

Structure Factor Check

2H88

Title: AVIAN MITOCHONDRIAL RESPIRATORY COMPLEX II AT 1.8 ANGSTROM R
Date: 06-JUN-06
PDB code: 2H88

Crystal

Cell parameters:

a: 119.97 A b: 199.39 A c: 68.06 A
 α : 90.00 β : 90.35 γ : 90.00

Space group: P 1 21 1

Model

19414 atoms (2030 water molecules)

Number of chains: 51

Volume not occupied by model: 47.5 %

 (for atomic model): 31.2 A²

σ (B): 14.45 A²

Matthews coefficient: 3.00

Corresponding solvent % : 58.61

Refinement

Program: CNS 1.1

Nominal resolution range: 45.1 – 1.74 A

Reported R-factor: 0.178

Number of reflections used: 291095

Reported Rfree: 0.21

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 45.1 – 1.70 A

Reflections in file: 304099

Unique reflections above 0: 304099

above 1 σ : 301680

above 3 σ : 224779

SF CHECK

Nominal resolution range: 45.1 – 1.74 A

\05max. from input data, min. from author\05

Used reflections: 295022

Reflections out of resolution: 9077

Completeness: 90.6 %

R_stand(F) = $\langle \sigma(F) \rangle / \langle F \rangle$: 0.061

Anisotropic distribution of Structure Factors

ratio of eigen values: 0.7341 1.0000 0.8149

B_overall (by Patterson): 27.A²

Optical resolution: 1.47 A

Expected opt. resol. for complete data set: 1.47 A

Estimated minimal error: 0.025 A

Model vs. Structure Factors

R-factor for all reflections: 0.185

Correlation factor: 0.957

R-factor: 0.188

for $F > 2.0 \sigma$

nom. resolution range: 45.14 – 1.74A

reflections used: 293276

Rfree: 0.212

Nfree: 14570

R-factor without free-refl.: 0.187

Non free-reflections: 278706

<u> (error in coords by Luzzati plot): 0.199 A

Estimated maximal error: 0.075 A

DPI: 0.091 A

Scaling

Scale: 1.273

Bdiff: -1.42

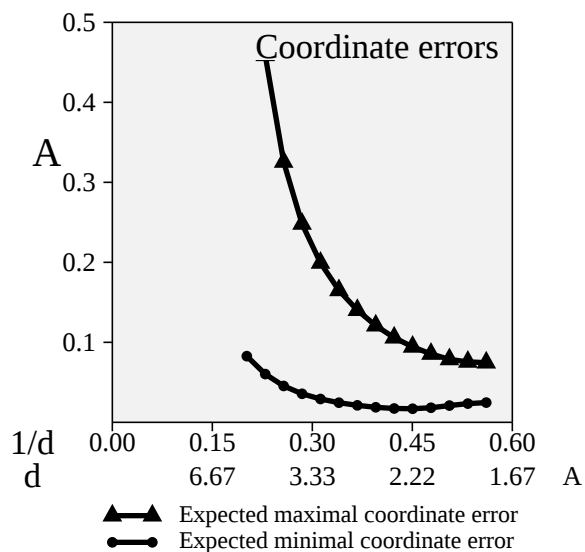
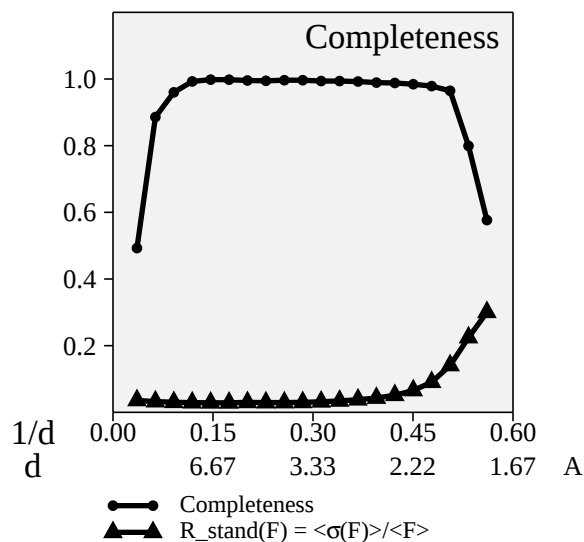
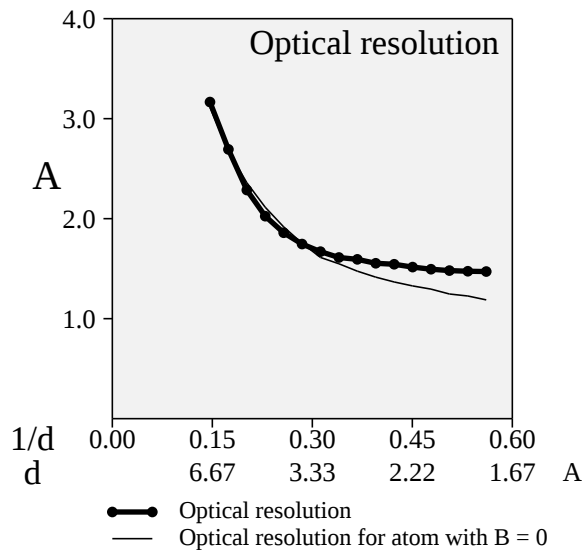
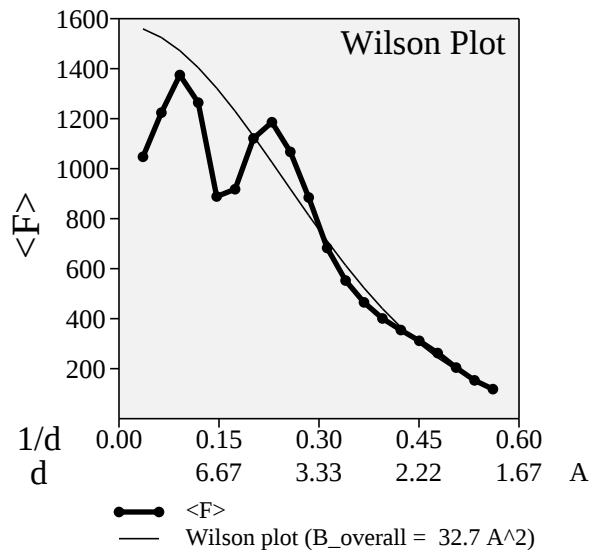
Anisothermal Scaling (Beta):

-0.2131 1.9139 0.2298 0.0000 0.2974 0.0000

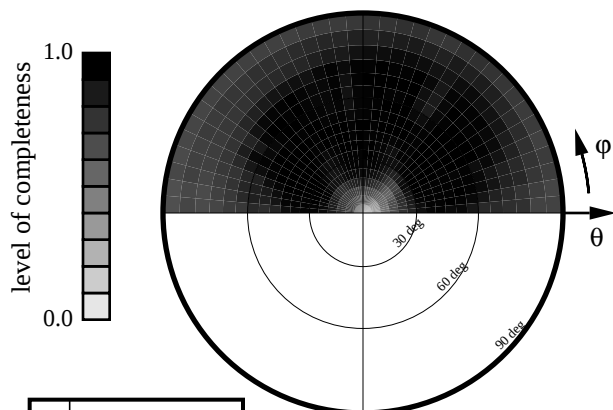
Solvent correction – Ks,Bs: 0.758 250.006

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2H88

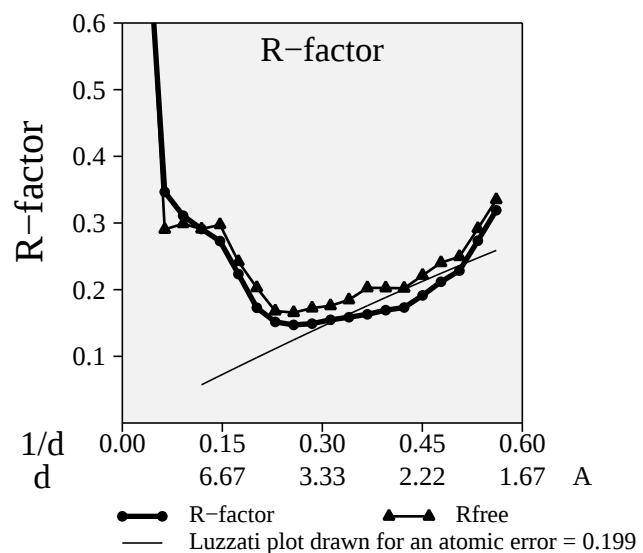


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	89.65	0.00
k	90.00	90.00
l	0.00	0.00

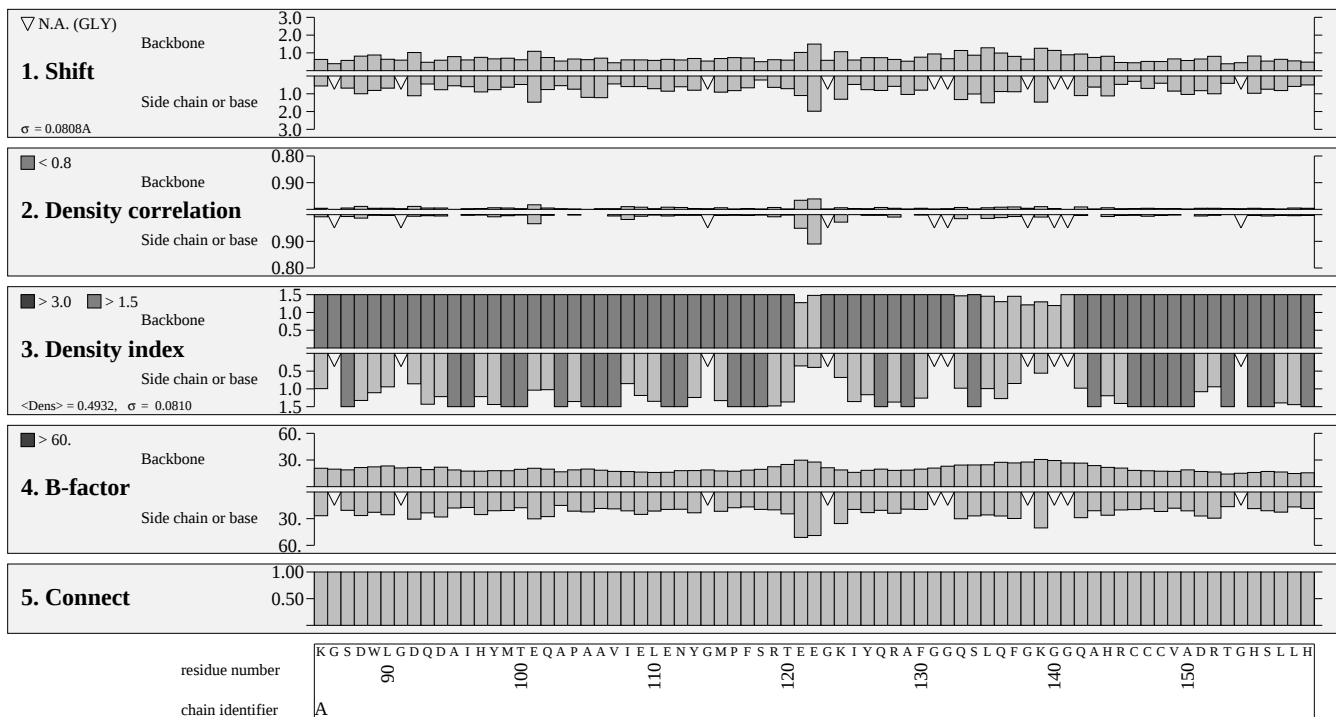
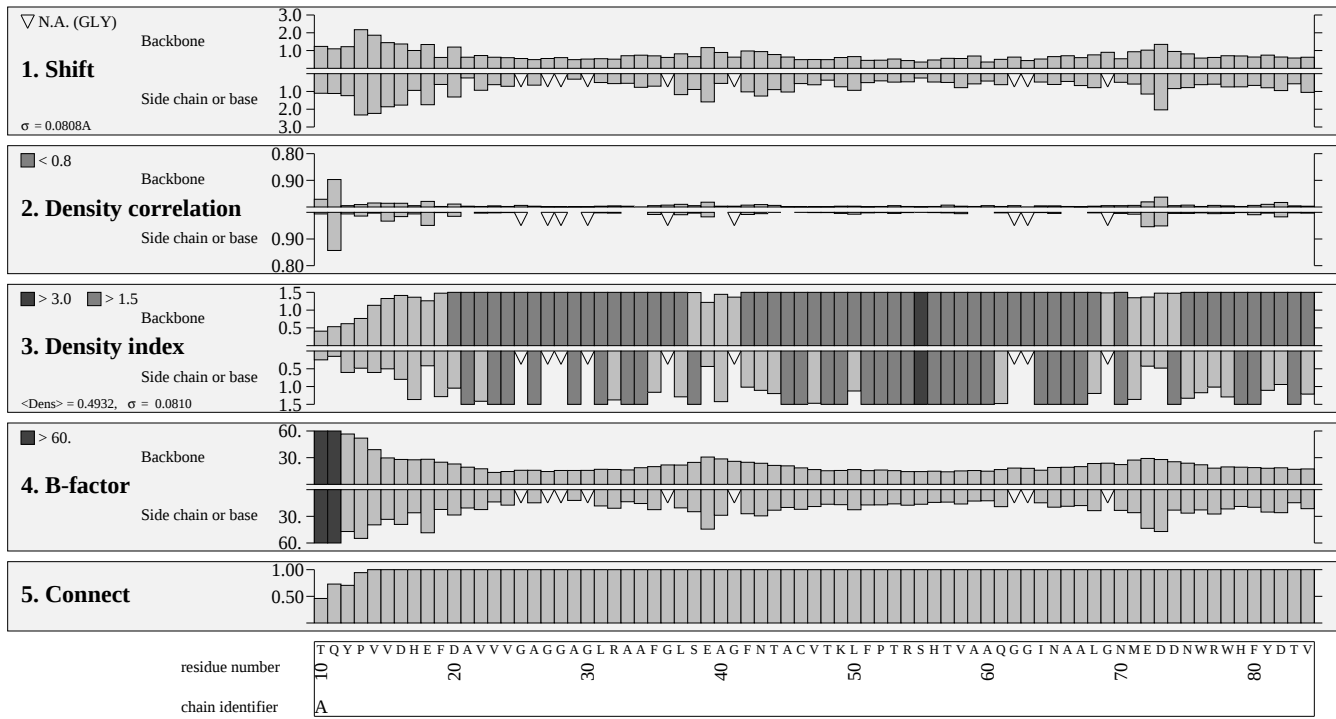
polar coordinates of the crystallographical axes



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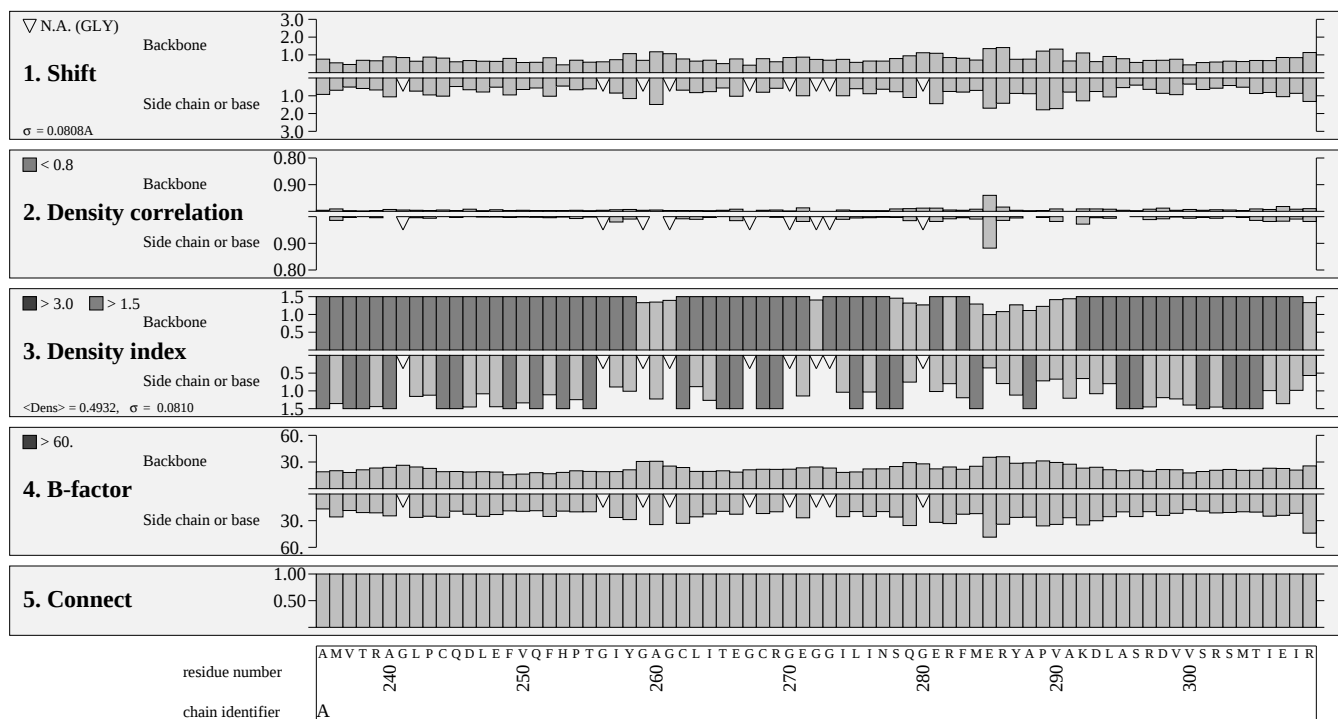
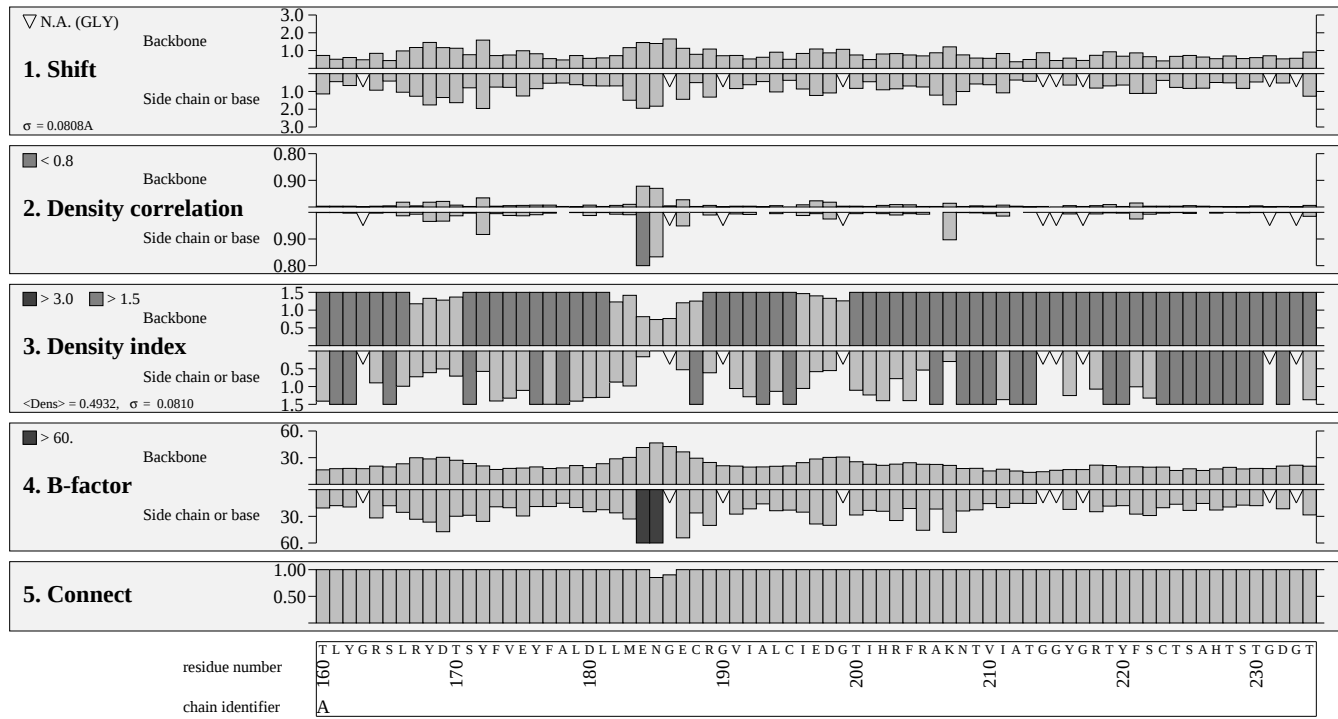
Local estimation



