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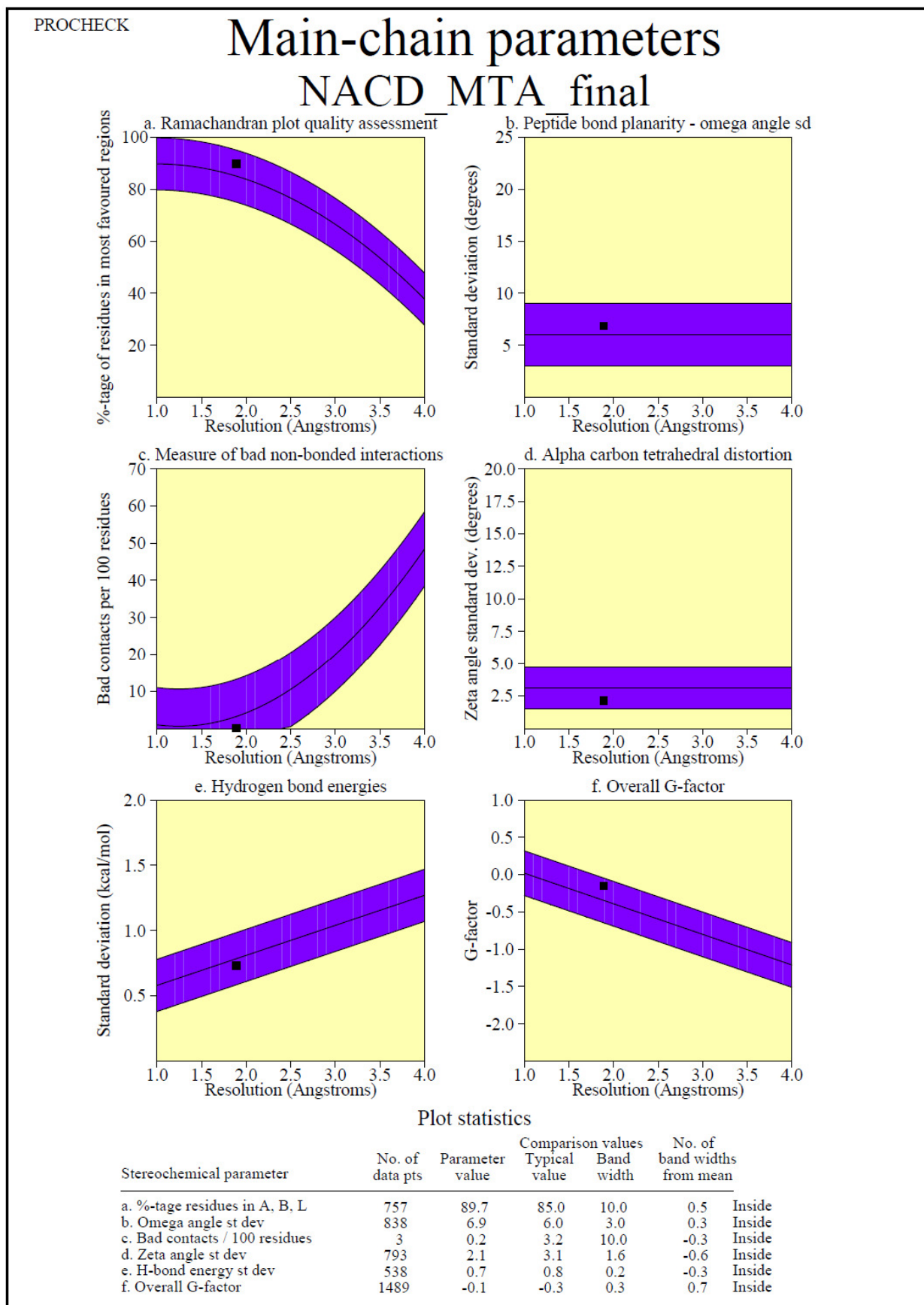
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Appendix I: PROCHECK results for the *Pf*SpdS-NACD-MTA crystal structure

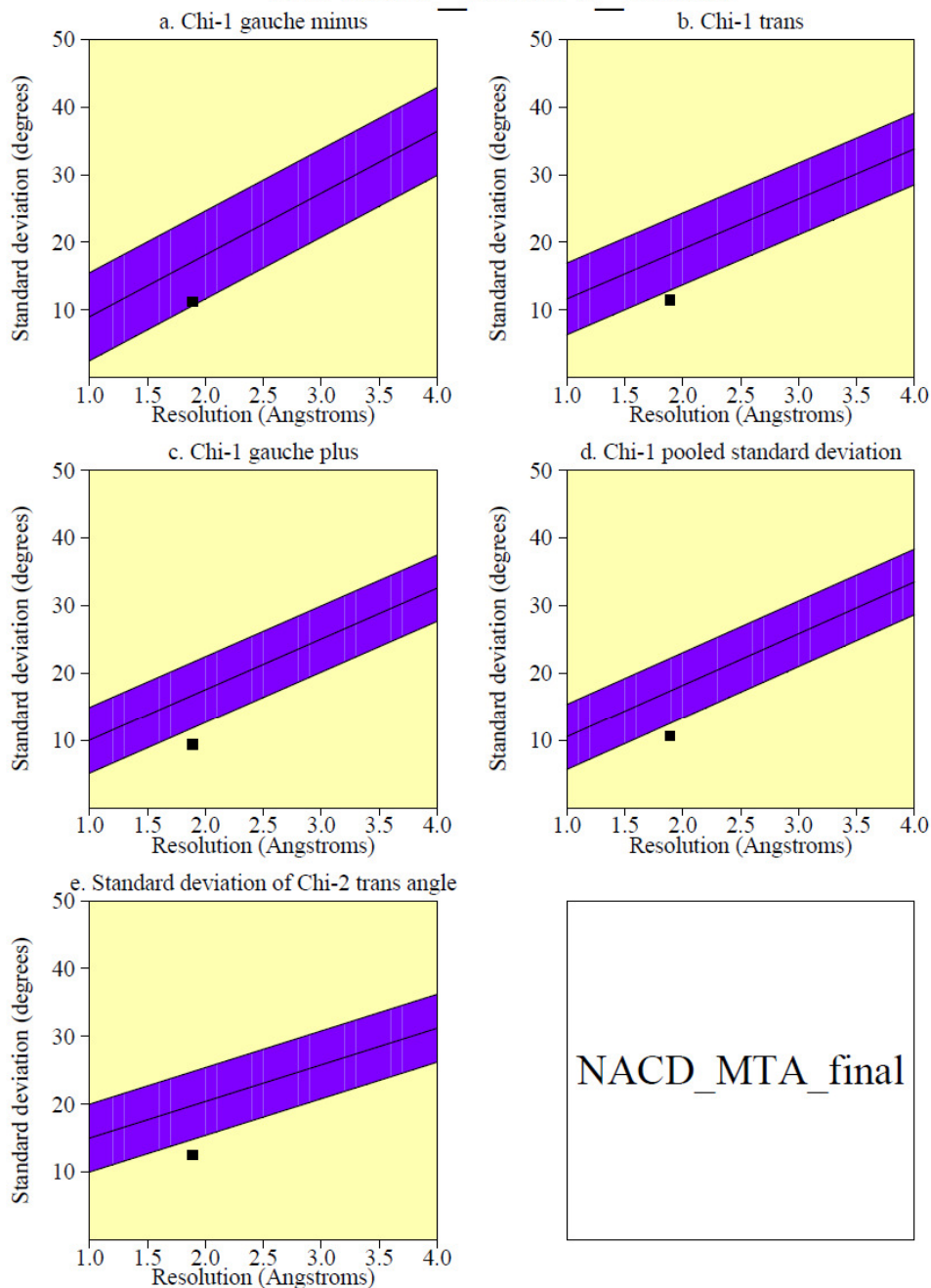




PROCHECK

Side-chain parameters

NACD_MTA_final



Plot statistics

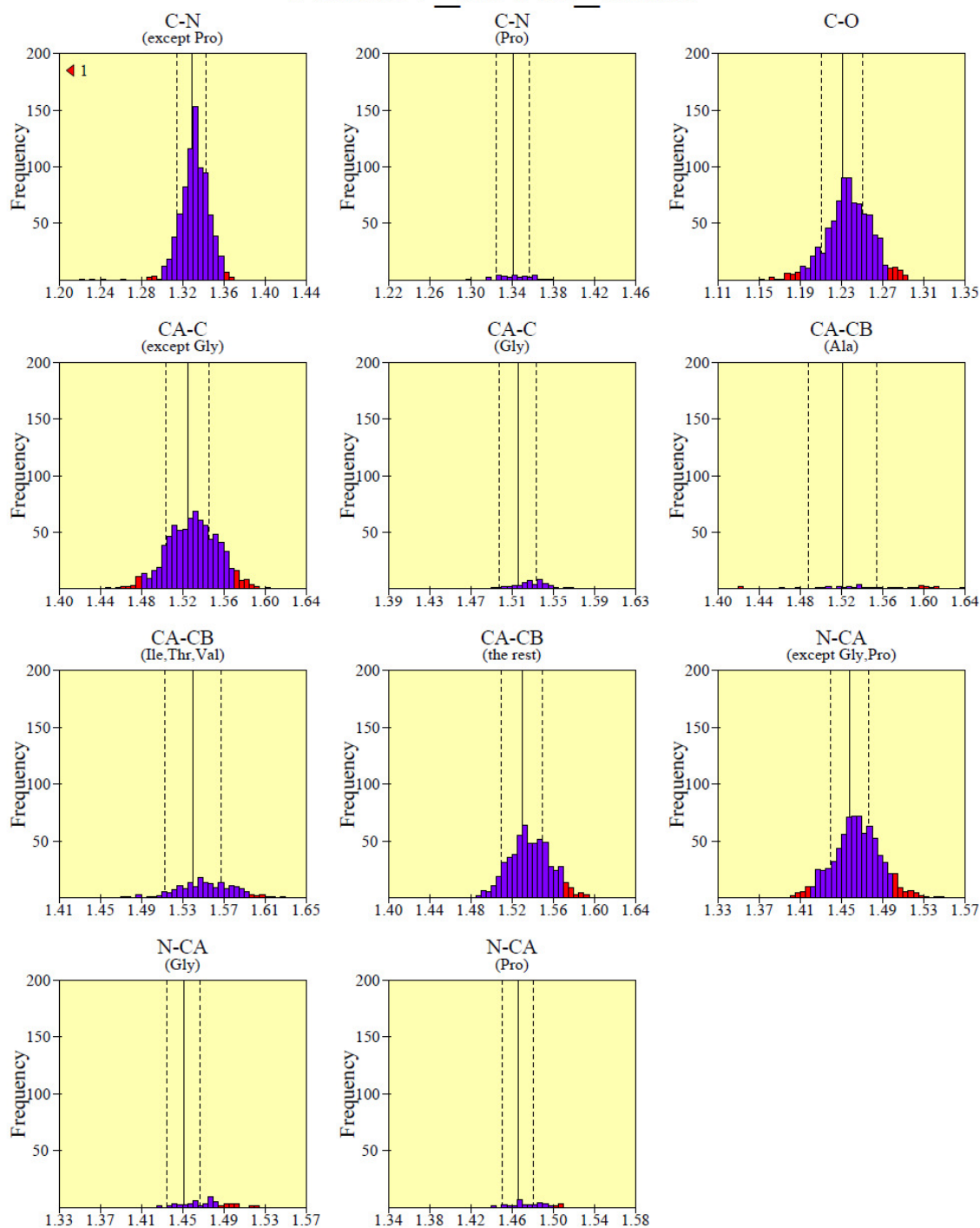
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. Chi-1 gauche minus st dev	125	11.2	17.1	6.5	-0.9	Inside
b. Chi-1 trans st dev	230	11.5	18.2	5.3	-1.3	BETTER
c. Chi-1 gauche plus st dev	371	9.3	16.7	4.9	-1.5	BETTER
d. Chi-1 pooled st dev	726	10.6	17.3	4.8	-1.4	BETTER
e. Chi-2 trans st dev	243	12.5	19.8	5.0	-1.5	BETTER

