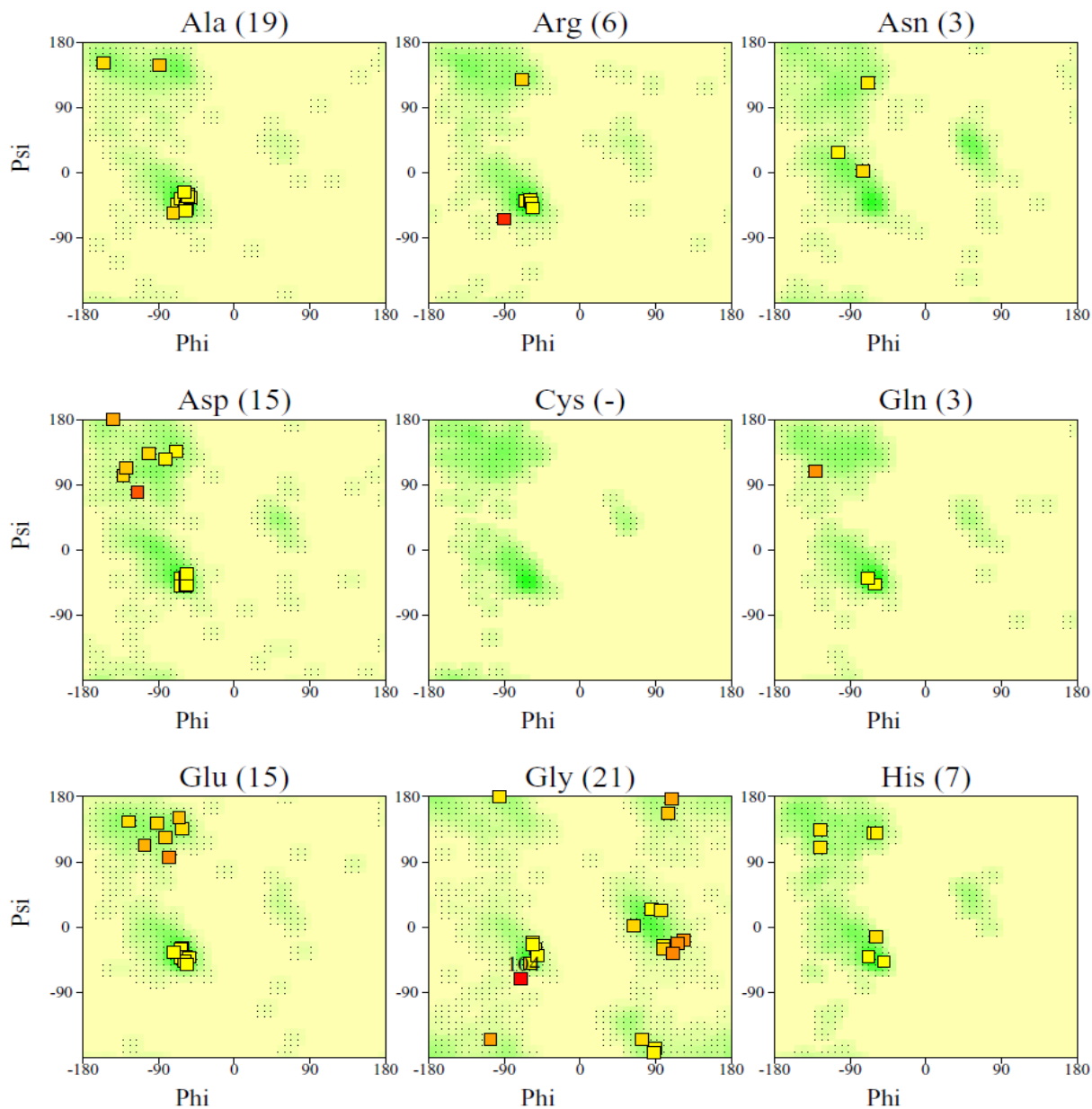
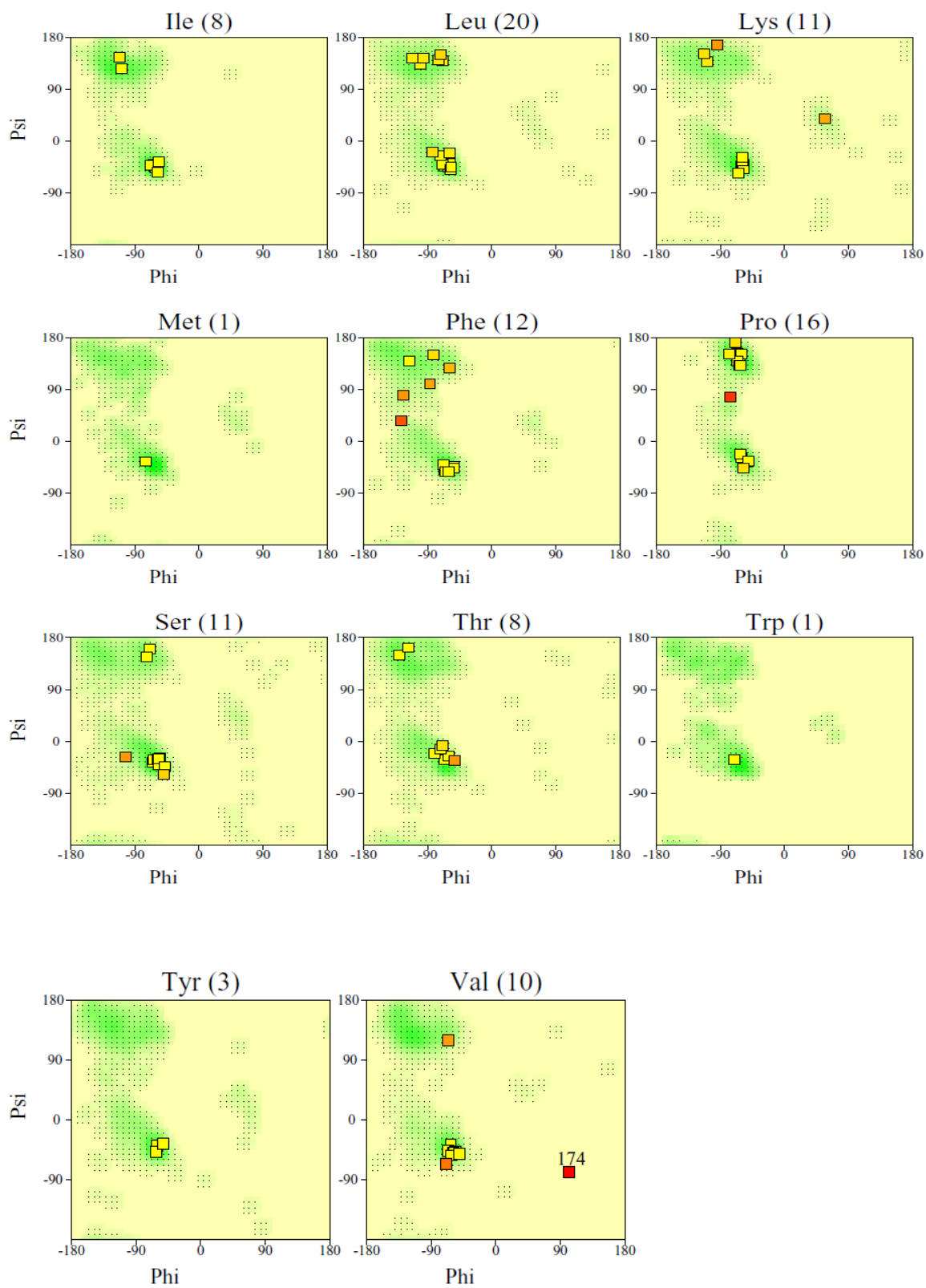


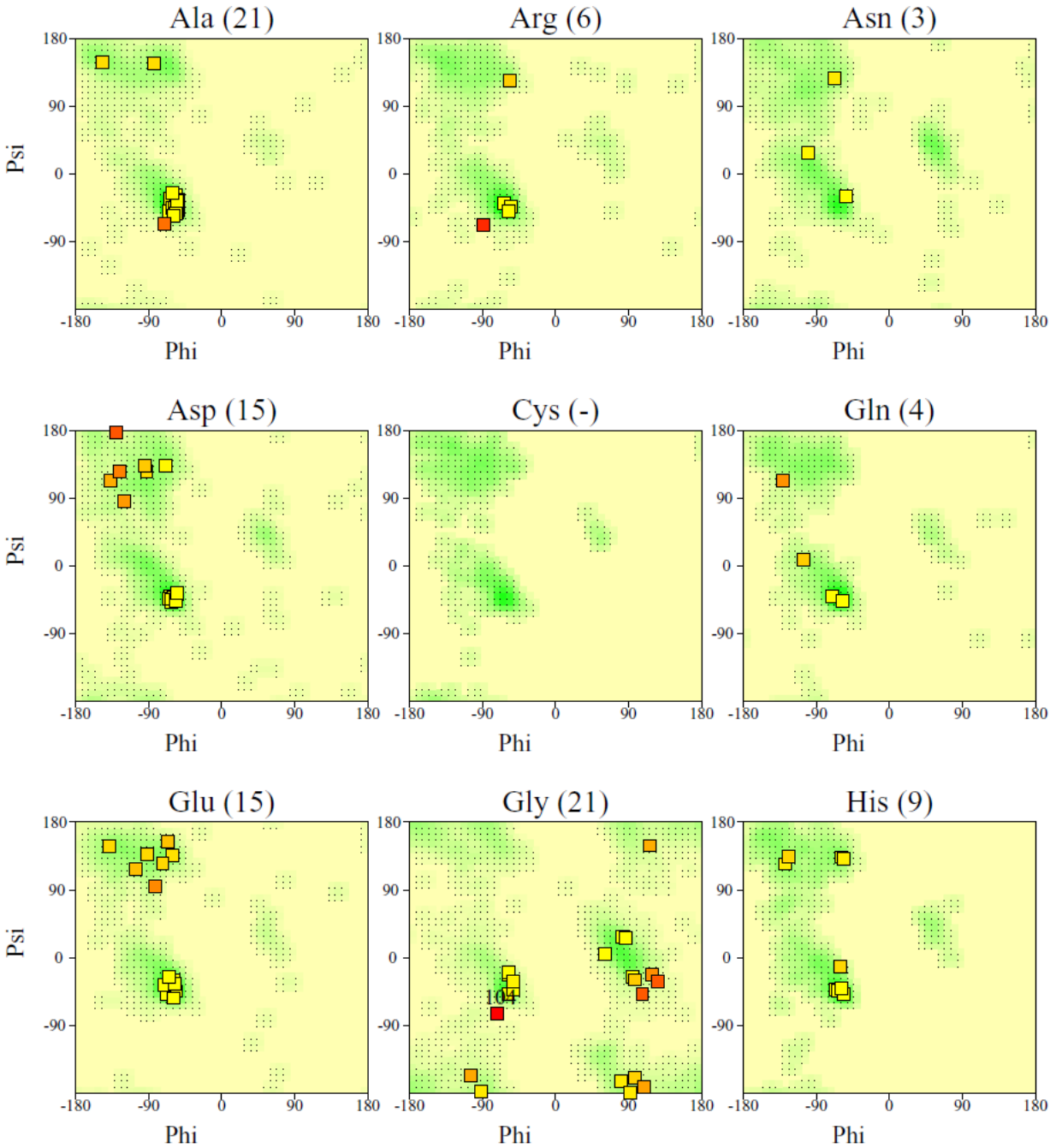
**Fig. S4:** Ramachandran plots of a) all residue types, b) main chain bond length, c) main chain properties, d) side chain properties, e) residue properties, f) RMS distance from planarity and g) chi1-chi2 plots in ICP 7035 and ICPL 84023