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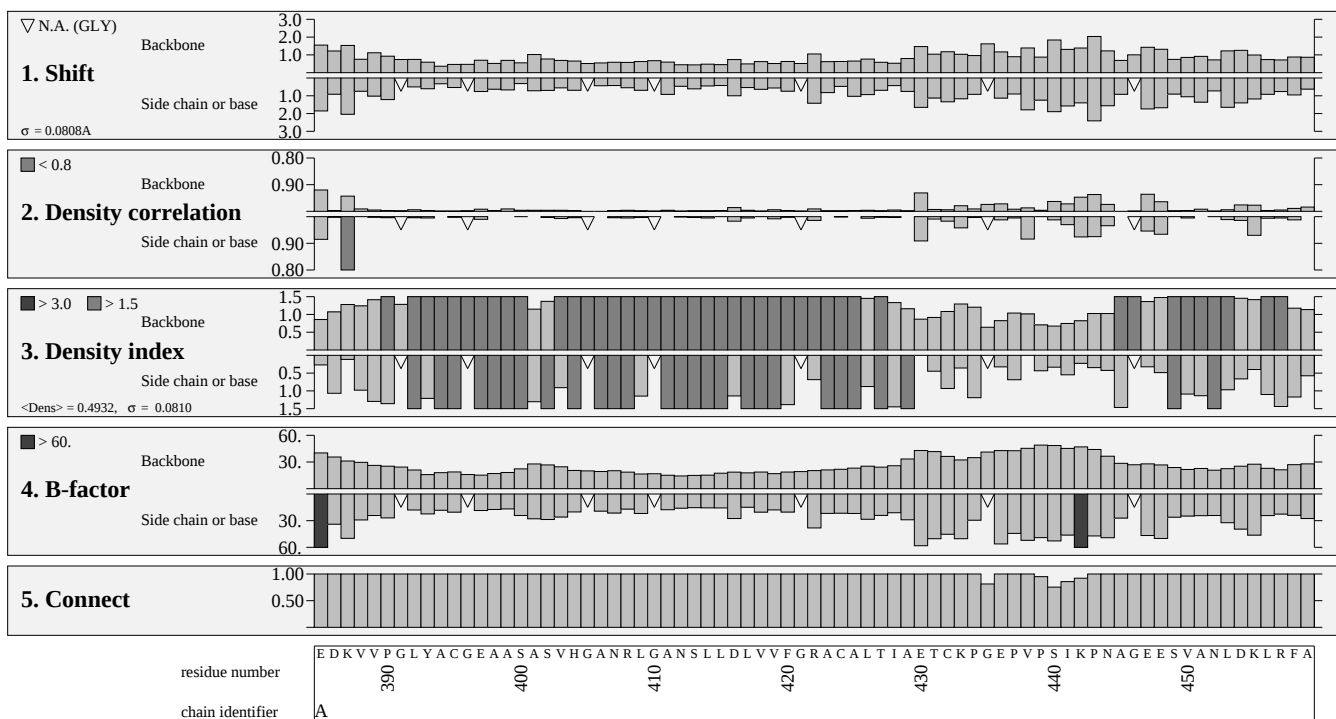
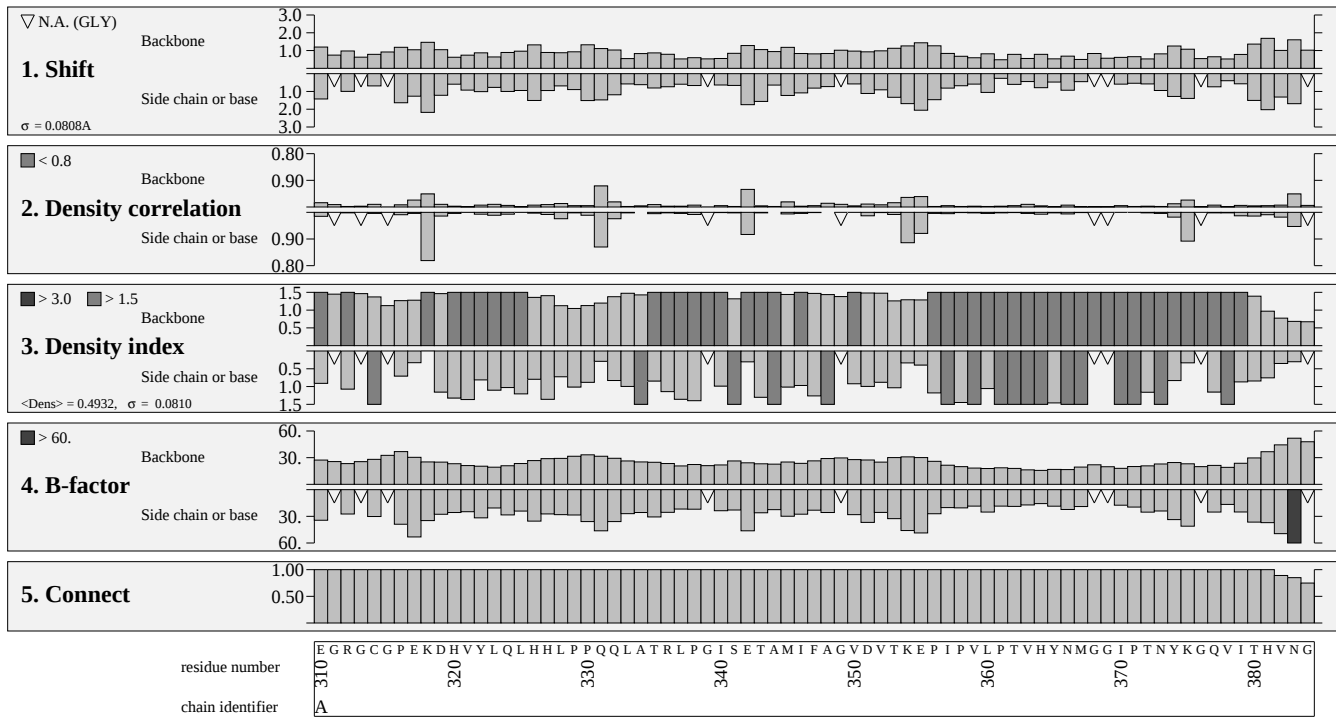
Local estimation (2)



Structure Factor Check

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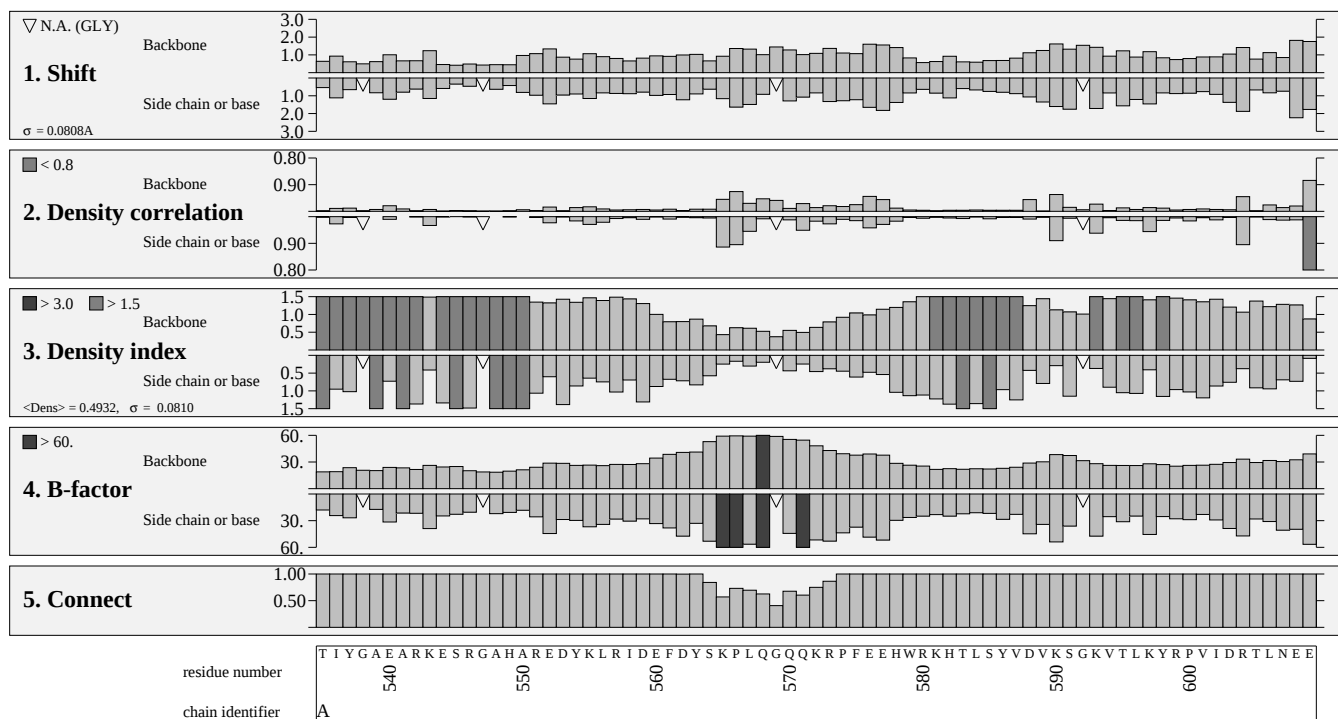
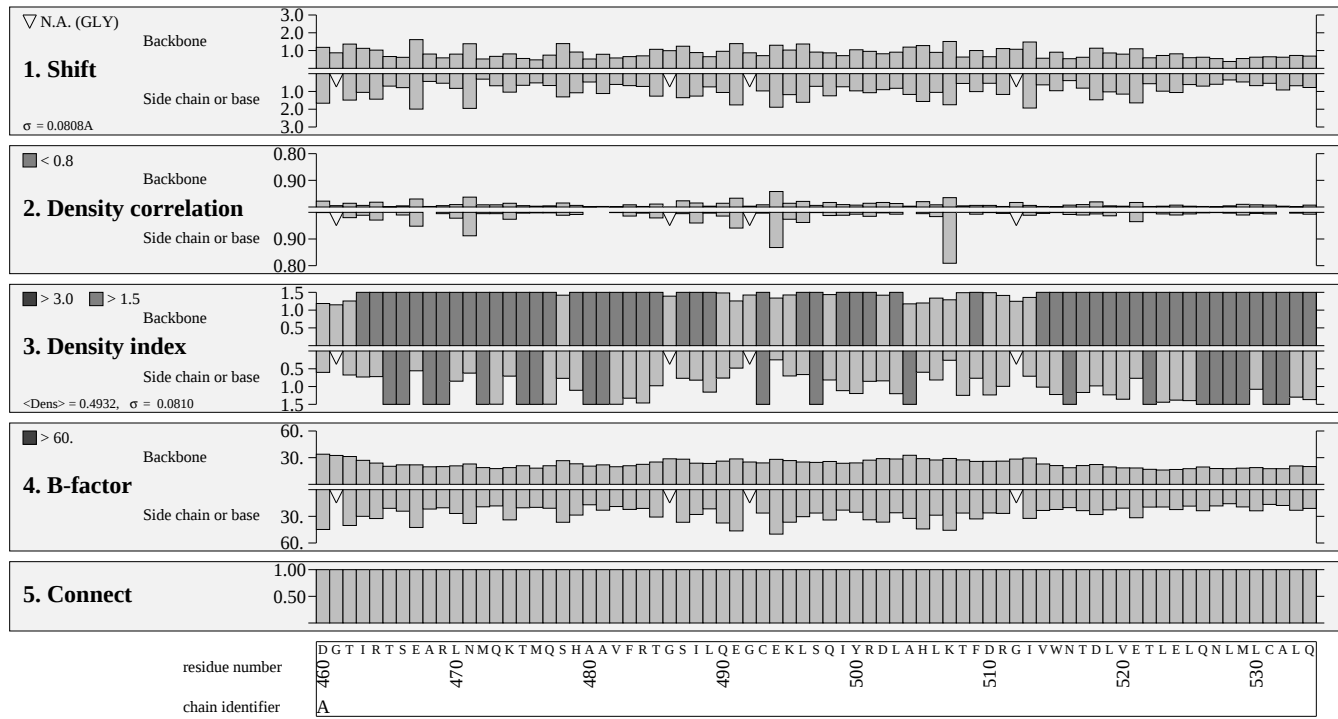
Local estimation (3)



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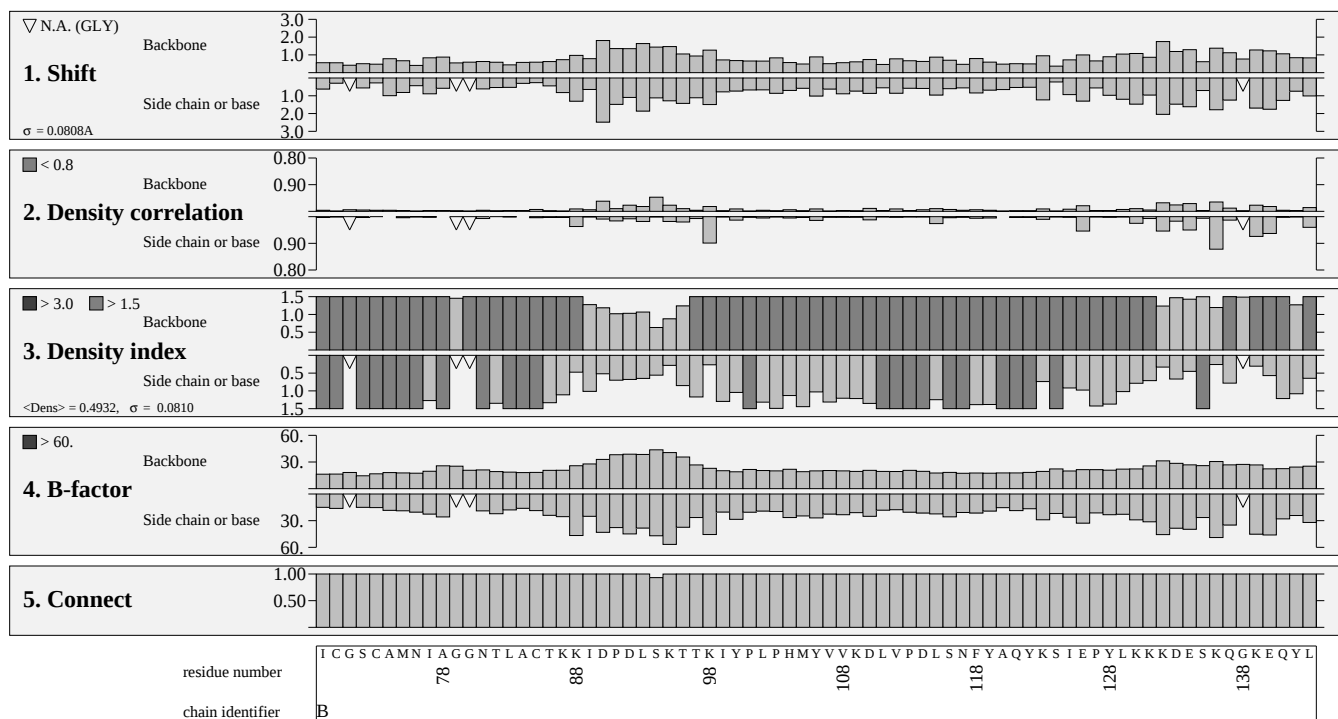
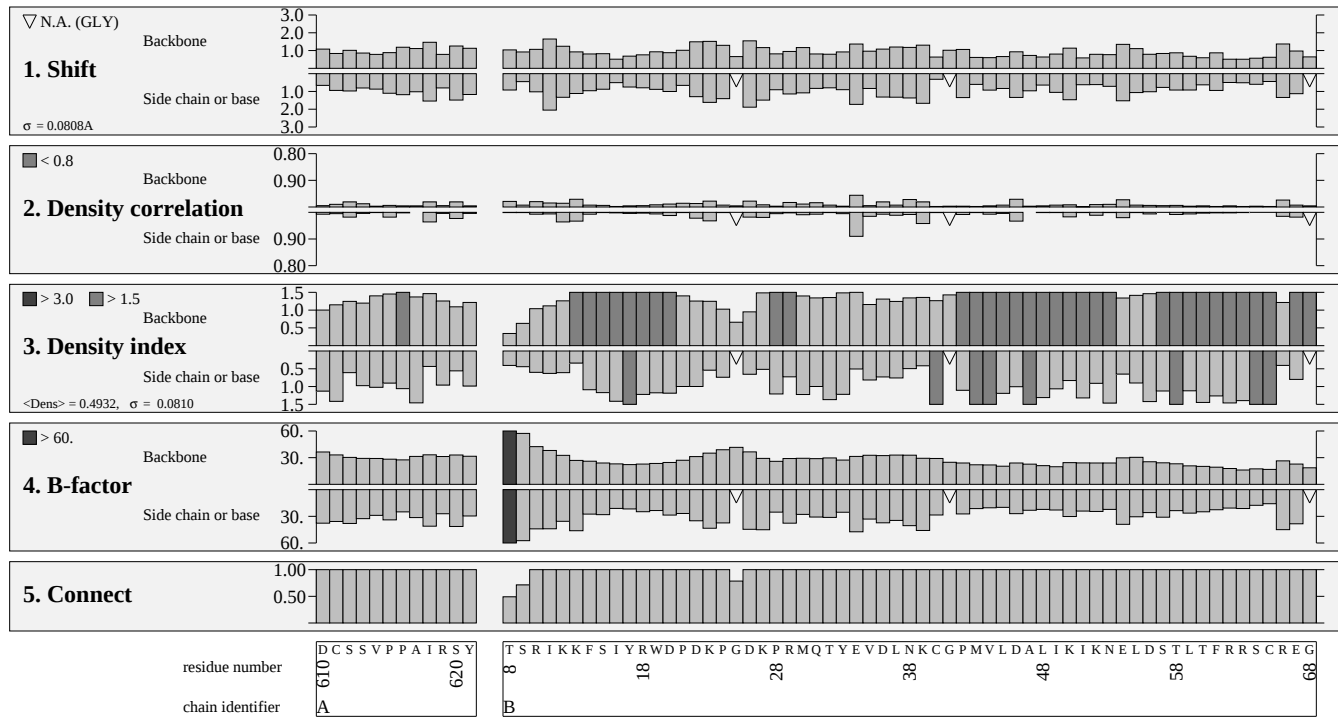
Local estimation (4)



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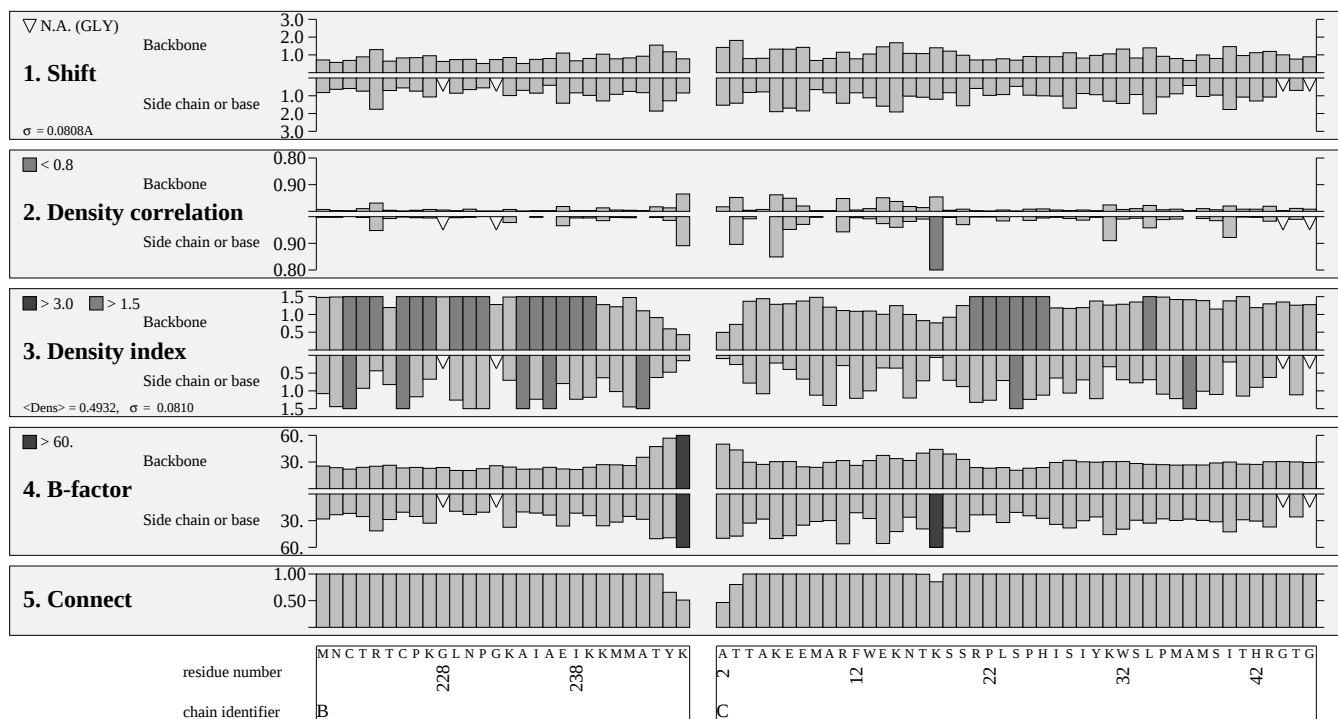
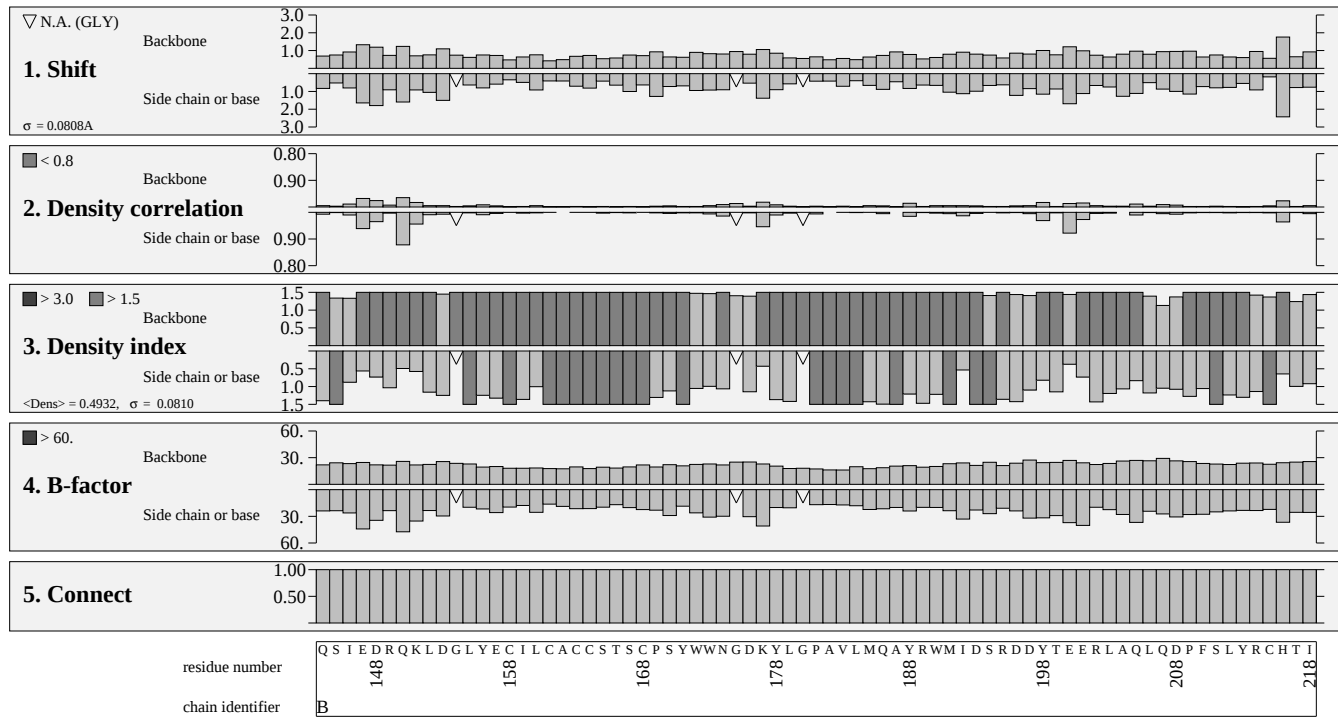
Local estimation (5)