PROCHECK

Page 1

Main-chain bond lengths

NACD_MTA_final



Black bars > 2.0 st. devs. from mean.

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

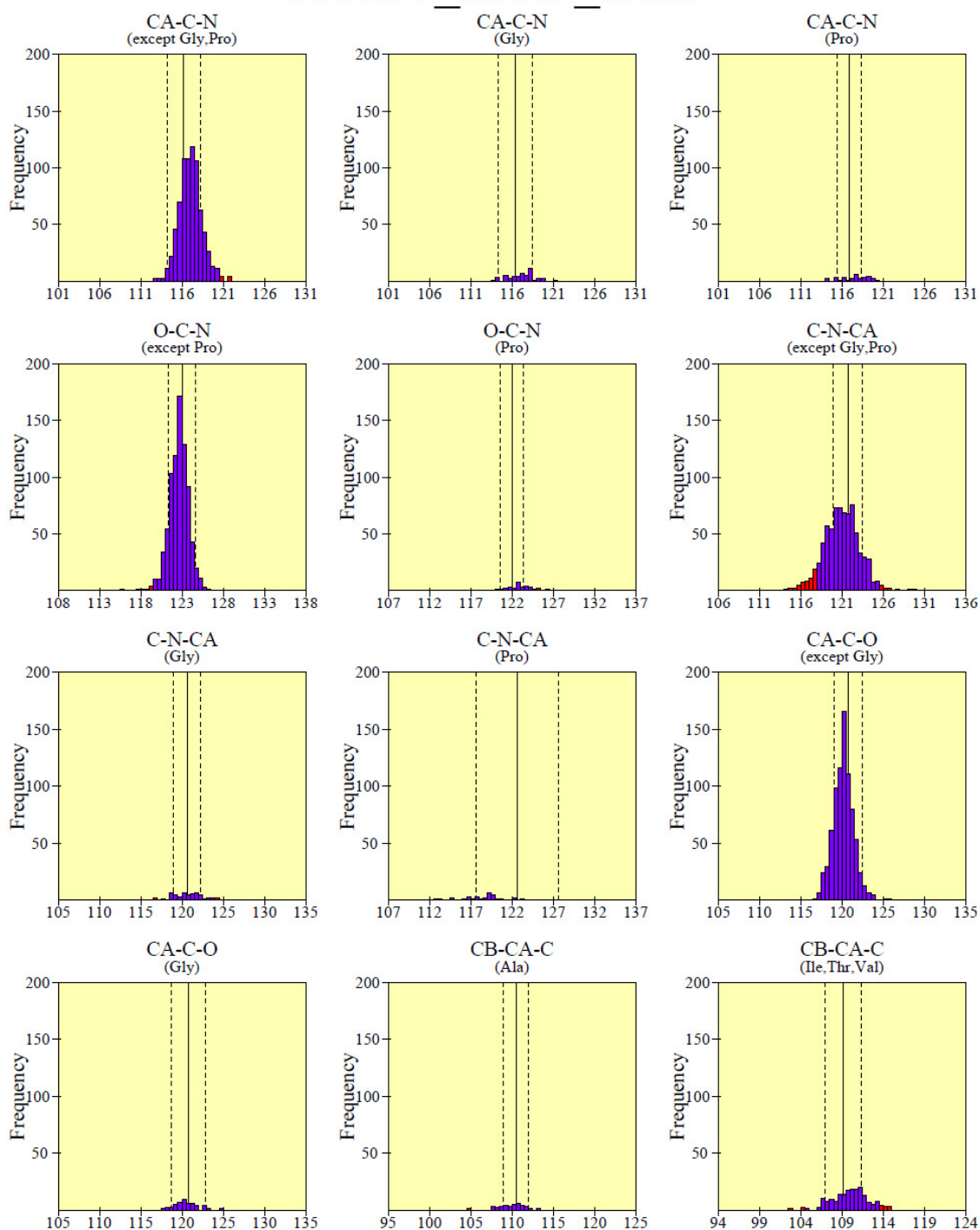
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

PROCHECK

Page 1

Main-chain bond angles

NACD_MTA_final



Black bars > 2.0 st. devs. from mean.

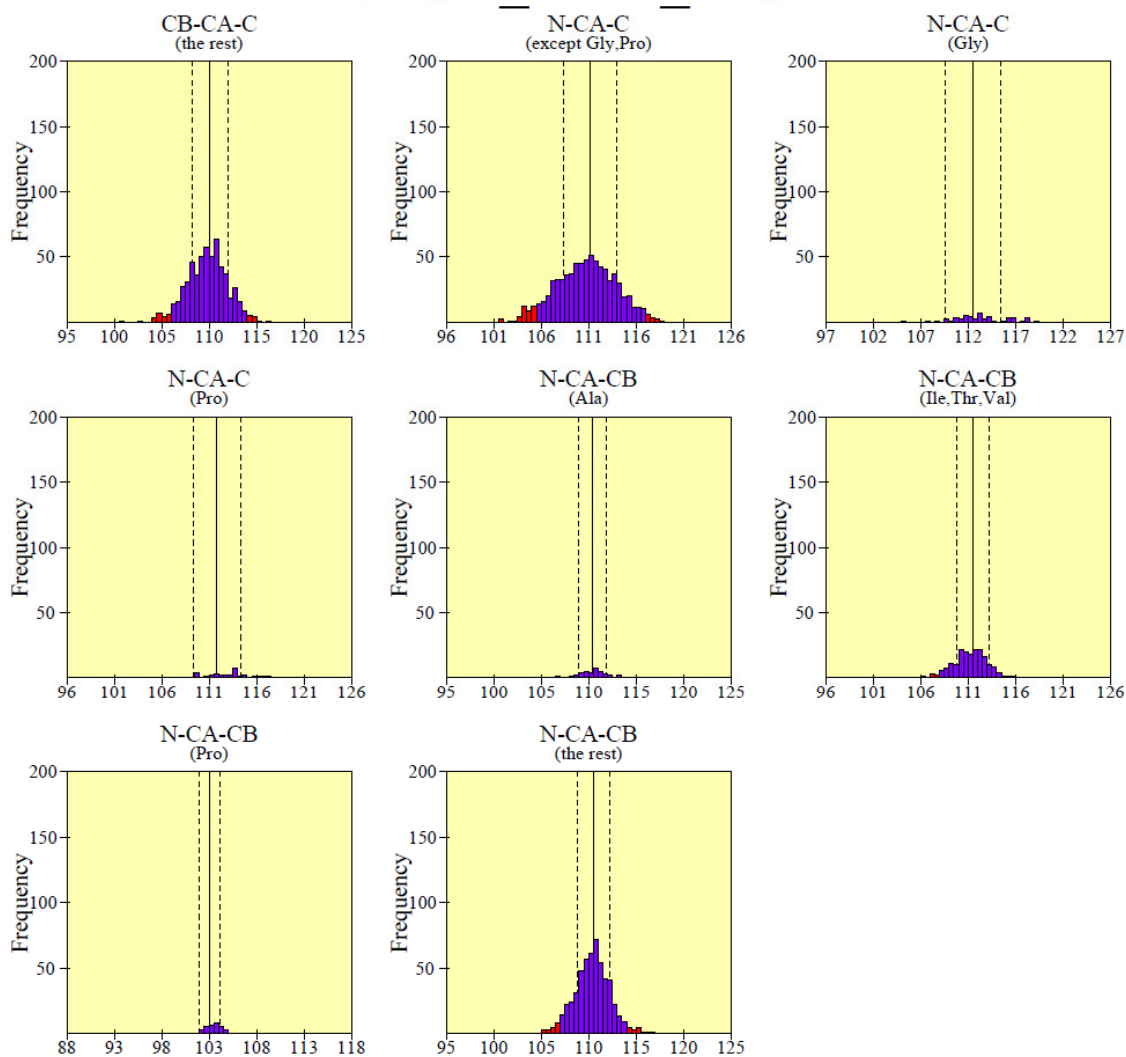
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.



PROCHECK

Page 2

Main-chain bond angles NACD_MTA_final



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.