**a) Ramachandran plots of all residue types in ICP 7035 in pigeon pea**

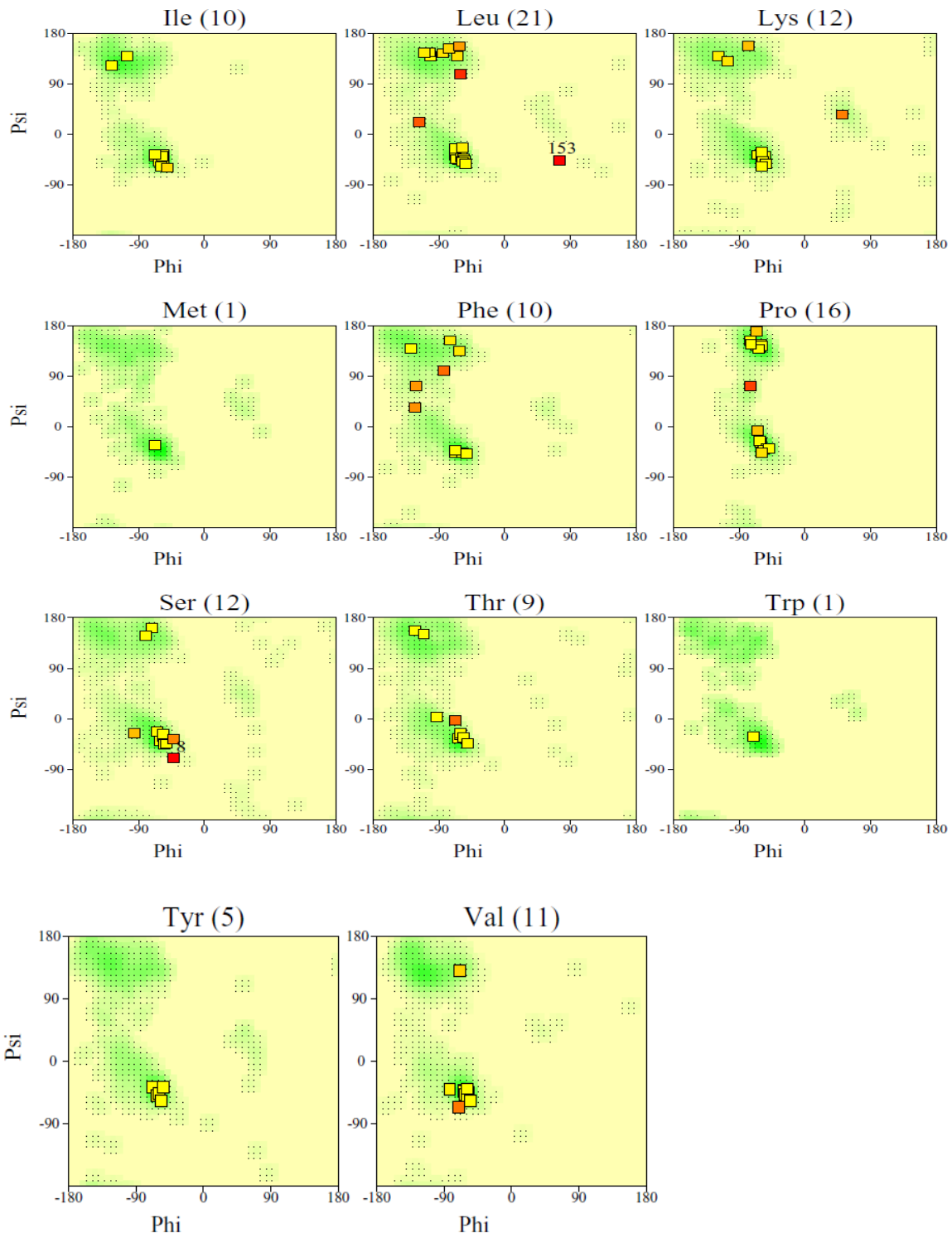


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0Å or better.

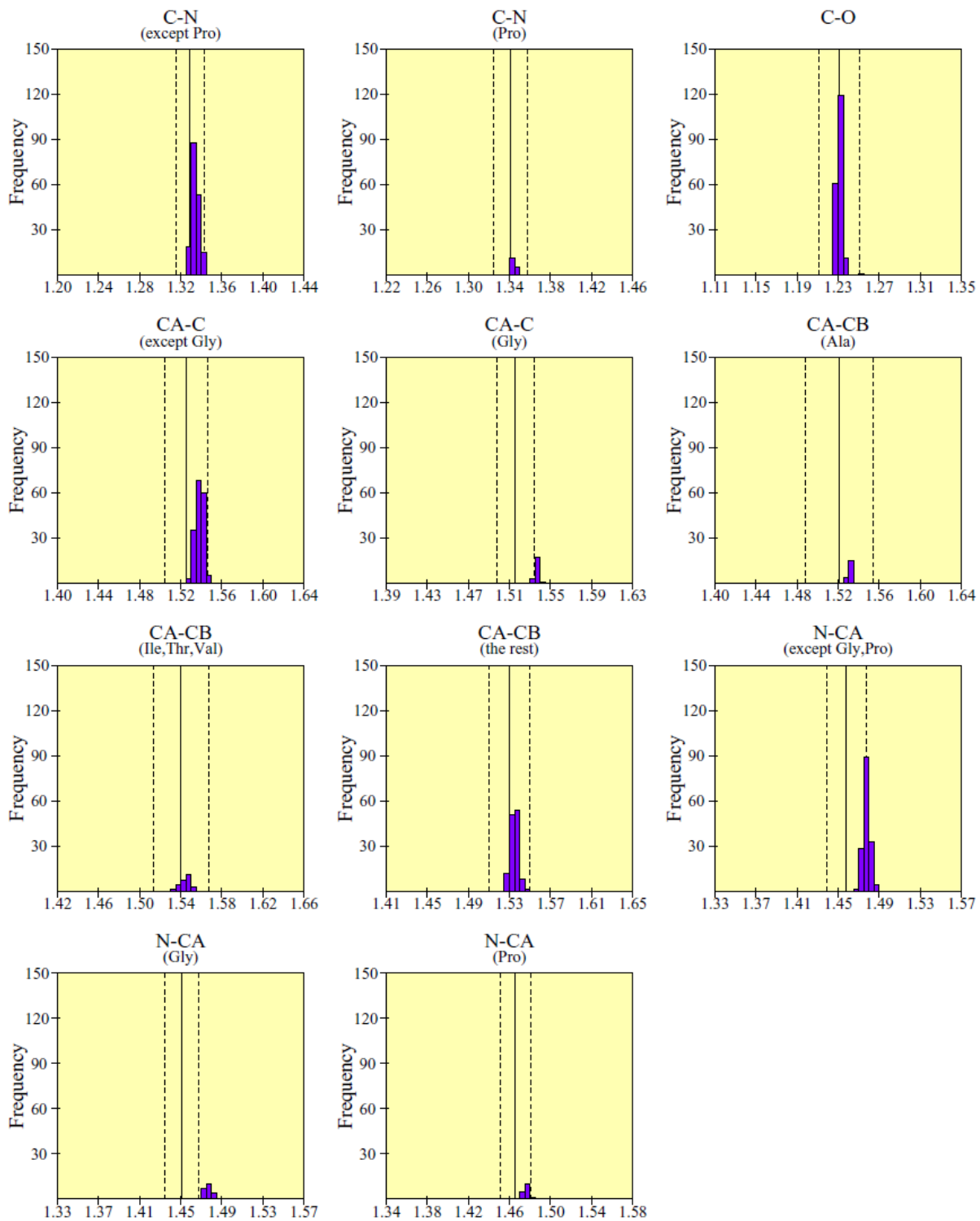




Numbers of residues are shown in brackets. Those in unfavourable conformations (score  $< -3.00$ ) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0Å or better.

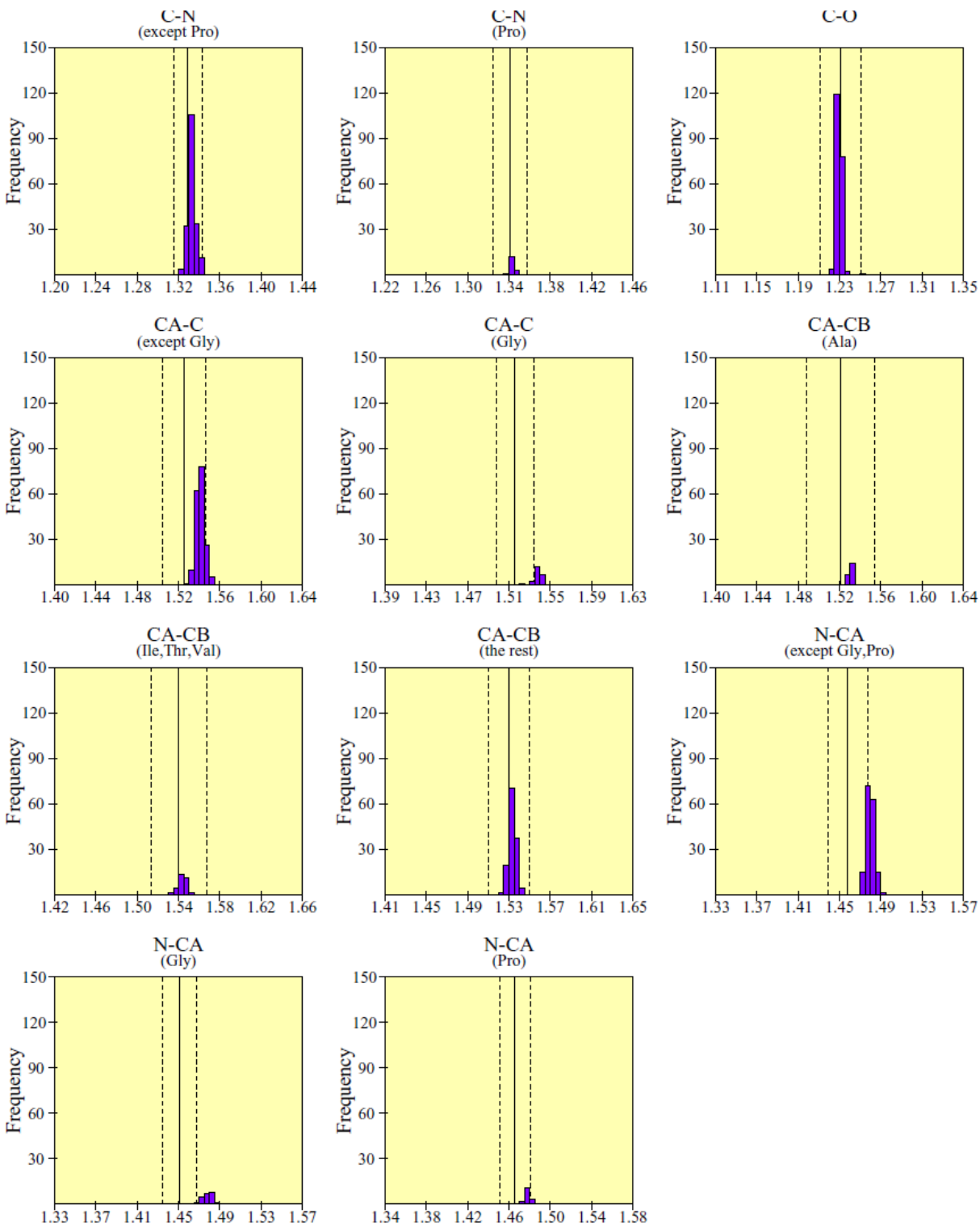


## b) Main chain bond length



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.

