

Structure Factor Check

3VRB

Title: MITOCHONDRIAL RHODOQUINOL-FUMARATE REDUCTASE FROM THE PARASITIC NEMATODE ASCARIS SUUM WITH THE SPECIFIC INHIBITOR FLUTOLANI SUBSTRATE FUMARATE
 Date: 07-APR-12
 PDB code: 3VRB

Crystal

Cell parameters:

a: 124.31 A b: 131.65 A c: 222.52 A
 α : 90.00 β : 90.00 γ : 90.00
 Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 35.4 – 2.91 A
 Reflections in file: 80656
 Unique reflections above 0: 59723
 above 1 σ : 59711
 above 3 σ : 43081
 Reflections > 0: 20933

SFCHECK

Nominal resolution range: 35.4 – 2.91 A
\05max. from input data, min. from author\05
 Used reflections: 59723
 Completeness: 74.0 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.061
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.8653 1.0000 0.8882
 B_{overall} (by Patterson): 58. A²
 Optical resolution: 2.26 A
 Expected opt. resol. for complete data set: 2.26 A
 Estimated minimal error: 0.061 A

Model

18242 atoms
 Number of chains: 24
 Volume not occupied by model: 56.4 %
 $\langle B \rangle$ (for atomic model): 84.5 A²
 $\sigma(B)$: 12.06 A²
 Matthews coefficient: 3.56
 Corresponding solvent % : 65.22

Model vs. Structure Factors

R-factor for all reflections: 0.261
 Correlation factor: 0.859
 R-factor: 0.272
 for $F > 2.0\sigma$
 nom. resolution range: 35.39 – 2.91A
 reflections used: 59707

Refinement

Program: REFMAC 5.5.0109
 Nominal resolution range: 35.4 – 2.91 A
 Reported R-factor: 0.204
 Number of reflections used: 56737
 Reported Rfree: 0.27
 Sigma cut-off: N.A.

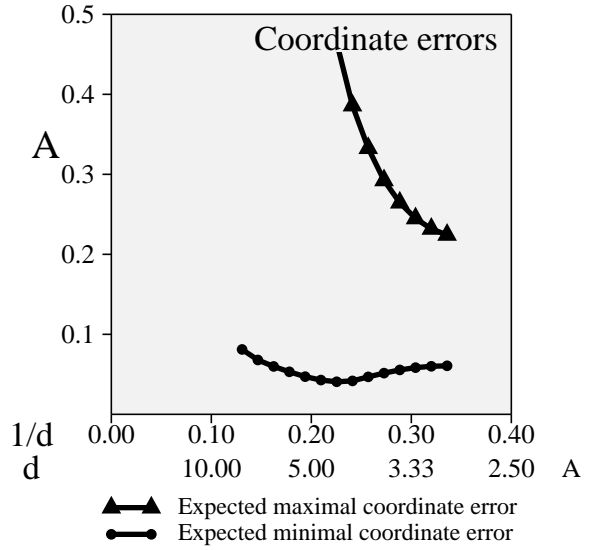
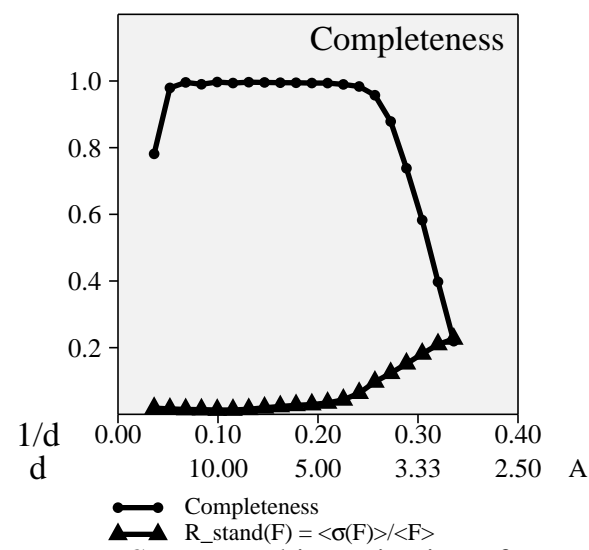
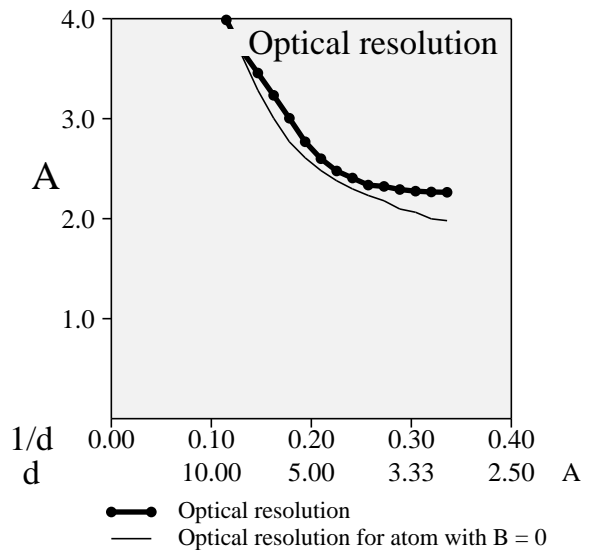
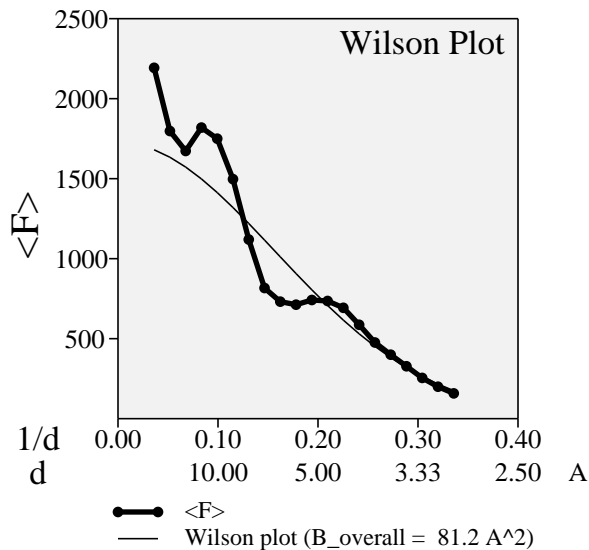
Rfree: 0.326
 Nfree: 2986
 R-factor without free-refl.: 0.270
 Non free-reflections: 56721
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.396 A
 Estimated maximal error: 0.224 A
 DPI: 0.483 A

Scaling

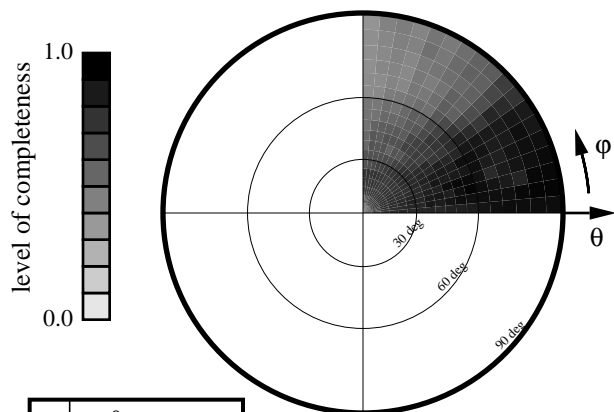
Scale: 0.878
 Bdiff: -3.98
 Anisothermal Scaling (Beta):
 -0.6359 1.4454 -0.1930 0.0000 0.0000 -0.0000
 Solvent correction – Ks,Bs: 0.478 250.021

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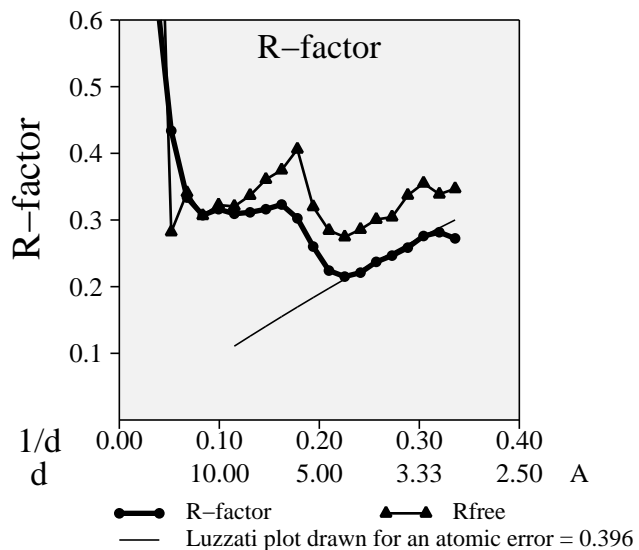


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

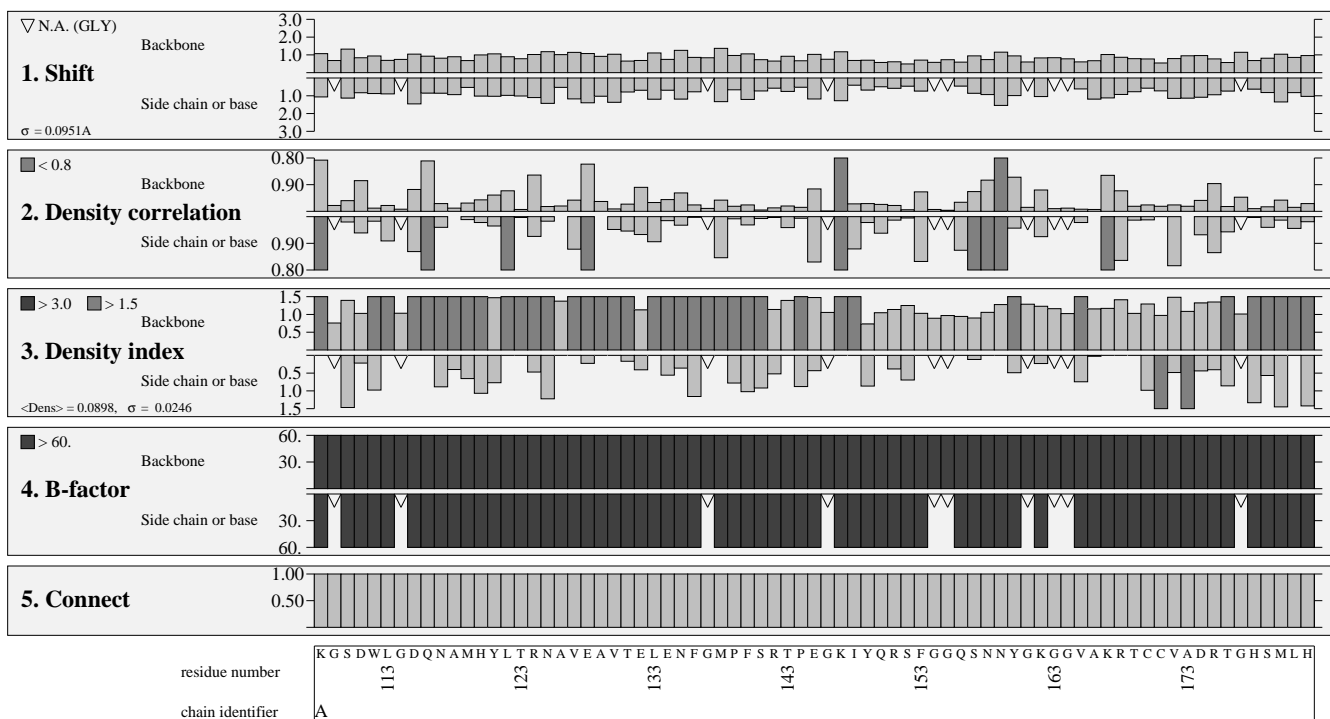
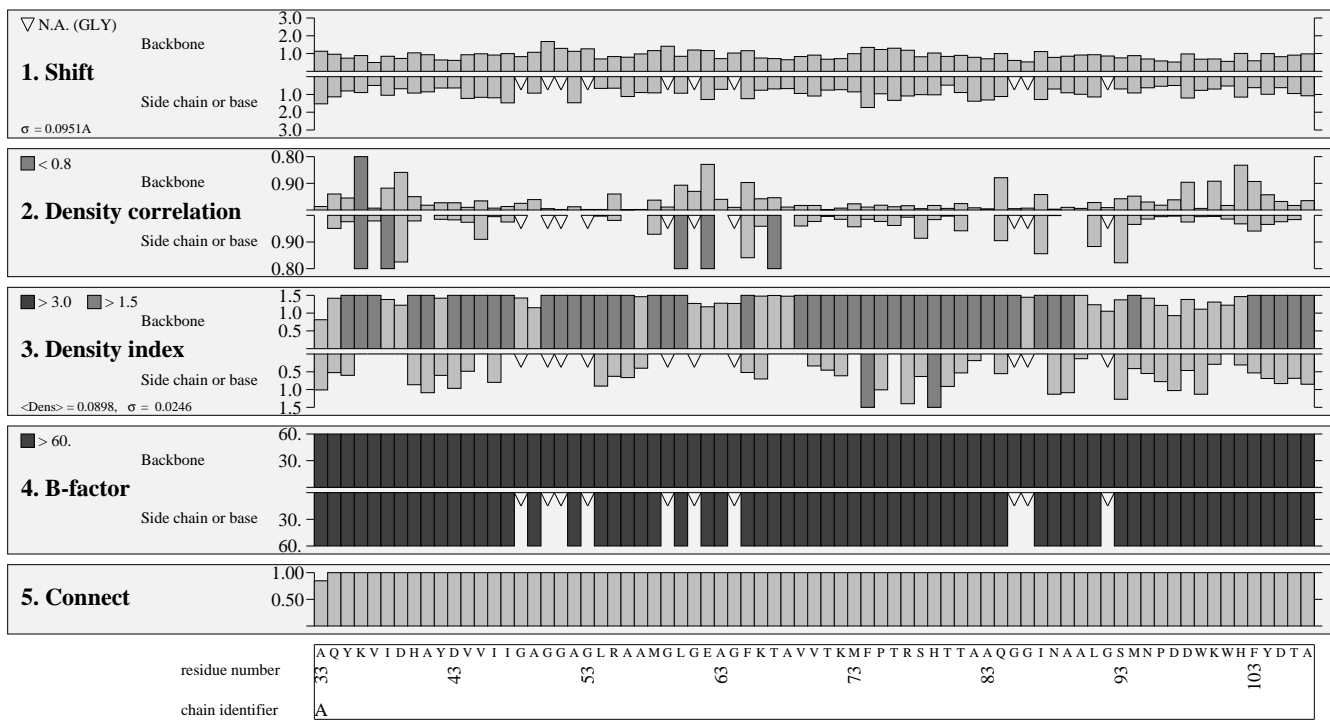
polar coordinates of the crystallographical axes



