

Structure Factor Check

3L74

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH FAMOXADONE BOUND
 Date: 28-DEC-09
 PDB code: 3L74

Crystal

Cell parameters:

a: 171.89 Å b: 181.69 Å c: 240.75 Å
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 58.7 – 2.70 Å
 Reflections in file: 199233
 Unique reflections above 0: 199233
 above 1 σ : 194835
 above 3 σ : 123637

SF CHECK

Nominal resolution range: 58.7 – 2.76 Å
 \05max. from input data, min. from author\05
 Used reflections: 189274
 Reflections out of resolution: 9959
 Completeness: 98.0 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.076
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.5632 0.7439
 B_{overall} (by Patterson): 45. Å²
 Optical resolution: 2.06 Å
 Expected opt. resol. for complete data set: 2.06 Å
 Estimated minimal error: 0.076 Å

Model

32703 atoms (28 water molecules)

Number of chains: 51
 Volume not occupied by model: 62.5 %
 $\langle B \rangle$ (for atomic model): 61.9 Å²
 $\sigma(B)$: 21.35 Å²
 Matthews coefficient: 4.11
 Corresponding solvent % : 69.81

Model vs. Structure Factors

R-factor for all reflections: 0.296
 Correlation factor: 0.857
 R-factor: 0.299
 for $F > 2.0 \sigma$
 nom. resolution range: 58.66 – 2.76 Å
 reflections used: 185359
 R_{free} : 0.319
 N_{free} : 3624
 R -factor without free-refl.: 0.299
 Non free-reflections: 181735
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.451 Å
 Estimated maximal error: 0.246 Å
 DPI: 0.315 Å

Refinement

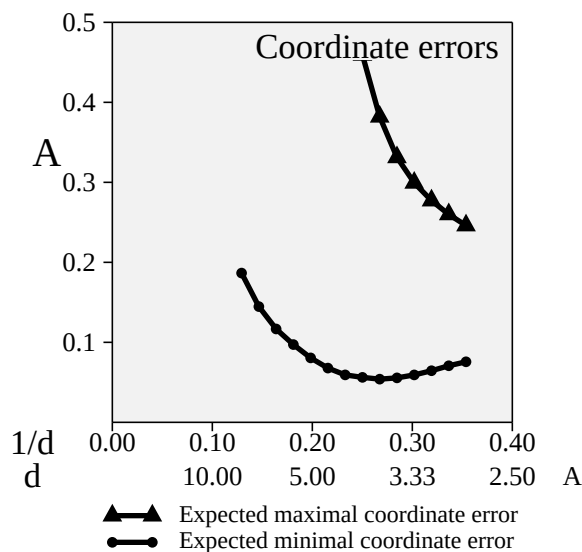
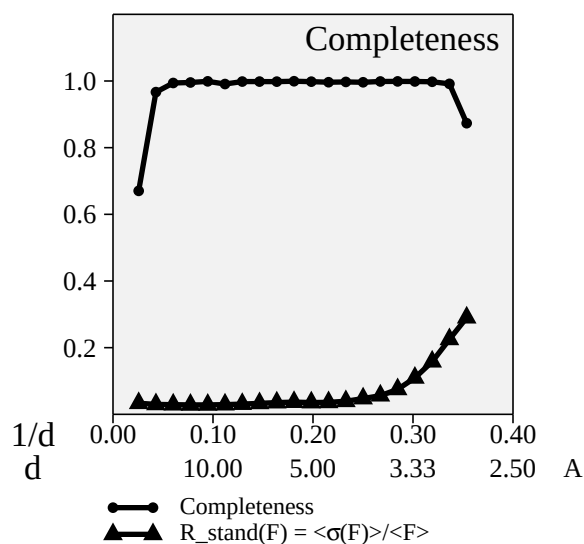
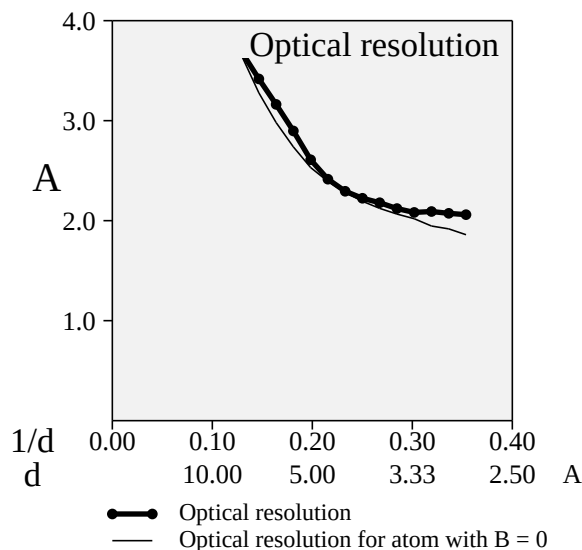
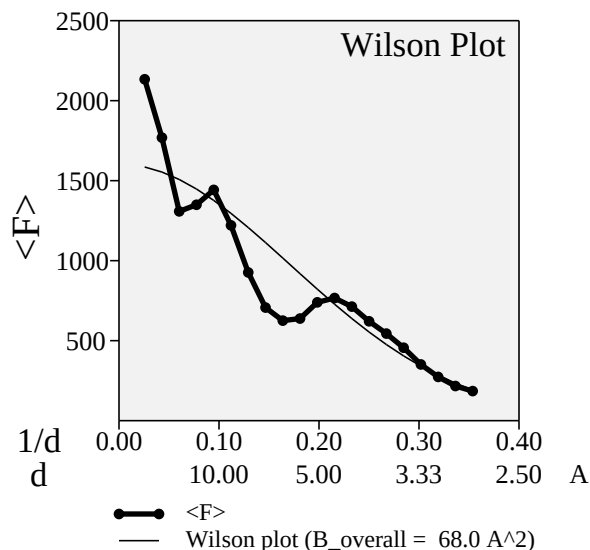
Program: CNS 1.1
 Nominal resolution range: 58.7 – 2.76 Å
 Reported R -factor: 0.259
 Number of reflections used: 189275
 Reported R_{free} : 0.29
 Sigma cut-off: N.A.