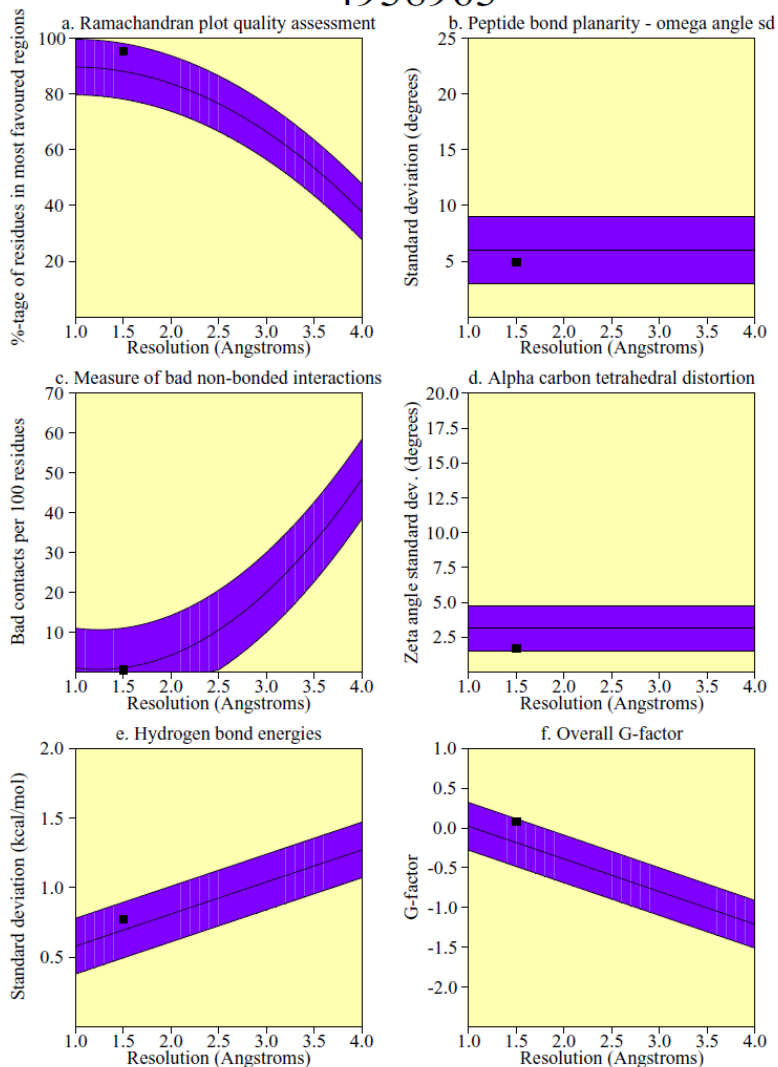


Black bars > 2.0 st. devs. from mean.

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

## c) Main chain properties

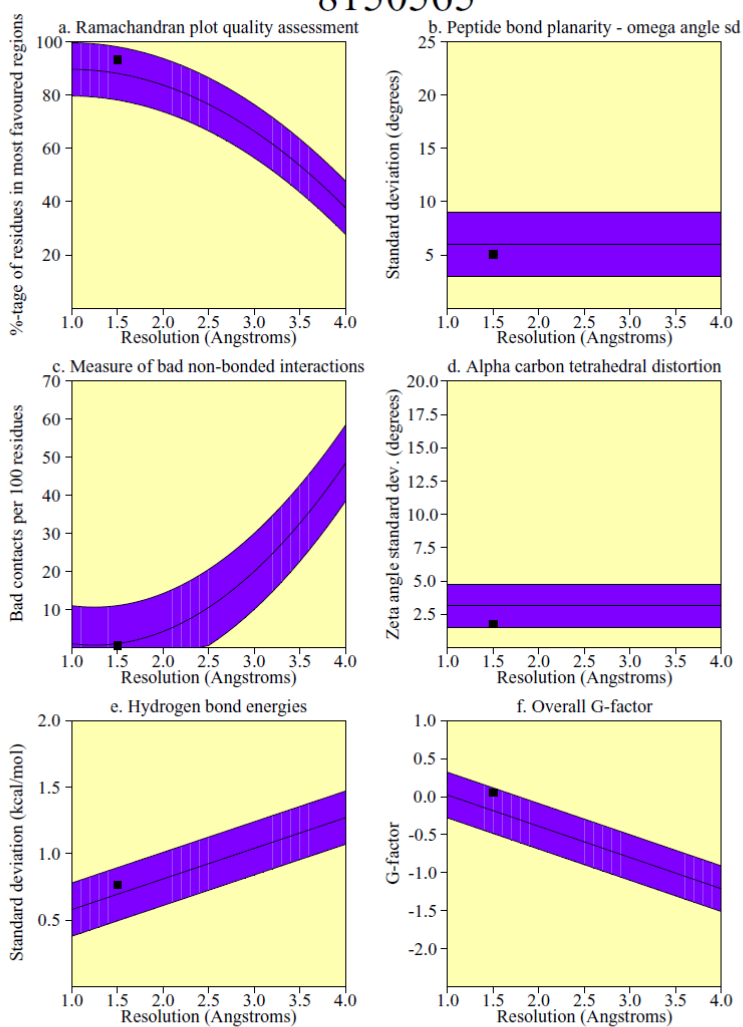
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Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. %-tage residues in A, B, L	153	95.4	88.2	10.0	0.7	Inside
b. Omega angle st dev	191	4.9	6.0	3.0	-0.4	Inside
c. Bad contacts / 100 residues	1	0.5	1.0	10.0	-0.1	Inside
d. Zeta angle st dev	171	1.7	3.1	1.6	-0.9	Inside
e. H-bond energy st dev	112	0.8	0.7	0.2	0.4	Inside
f. Overall G-factor	192	0.1	-0.2	0.3	0.9	Inside

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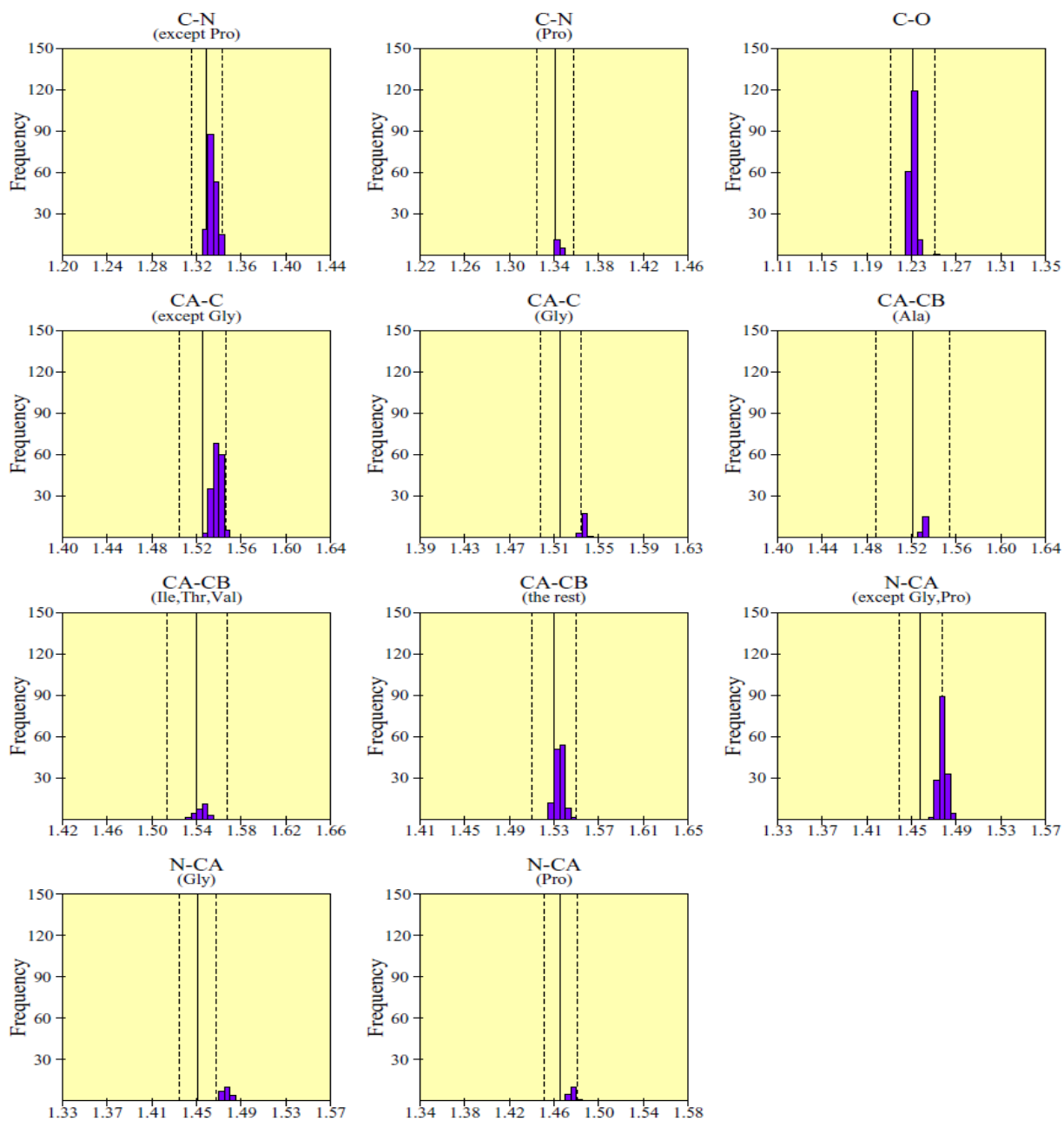


Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. %-tage residues in A, B, L	165	93.3	88.2	10.0	0.5	Inside
b. Omega angle st dev	203	5.1	6.0	3.0	-0.3	Inside
c. Bad contacts / 100 residues	1	0.5	1.0	10.0	-0.1	Inside
d. Zeta angle st dev	182	1.8	3.1	1.6	-0.8	Inside
e. H-bond energy st dev	120	0.8	0.7	0.2	0.3	Inside
f. Overall G-factor	204	0.1	-0.2	0.3	0.8	Inside

