

Structure Factor Check

3SFD

Title: CRYSTAL STRUCTURE OF PORCINE MITOCHONDRIAL RESPIRATORY COMPL
BOUND WITH OXALOACETATE AND PENTACHLOROPHENOL
Date: 13-JUN-11
PDB code: 3SFD

Crystal

Cell parameters:

a: 70.31 A b: 83.36 A c: 293.10 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 48.9 – 2.61 A
 Reflections in file: 53815
 Unique reflections above 0: 40348
 Reflections > 0: 13467

SFCHECK

Nominal resolution range: 48.9 – 2.61 A
\05max. from input data, min. from author\05
 Used reflections: 40347
 Reflections out of resolution: 1
 Completeness: 75.5 %
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.8922 1.0000 0.7914
 B_overall (by Patterson): 44.A^2
 Optical resolution: 1.99 A
 Expected opt. resol. for complete data set: 1.99 A
 Estimated minimal error: 0.027 A

Model

8746 atoms (130 water molecules)

Number of chains: 15
 Volume not occupied by model: 56.3 %
 (for atomic model): 59.9 A^2
 σ (B): 15.28 A^2
 Matthews coefficient: 3.51
 Corresponding solvent % : 64.66

Model vs. Structure Factors

R-factor for all reflections: 0.300
 Correlation factor: 0.825
 R-factor: 0.342
 for $F > 2.0\sigma$
 nom. resolution range: 50.00 – 2.61A
 reflections used: 40344
 Rfree: 0.368
 Nfree: 2054
 R-factor without free-refl.: 0.341
 Non free-reflections: 38290
 <u> (error in coords by Luzzati plot): 0.421 A
 Estimated maximal error: 0.169 A
 DPI: 0.381 A

Refinement

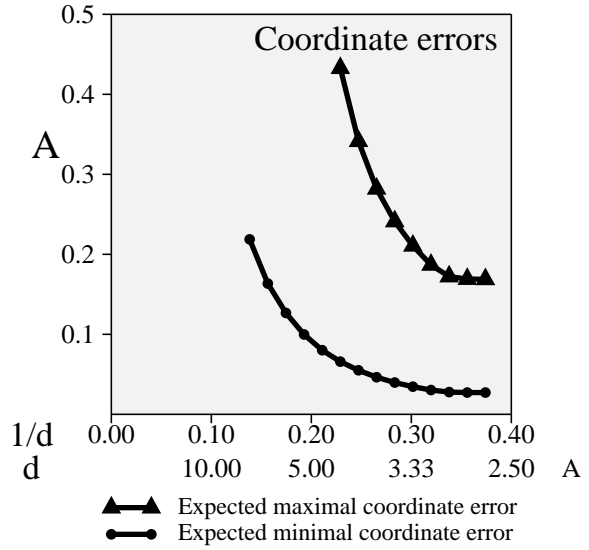
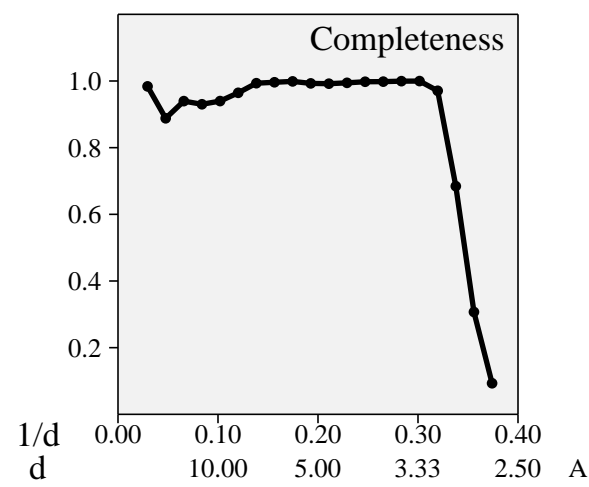
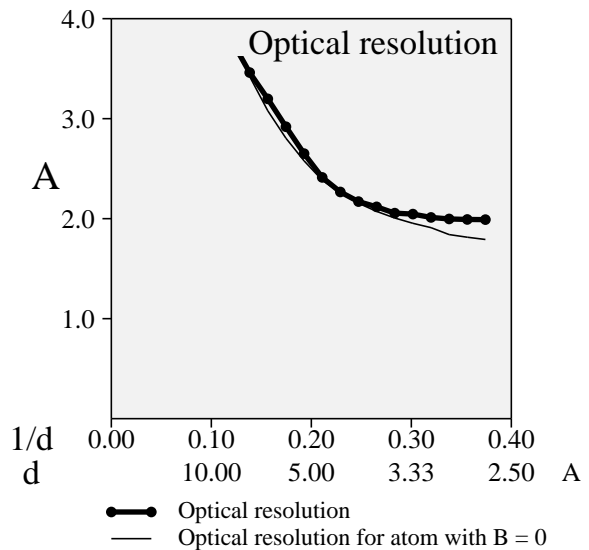
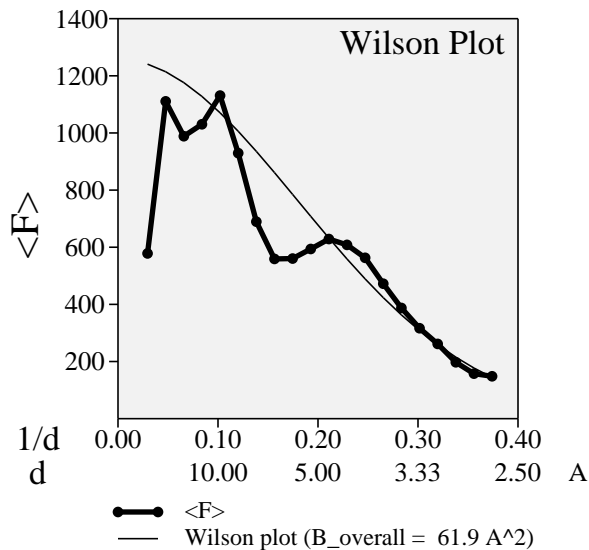
Program: REFMAC 5.5.0088
 Nominal resolution range: 50.0 – 2.61 A
 Reported R-factor: 0.242
 Number of reflections used: 38294
 Reported Rfree: 0.29
 Sigma cut-off: N.A.

Scaling

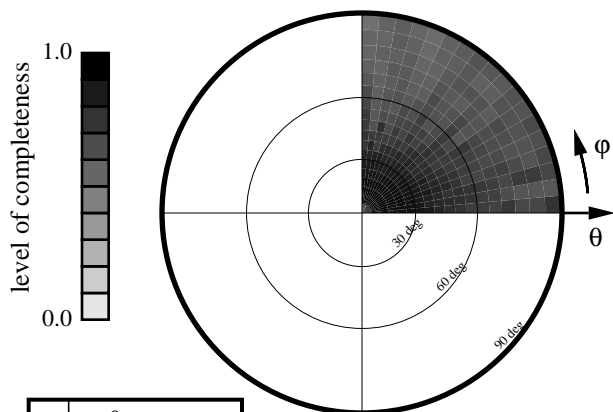
Scale: 0.895
 Bdiff: -5.47

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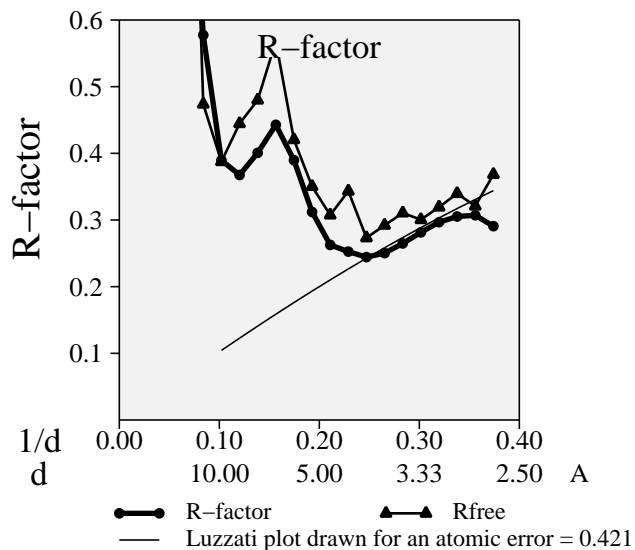


