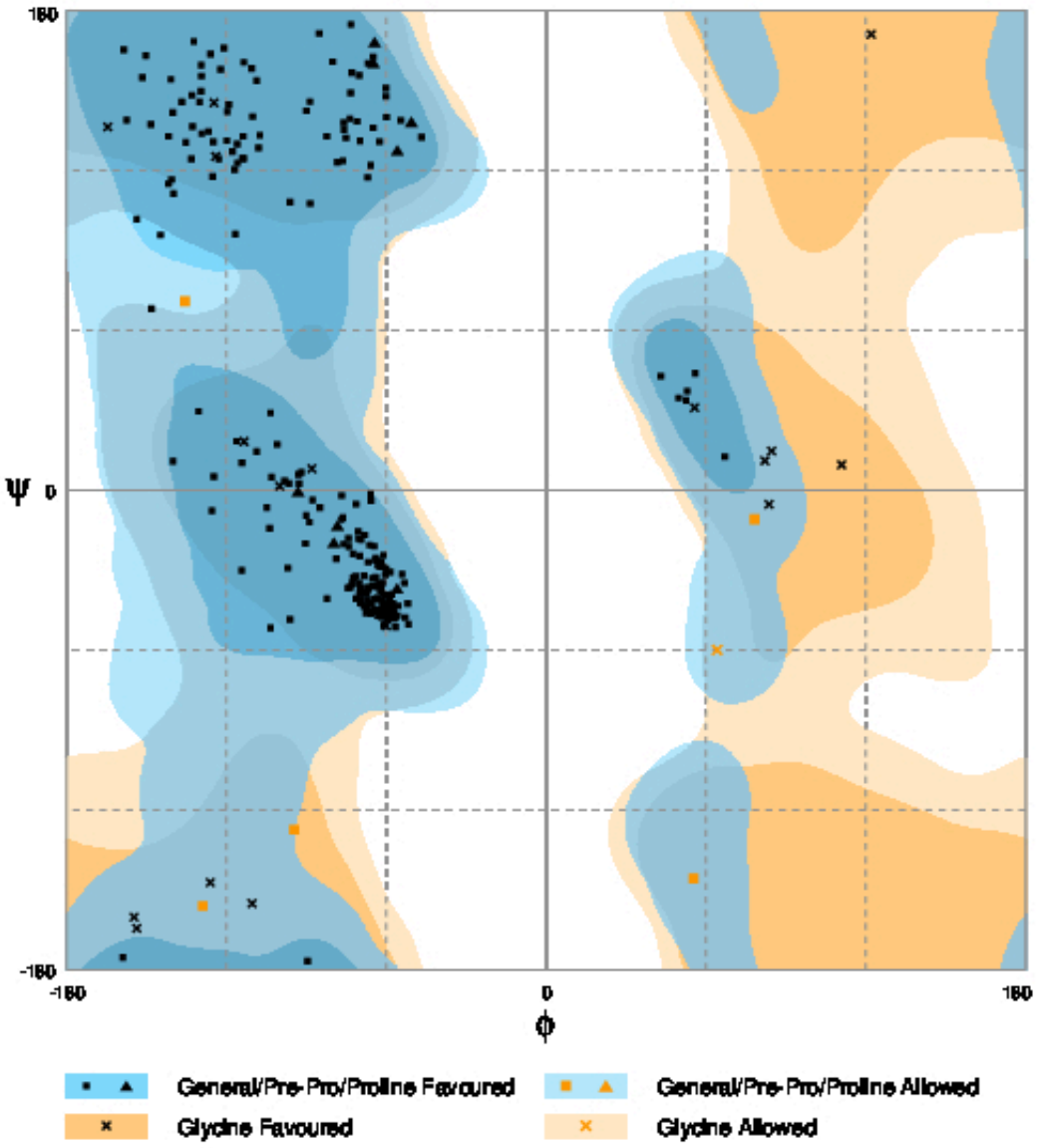
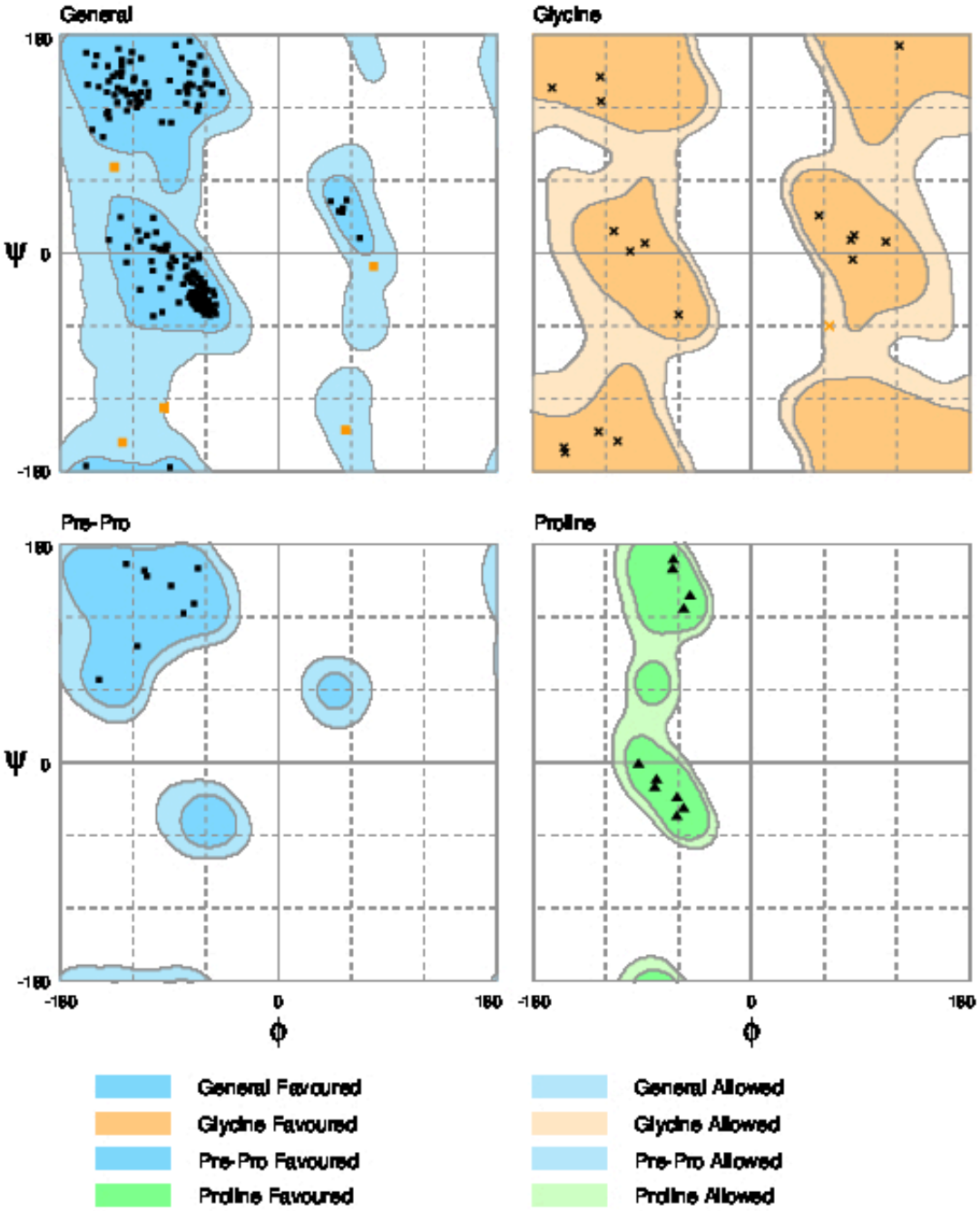
RAMPAGE I Information MolProbity I Crystallography and Bioinformatics Group

