

Structure Factor Check

3L72

Title: CHICKEN CYTOCHROME BC1 COMPLEX WITH KRESOXYM-I-DIMETHYL BOUN
 Date: 27-DEC-09
 PDB code: 3L72

Crystal

Cell parameters:

a: 172.61 A b: 181.55 A c: 241.03 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Model

32648 atoms (18 water molecules)

Number of chains: 51

Volume not occupied by model: 62.6 %

 (for atomic model): 75.1 A²

σ (B): 20.12 A²

Matthews coefficient: 4.13

Corresponding solvent % : 69.99

Refinement

Program: CNS 1.1

Nominal resolution range: 28.9 – 3.06 A

Reported R-factor: 0.264

Number of reflections used: 133892

Reported Rfree: 0.29

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 49.9 – 3.00 A

Reflections in file: 141090

Unique reflections above 0: 141090

above 1 σ : 136498

above 3 σ : 67537

SF CHECK

Nominal resolution range: 49.9 – 3.06 A

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

Used reflections: 133914

Reflections out of resolution: 7176

Completeness: 93.7 %

R_stand(F) = $\langle \sigma(F) \rangle / \langle F \rangle$: 0.110

Anisotropic distribution of Structure Factors

ratio of eigen values: 1.0000 0.4881 0.5169

B_overall (by Patterson): 52.A²

Optical resolution: 2.24 A

Expected opt. resol. for complete data set: 2.24 A

Estimated minimal error: 0.148 A

Model vs. Structure Factors

R-factor for all reflections: 0.315

Correlation factor: 0.833

R-factor: 0.316

for $F > 2.0 \sigma$

nom. resolution range: 28.93 – 3.06A

reflections used: 130194

Rfree: 0.345

Nfree: 2577

R-factor without free-refl.: 0.315

Non free-reflections: 127617

<u> (error in coords by Luzzati plot): 0.635 A

Estimated maximal error: 0.355 A

DPI: 0.433 A

Scaling

Scale: 0.477

Bdiff: -6.65

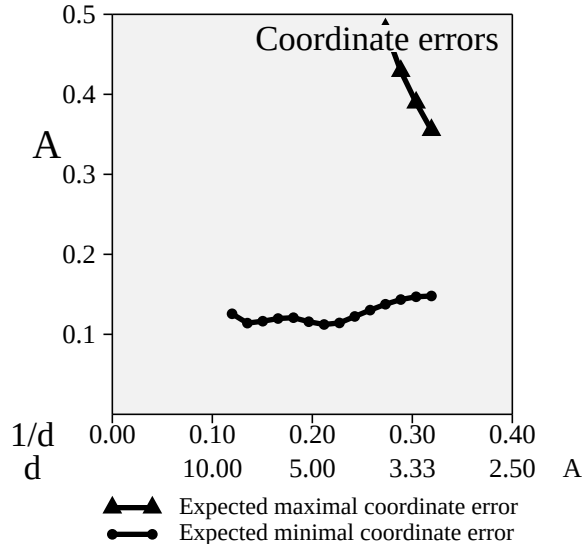
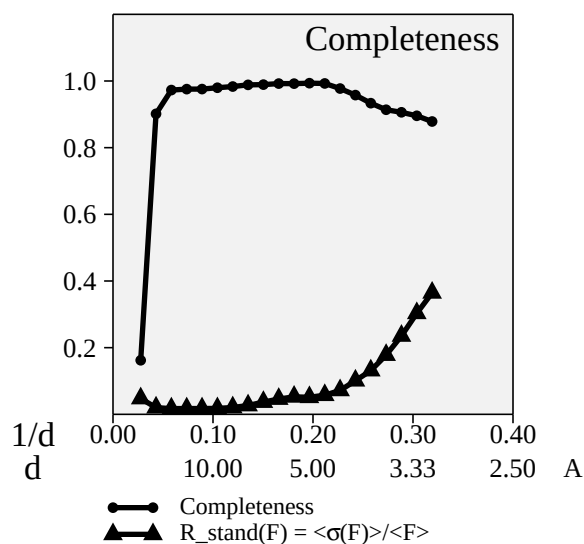
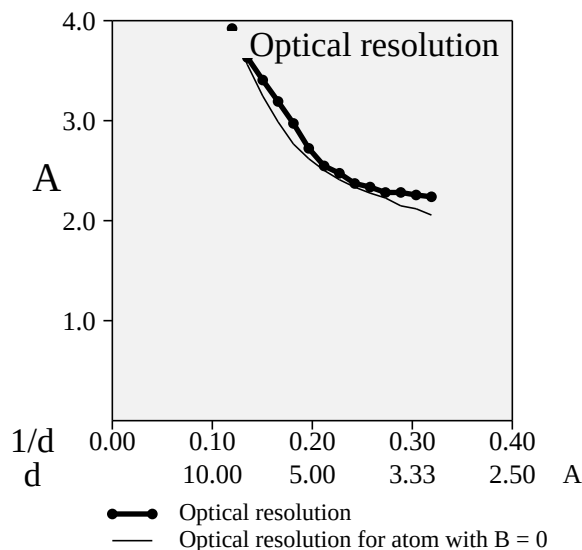
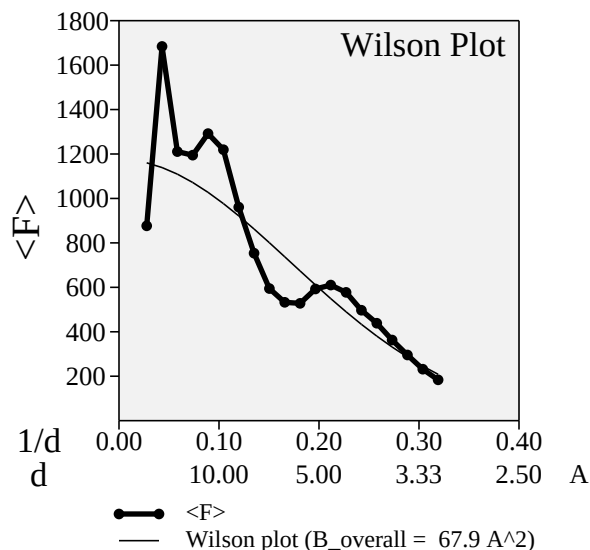
Anisothermal Scaling (Beta):

9.7786 -2.1368 -0.8960 0.0000 0.0000 0.0000

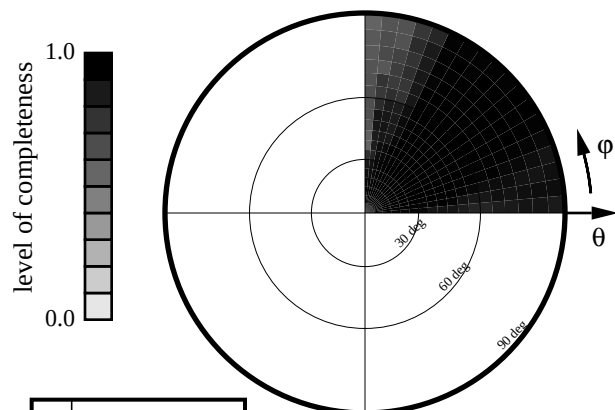
Solvent correction – Ks,Bs: 0.695 250.139

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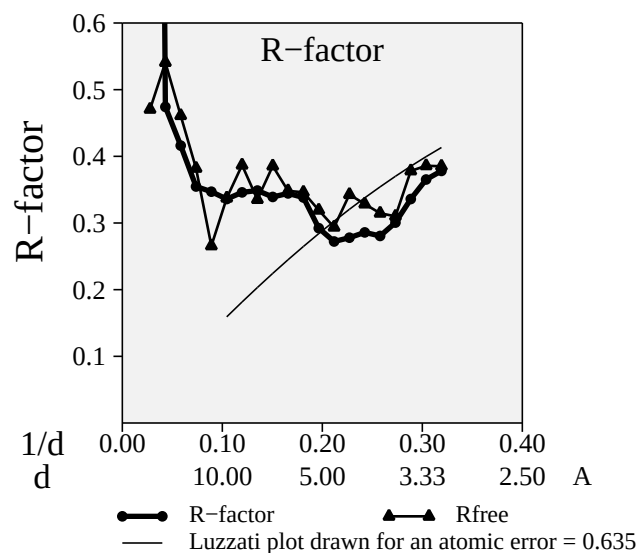


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

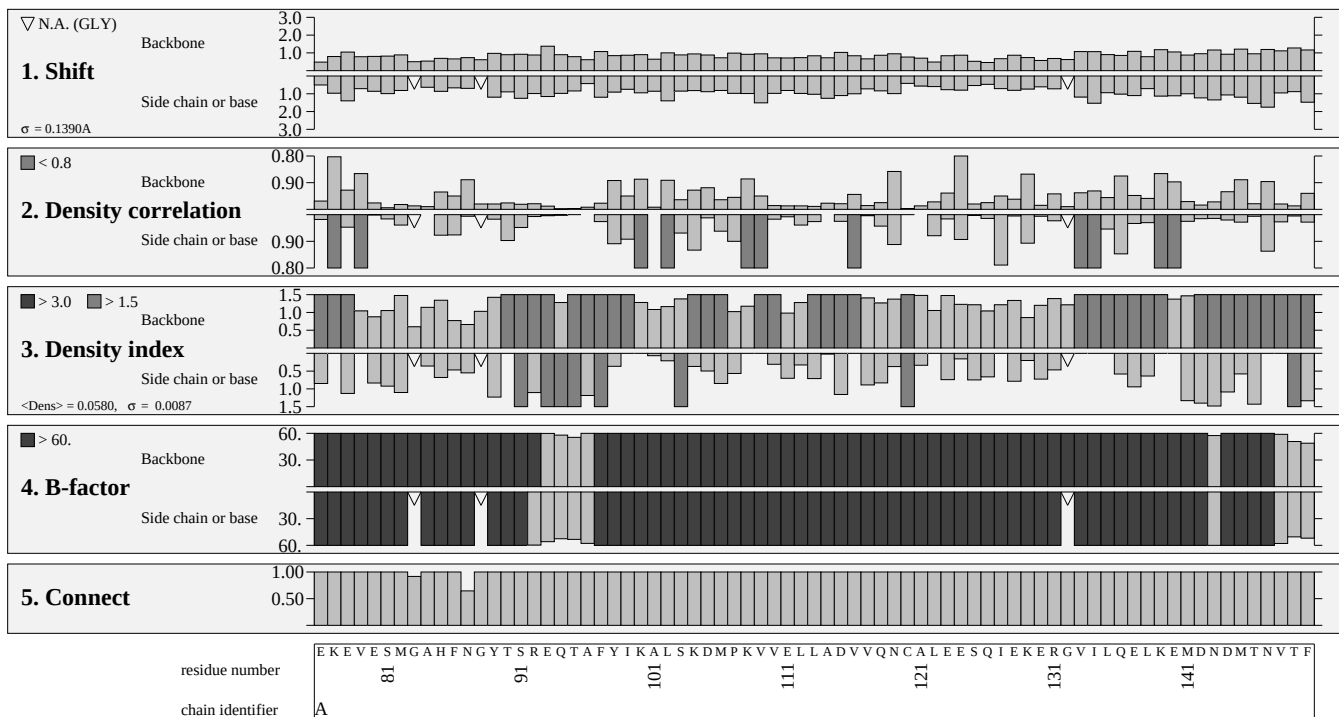
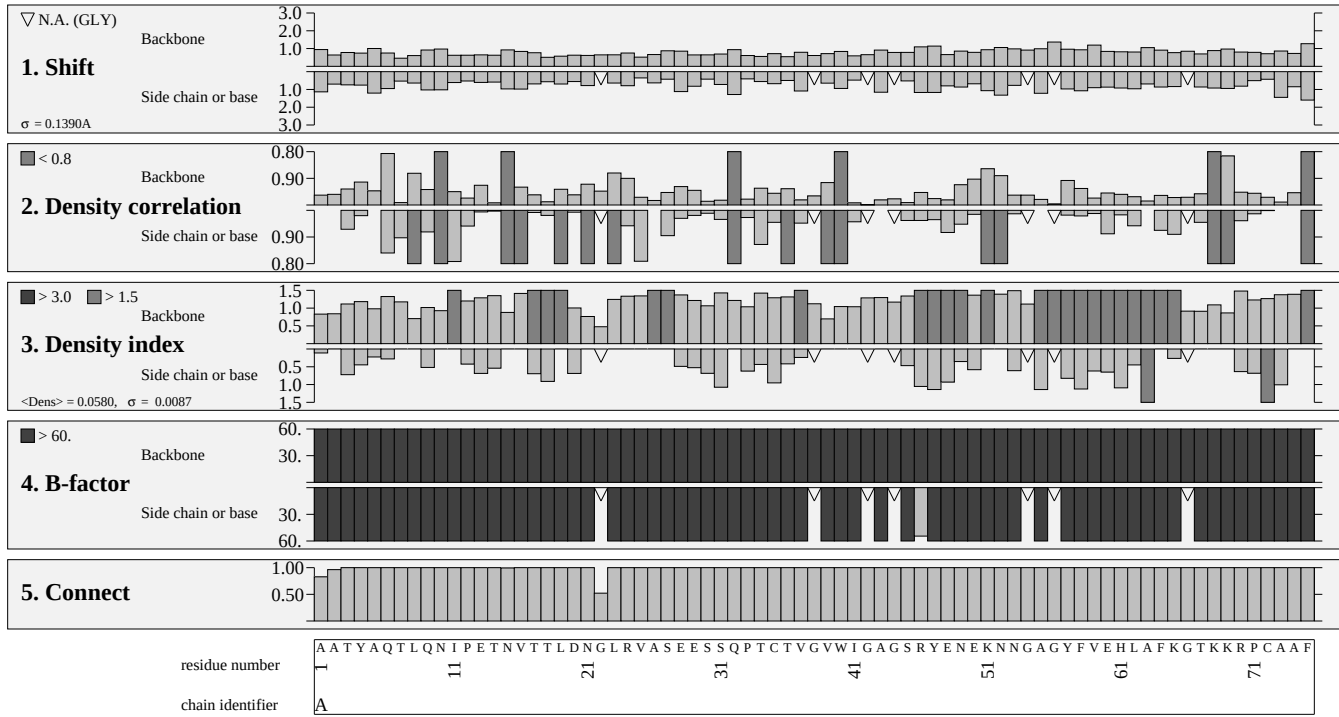
polar coordinates of the crystallographical axes



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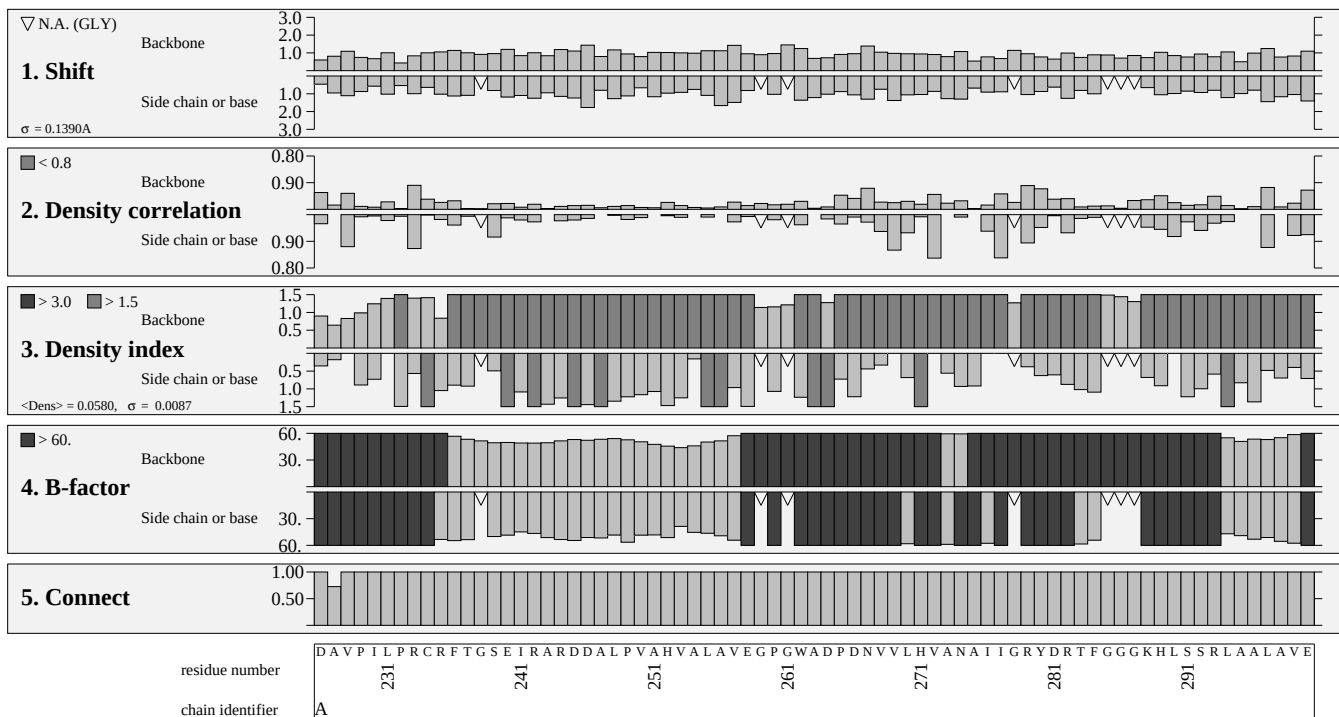
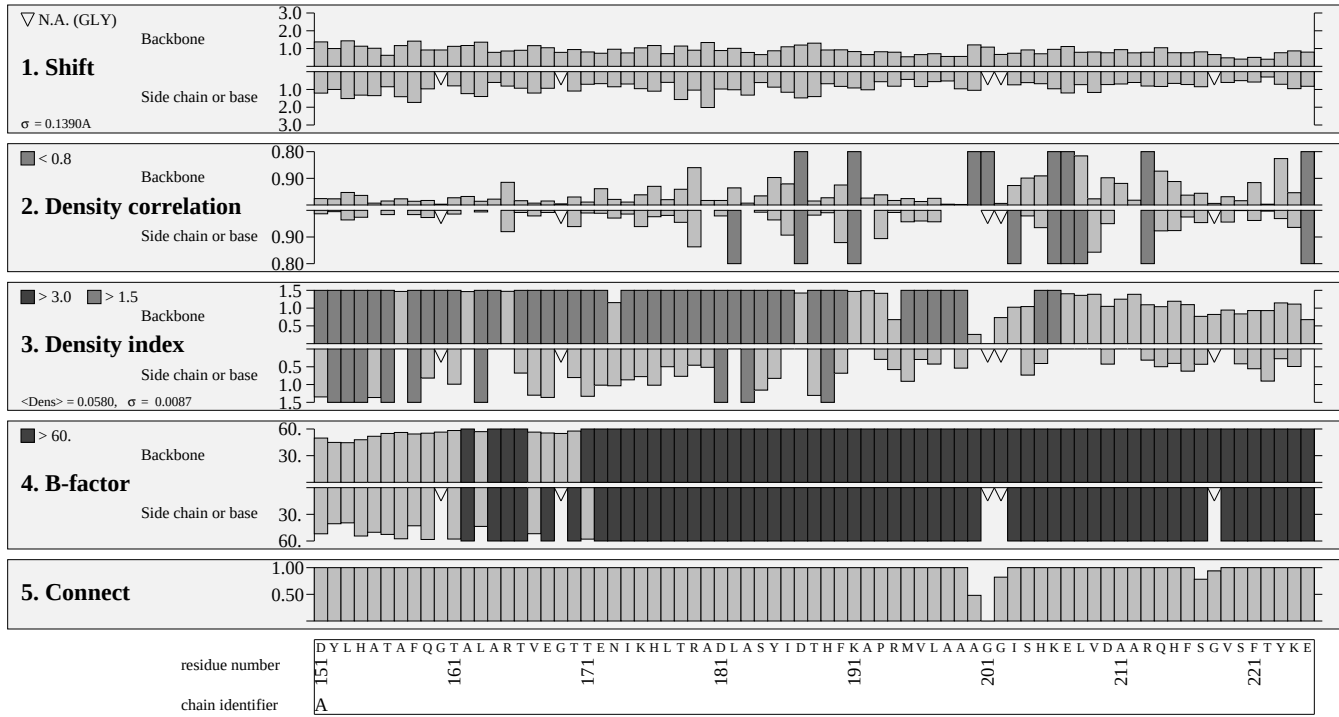
Local estimation