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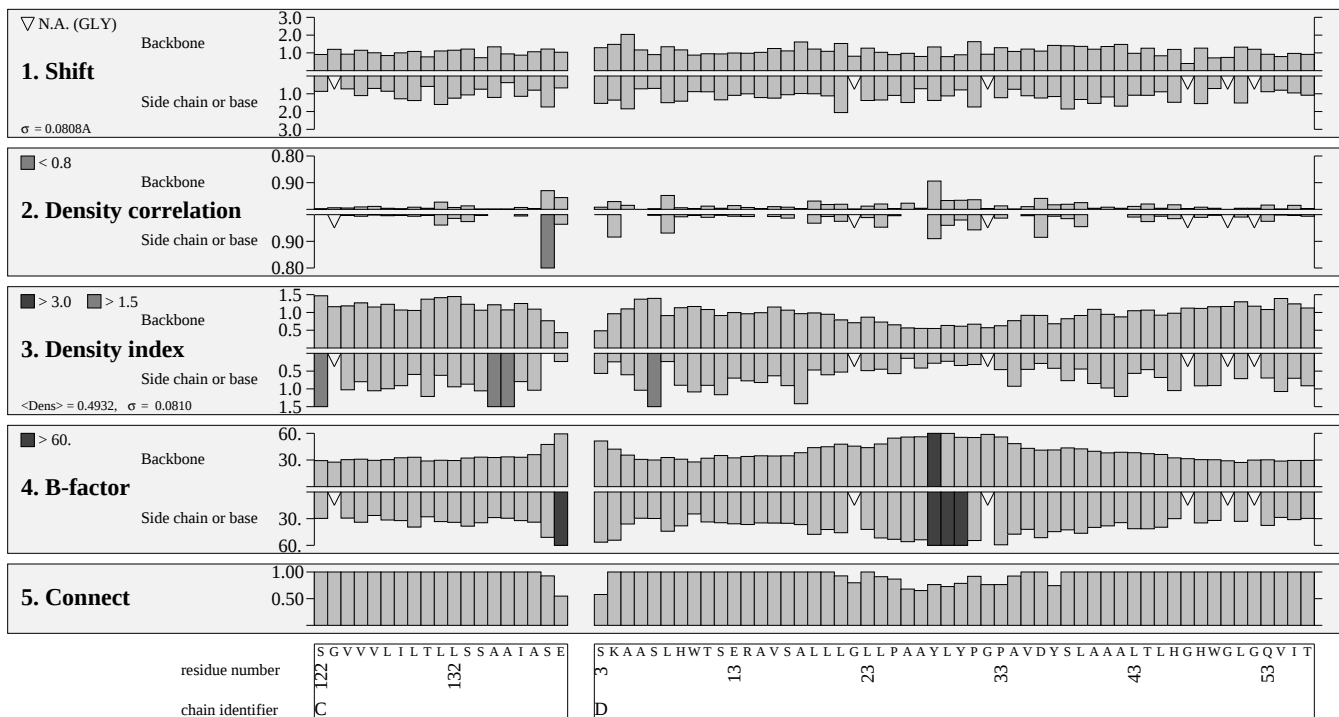
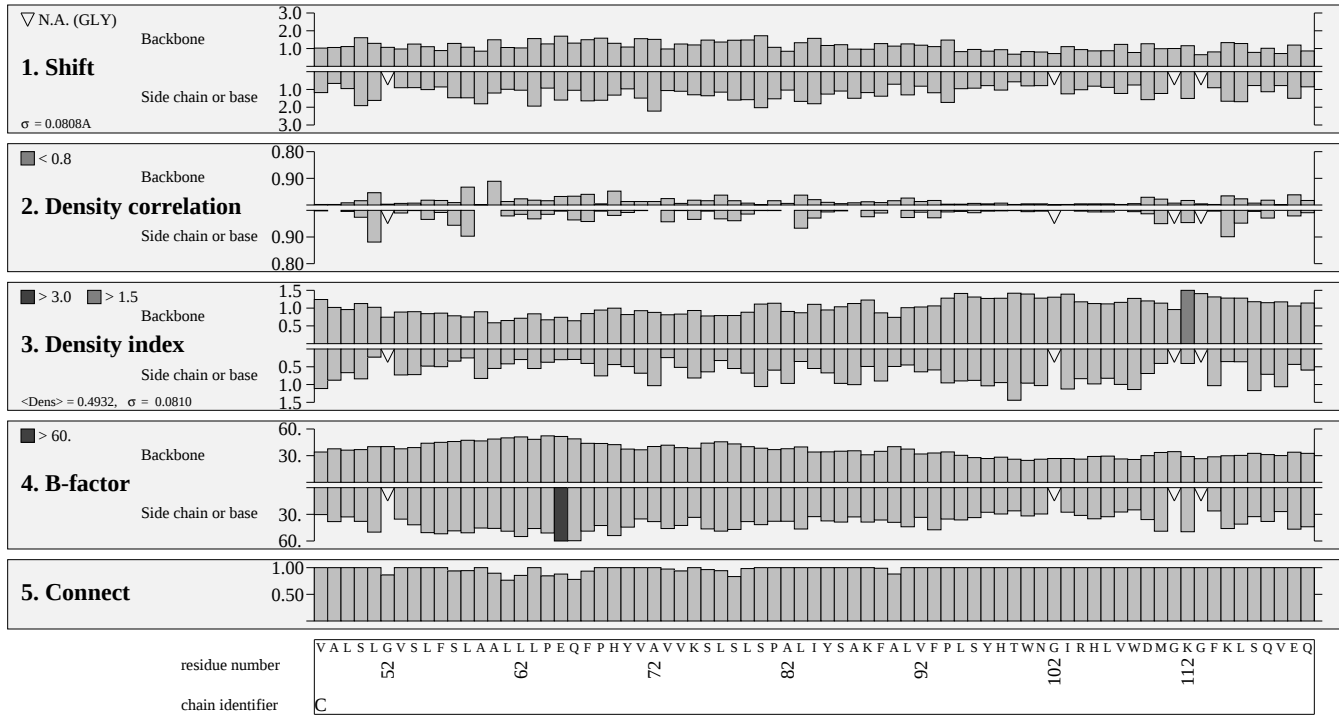
Local estimation (6)



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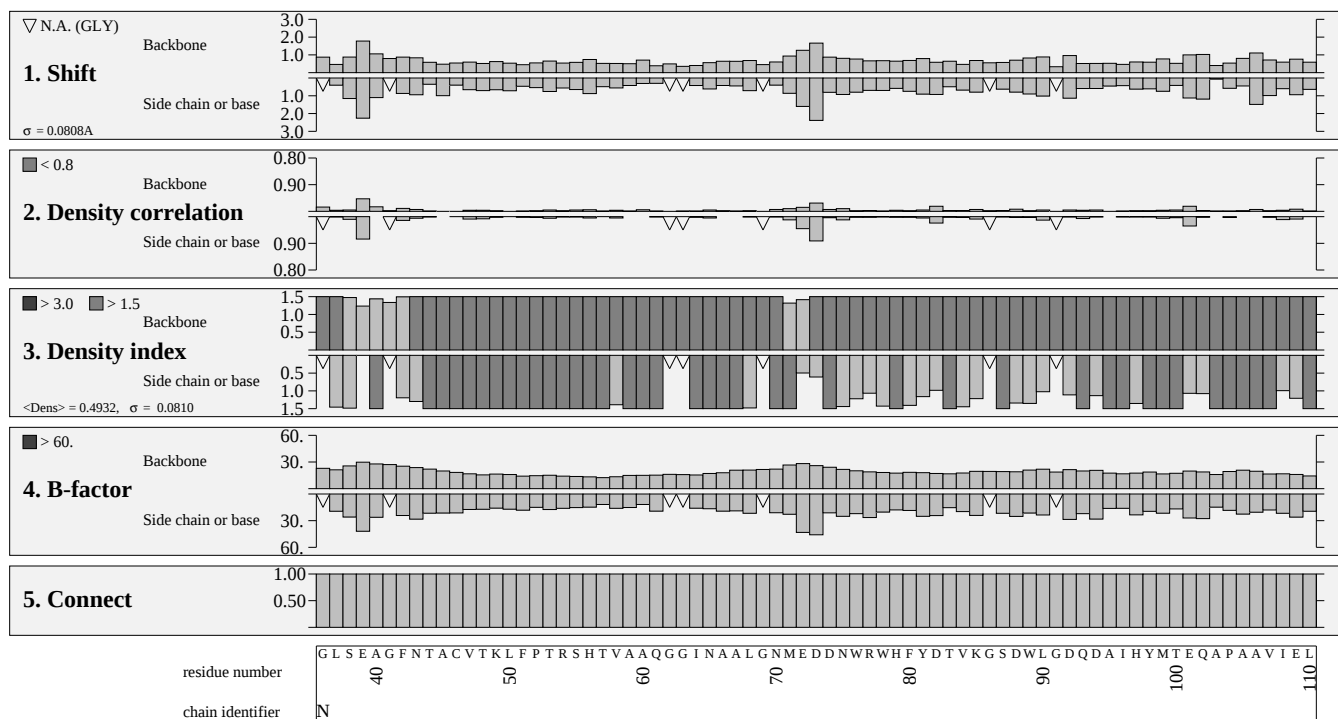
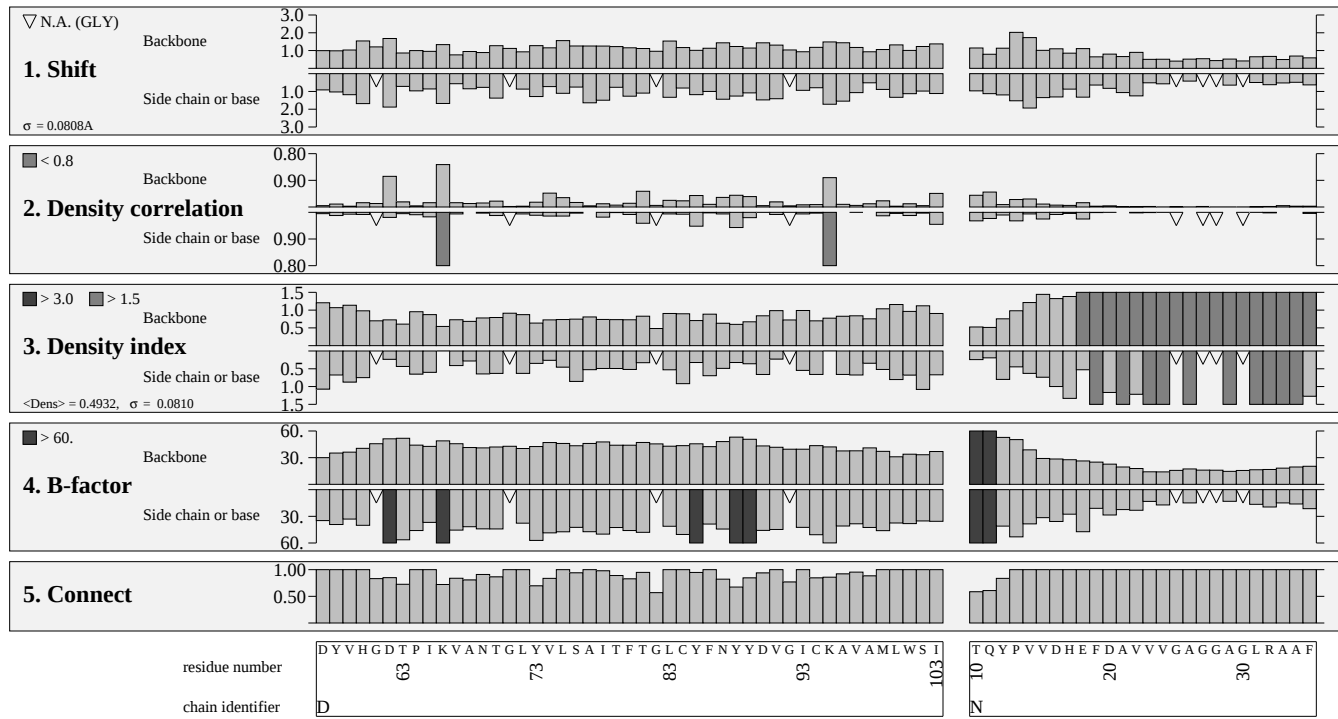
Local estimation (7)



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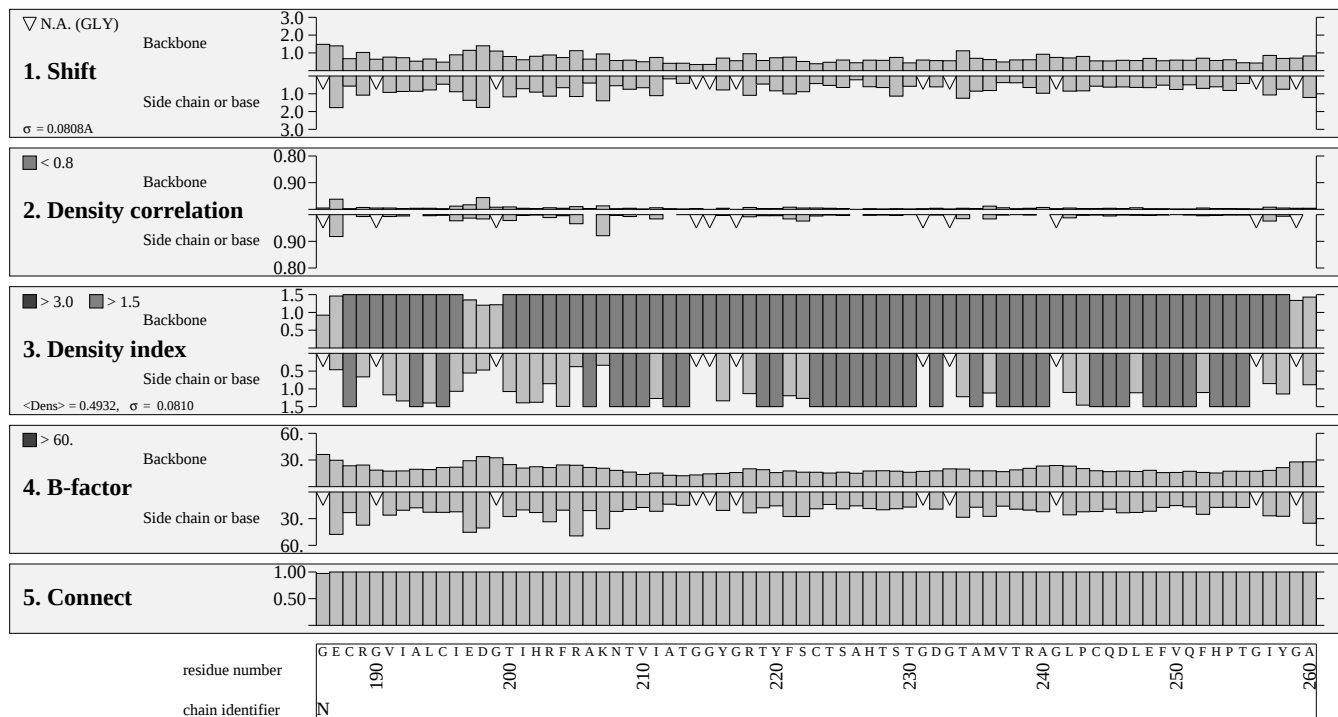
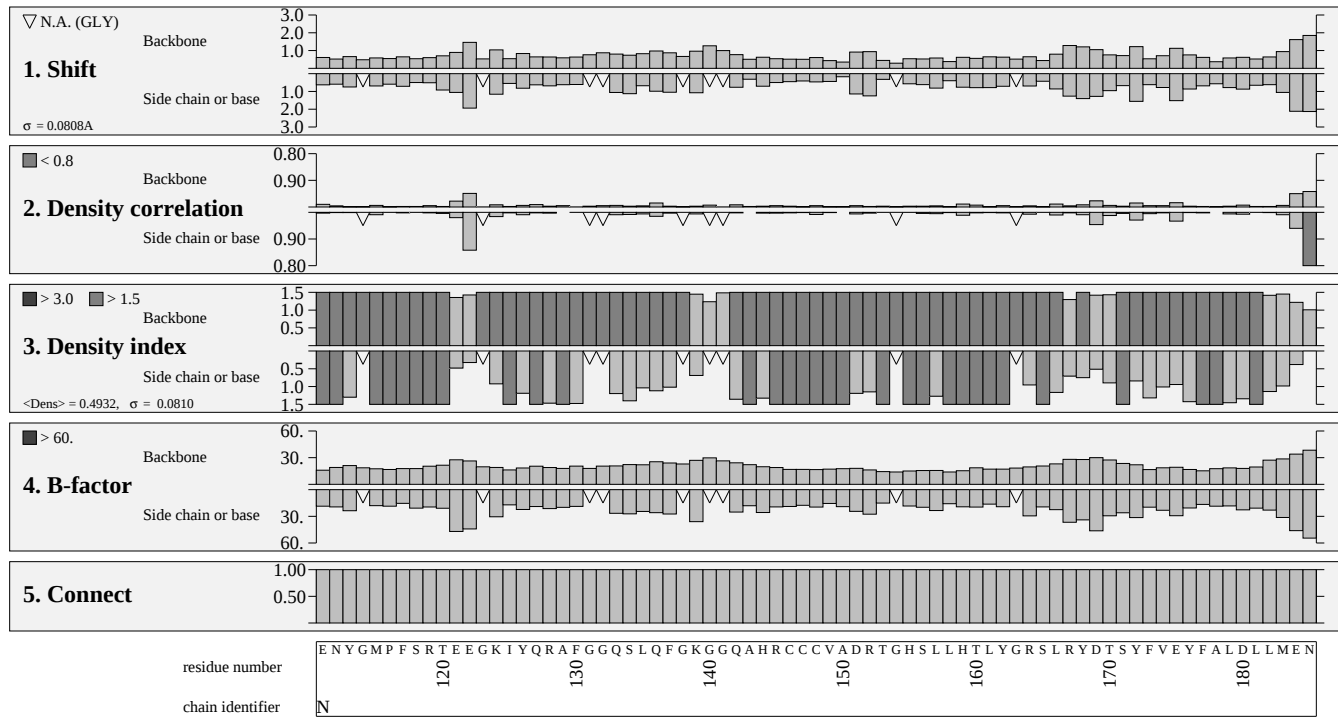
Local estimation (8)



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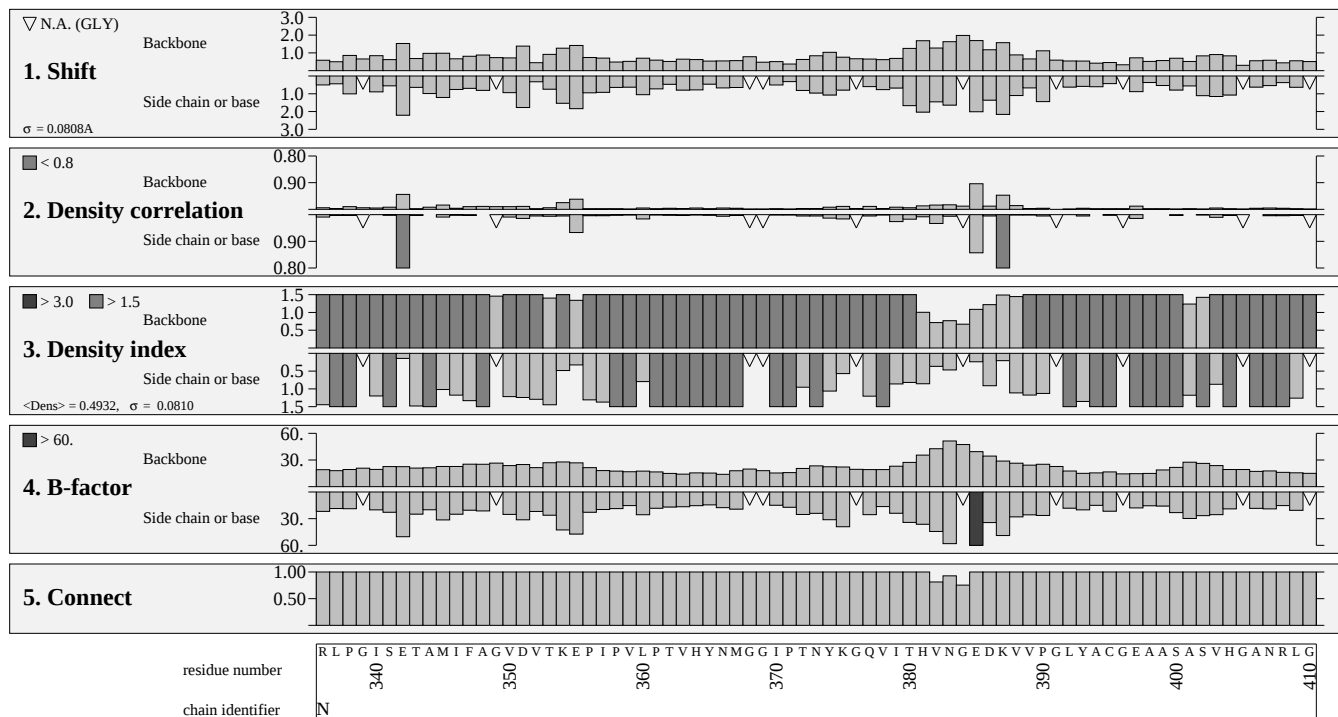
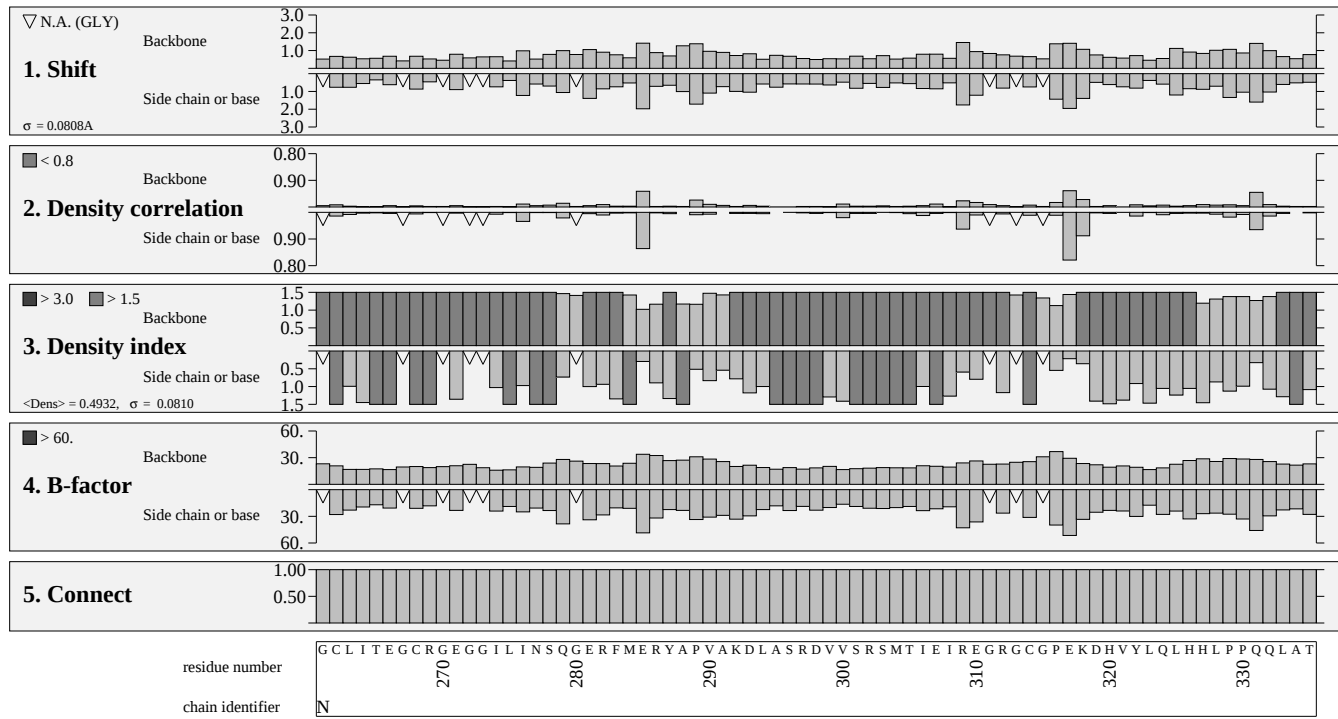
Local estimation (9)