RAMPAGE: Assessment of the Ramachandran Plot

File: LPG3.pdb

For high-resolution output, you can download a Adobe PDF or PostScript file

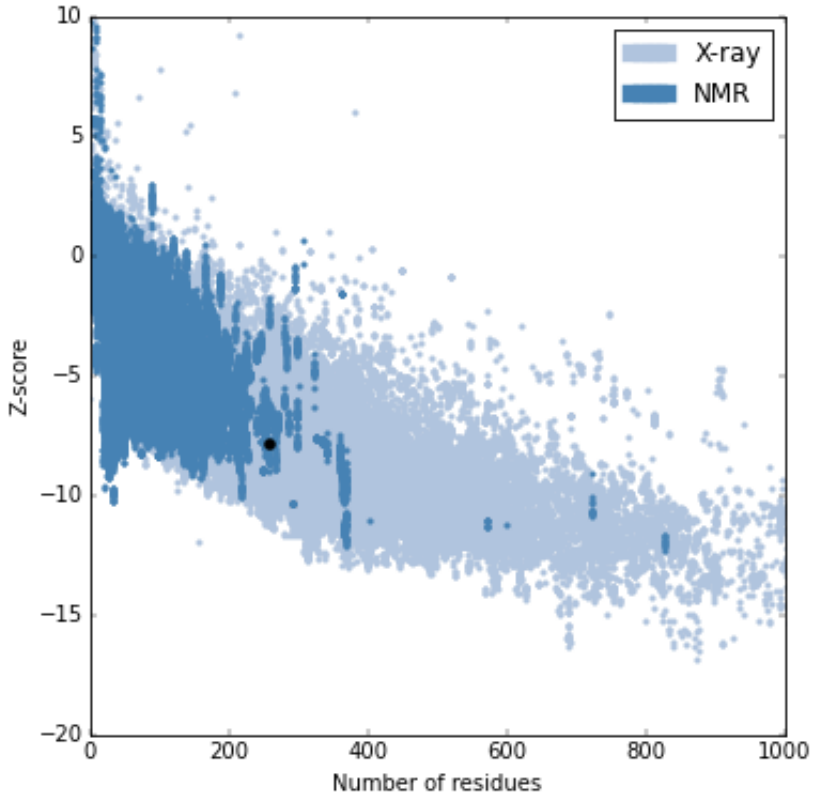




Evaluation of residues

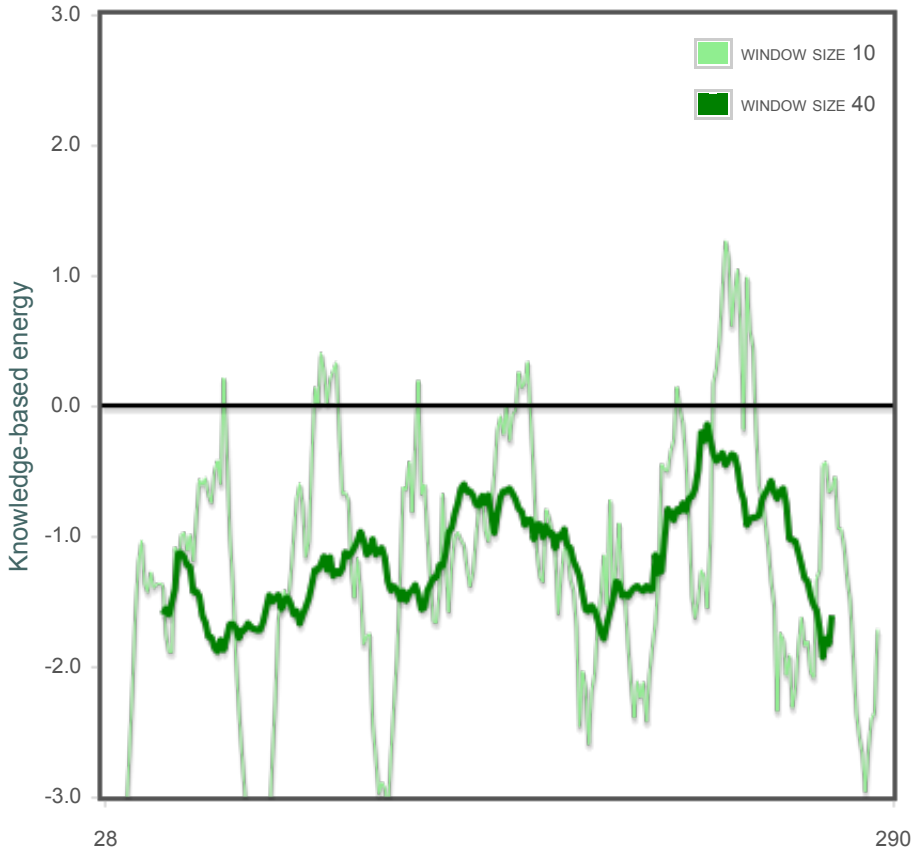
```
Residue [A  69 :CYS] (  55.42,-145.70) in Allowed region
Residue [A 103 :VAL] (-128.83,-156.00) in Allowed region
Residue [A 114 :ASN] (  78.33, -10.86) in Allowed region
Residue [A 220 :SER] ( -94.49,-127.38) in Allowed region
Residue [A 275 :ARG] (-135.48,  70.92) in Allowed region
Residue [A 289 :GLY] (  64.28, -59.97) in Allowed region
Number of residues in favoured region    (~98.0% expected)  :  252 ( 97.7%)
Number of residues in allowed region     ( ~2.0% expected)  :    6 (  2.3%)
Number of residues in outlier region                        :    0 (  0.0%)
```

RAMPAGE by Paul de Bakker and Simon Lovell.