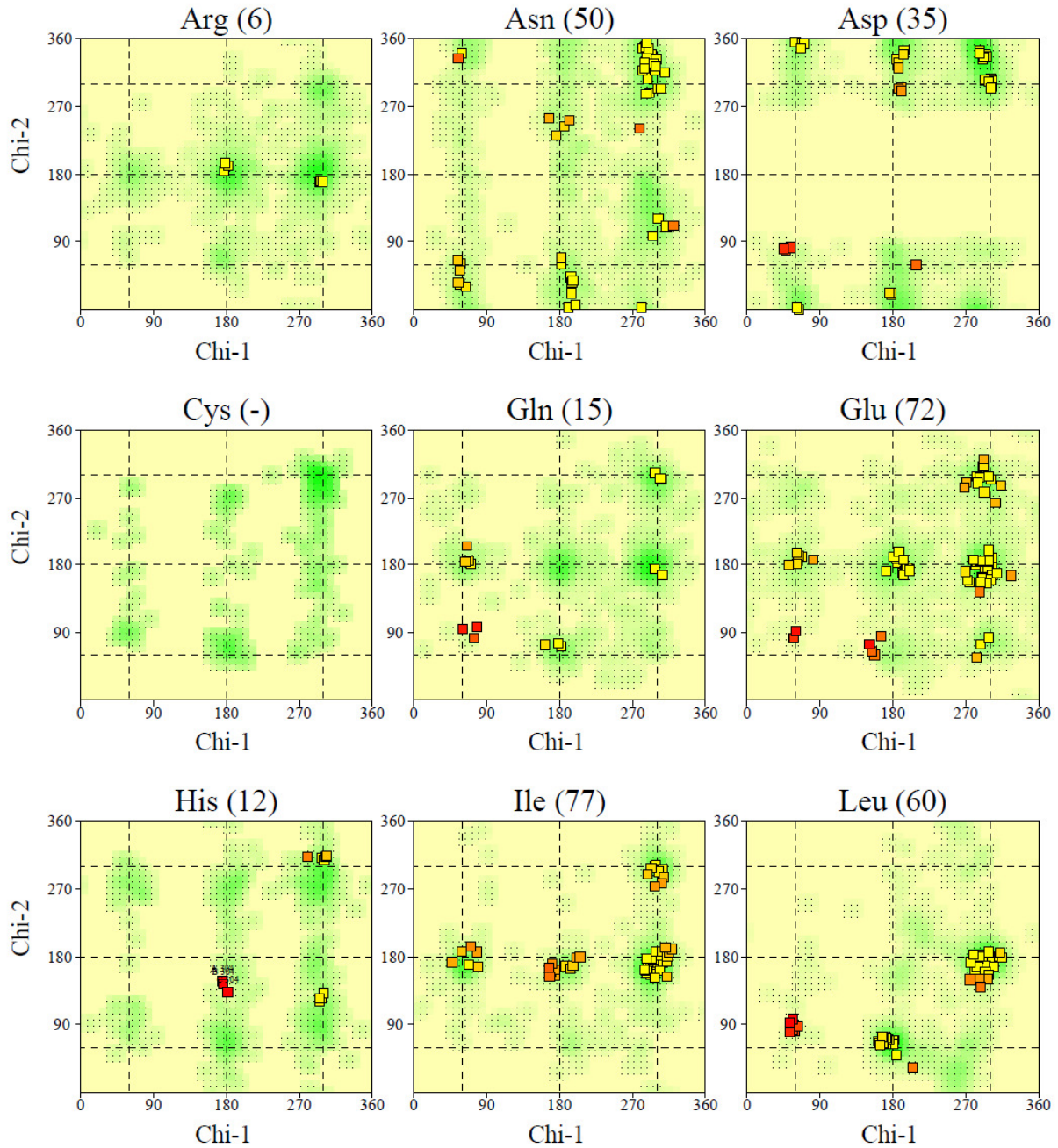


PROCHECK

Page 1

Chi1-Chi2 plots

NACD_MTA_final



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.

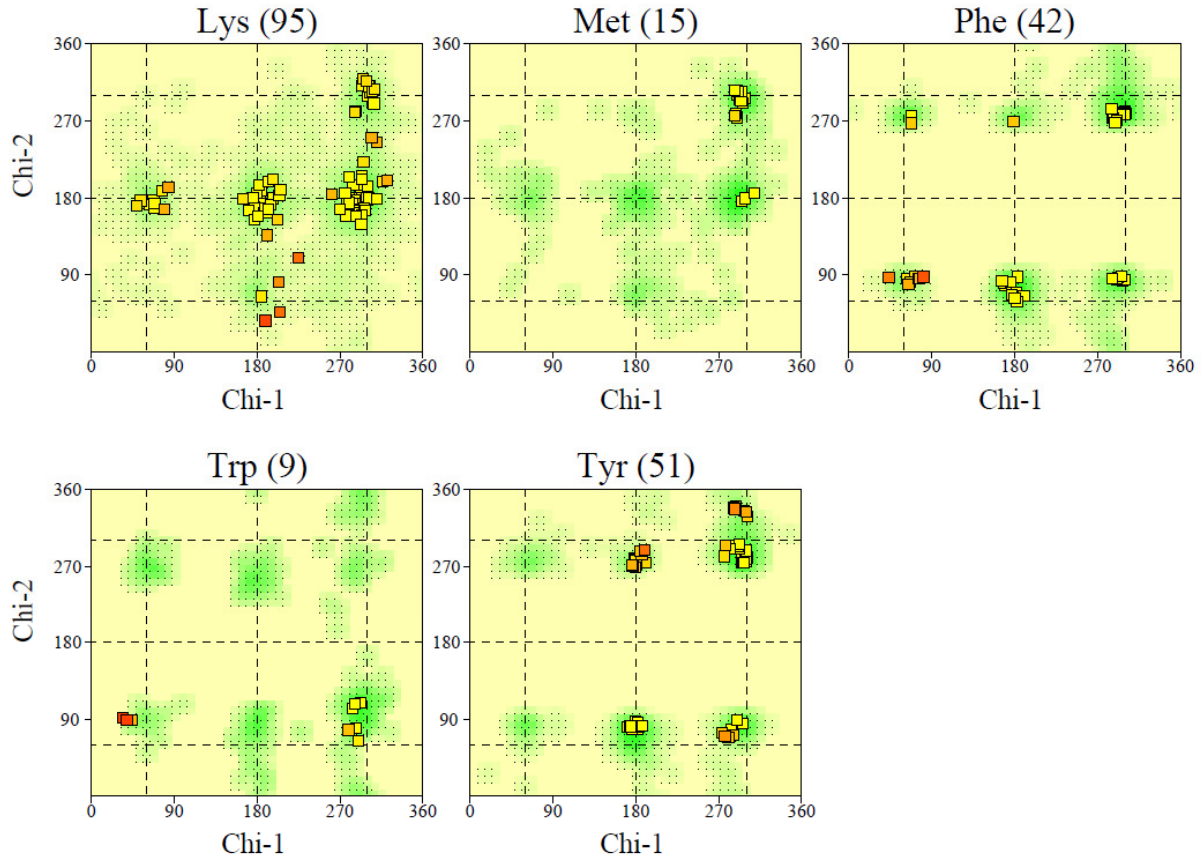


PROCHECK

Page 2

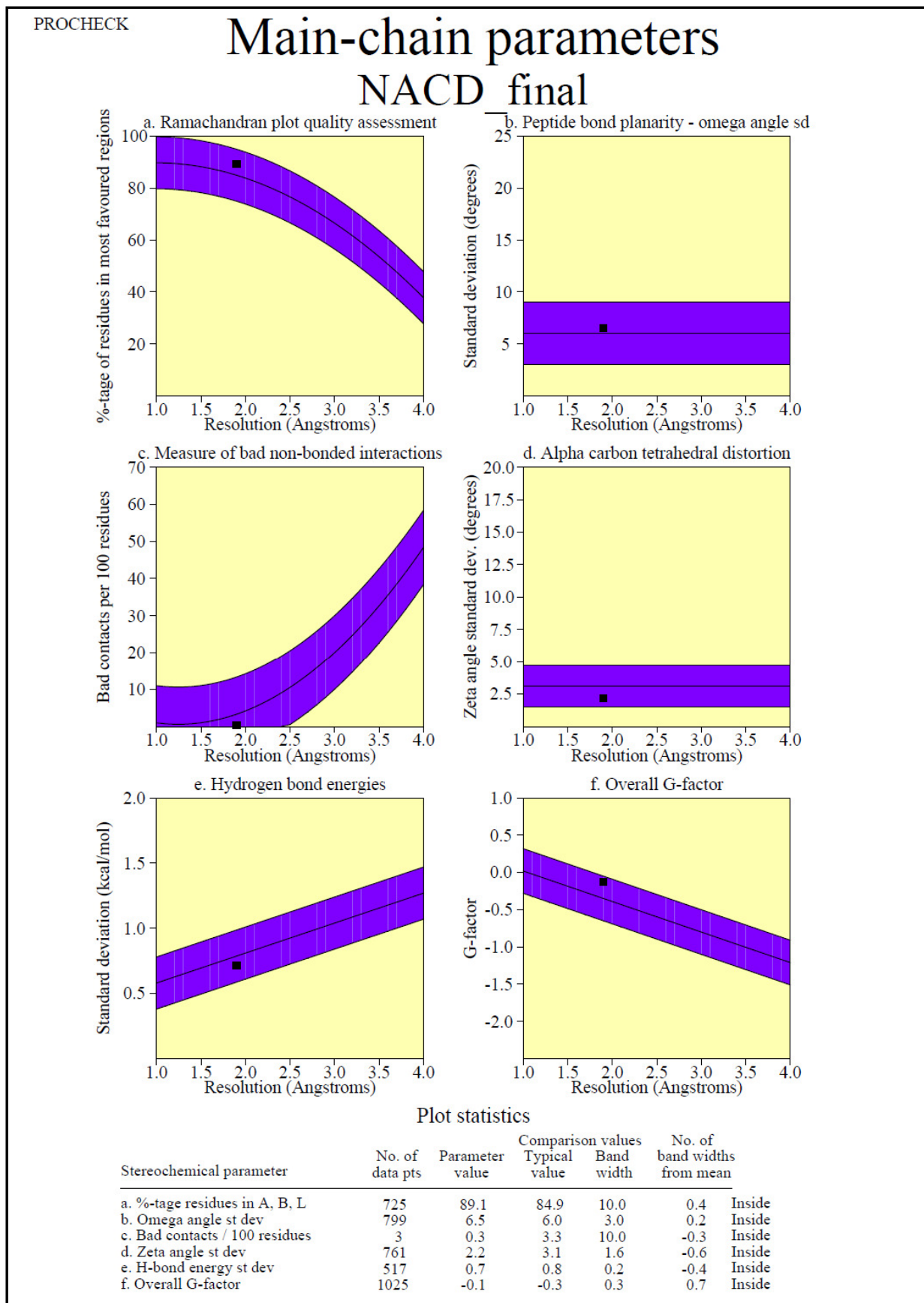
Chi1-Chi2 plots

NACD_MTA_final



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.