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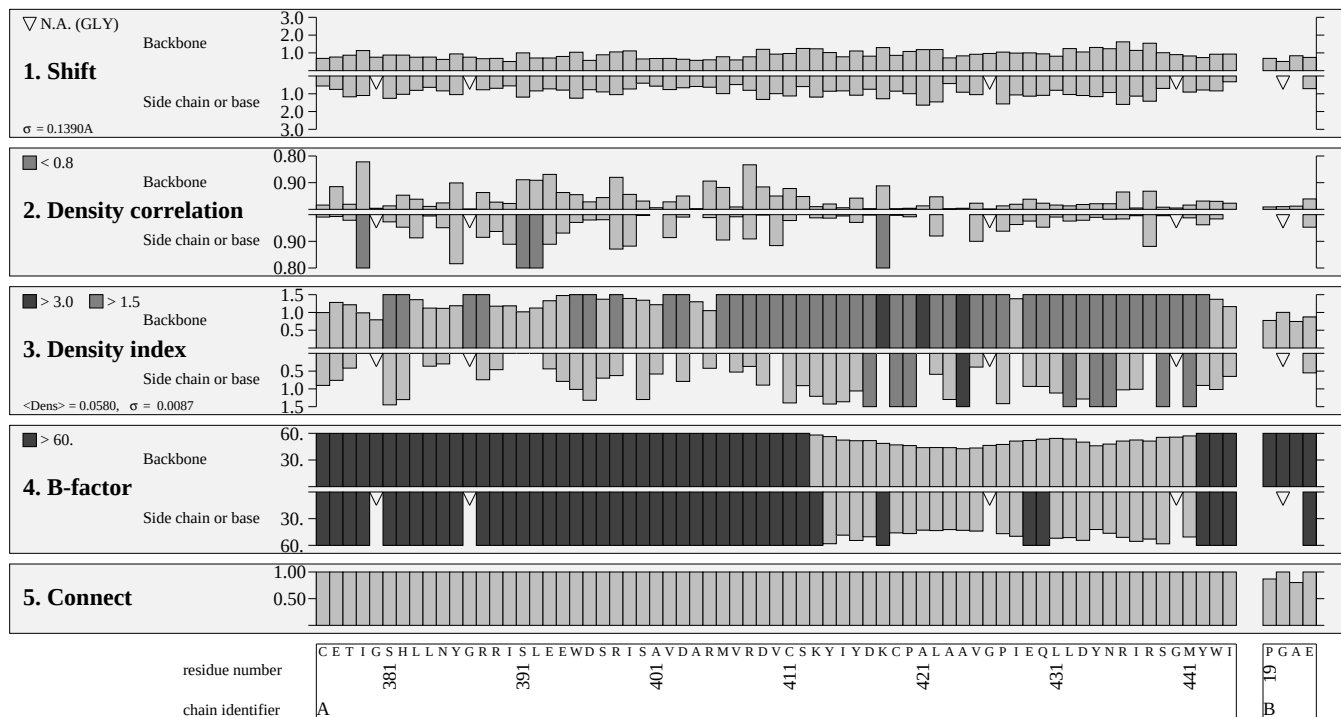
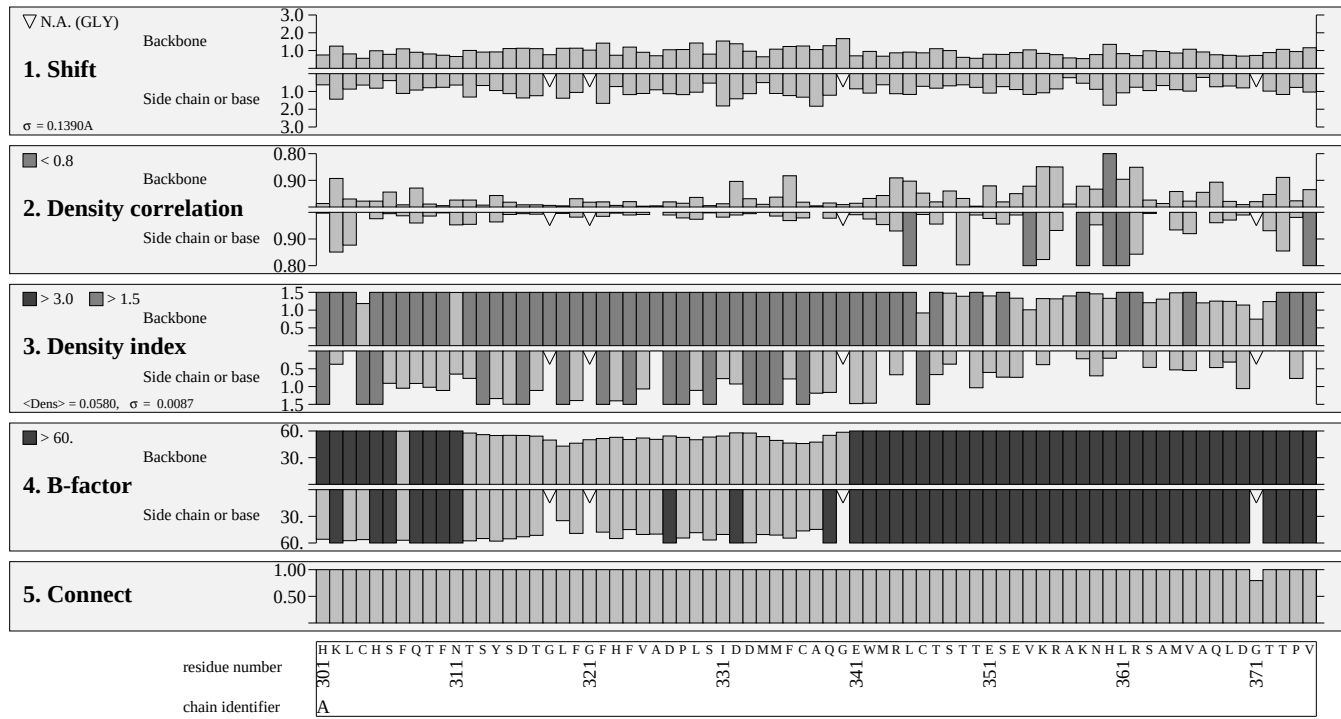
Local estimation (2)



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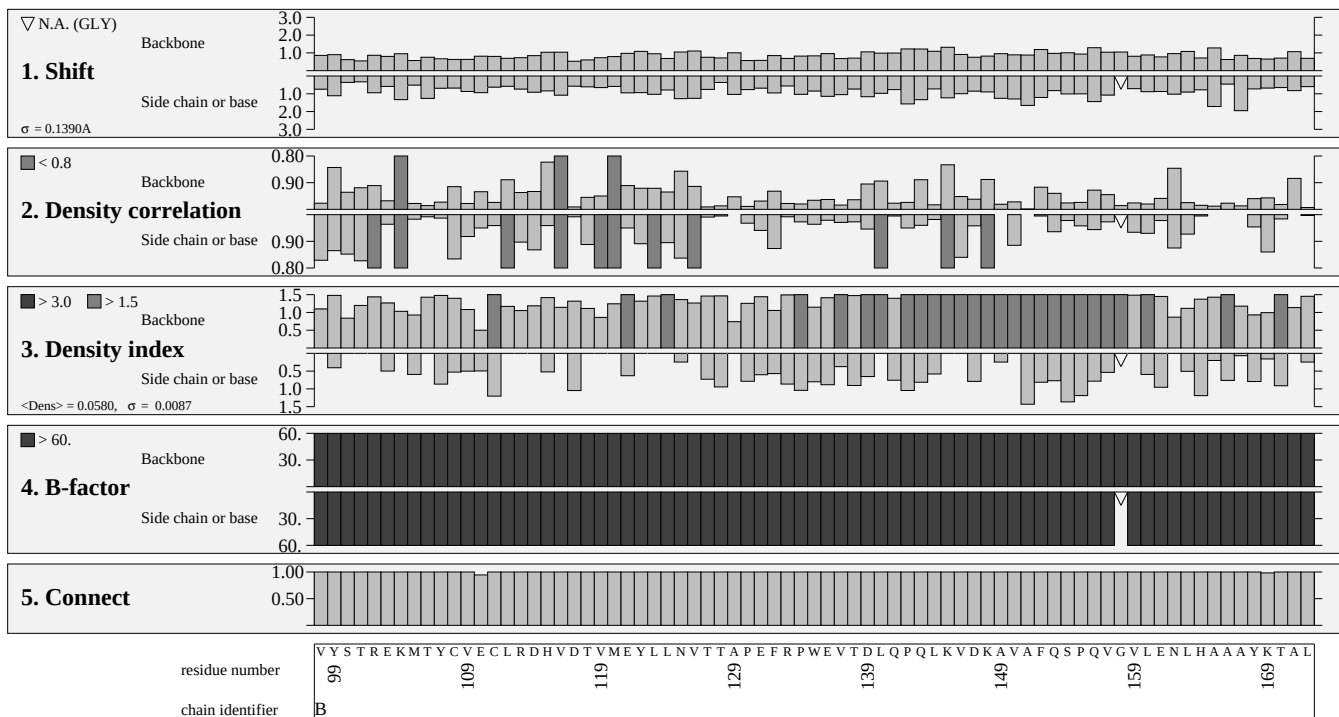
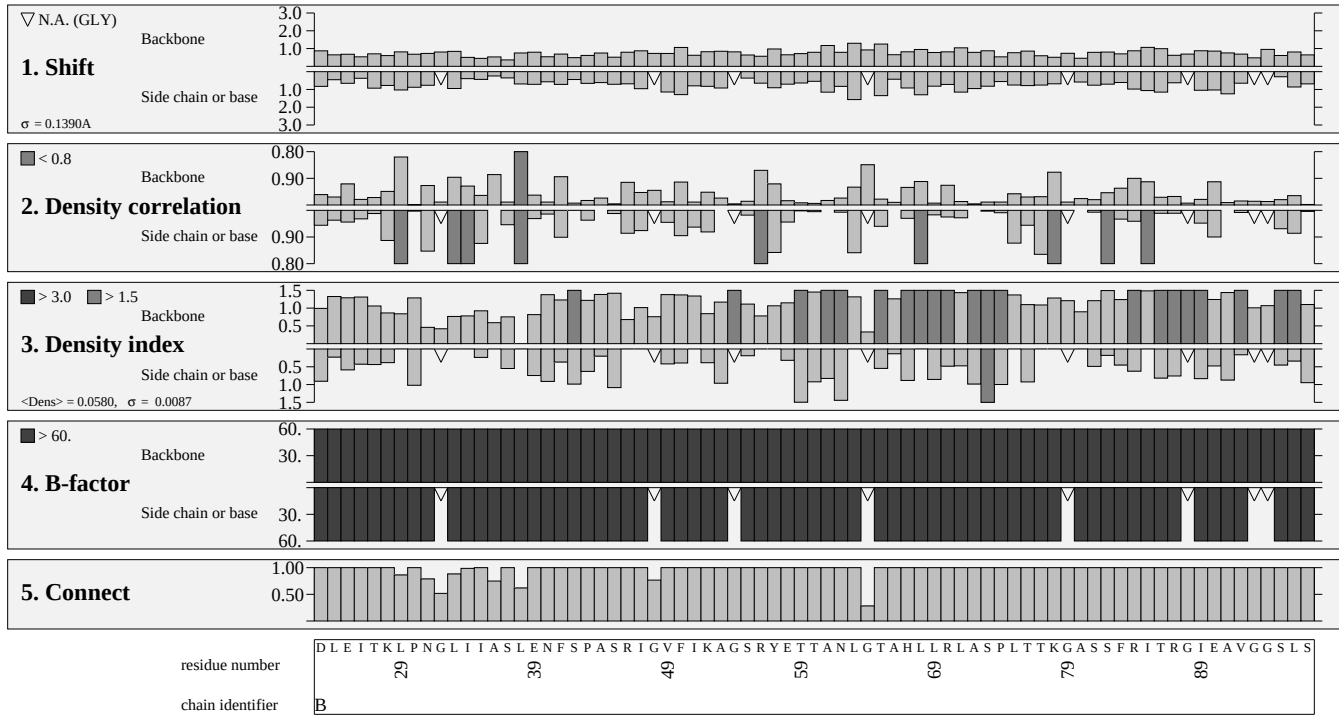
Local estimation (3)



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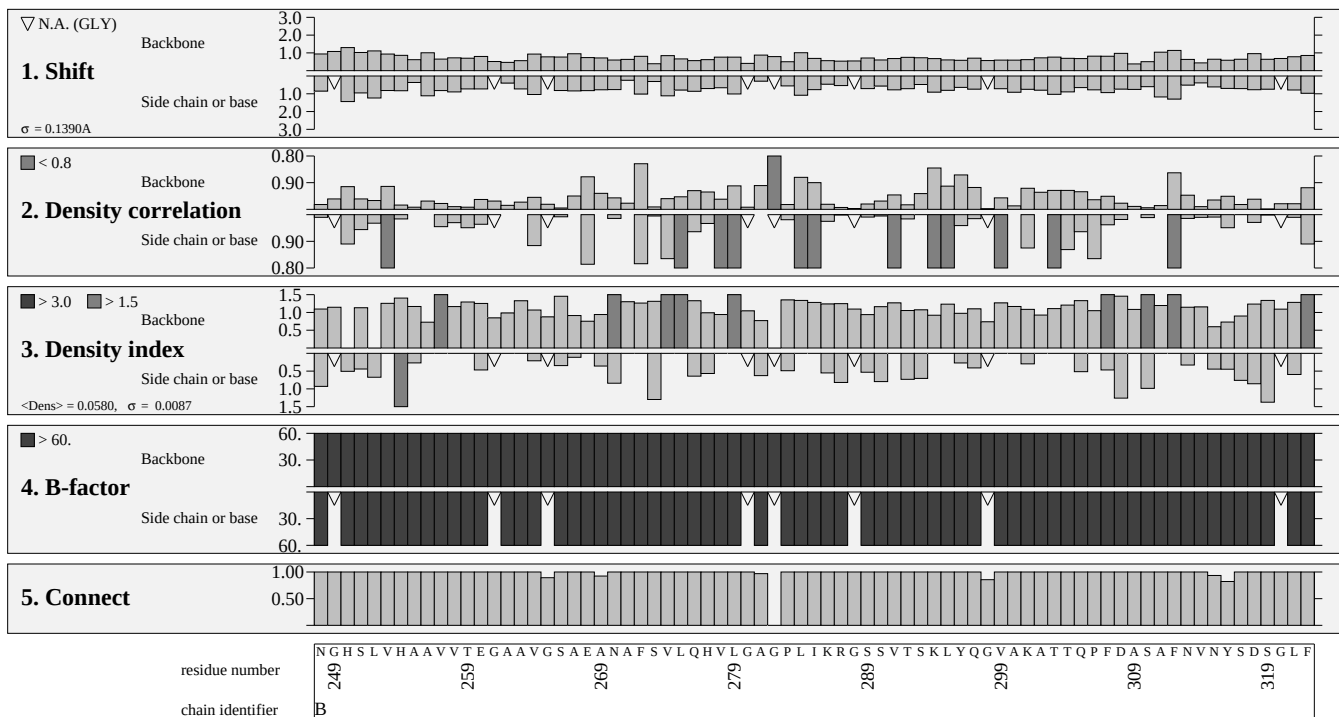
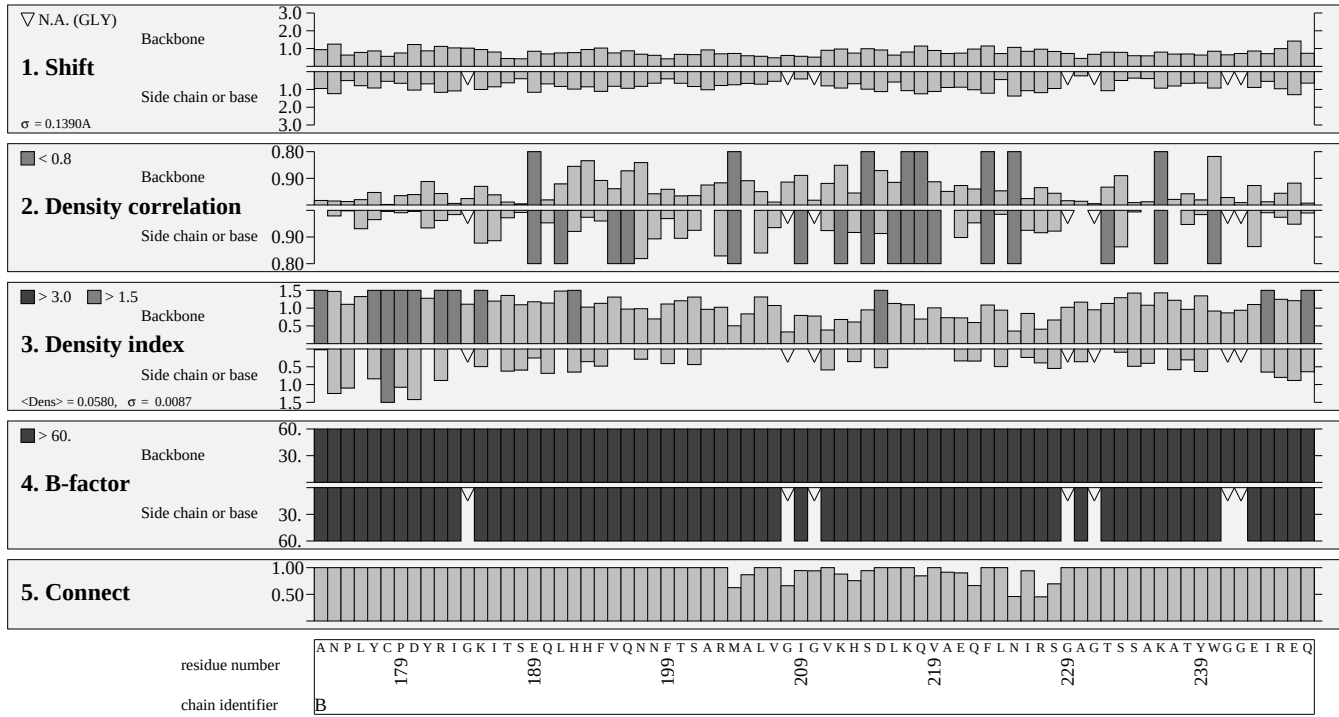
Local estimation (4)



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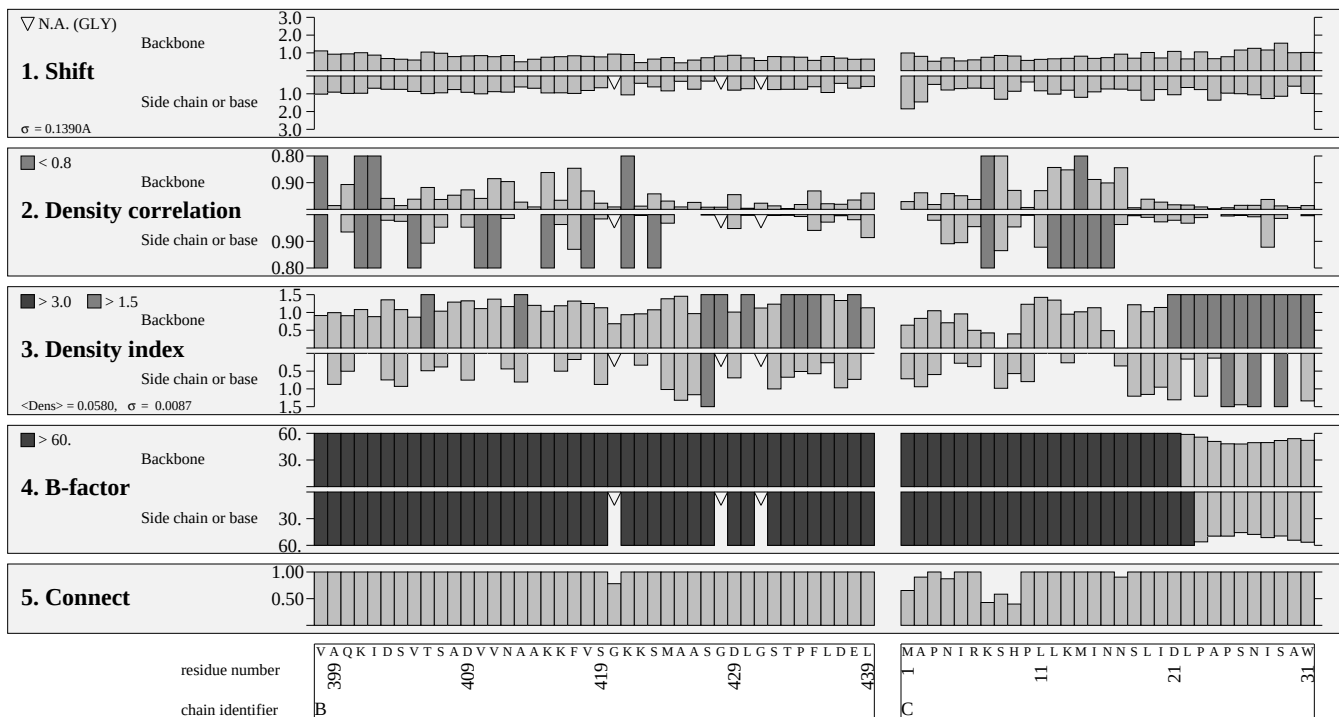
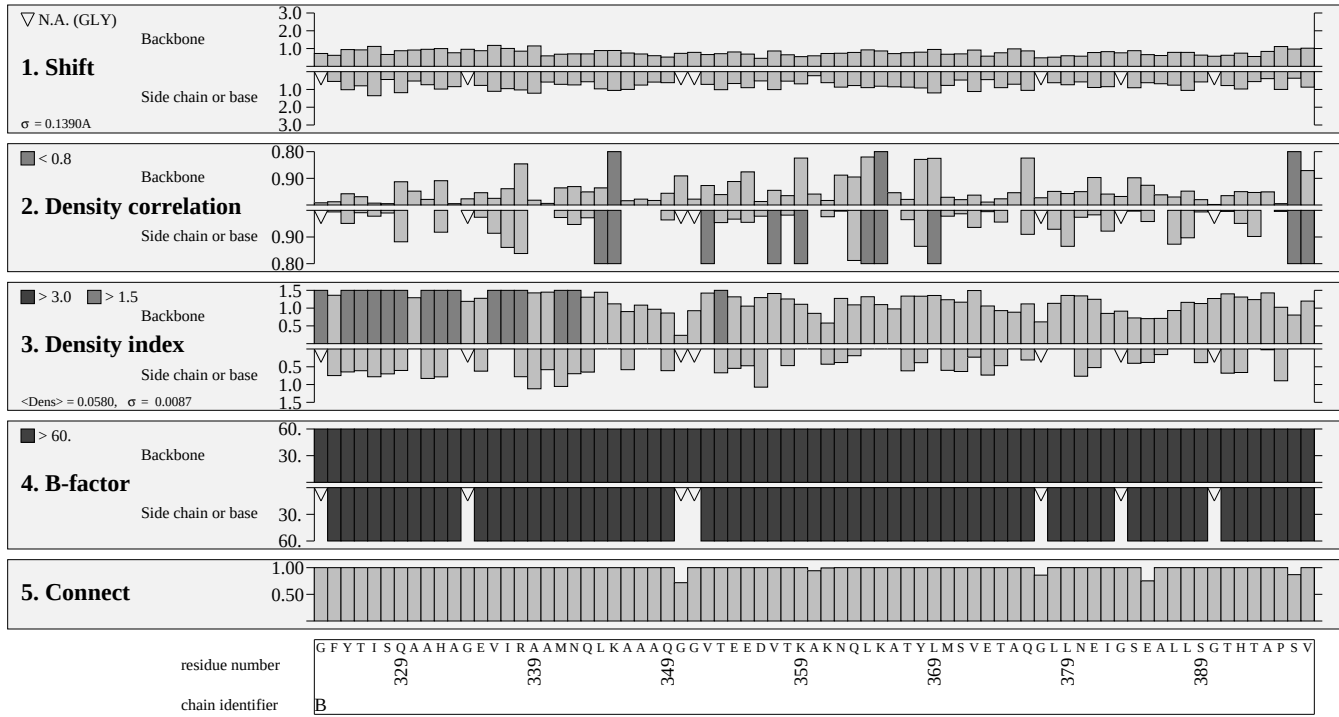
Local estimation (5)