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

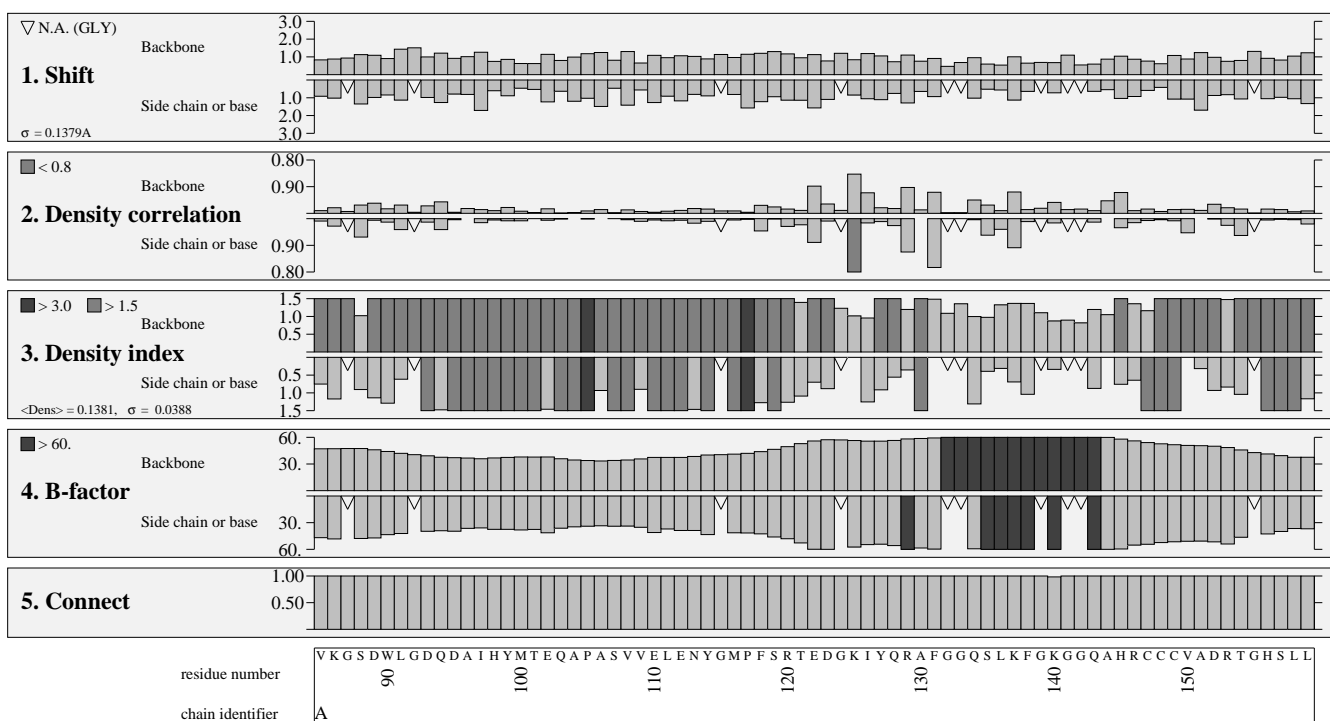
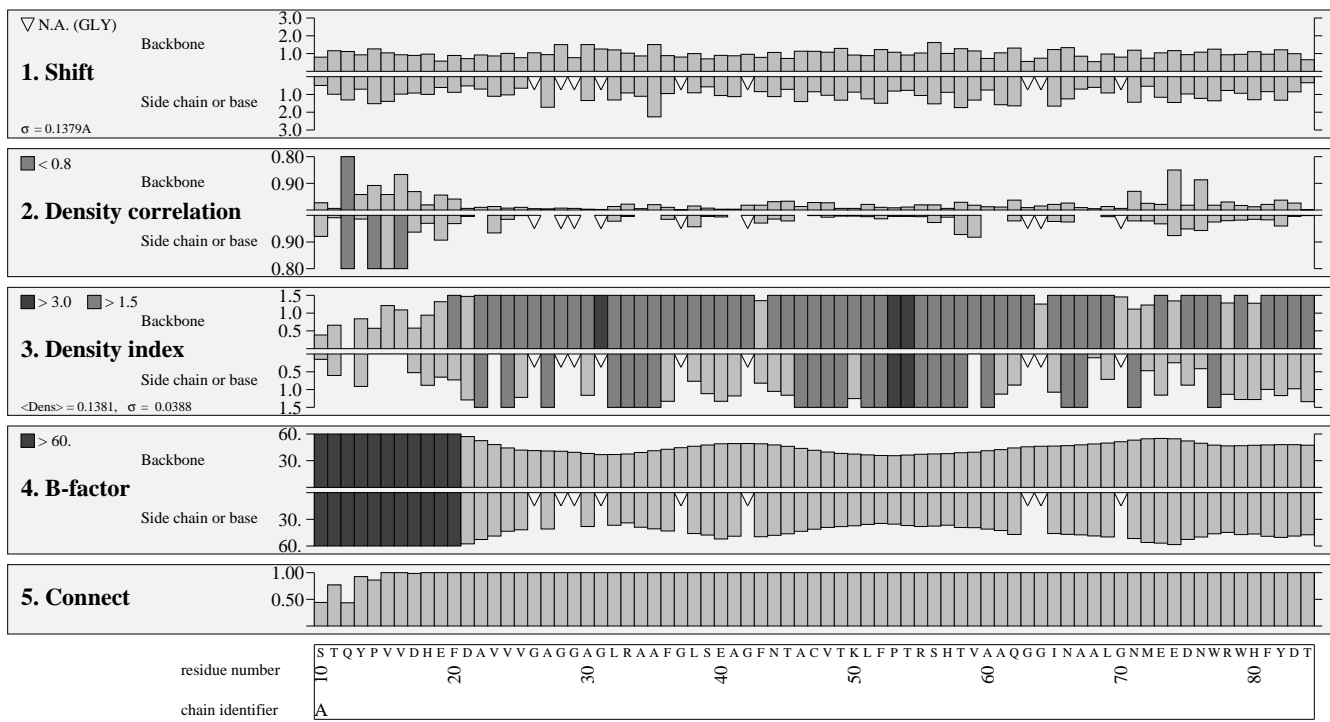
polar coordinates of the crystallographical axes