Scaling

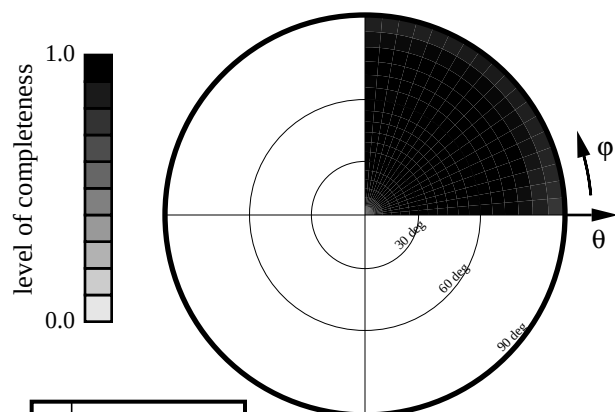
Scale: 0.528
 B_{diff} : -6.52
 Anisothermal Scaling (Beta):
 6.7161 -2.6140 1.8346 0.0000 0.0000 0.0000
 Solvent correction – K_s, B_s : 0.710 250.093

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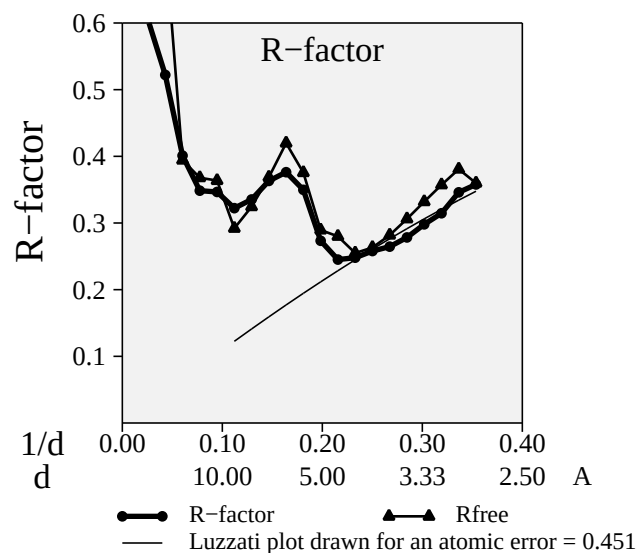