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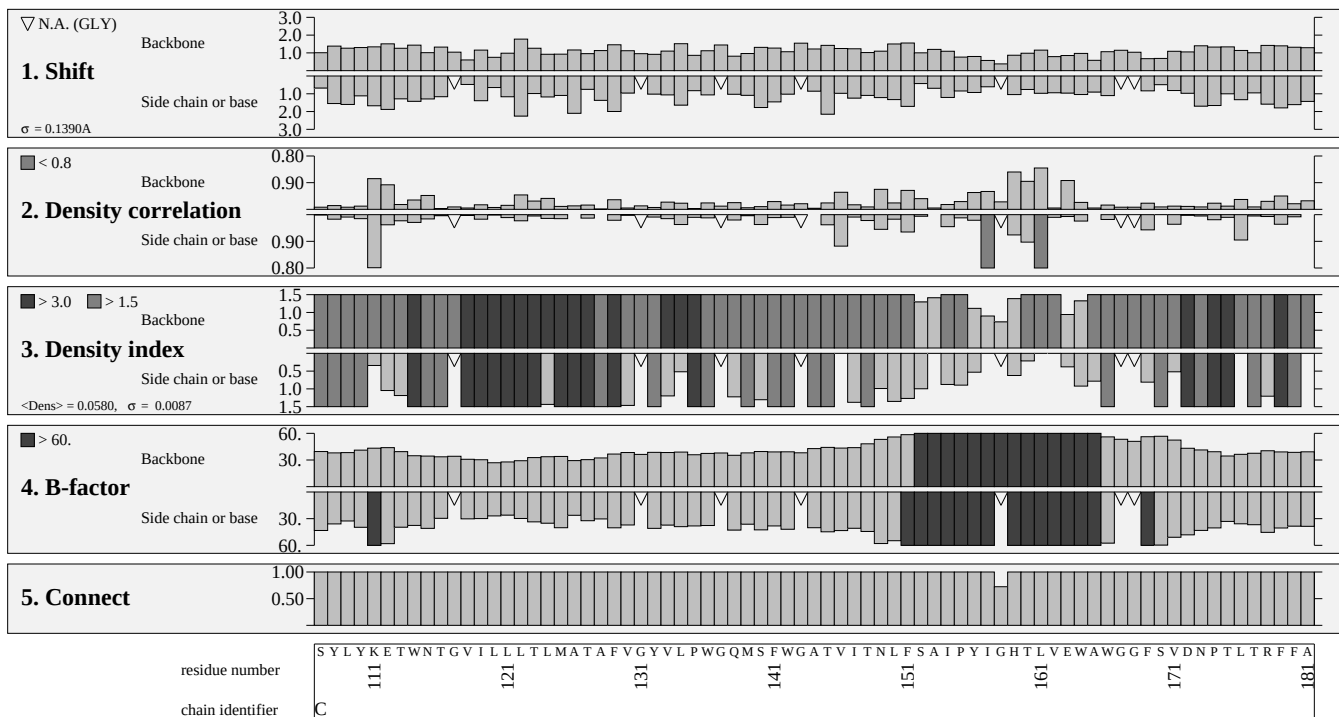
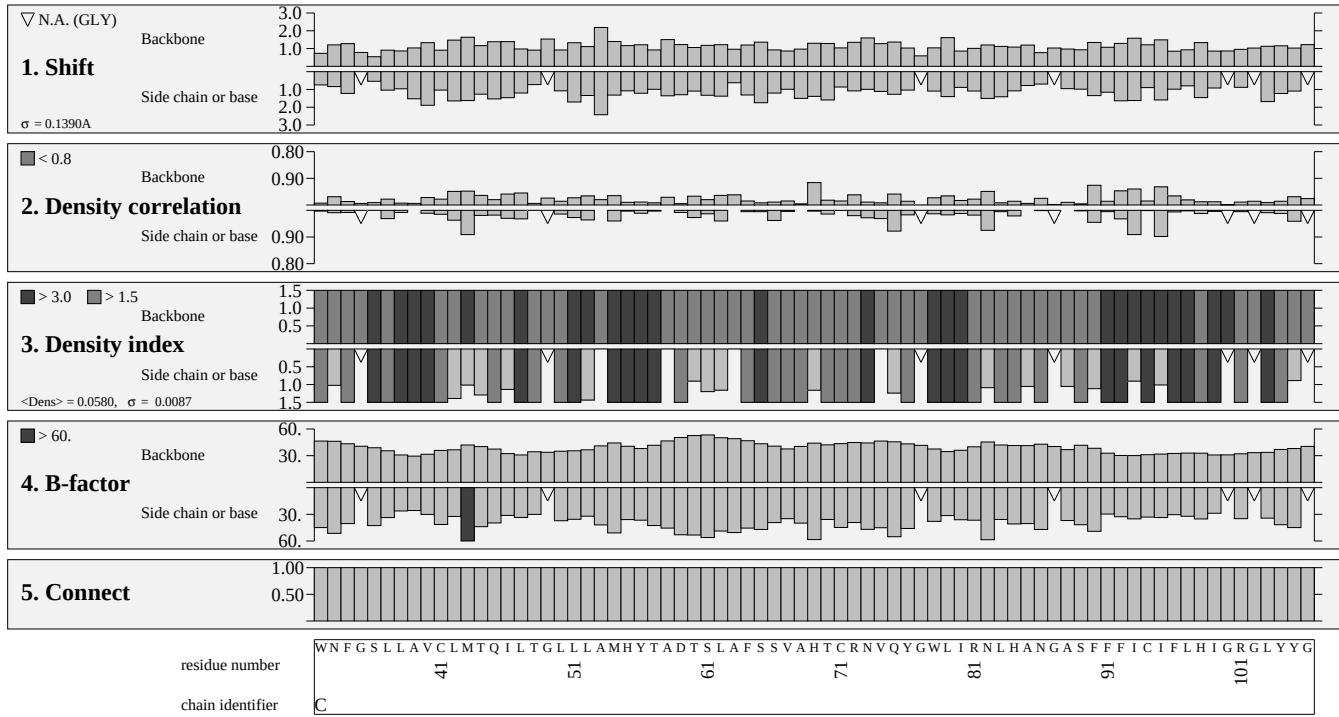
Local estimation (6)



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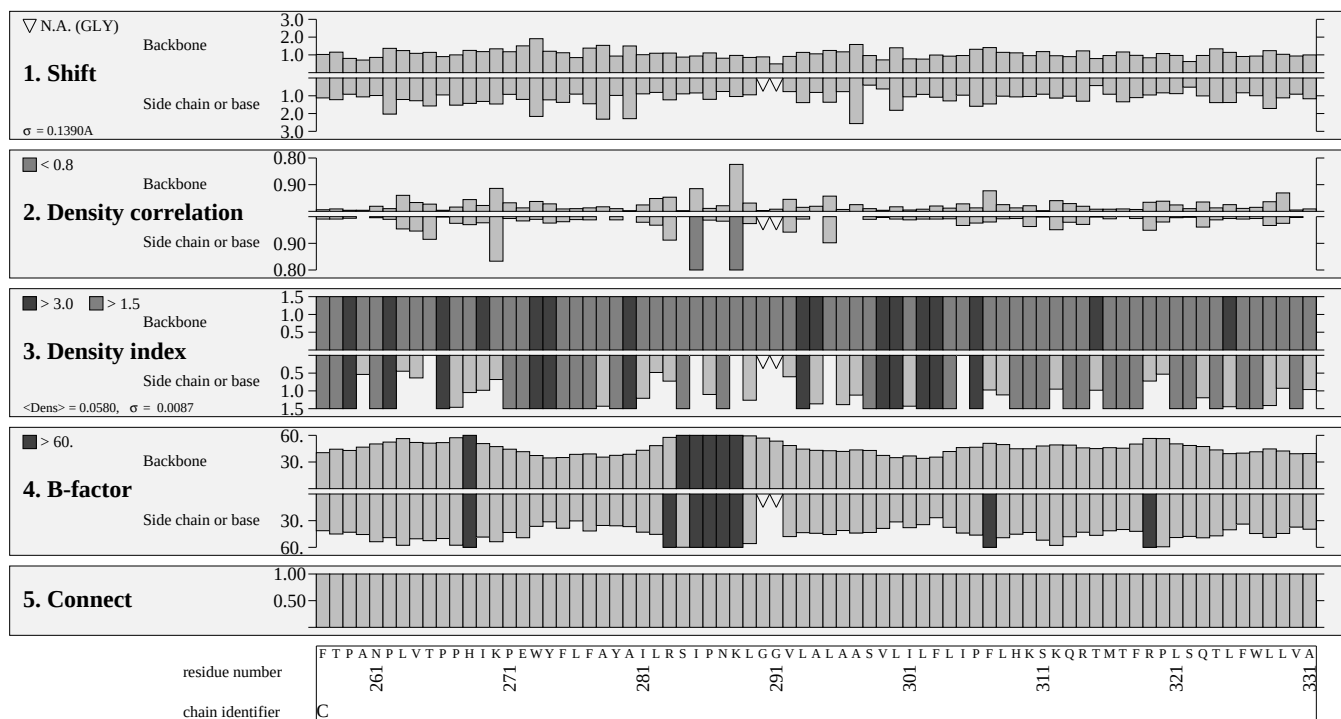
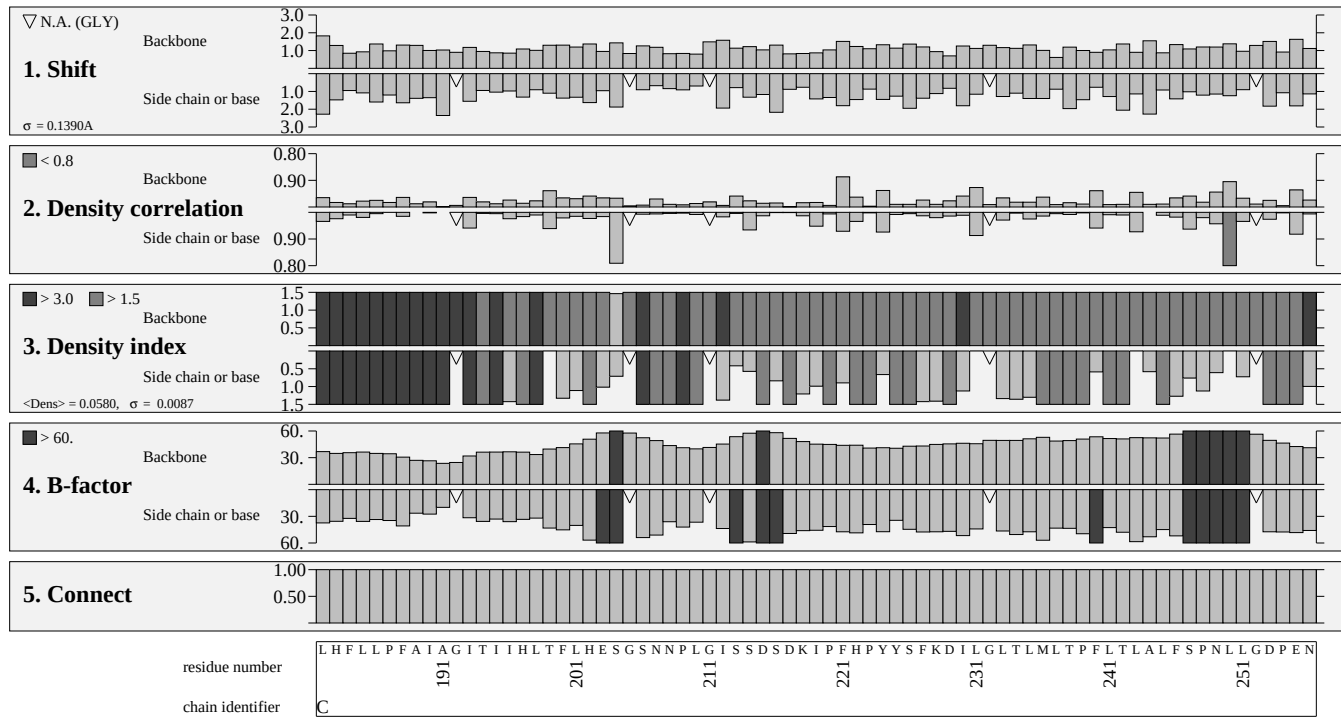
Local estimation (7)



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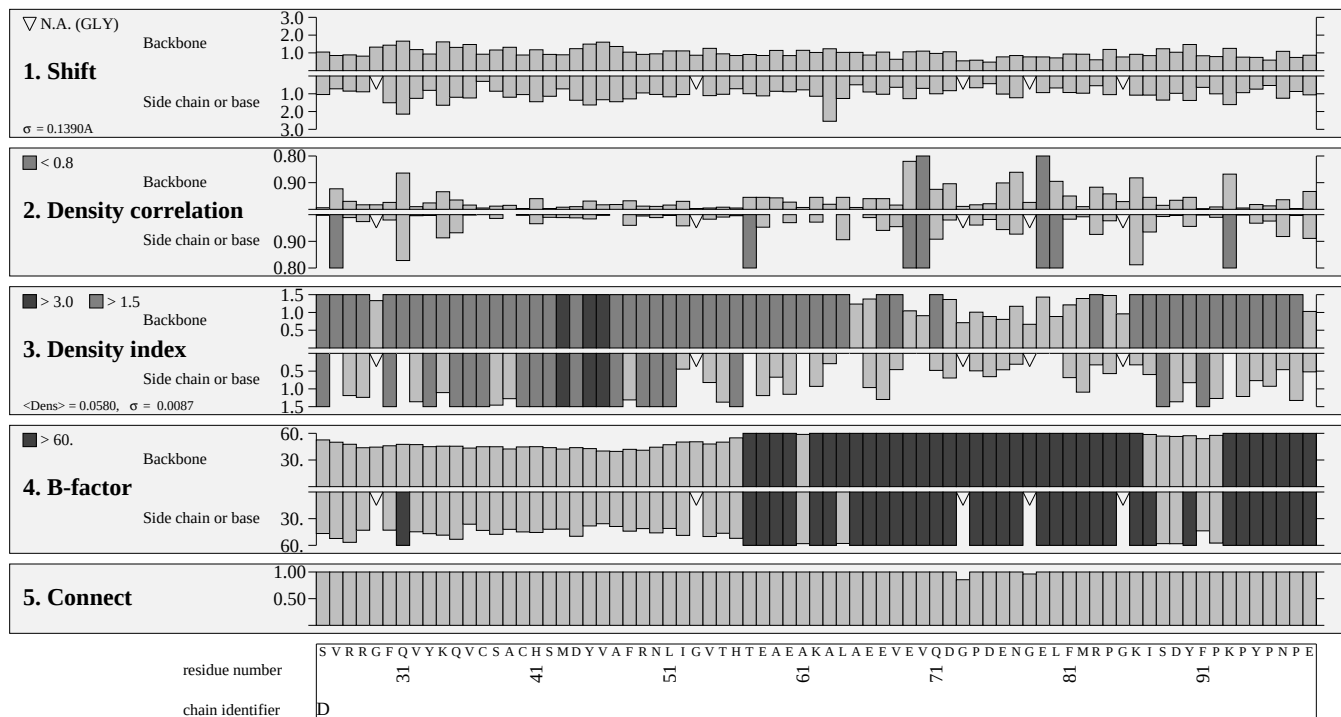
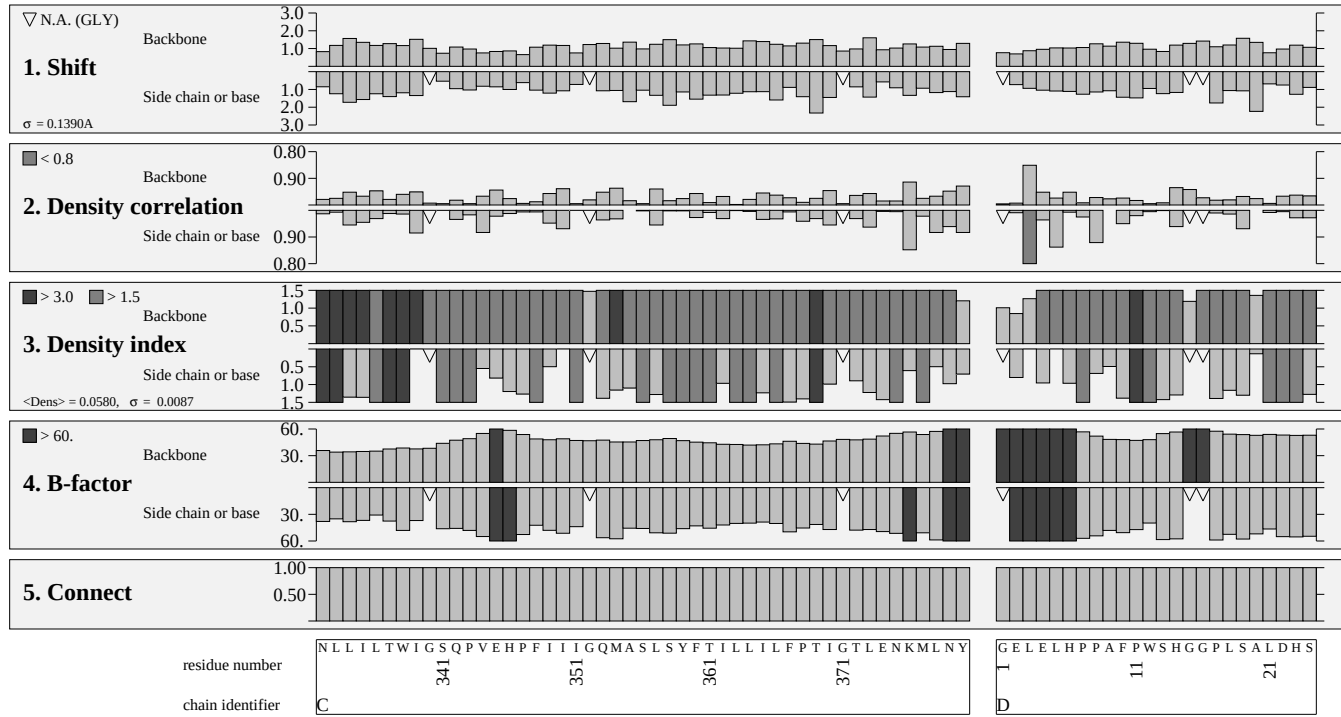
Local estimation (8)



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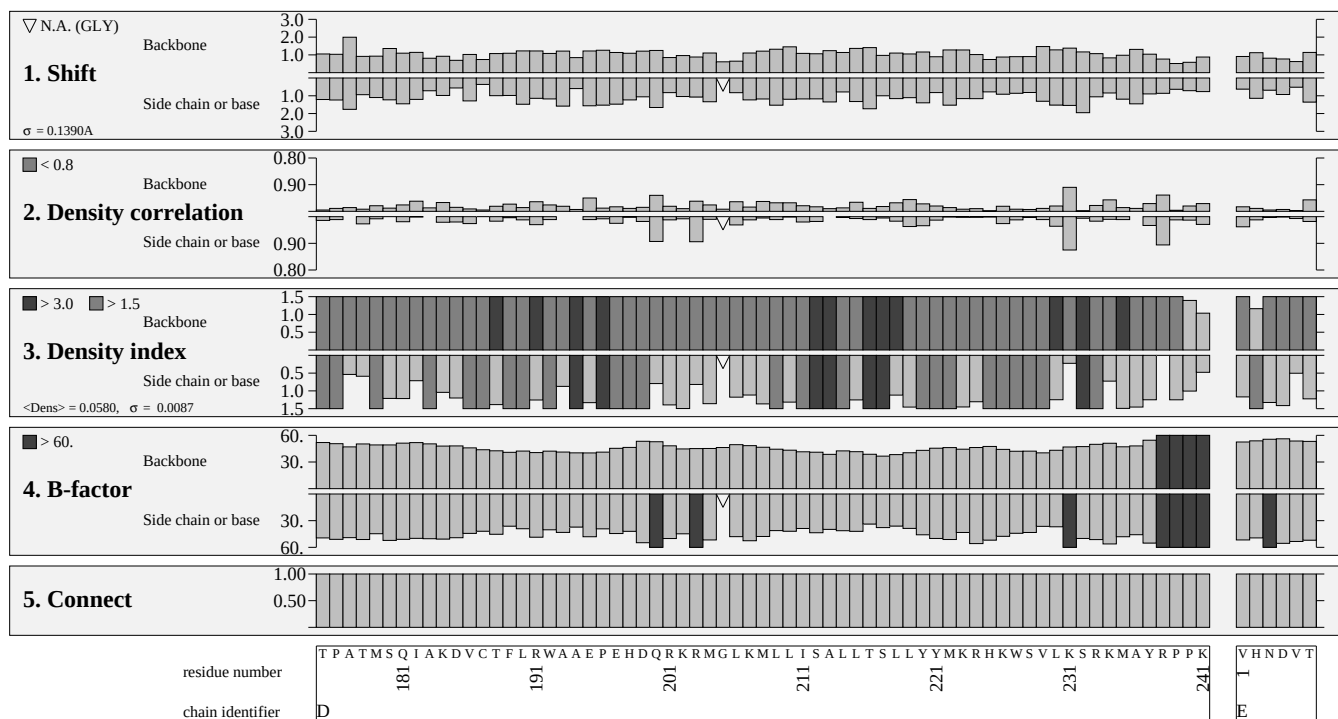
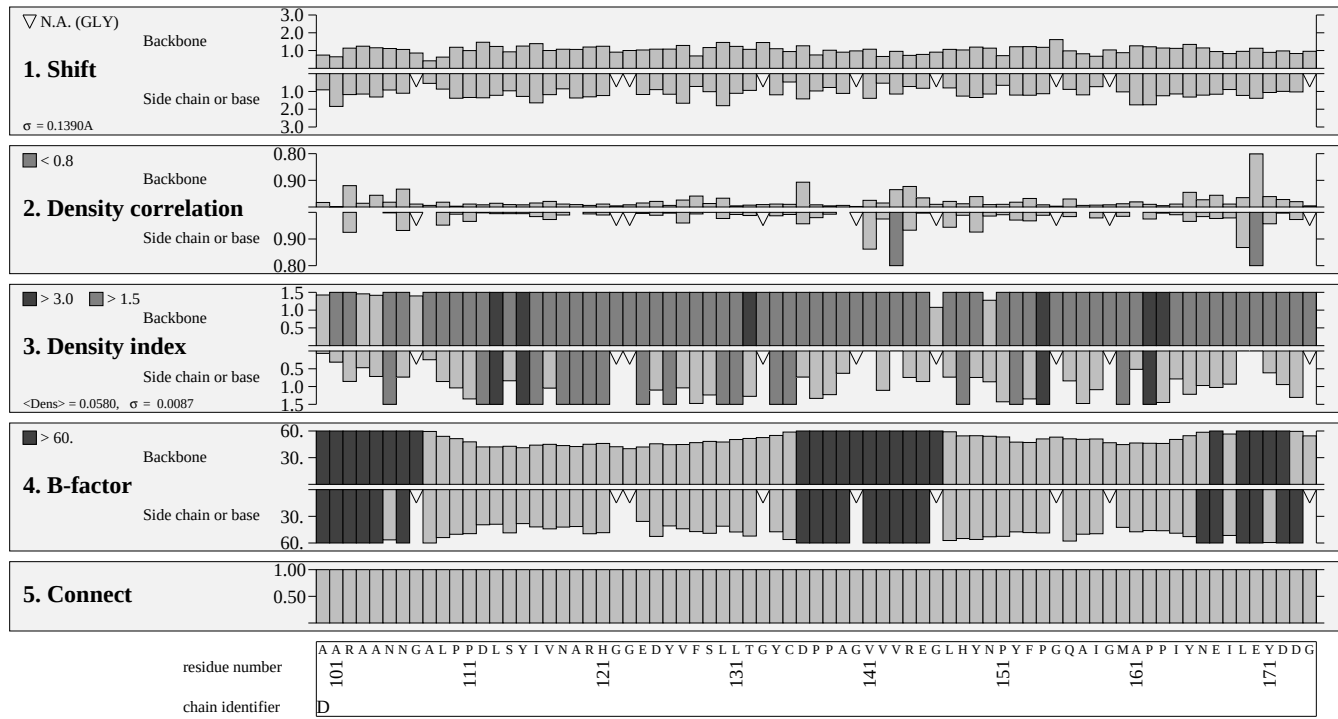
Local estimation (9)