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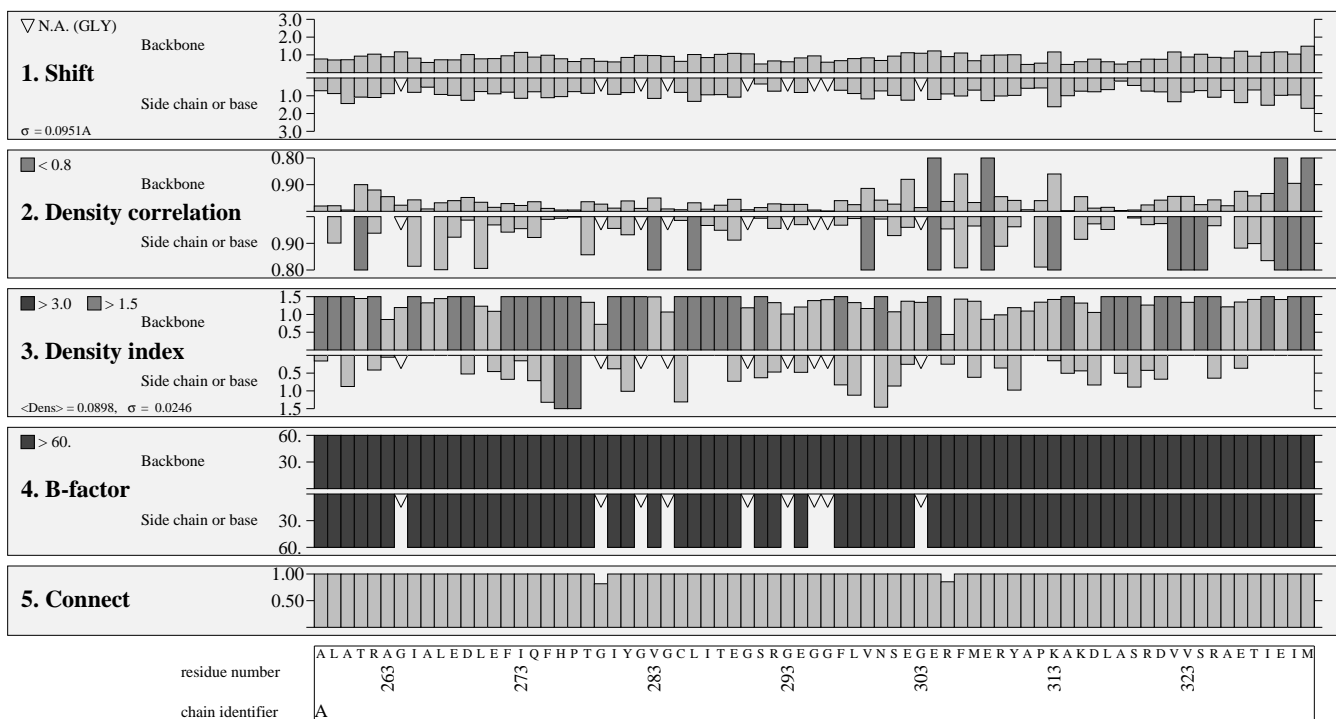
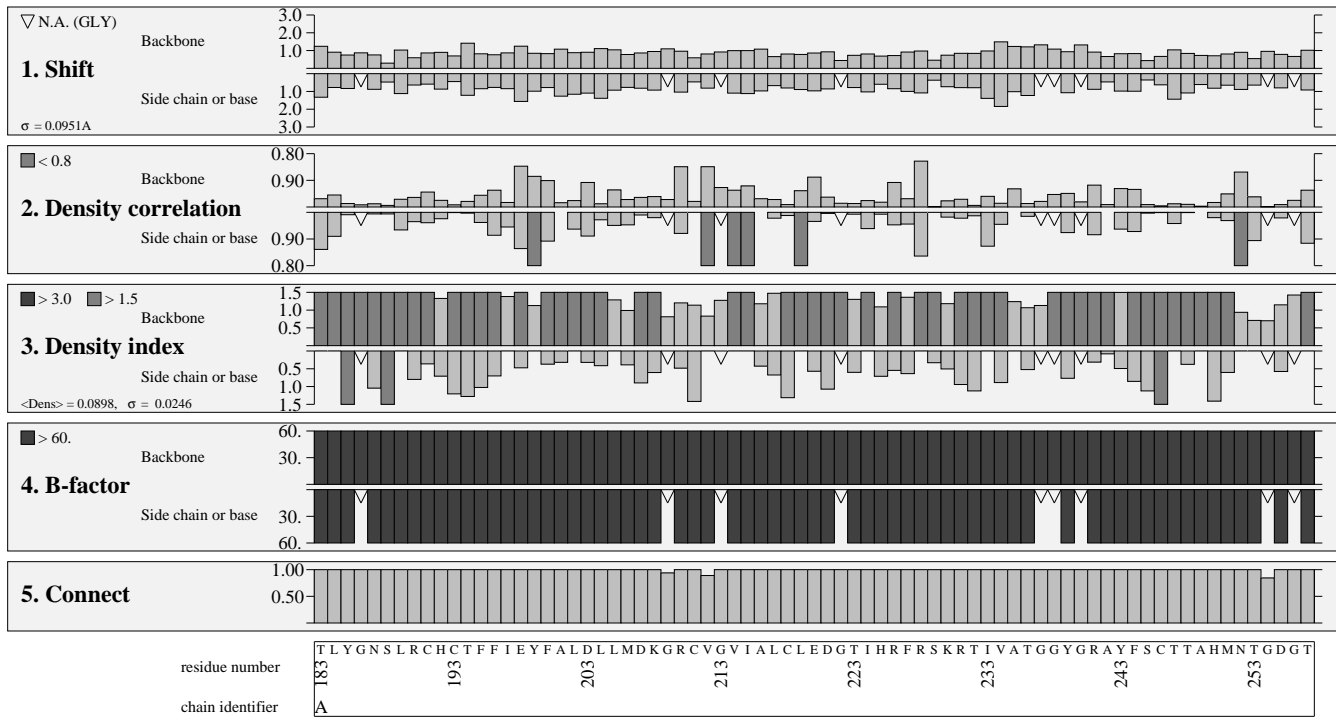
Local estimation



Structure Factor Check

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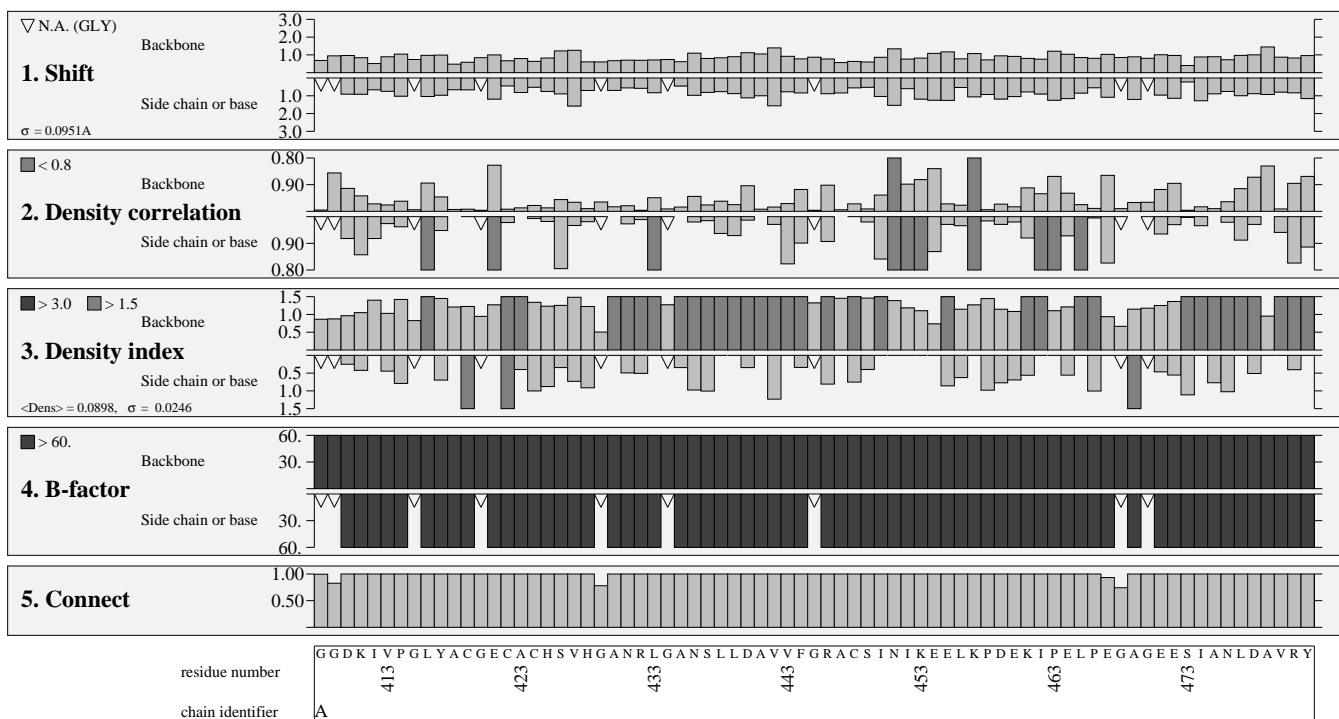
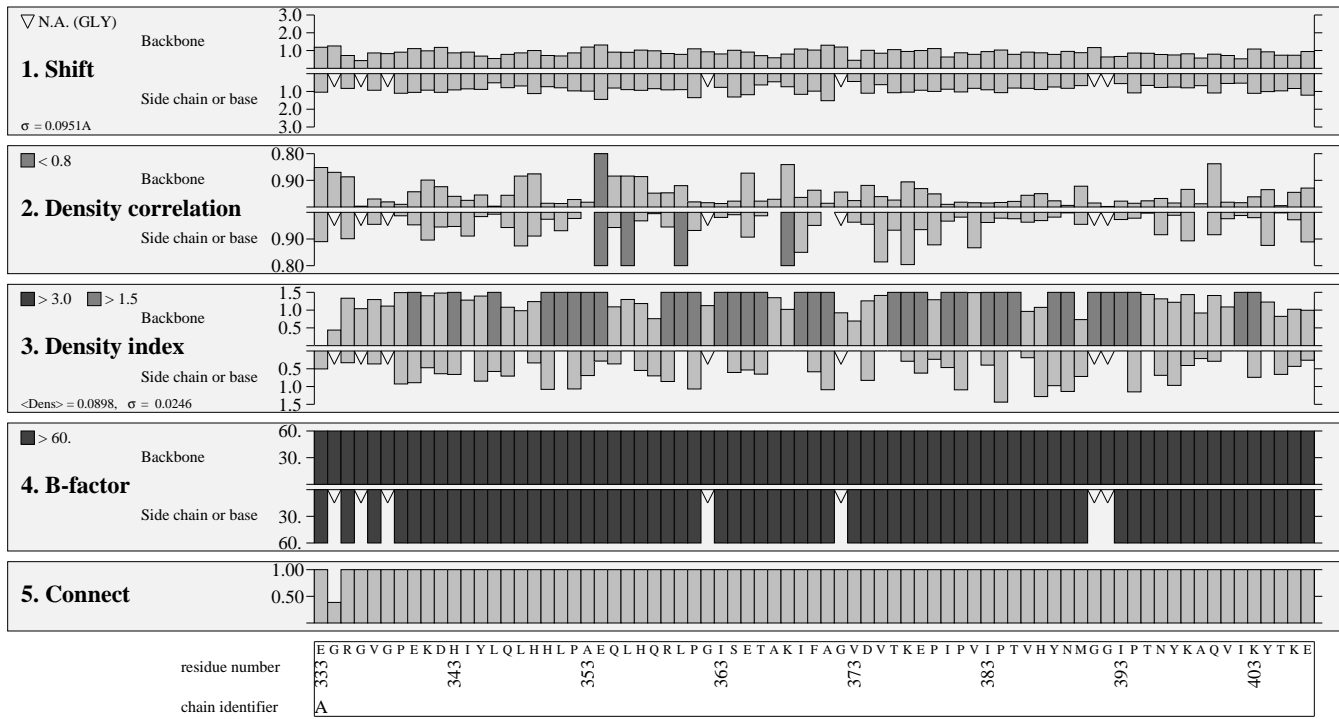
Local estimation (2)



