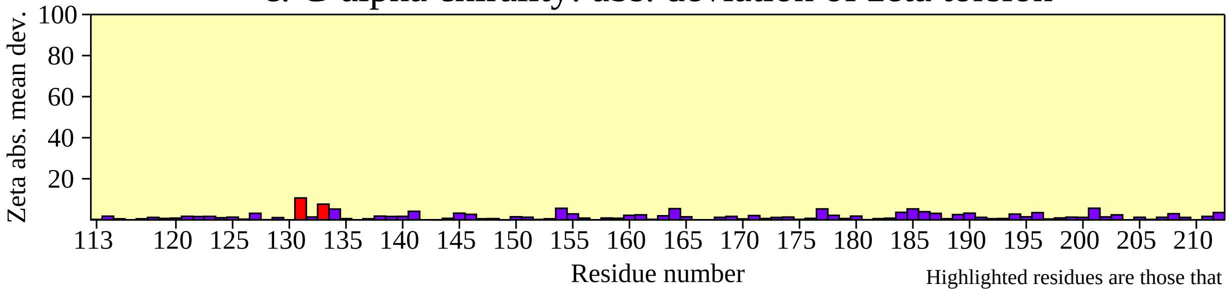
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

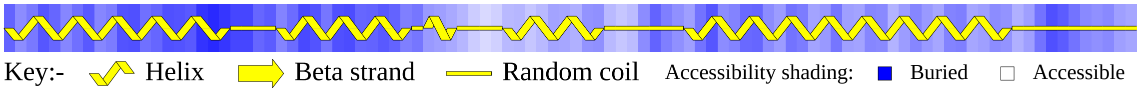


c. C-alpha chirality: abs. deviation of zeta torsion

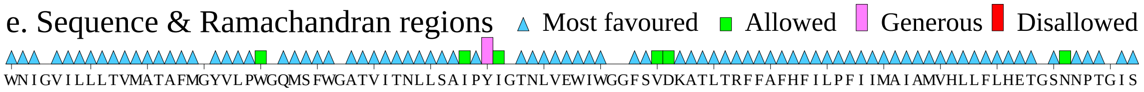


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

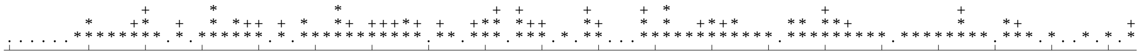
d. Secondary structure & estimated accessibility



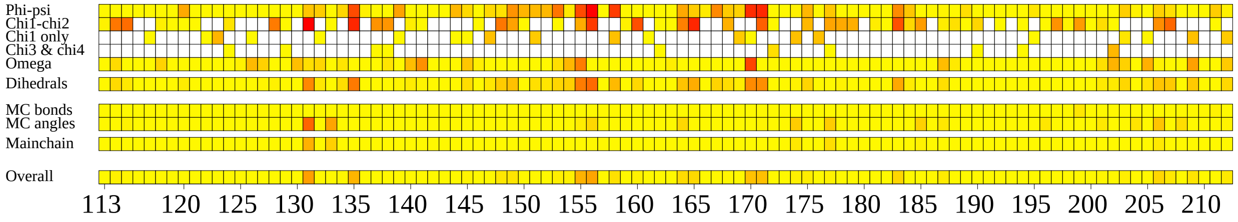
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



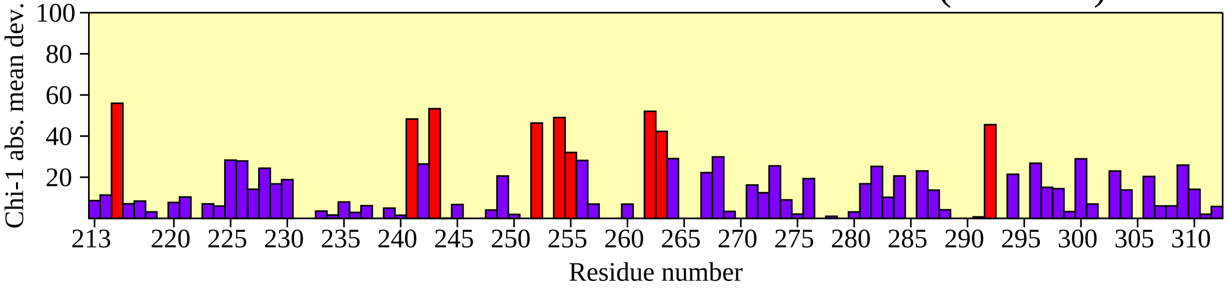
g. G-factors



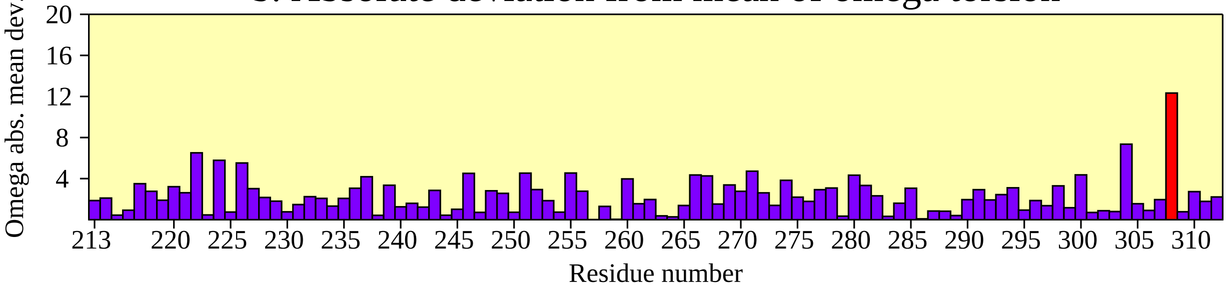
Residue properties

1ntm

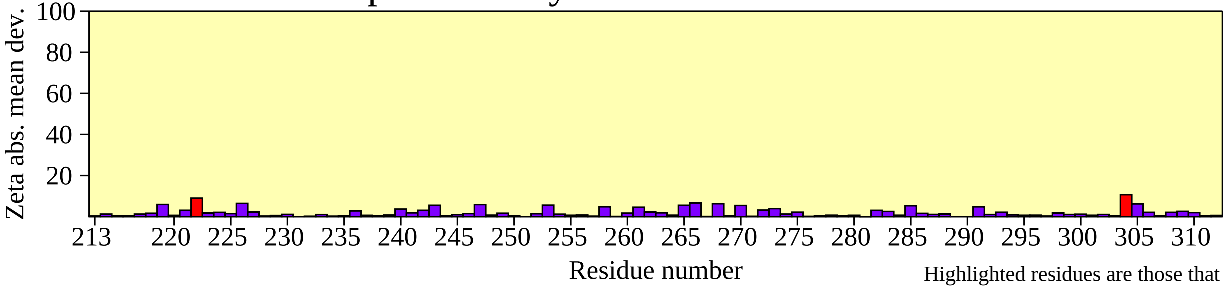
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

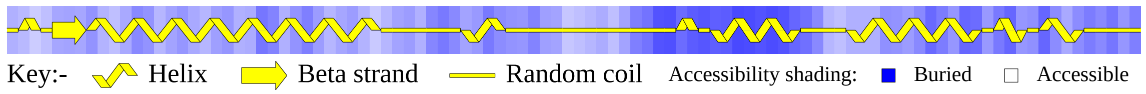


c. C-alpha chirality: abs. deviation of zeta torsion

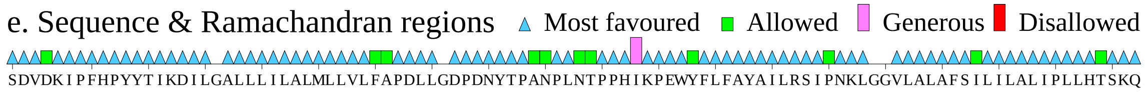


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

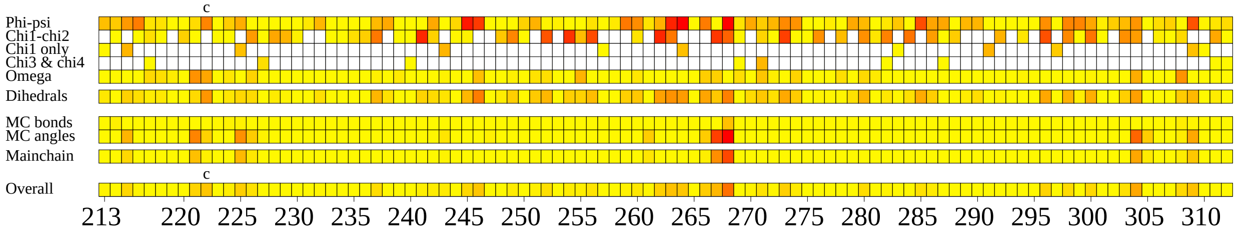


e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

g. G-factors

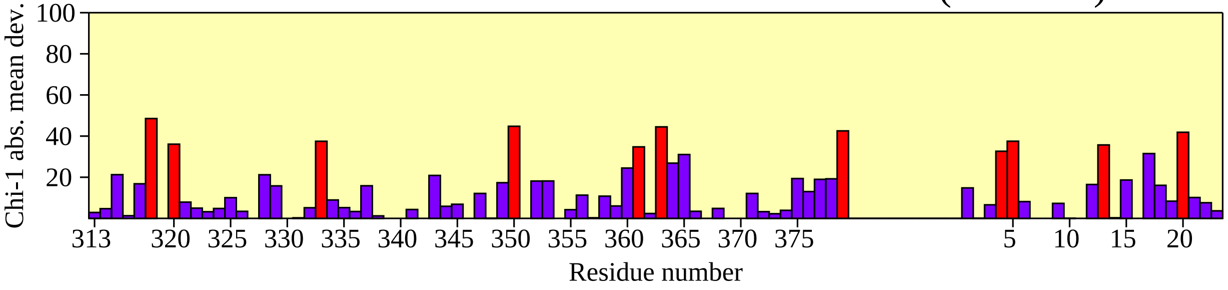


c = cis-peptide

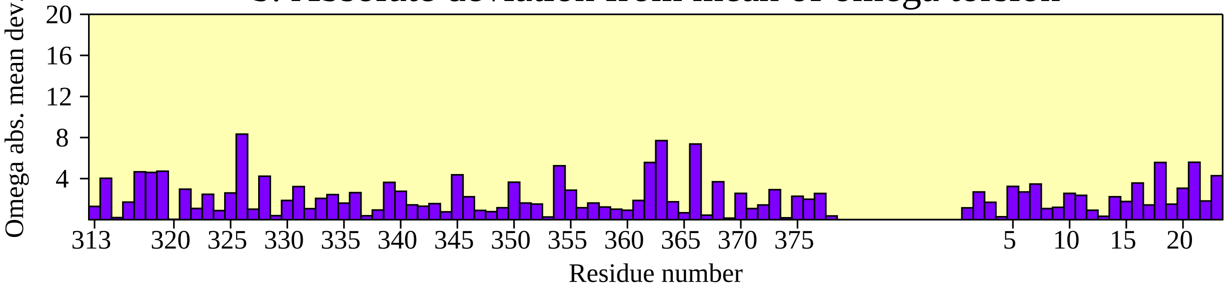
Residue properties

1ntm

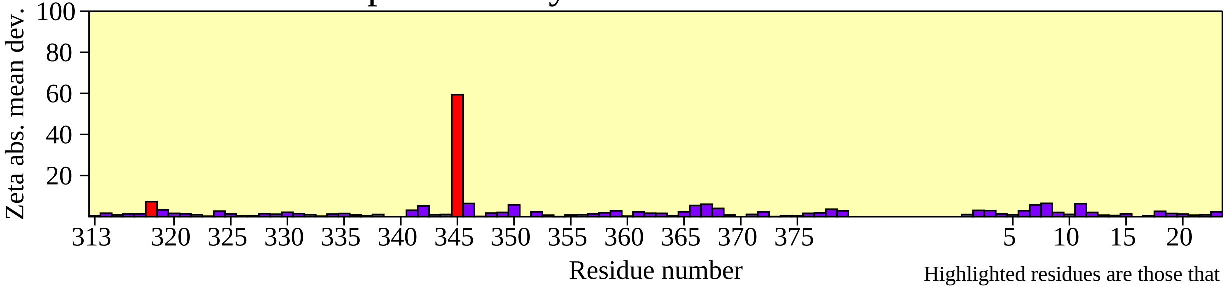
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