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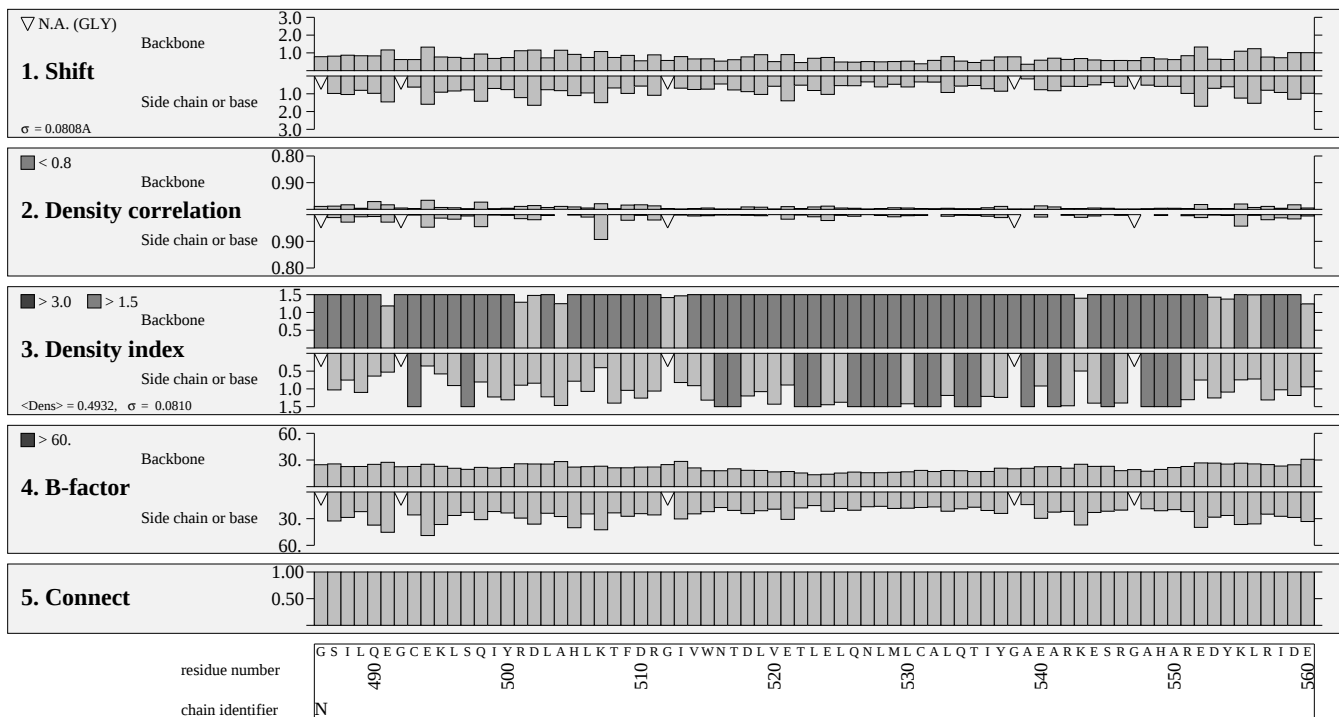
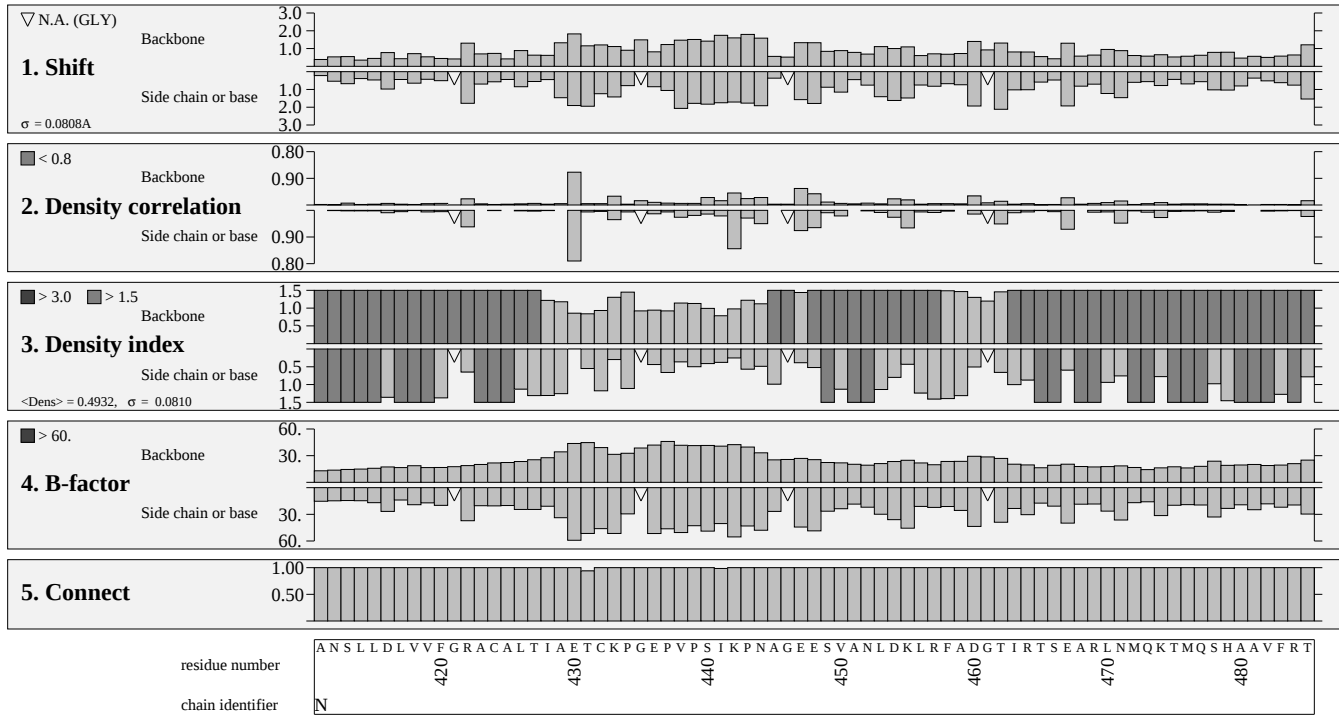
Local estimation (10)



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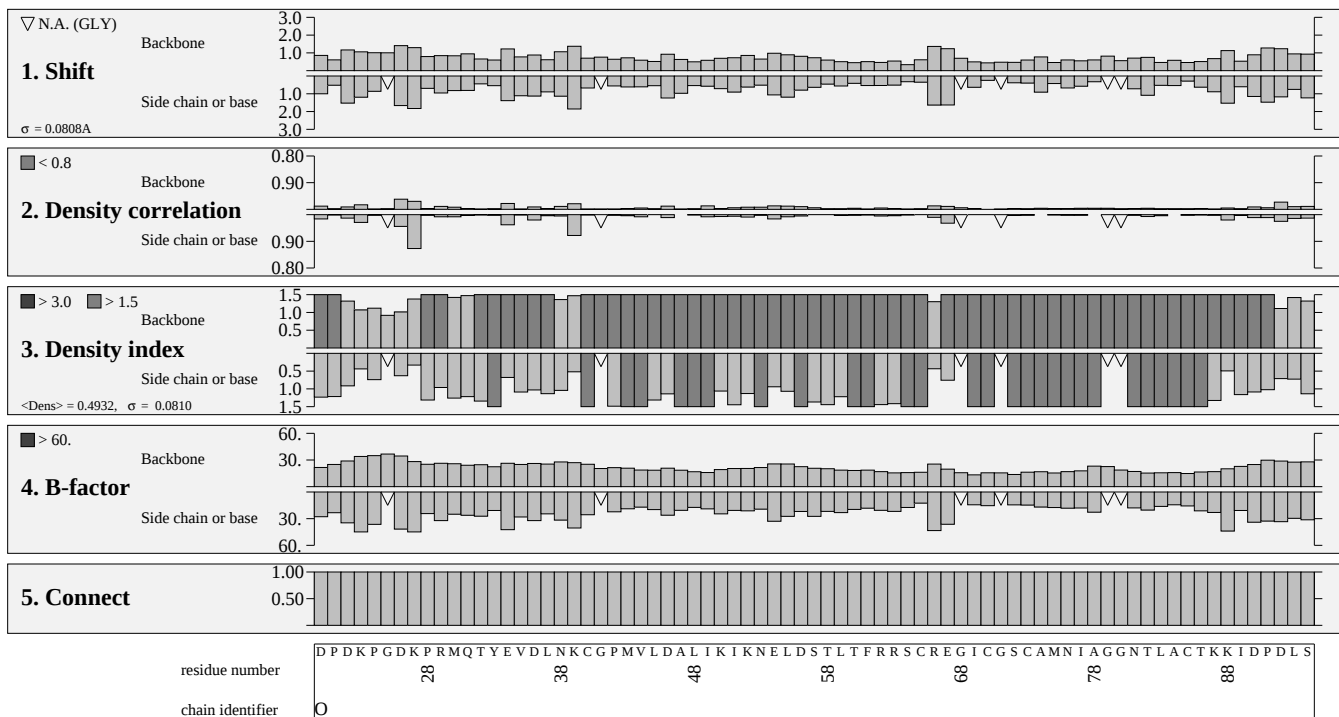
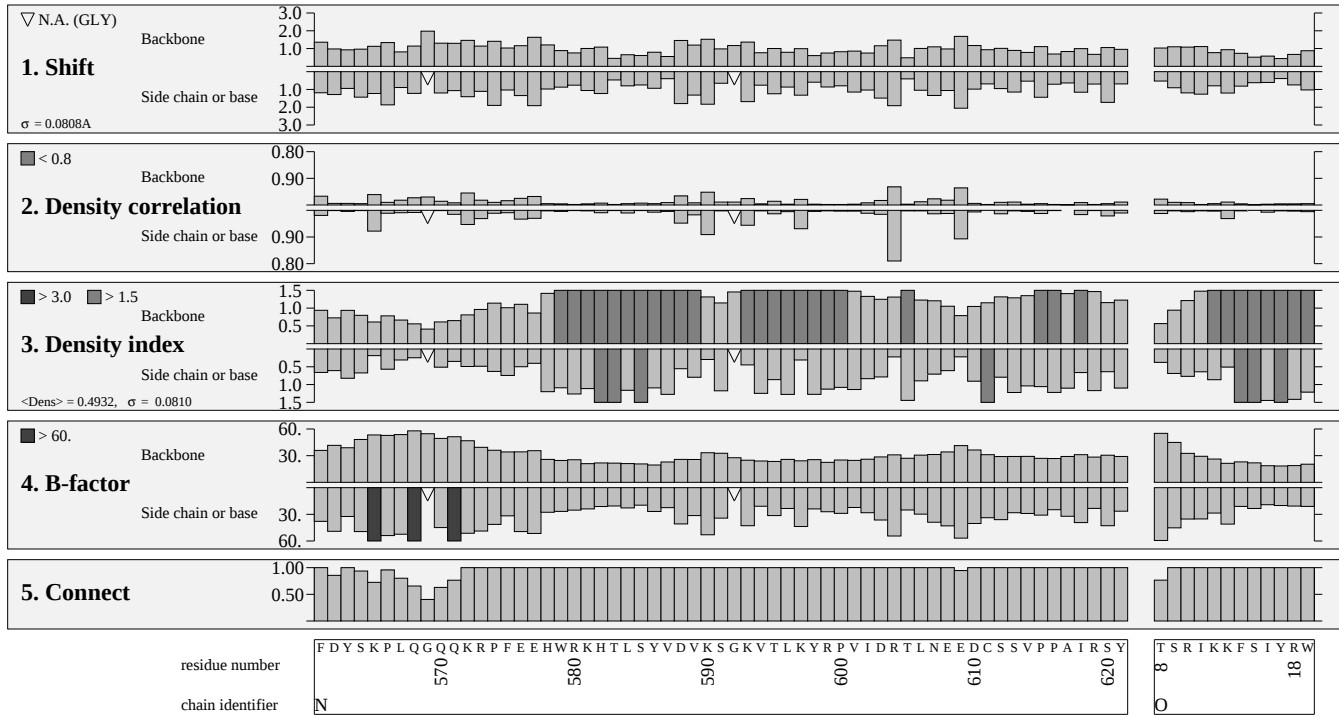
Local estimation (11)



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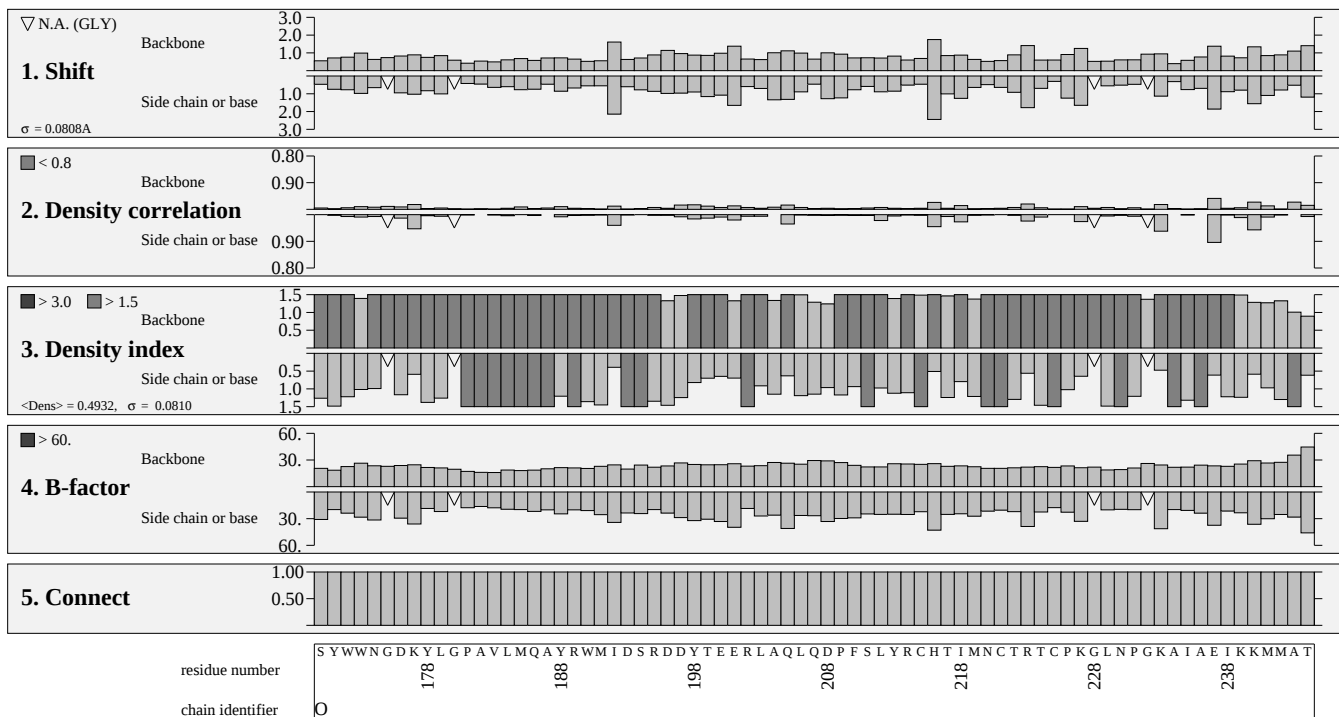
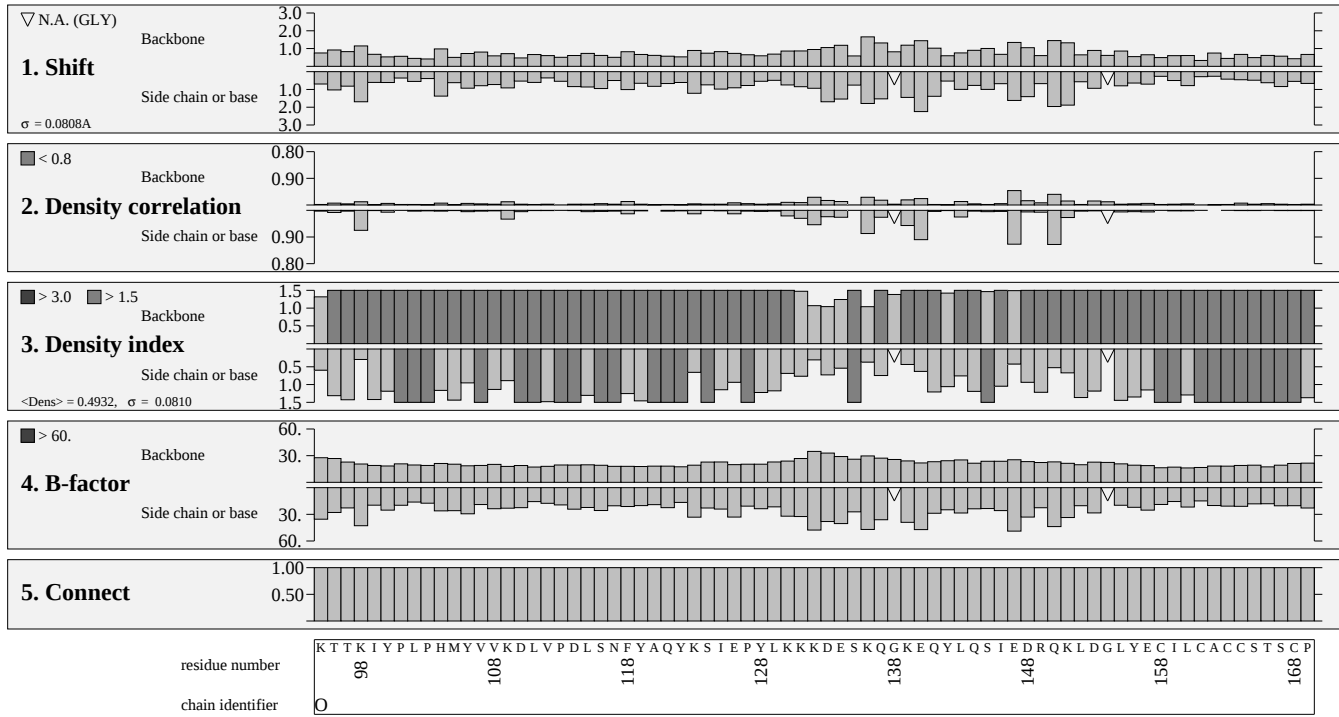
Local estimation (12)



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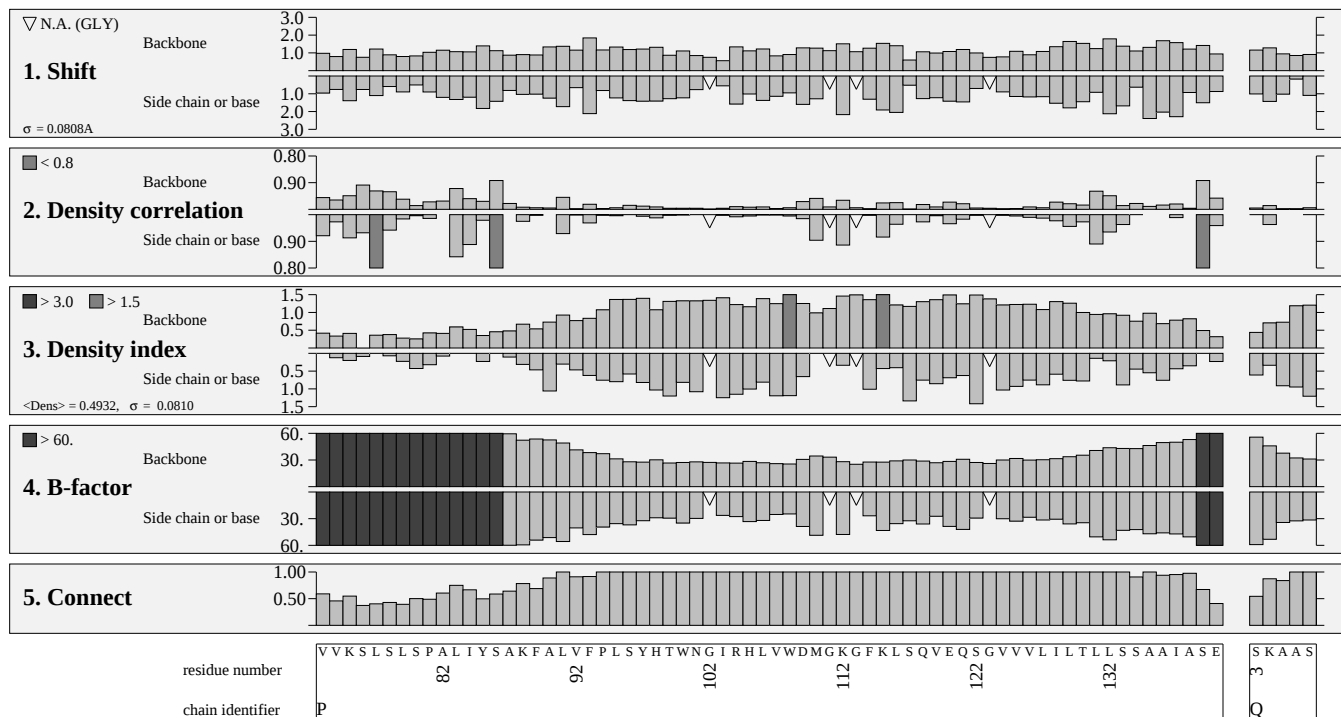
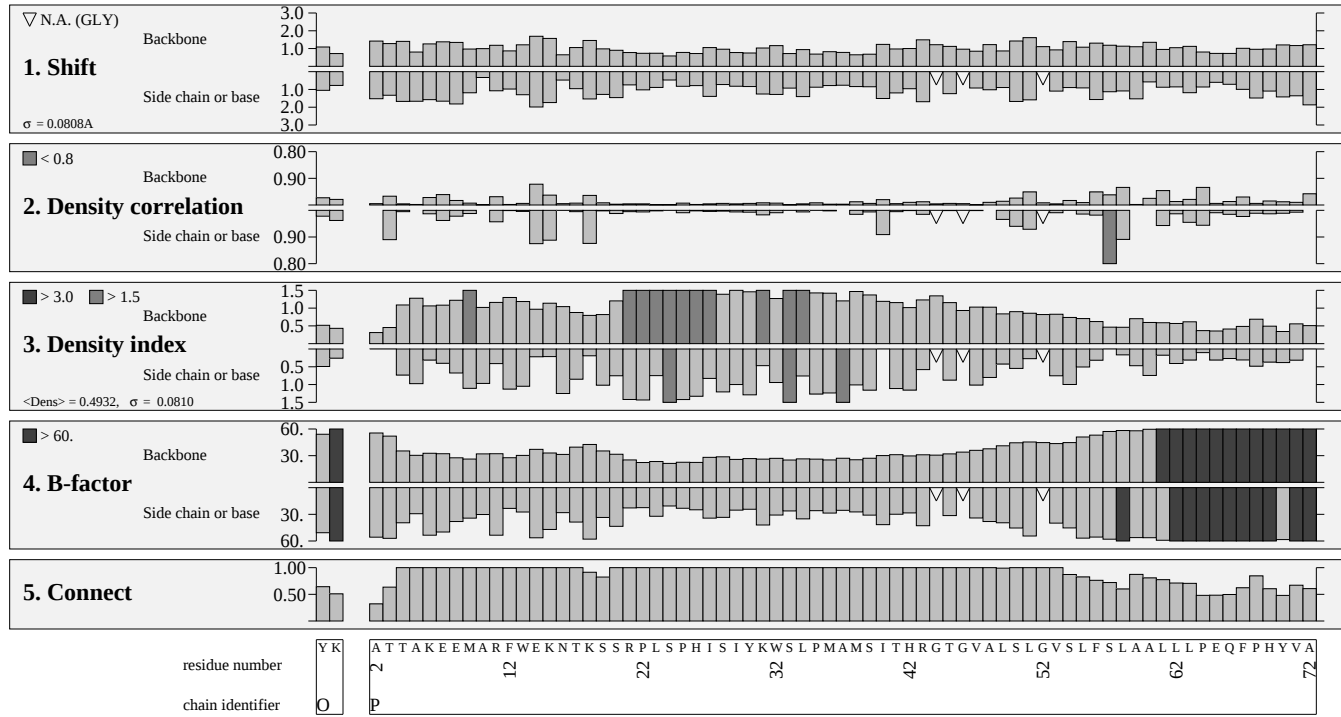
Local estimation (13)