Structure Factor Check

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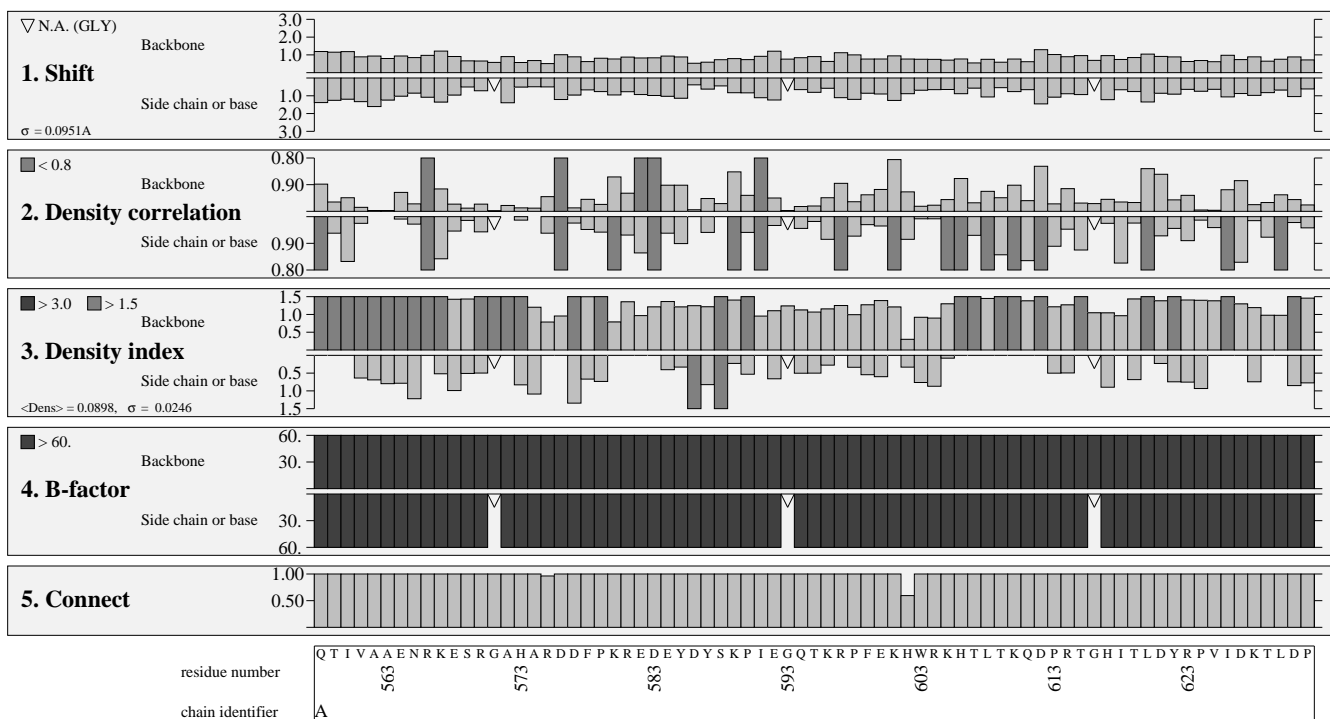
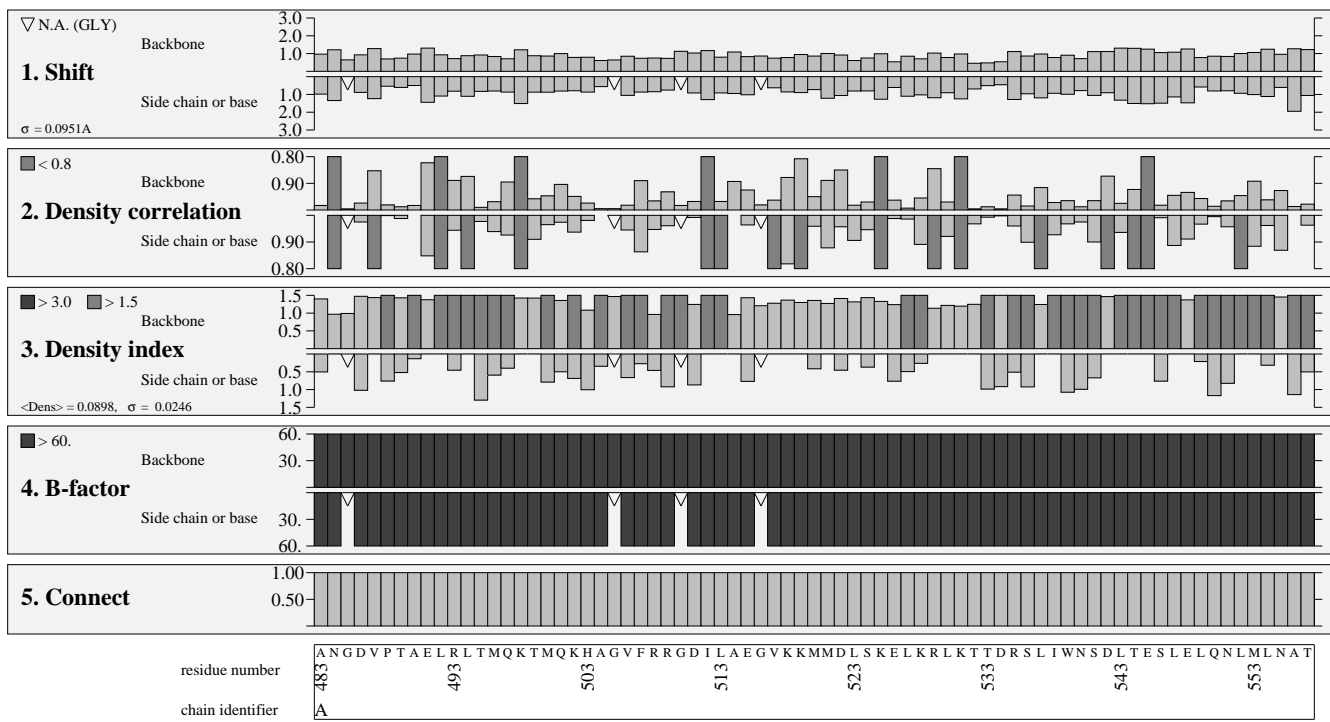
Local estimation (3)



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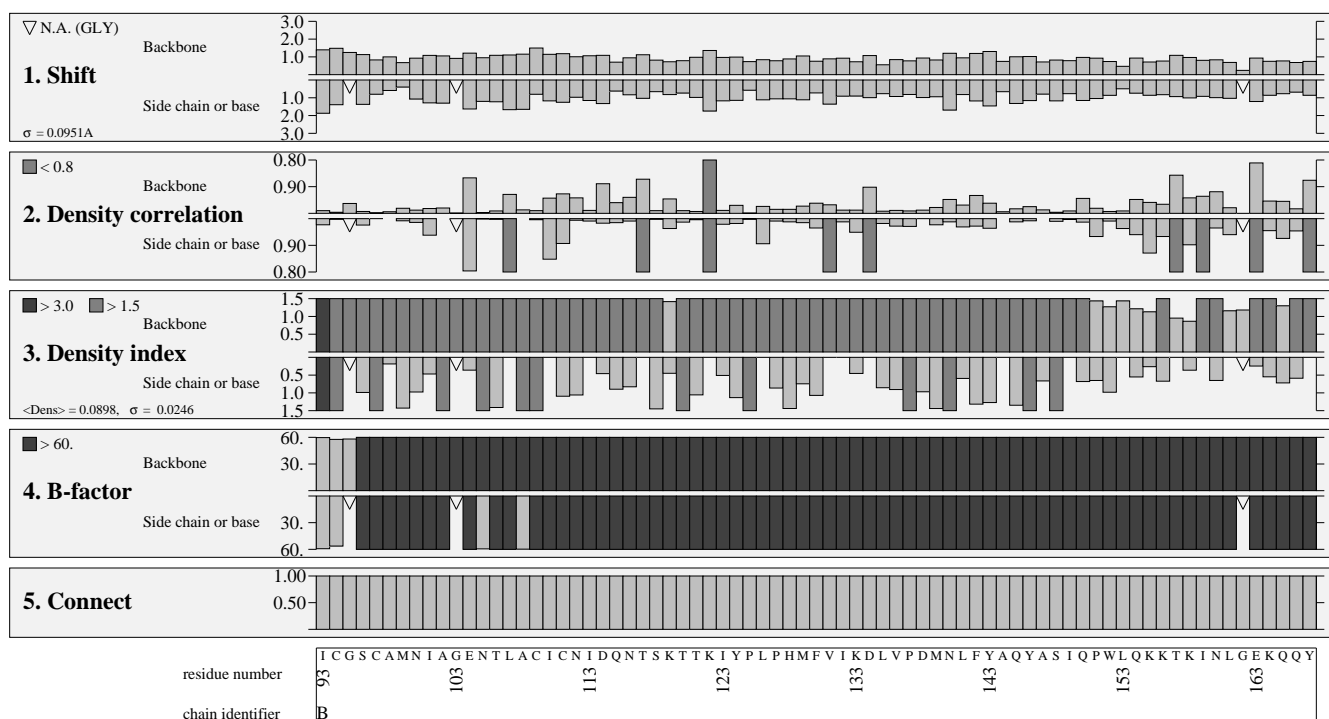
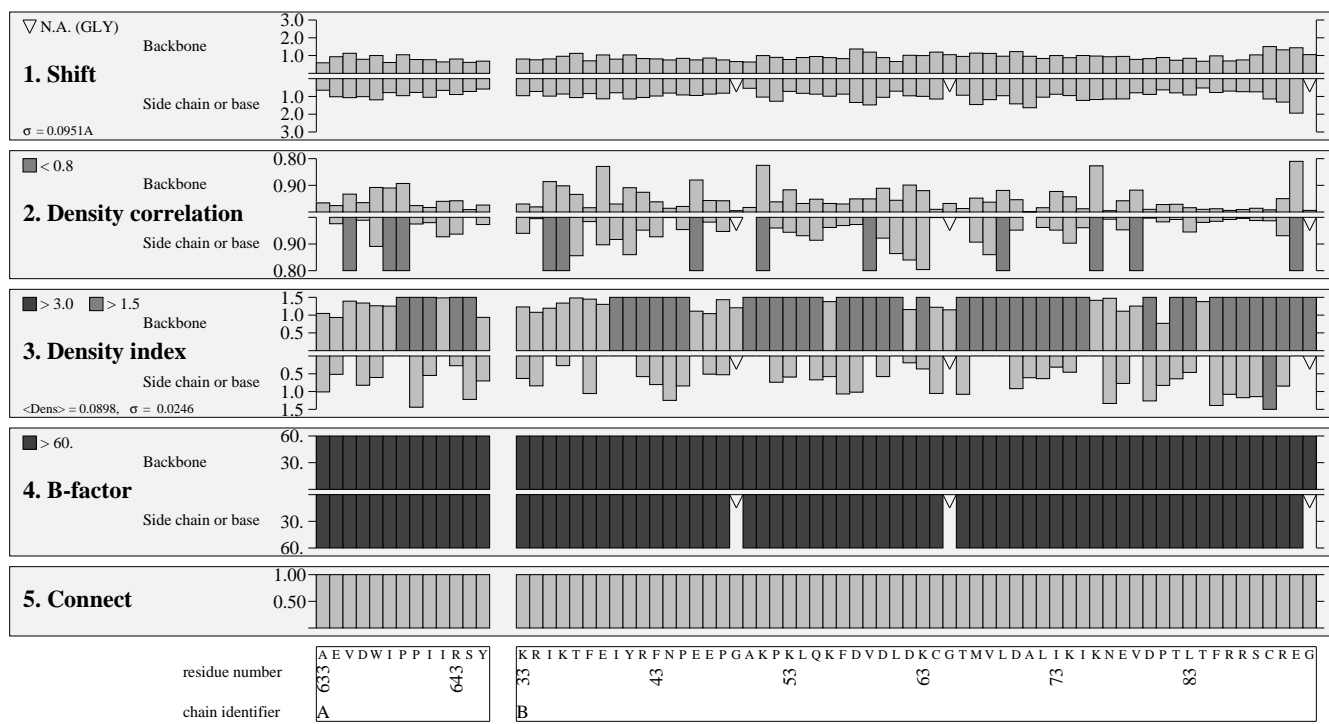
Local estimation (4)