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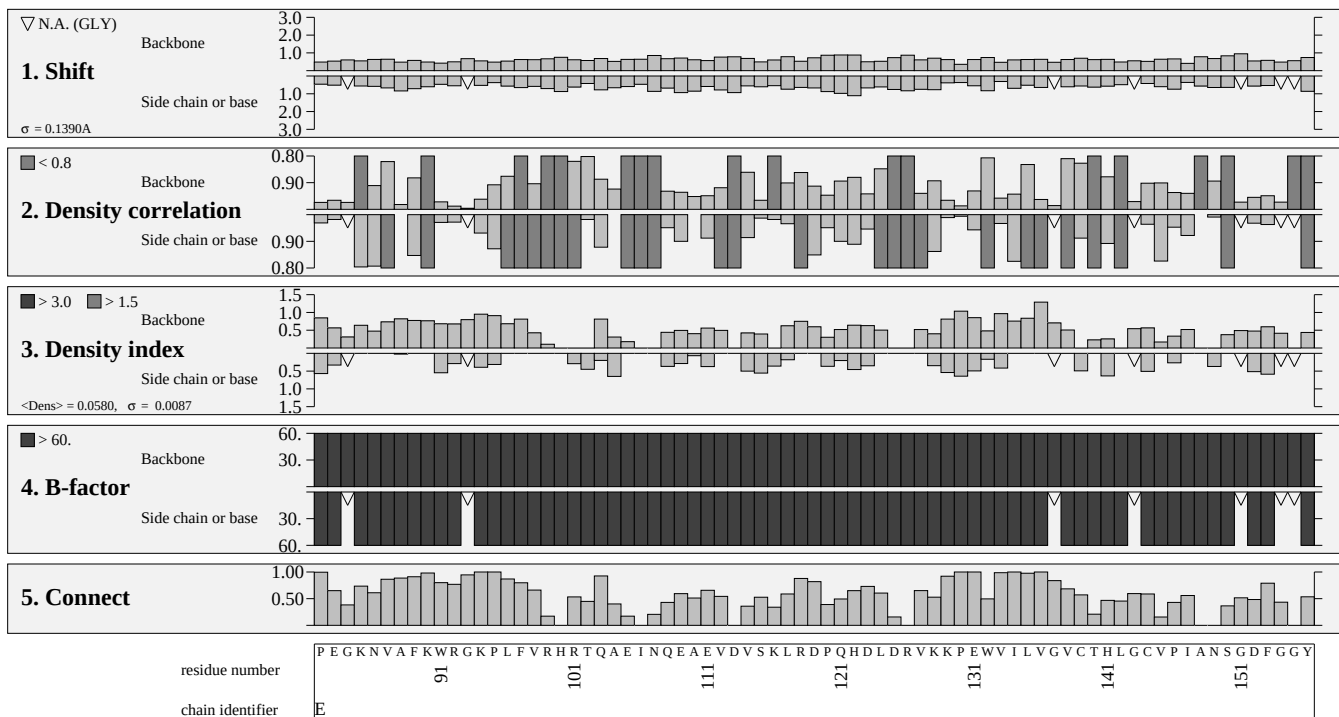
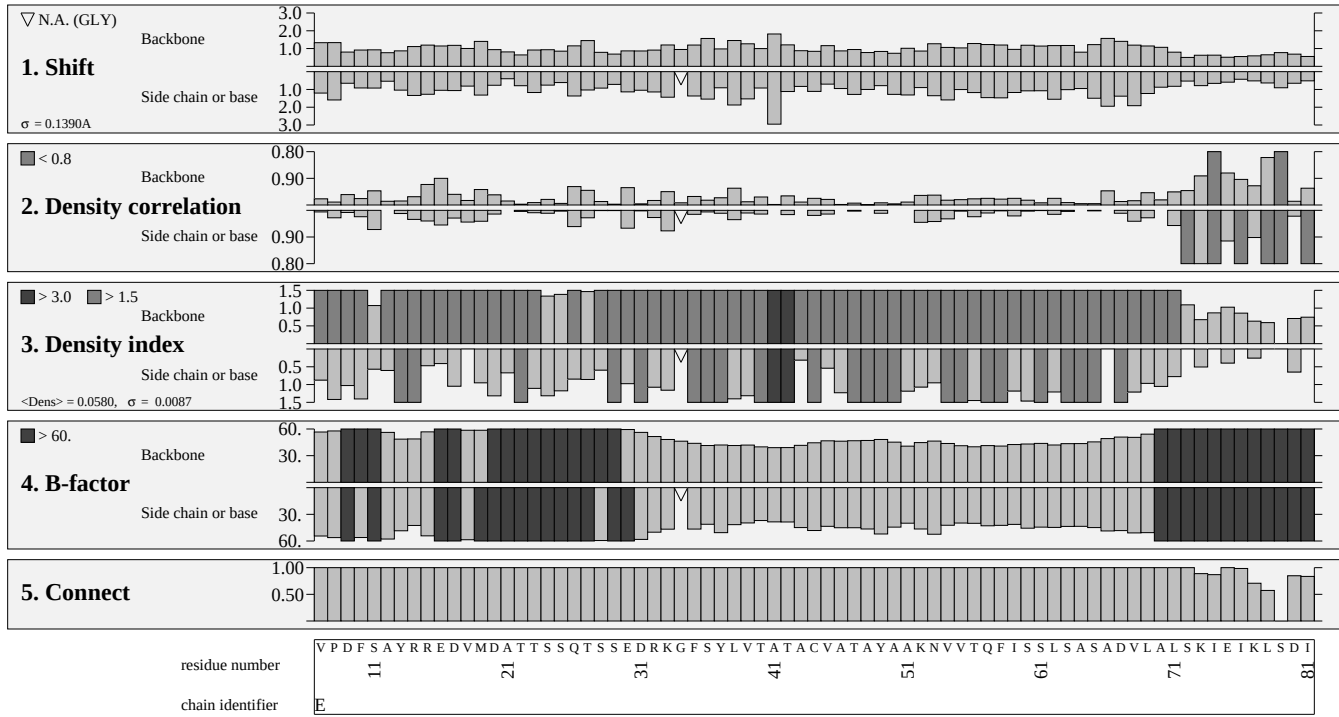
Local estimation (10)



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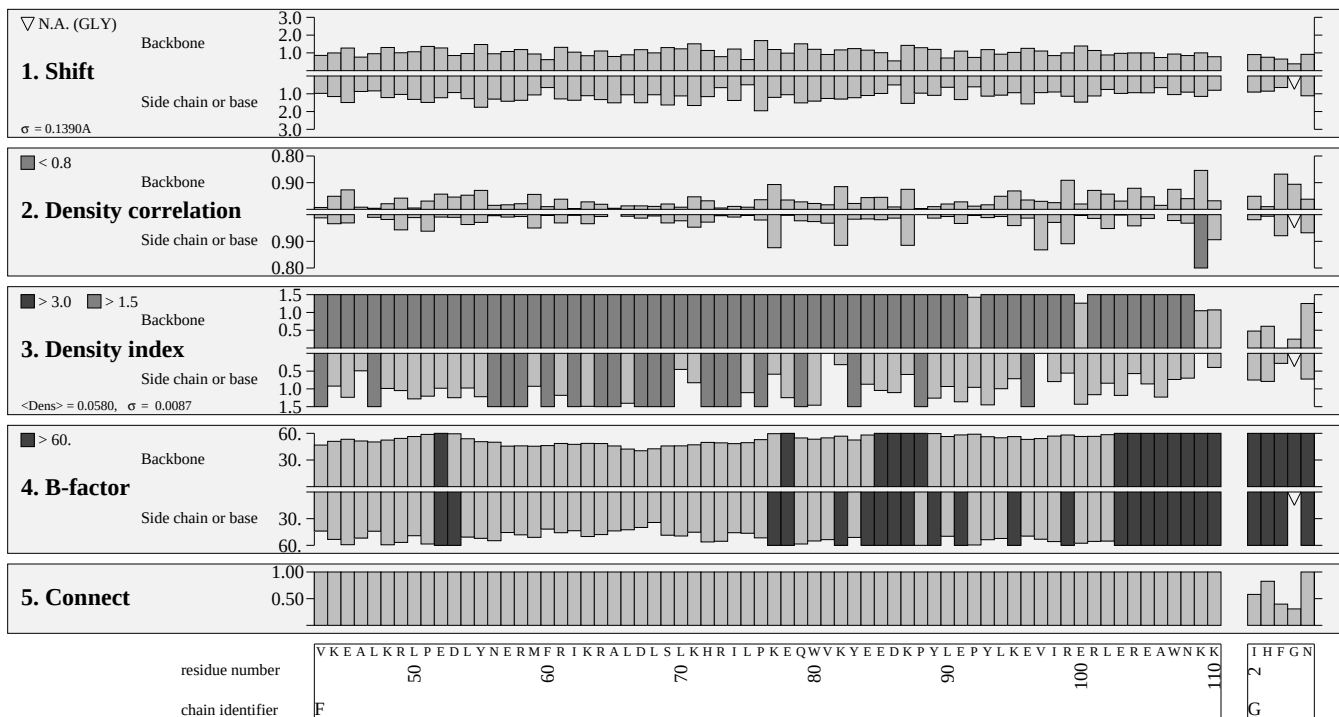
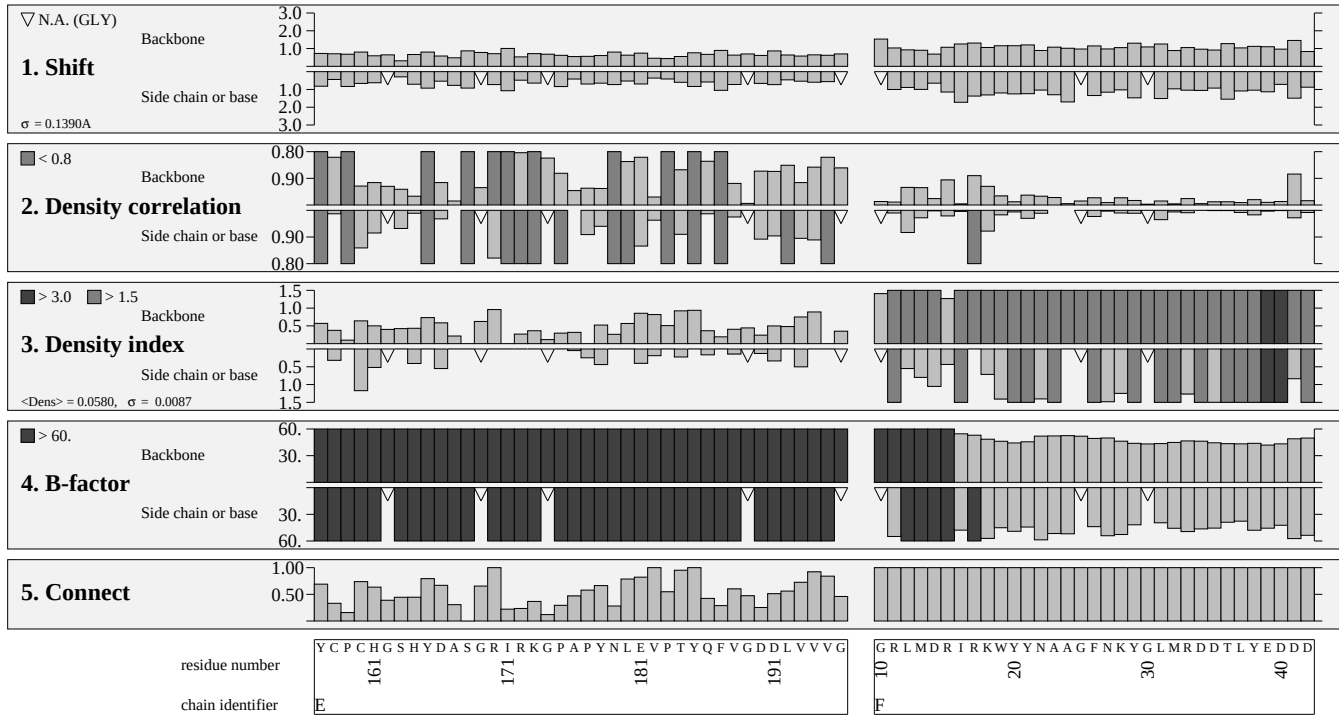
Local estimation (11)



Structure Factor Check

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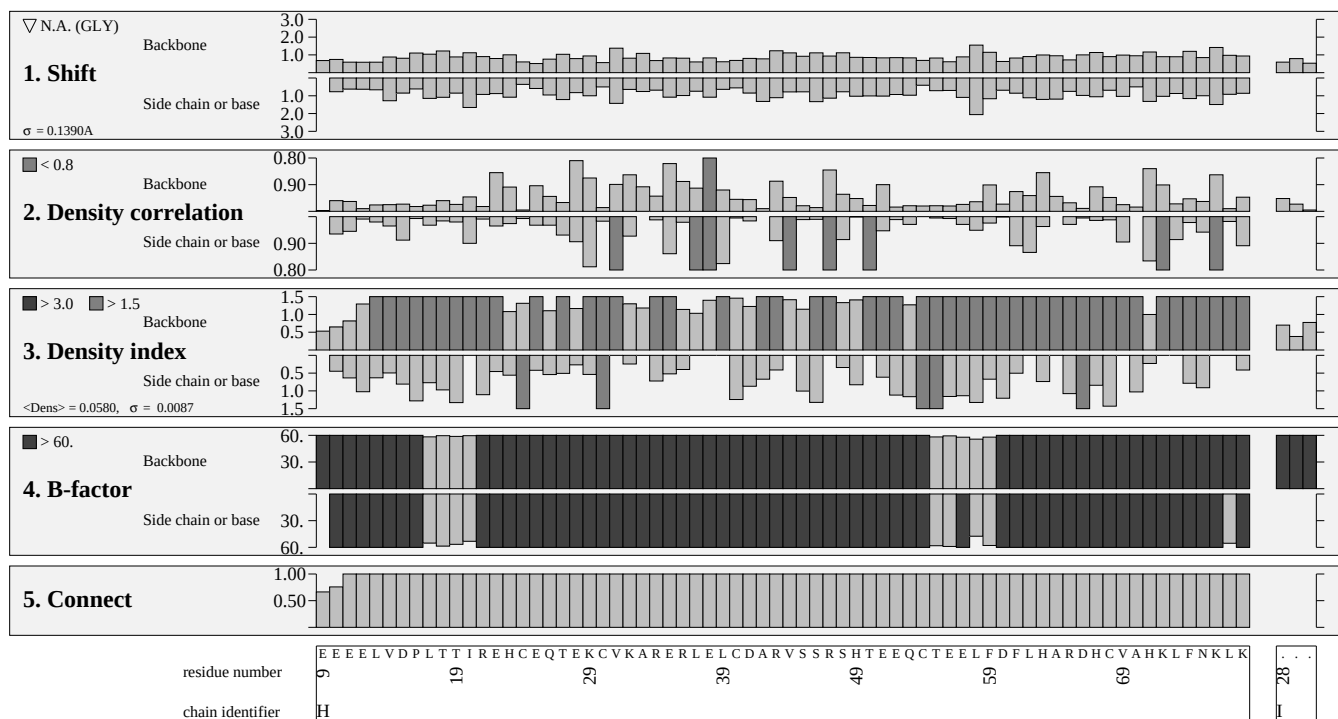
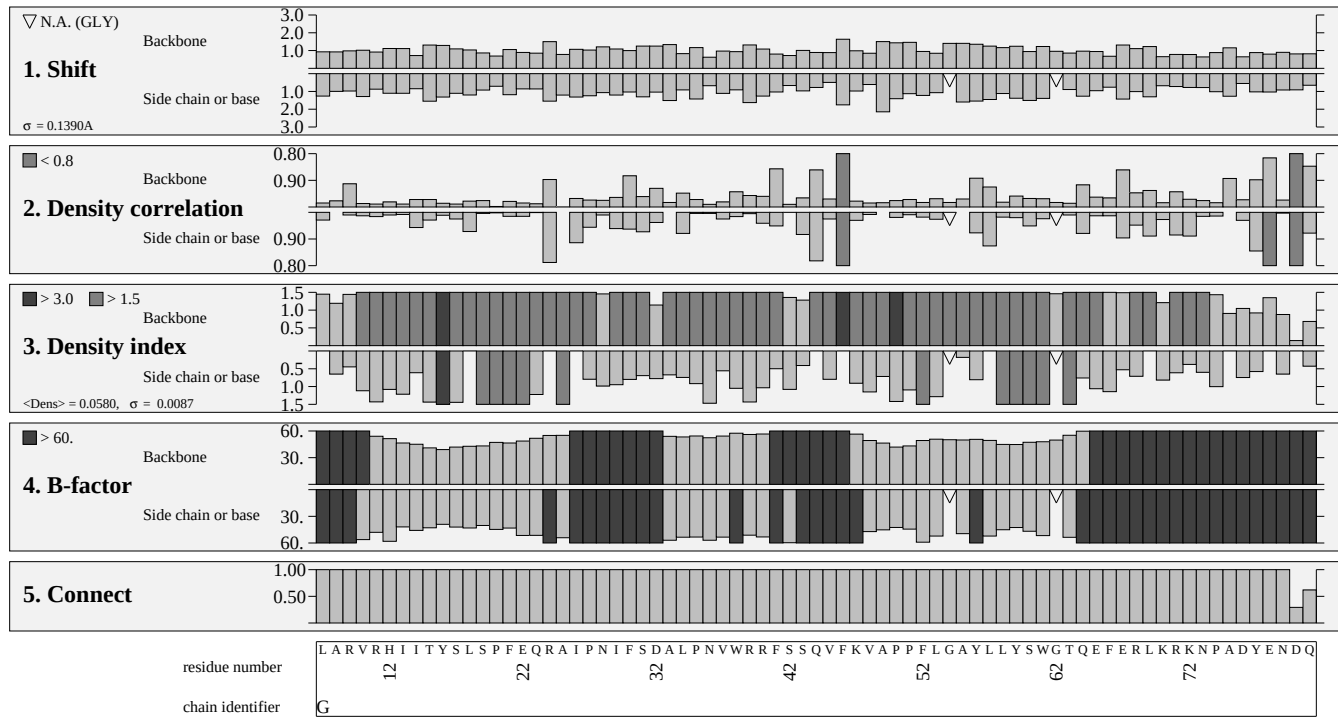
Local estimation (12)



Structure Factor Check

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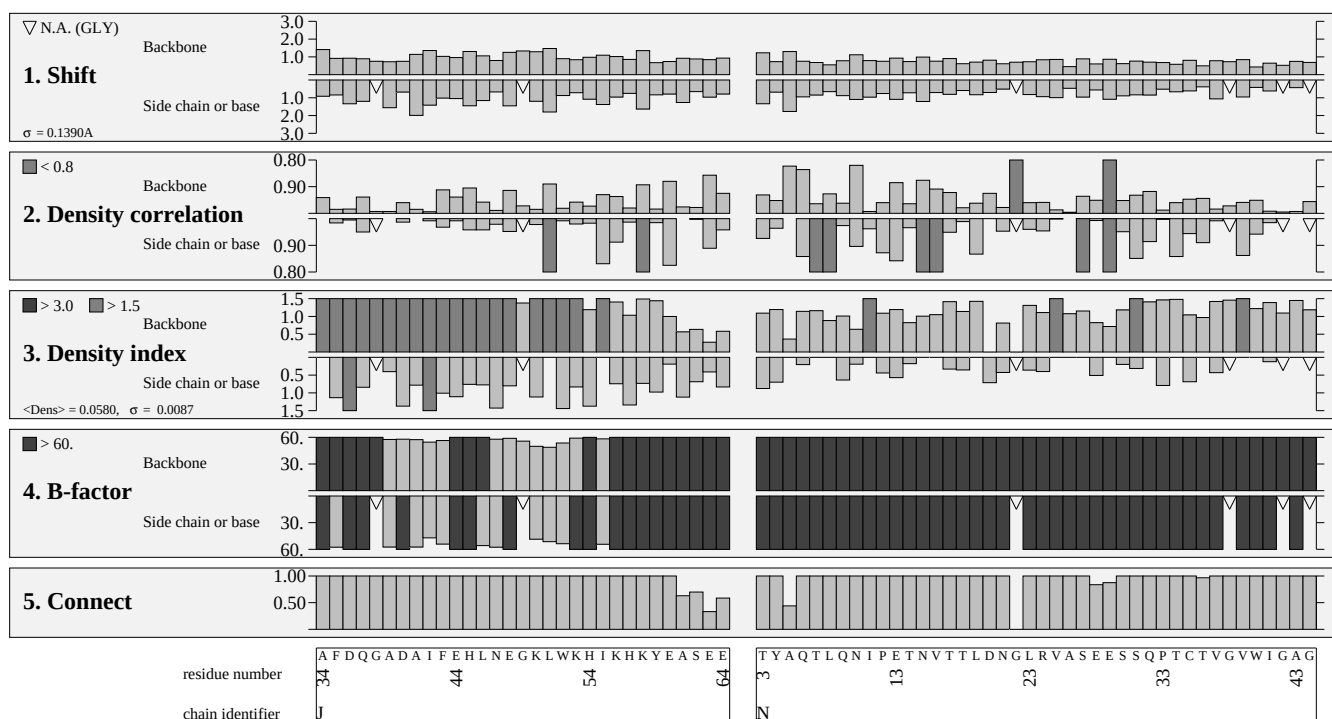
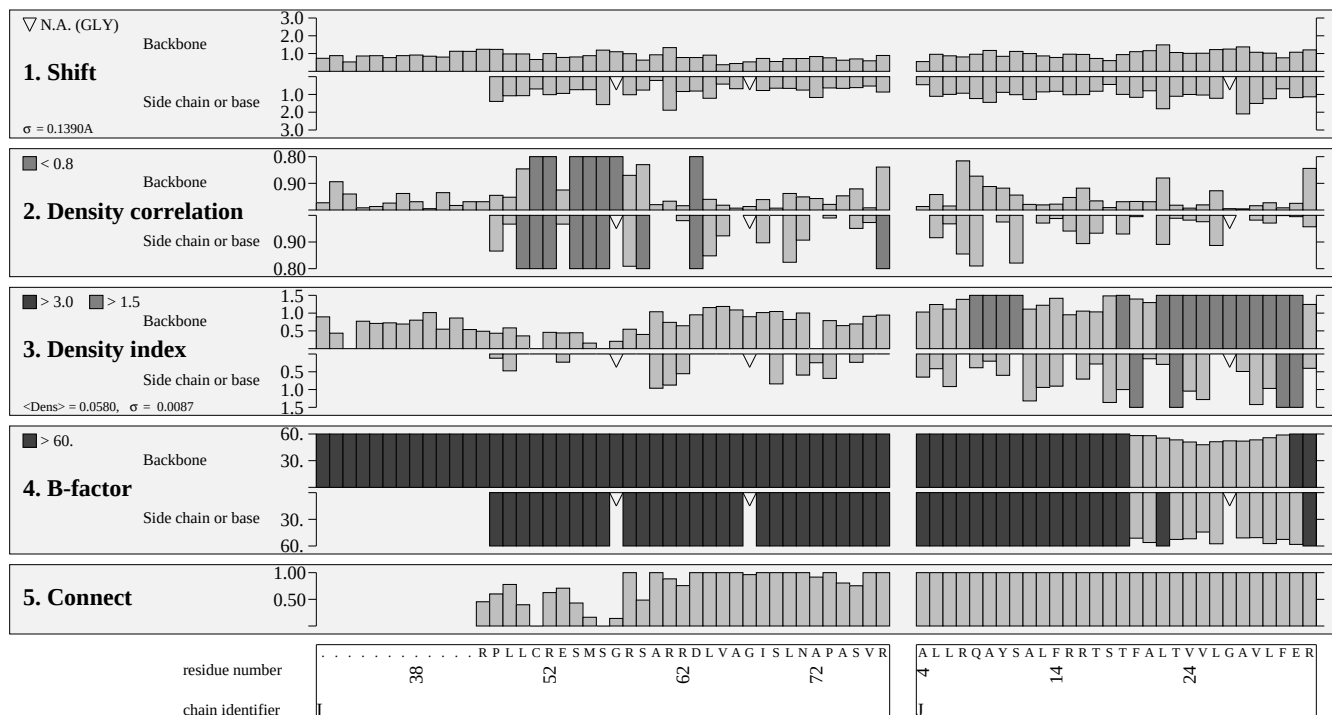
Local estimation (13)