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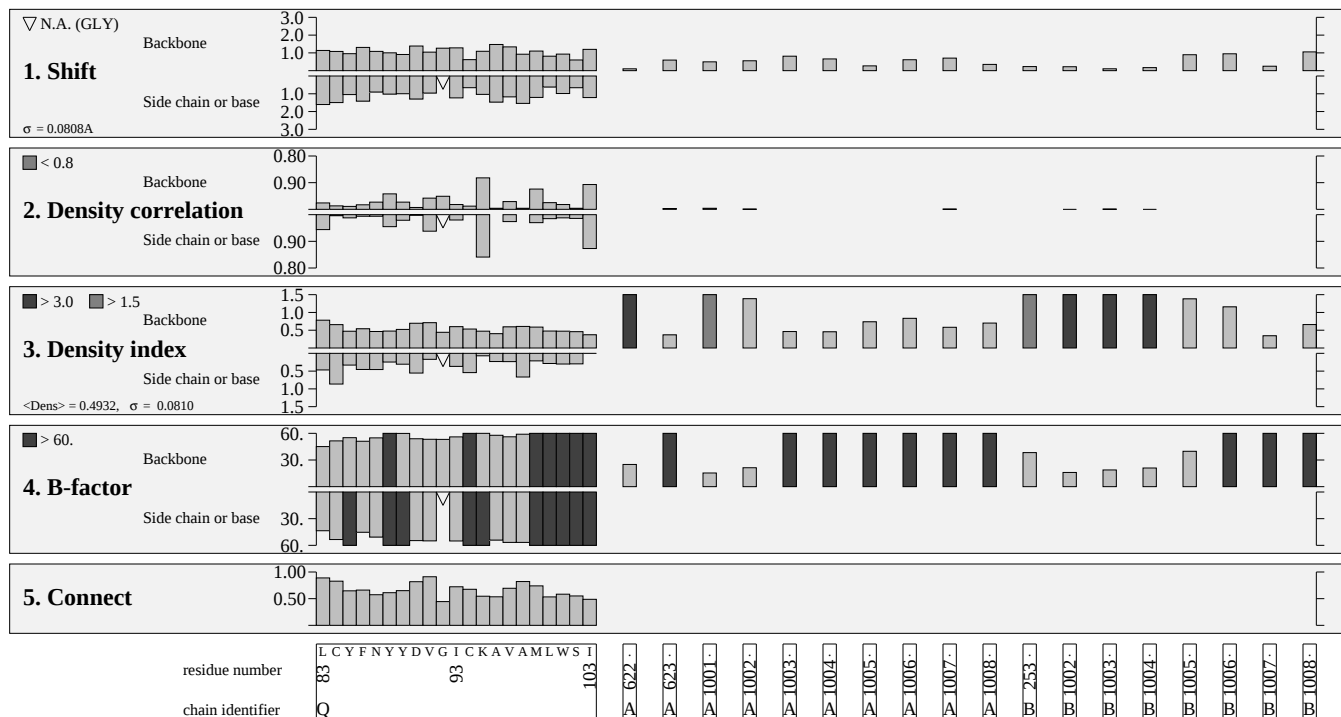
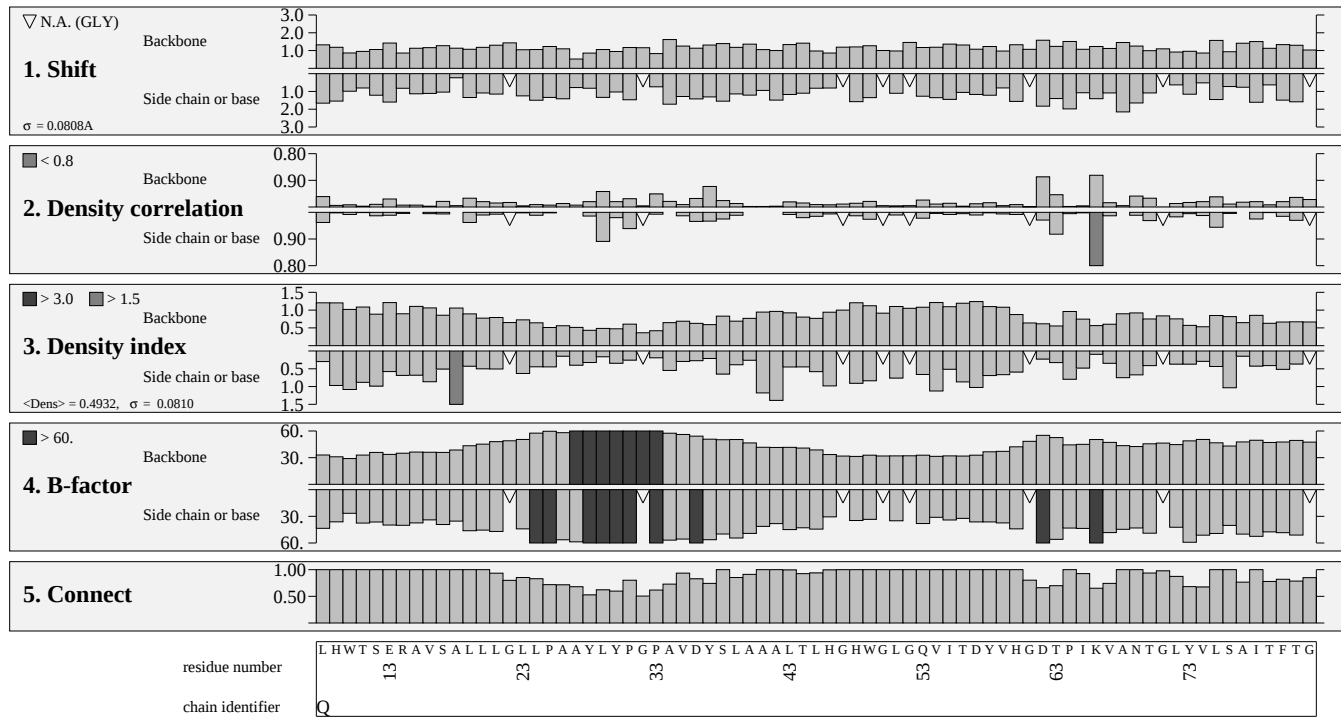
Local estimation (14)



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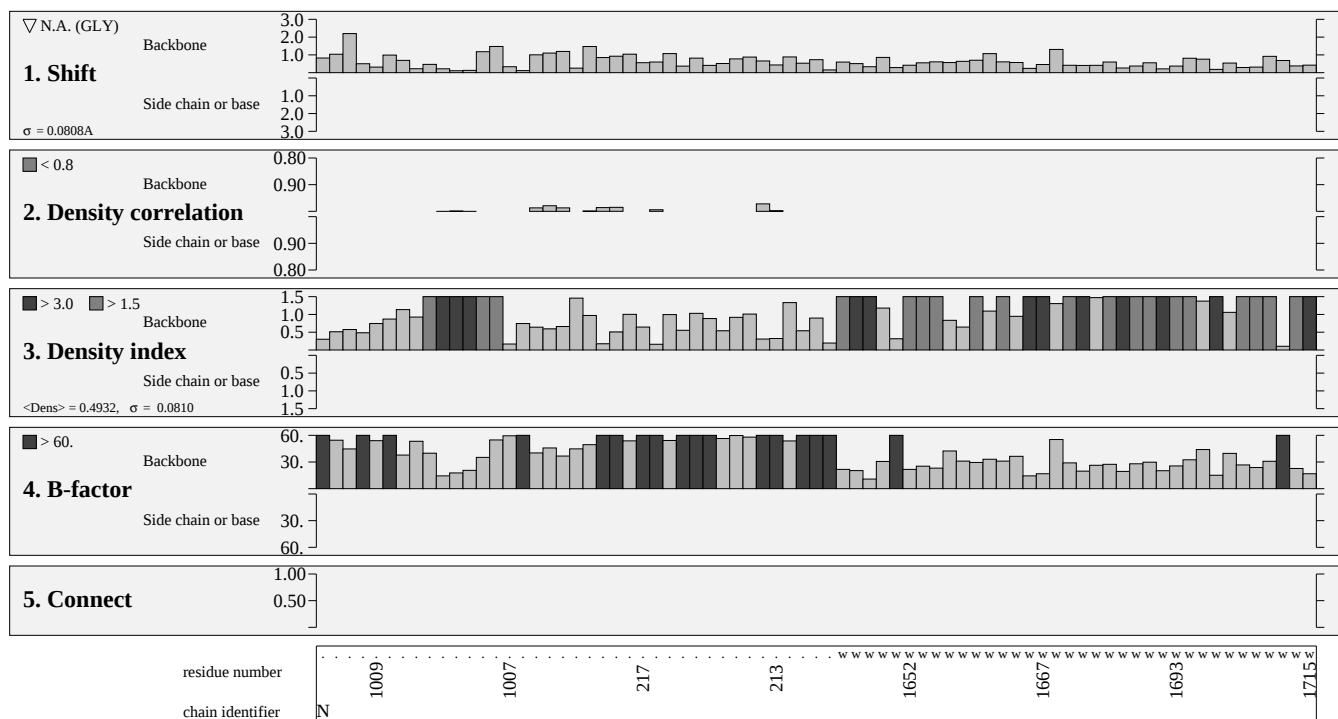
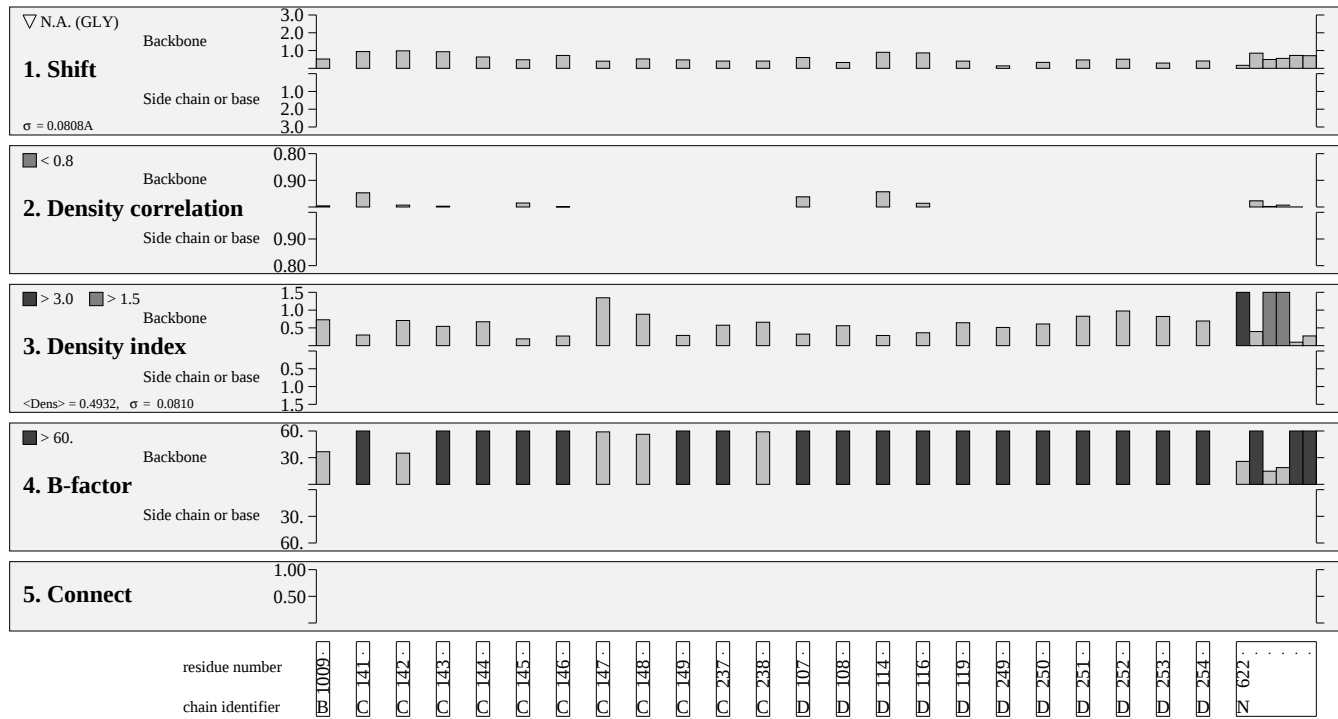
Local estimation (15)



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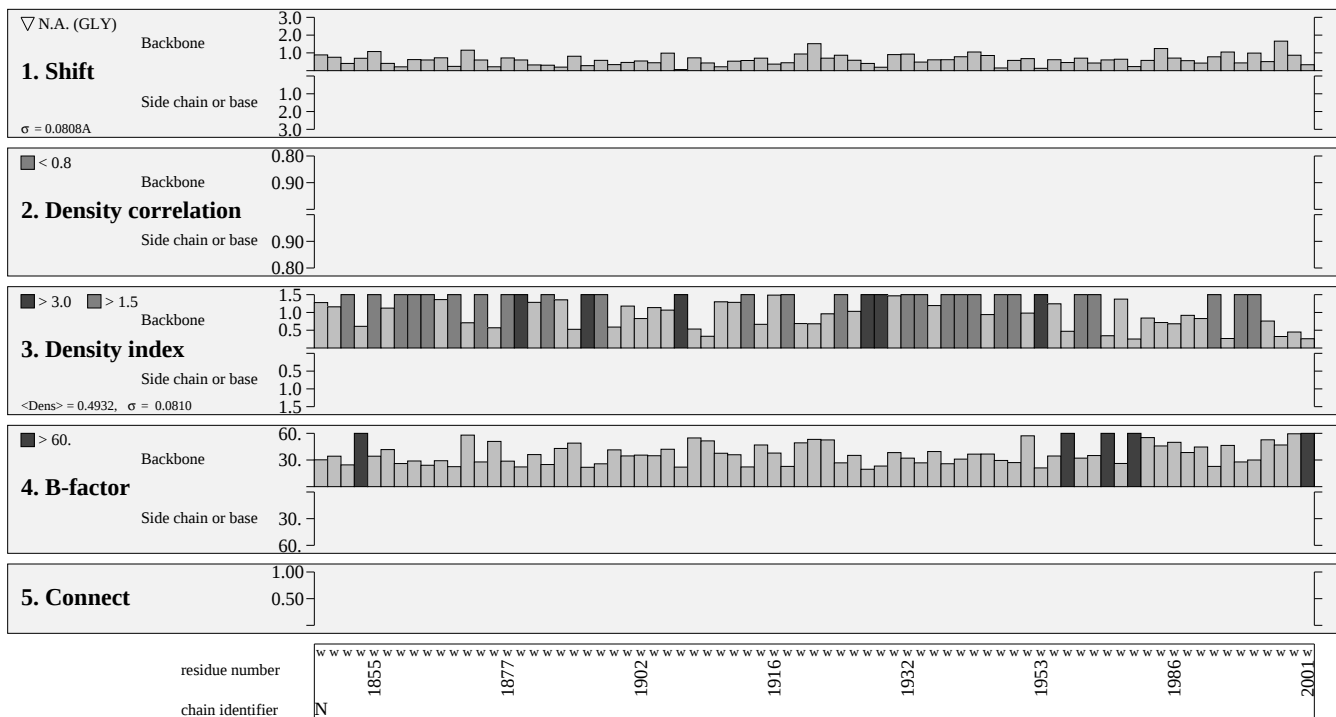
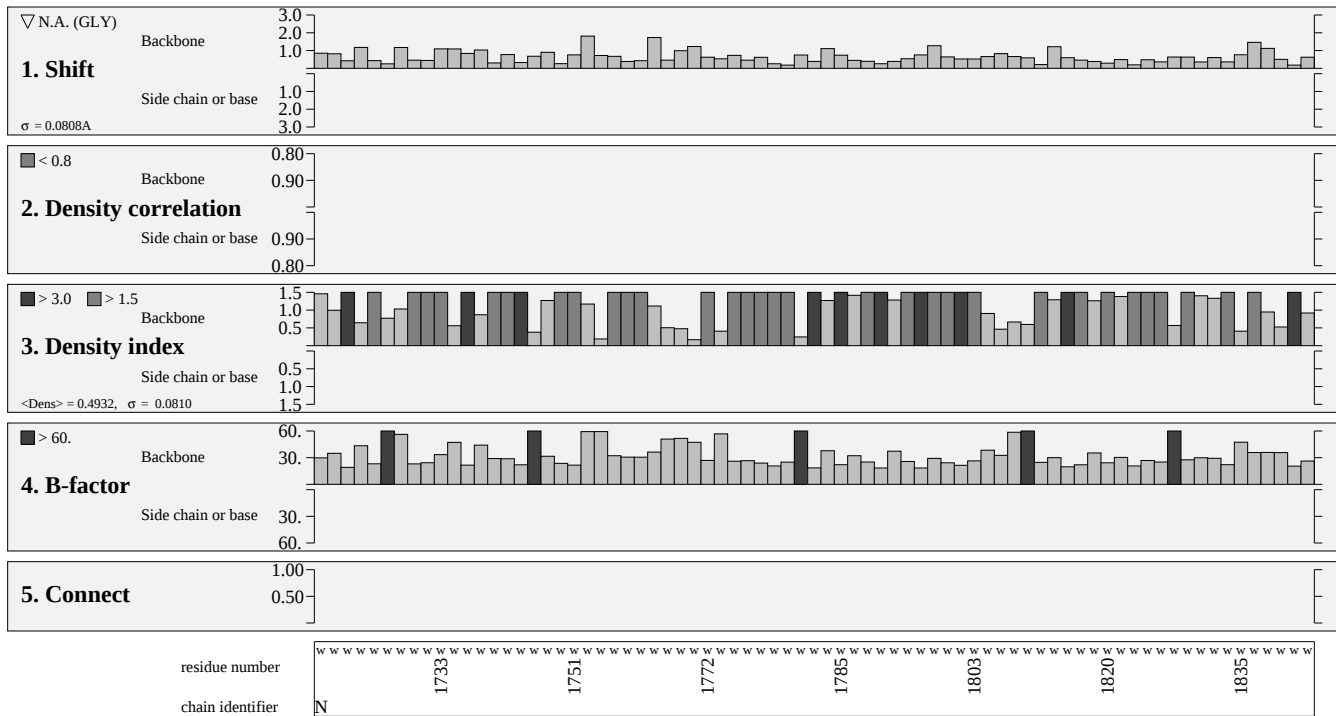
Local estimation (16)



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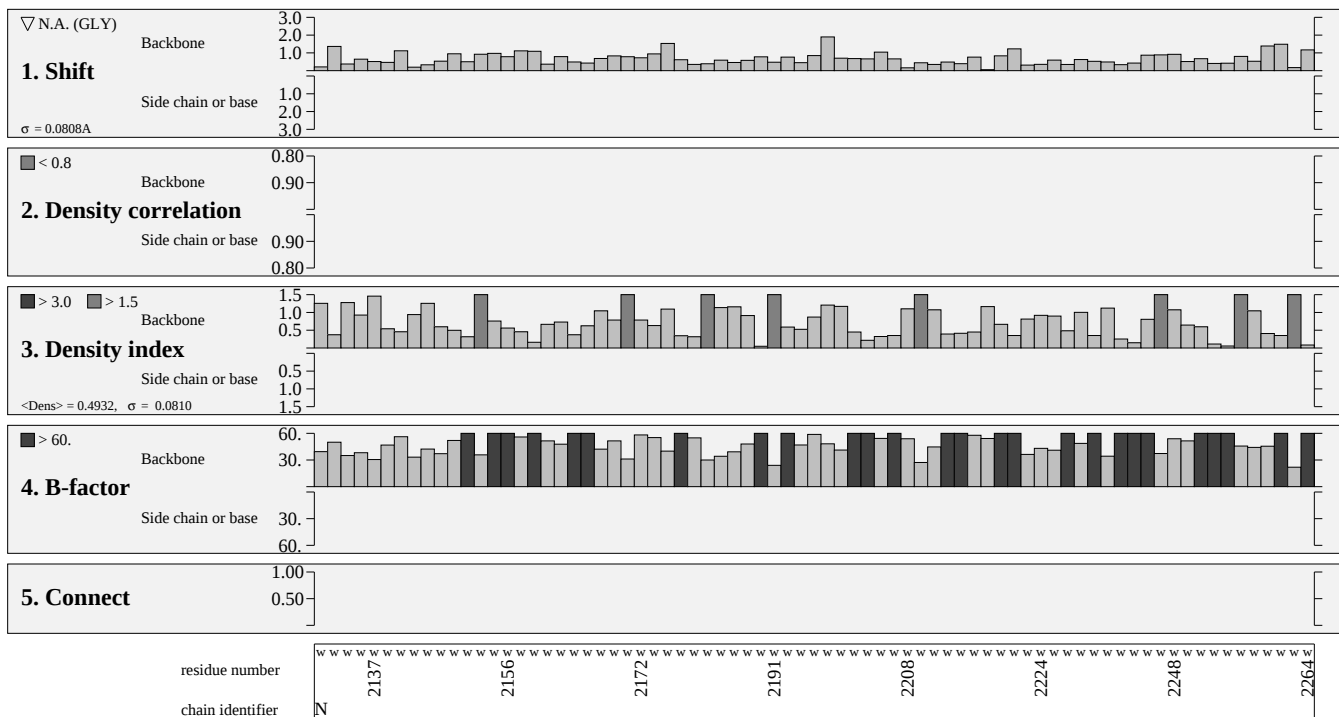
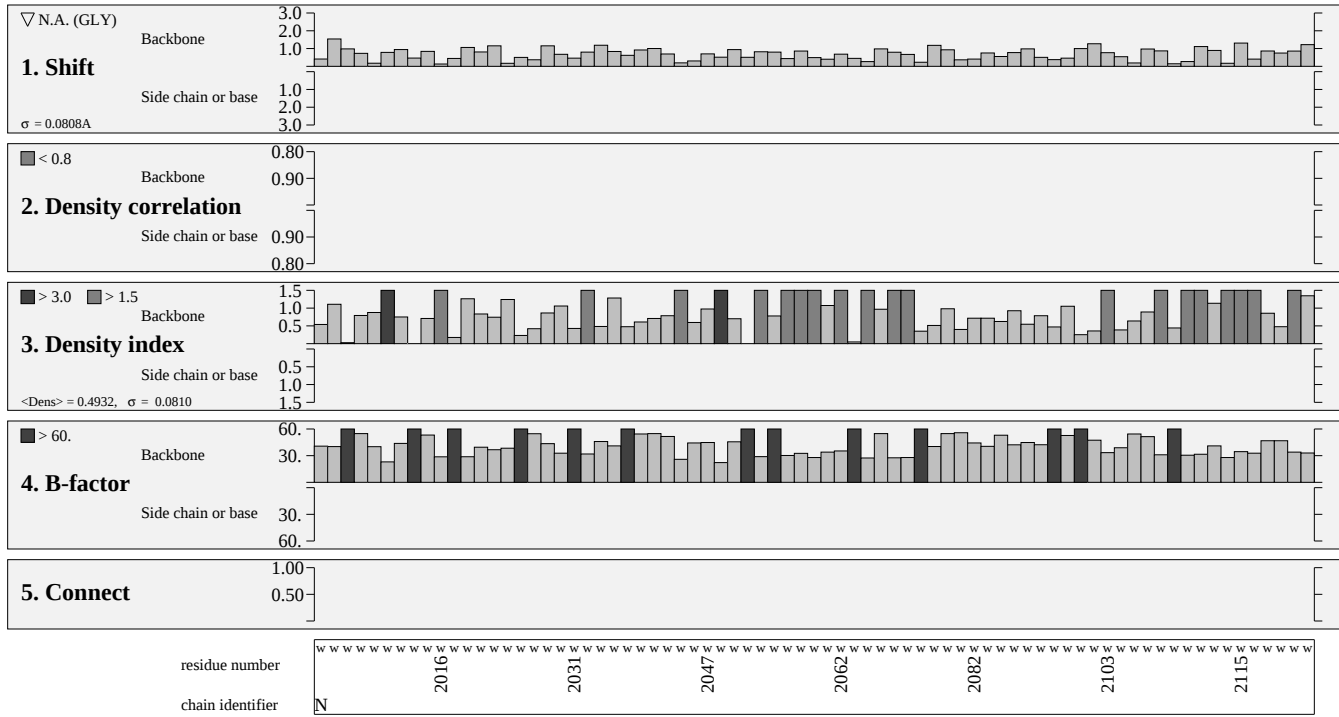
Local estimation (17)