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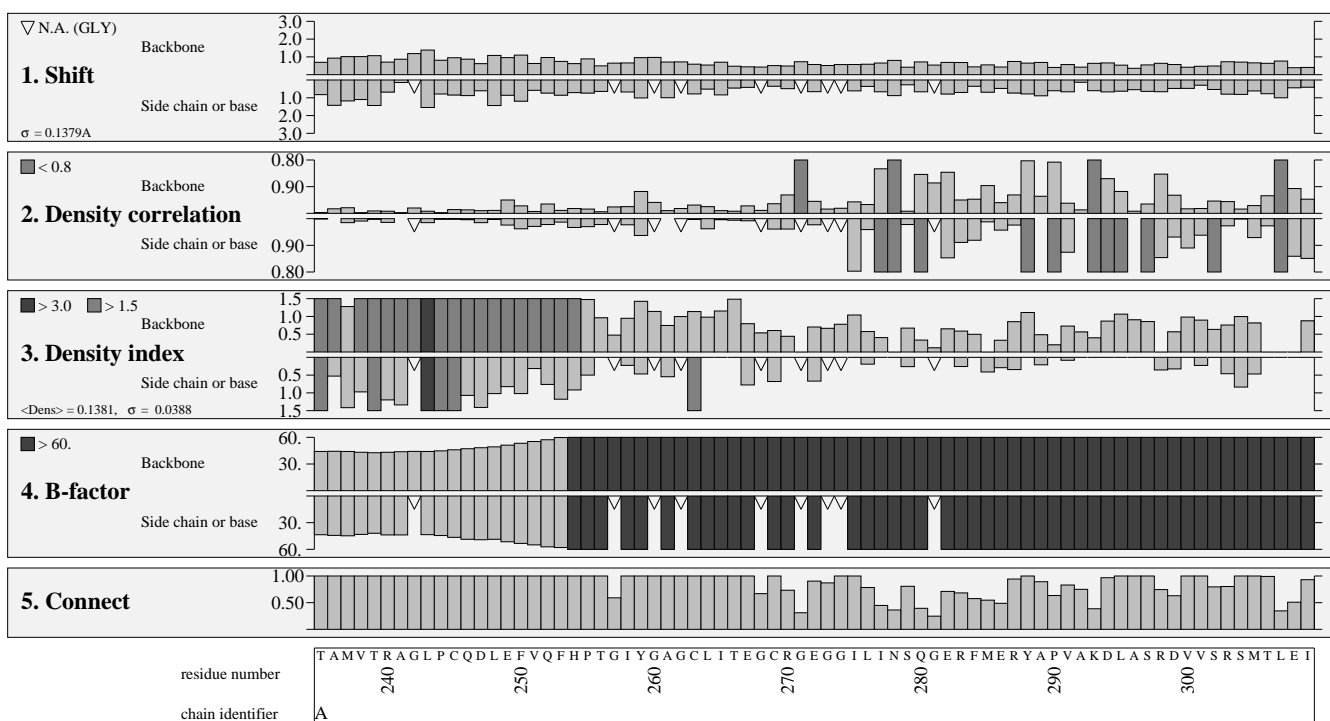
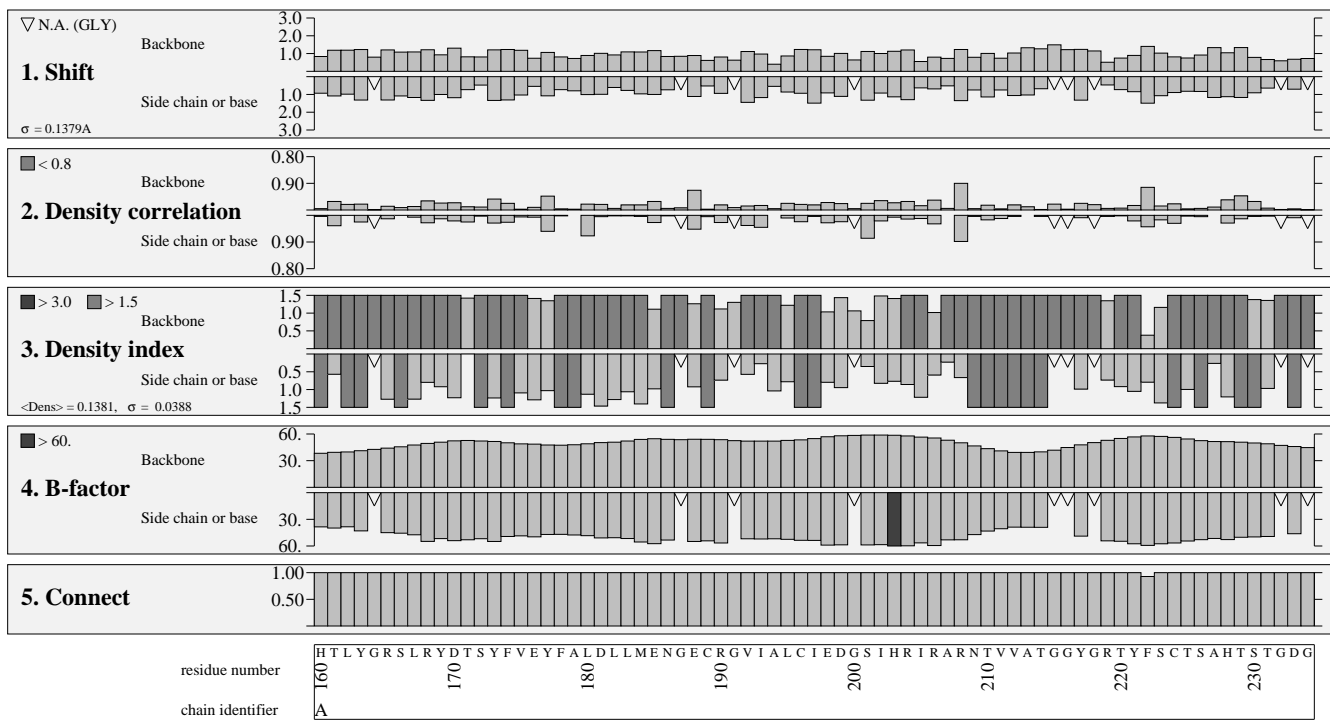
Local estimation