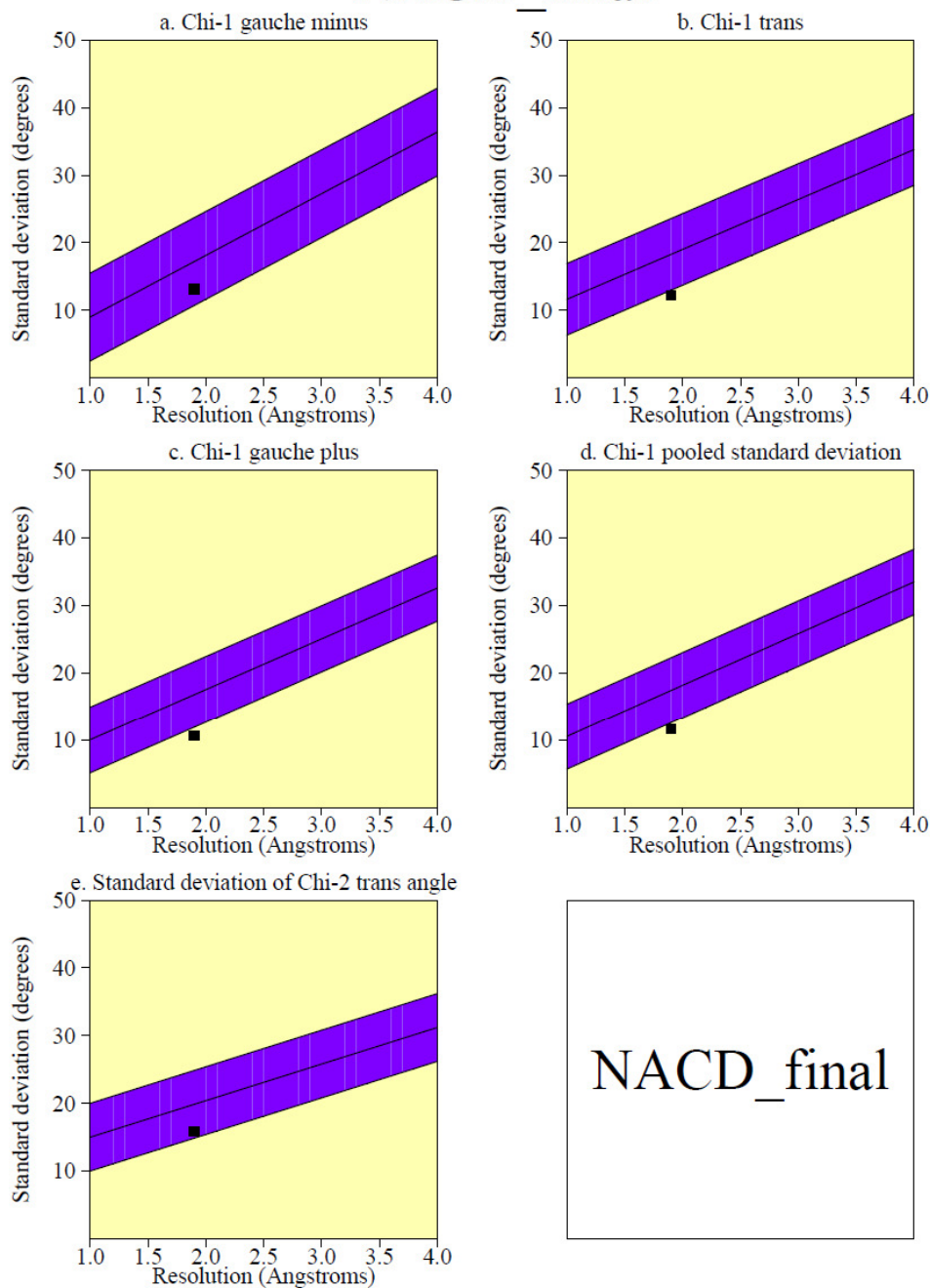
Appendix II: PROCHECK results for the *PfSpdS*-NACD crystal structure



PROCHECK

Side-chain parameters

NACD_final



NACD_final

Plot statistics

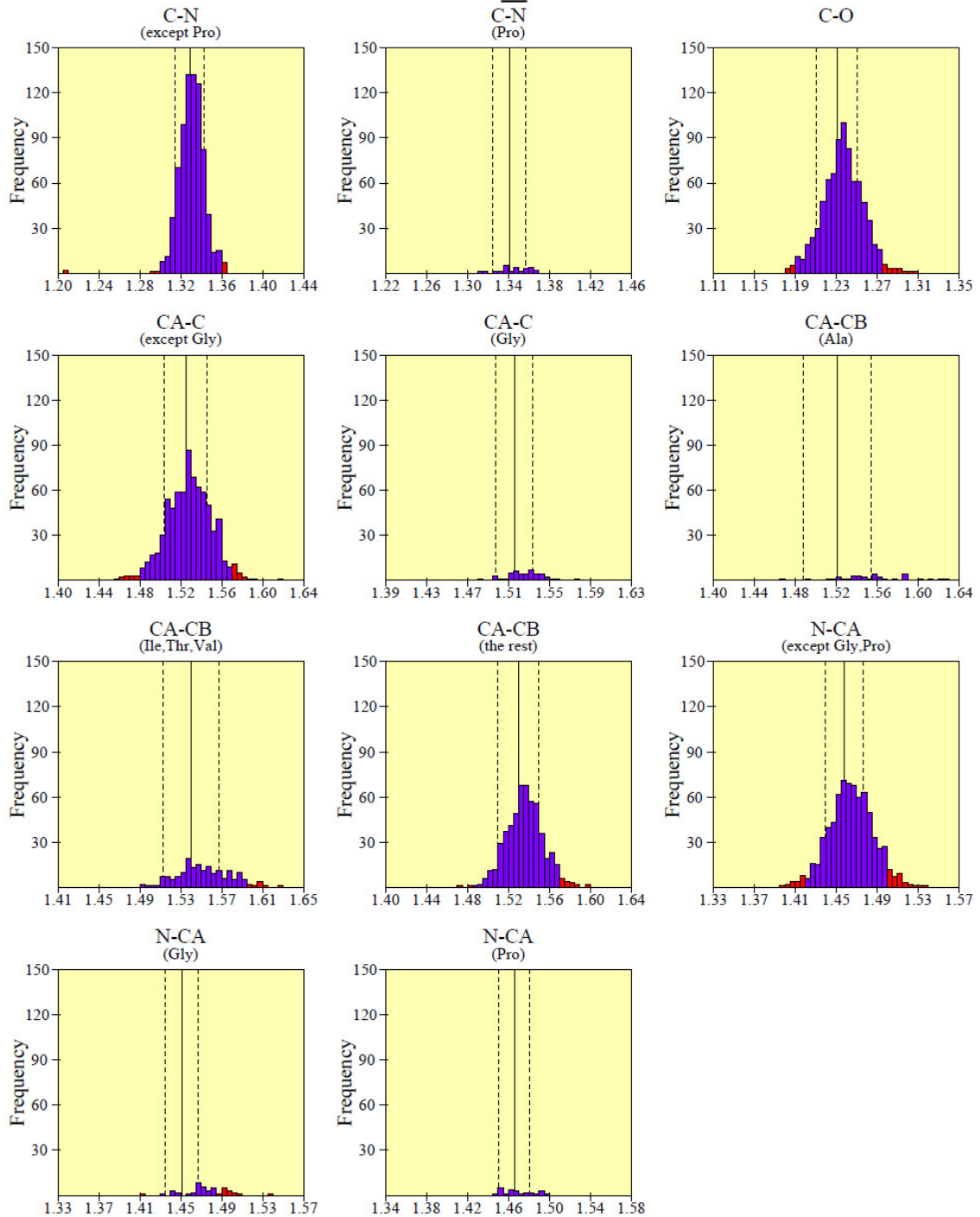
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. Chi-1 gauche minus st dev	108	13.1	17.2	6.5	-0.6	Inside
b. Chi-1 trans st dev	233	12.3	18.3	5.3	-1.1	BETTER
c. Chi-1 gauche plus st dev	363	10.7	16.8	4.9	-1.2	BETTER
d. Chi-1 pooled st dev	704	11.7	17.4	4.8	-1.2	BETTER
e. Chi-2 trans st dev	236	15.9	19.9	5.0	-0.8	Inside



PROCHECK

Page 1

Main-chain bond lengths NACD_final



Black bars > 2.0 st. devs. from mean.