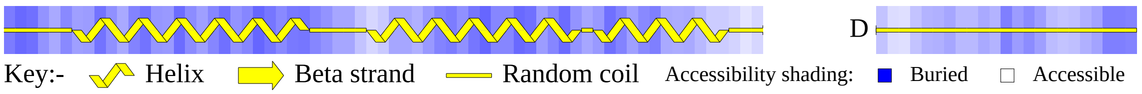


c. C-alpha chirality: abs. deviation of zeta torsion

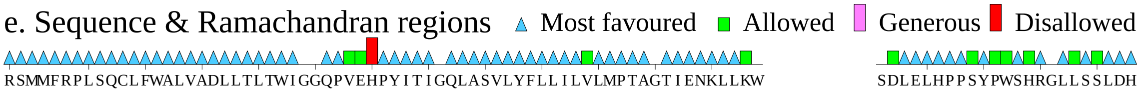


Highlighted residues are those that
deviate by more than 2.0 st. devs. from ideal

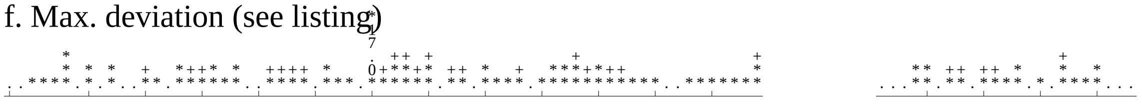
d. Secondary structure & estimated accessibility



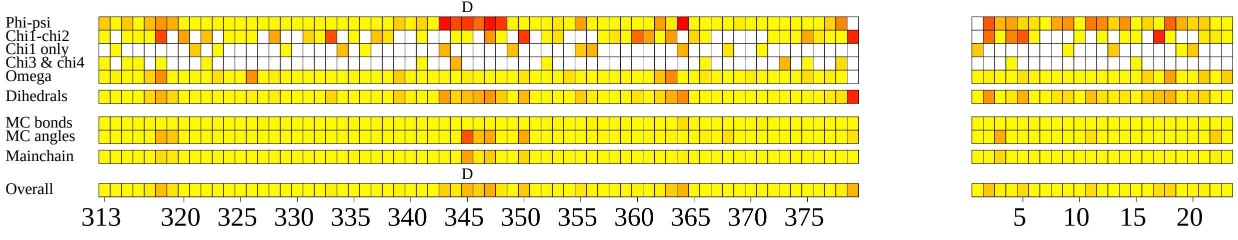
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

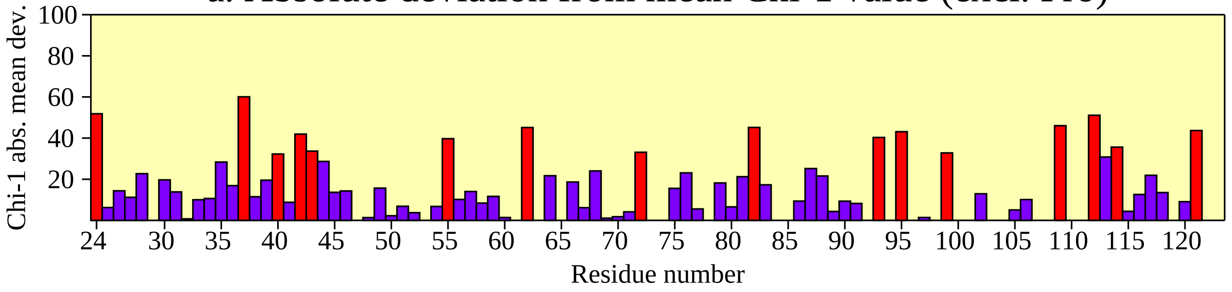


D = D-amino acid

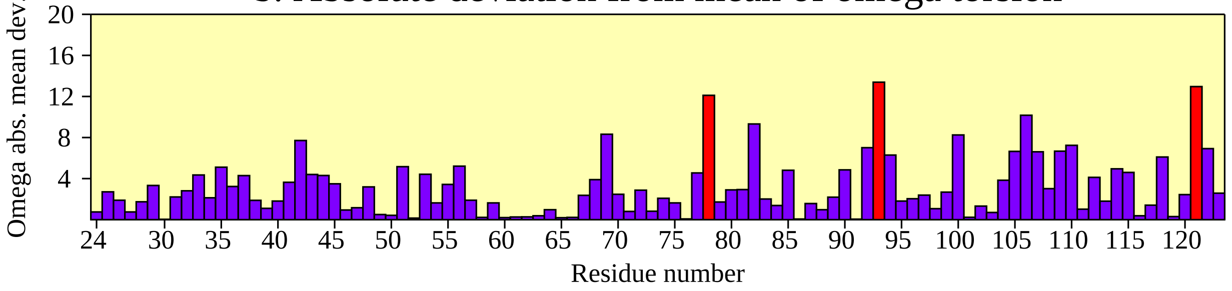
Residue properties

1ntm

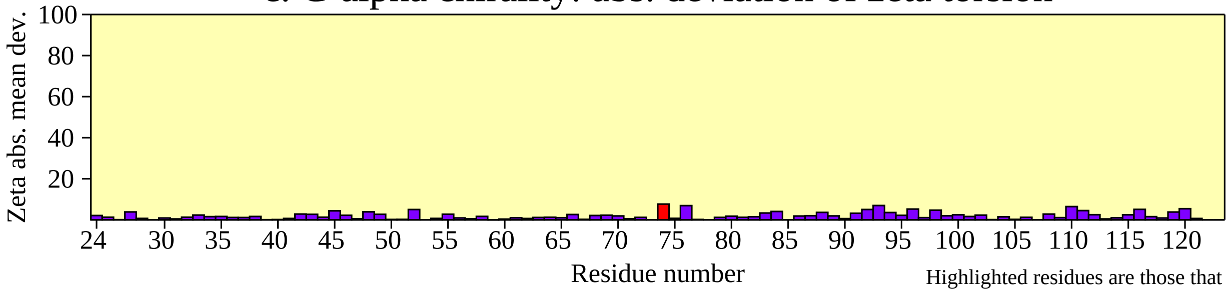
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

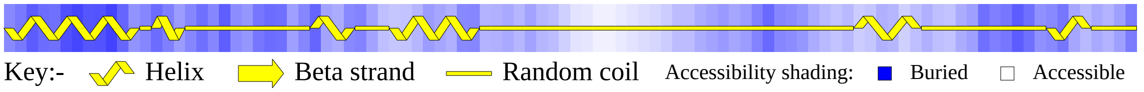


c. C-alpha chirality: abs. deviation of zeta torsion

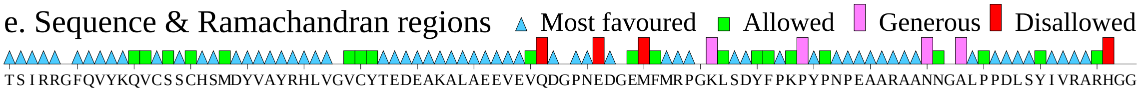


Highlighted residues are those that
deviate by more than 2.0 st. devs. from ideal

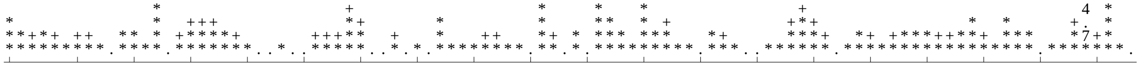
d. Secondary structure & estimated accessibility



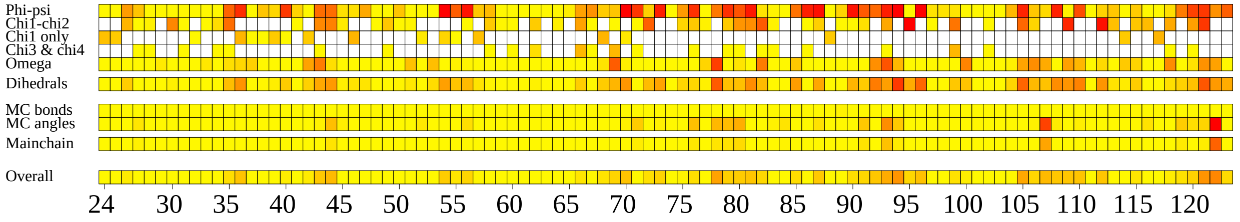
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



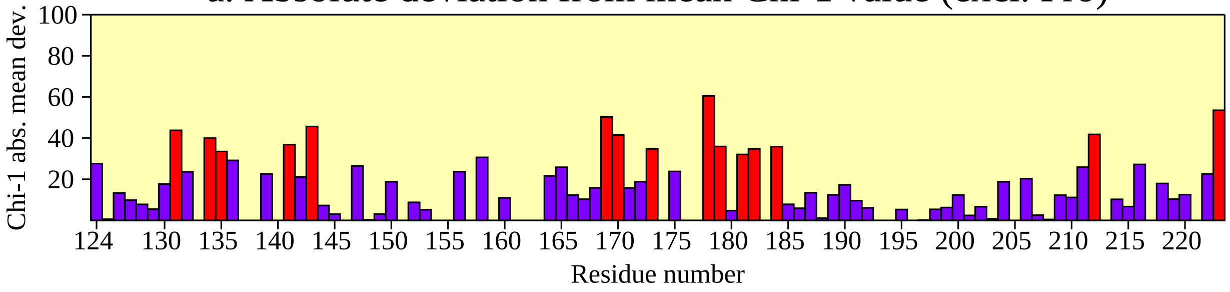
g. G-factors



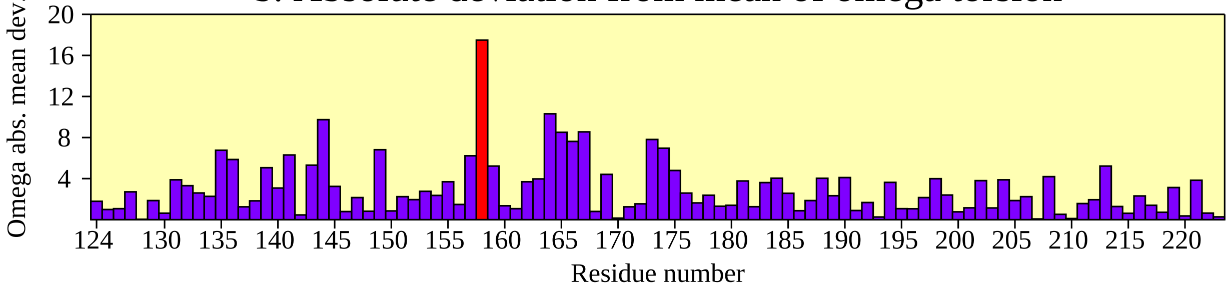
Residue properties

1ntm

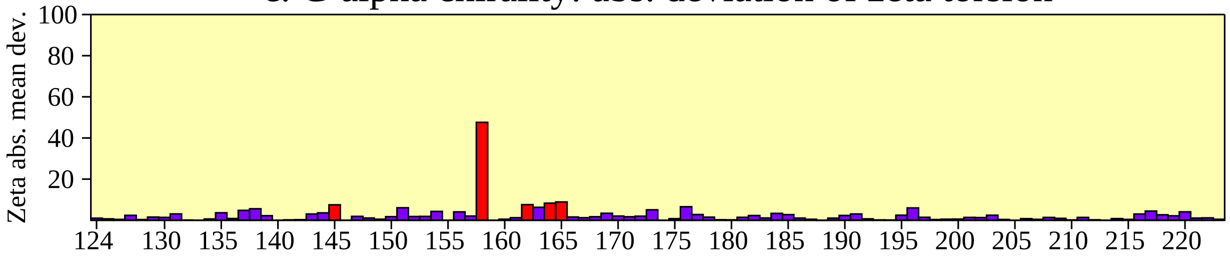
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