Structure Factor Check

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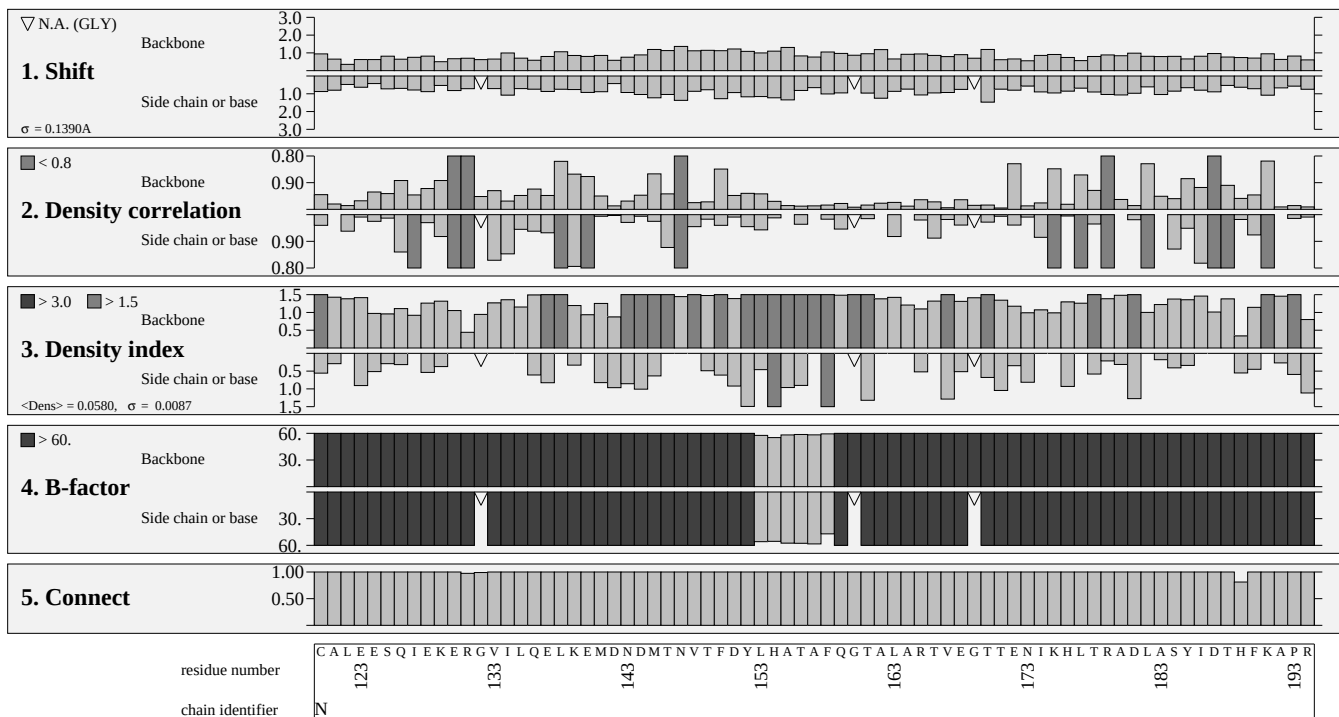
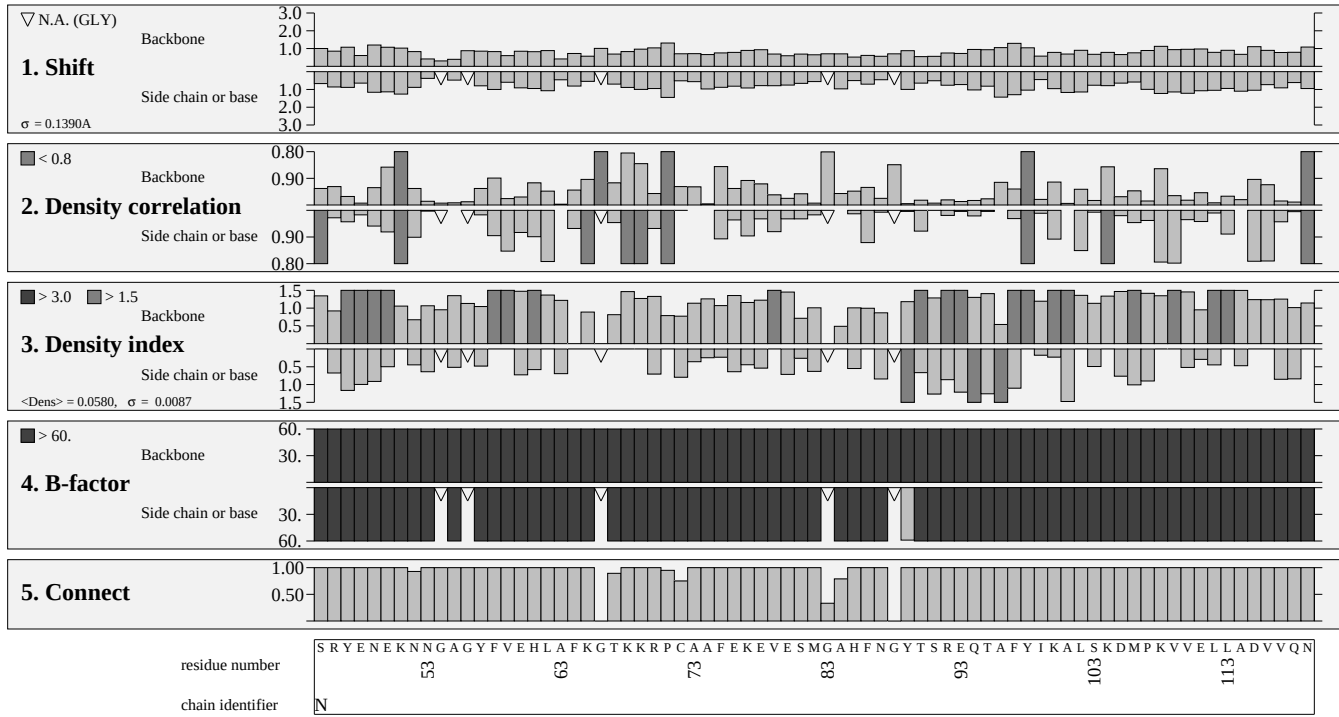
Local estimation (14)



Structure Factor Check

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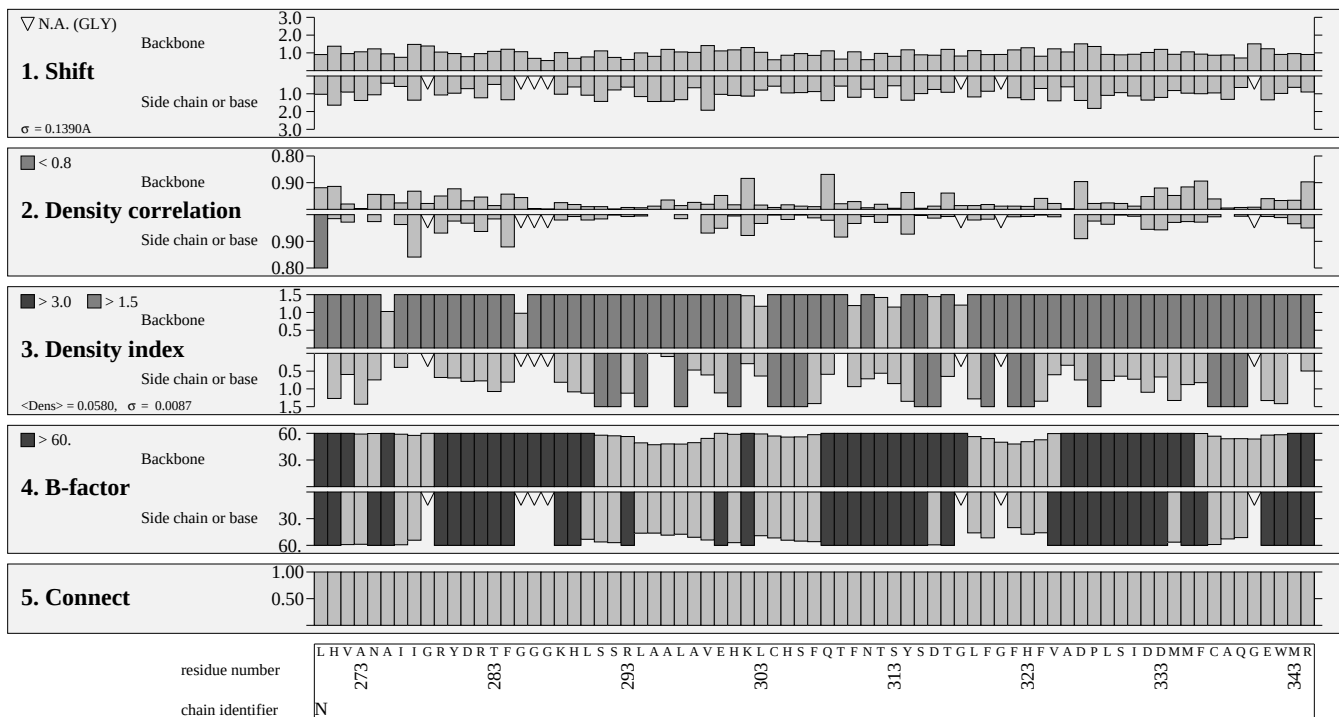
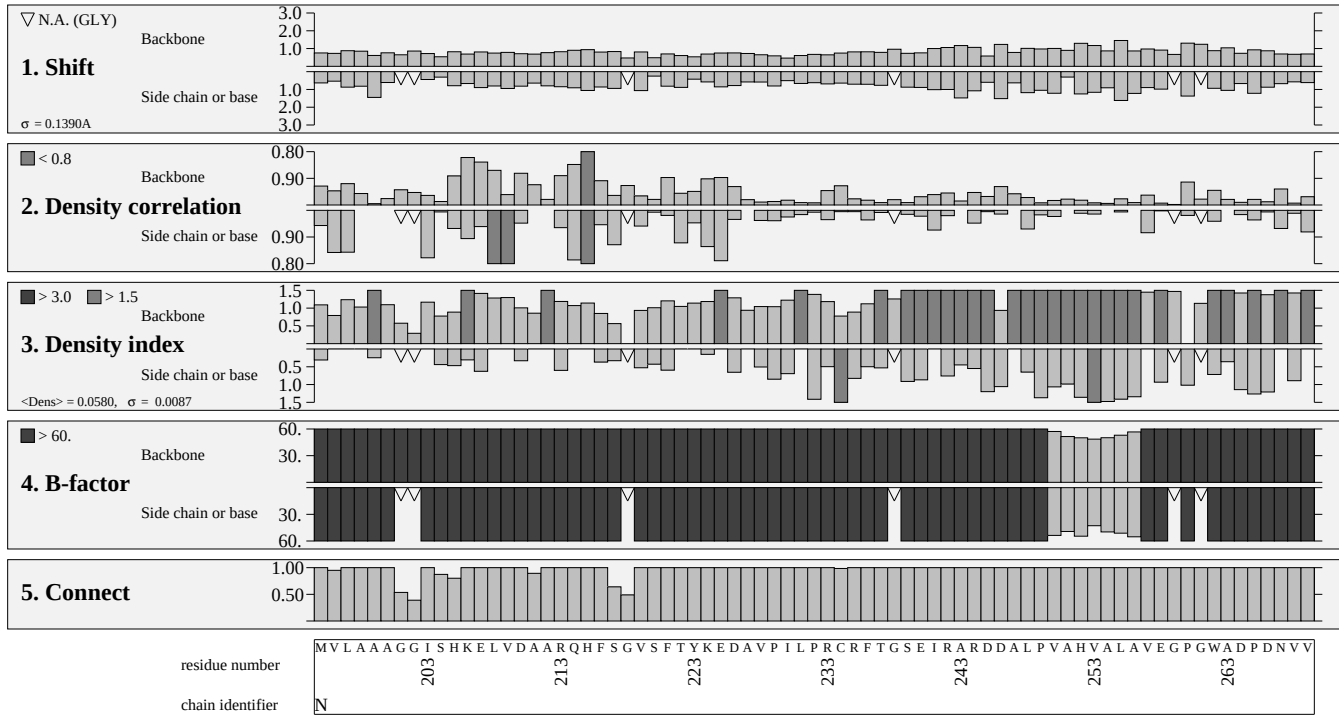
Local estimation (15)



Structure Factor Check

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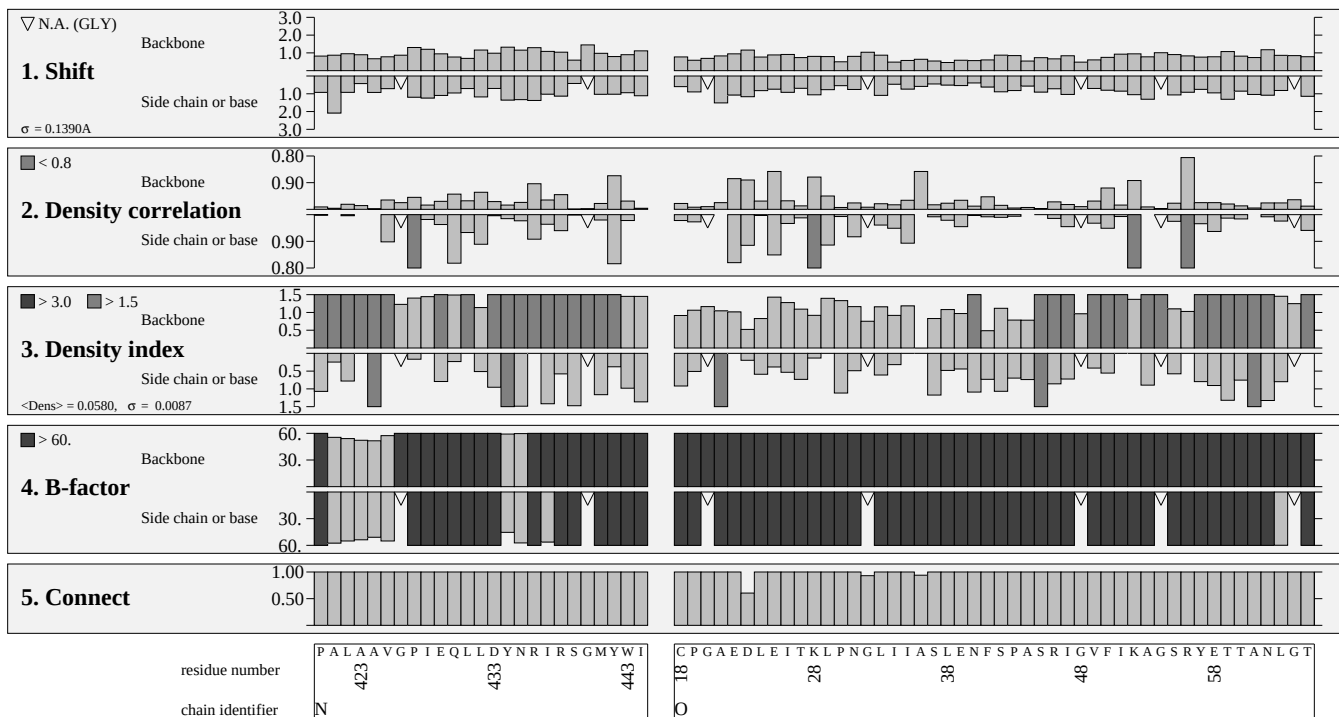
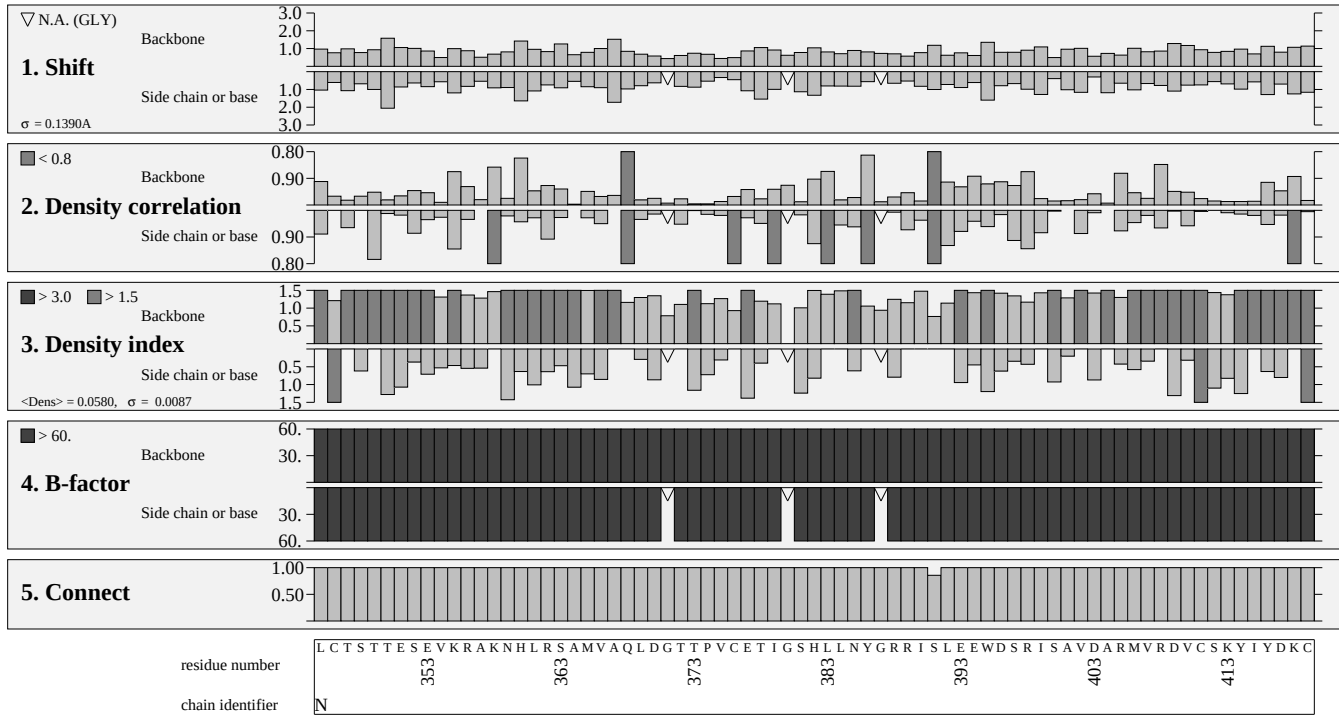
Local estimation (16)