Structure Factor Check

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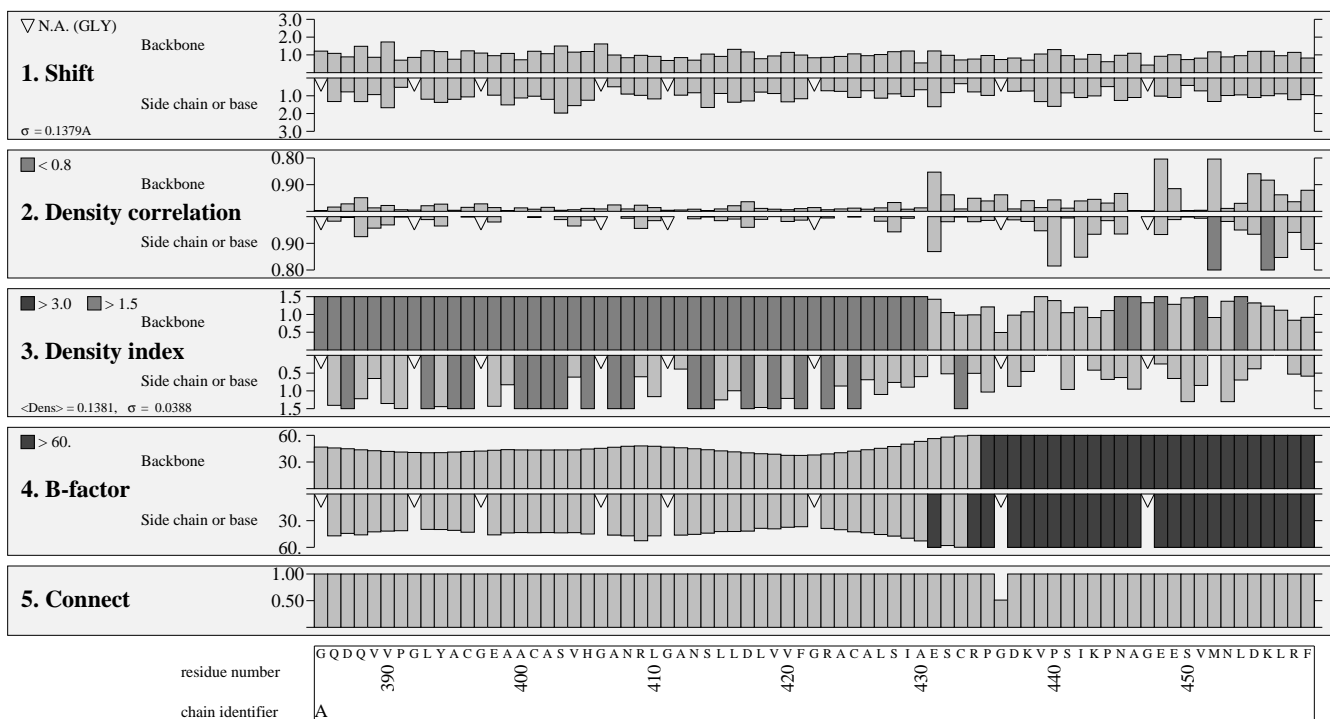
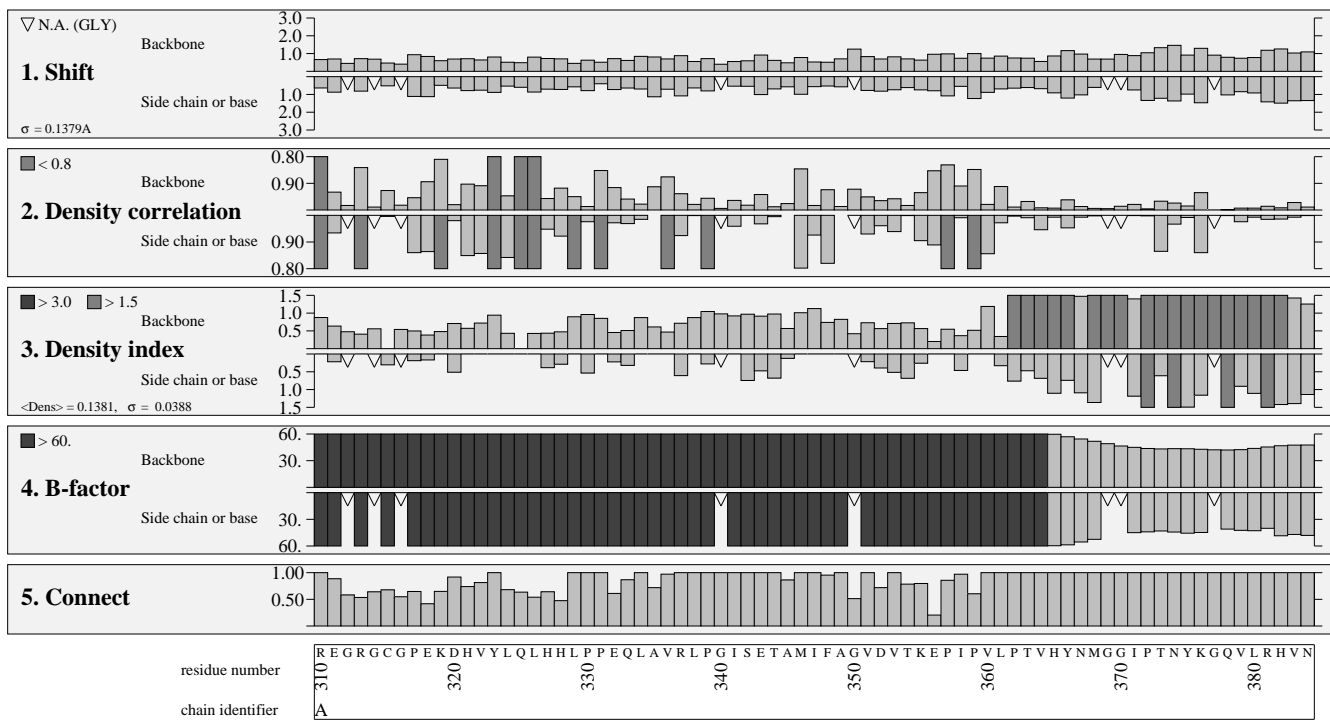
Local estimation (2)