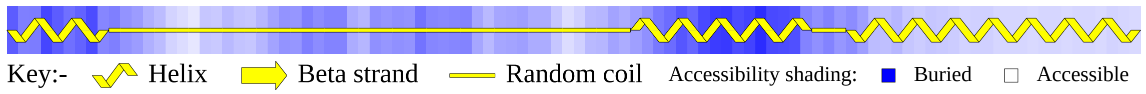


c. C-alpha chirality: abs. deviation of zeta torsion

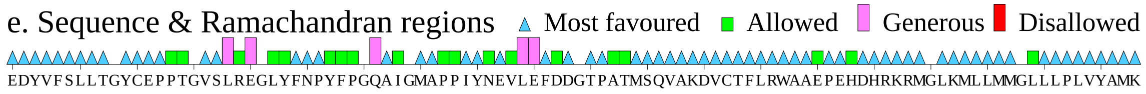


Highlighted residues are those that
deviate by more than 2.0 st. devs. from ideal

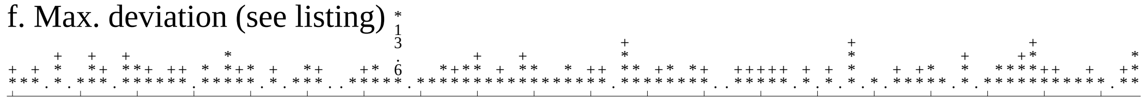
d. Secondary structure & estimated accessibility



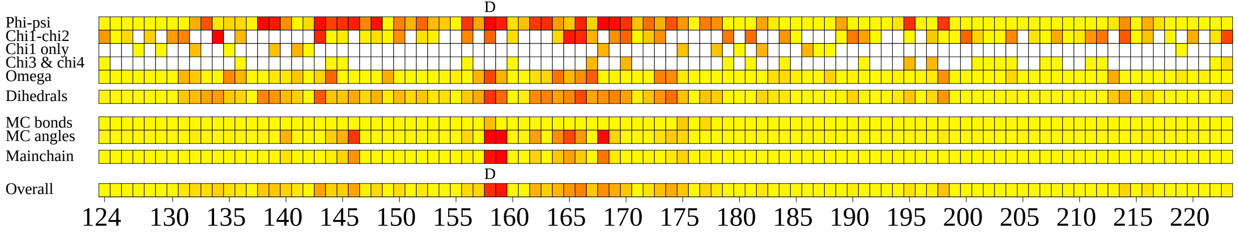
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

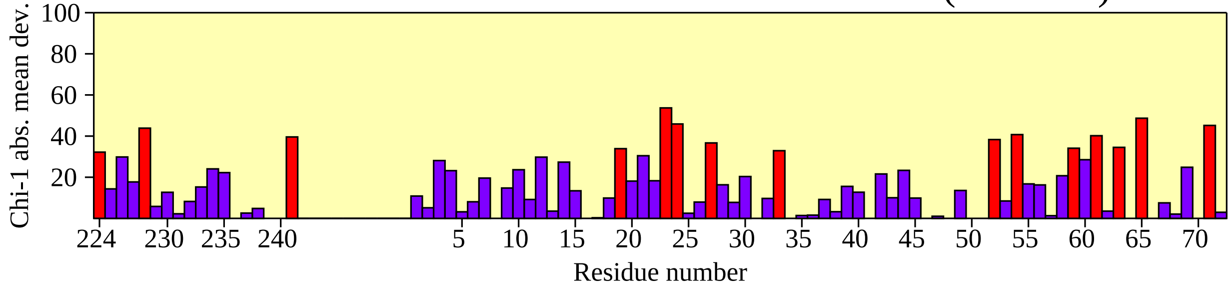


D = D-amino acid

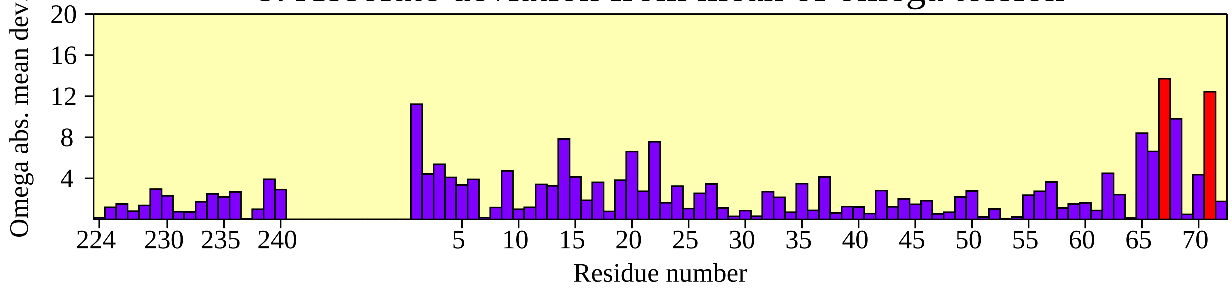
Residue properties

1ntm

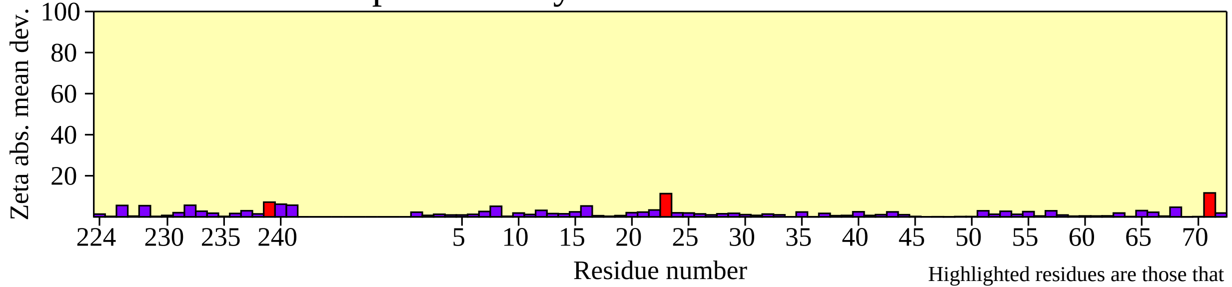
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

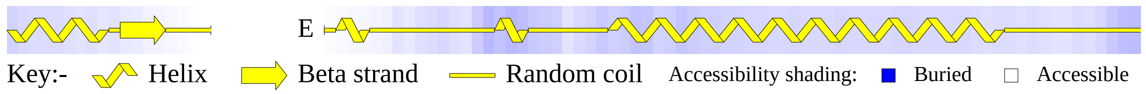


c. C-alpha chirality: abs. deviation of zeta torsion

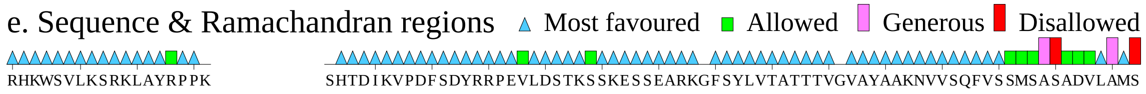


Highlighted residues are those that
deviate by more than 2.0 st. devs. from ideal

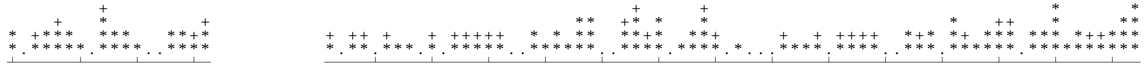
d. Secondary structure & estimated accessibility



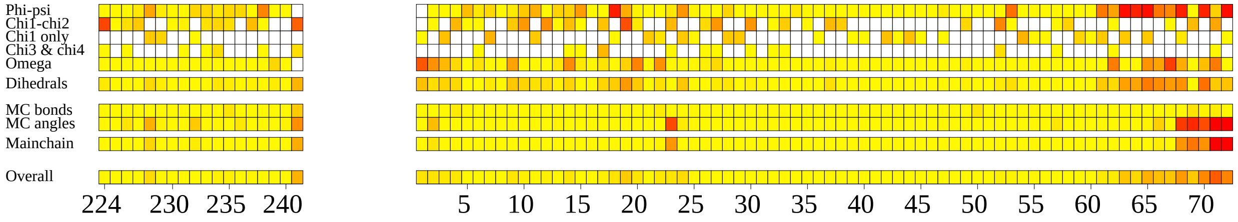
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



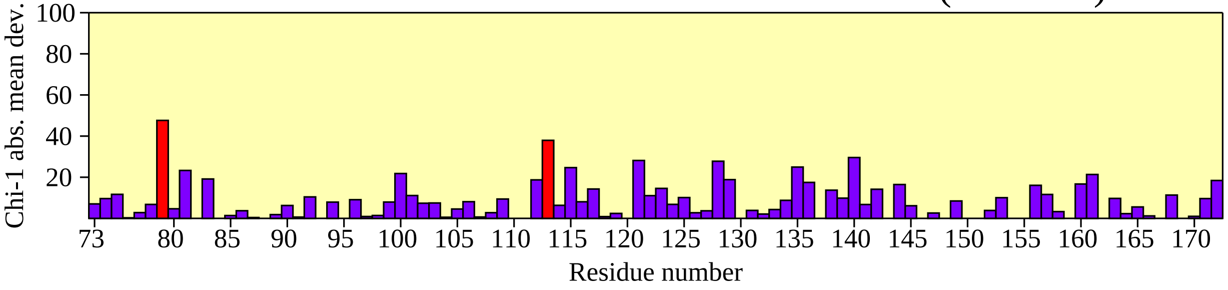
g. G-factors



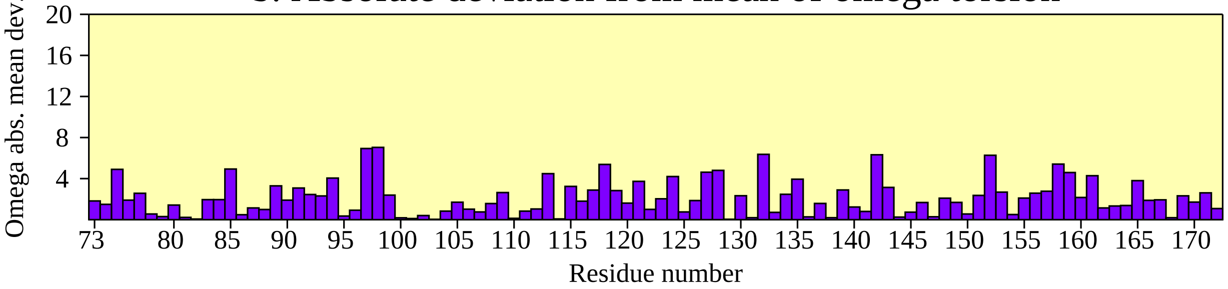
Residue properties

1ntm

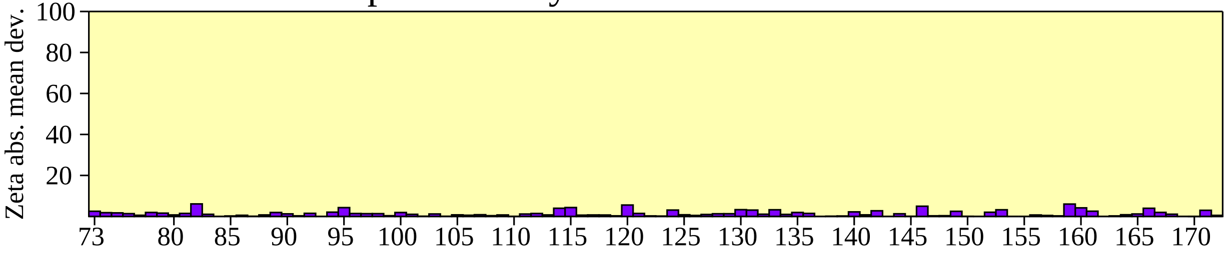
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