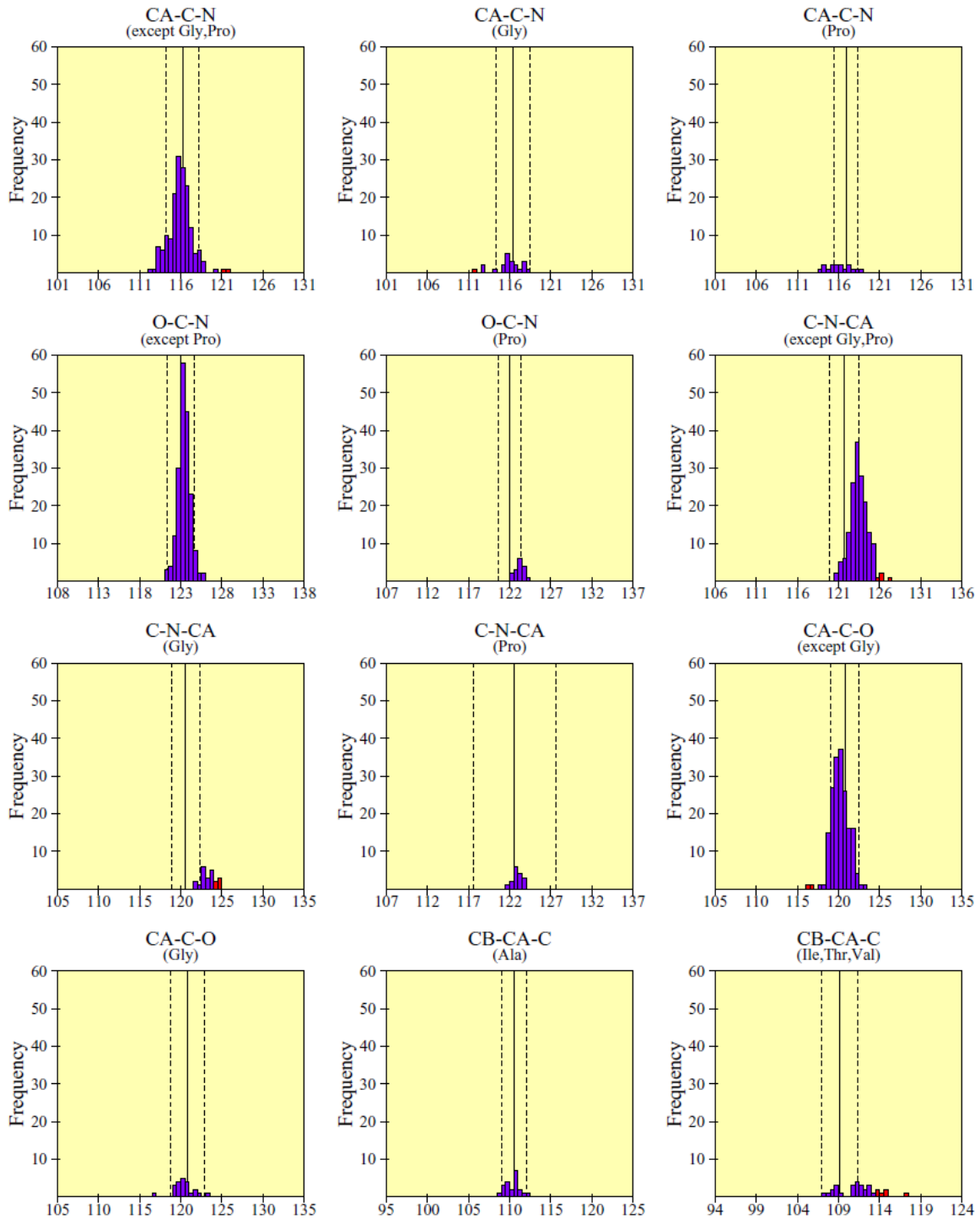


## Main chain bond angle of ICP 7035



Black bars > 2.0 st. devs. from mean.

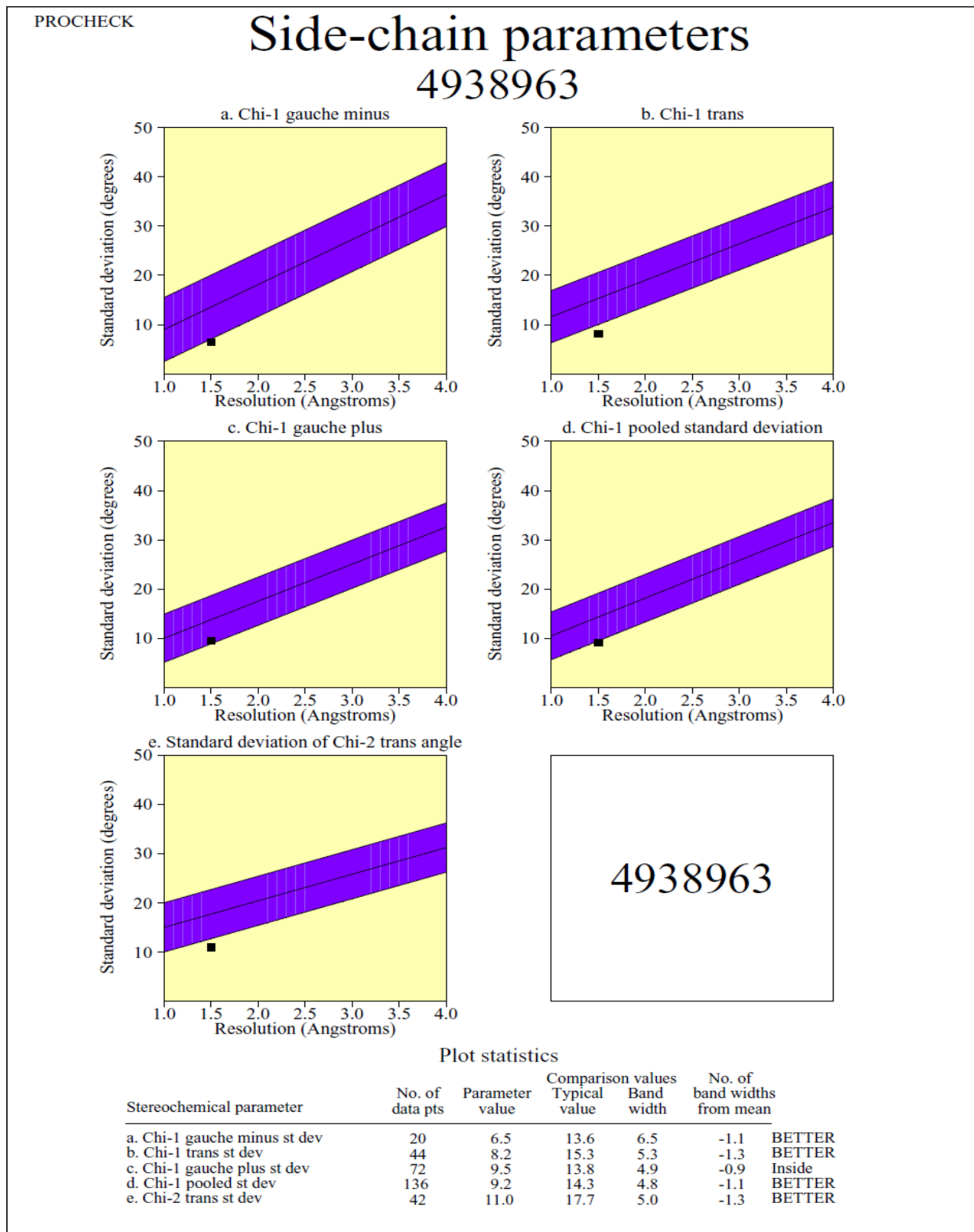
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.



Black bars > 2.0 st. devs. from mean.

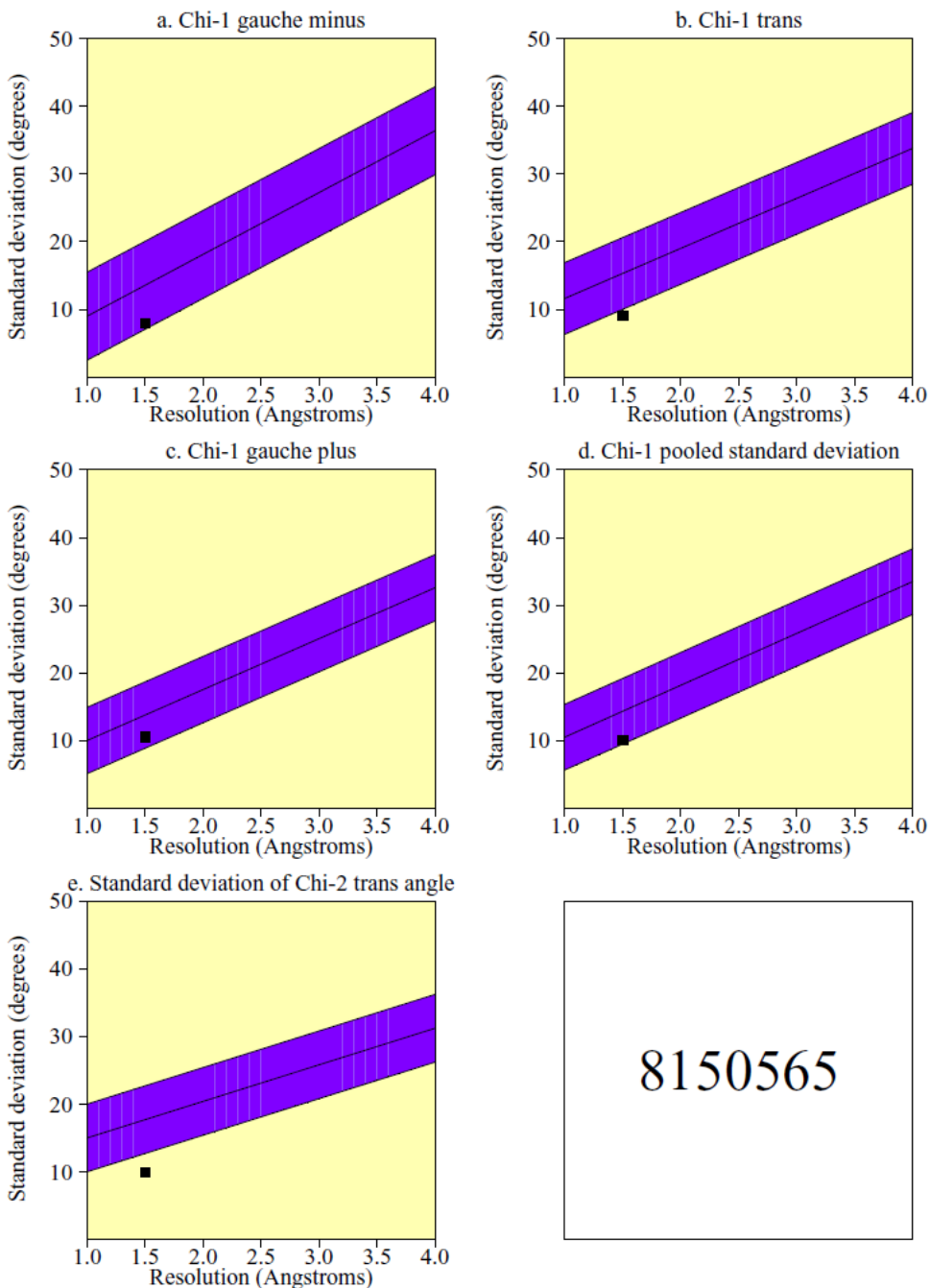
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