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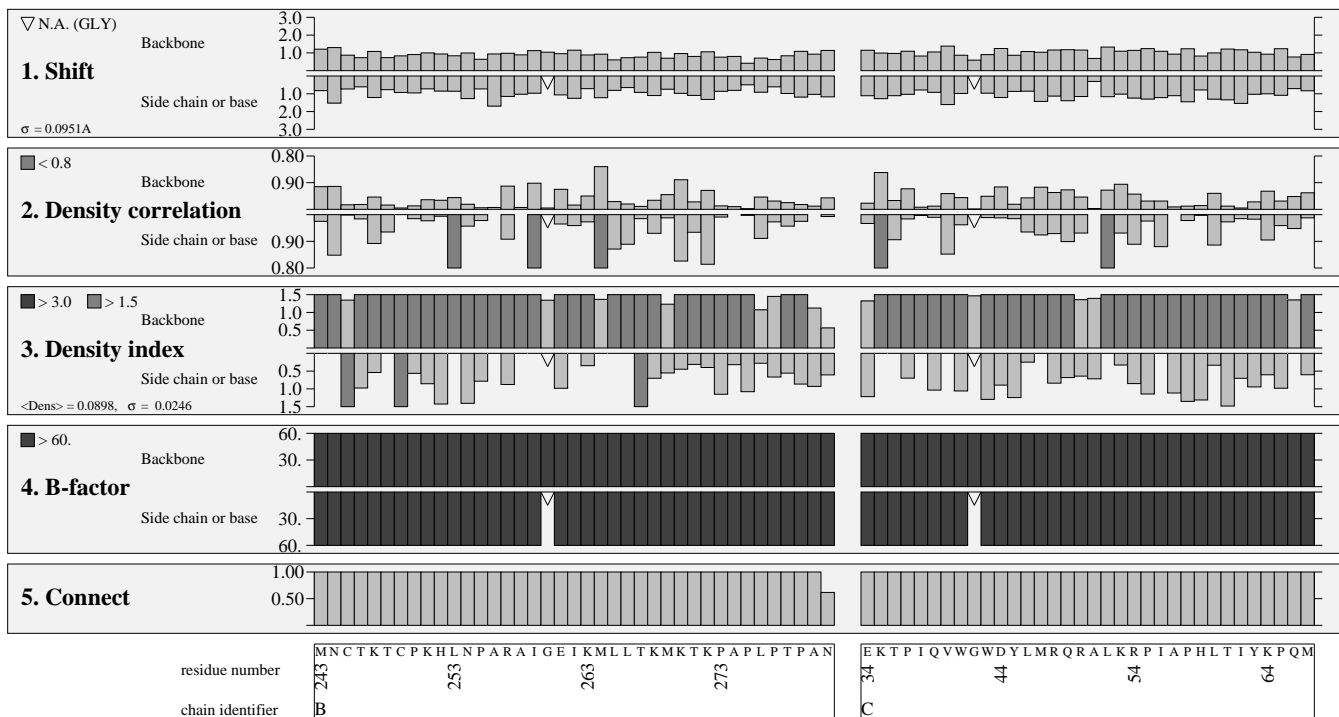
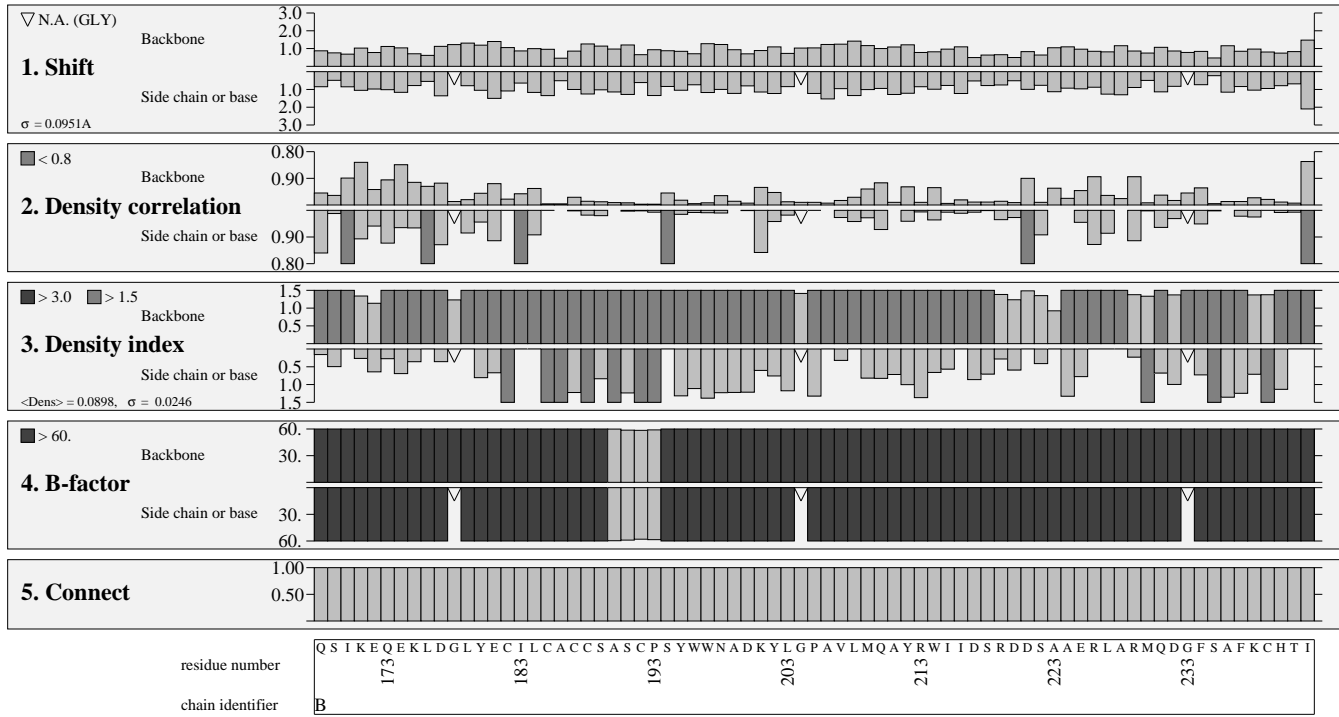
Local estimation (5)



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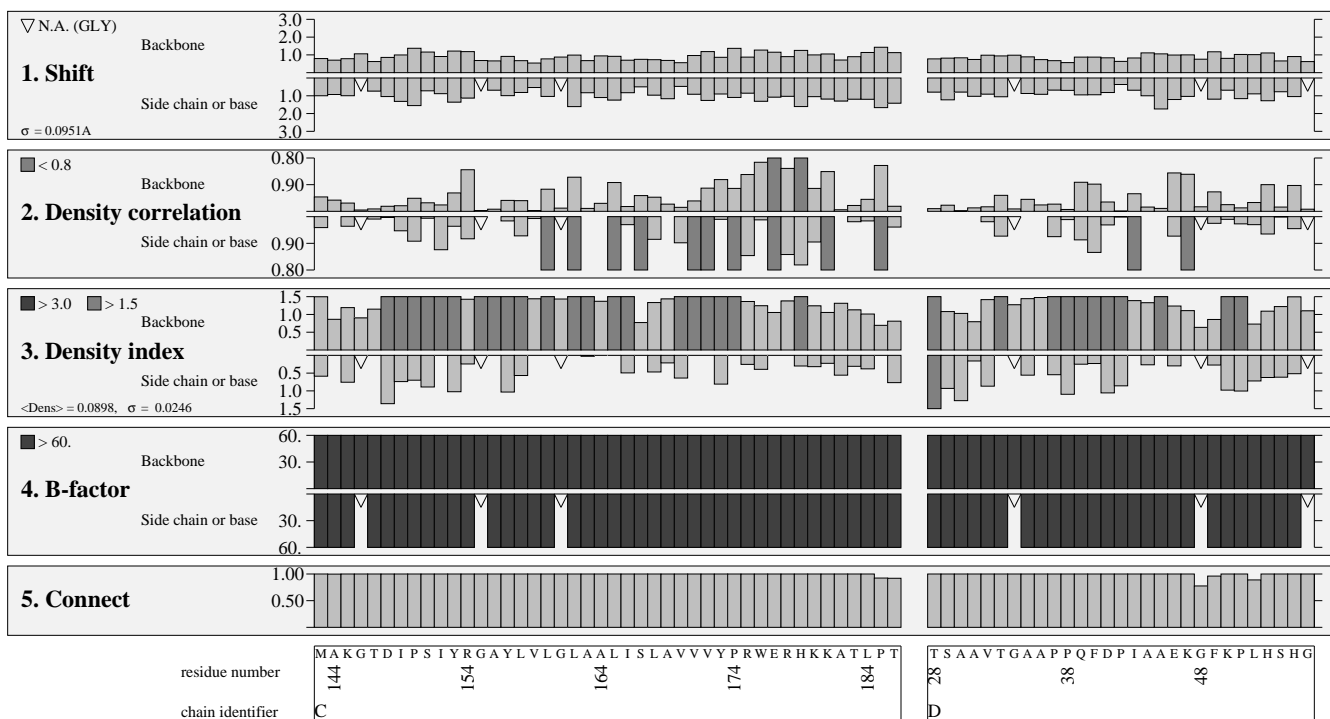
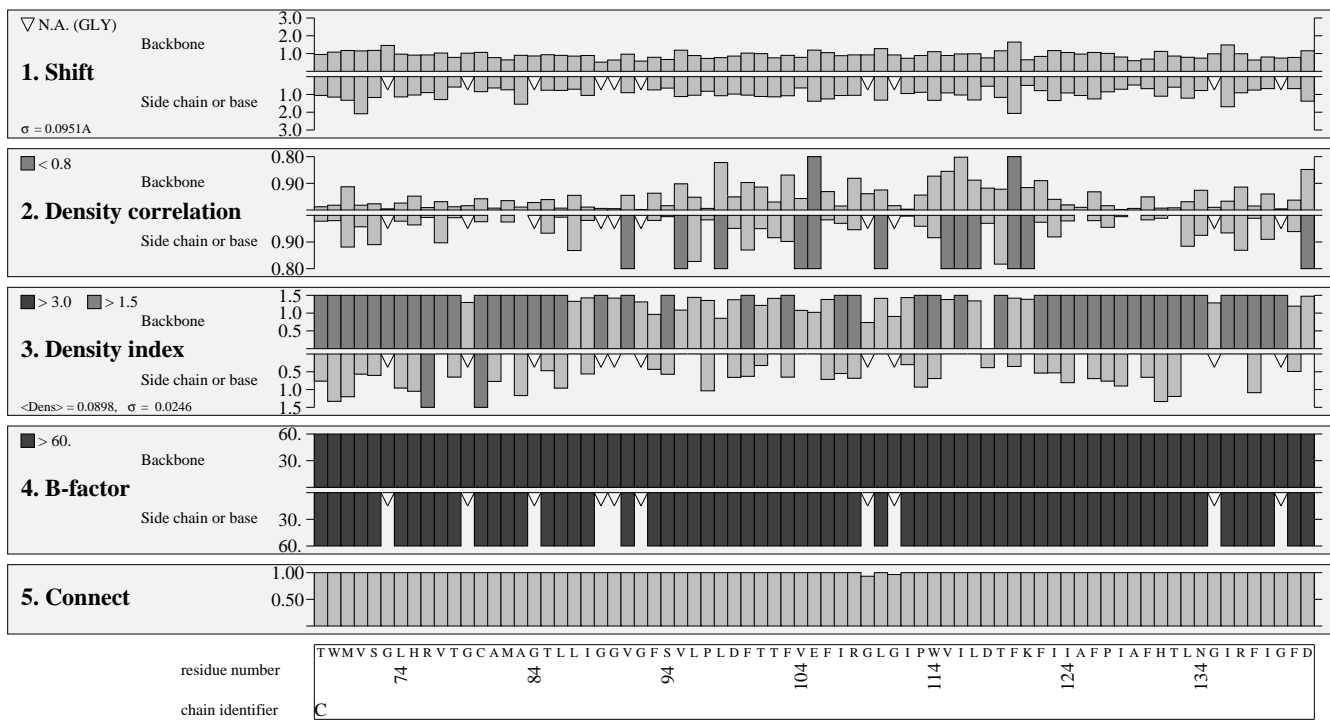
Local estimation (6)