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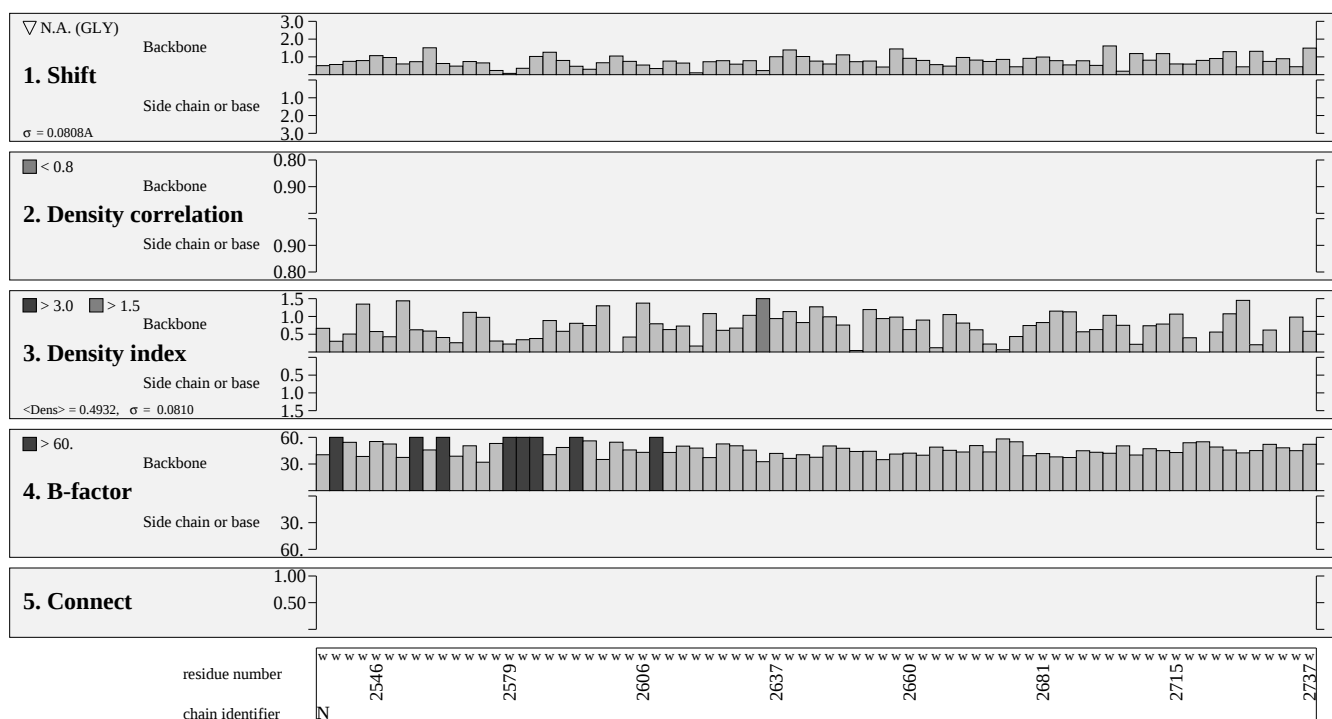
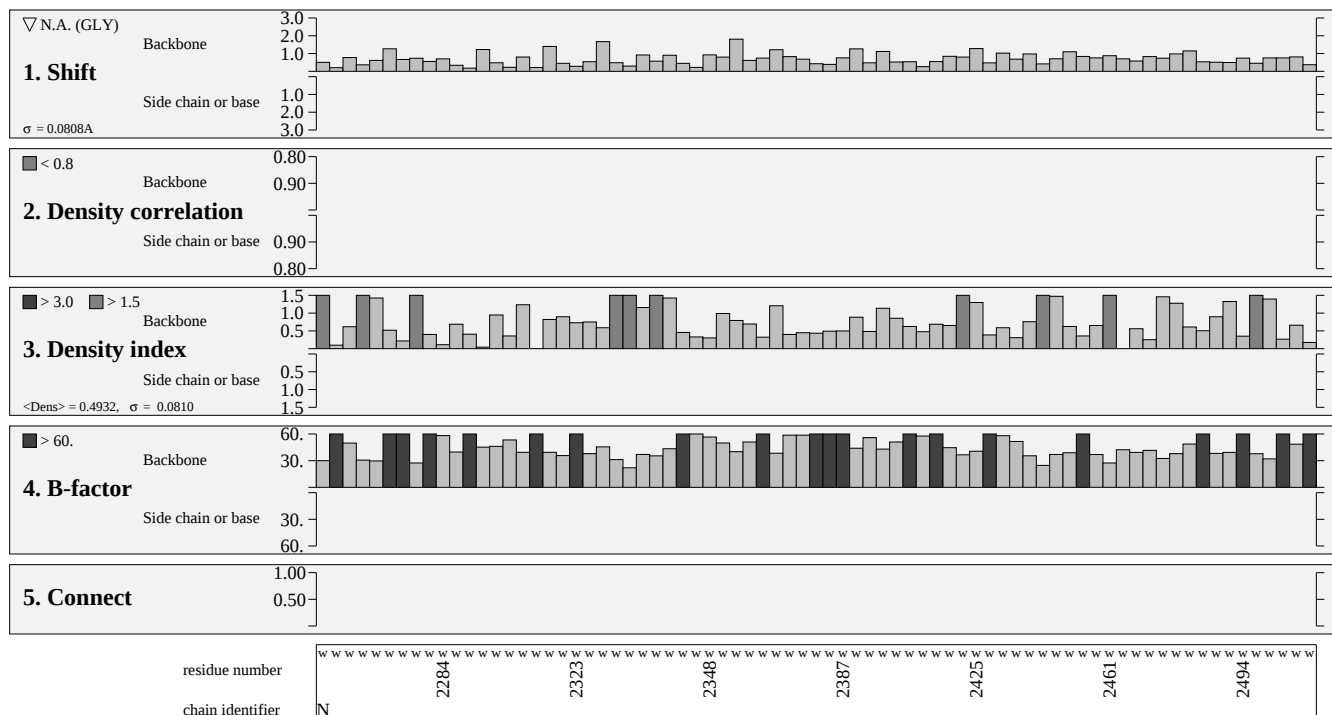
Local estimation (18)



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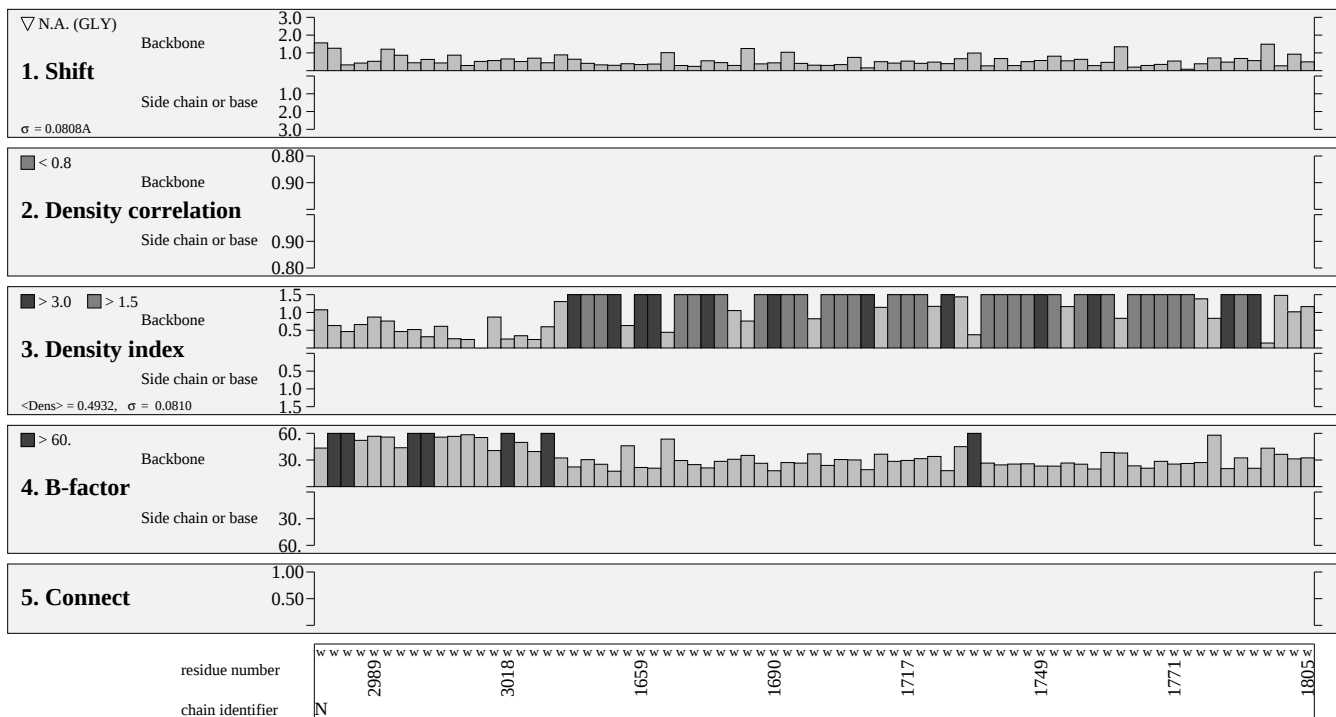
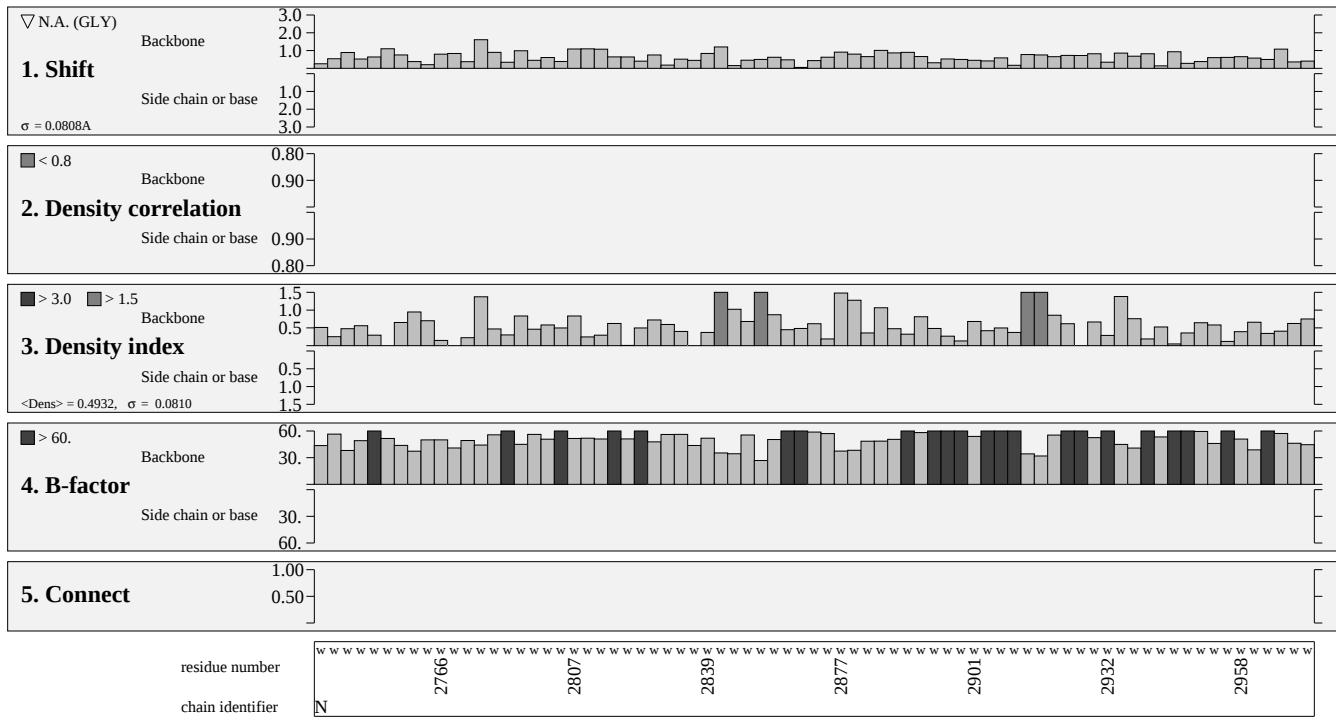
Local estimation (19)



Structure Factor Check

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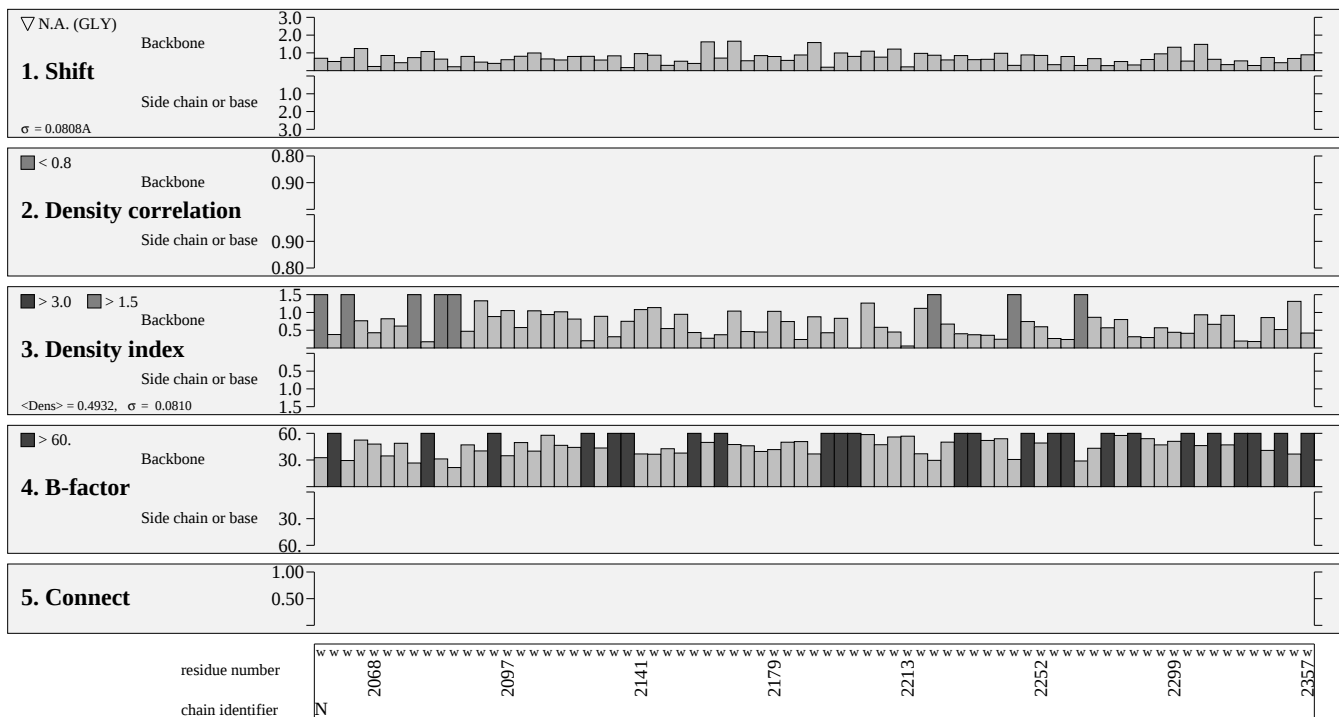
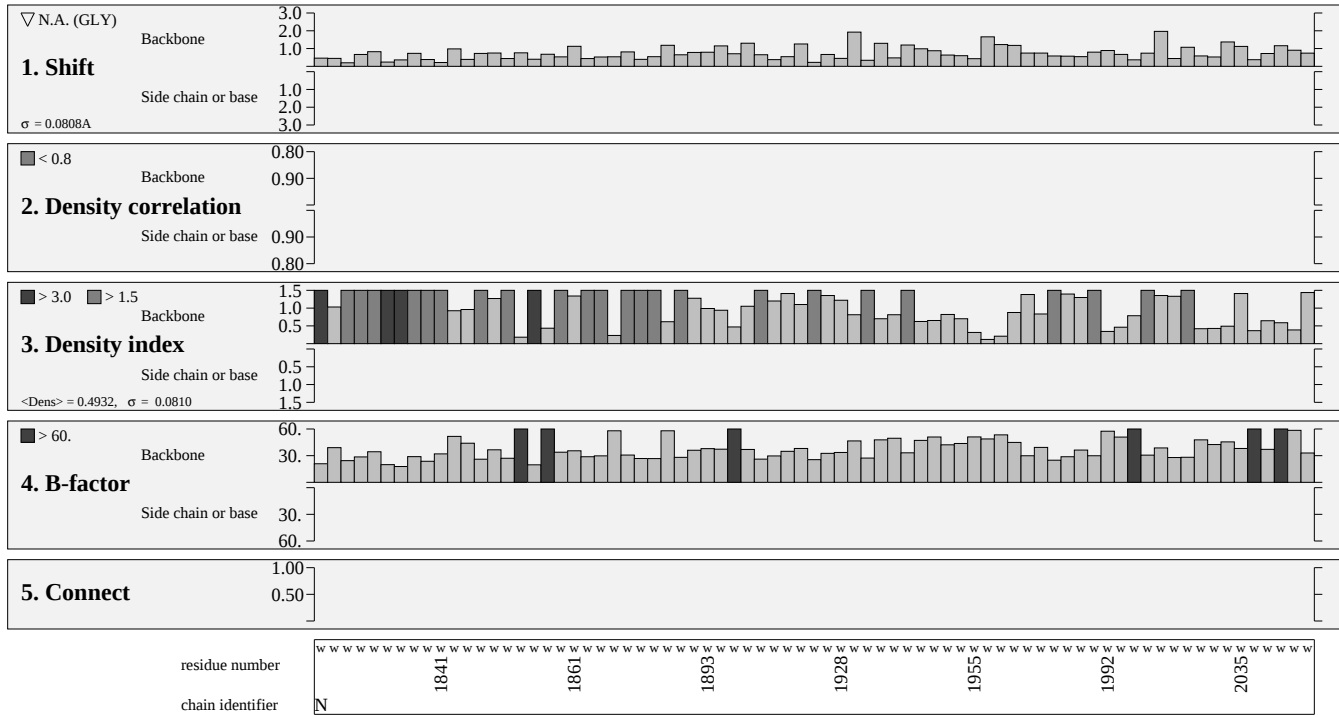
Local estimation (20)