## d) Side chain properties



# Side-chain parameters

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Plot statistics

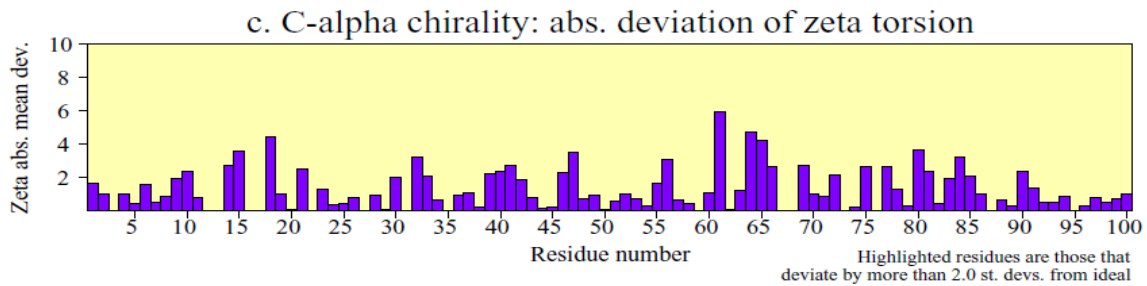
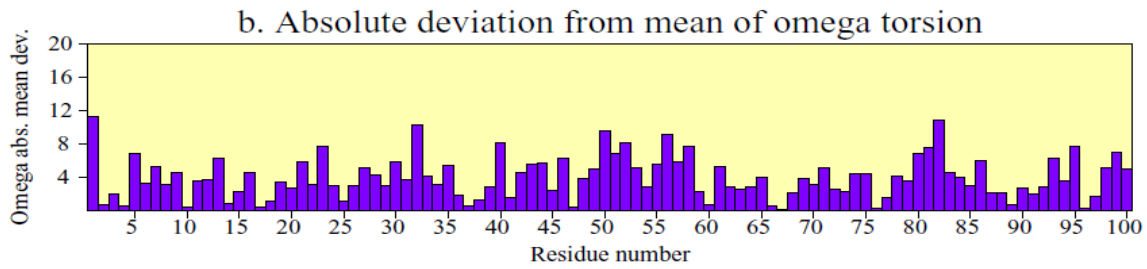
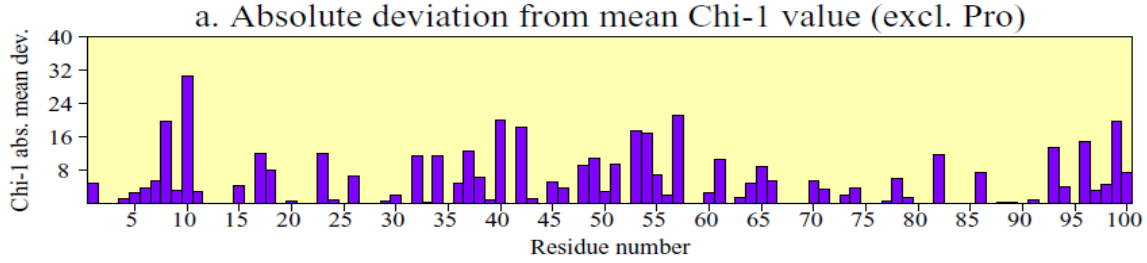
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. Chi-1 gauche minus st dev	19	8.0	13.6	6.5	-0.9	Inside
b. Chi-1 trans st dev	49	9.1	15.3	5.3	-1.2	BETTER
c. Chi-1 gauche plus st dev	77	10.5	13.8	4.9	-0.7	Inside
d. Chi-1 pooled st dev	145	10.1	14.3	4.8	-0.9	Inside
e. Chi-2 trans st dev	48	9.9	17.7	5.0	-1.6	BETTER

e) Residue properties

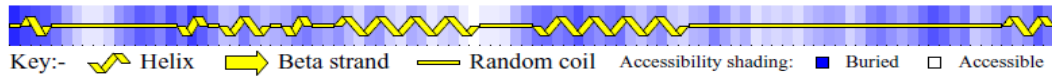
# Residue properties

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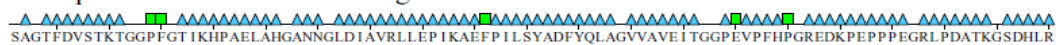
1000



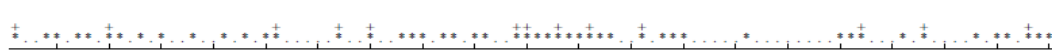
d. Secondary structure & estimated accessibility



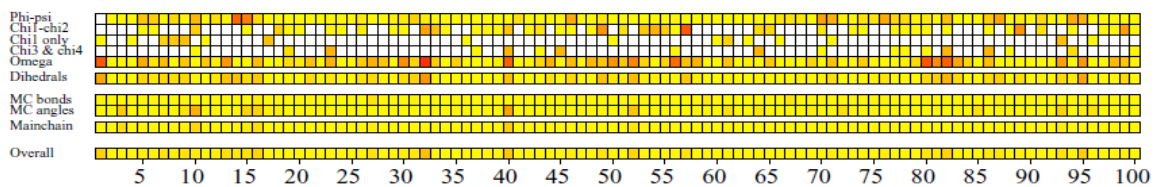
e. Sequence & Ramachandran regions

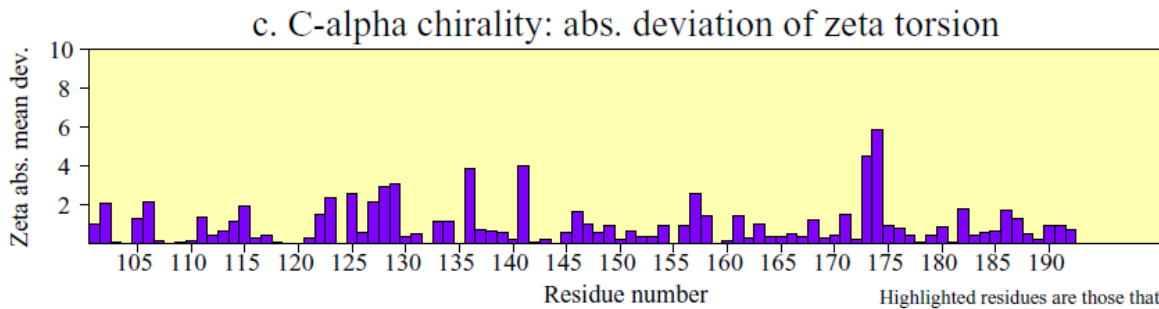
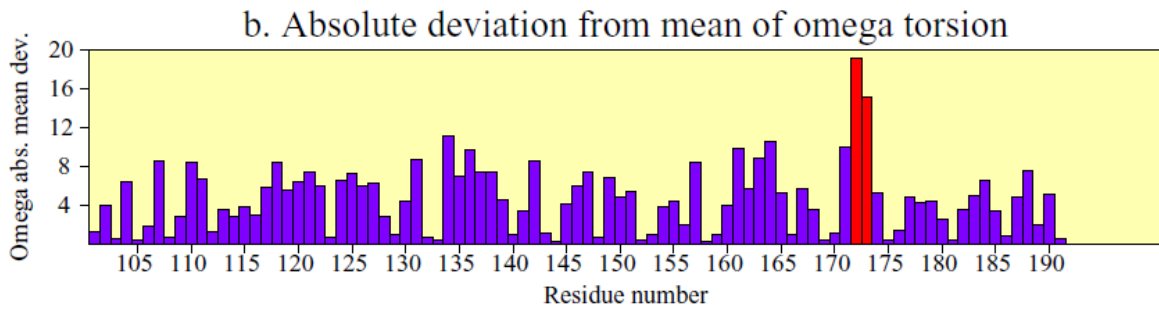
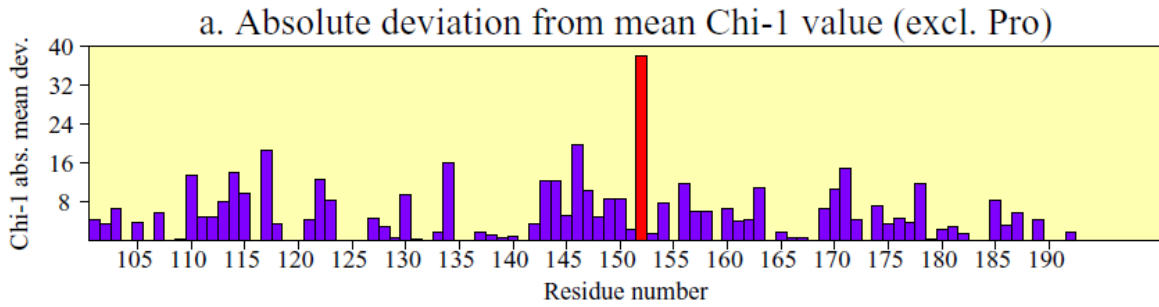


f. Max. deviation (see listing)

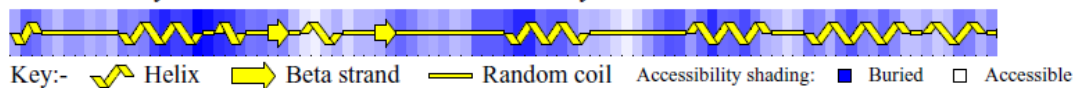


g. G-factors

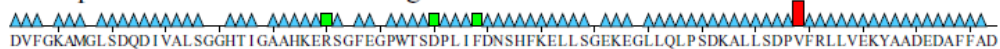




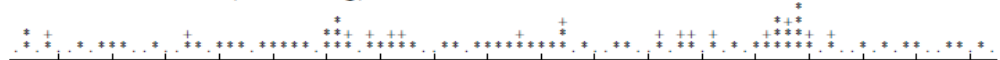
d. Secondary structure & estimated accessibility



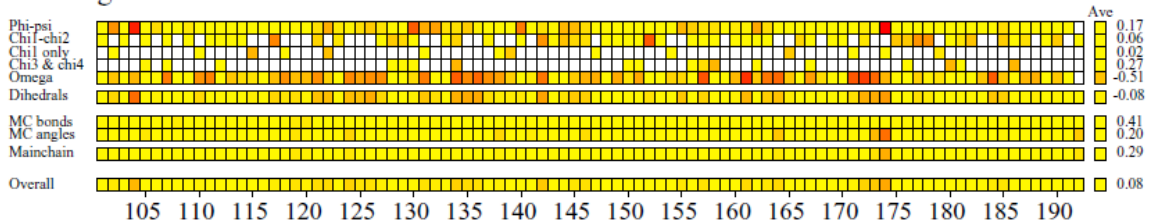
e. Sequence & Ramchandran regions



f. Max. deviation (see listing)