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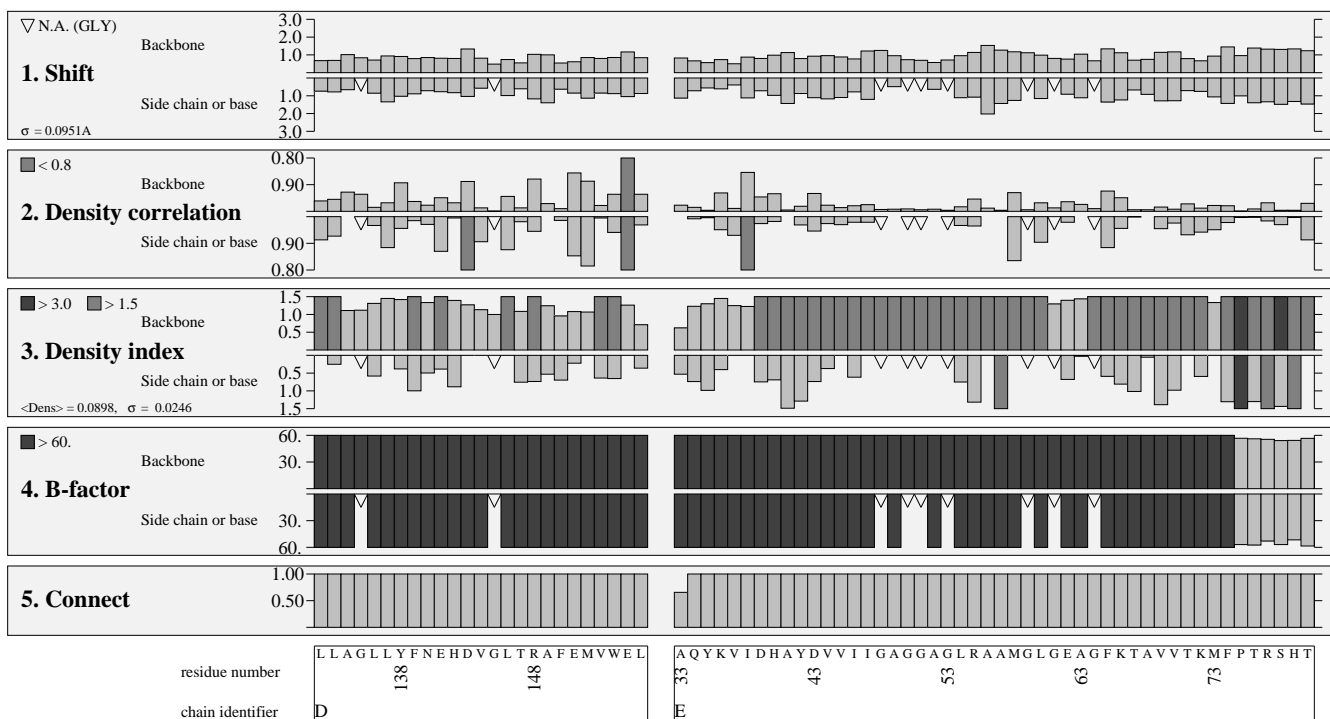
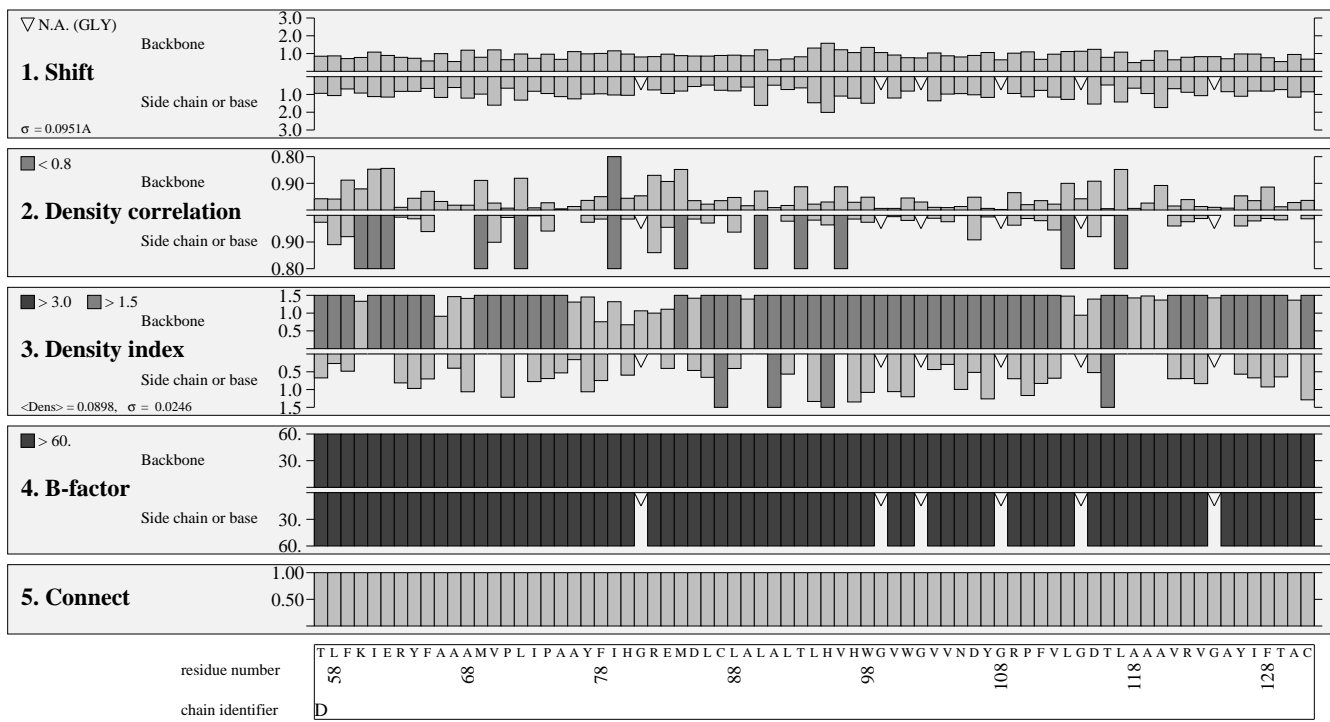
Local estimation (7)



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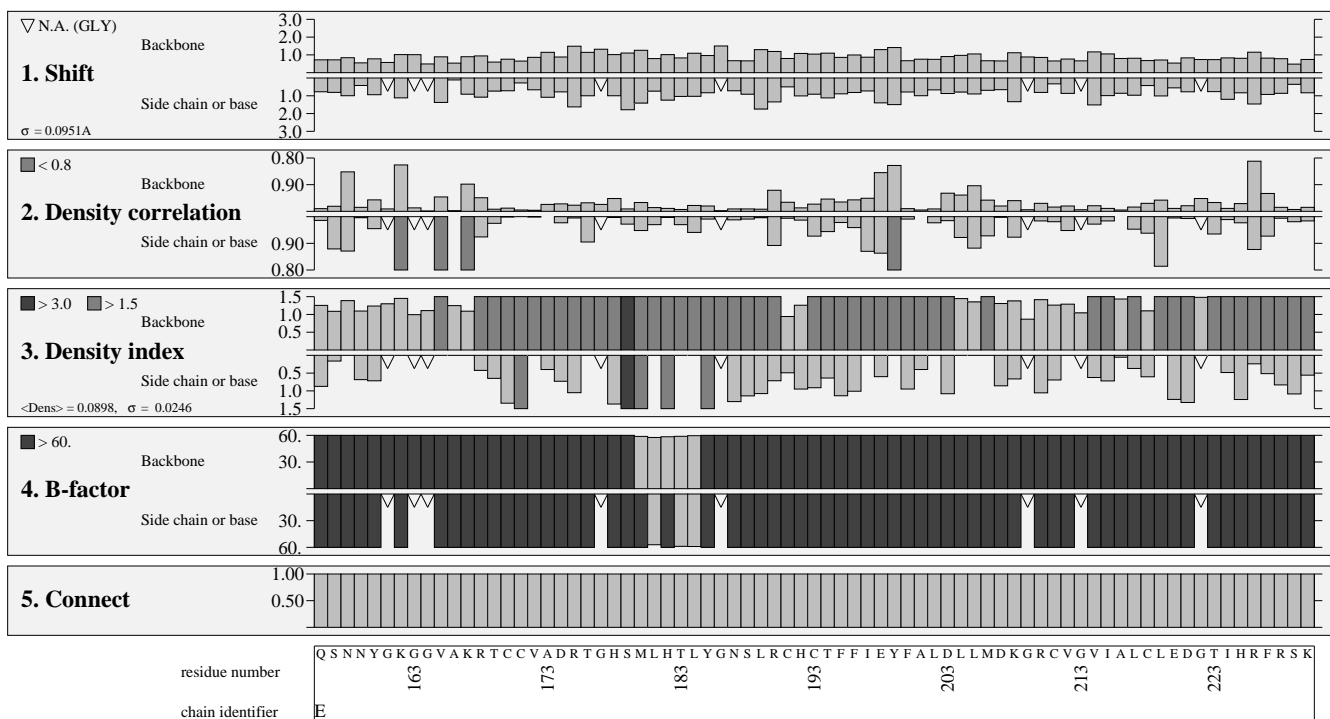
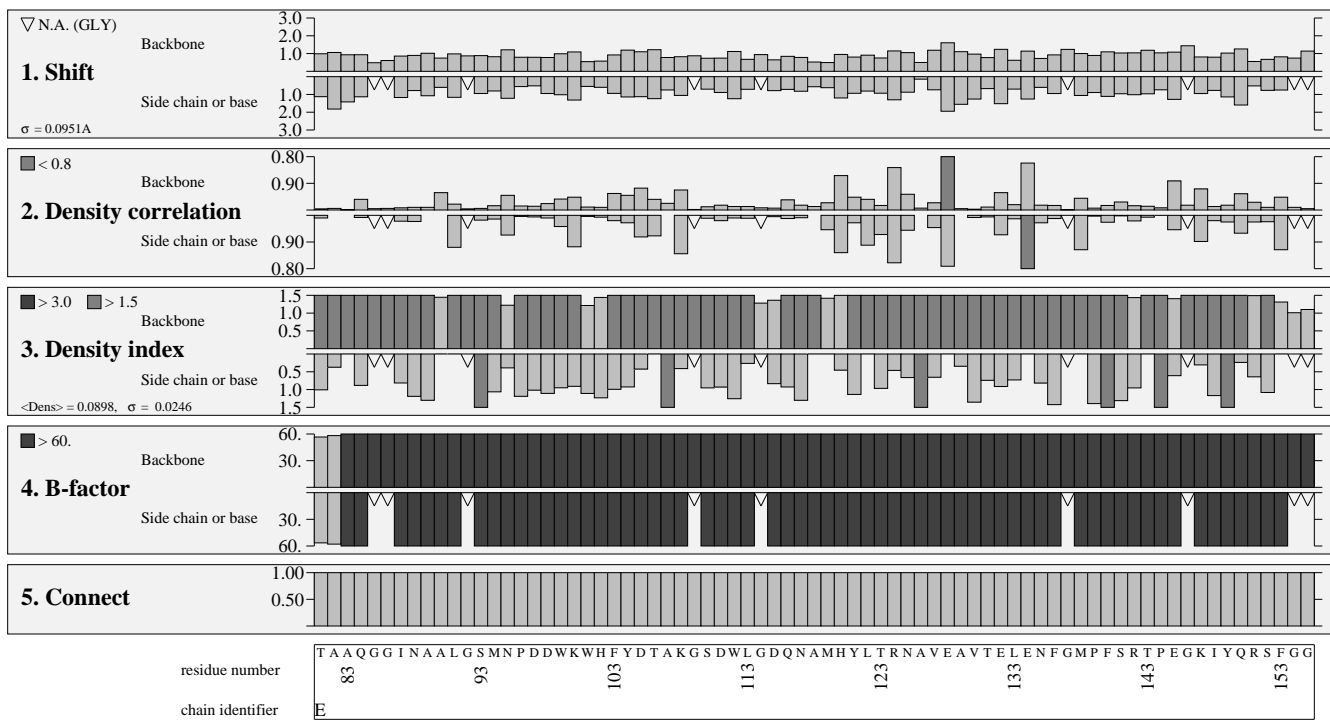
Local estimation (8)