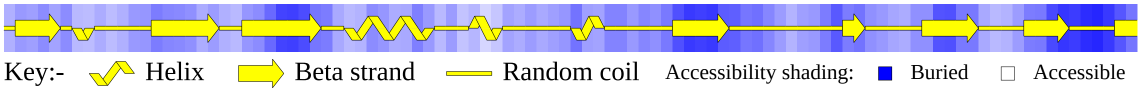


c. C-alpha chirality: abs. deviation of zeta torsion

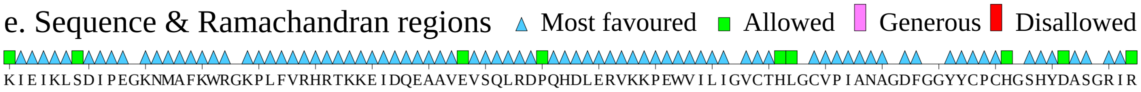


Highlighted residues are those that
deviate by more than 2.0 st. devs. from ideal

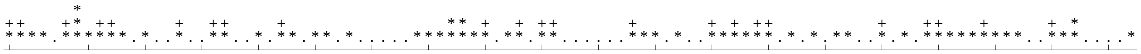
d. Secondary structure & estimated accessibility



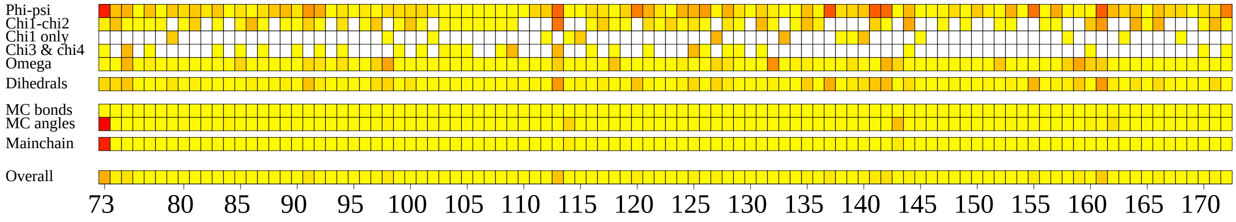
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



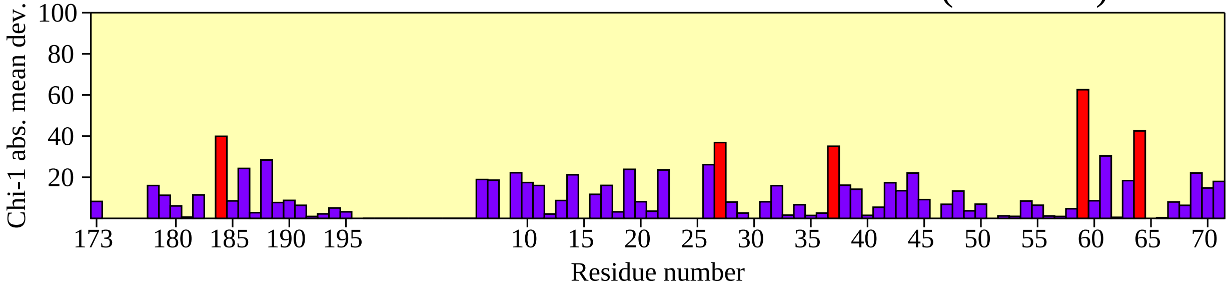
g. G-factors



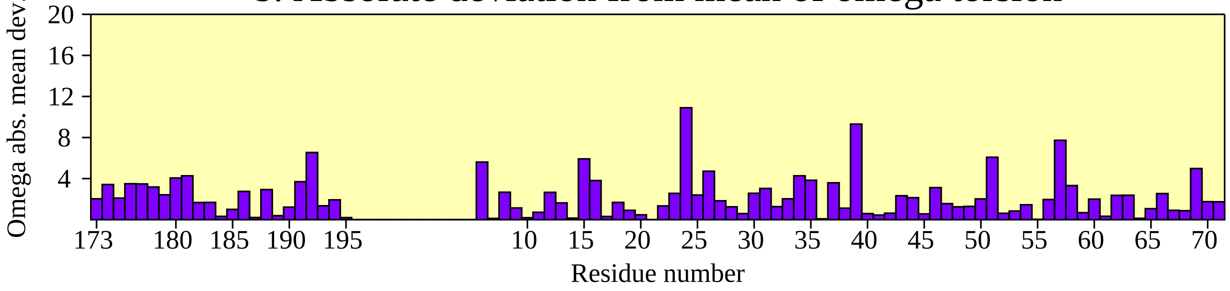
Residue properties

1ntm

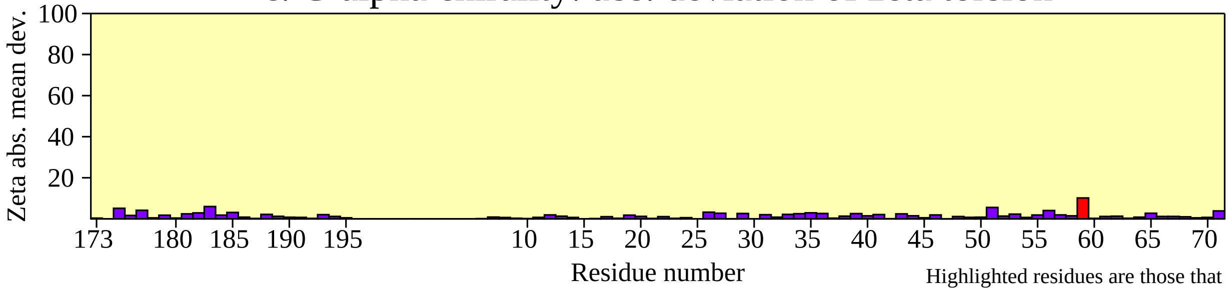
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

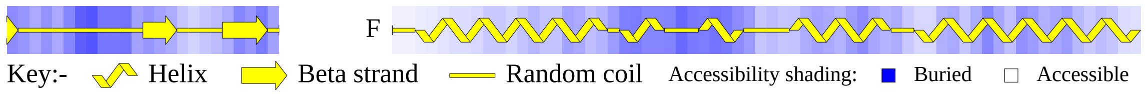


c. C-alpha chirality: abs. deviation of zeta torsion



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

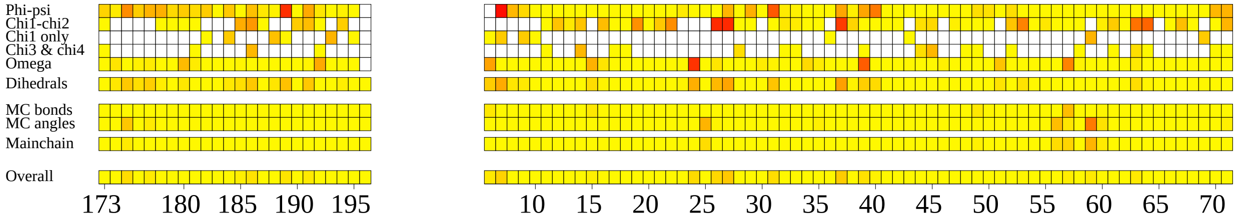
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions

f. Max. deviation (see listing)

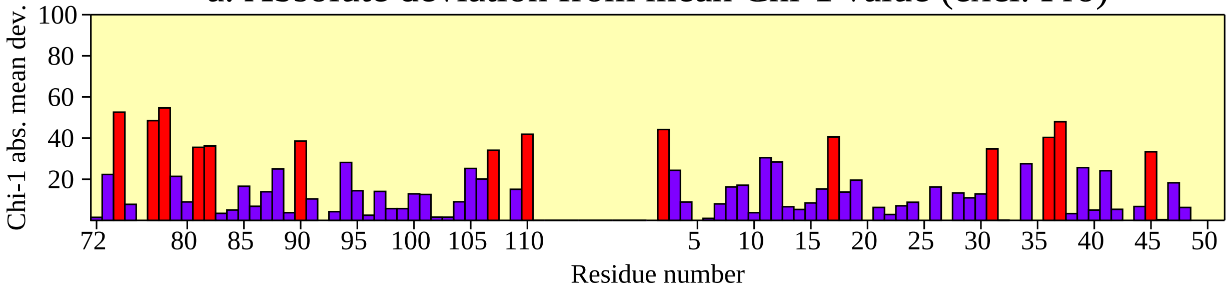
g. G-factors



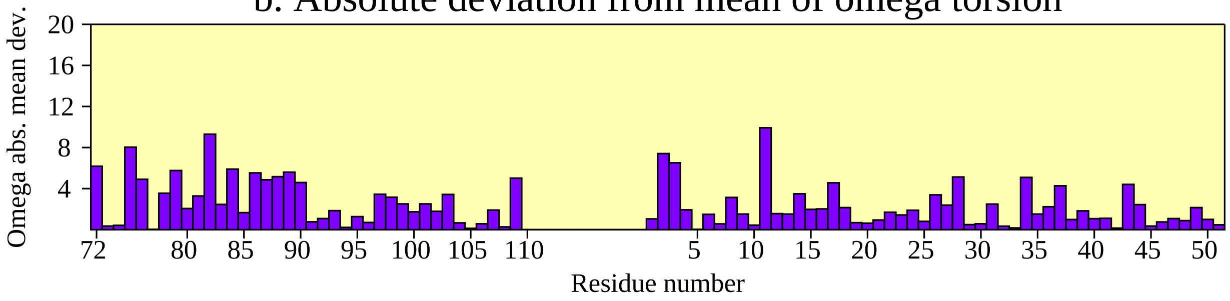
Residue properties

1ntm

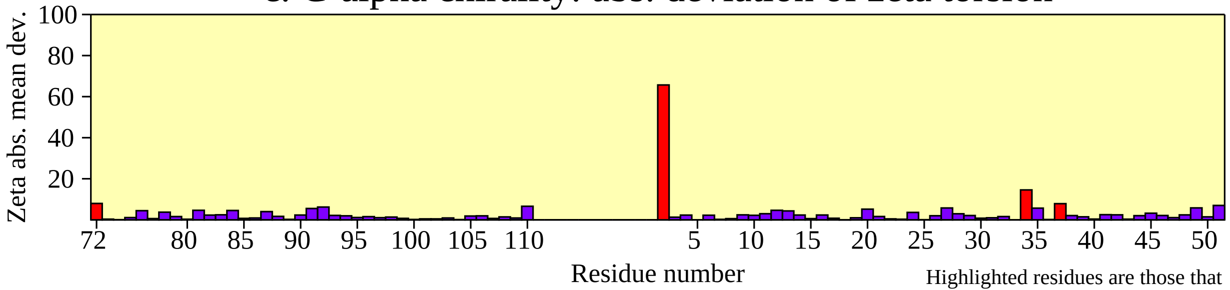
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