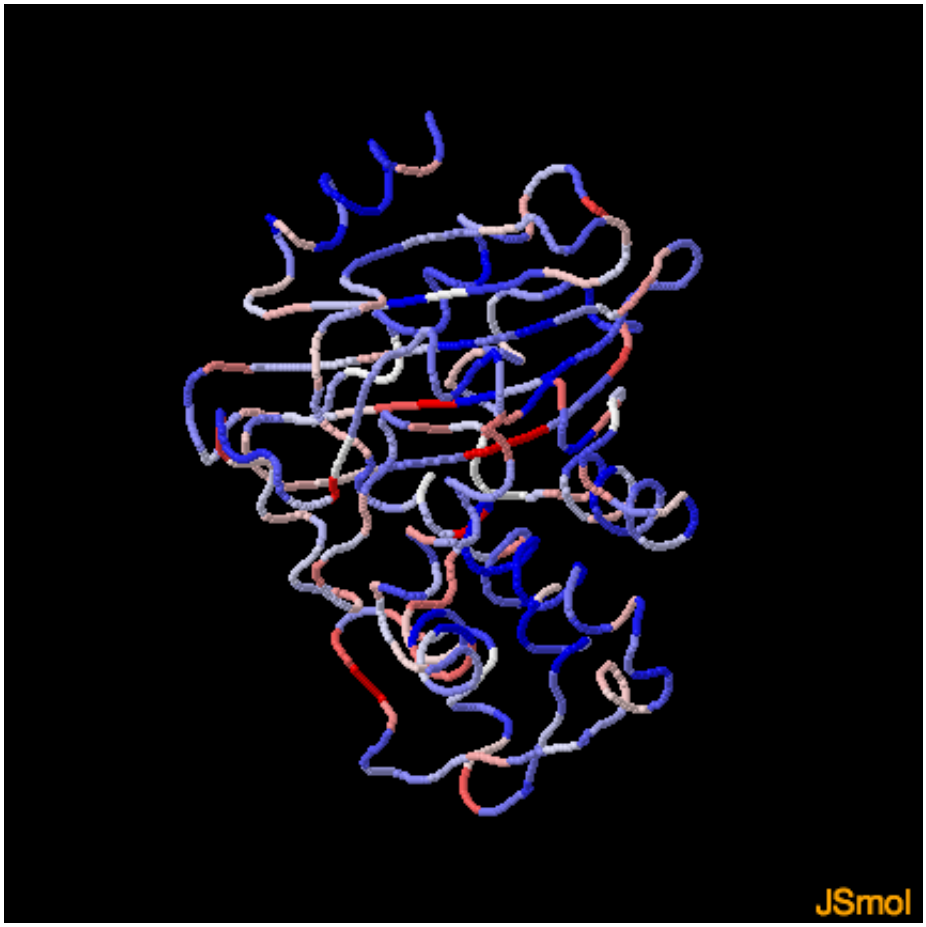


Local model quality

HELP



Sequence position



Lowest energy Highest energy

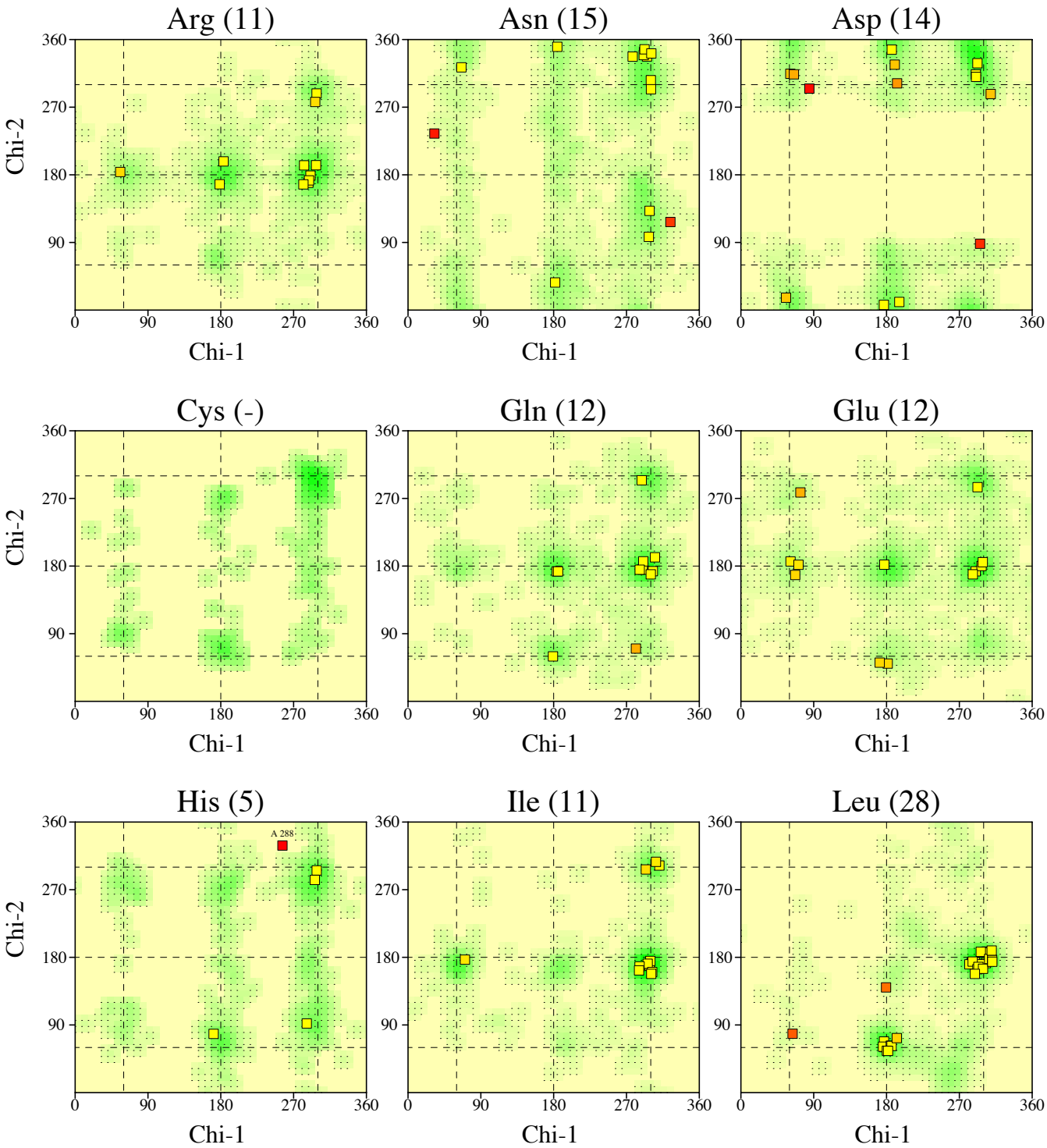
Please cite the following articles if you publish results using ProSA-web:

- Wiederstein & Sippl (2007)
  ProSA-web: interactive web service for the recognition of errors in three-dimensional structures of proteins.
  Nucleic Acids Research 35, W407-W410. [view]
- Sippl, M.J. (1993)
  Recognition of Errors in Three-Dimensional Structures of Proteins.
  Proteins 17, 355-362. [view]

This site is maintained by Markus Wiederstein. For comments and suggestions please contact prosa@came.sbg.ac.at