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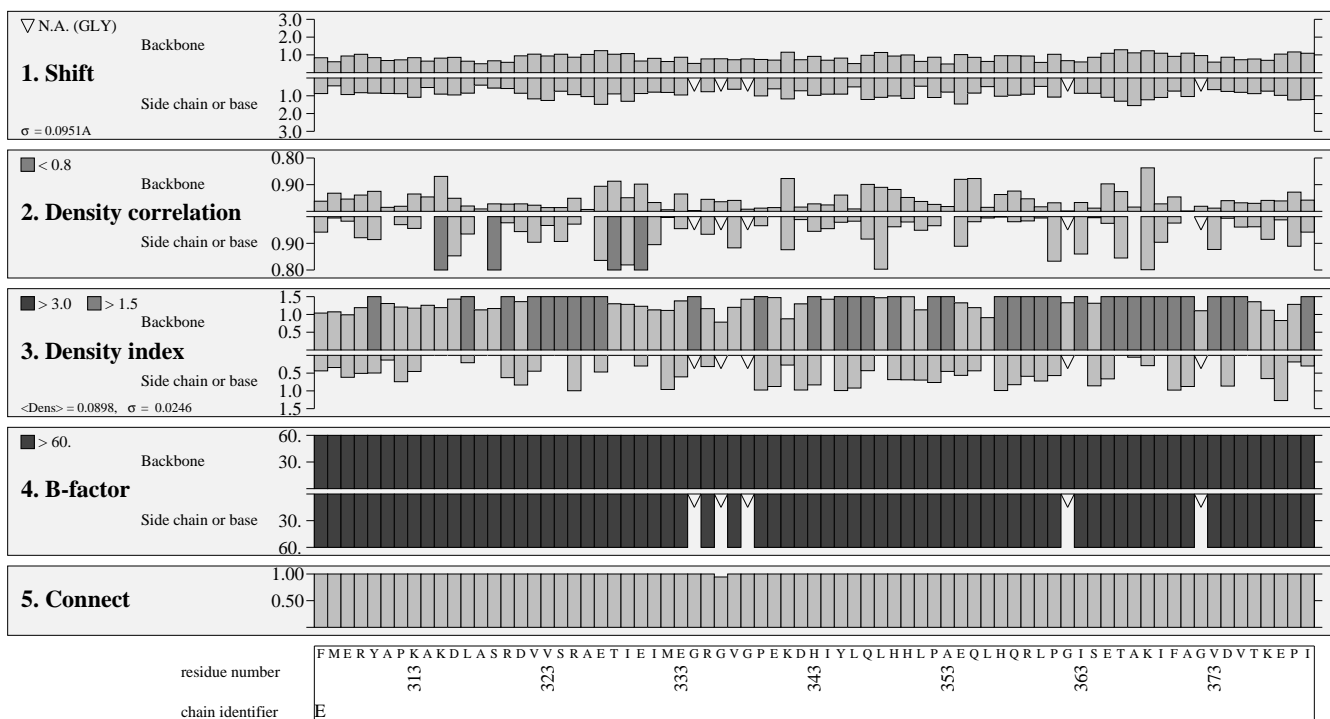
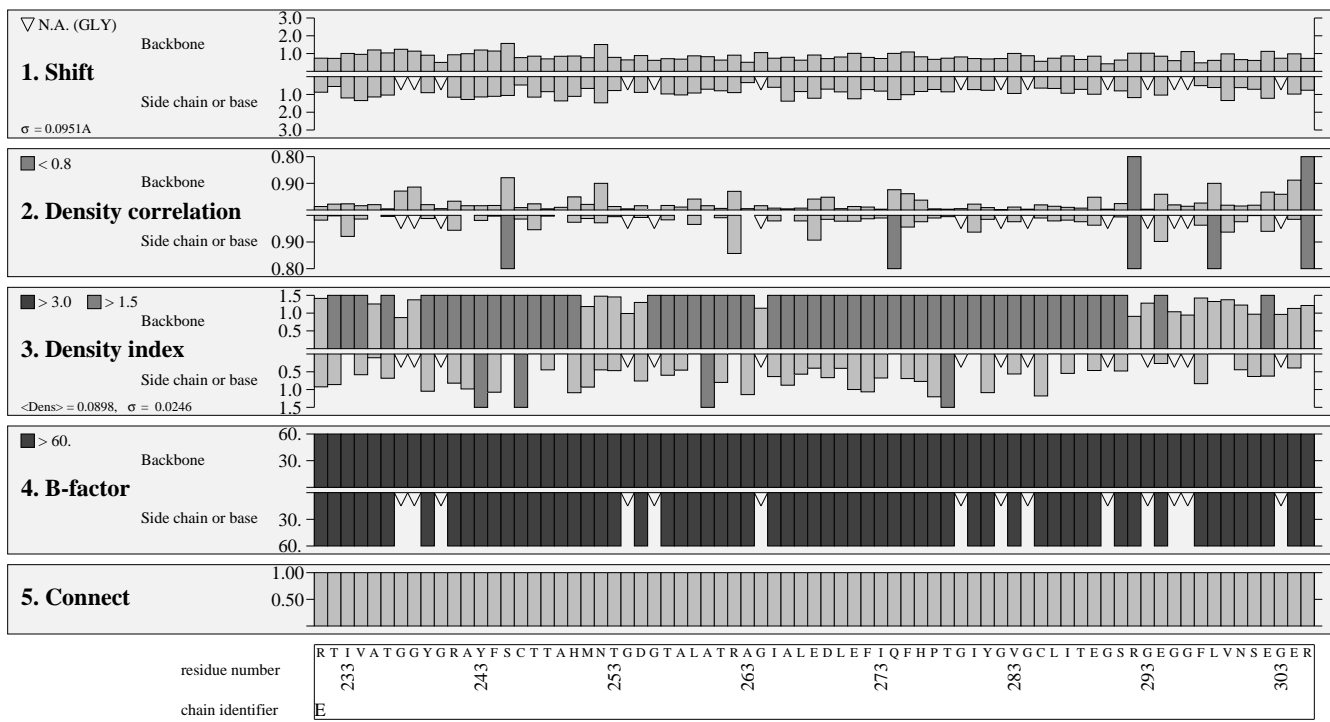
Local estimation (9)



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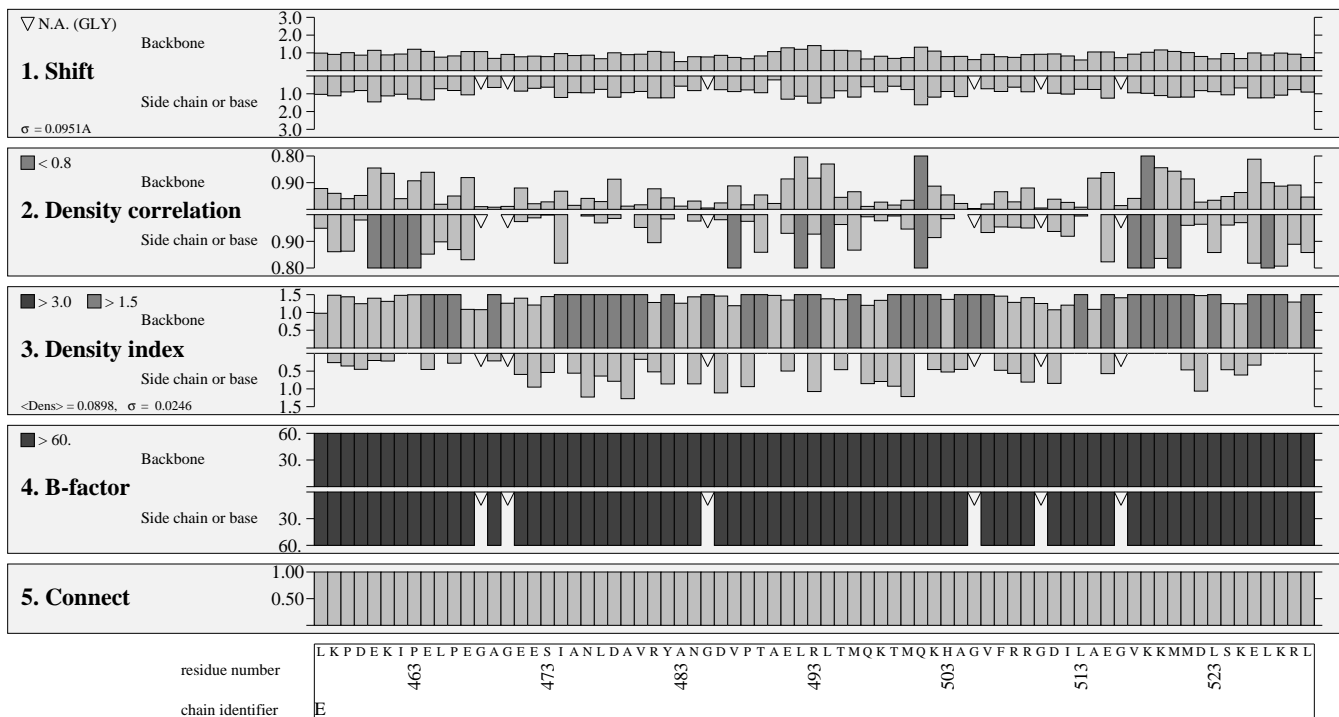
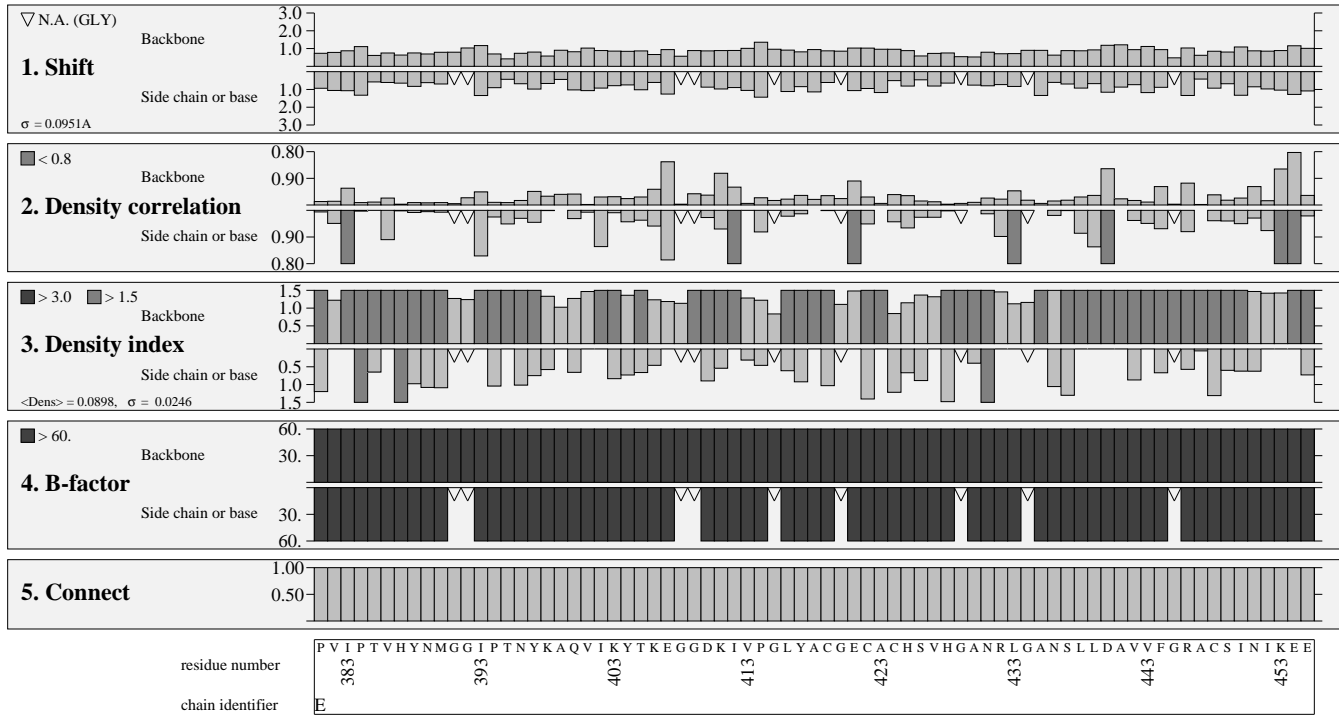
Local estimation (10)