Structure Factor Check

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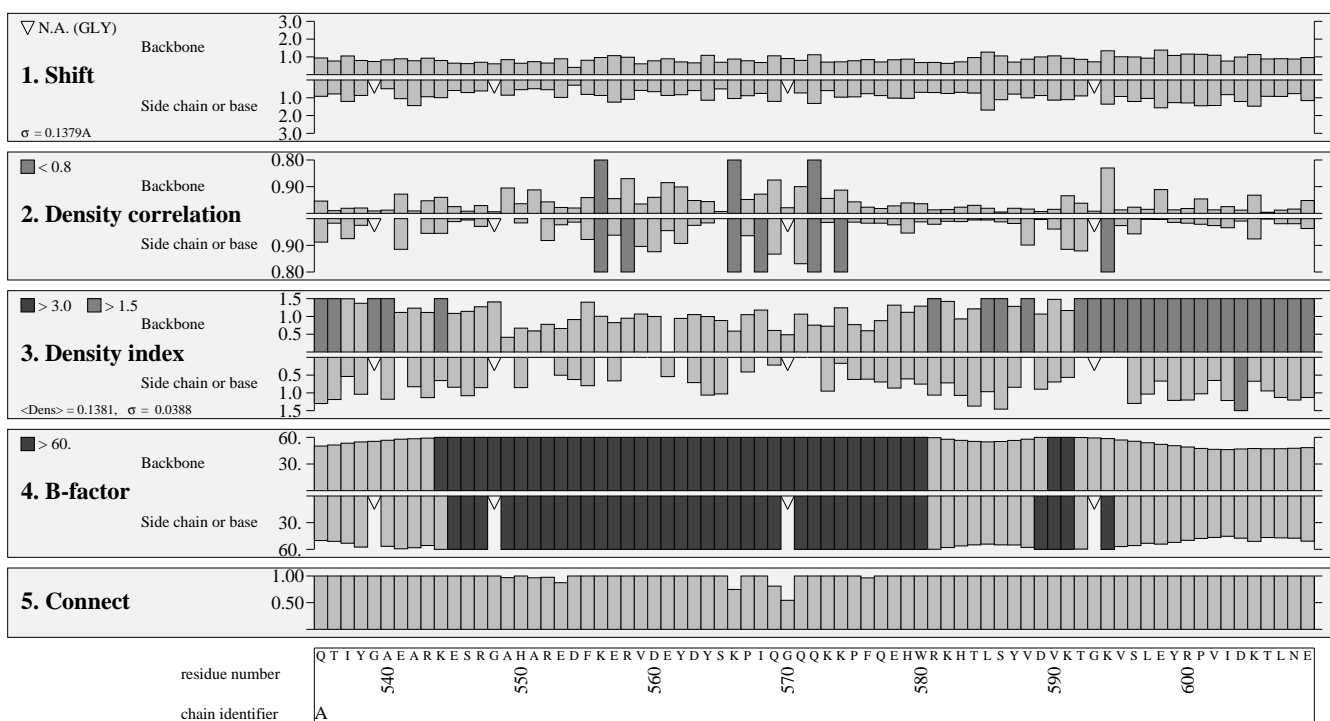
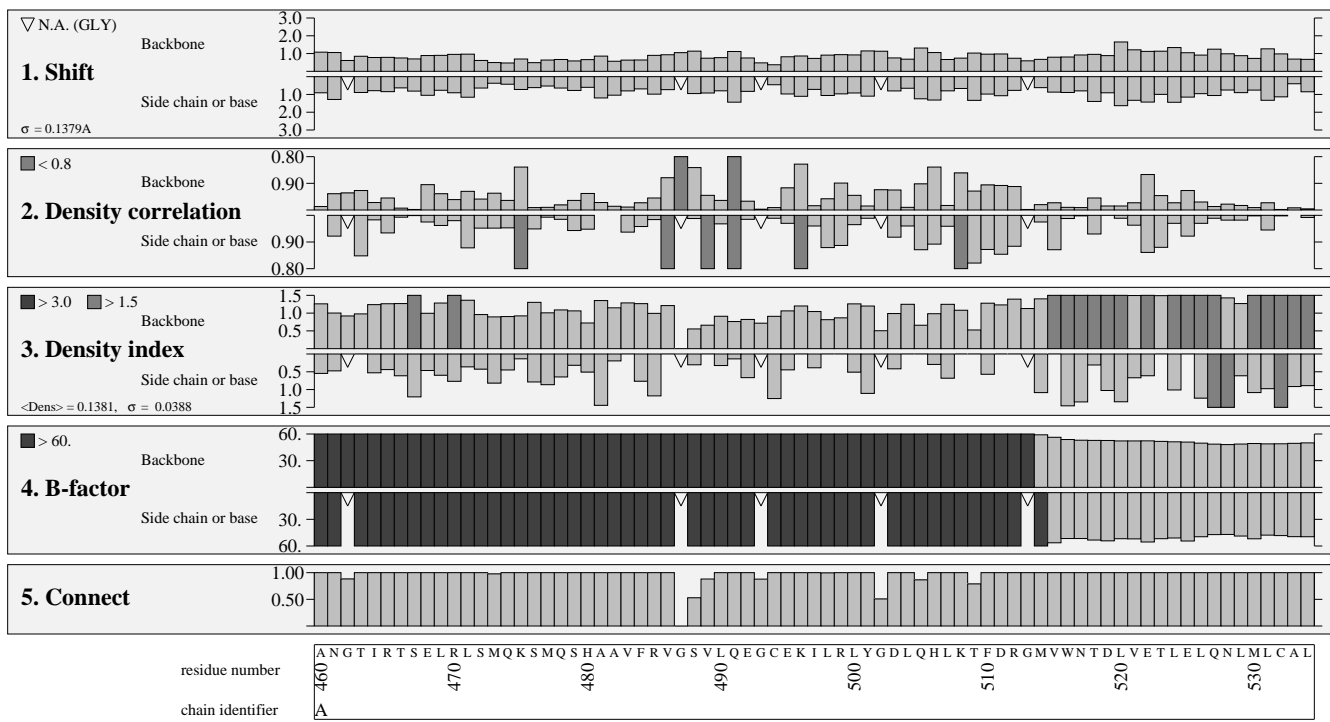
Local estimation (3)



Structure Factor Check

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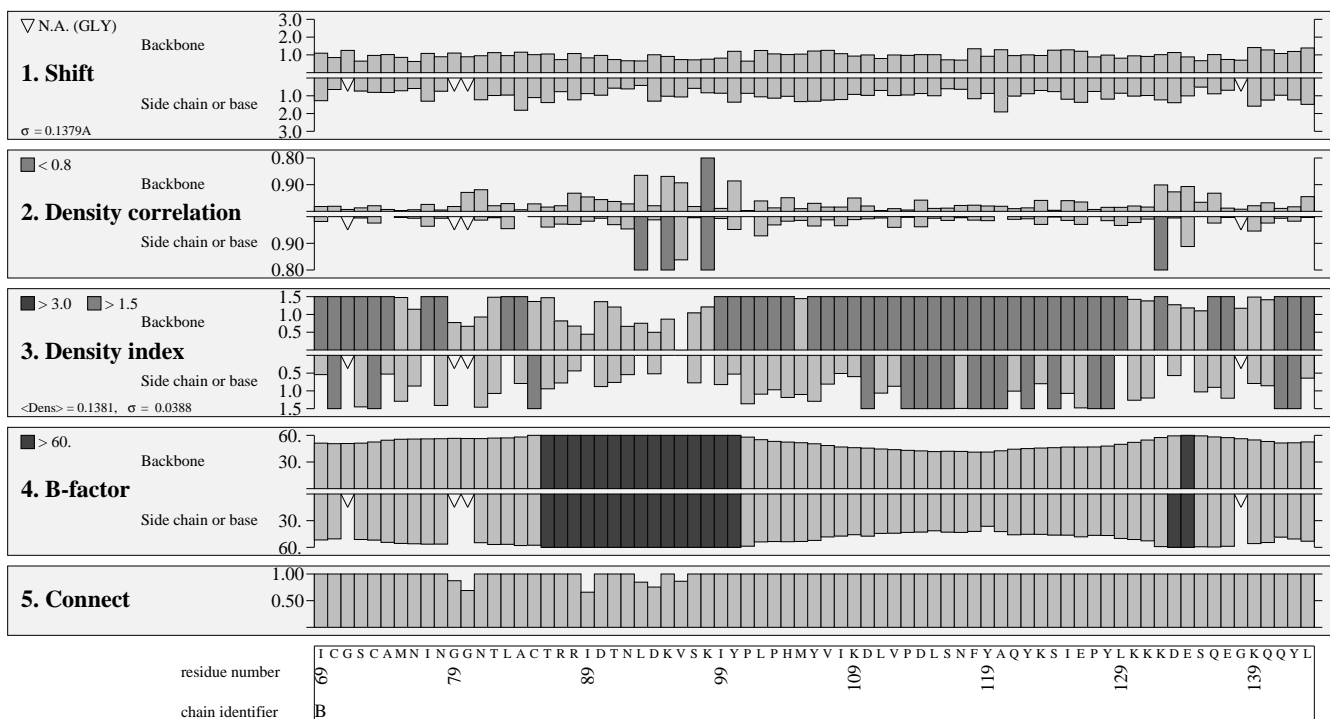
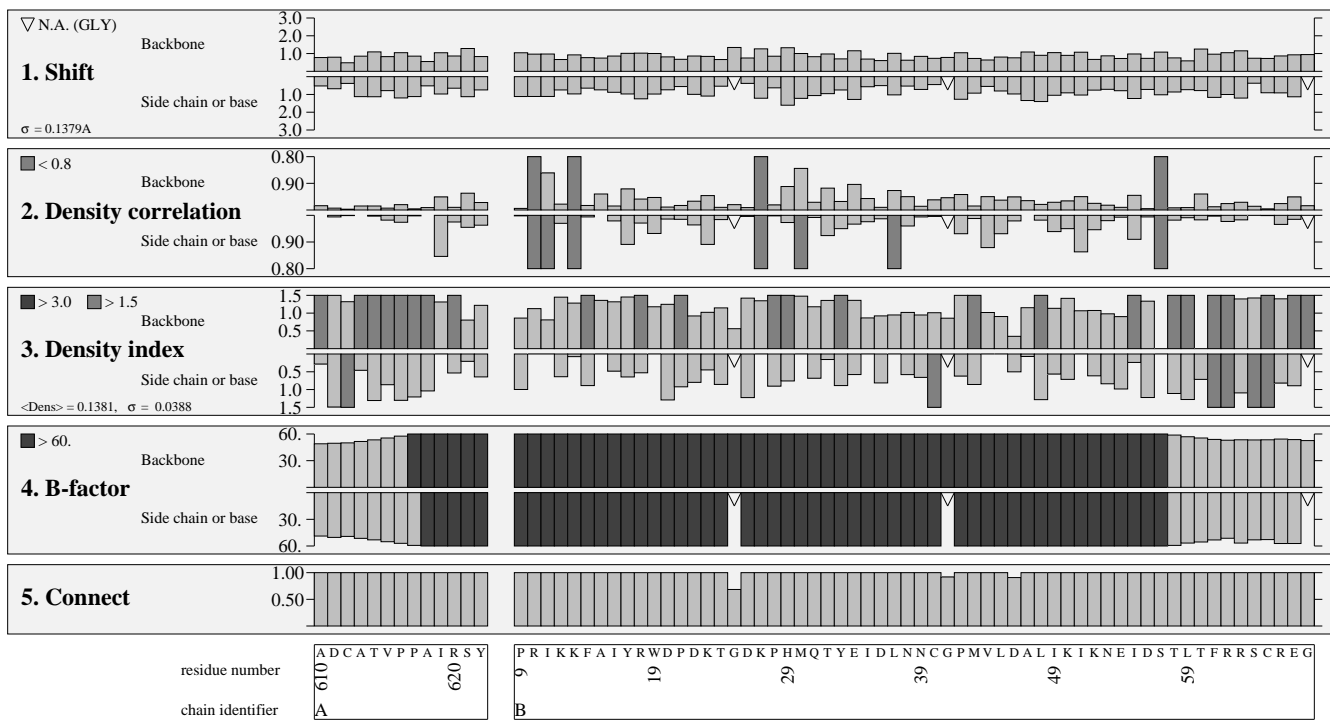
Local estimation (4)