Chi1-Chi2 plots

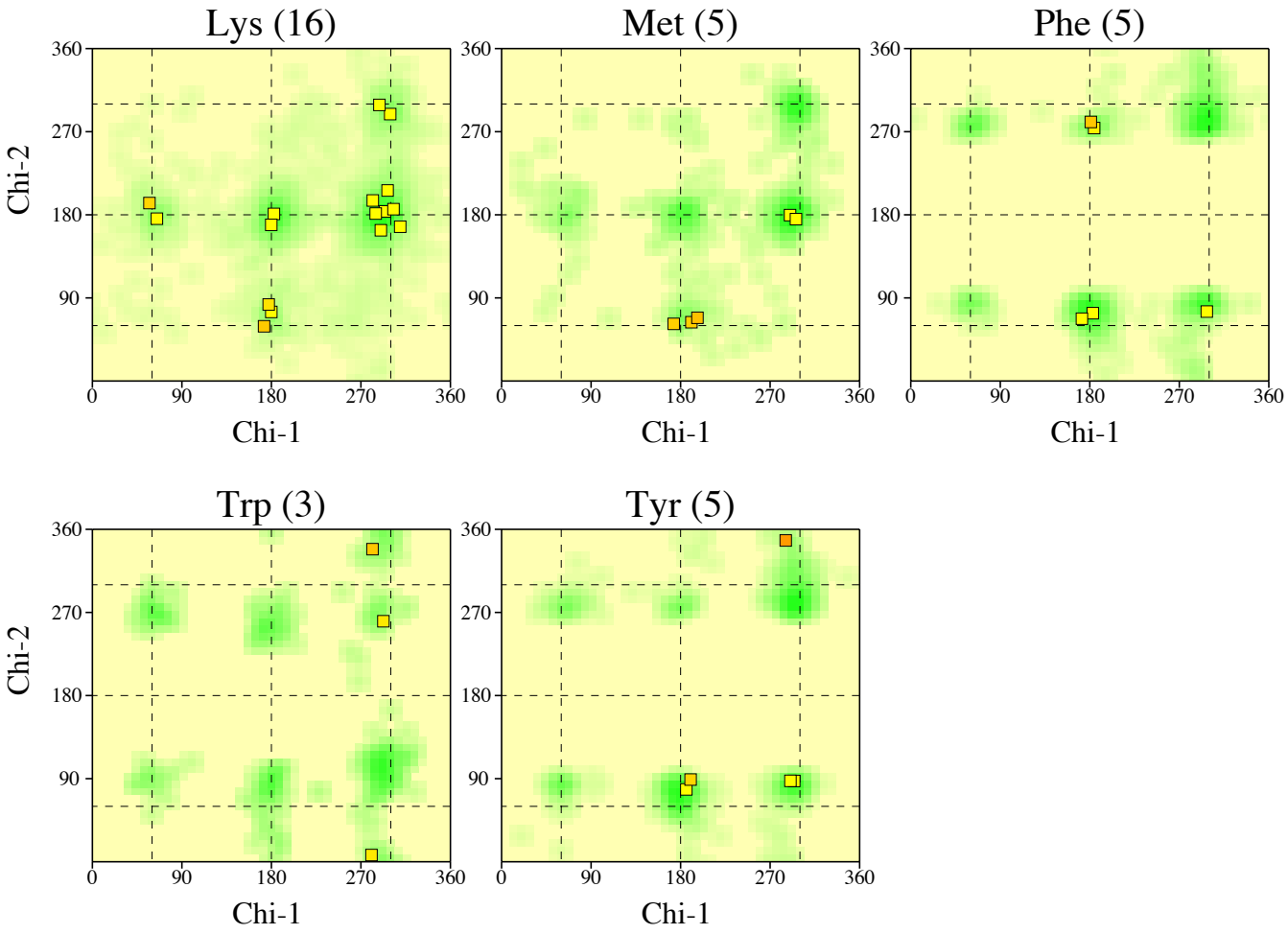
LPG3 - Chain A



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

LPG3 - Chain A



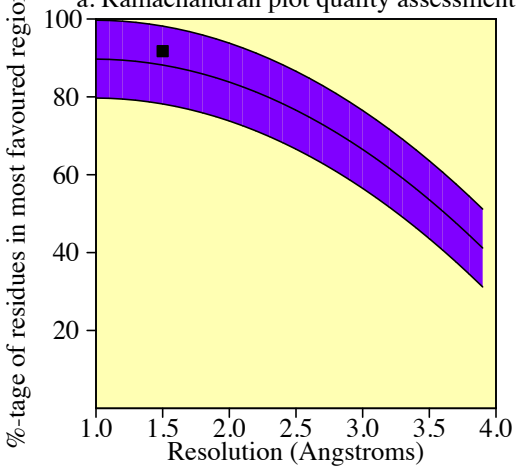
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

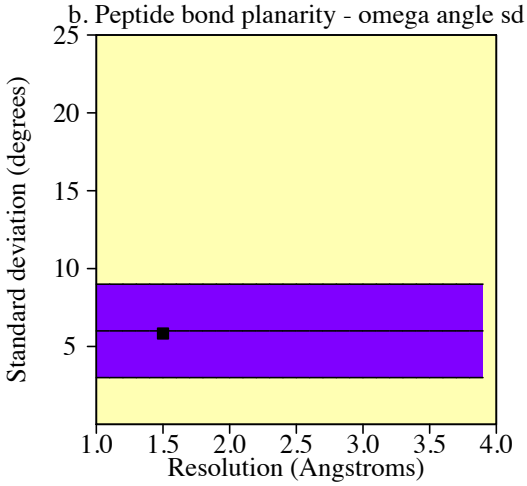
Main-chain parameters

LPG3 - Chain A

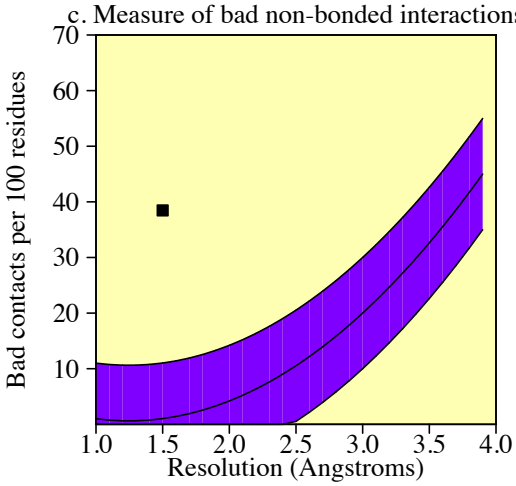
a. Ramachandran plot quality assessment



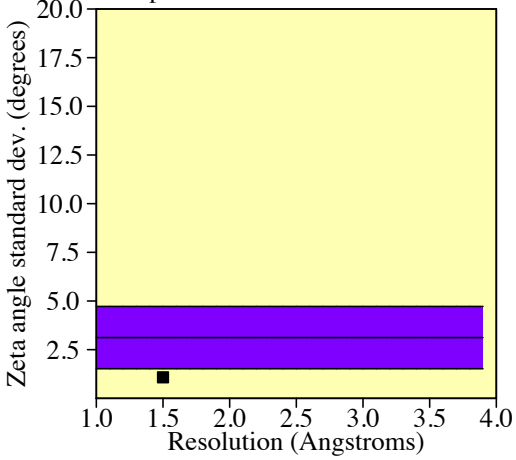
b. Peptide bond planarity - omega angle sd



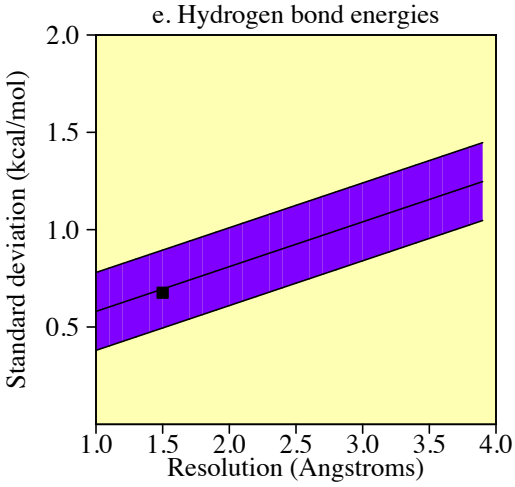
c. Measure of bad non-bonded interactions



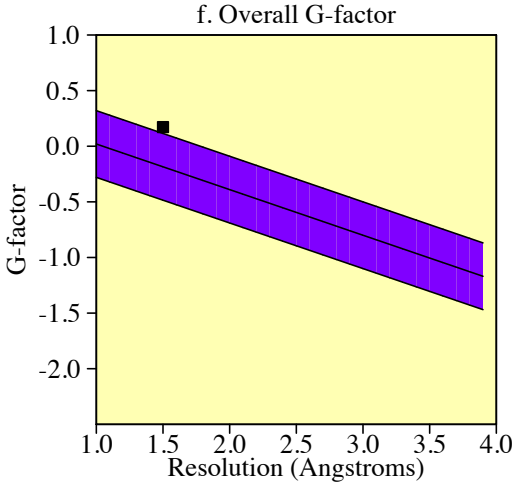
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor



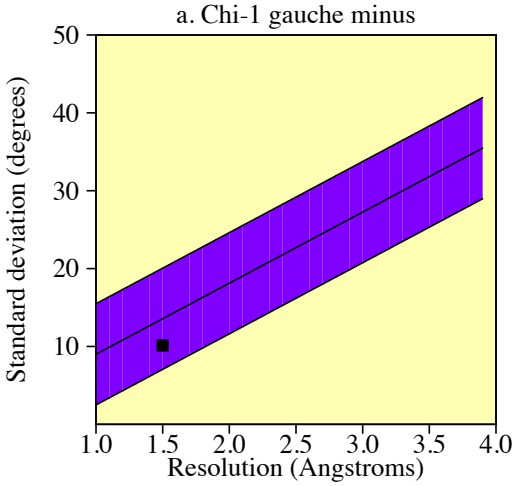
Plot statistics

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	230	91.7	88.2	10.0	0.4	Inside
b. Omega angle st dev	258	5.8	6.0	3.0	-0.1	Inside
c. Bad contacts / 100 residues	100	38.5	1.0	10.0	3.7	WORSE
d. Zeta angle st dev	242	1.1	3.1	1.6	-1.3	BETTER
e. H-bond energy st dev	169	0.7	0.7	0.2	-0.1	Inside
f. Overall G-factor	260	0.2	-0.2	0.3	1.2	BETTER