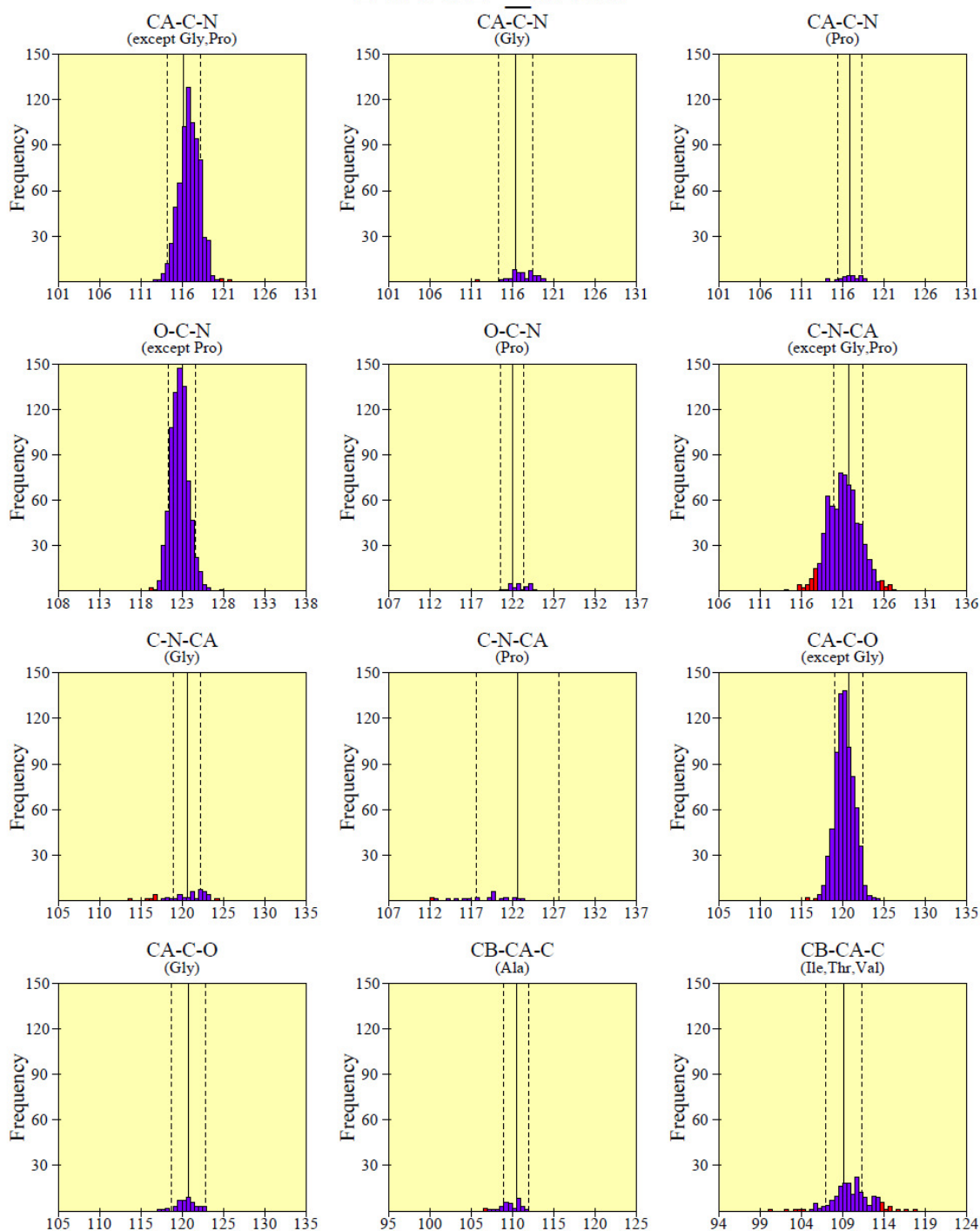
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

PROCHECK

Page 1

Main-chain bond angles

NACD_final



Black bars > 2.0 st. devs. from mean.

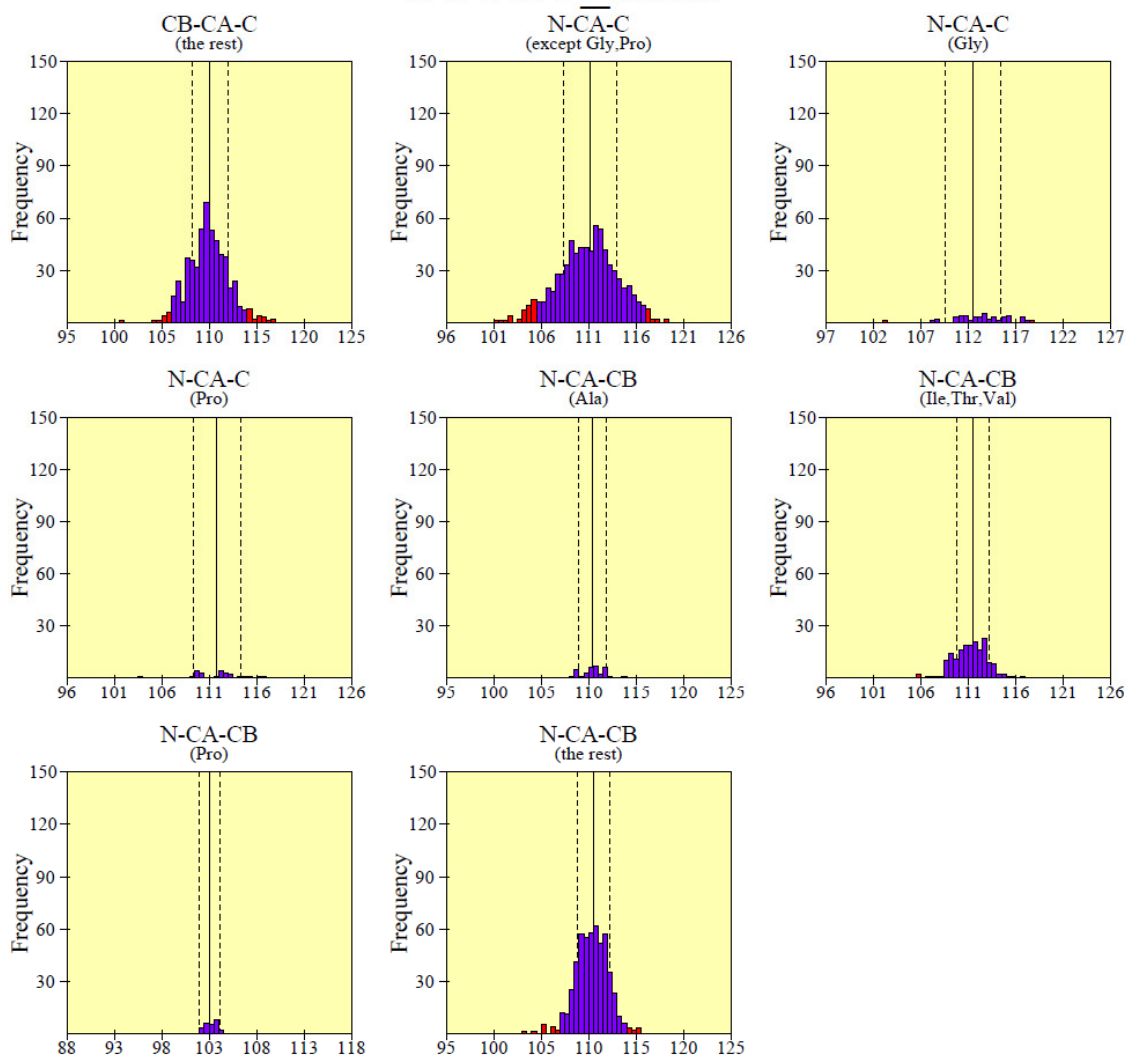
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.



PROCHECK

Page 2

Main-chain bond angles NACD_final



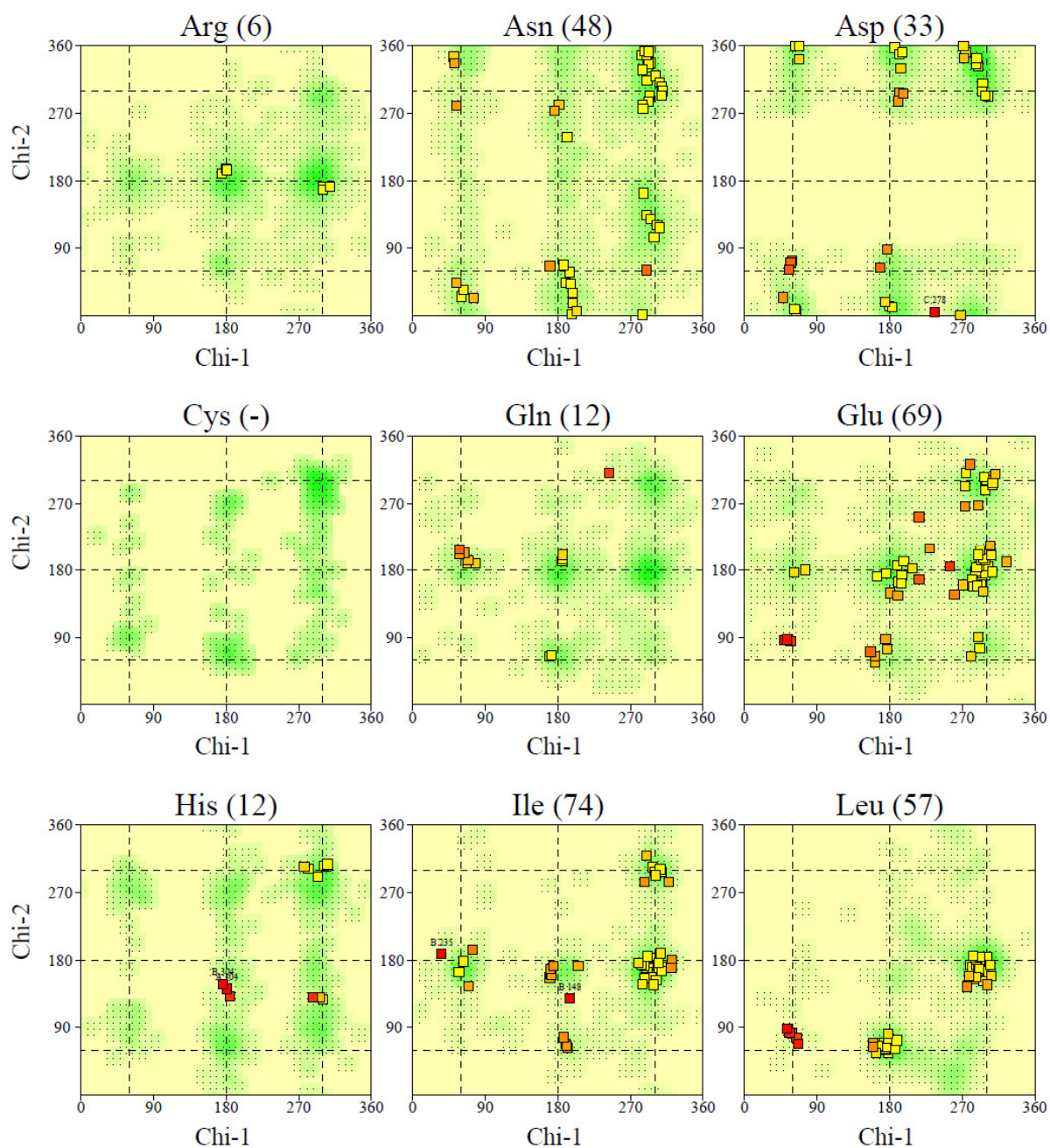
Black bars > 2.0 st. devs. from mean.

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

PROCHECK

Page 1

Chi1-Chi2 plots NACD_final



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.