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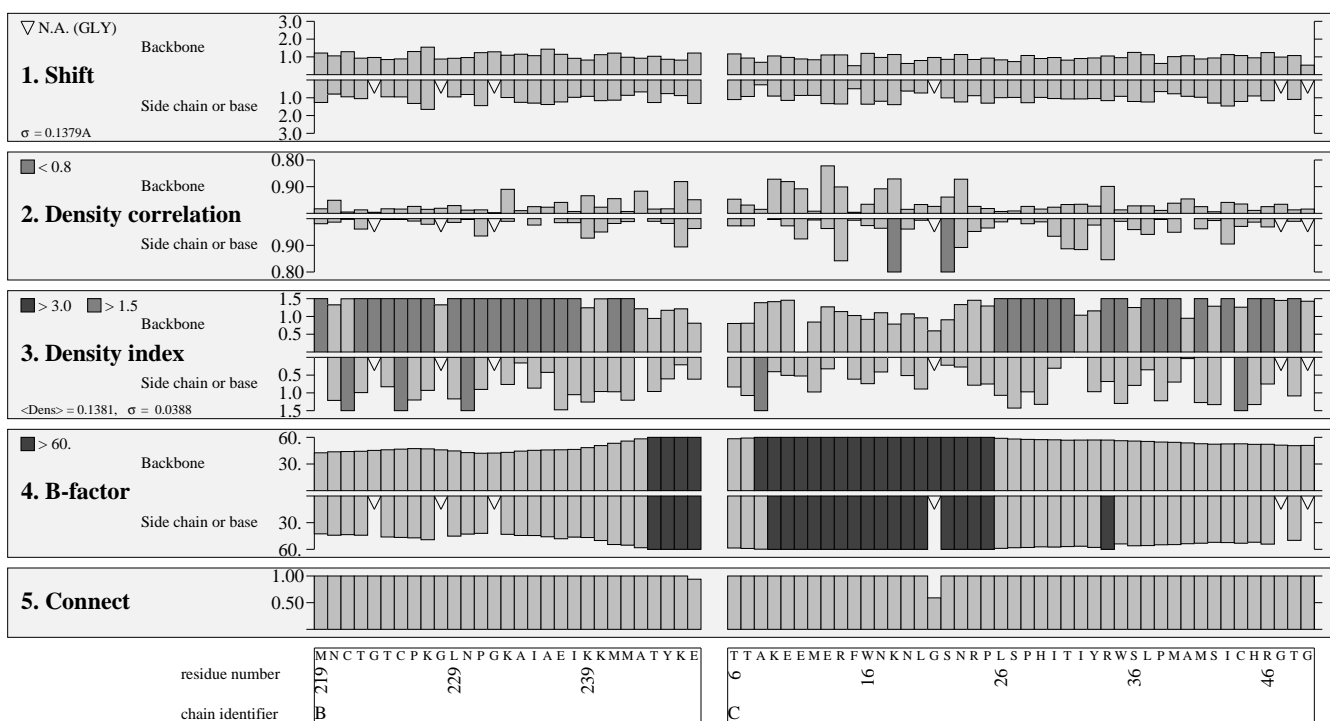
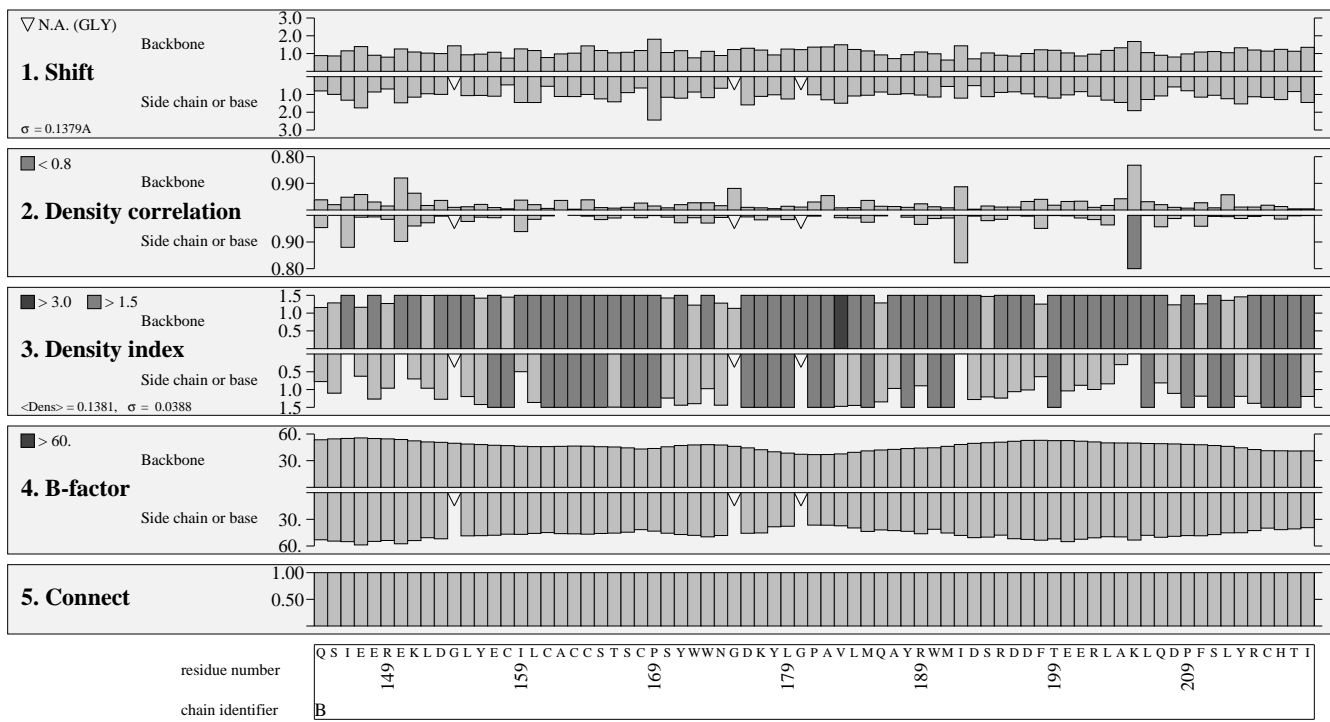
Local estimation (5)