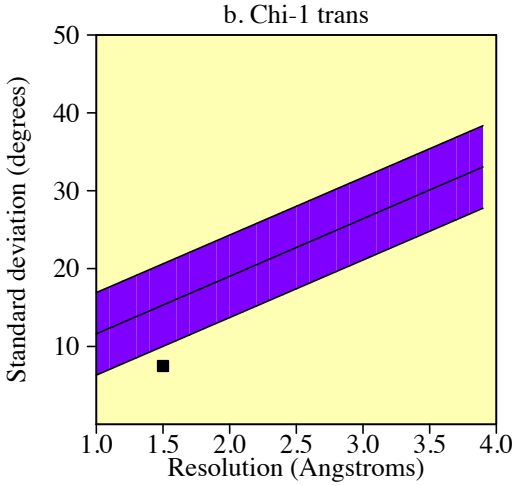
Side-chain parameters

LPG3 - Chain A

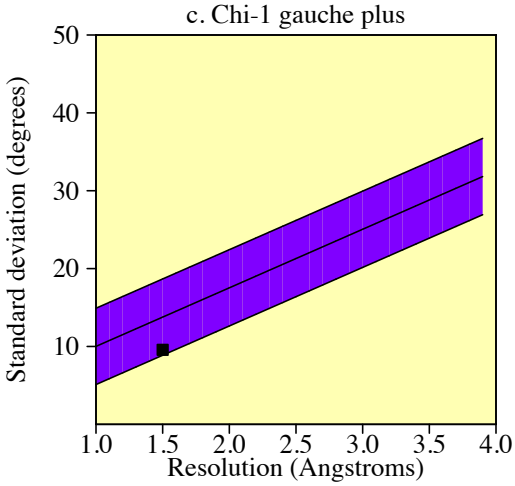
a. Chi-1 gauche minus



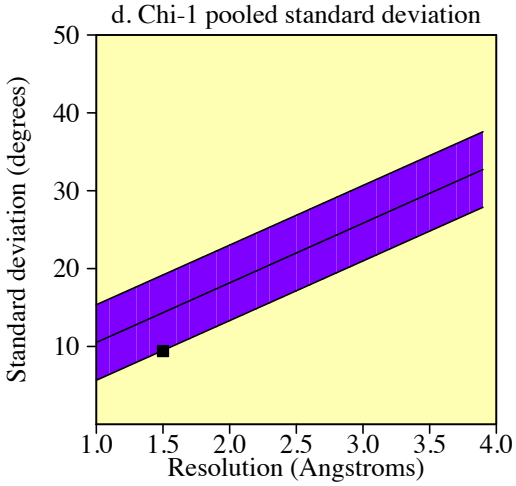
b. Chi-1 trans



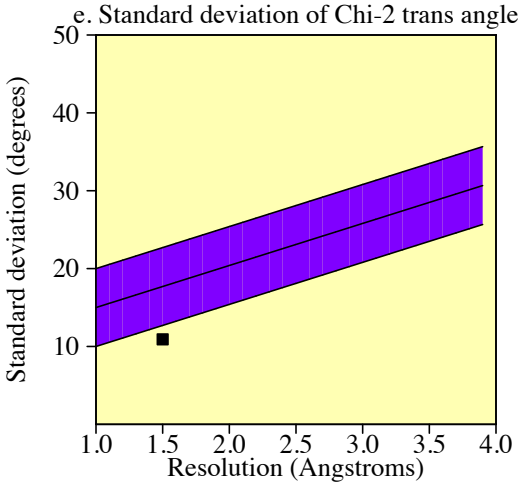
c. Chi-1 gauche plus



d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



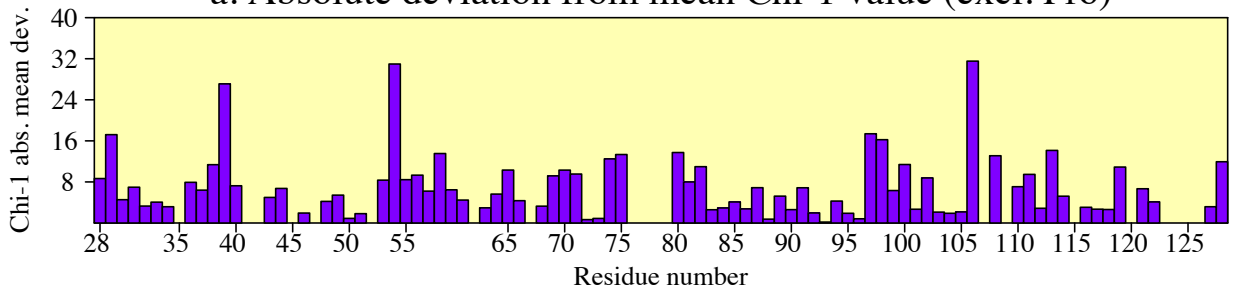
LPG3 - Chain A

Plot statistics

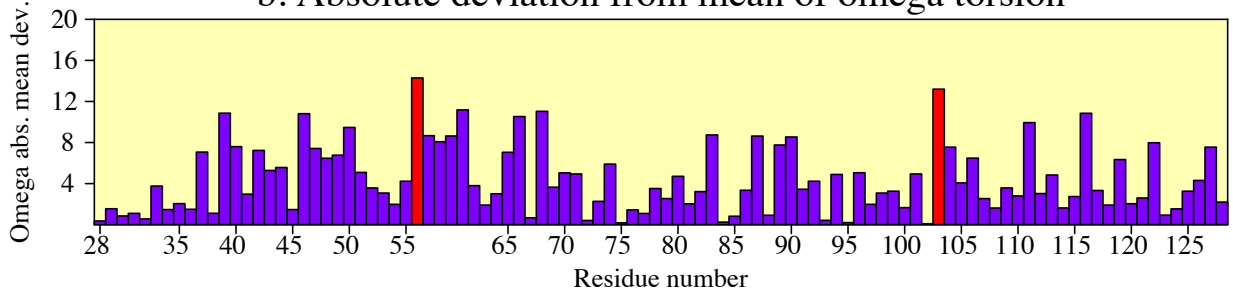
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	41	10.1	13.6	6.5	-0.5	Inside
b. Chi-1 trans st dev	56	7.5	15.3	5.3	-1.5	BETTER
c. Chi-1 gauche plus st dev	101	9.6	13.8	4.9	-0.9	Inside
d. Chi-1 pooled st dev	198	9.4	14.3	4.8	-1.0	BETTER
e. Chi-2 trans st dev	66	10.9	17.7	5.0	-1.4	BETTER

Residue properties
LPG3 - Chain A

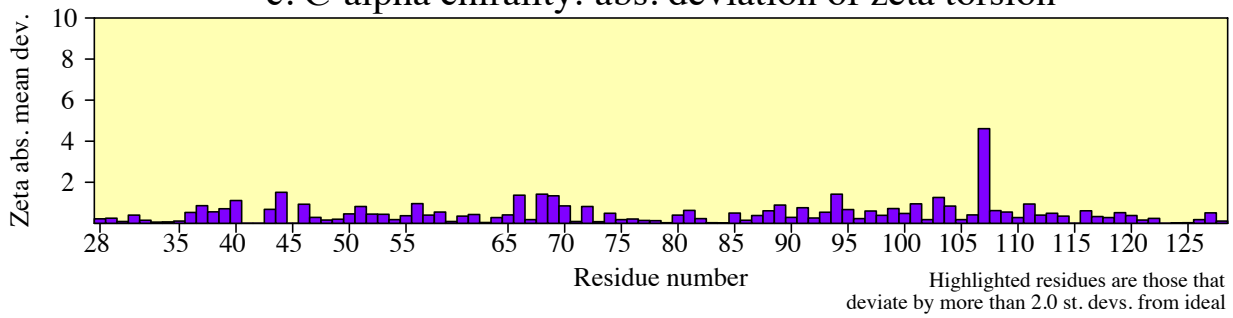
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