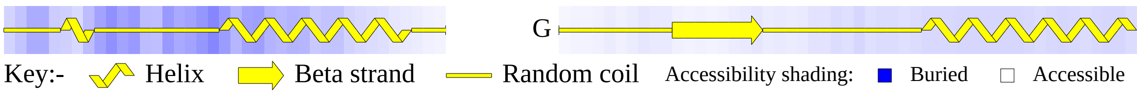


c. C-alpha chirality: abs. deviation of zeta torsion

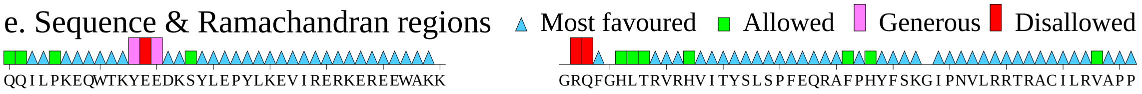


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

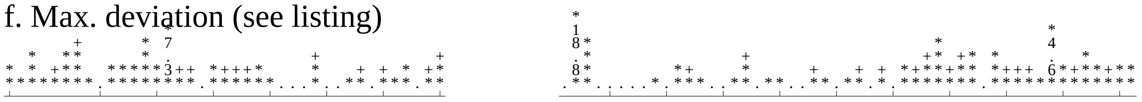
d. Secondary structure & estimated accessibility



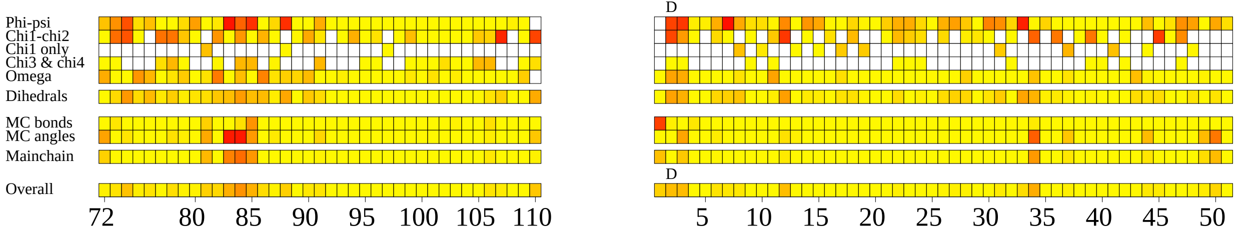
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

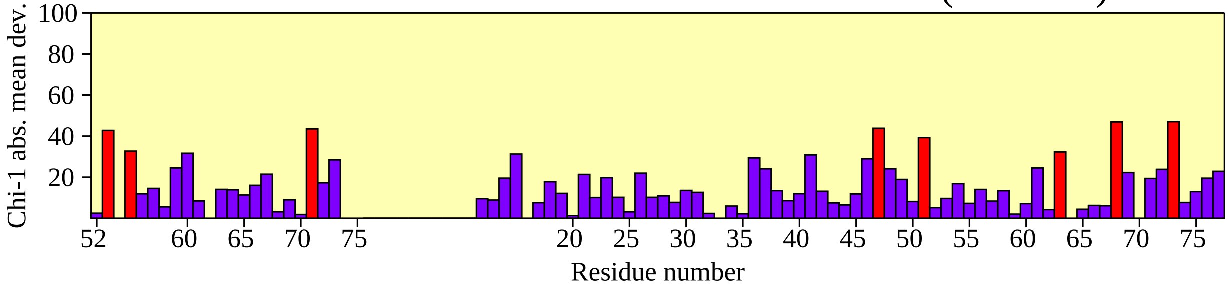


D = D-amino acid

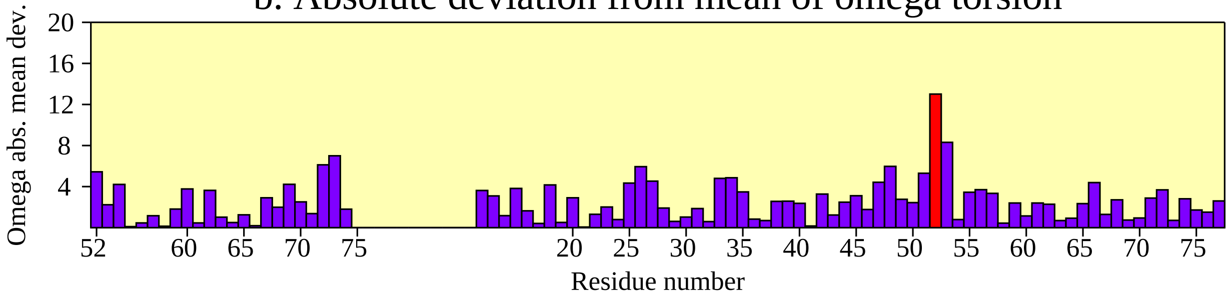
Residue properties

1ntm

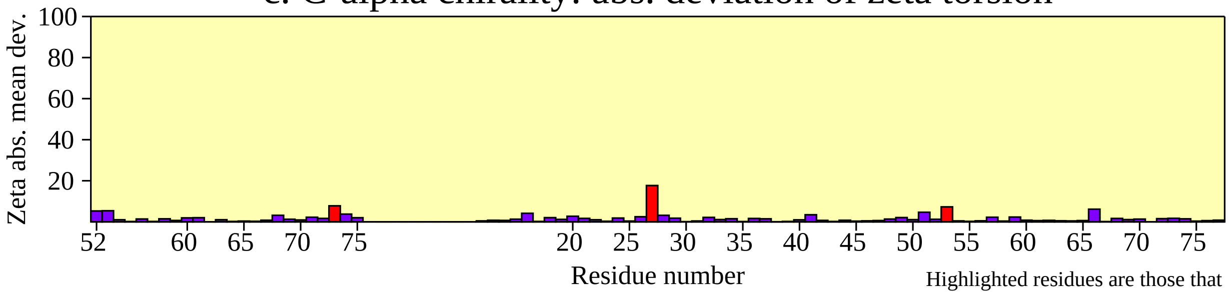
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

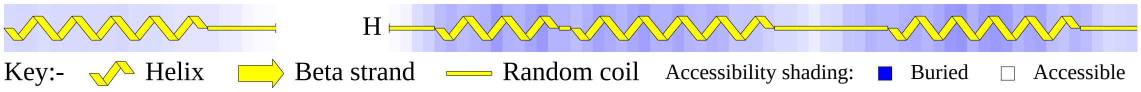


c. C-alpha chirality: abs. deviation of zeta torsion

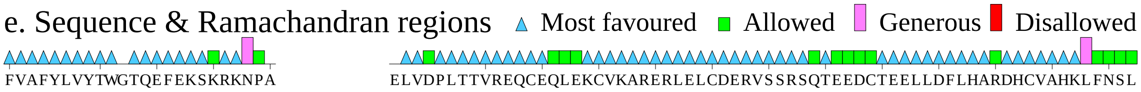


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

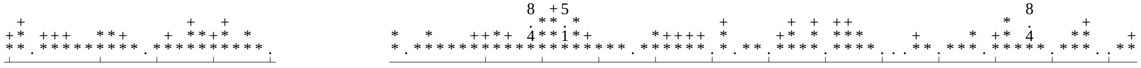
d. Secondary structure & estimated accessibility



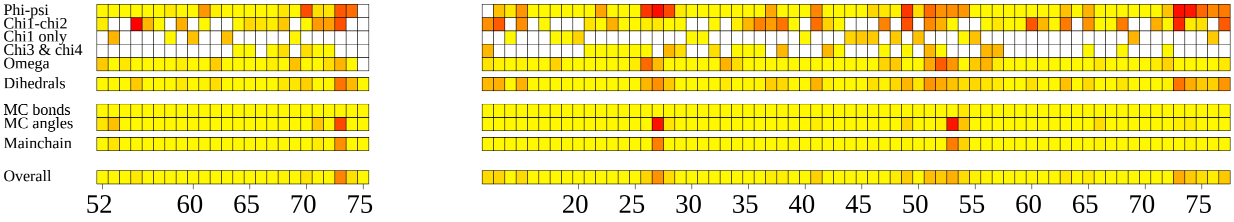
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



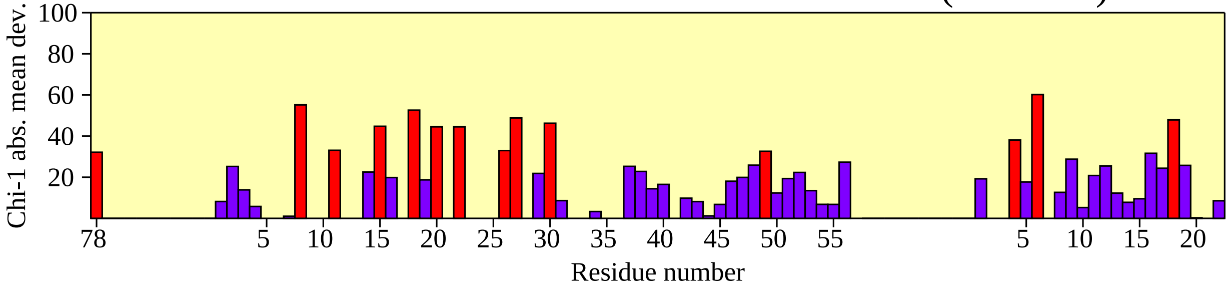
g. G-factors



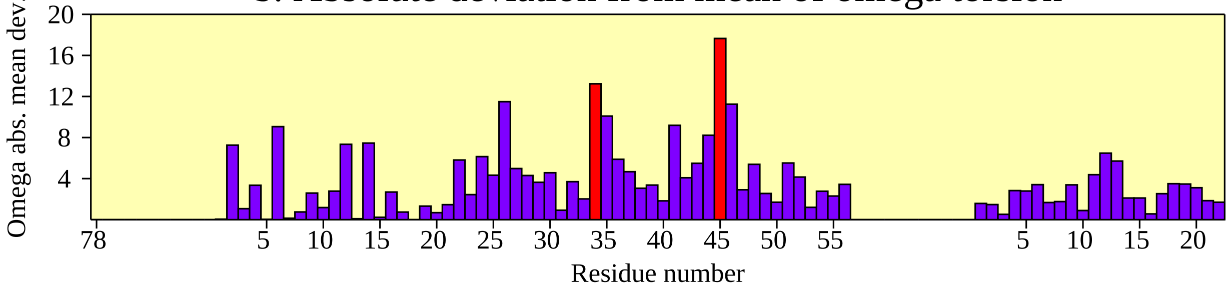
Residue properties

1ntm

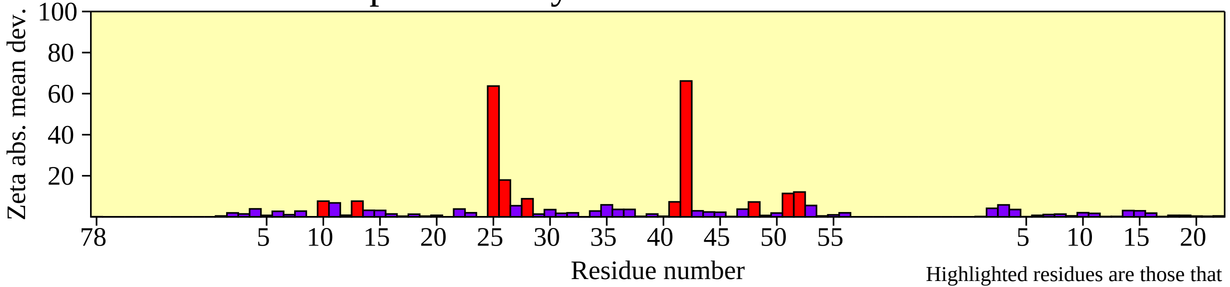
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