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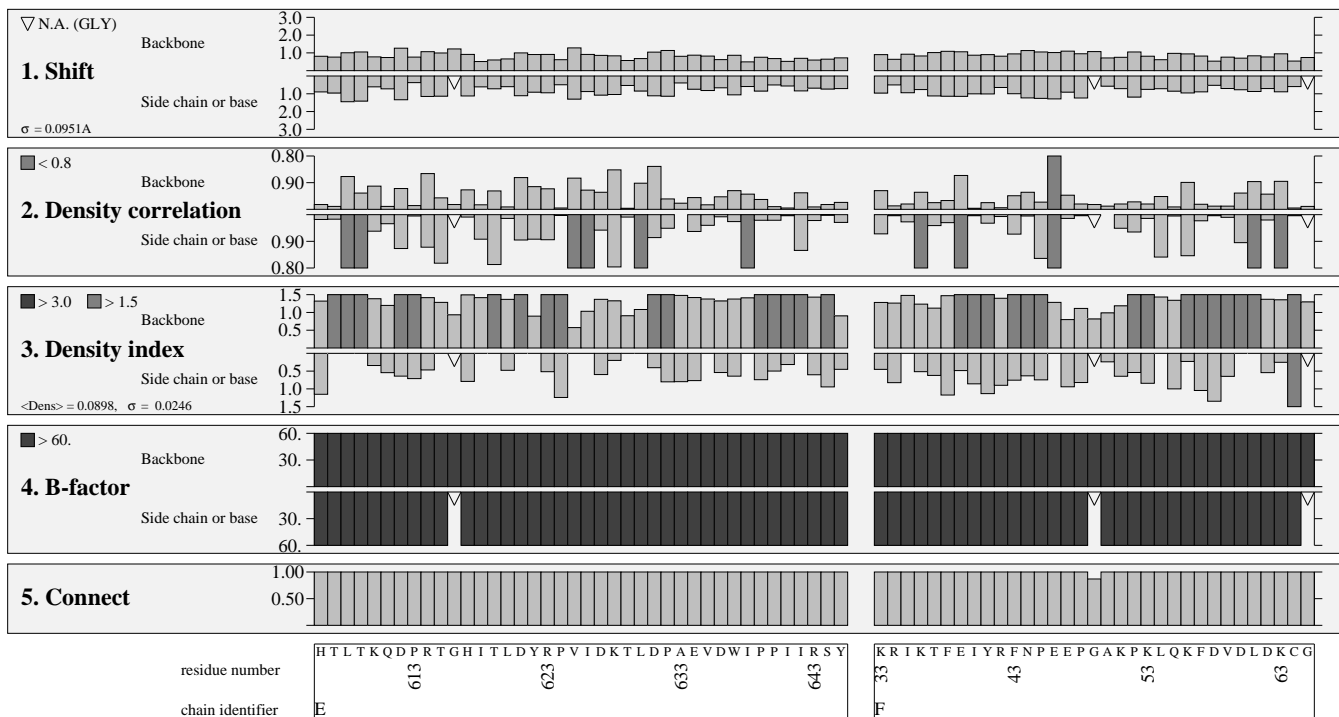
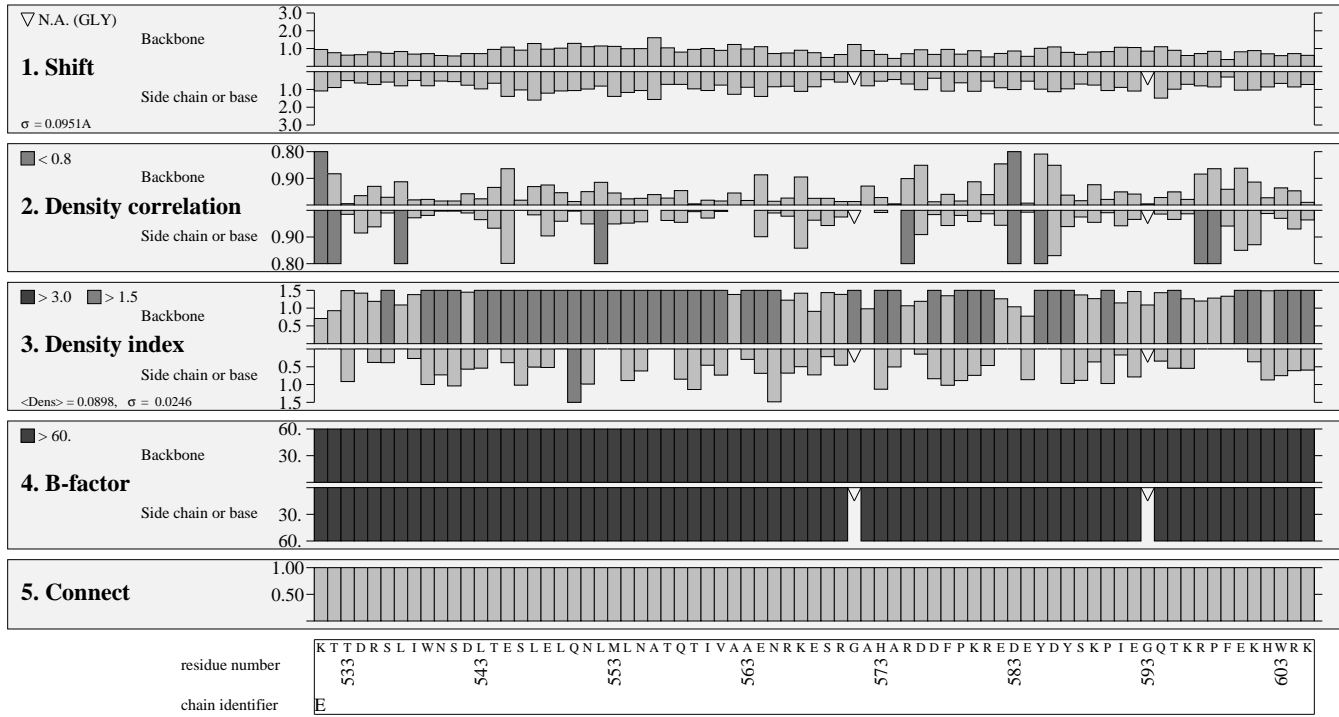
Local estimation (11)



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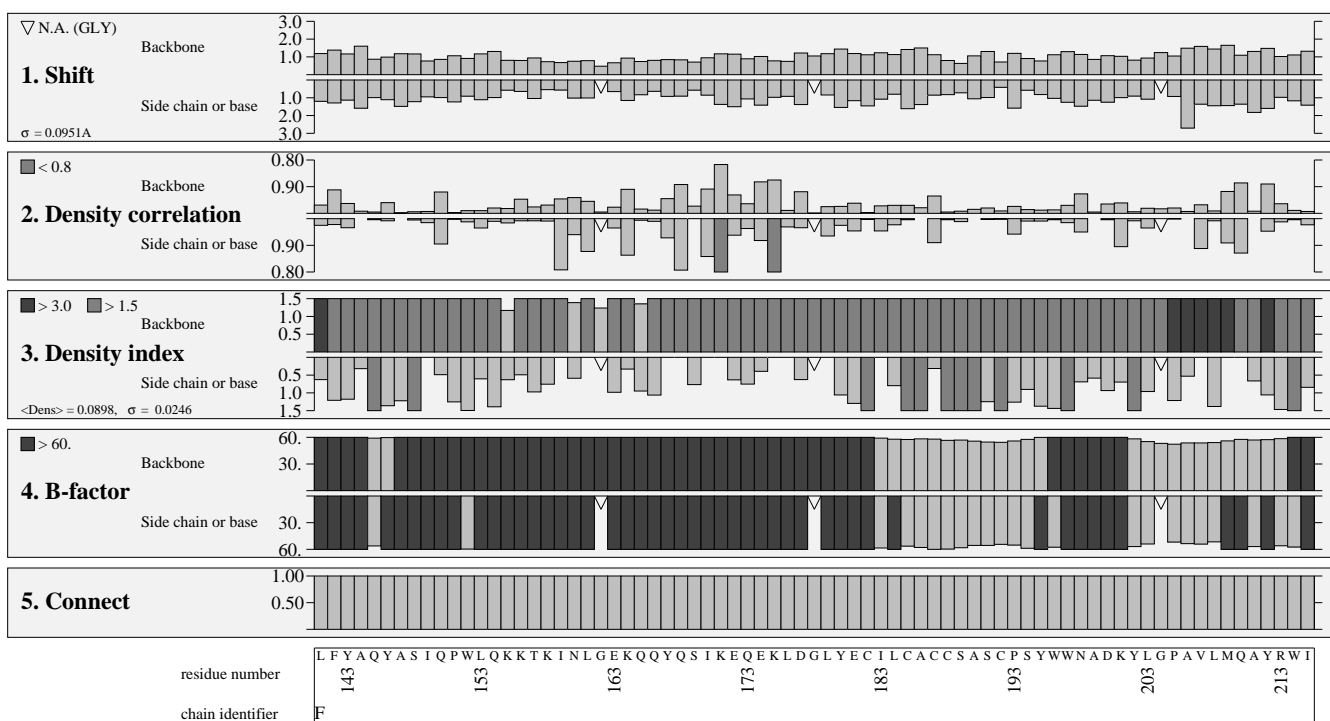
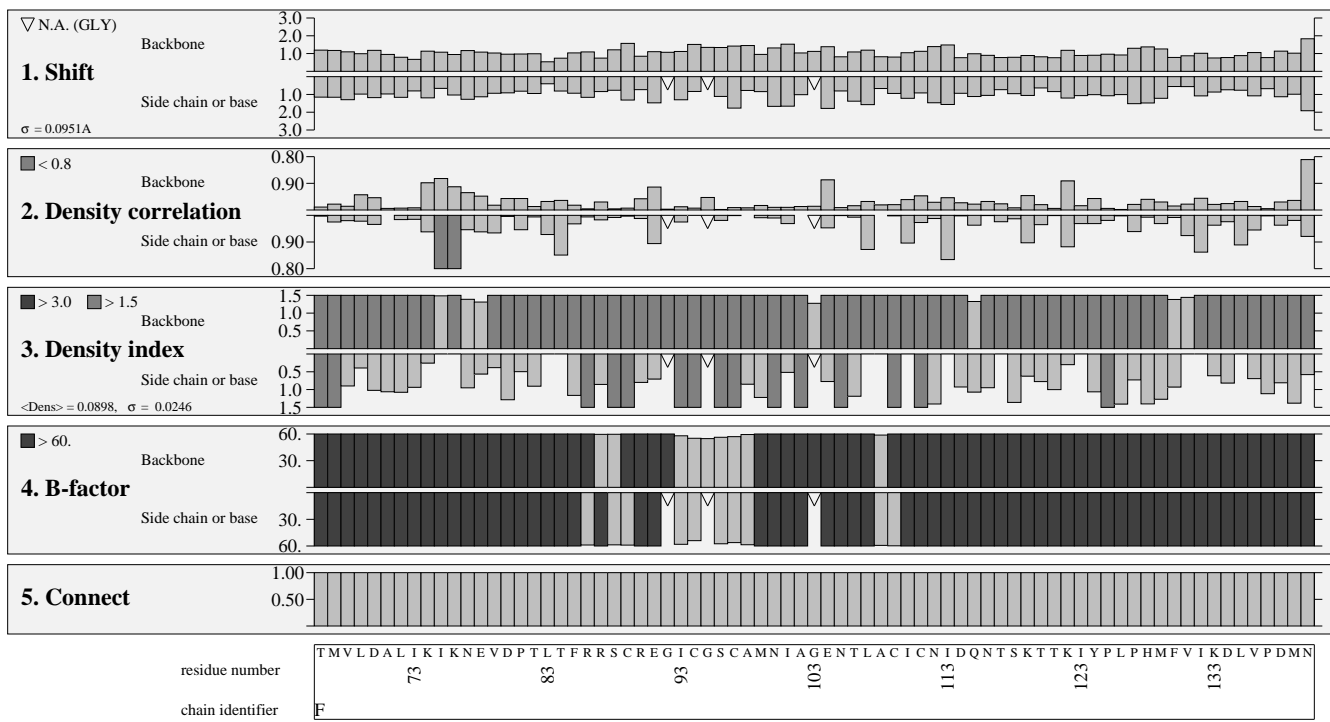
Local estimation (12)