Structure Factor Check

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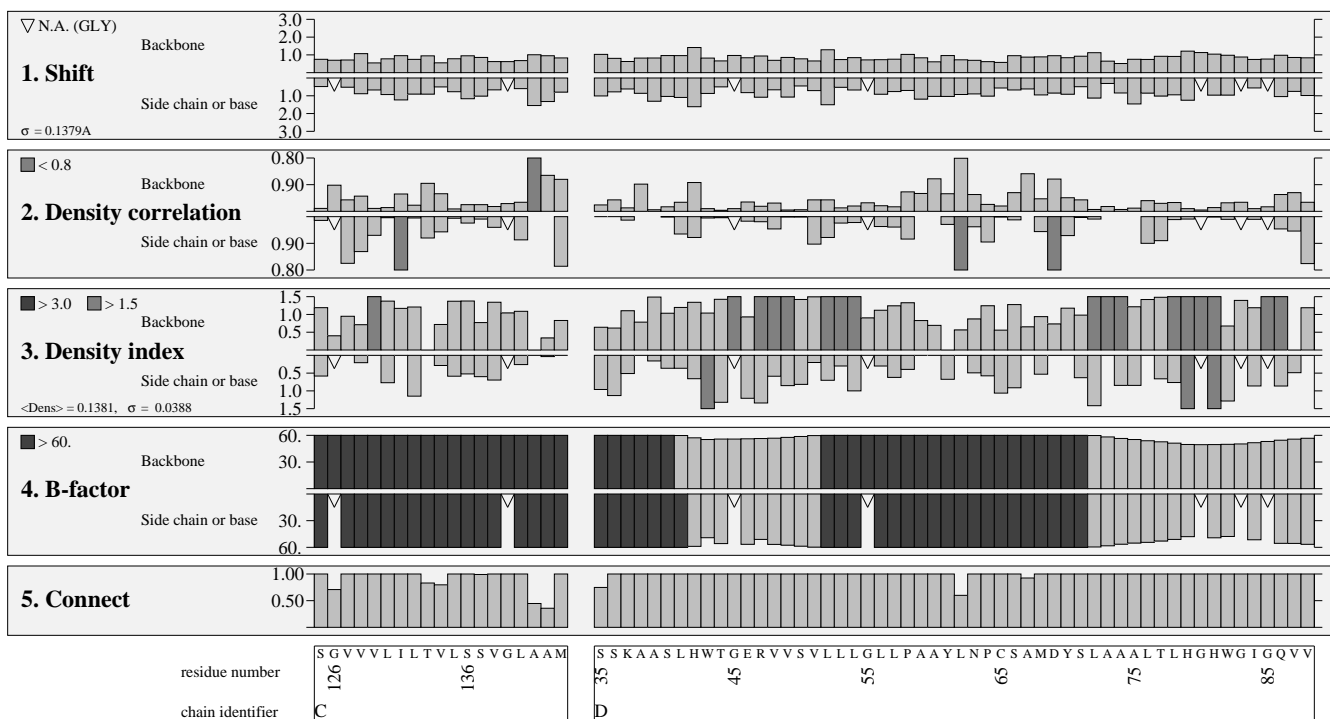
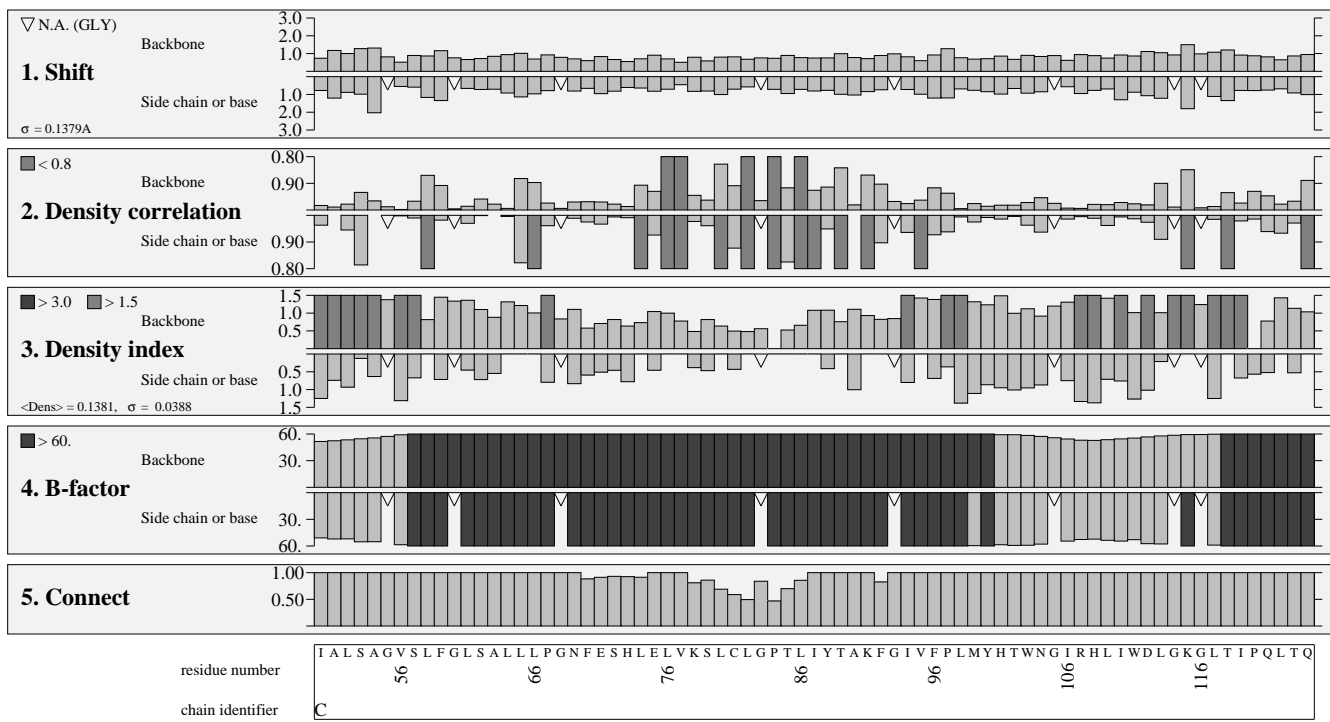
Local estimation (6)