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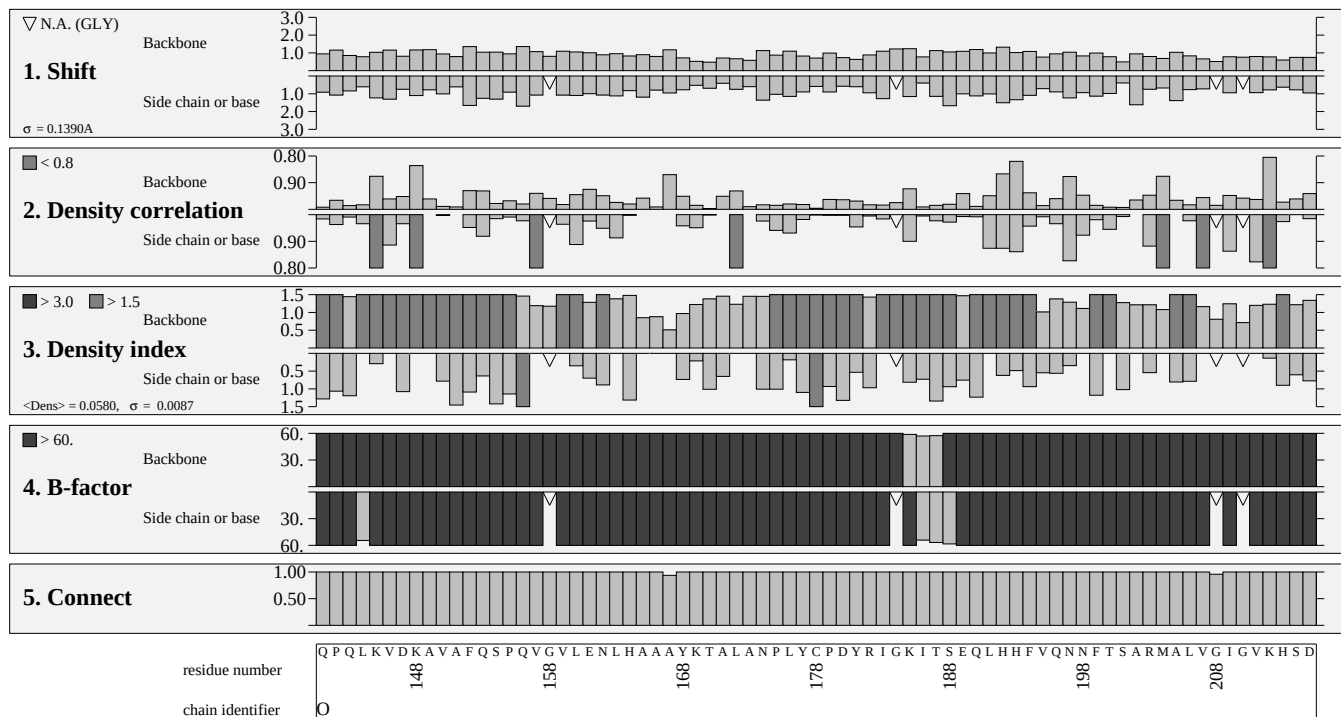
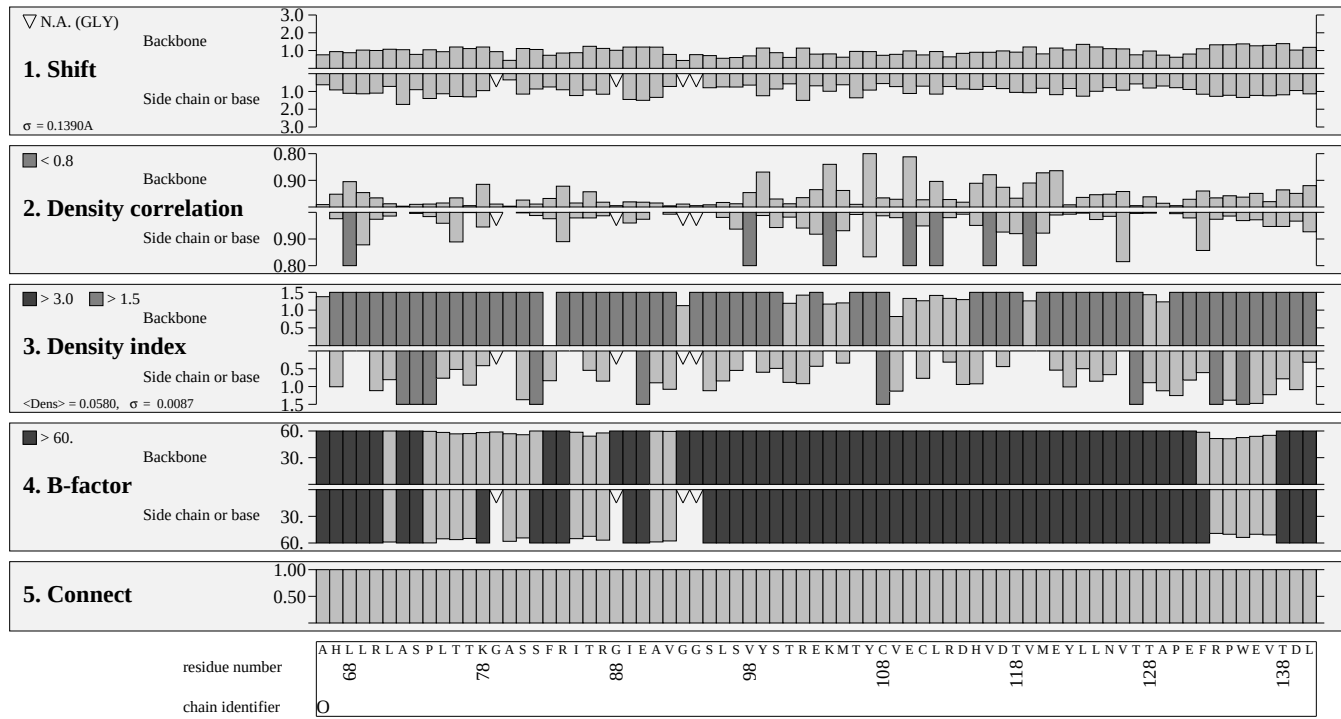
Local estimation (17)



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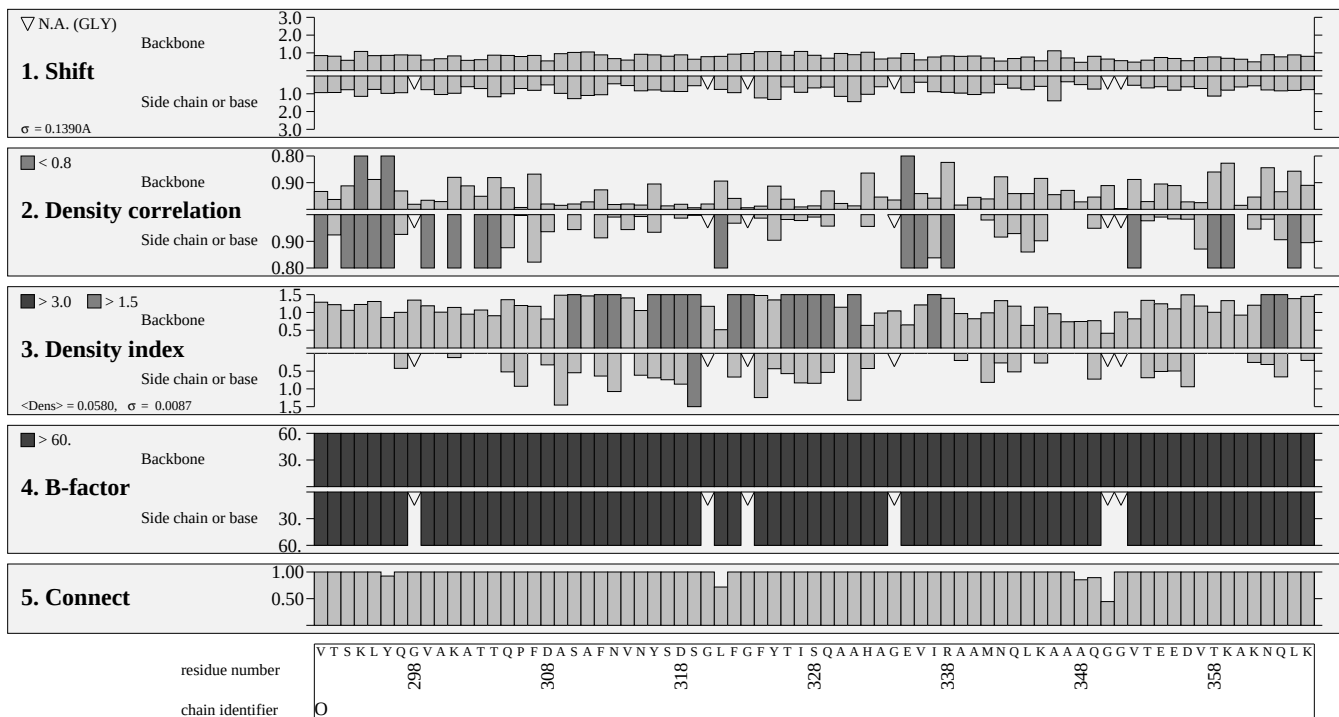
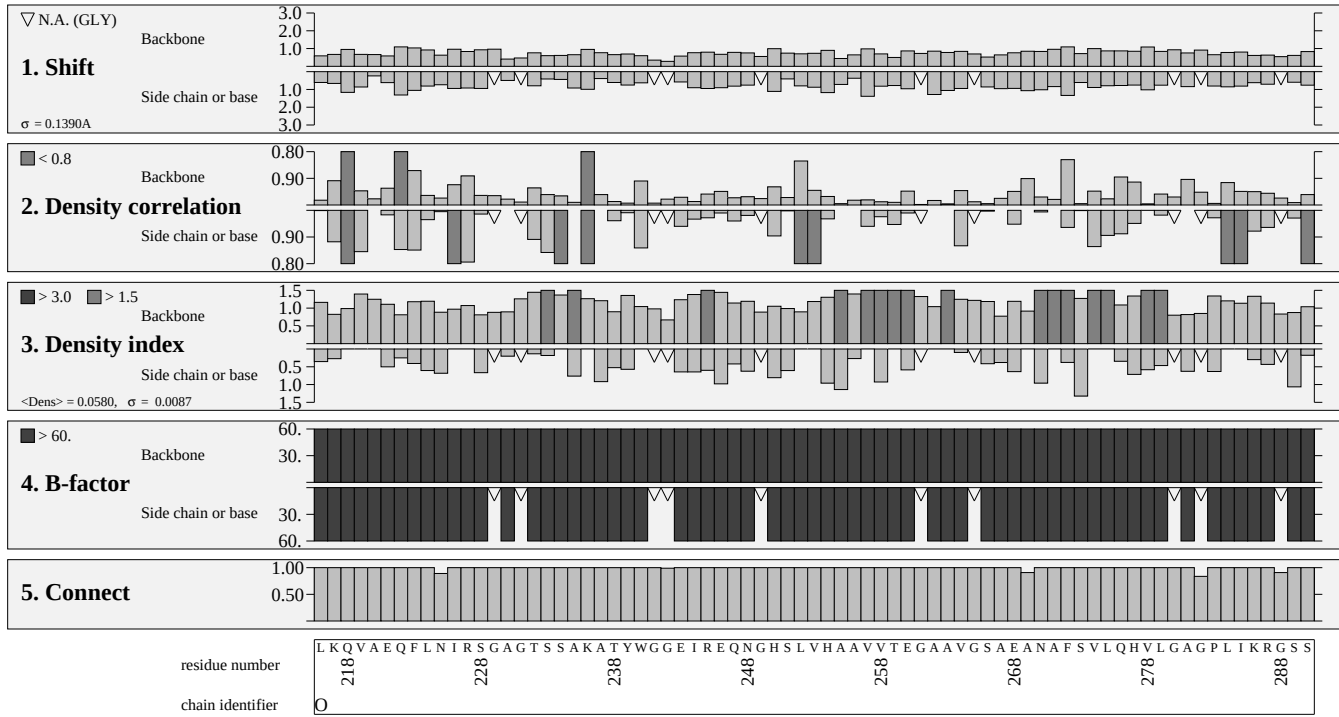
Local estimation (18)



Structure Factor Check

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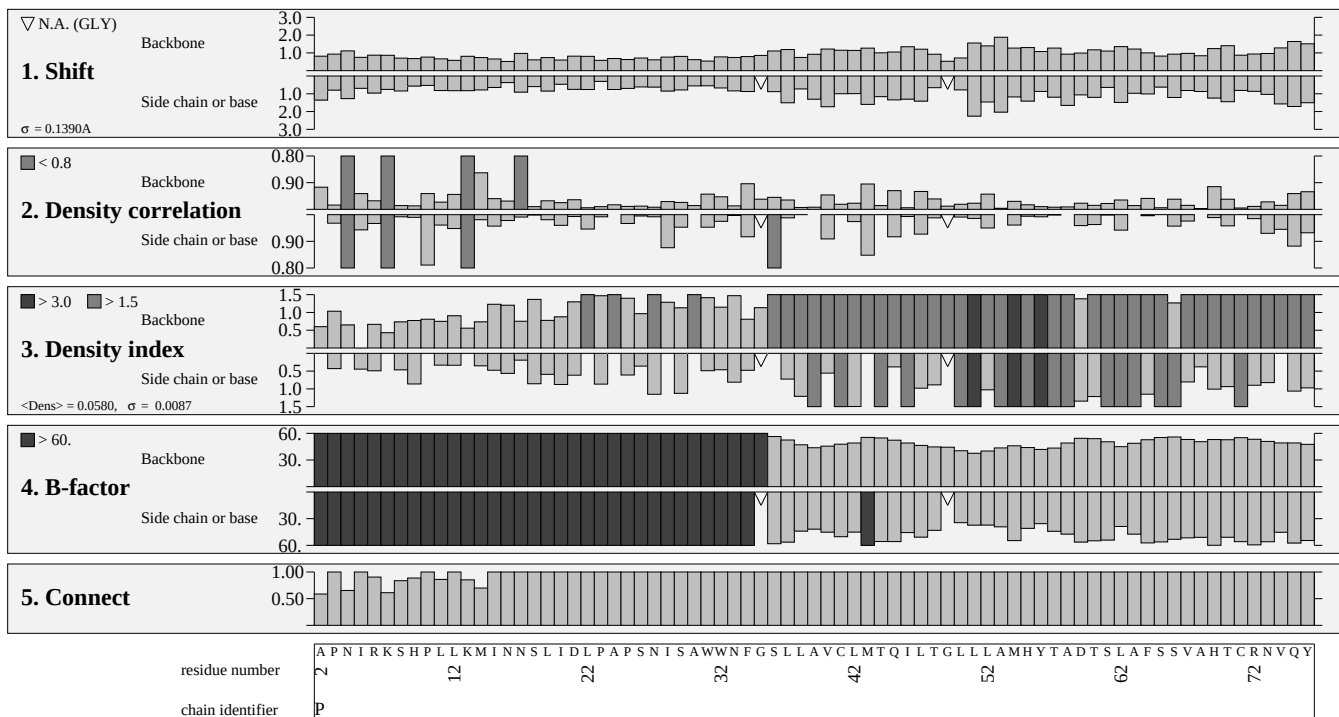
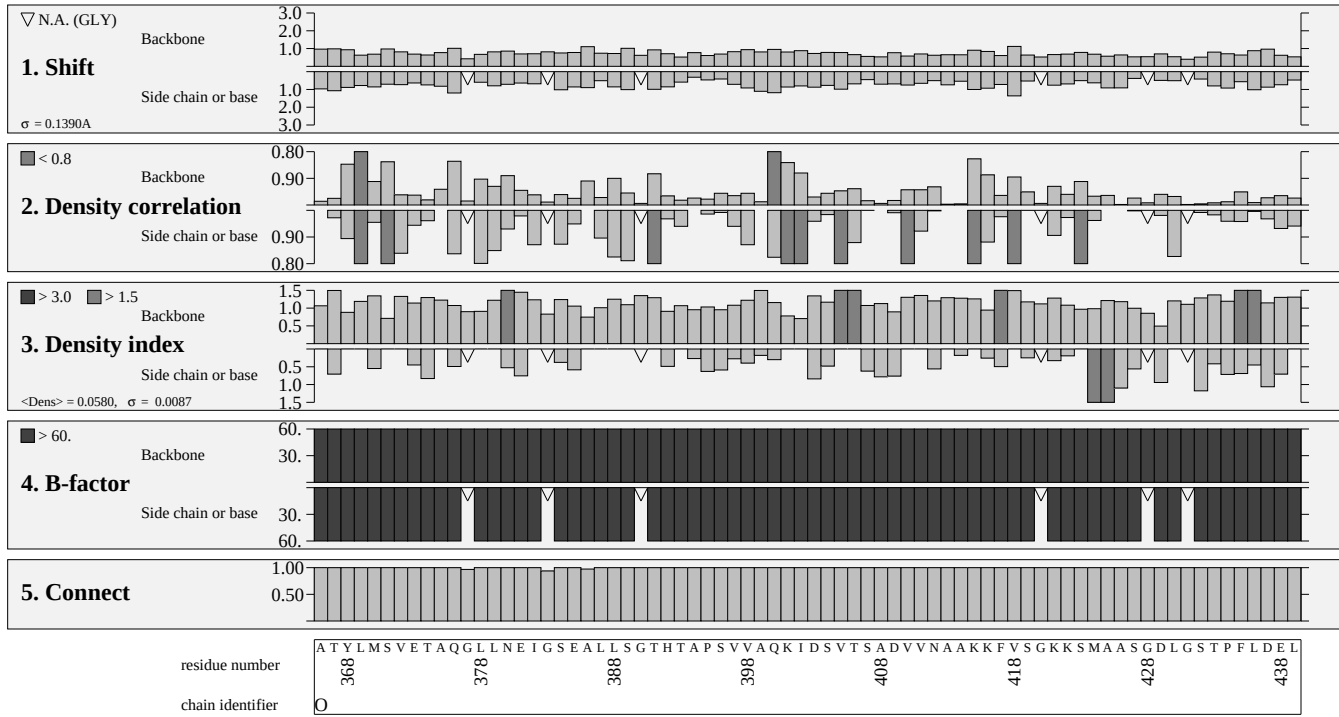
Local estimation (19)



Structure Factor Check

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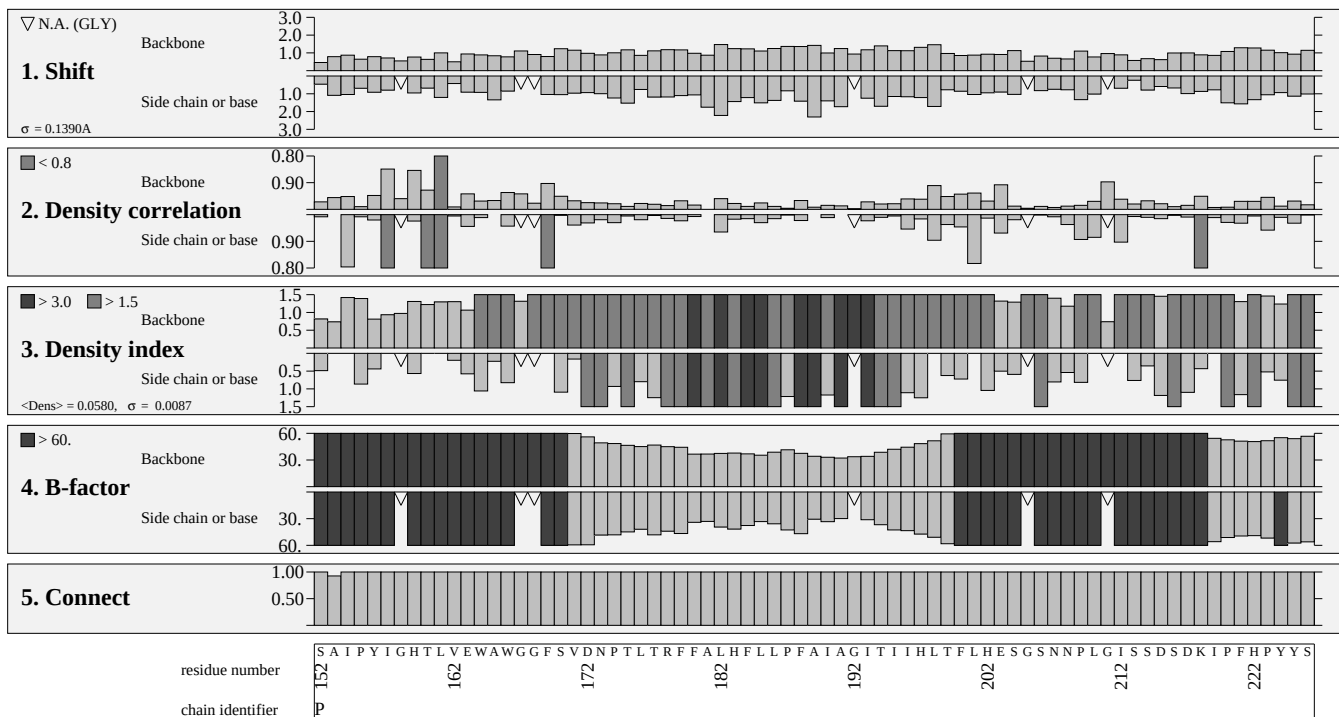
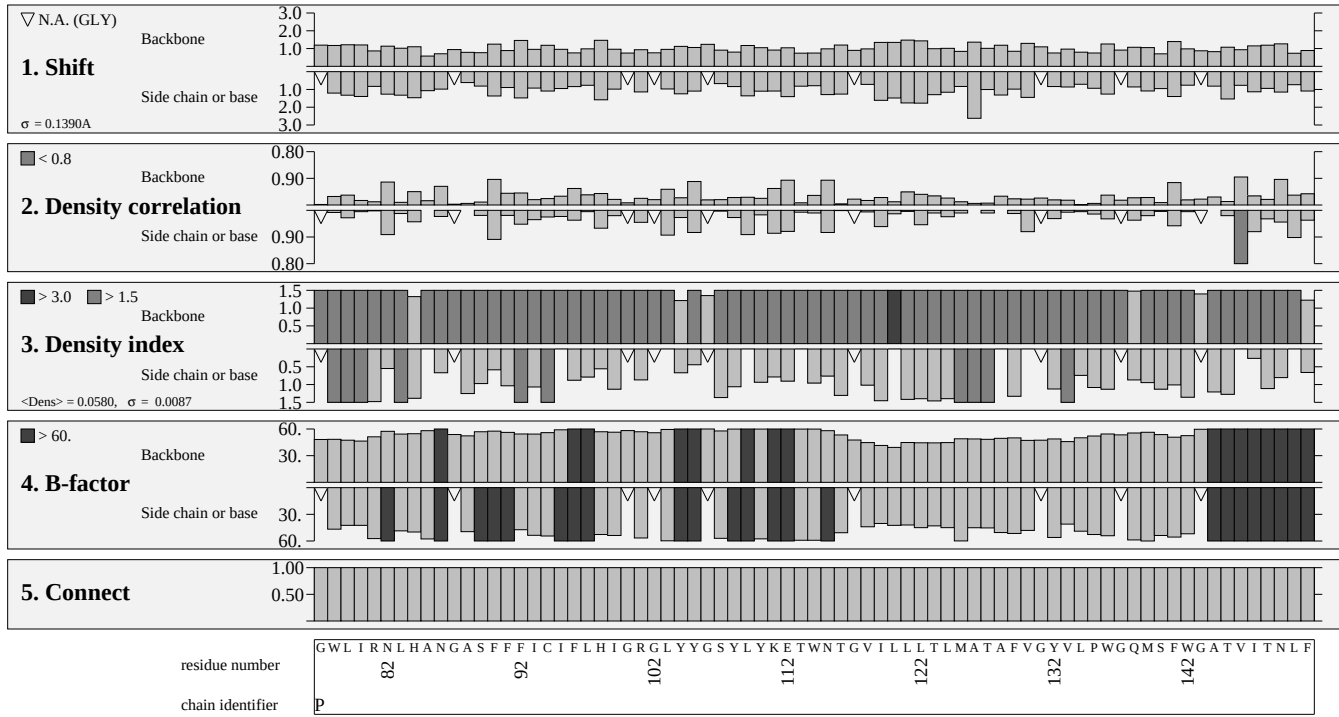
Local estimation (20)