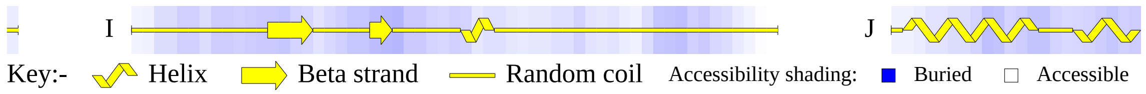


c. C-alpha chirality: abs. deviation of zeta torsion

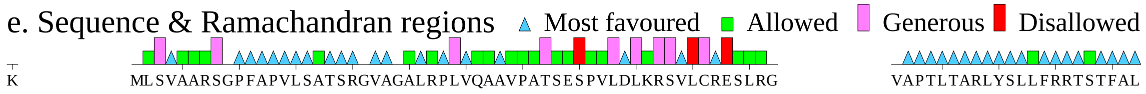


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

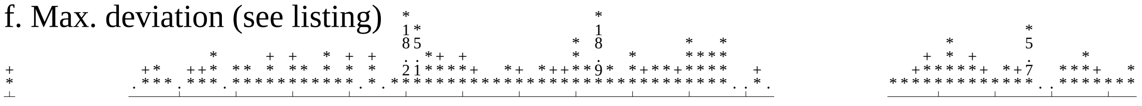
d. Secondary structure & estimated accessibility



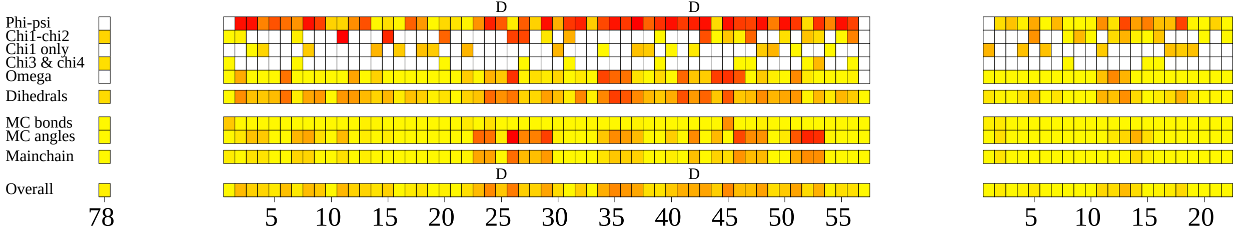
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

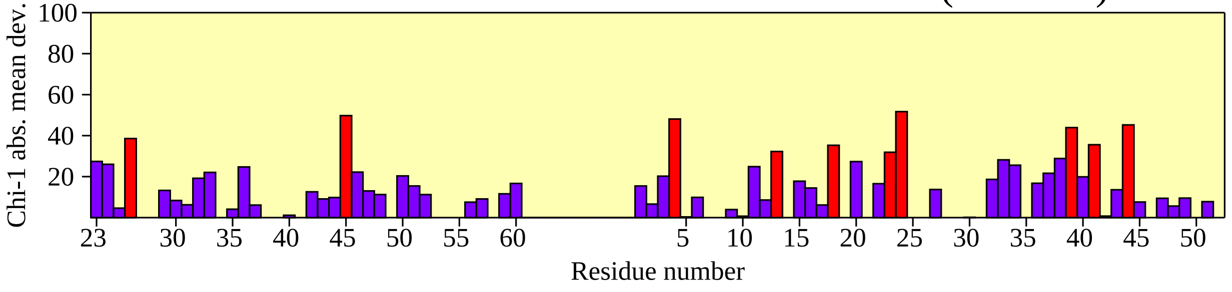


D = D-amino acid

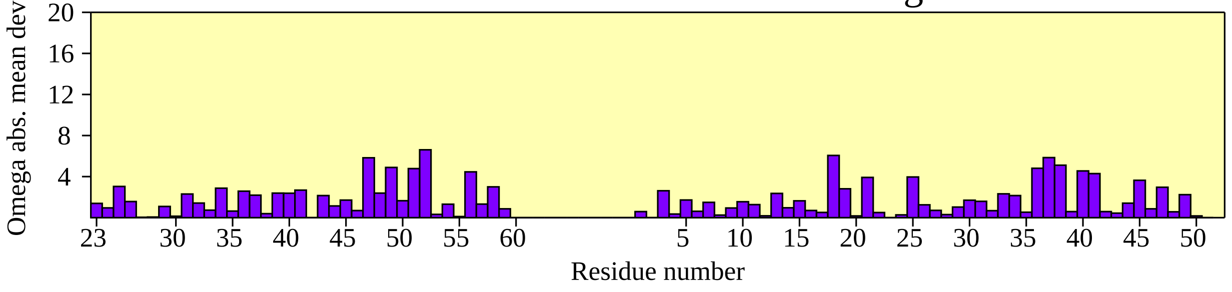
Residue properties

1ntm

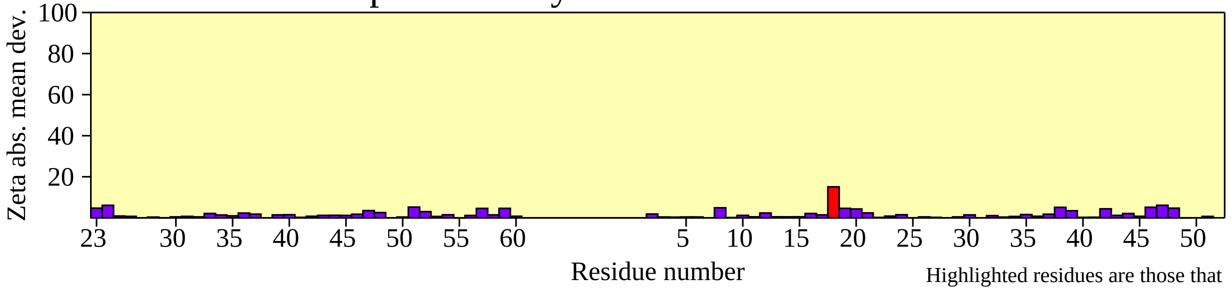
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

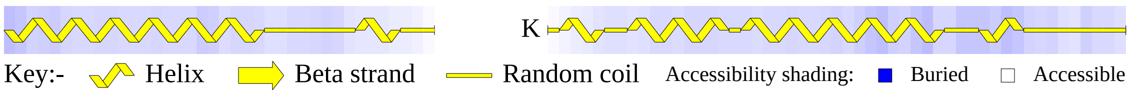


c. C-alpha chirality: abs. deviation of zeta torsion

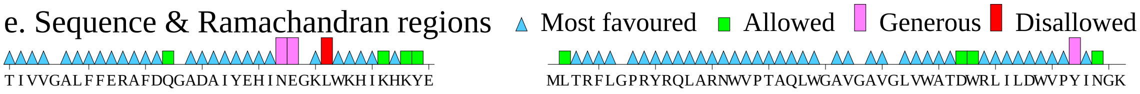


Highlighted residues are those that
deviate by more than 2.0 st. devs. from ideal

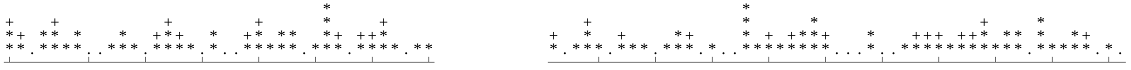
d. Secondary structure & estimated accessibility



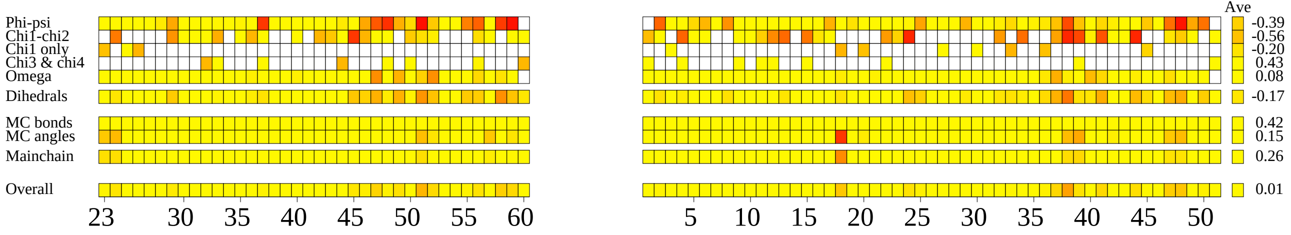
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



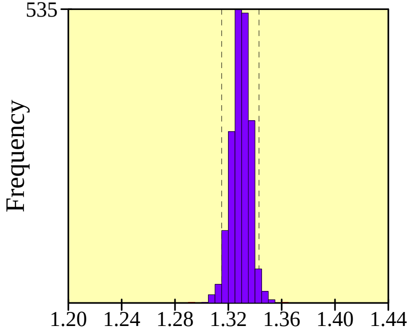
g. G-factors



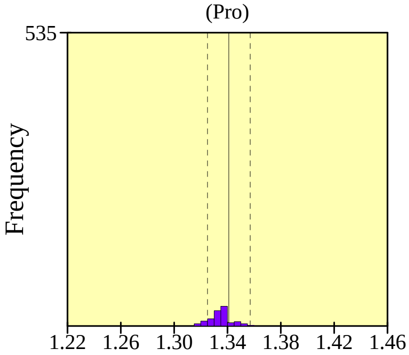
Main-chain bond lengths

1ntm

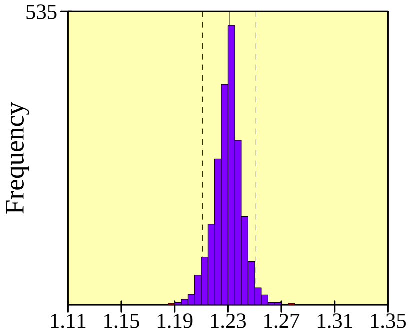
C-N
(except Pro)



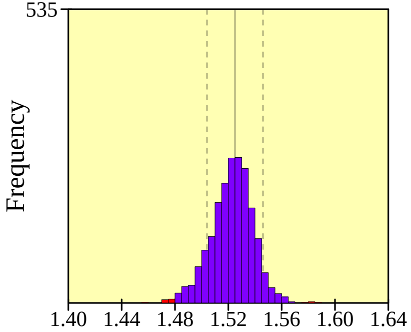
C-N
(Pro)