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

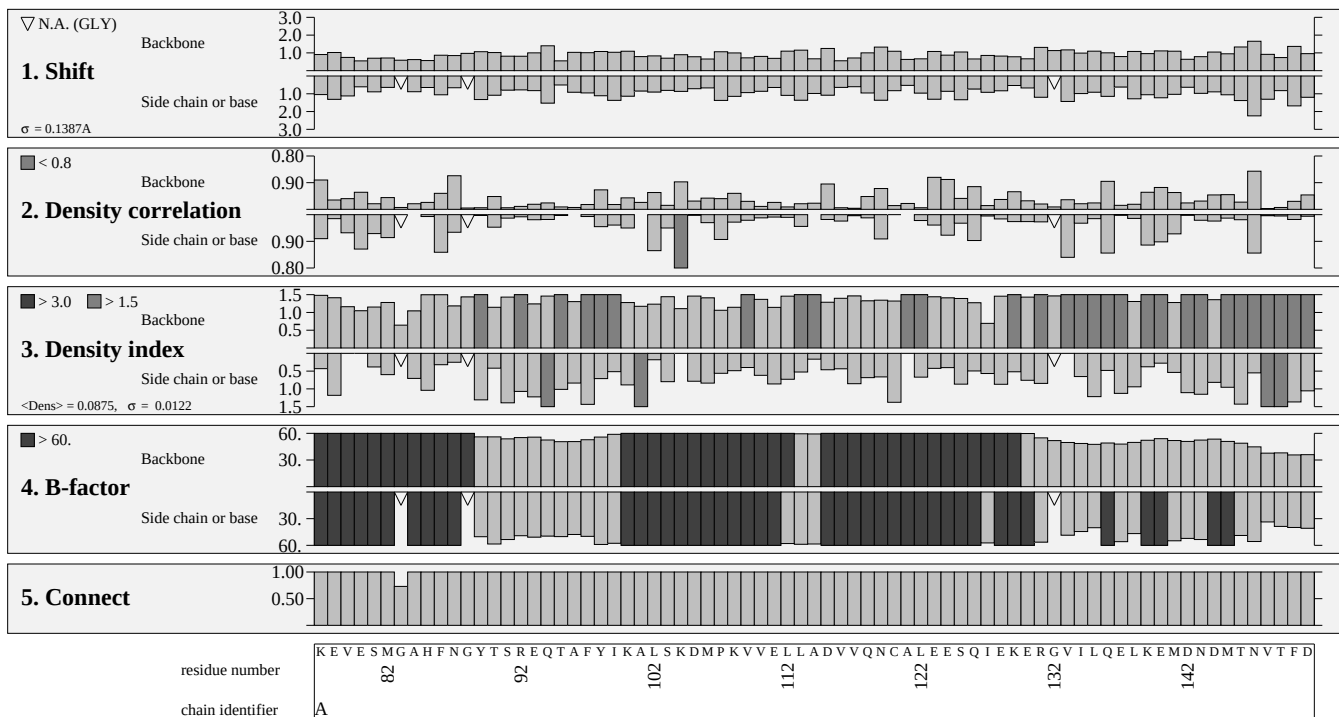
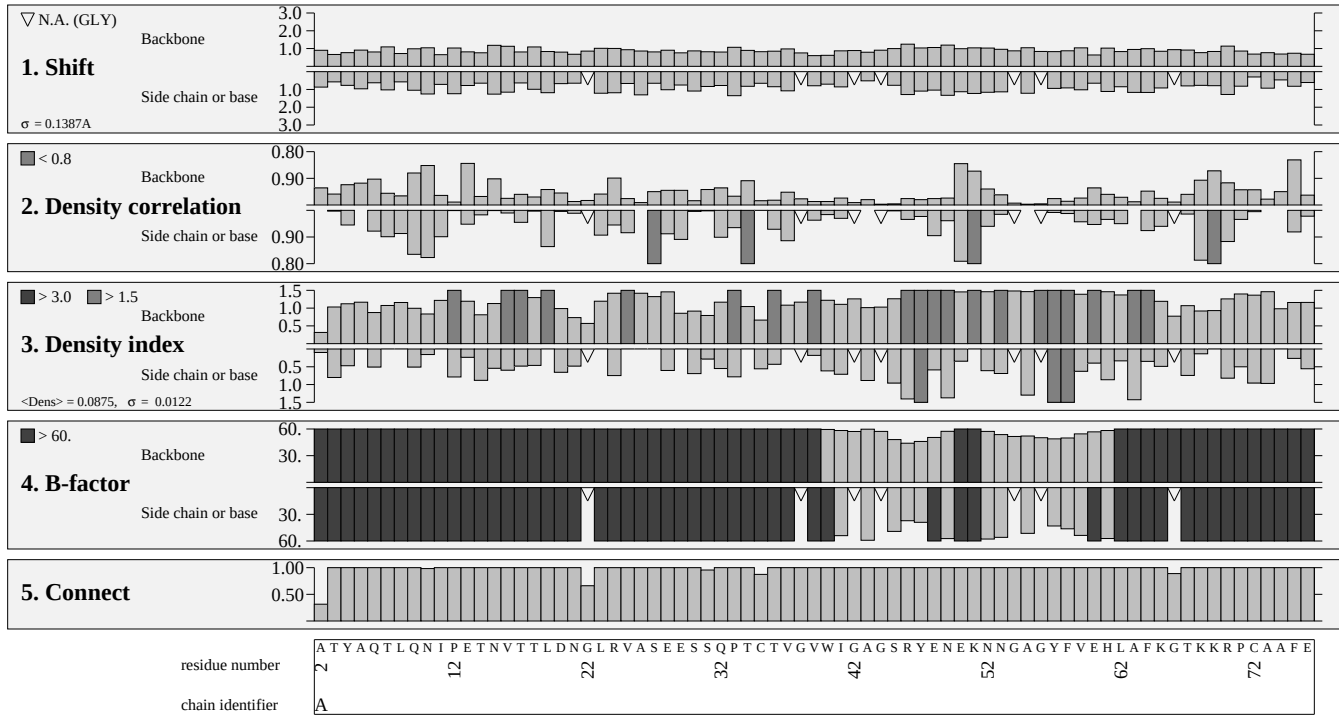
polar coordinates of the crystallographical axes