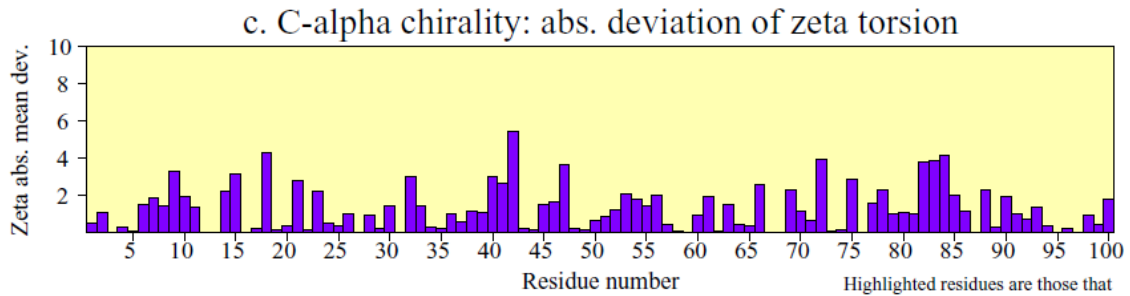
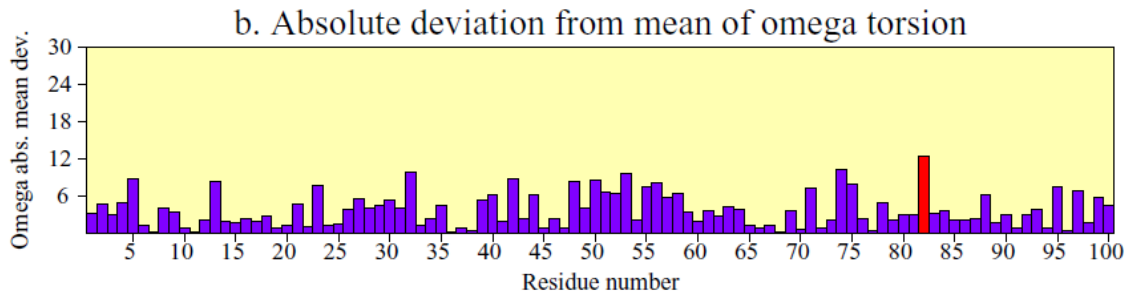
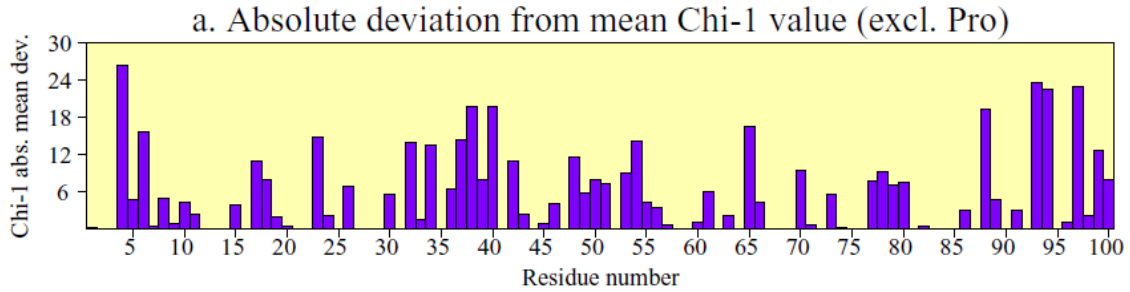


g. G-factors



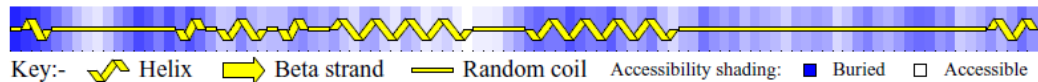
# Residue properties

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

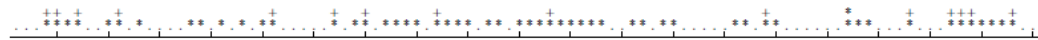
d. Secondary structure & estimated accessibility



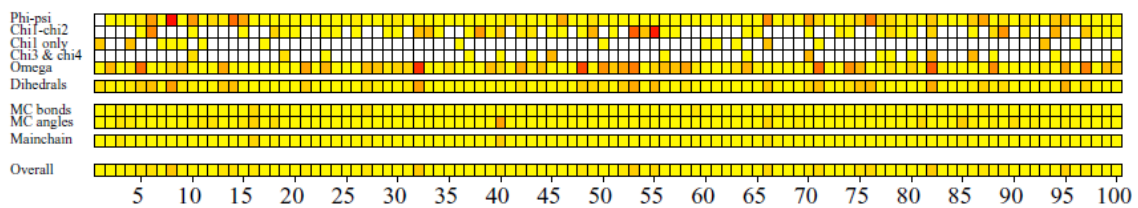
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

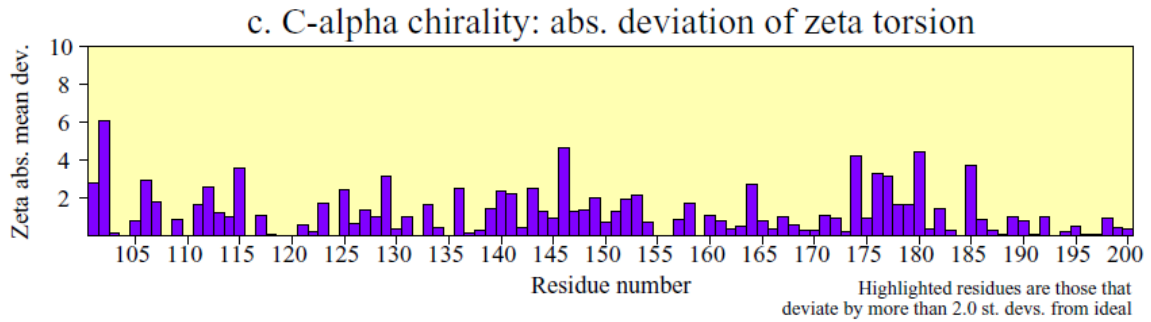
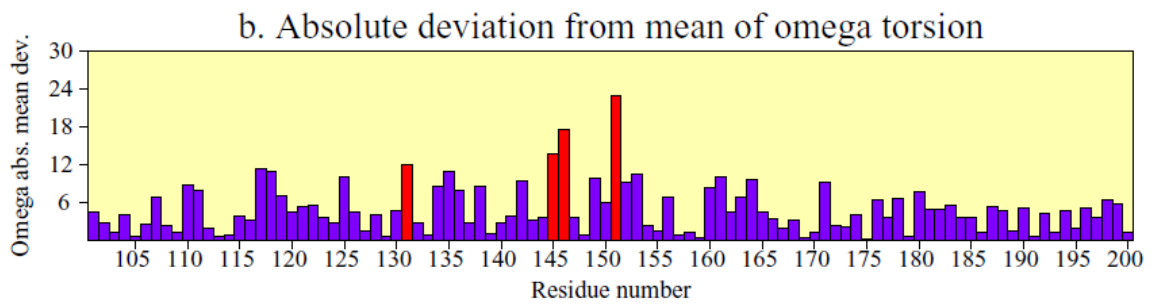
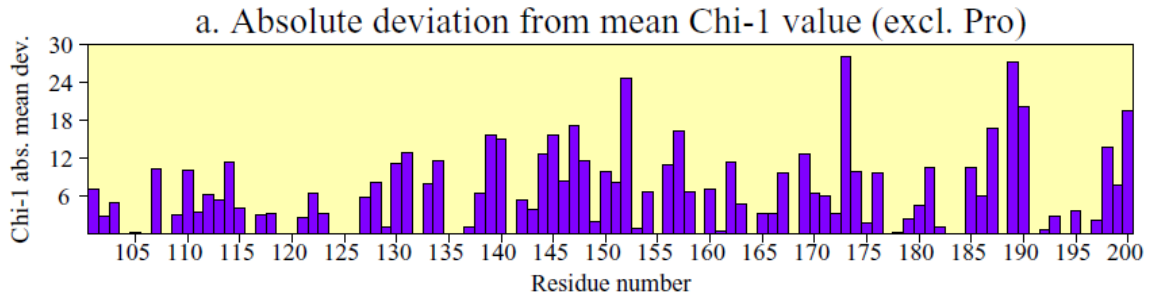
SAGTFDVKSTKTGGPFGT IKHPAELAHGANNGLDI AVRLLLEPIKAEFPI LSAYAFYQLAGVVAVEI TGGPEVPPFHPGREDKPEPPPEGRLP DATKGS DHLR

f. Max. deviation (see listing)

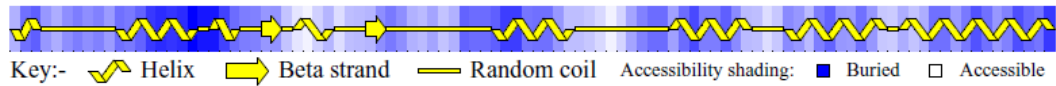


g. G-factors

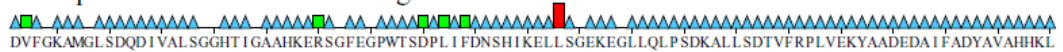




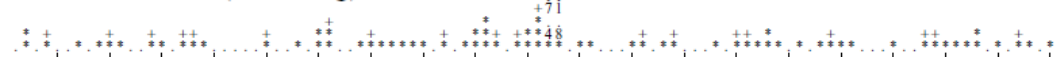
d. Secondary structure & estimated accessibility