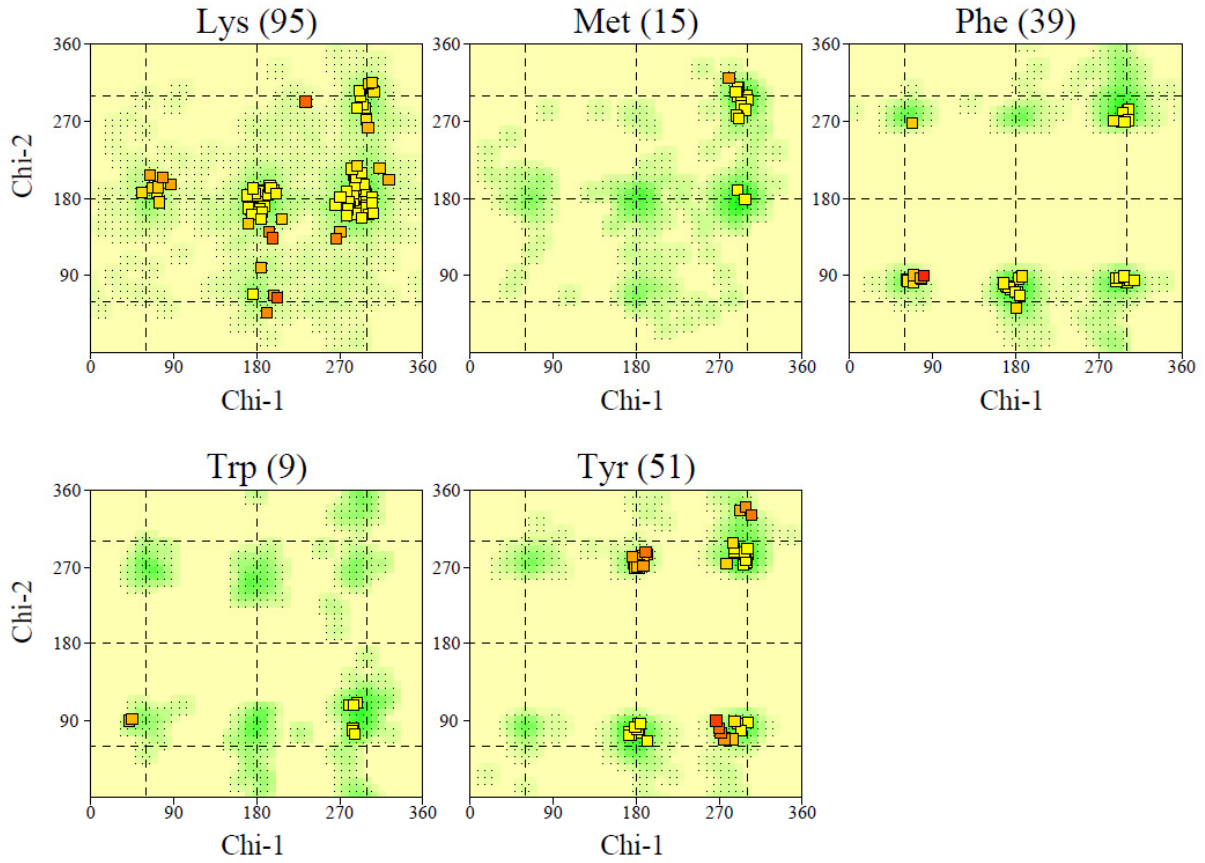


PROCHECK

Page 2

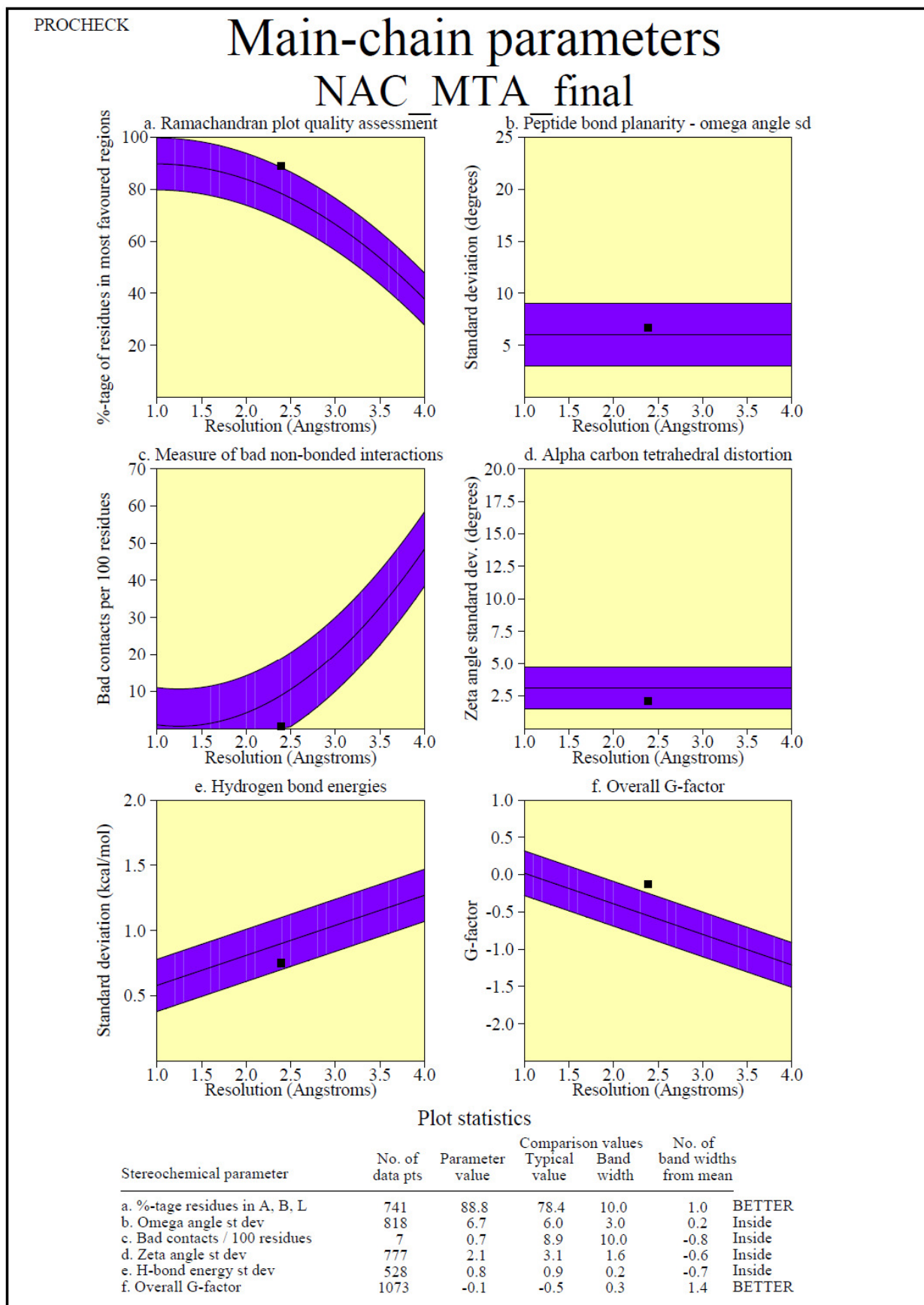
Chi1-Chi2 plots

NACD_final



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.

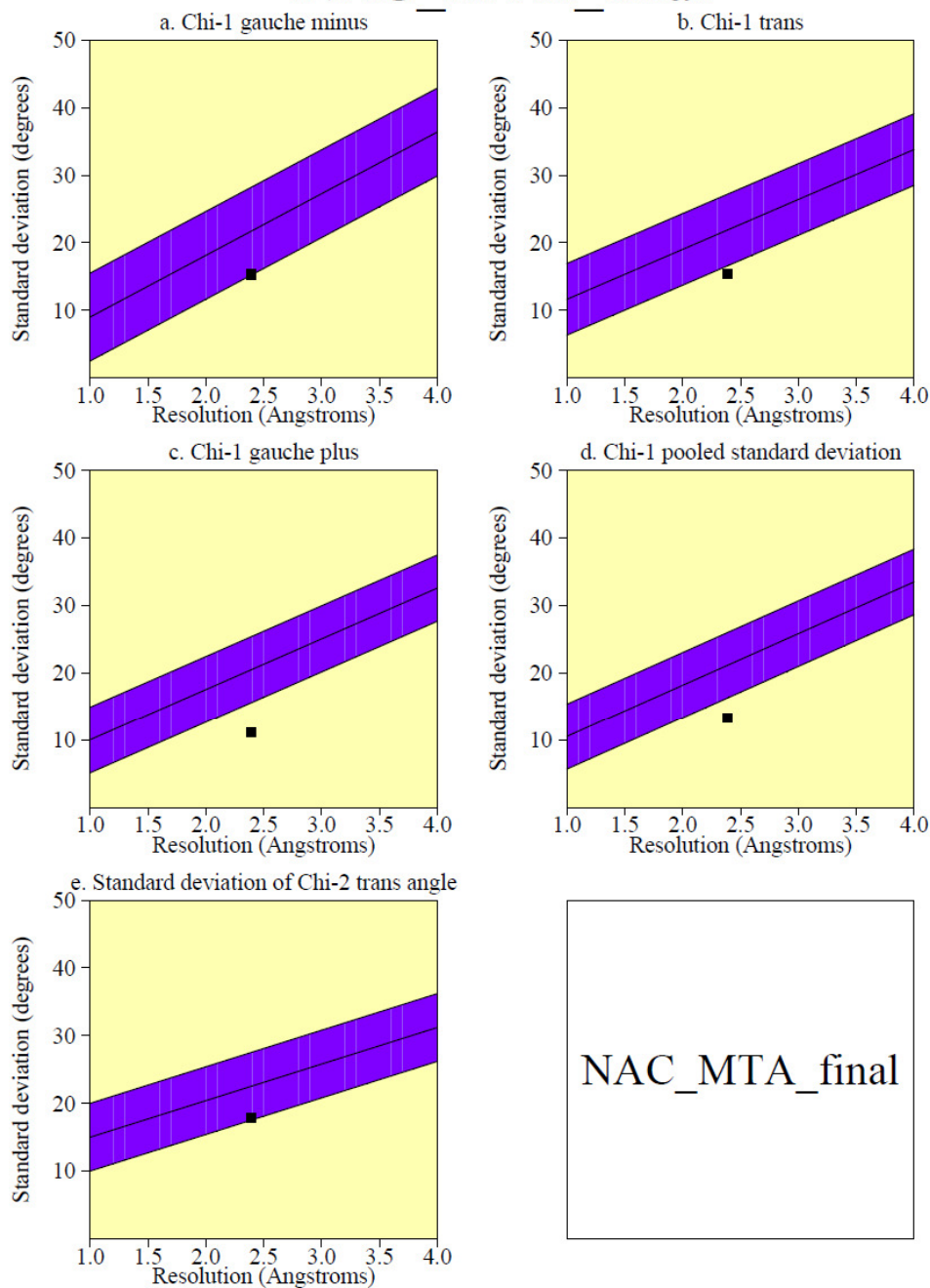
Appendix III: PROCHECK results for the *Pf*SpdS-NAC-MTA crystal structure