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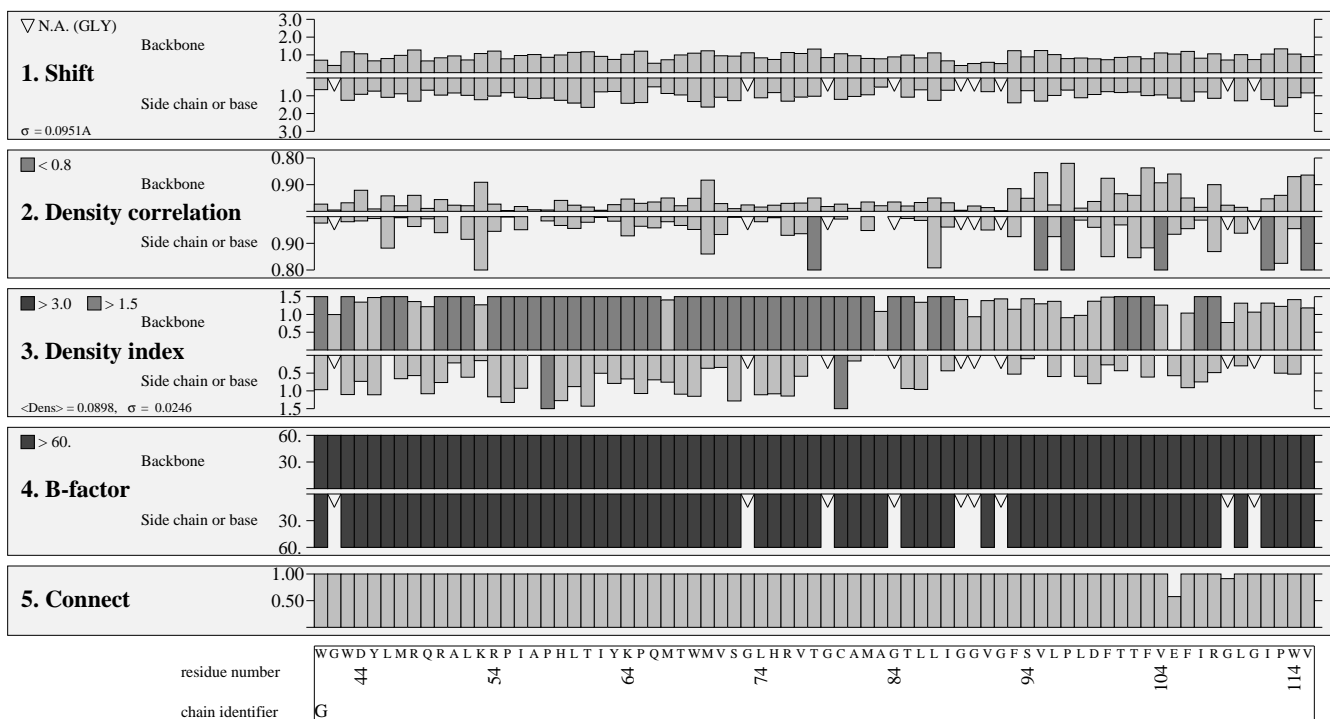
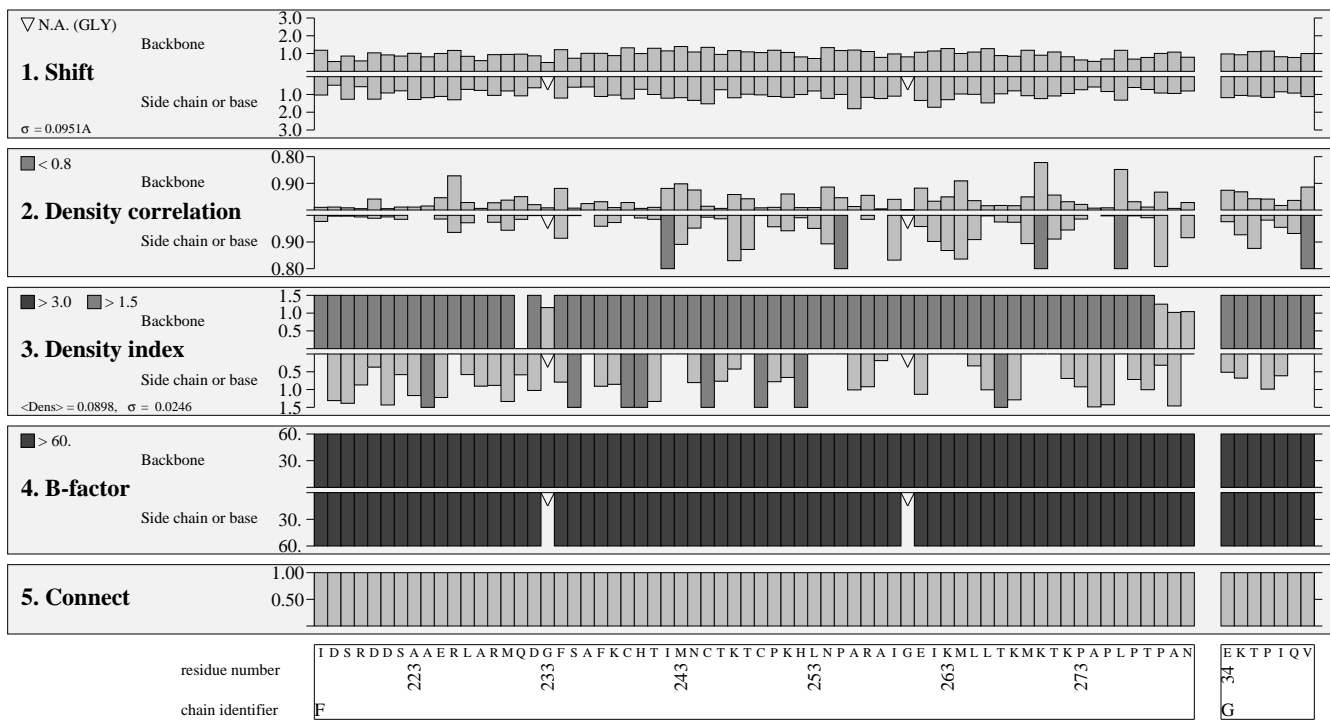
Local estimation (13)



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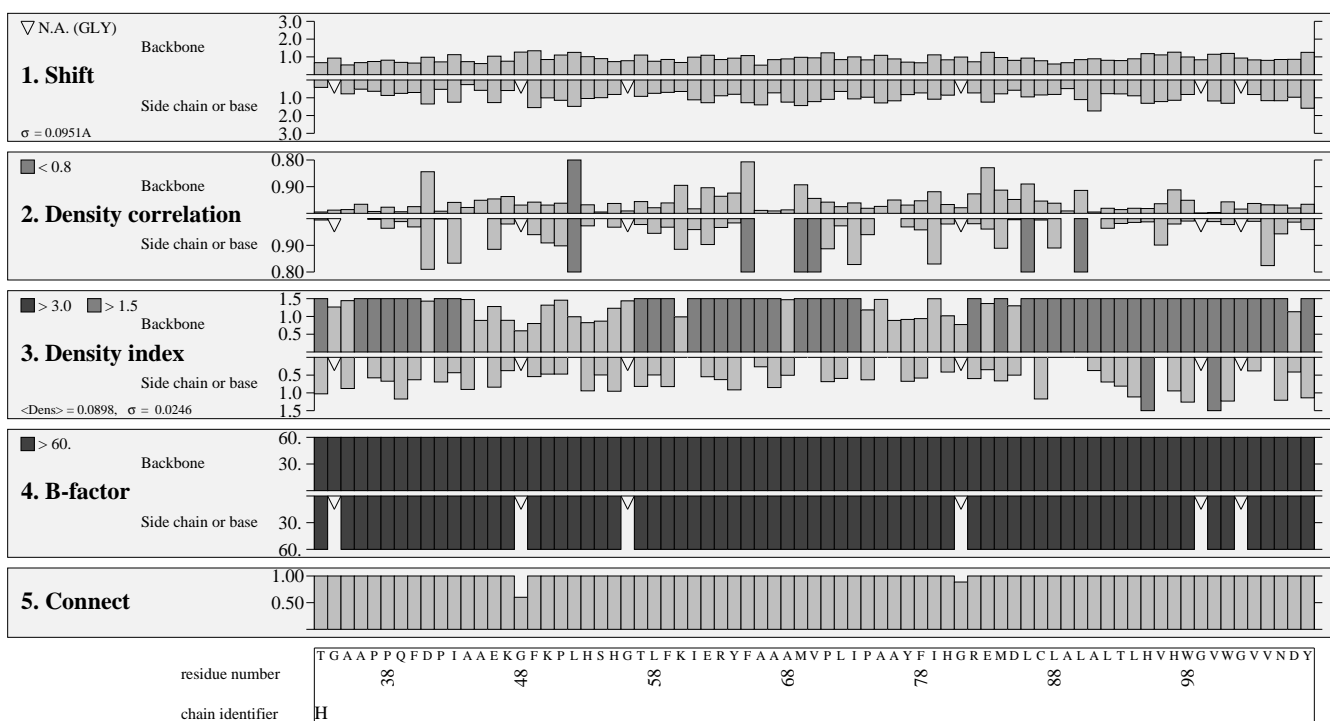
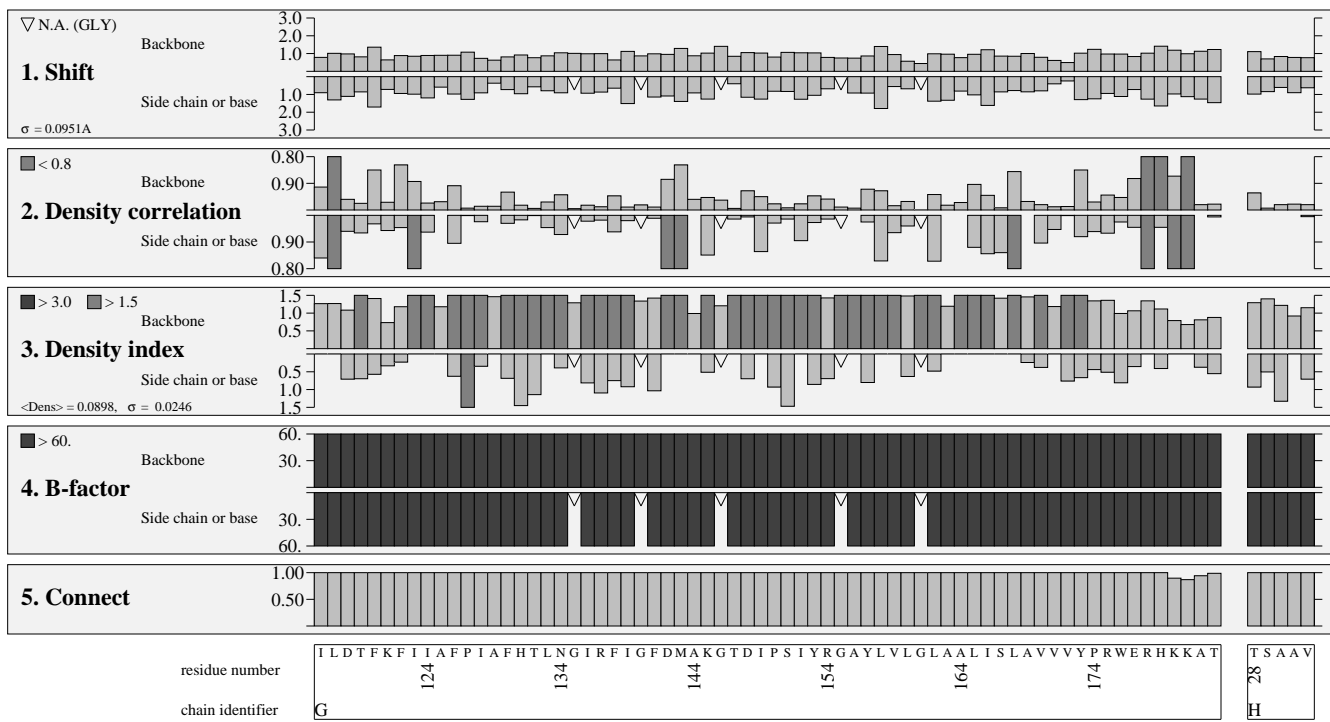
Local estimation (14)



Structure Factor Check

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Local estimation (15)



Structure Factor Check

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Local estimation (16)