Structure Factor Check

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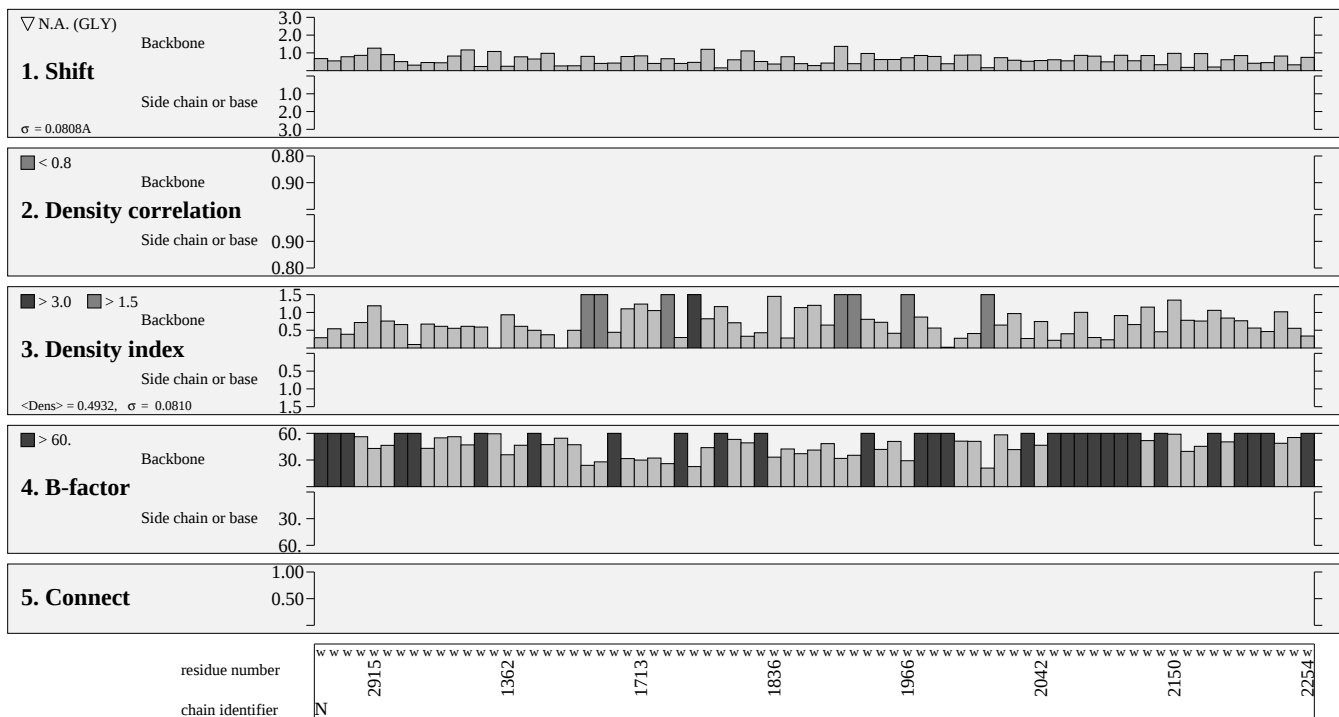
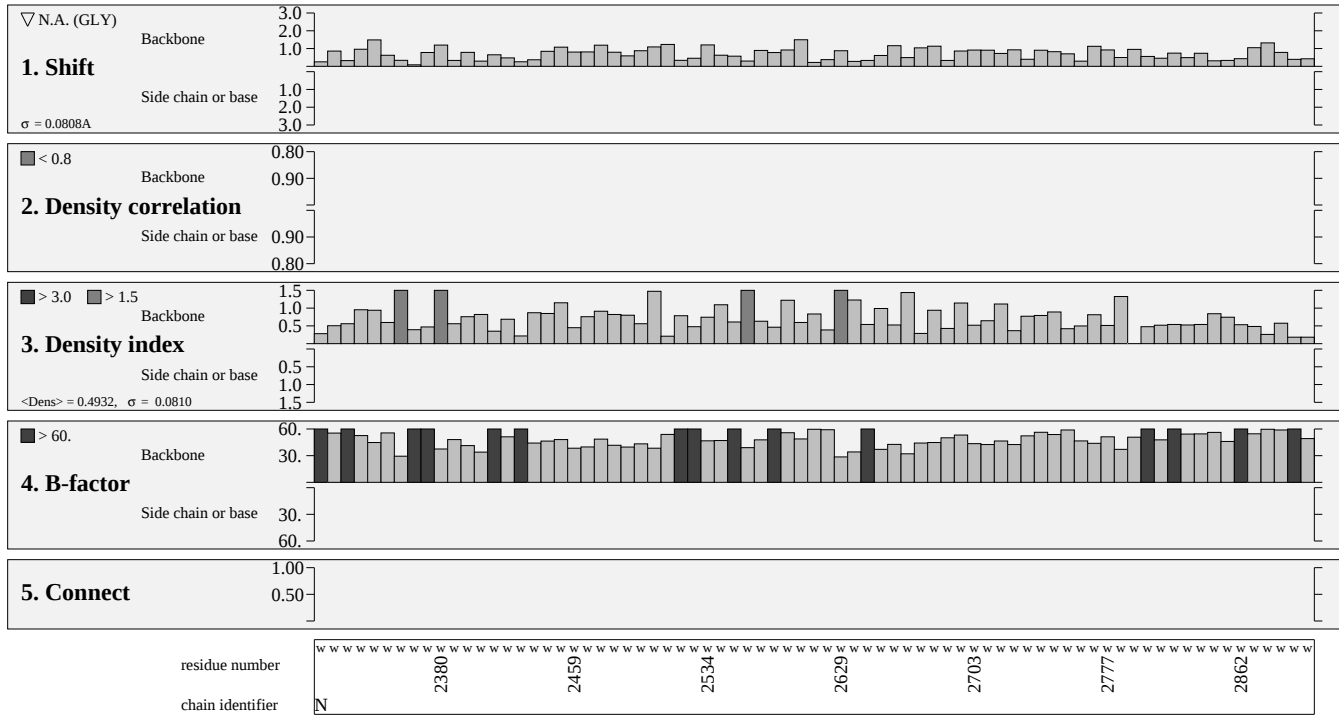
Local estimation (21)



Structure Factor Check

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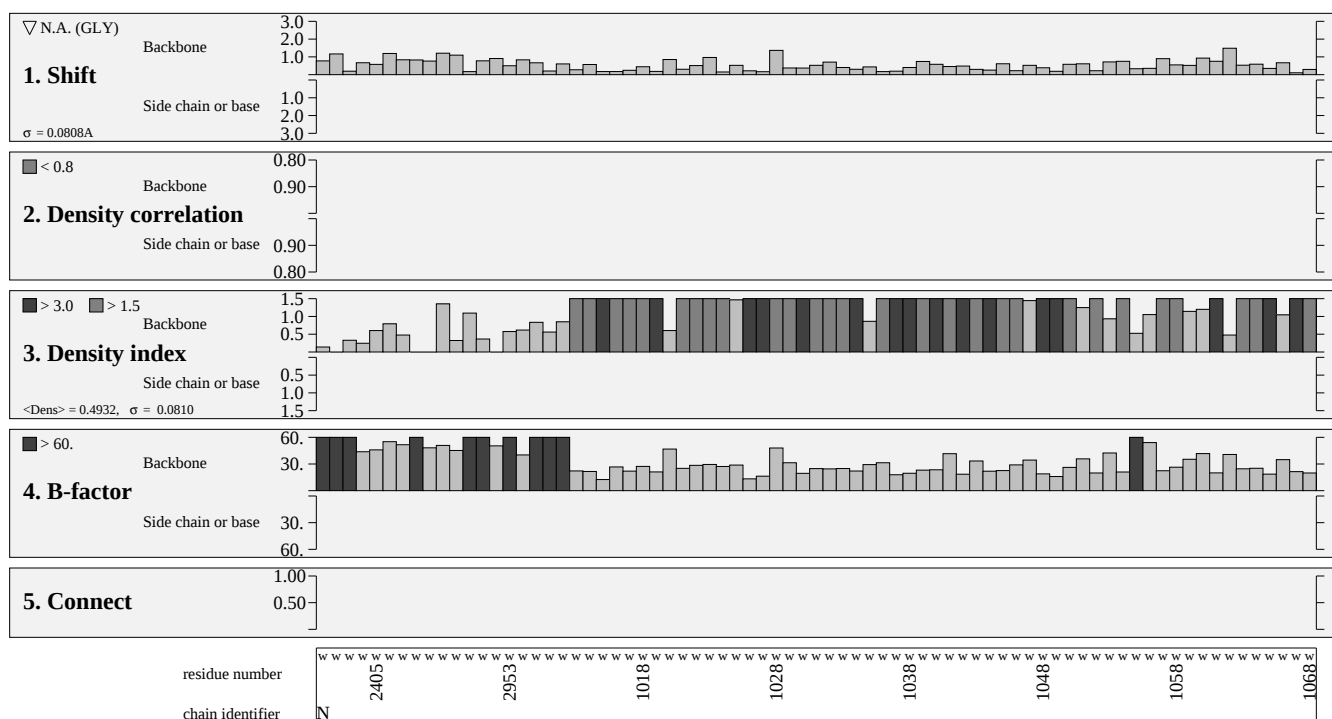
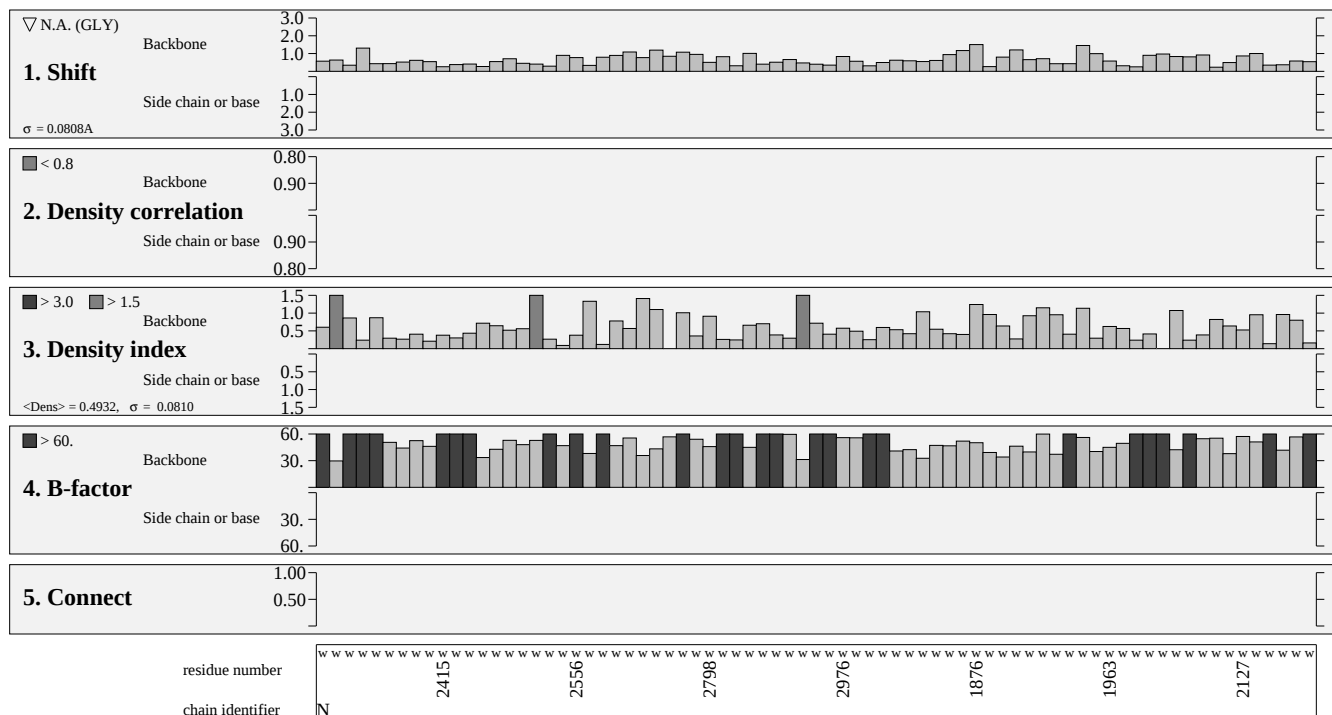
Local estimation (22)



Structure Factor Check

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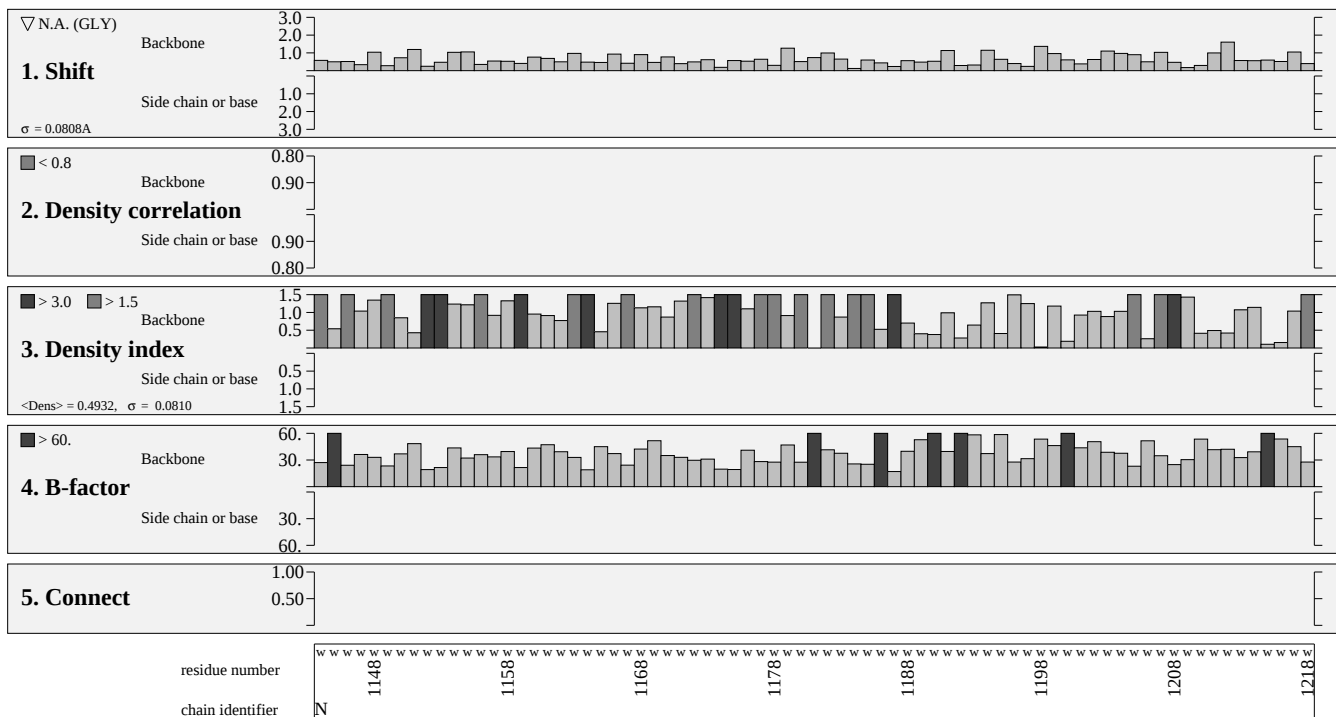
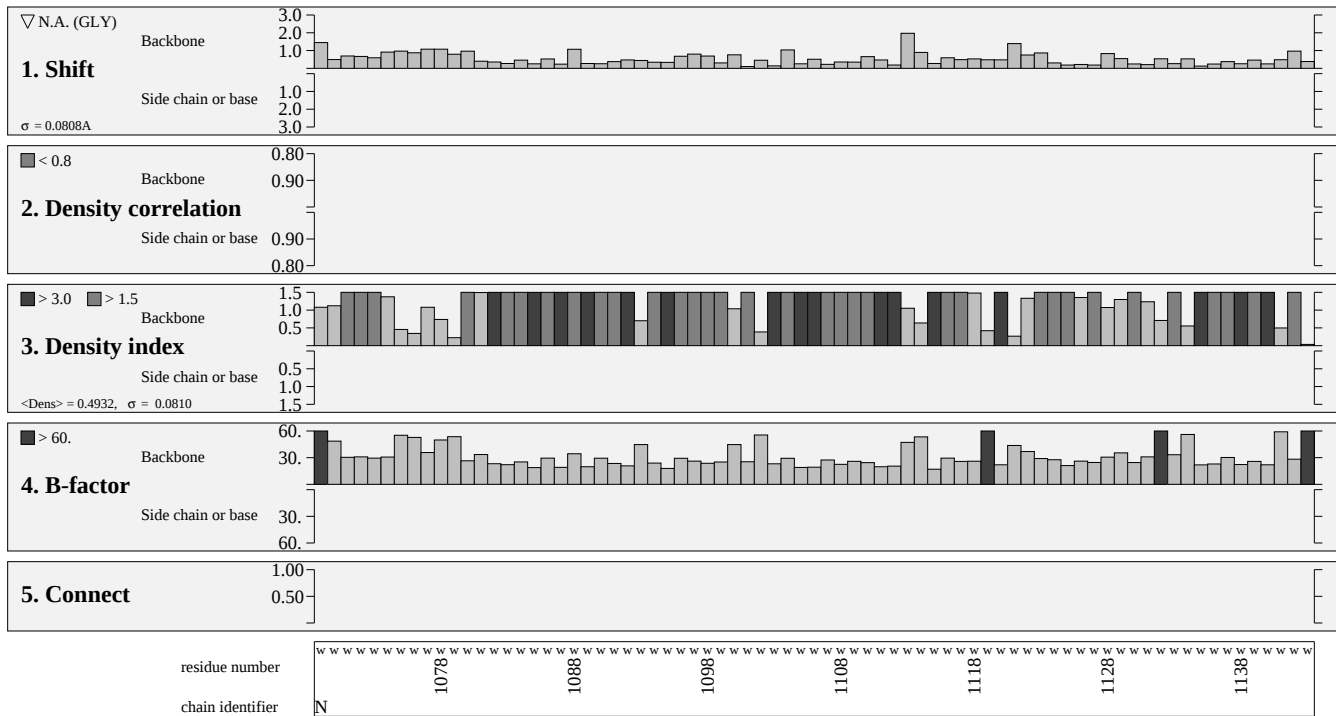
Local estimation (23)



Structure Factor Check

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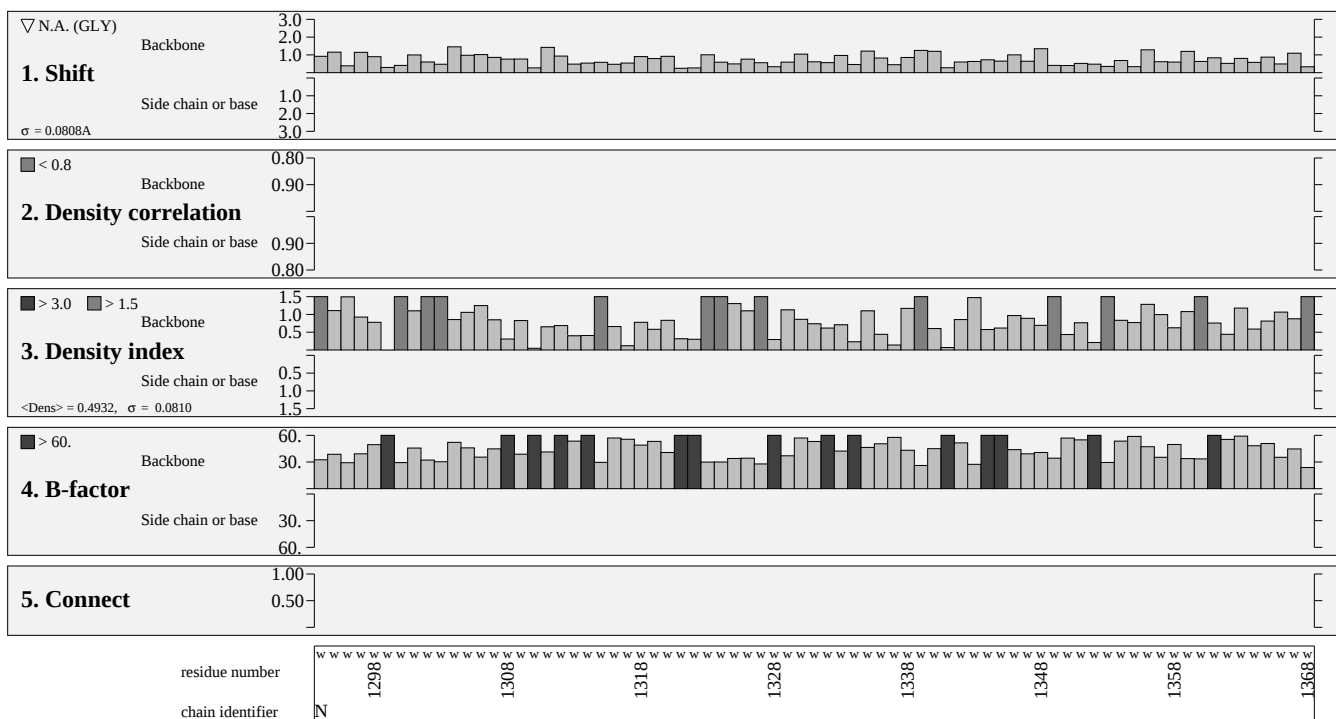
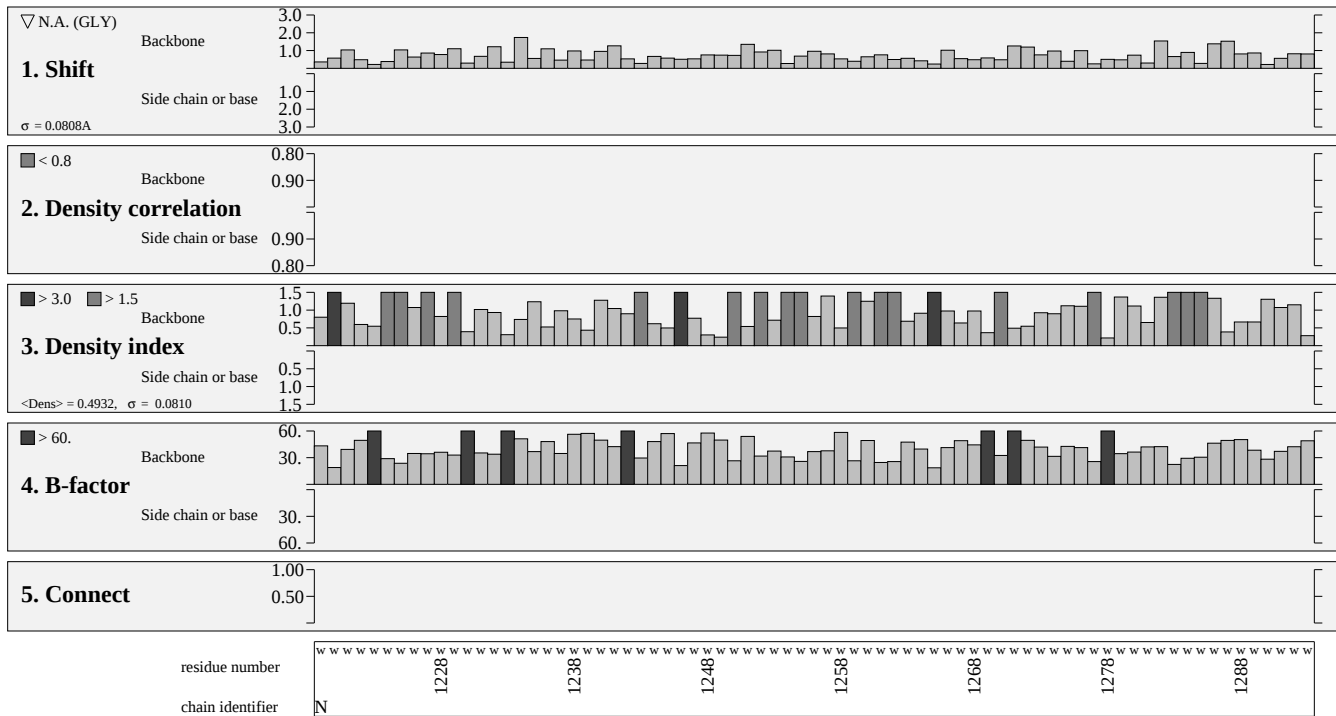
Local estimation (24)