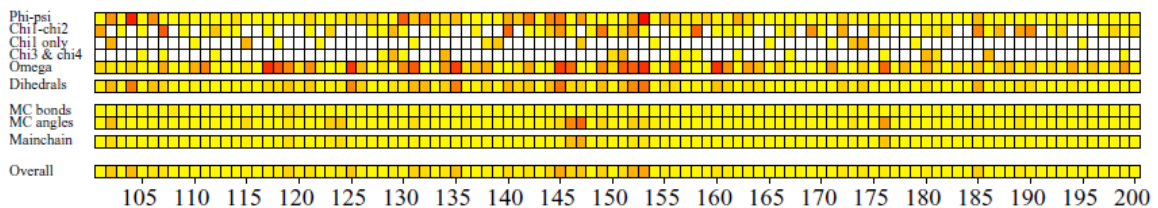
e. Sequence & Ramachandran regions



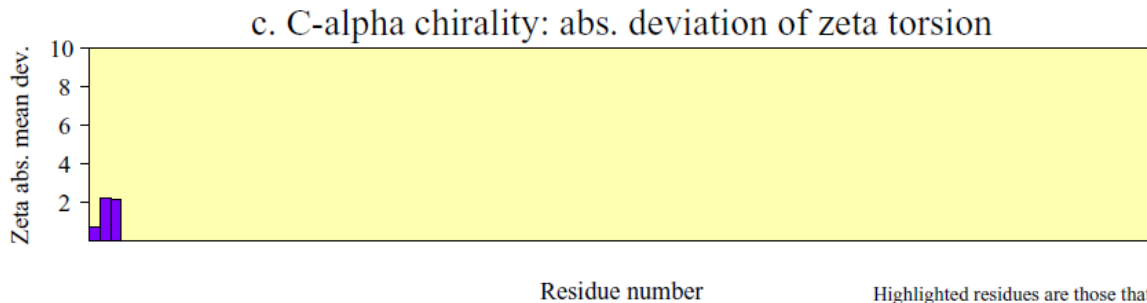
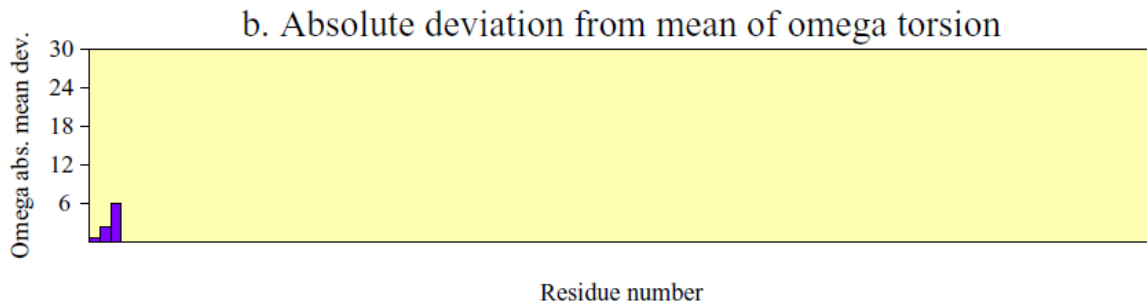
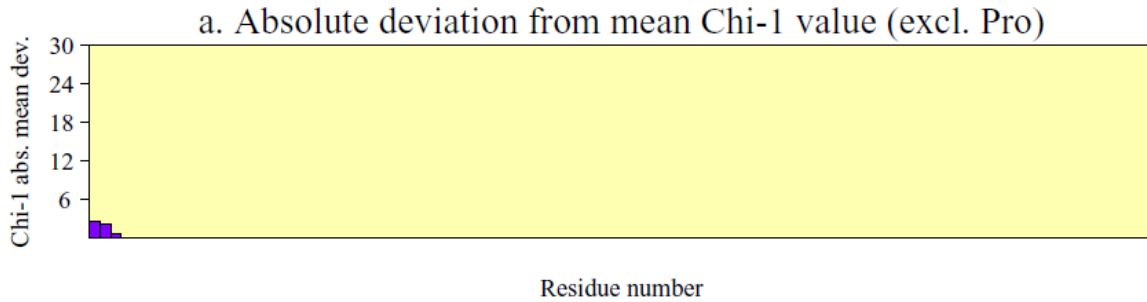
f. Max. deviation (see listing)



g. G-factors







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)

\* . \*

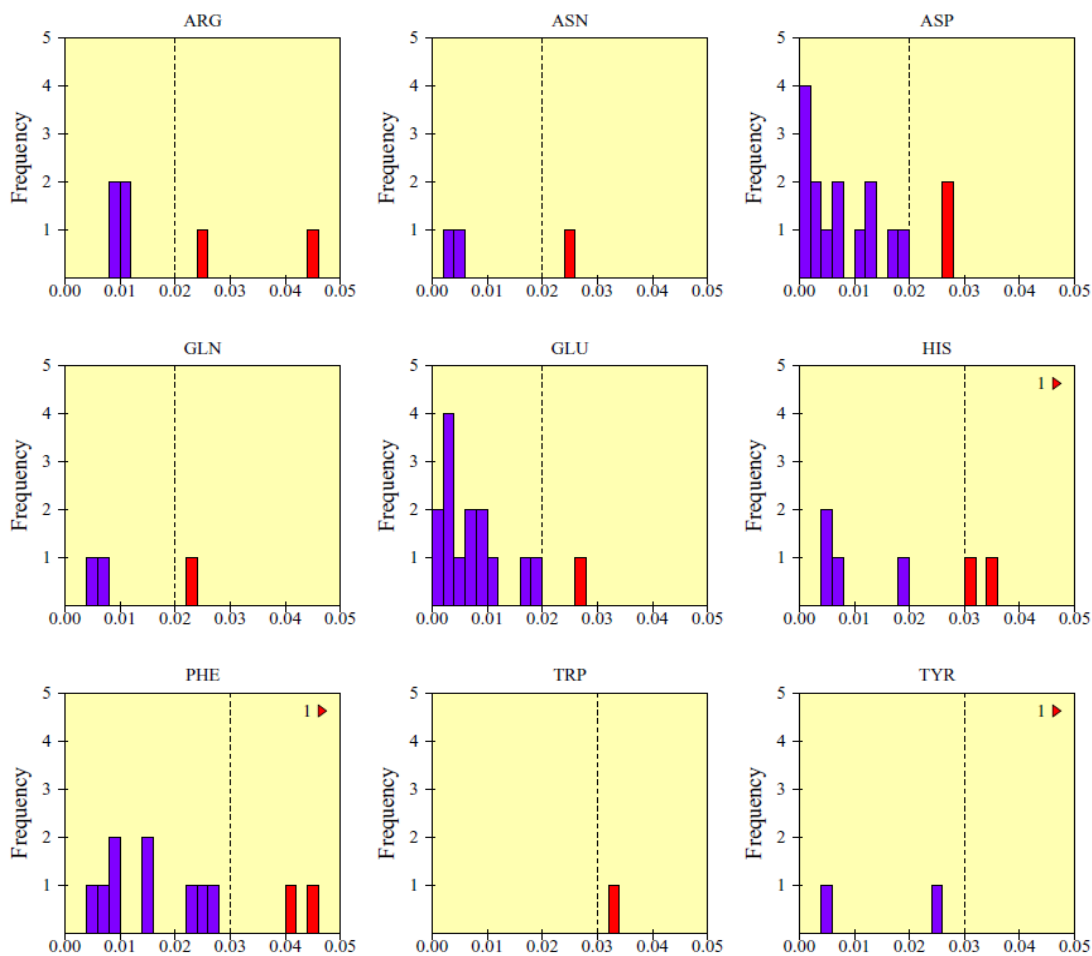
g. G-factors

	Ave
Phi-psi	0.11
Chi1-chi2	-0.05
Chi1 only	0.04
Chi3 & chi4	0.37
Omega	-0.42
Dihedrals	-0.08
MC bonds	0.36
MC angles	0.13
Mainchain	0.23
Overall	0.05

f) RMS distance from planarity

# RMS distances from planarity

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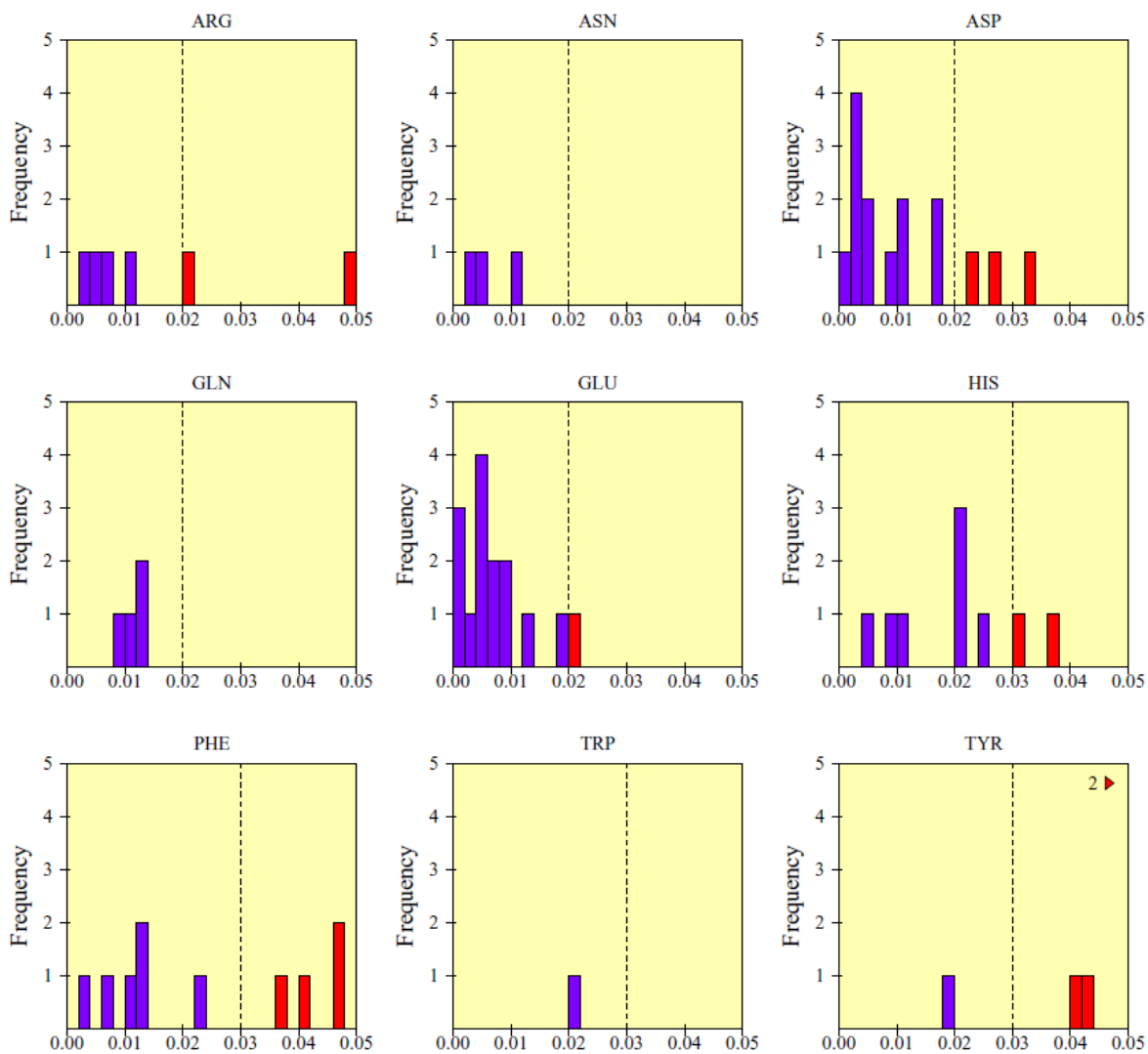


Histograms showing RMS distances of planar atoms from best-fit plane. Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