Structure Factor Check

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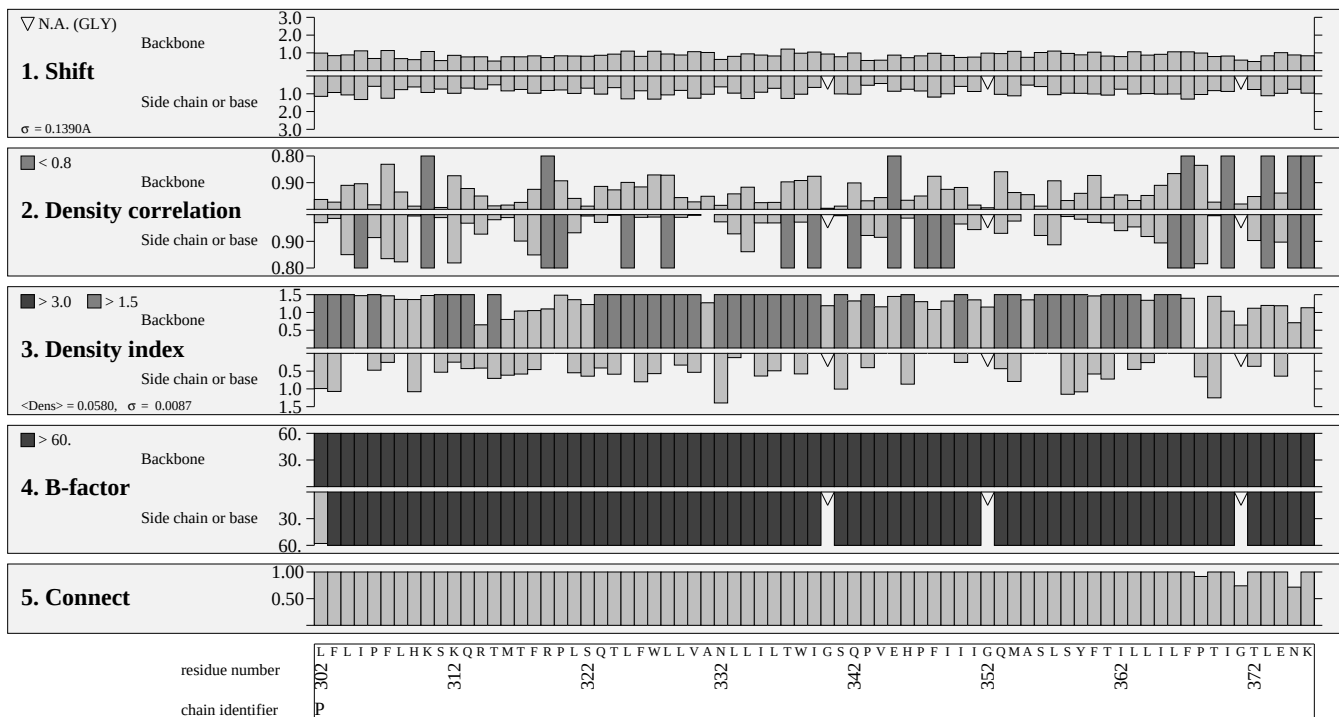
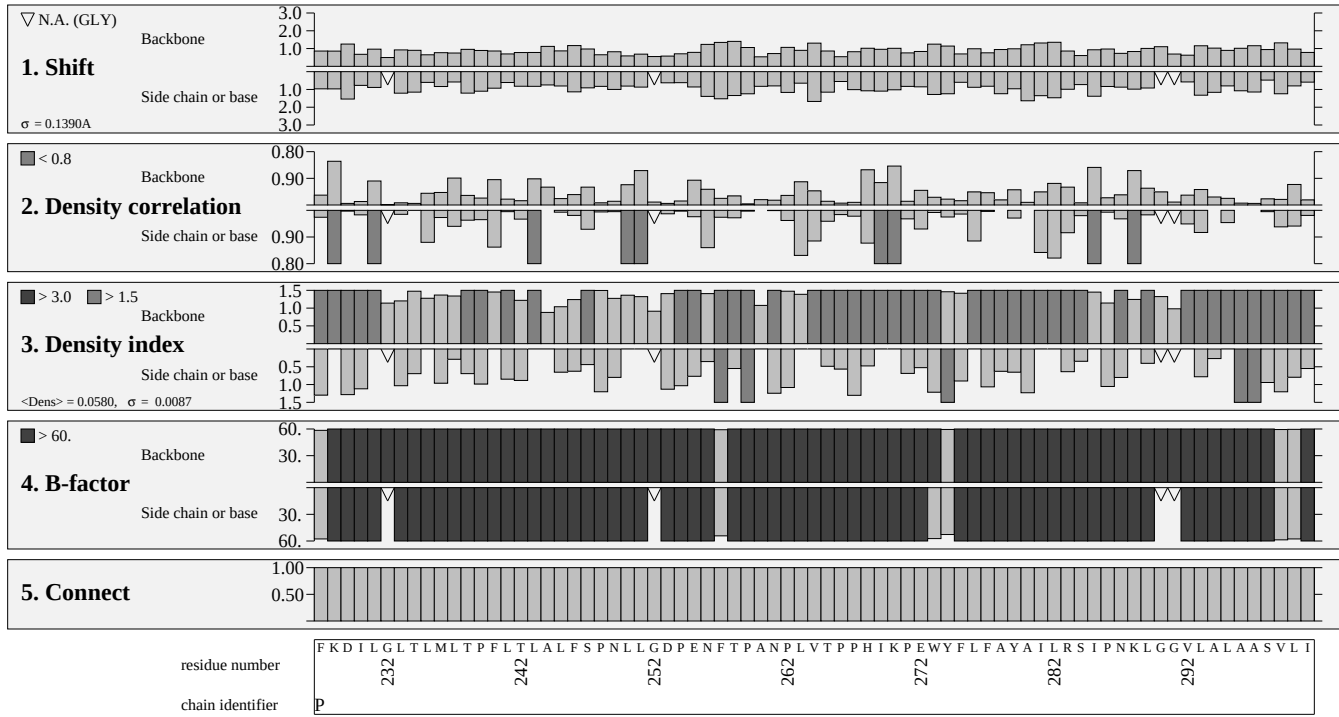
Local estimation (21)



Structure Factor Check

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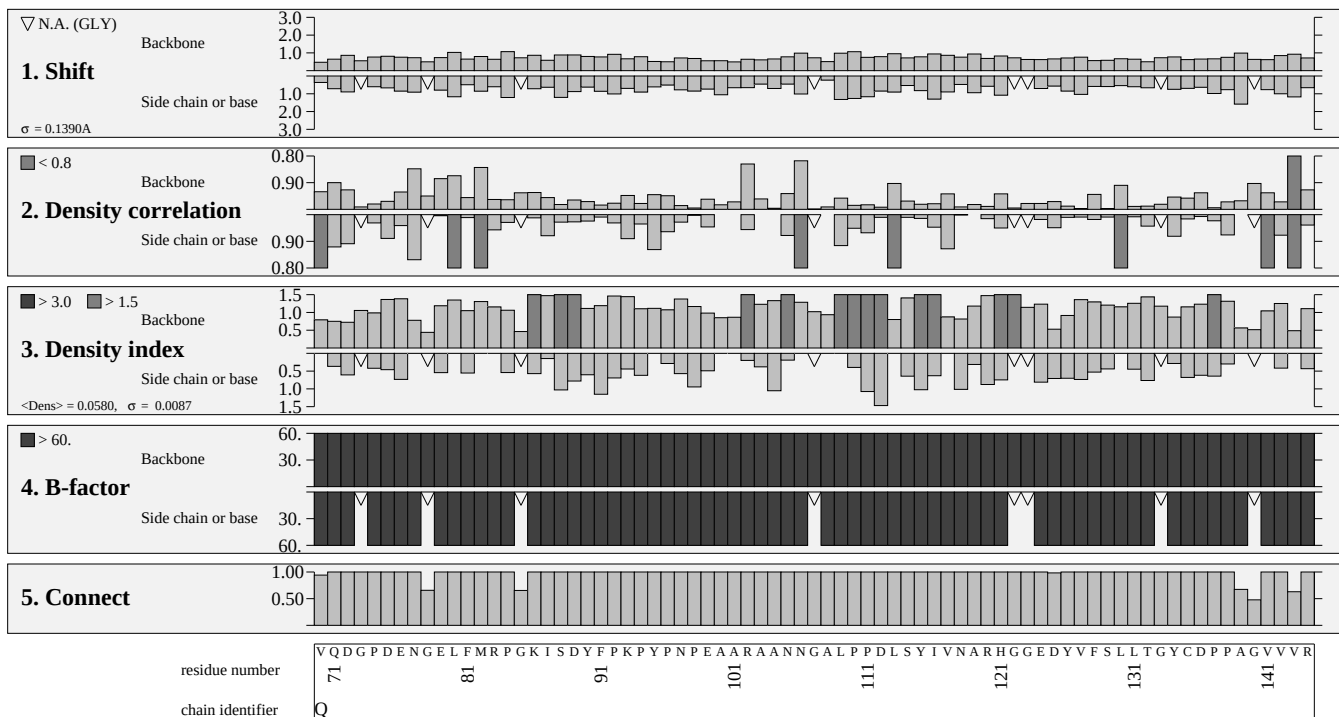
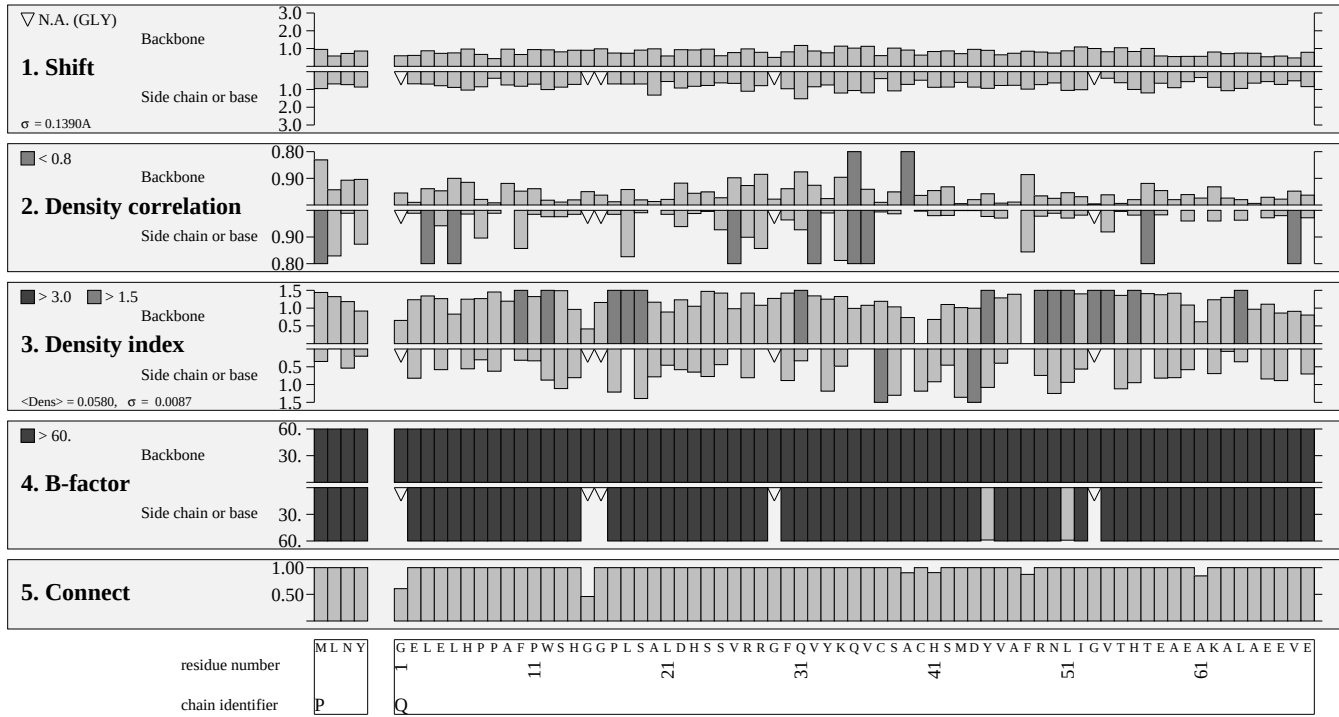
Local estimation (22)



Structure Factor Check

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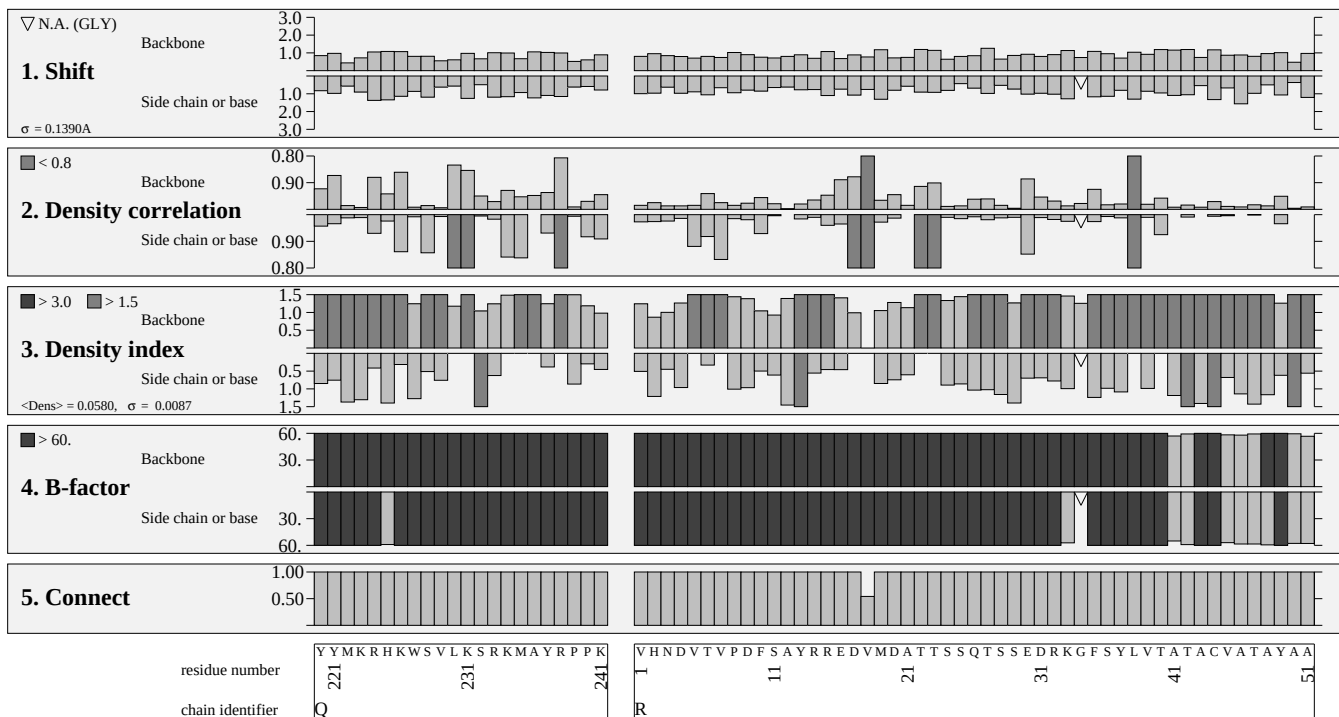
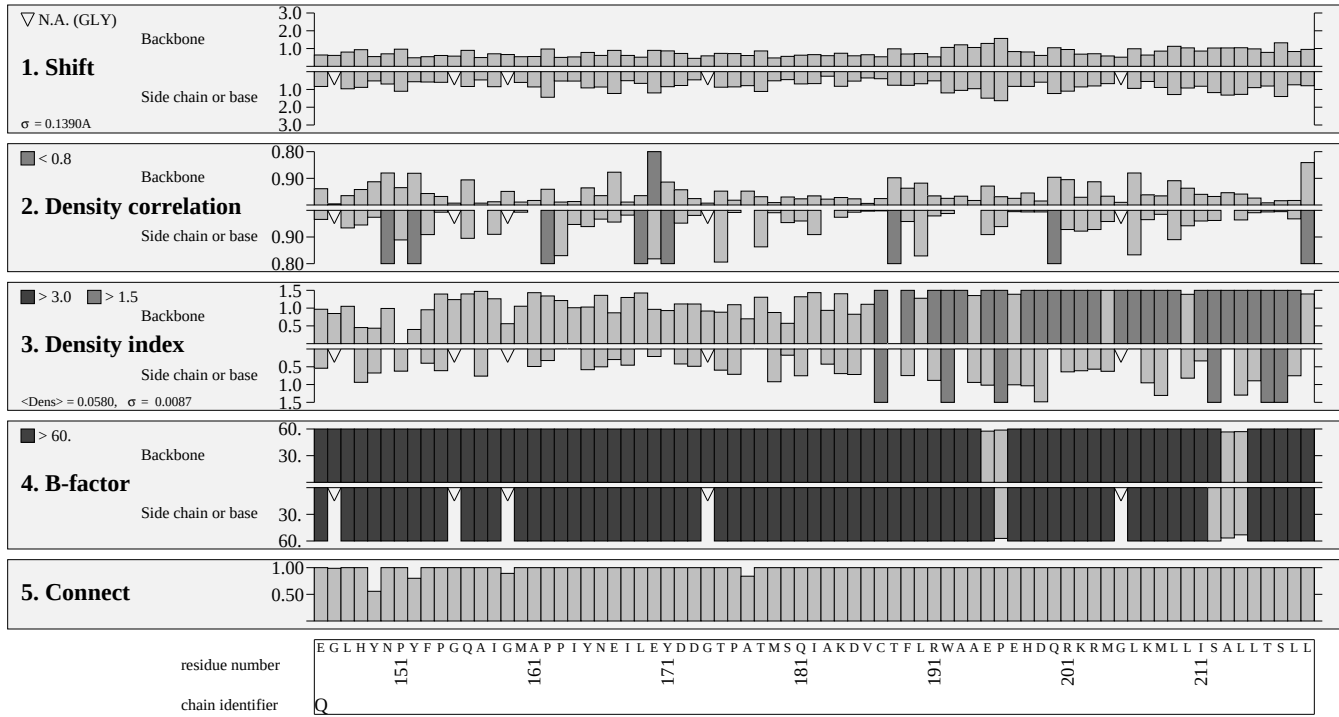
Local estimation (23)



Structure Factor Check

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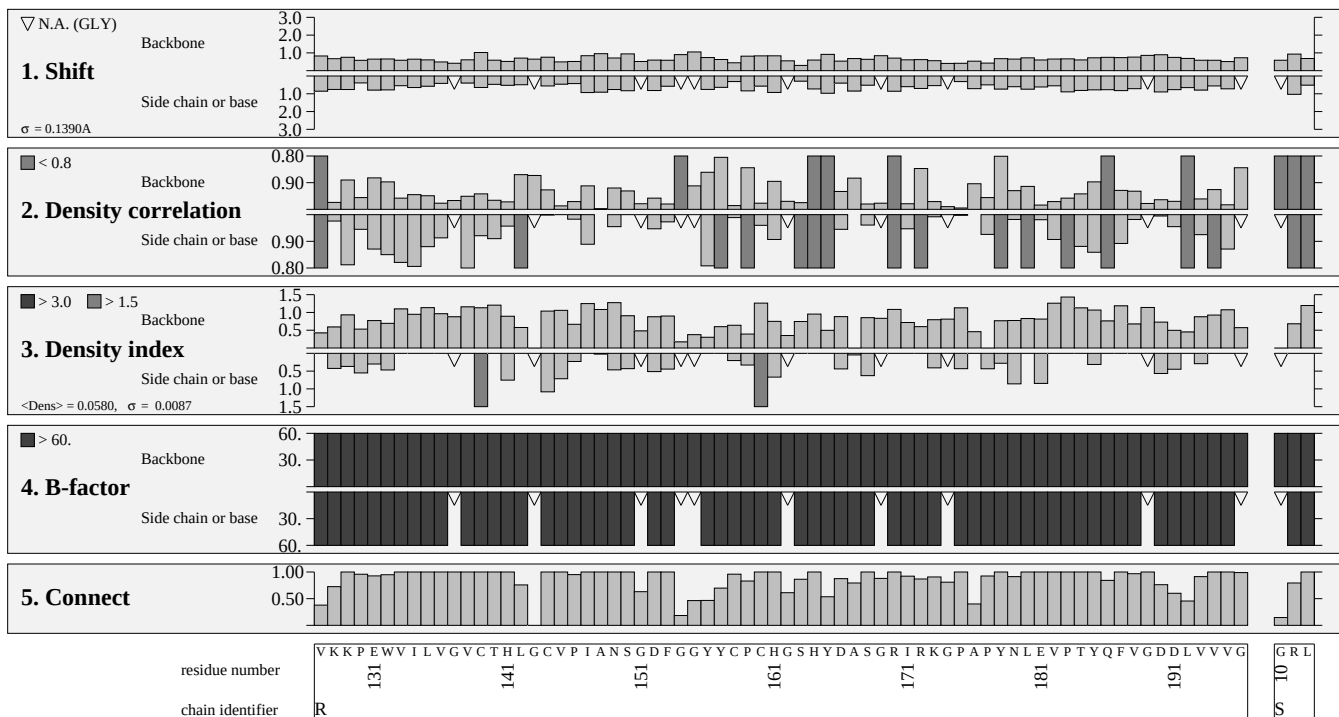
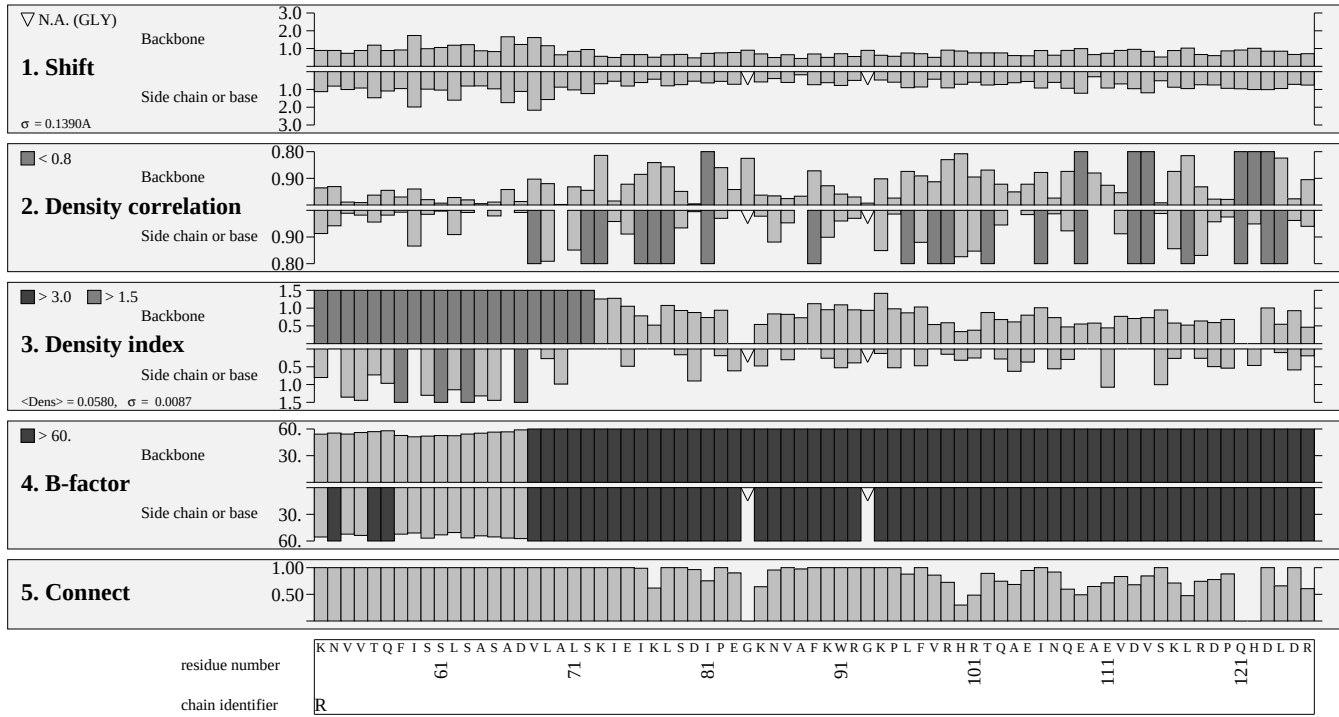
Local estimation (24)