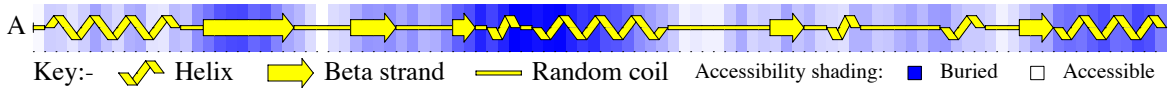


c. C-alpha chirality: abs. deviation of zeta torsion



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

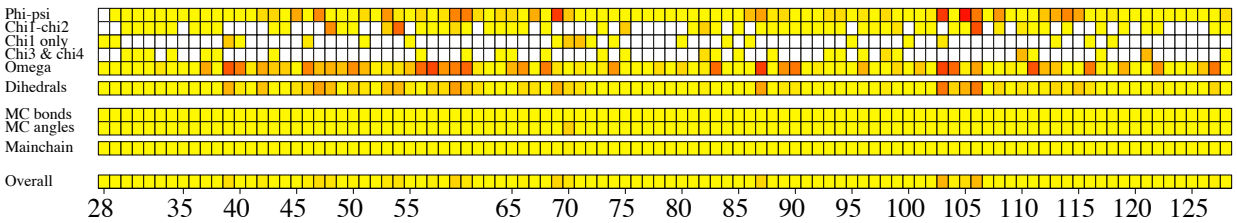
d. Secondary structure & estimated accessibility



e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

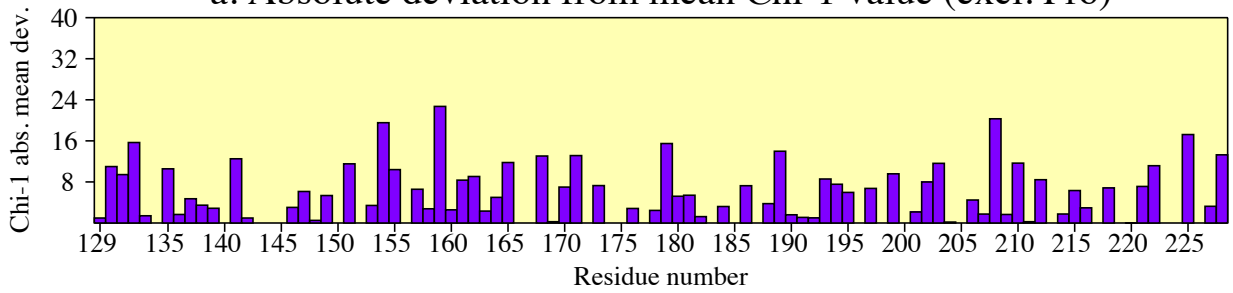
f. Max. deviation (see listing)

g. G-factors

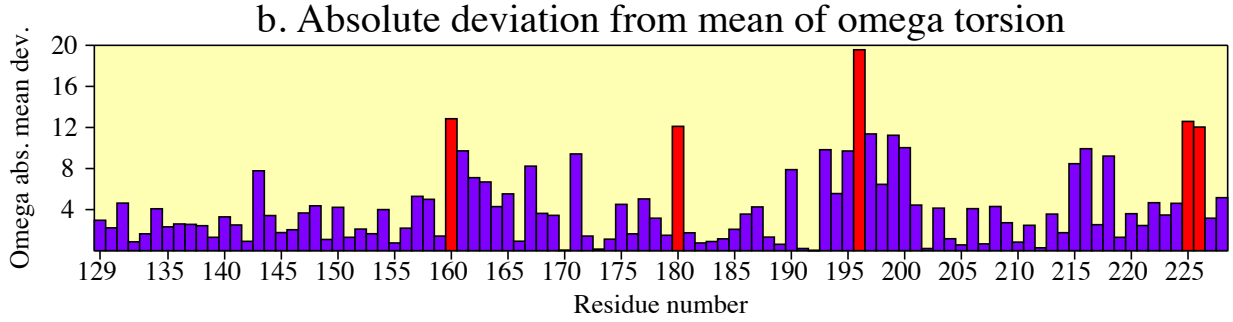


Residue properties
LPG3 - Chain A

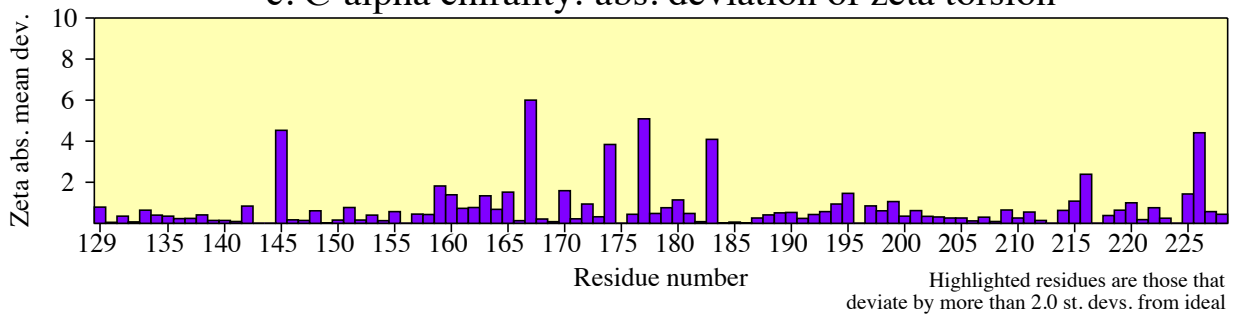
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

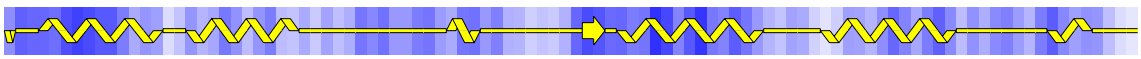


c. C-alpha chirality: abs. deviation of zeta torsion



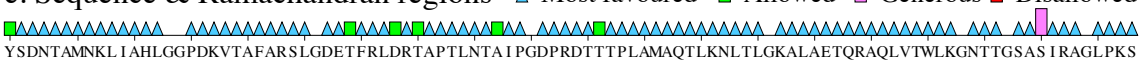
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



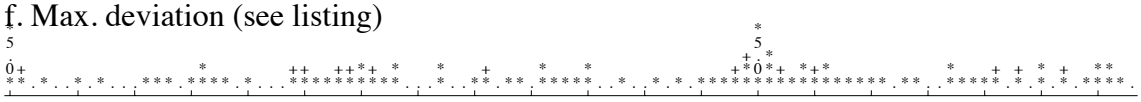
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

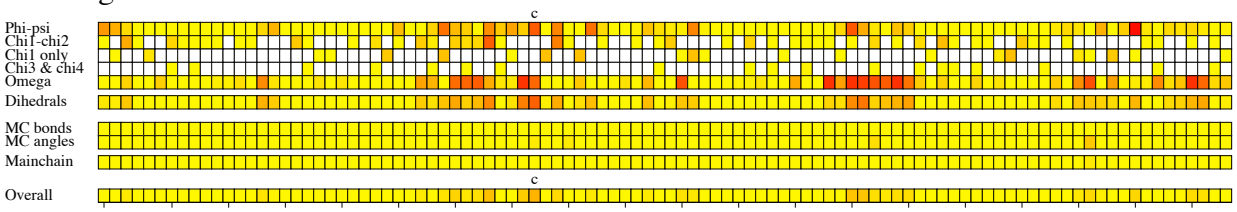


YSDNTAMNKL I AHLGGPDKVTAFARS LGDETFRLDRTAPTLNTA I PGDPRDTTTPLAMAQTLKNLTLGKALAETQRAQLVTWLKGNTTGSAS I RAGLPKS

f. Max. deviation (see listing)