Structure Factor Check

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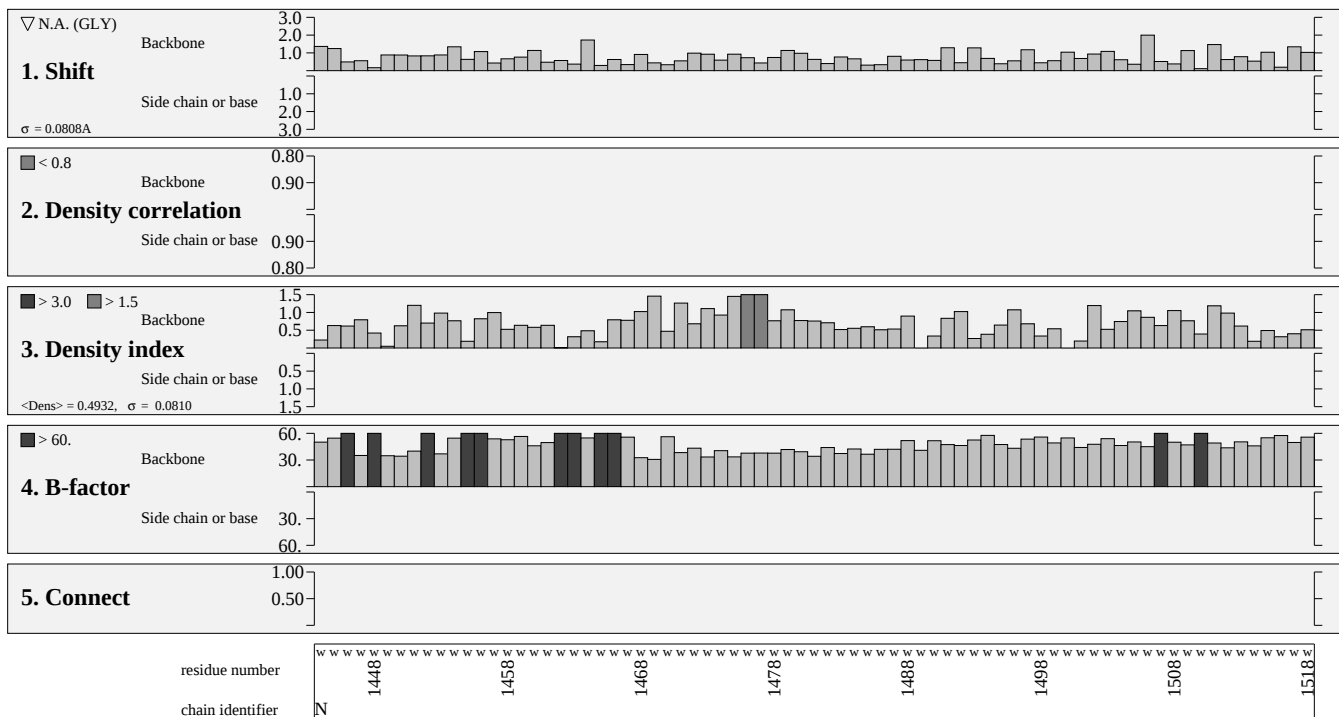
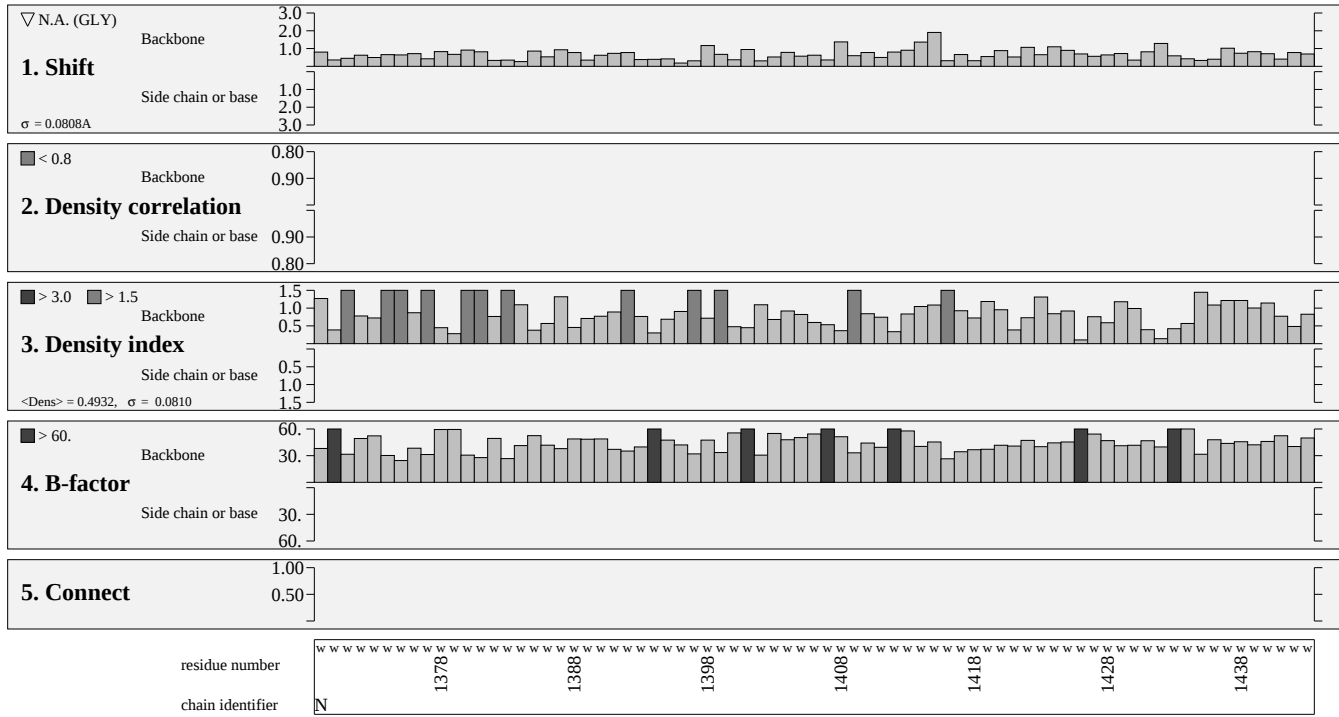
Local estimation (25)



Structure Factor Check

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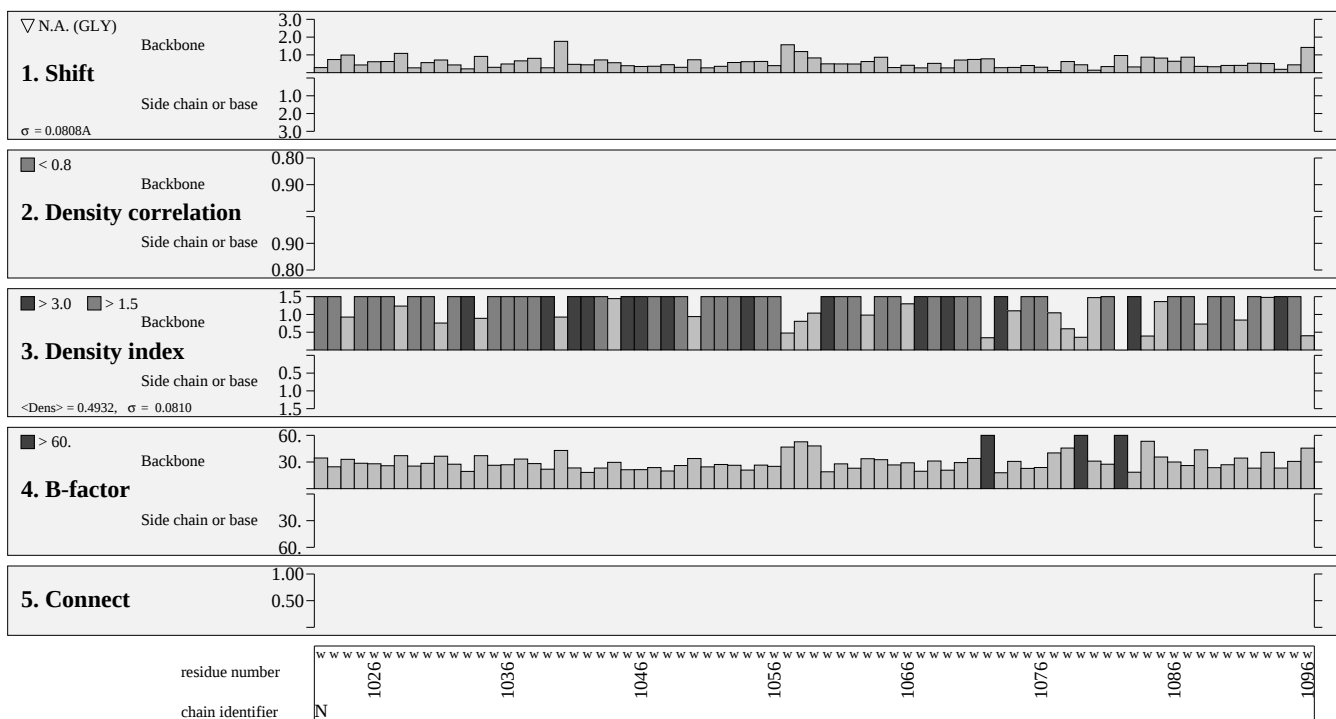
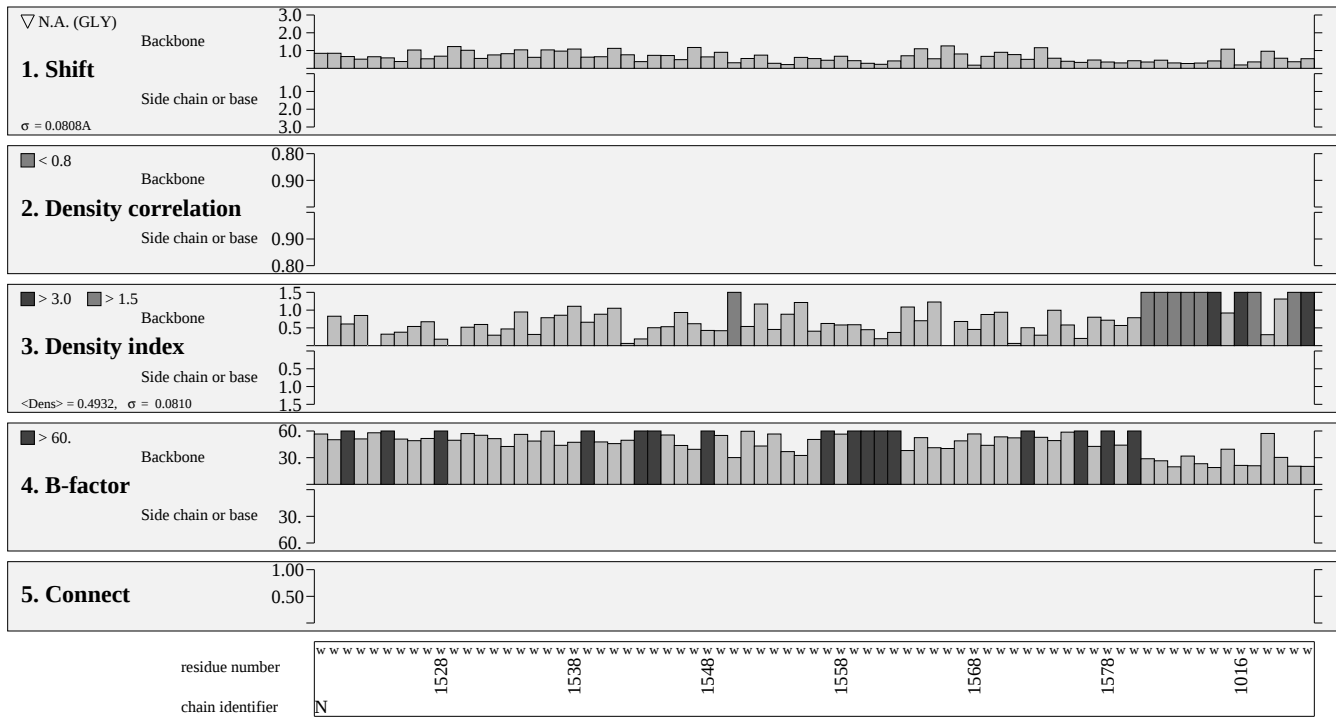
Local estimation (26)



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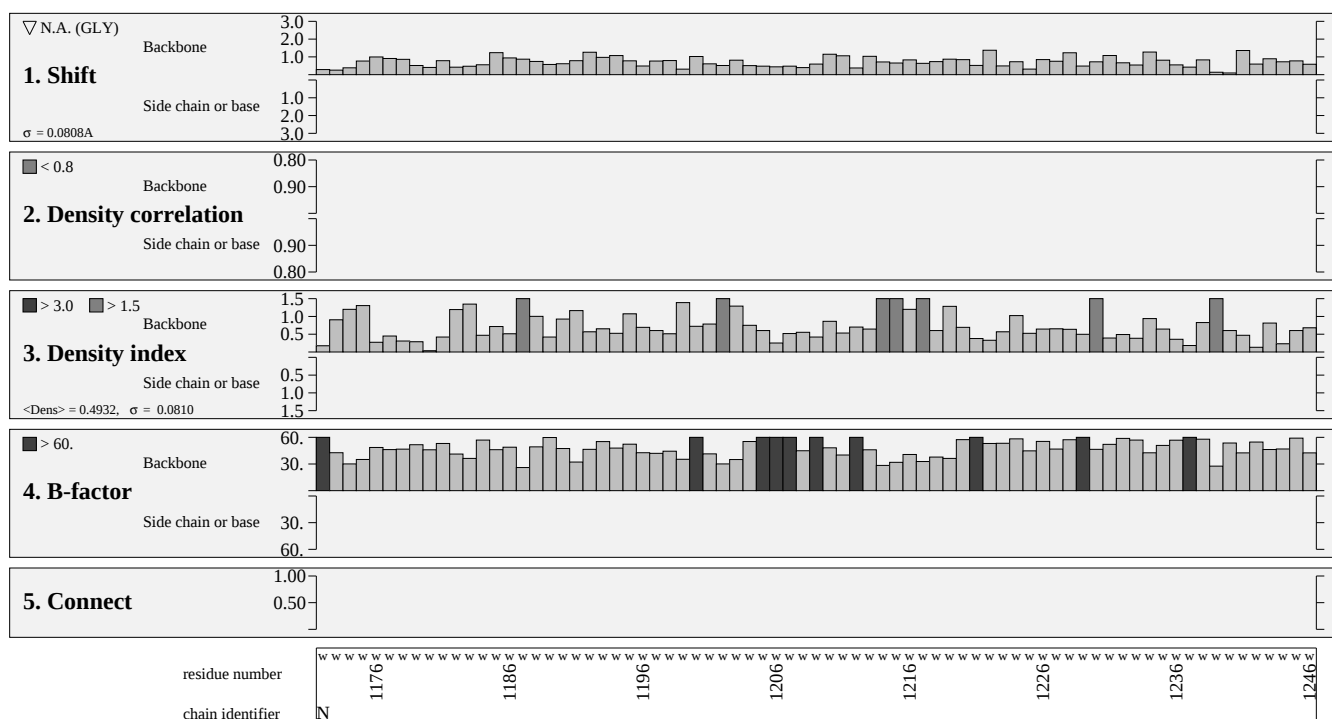
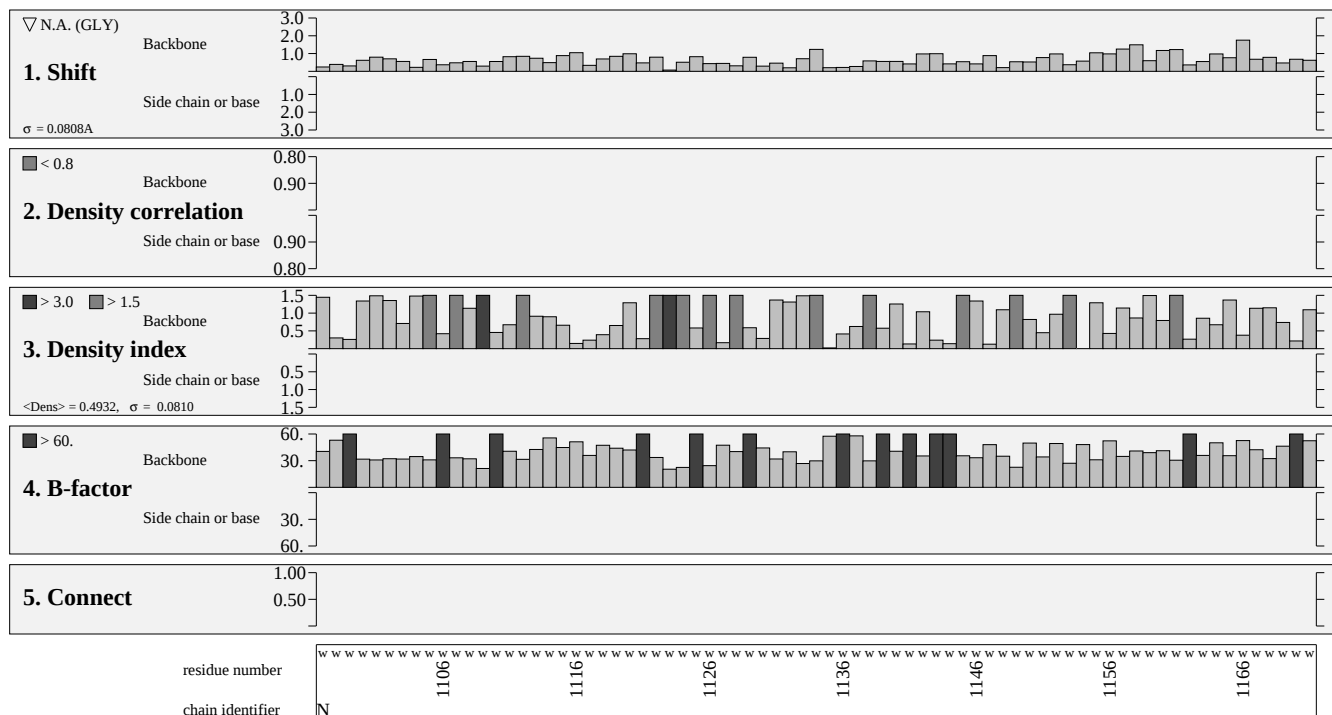
Local estimation (27)



Structure Factor Check

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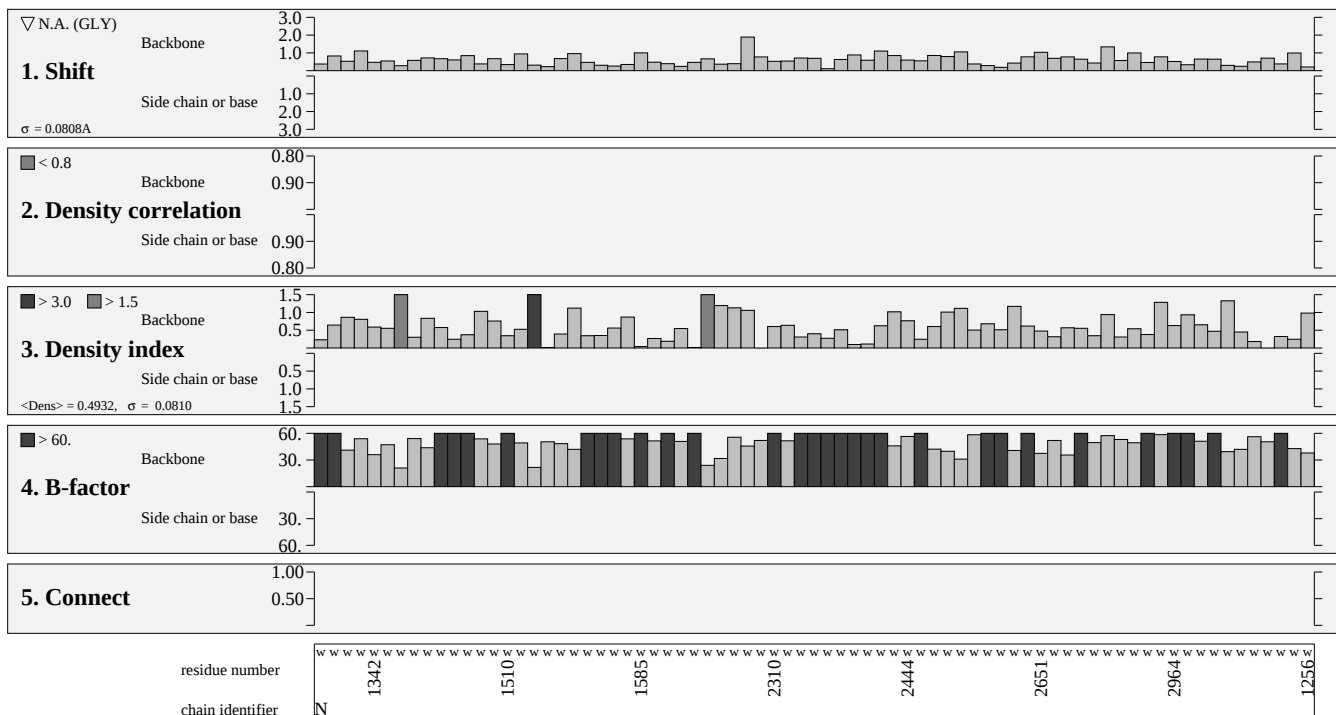
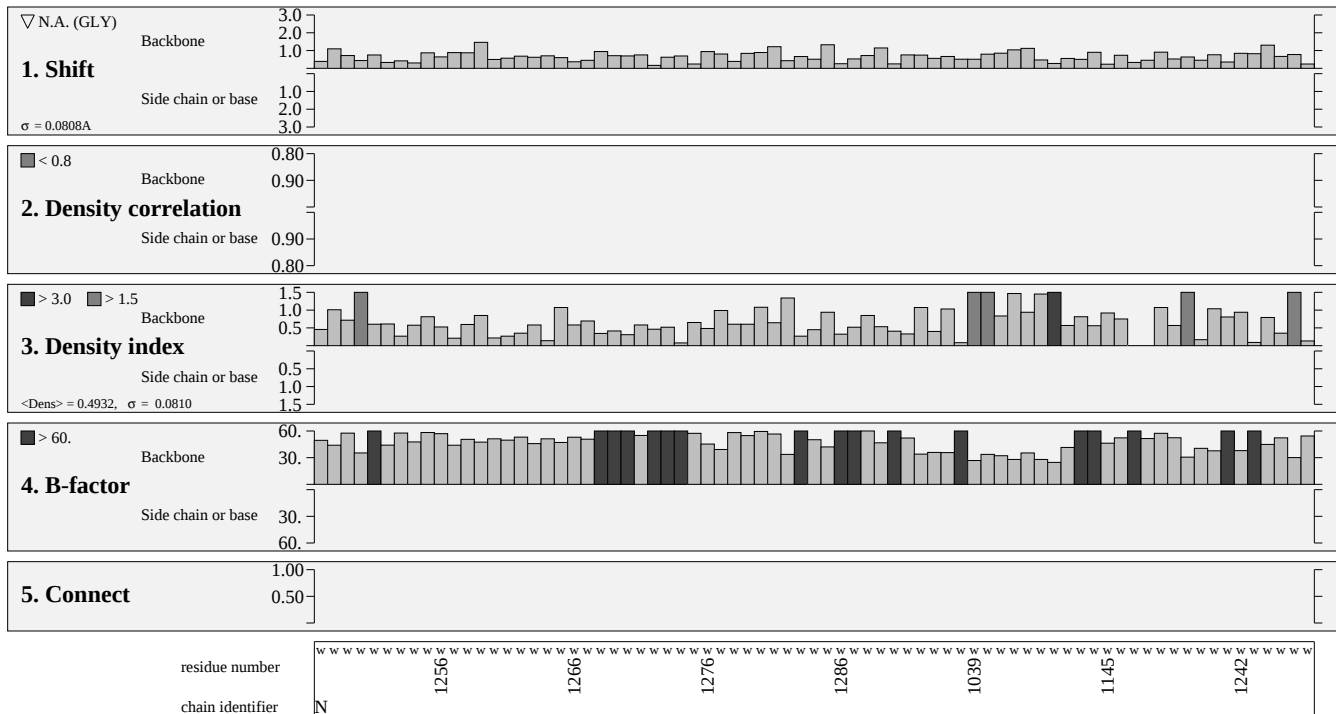
Local estimation (28)



Structure Factor Check

2H88

Local estimation (29)



Local estimation (30)