Structure Factor Check

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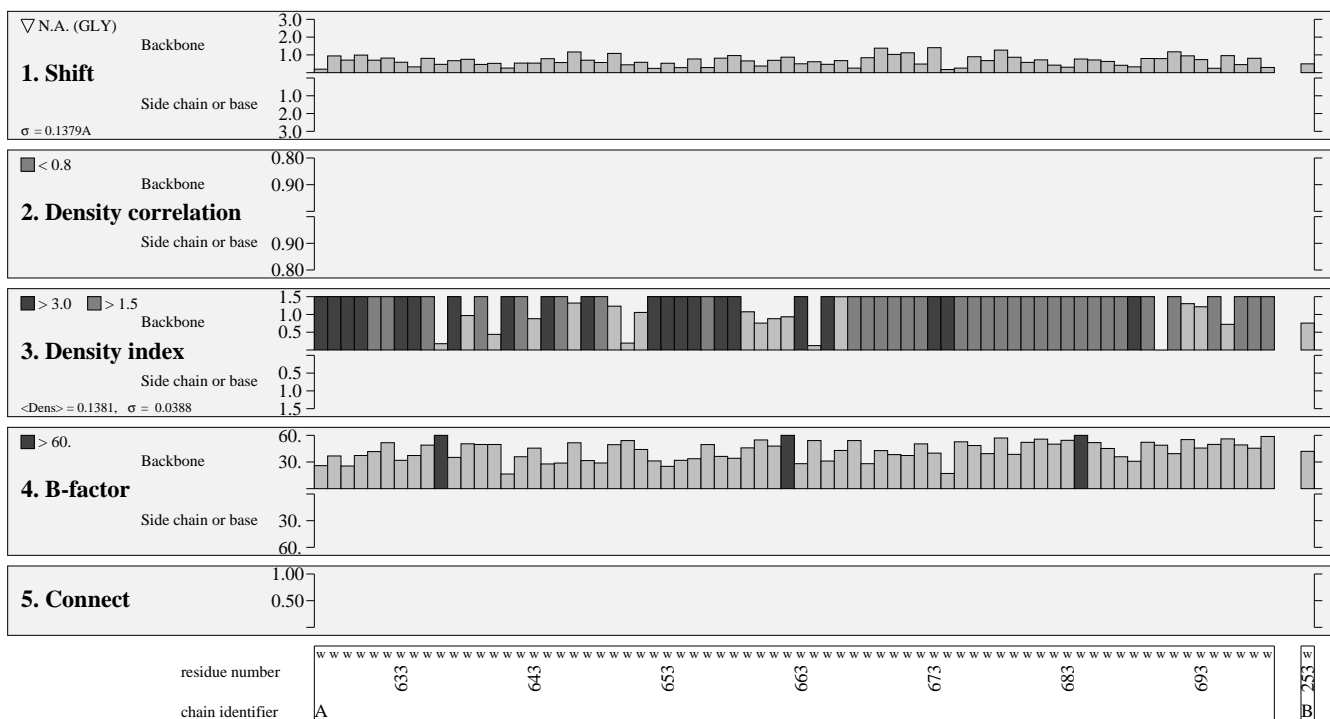
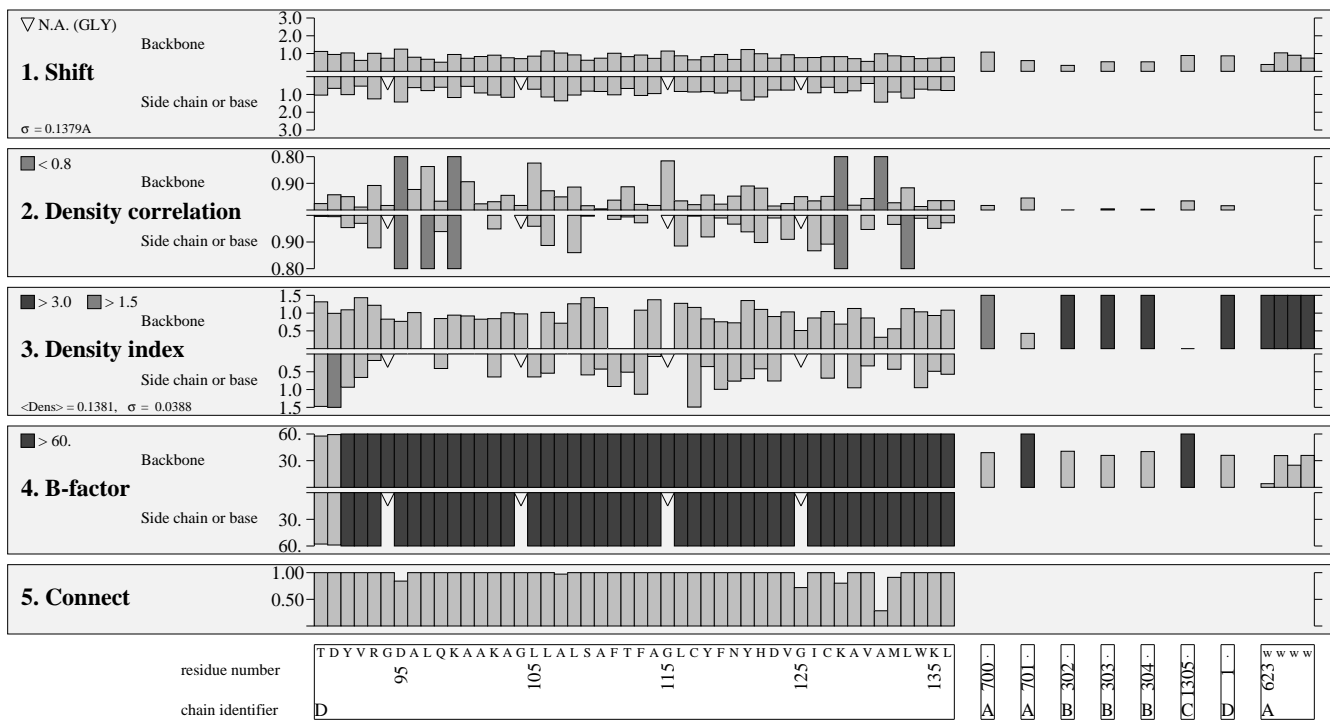
Local estimation (7)



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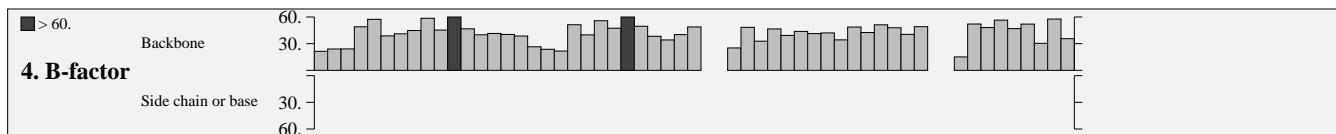
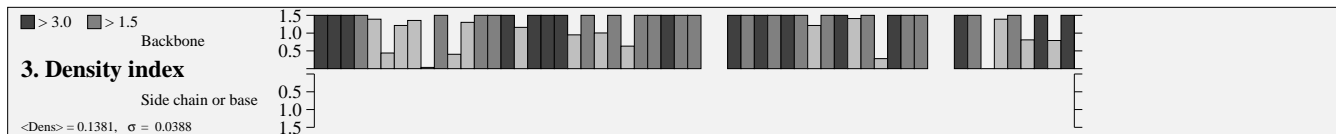
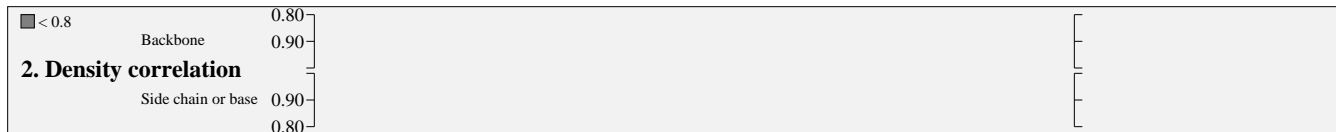
Local estimation (8)



Structure Factor Check

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Local estimation (9)



residue number	ww	ww	ww
	263	273	
chain identifier	B	C	D