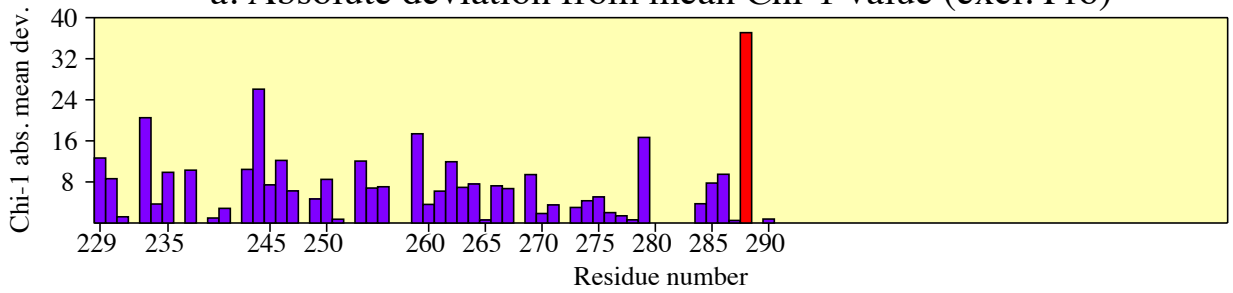
g. G-factors



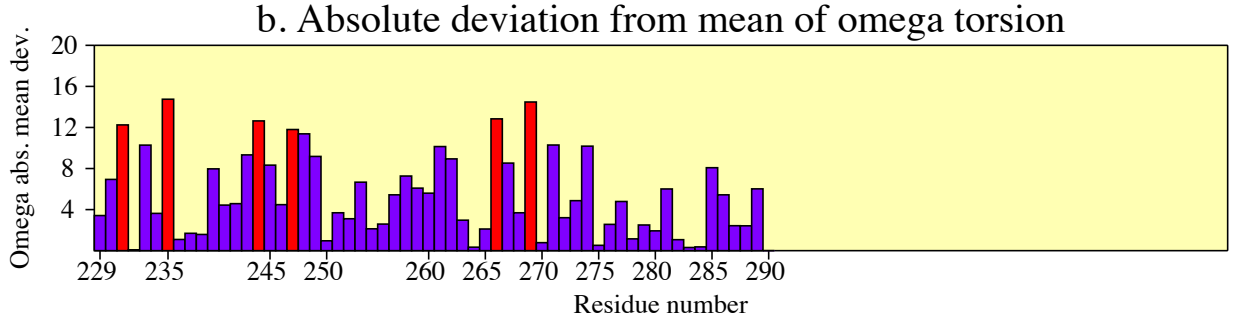
c = cis-peptide

Residue properties
LPG3 - Chain A

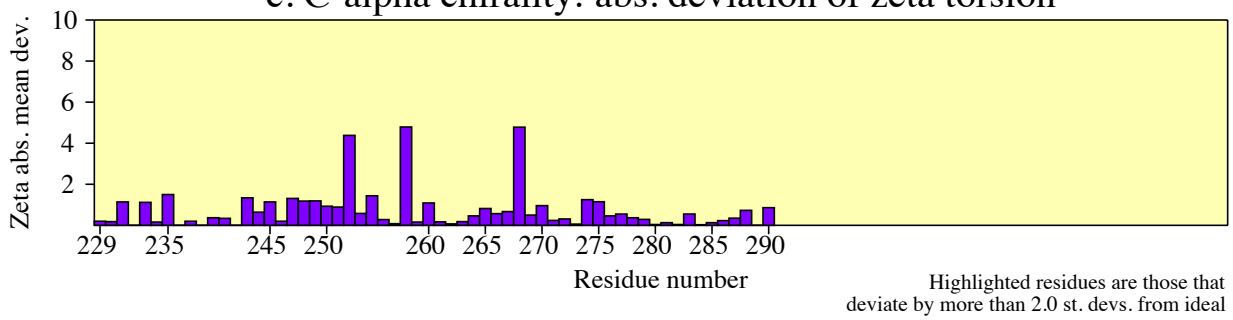
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

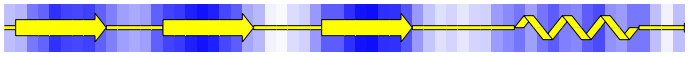


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

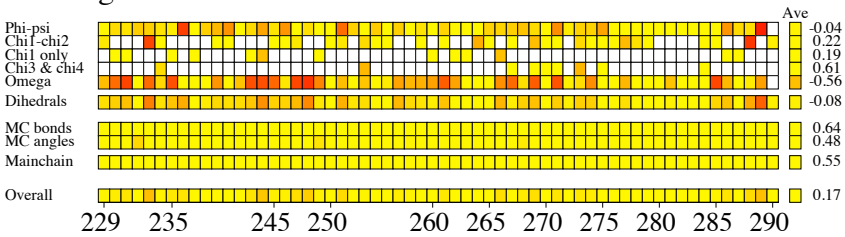


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

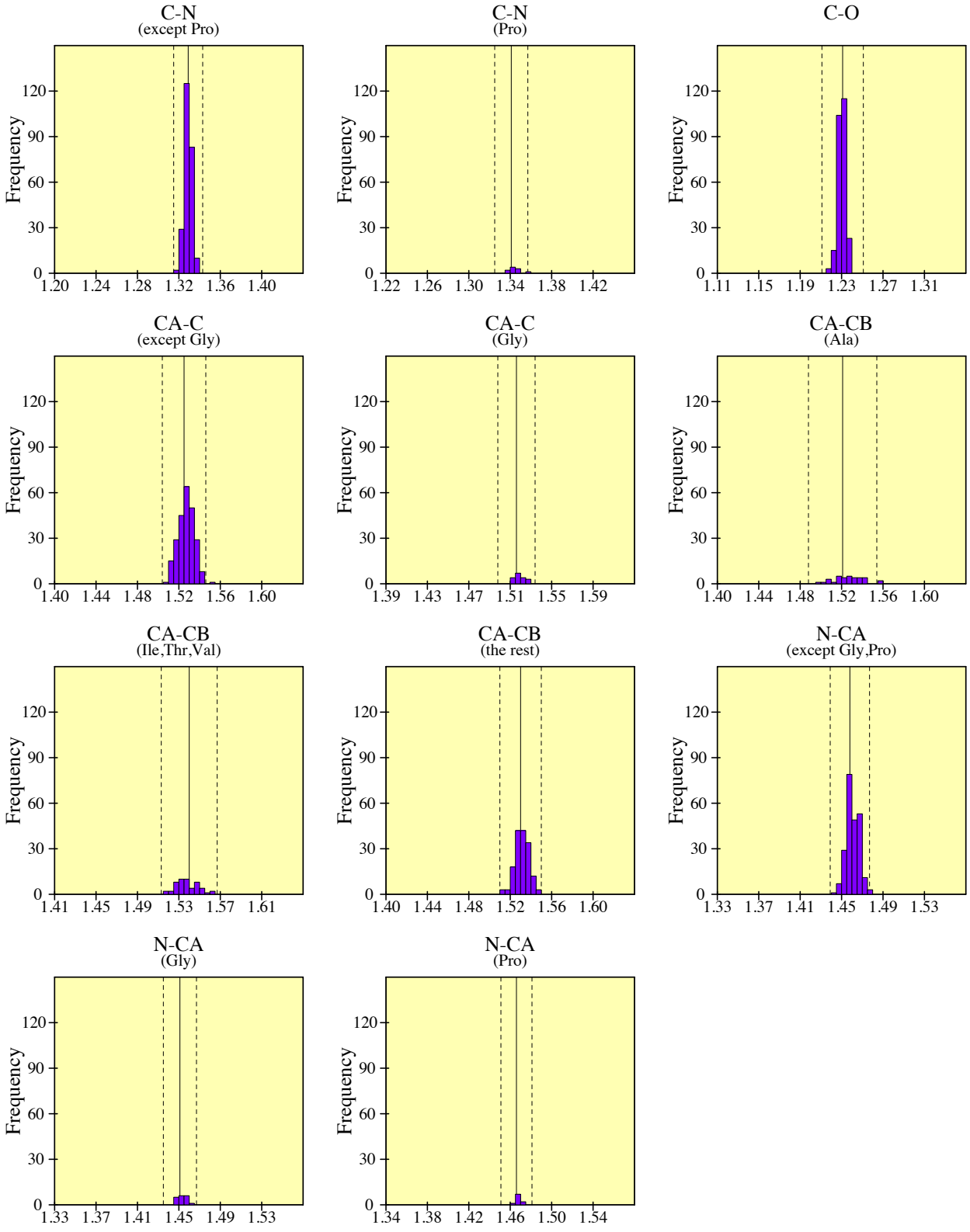
f. Max. deviation (see listing)