PROCHECK

Side-chain parameters

NAC_MTA_final



NAC_MTA_final

Plot statistics

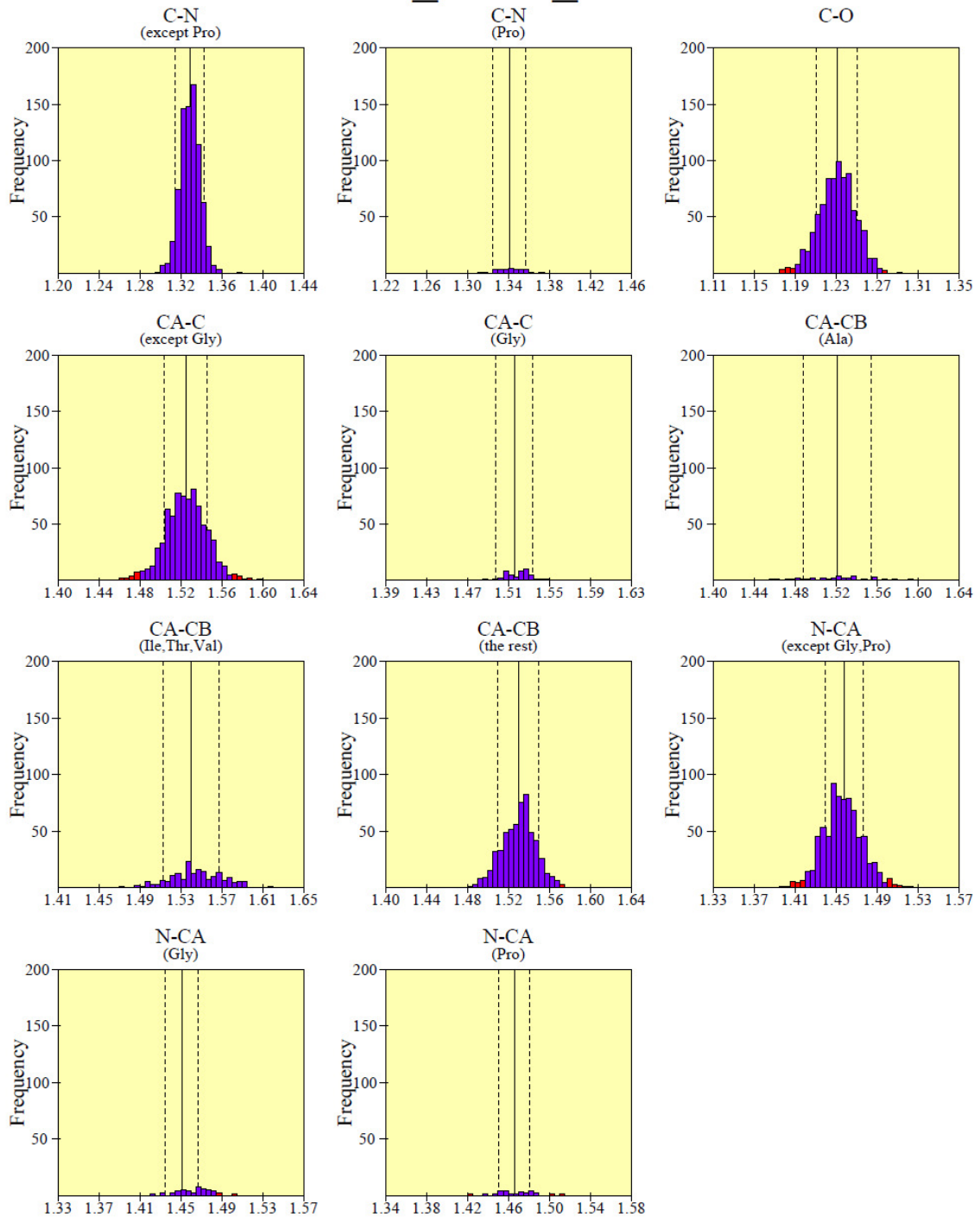
Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. Chi-1 gauche minus st dev	123	15.3	21.7	6.5	-1.0	Inside
b. Chi-1 trans st dev	234	15.3	21.9	5.3	-1.2	BETTER
c. Chi-1 gauche plus st dev	360	11.2	20.5	4.9	-1.9	BETTER
d. Chi-1 pooled st dev	717	13.3	21.2	4.8	-1.6	BETTER
e. Chi-2 trans st dev	238	17.9	22.5	5.0	-0.9	Inside



PROCHECK

Page 1

Main-chain bond lengths NAC_MTA_final



Black bars > 2.0 st. devs. from mean.

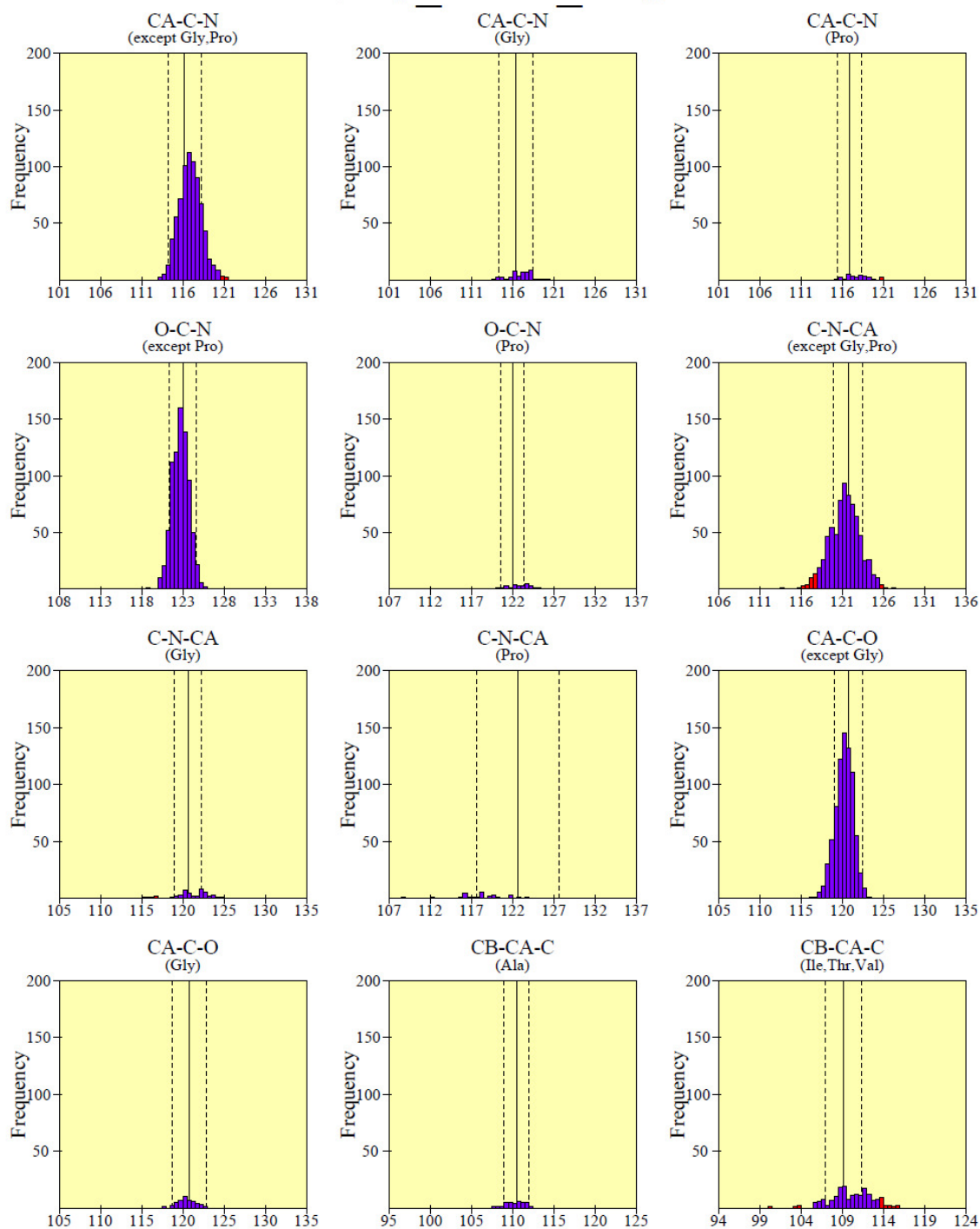
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

PROCHECK

Page 1

Main-chain bond angles

NAC_MTA_final



Black bars > 2.0 st. devs. from mean.