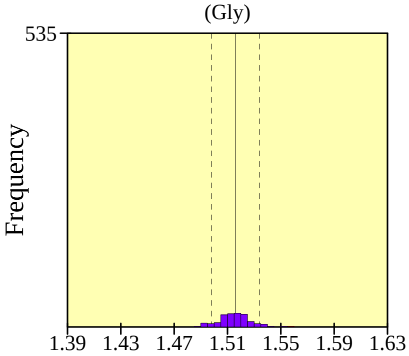
C-O



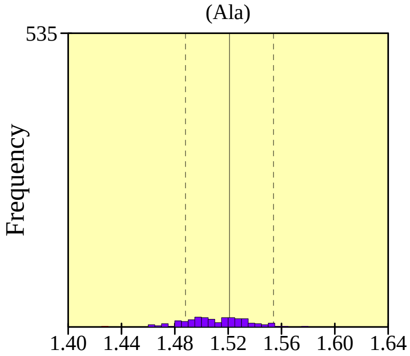
CA-C
(except Gly)



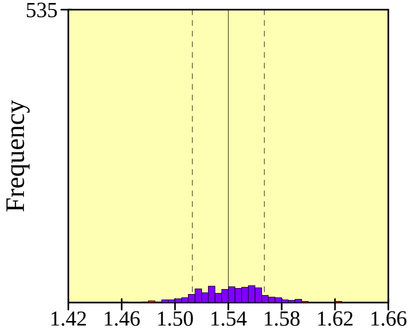
CA-C
(Gly)



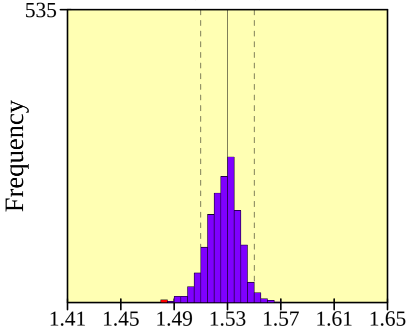
CA-CB
(Ala)



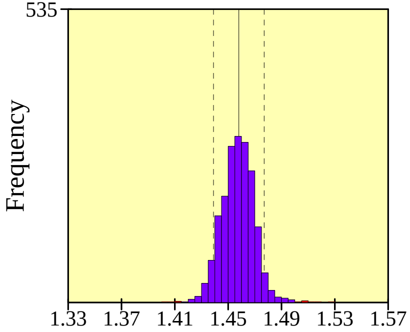
CA-CB
(Ile,Thr,Val)



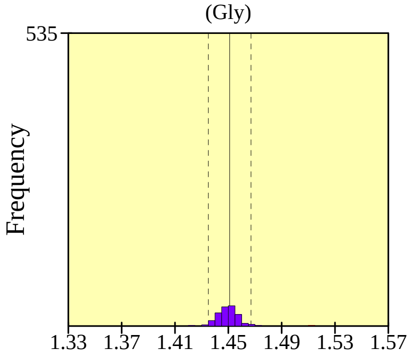
CA-CB
(the rest)



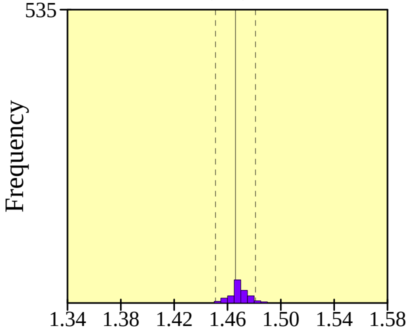
N-CA
(except Gly,Pro)



N-CA
(Gly)



N-CA
(Pro)

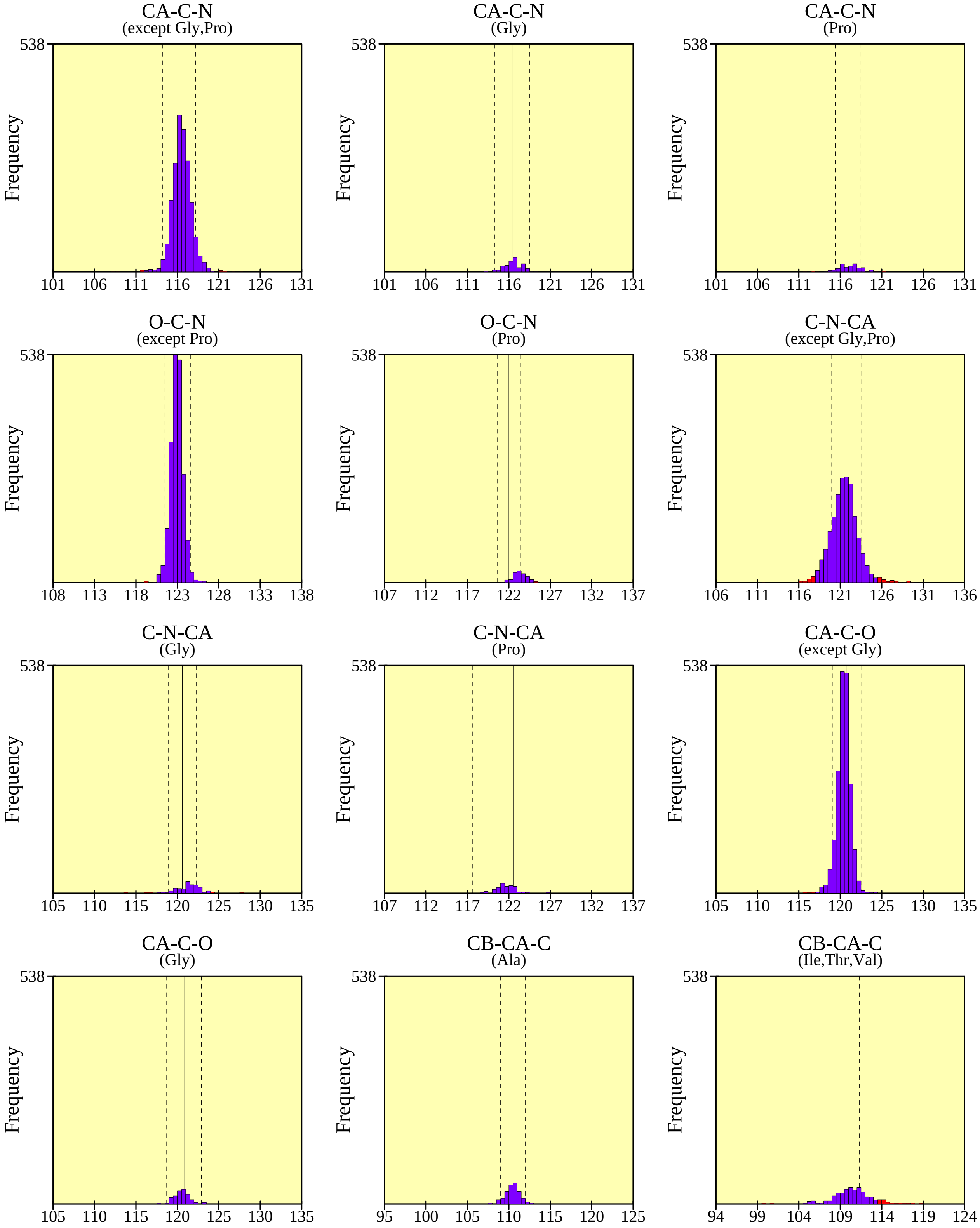


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

1ntm



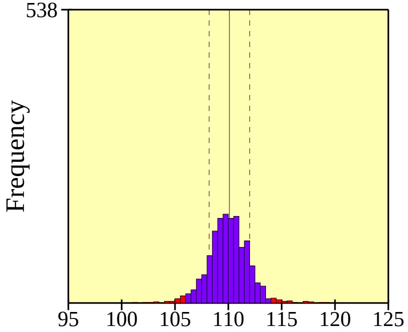
Black bars > 2.0 st. devs. from mean.

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

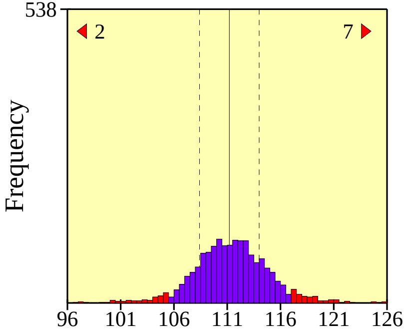
Main-chain bond angles

1ntm

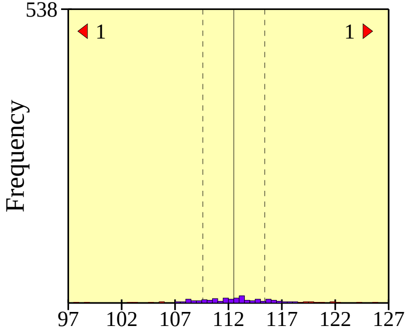
CB-CA-C
(the rest)



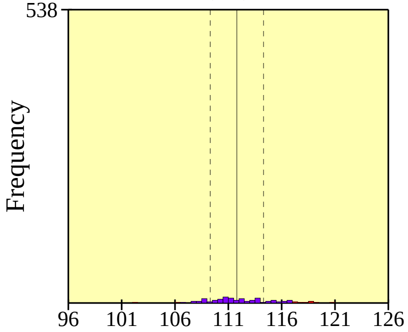
N-CA-C
(except Gly,Pro)



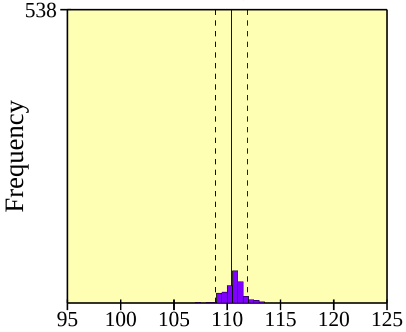
N-CA-C
(Gly)



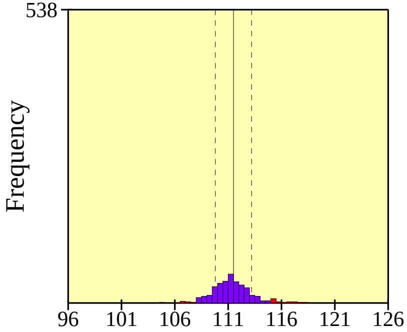
N-CA-C
(Pro)



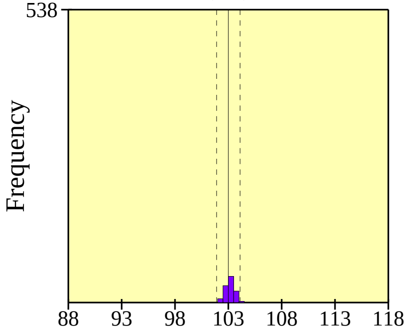
N-CA-CB
(Ala)



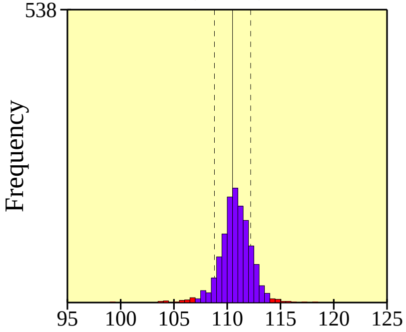
N-CA-CB
(Ile,Thr,Val)



N-CA-CB
(Pro)