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

# RMS distances from planarity

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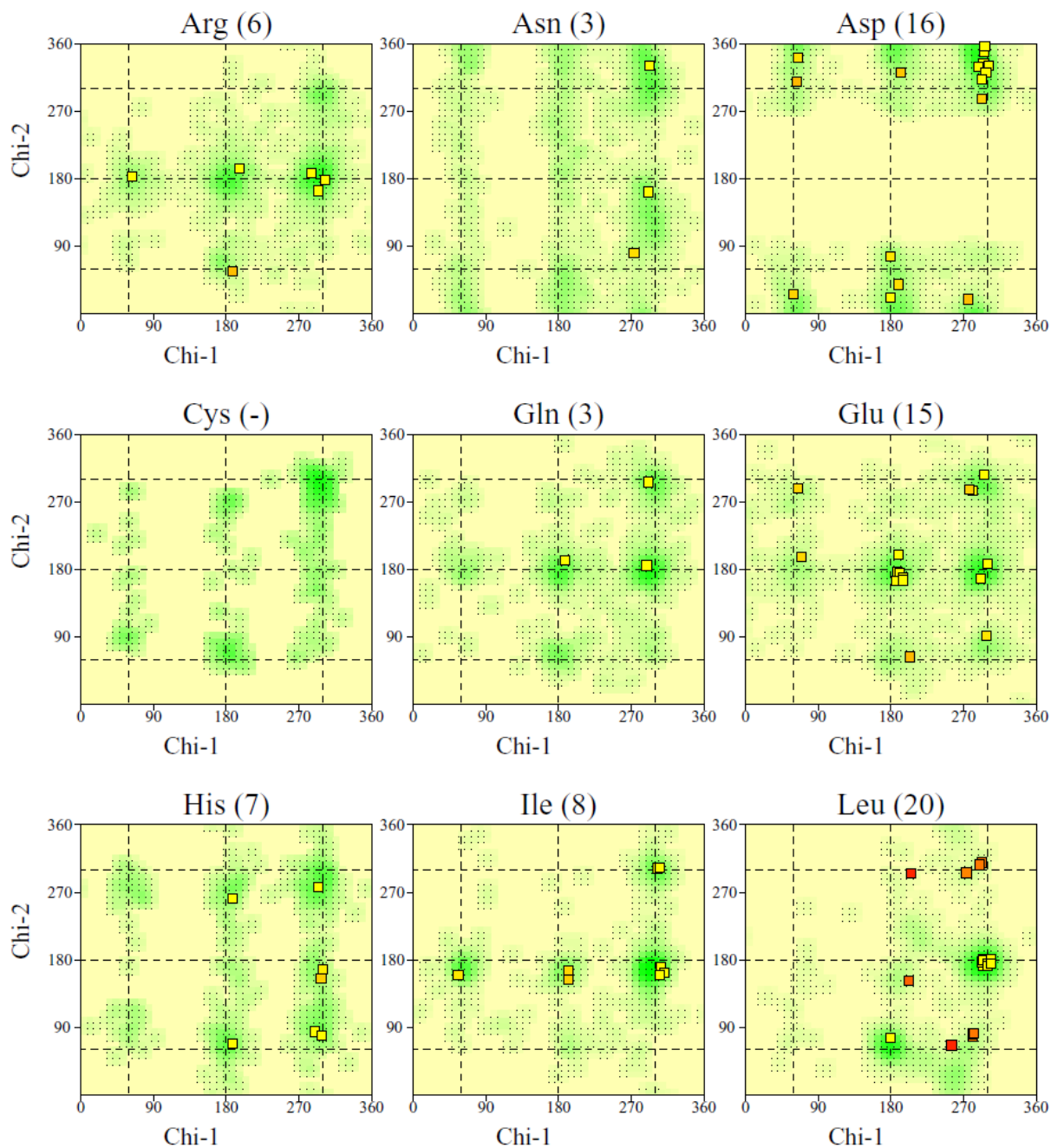
Histograms showing RMS distances of planar atoms from best-fit plane.  
 Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

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

g) All Chi1-Chi2 plots of ICP 7035 and ICPL 84023 in pigeon pea

## Chi1-Chi2 plots

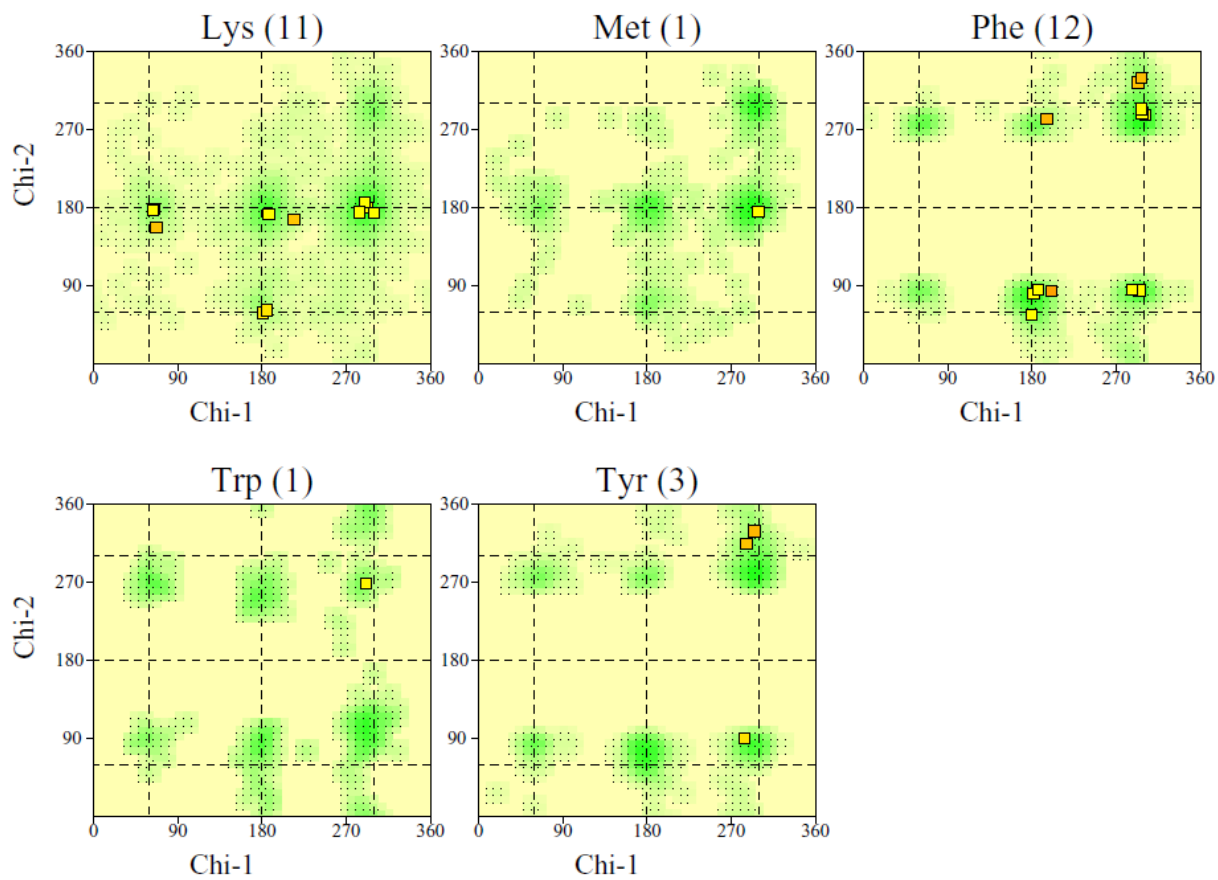
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Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0Å or better.

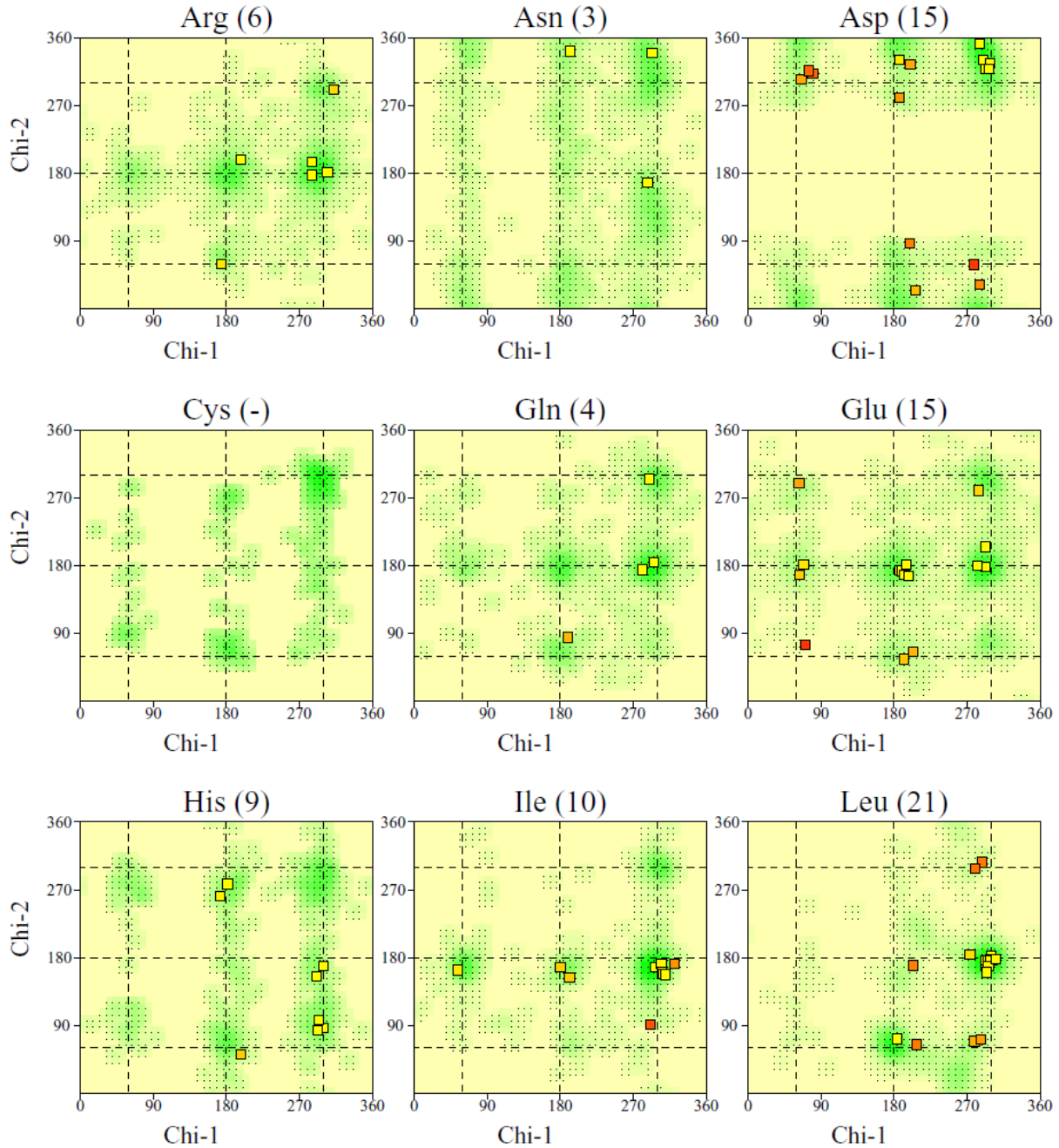
# Chi1-Chi2 plots

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# Chi1-Chi2 plots

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

# Chi1-Chi2 plots

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