g. G-factors



Main-chain bond lengths

LPG3 - Chain A

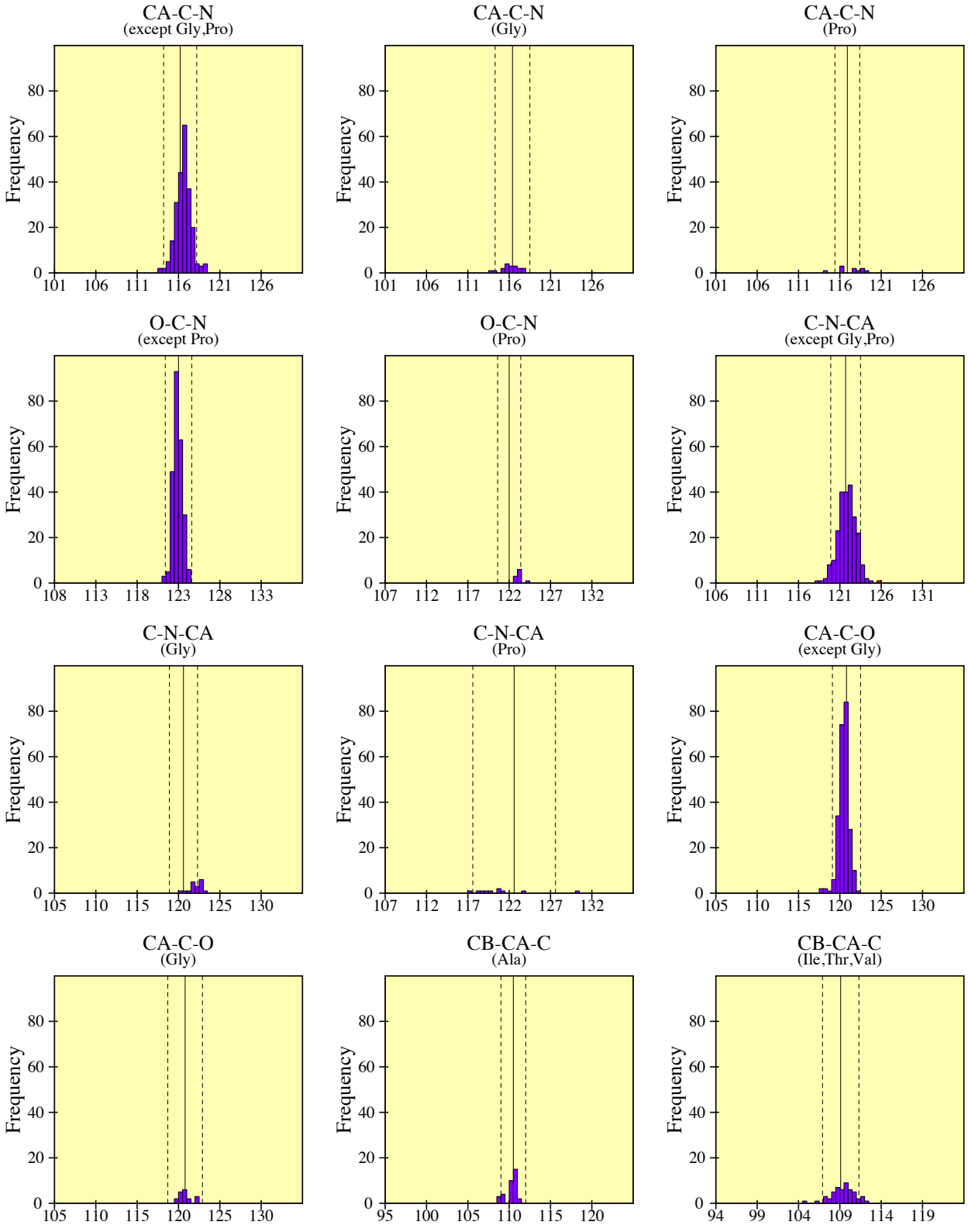


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

LPG3 - Chain A

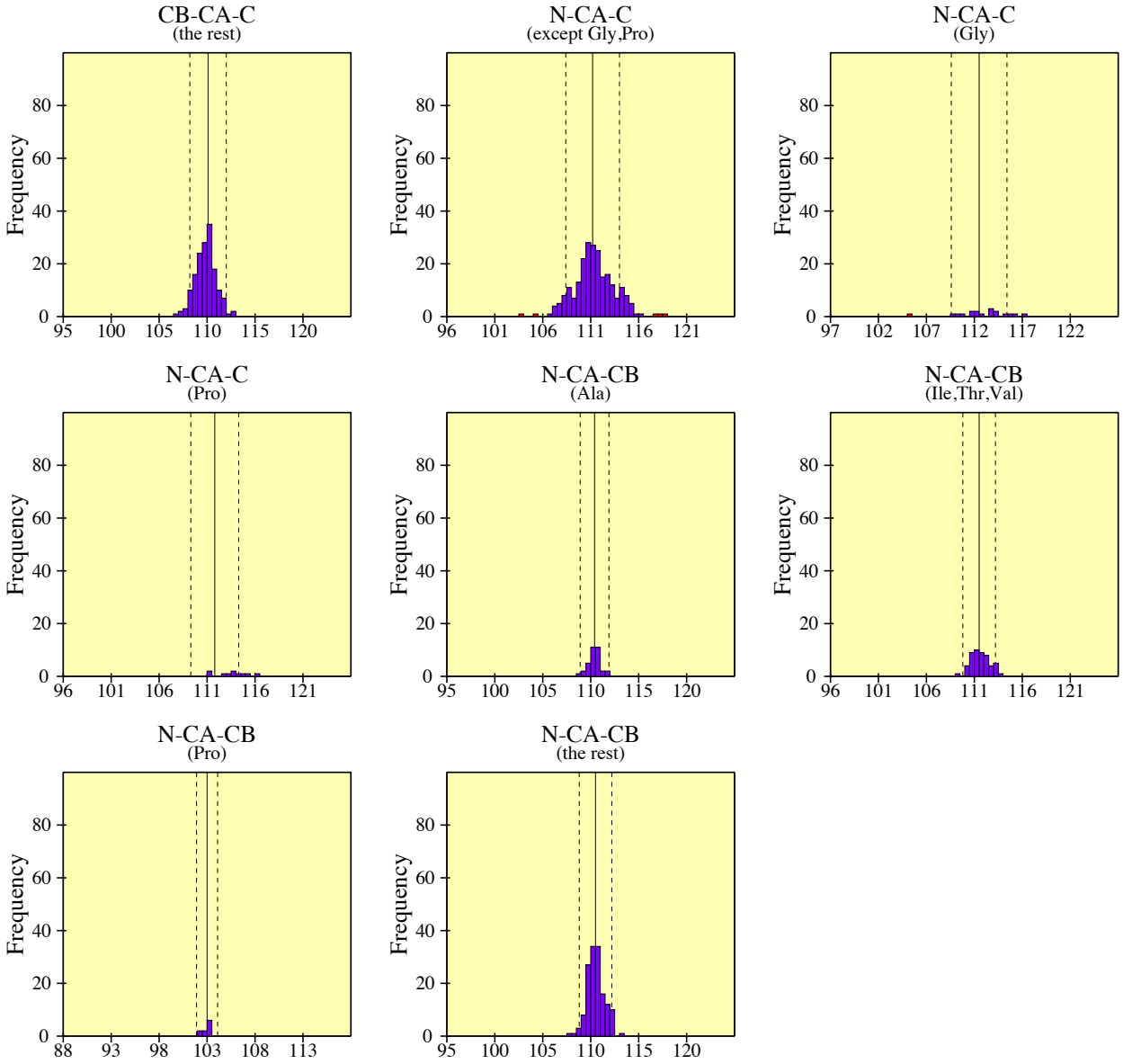


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

LPG3 - Chain A



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.