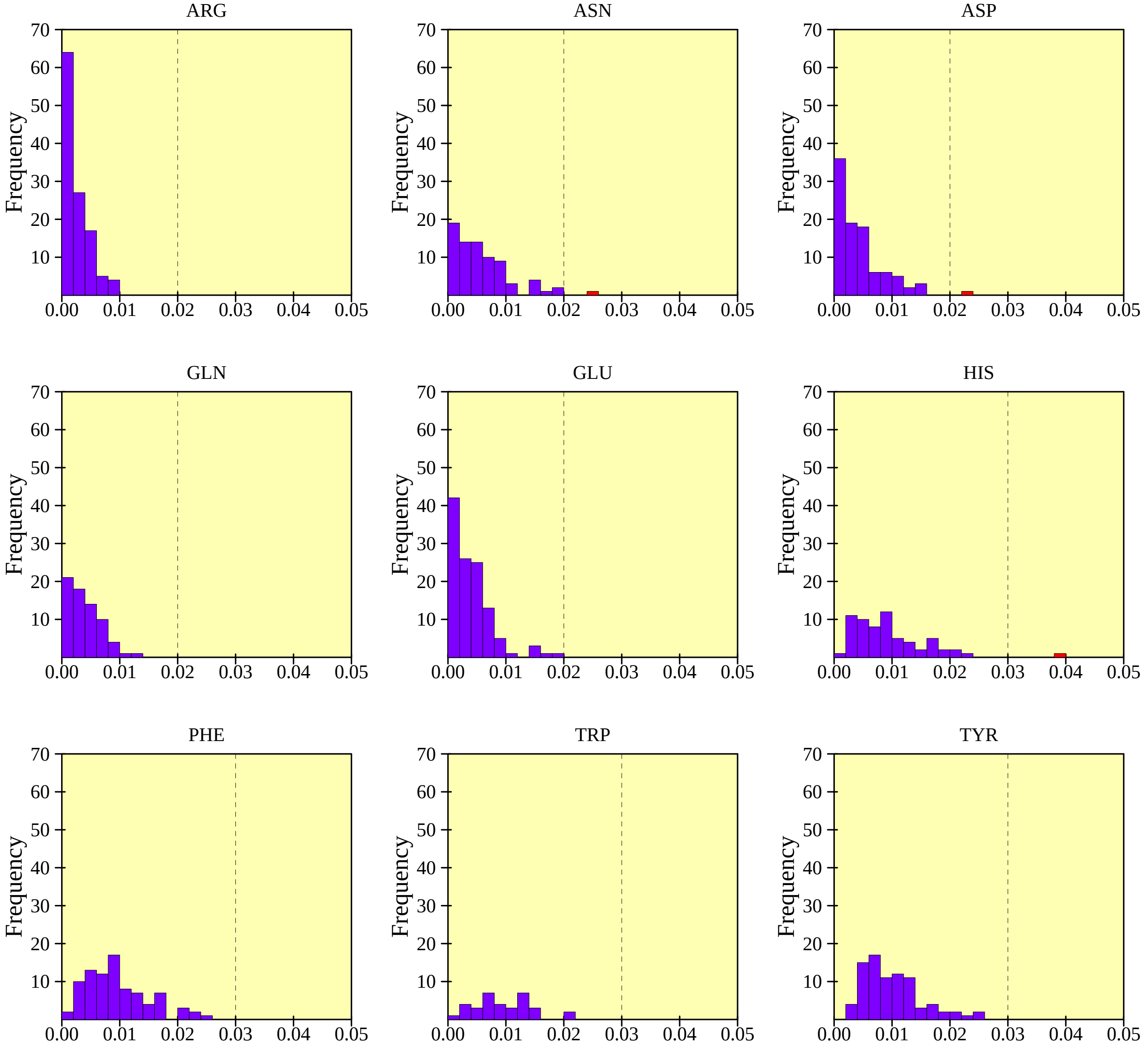
N-CA-CB
(the rest)



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

1ntm

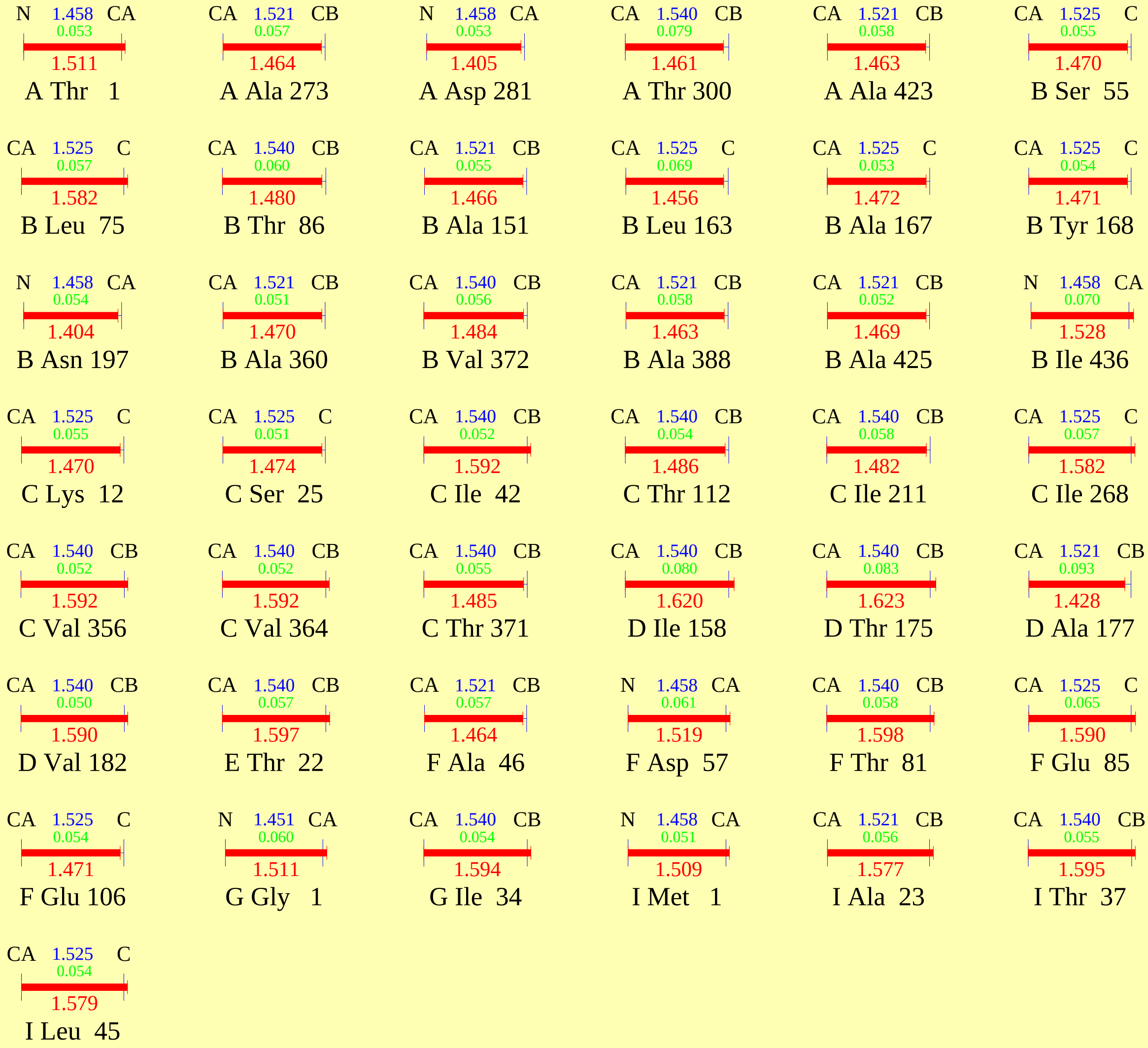


Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

Distorted geometry

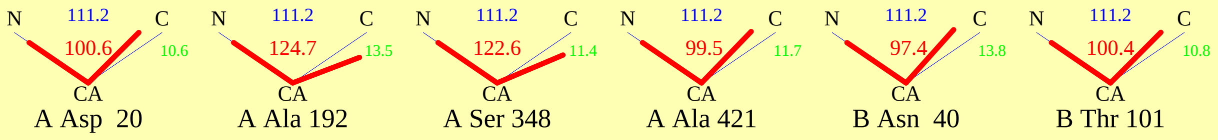
1ntm

Main-chain bond lengths



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

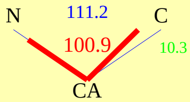
Main-chain bond angles



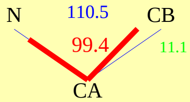
Distorted geometry

1ntm

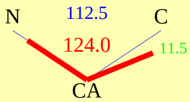
Main-chain bond angles (contd)



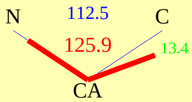
B Met 105



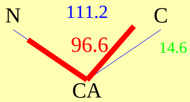
B Asn 170



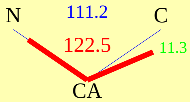
B Gly 231



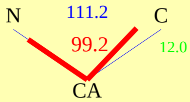
B Gly 234



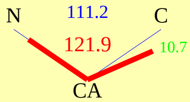
B Ala 235



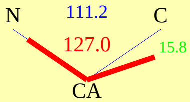
B Phe 435



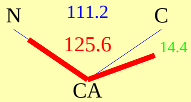
B Ile 436



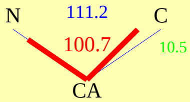
C Asn 26



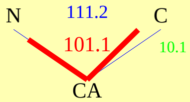
C Ile 268



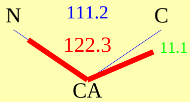
C His 345



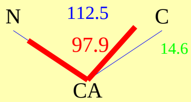
D Leu 3



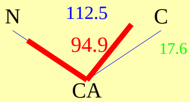
D Asp 22



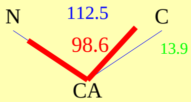
D Lys 93



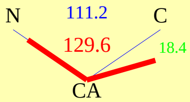
D Gly 107



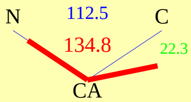
D Gly 122



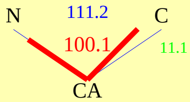
D Gly 146



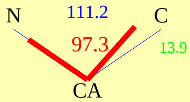
D Ile 158



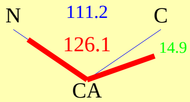
D Gly 159



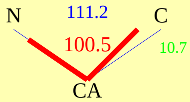
D Asn 166



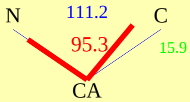
D Val 168



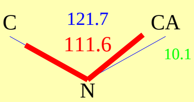
E Lys 23



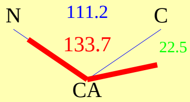
E Val 68



E Leu 69



E Ala 70 - E Met 71



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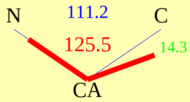
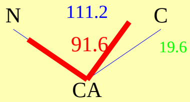
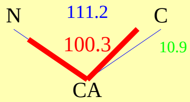


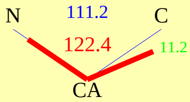
E Ser 72



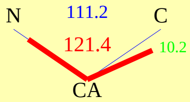
E Lys 73



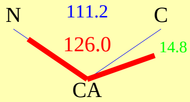
F Tyr 83



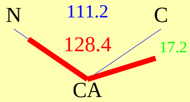
F Glu 85



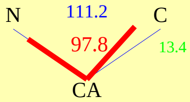
G Gln 3



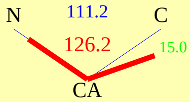
H Leu 27



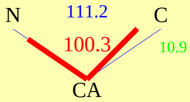
H Asp 53



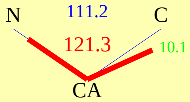
I Ala 23



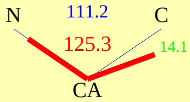
I Leu 26



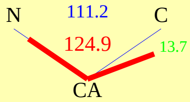
I Leu 29



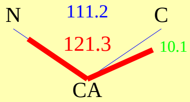
I Ala 36



I Lys 46



I Arg 52



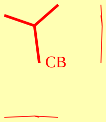
J Phe 14

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

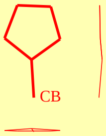
Distorted geometry

1ntm

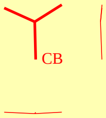
Planar groups



0.022
A Asp 378



0.039
B His 158



0.024
F Asn 27

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