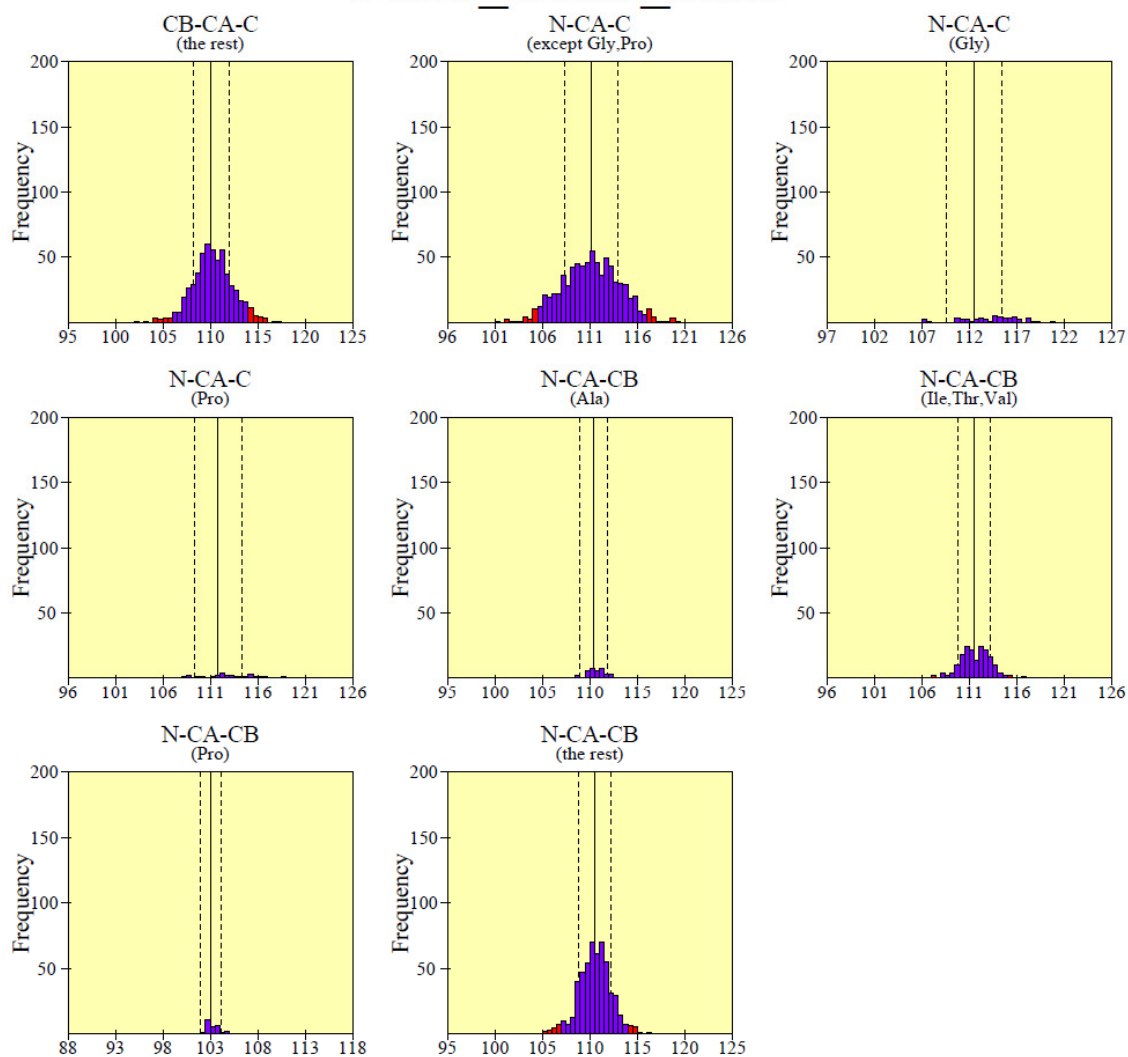
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.



PROCHECK

Page 2

Main-chain bond angles NAC_MTA_final



Black bars > 2.0 st. devs. from mean.

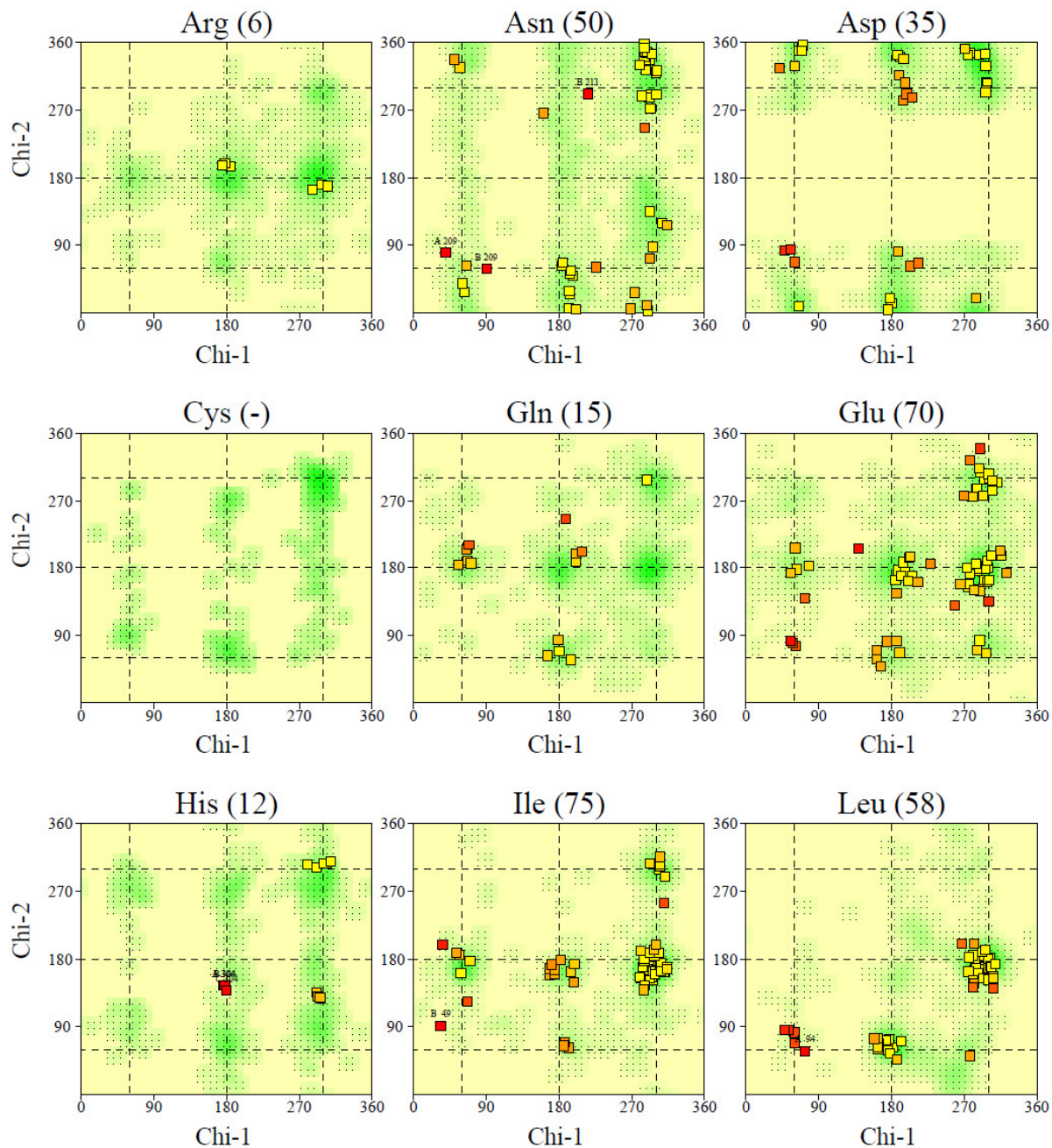
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

PROCHECK

Page 1

Chi1-Chi2 plots

NAC_MTA_final



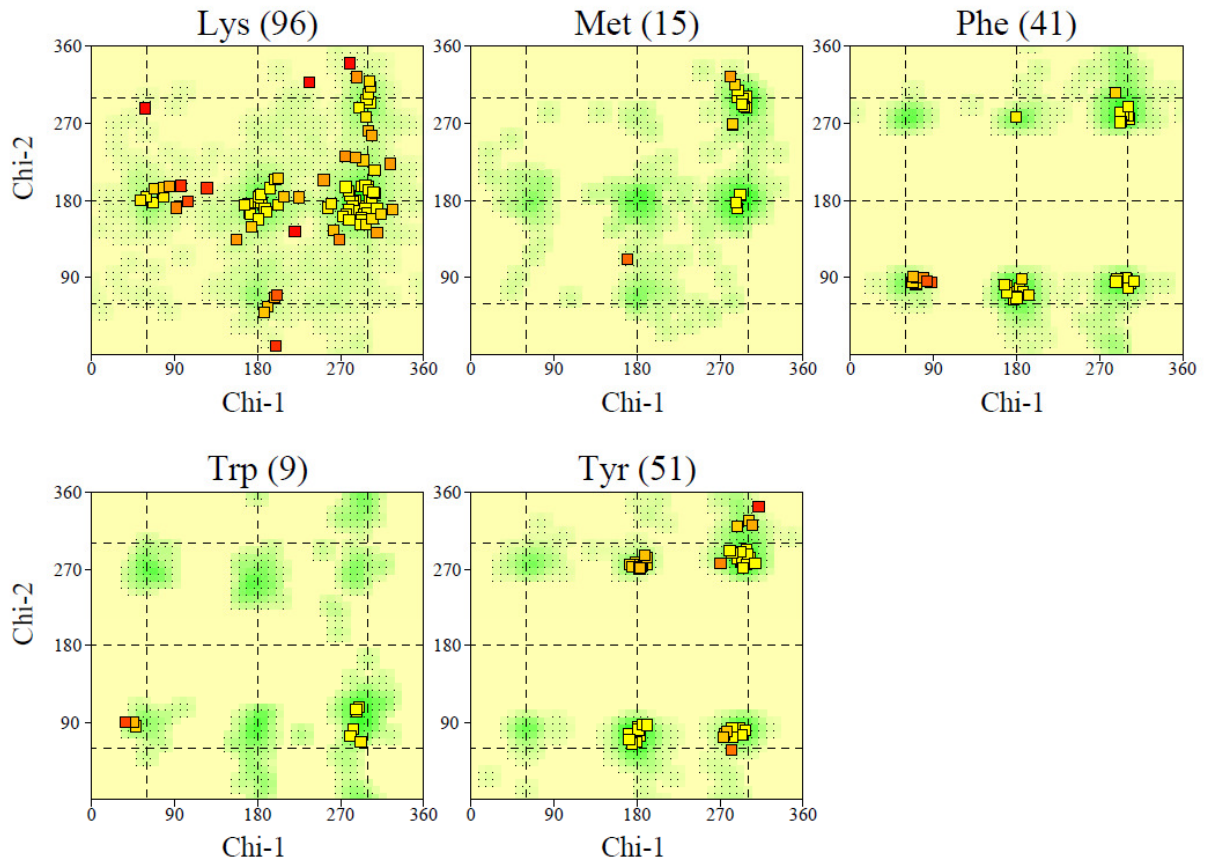
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled. Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0Å or better.

PROCHECK

Page 2

Chi1-Chi2 plots

NAC_MTA_final



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.