Structure Factor Check

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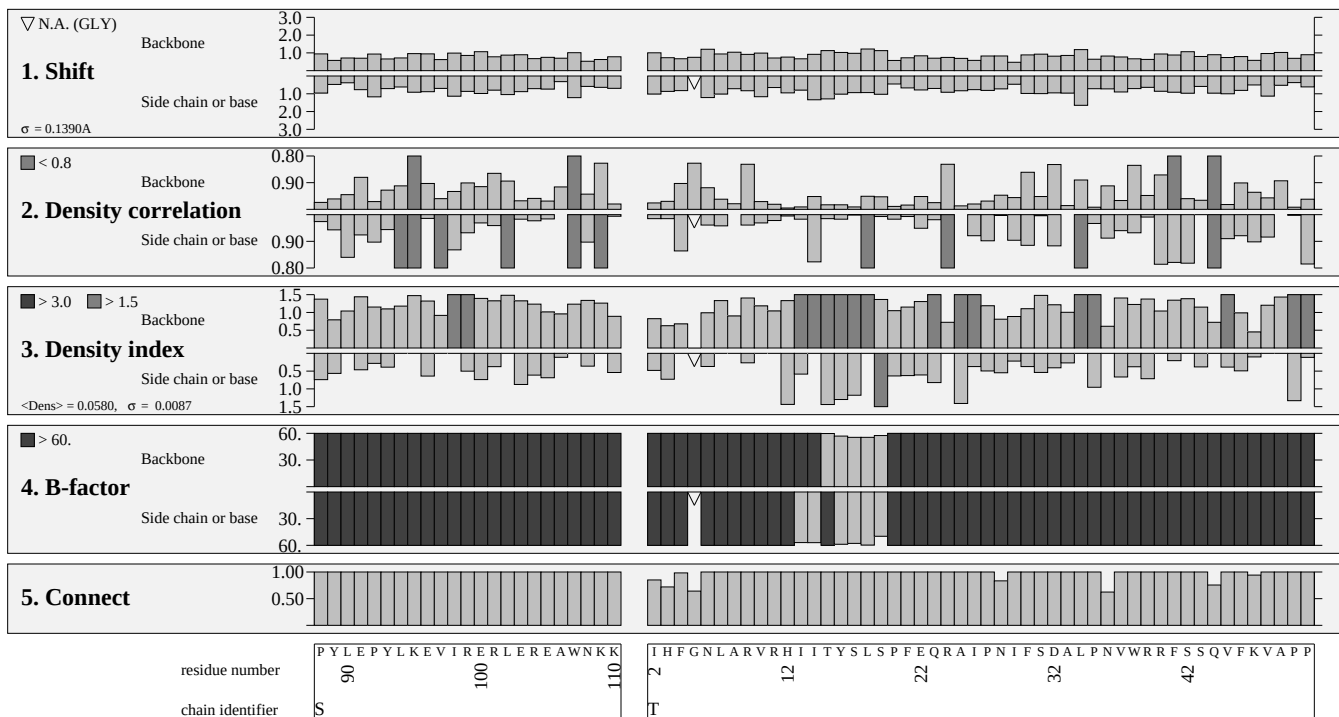
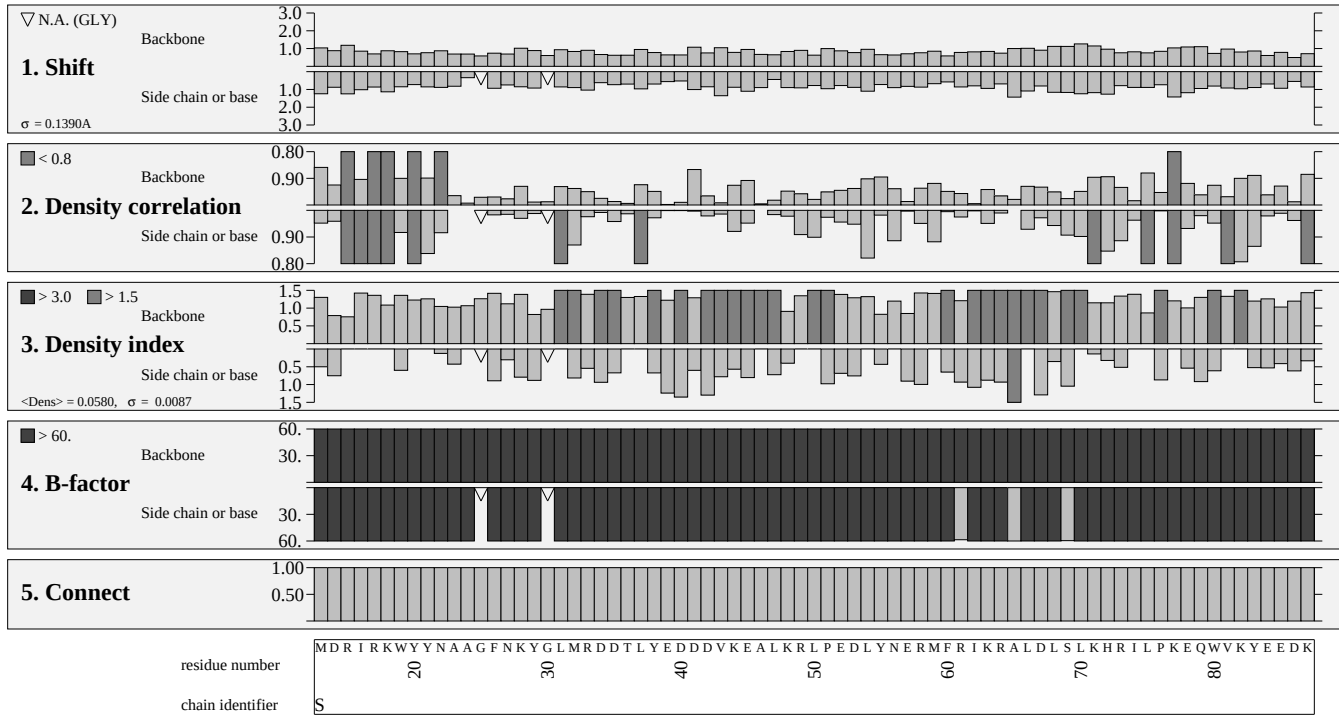
Local estimation (25)



Structure Factor Check

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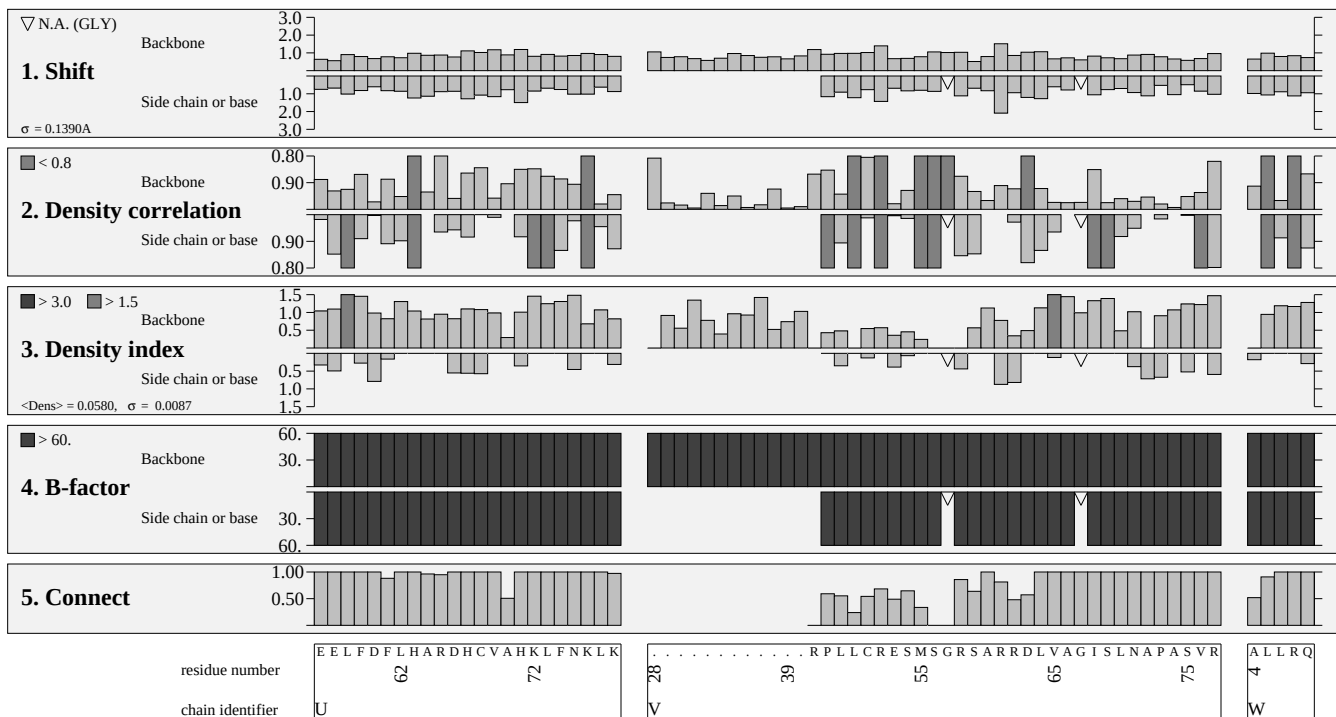
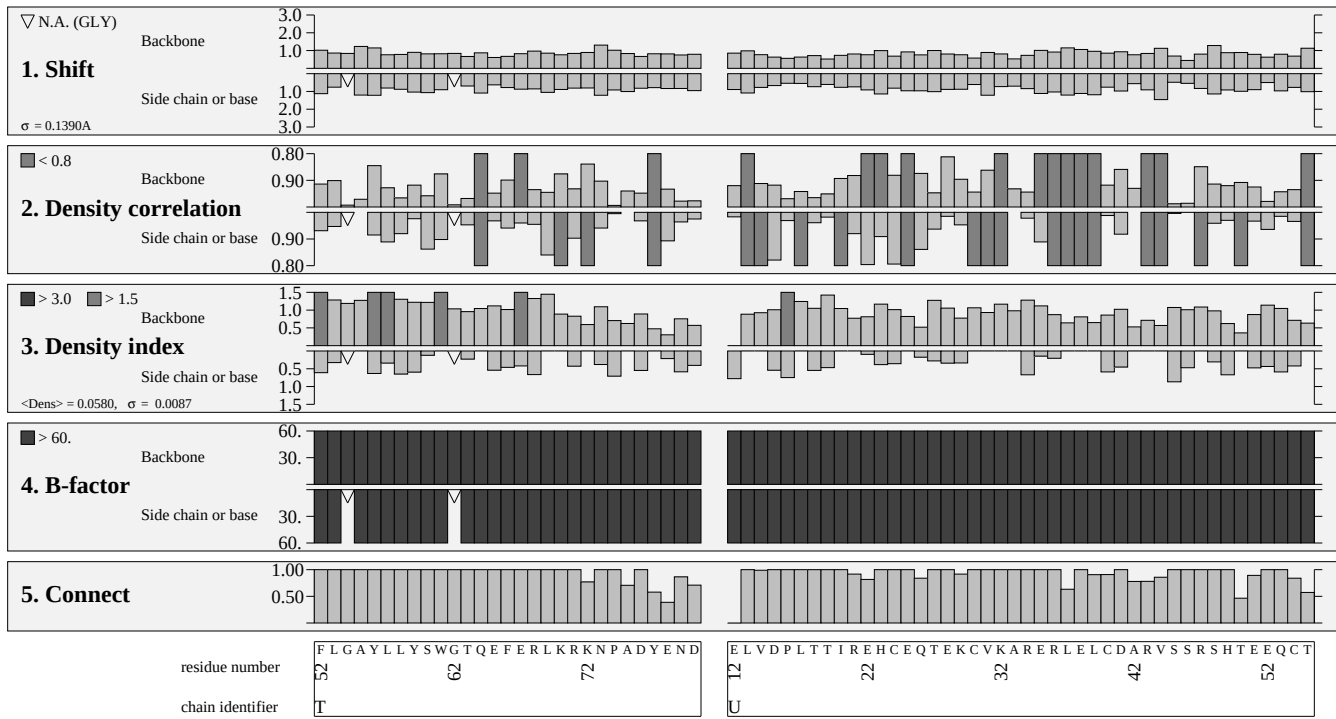
Local estimation (26)



Structure Factor Check

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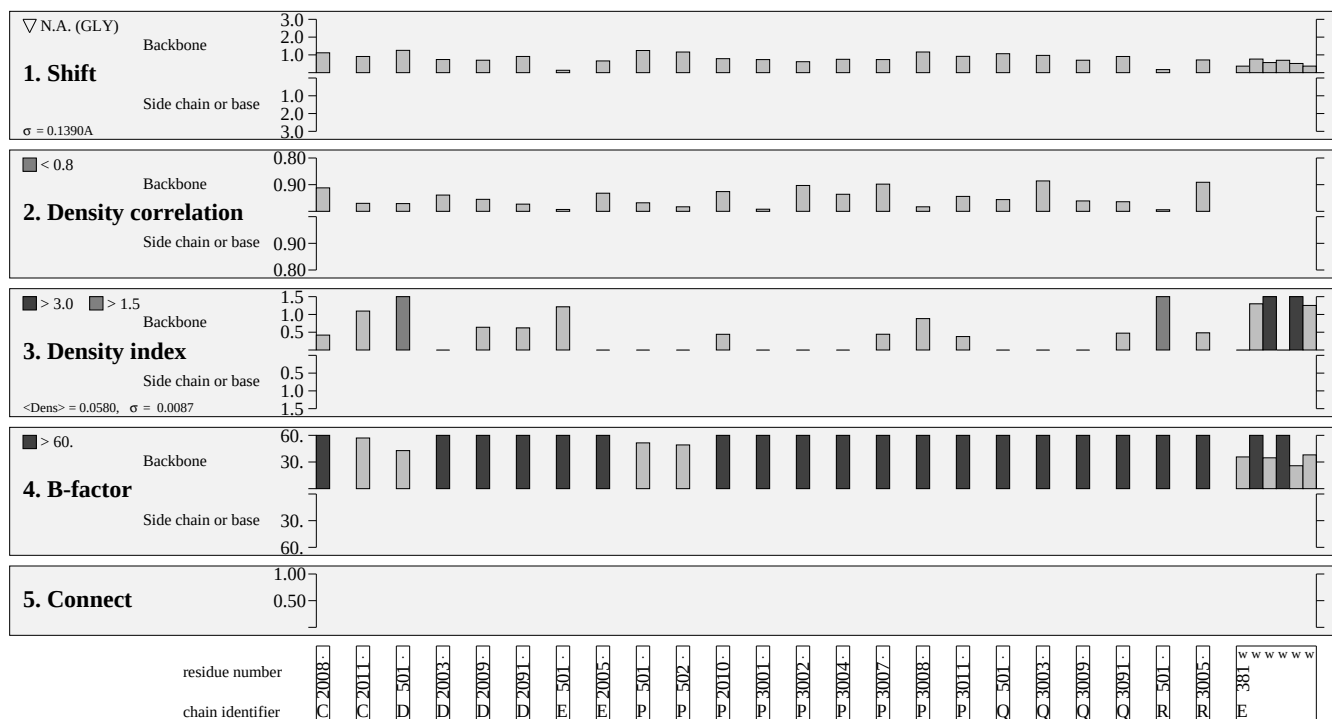
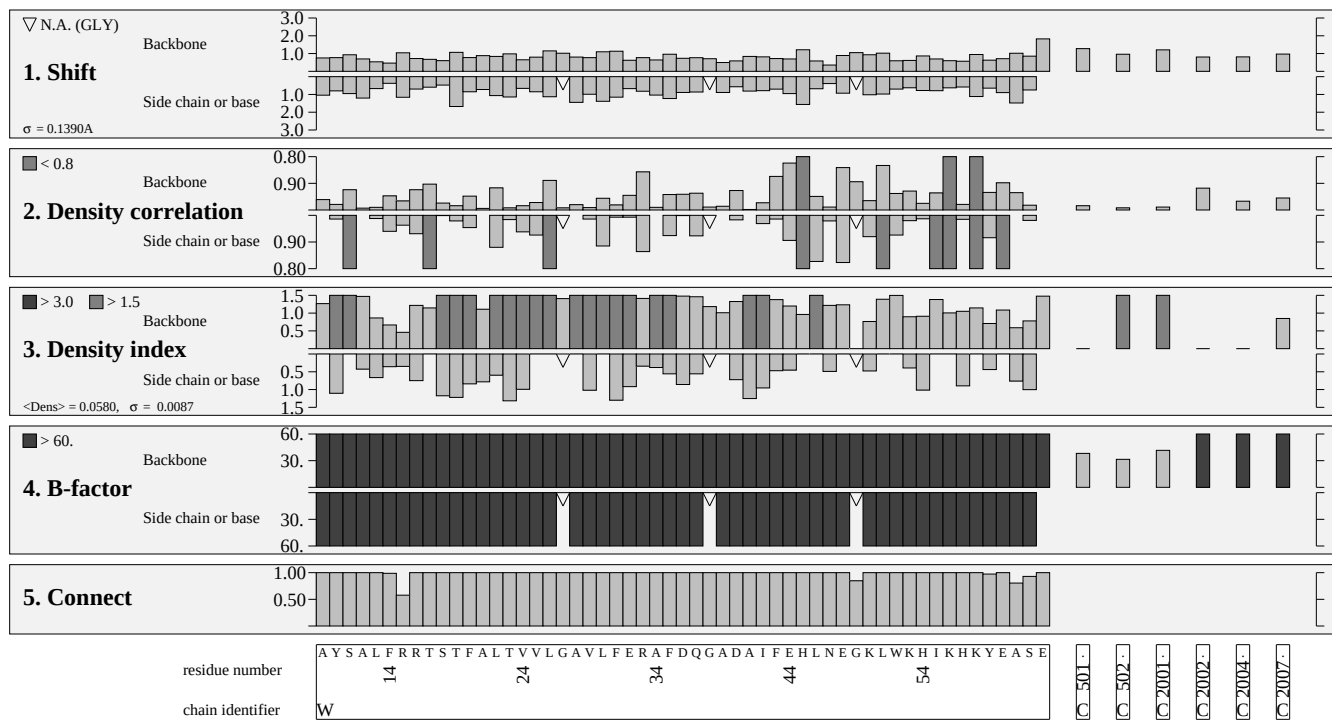
Local estimation (27)



Structure Factor Check

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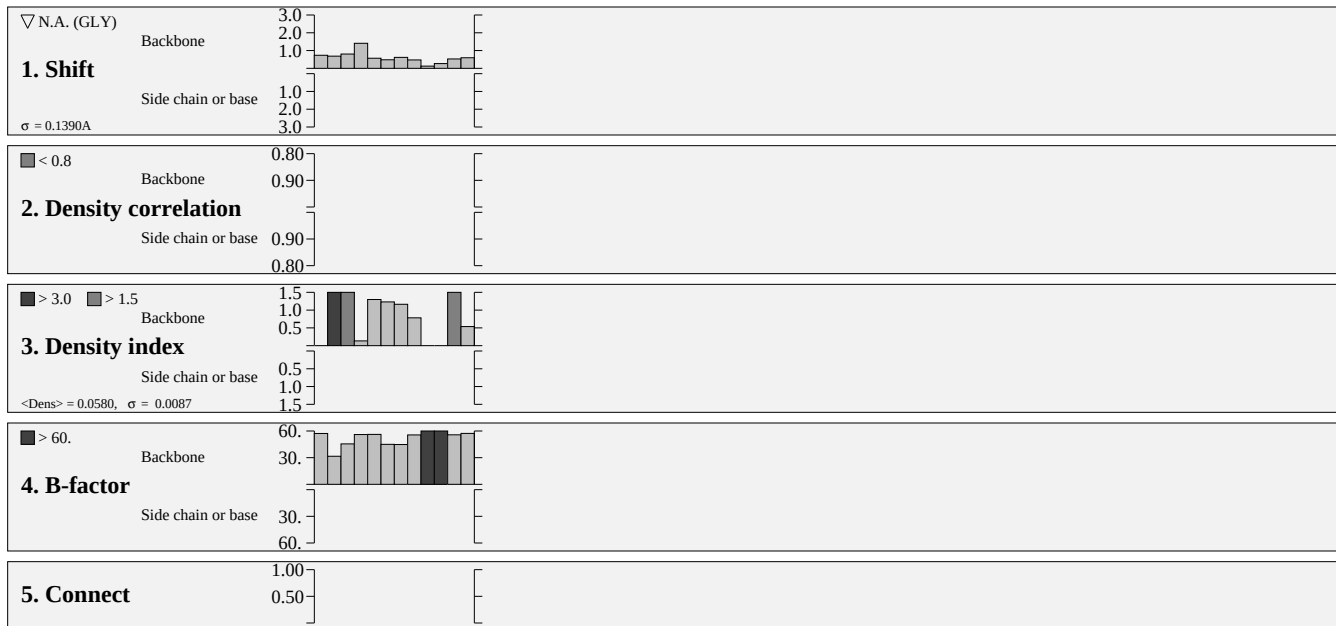
Local estimation (28)



Structure Factor Check

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Local estimation (29)



residue number

chain identifier

382
E