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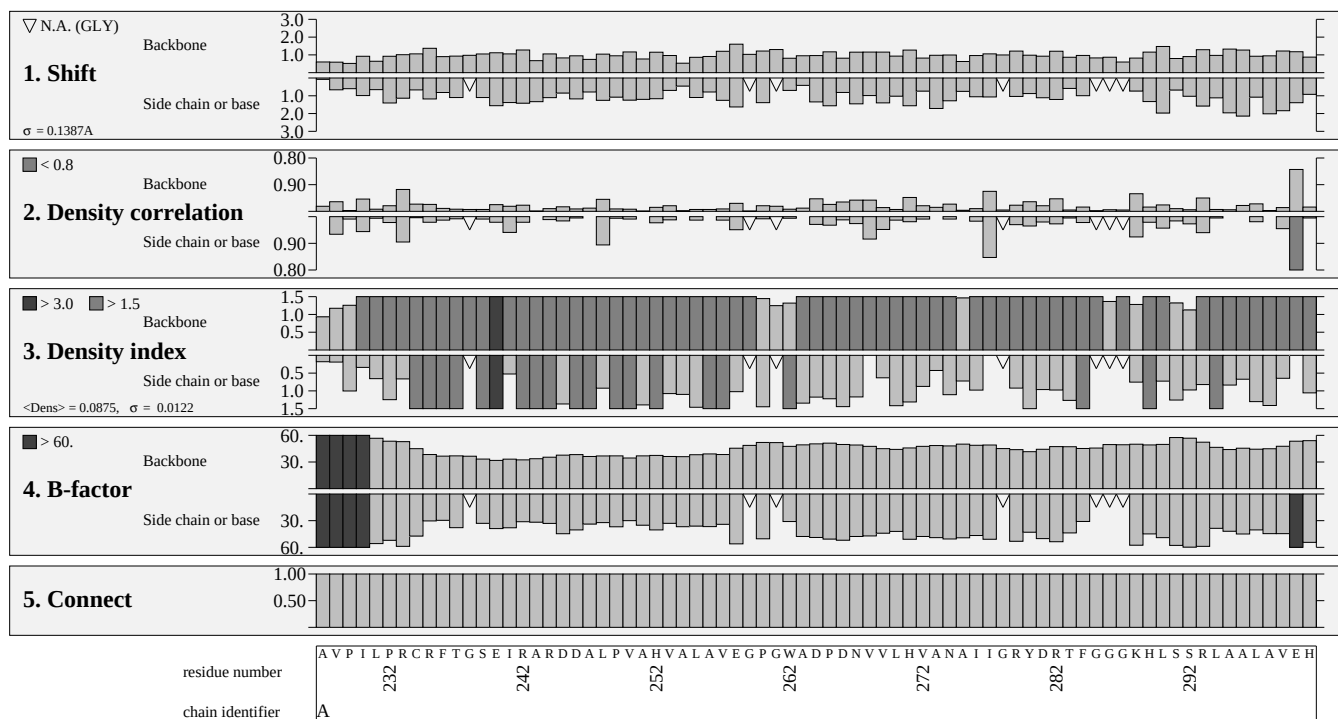
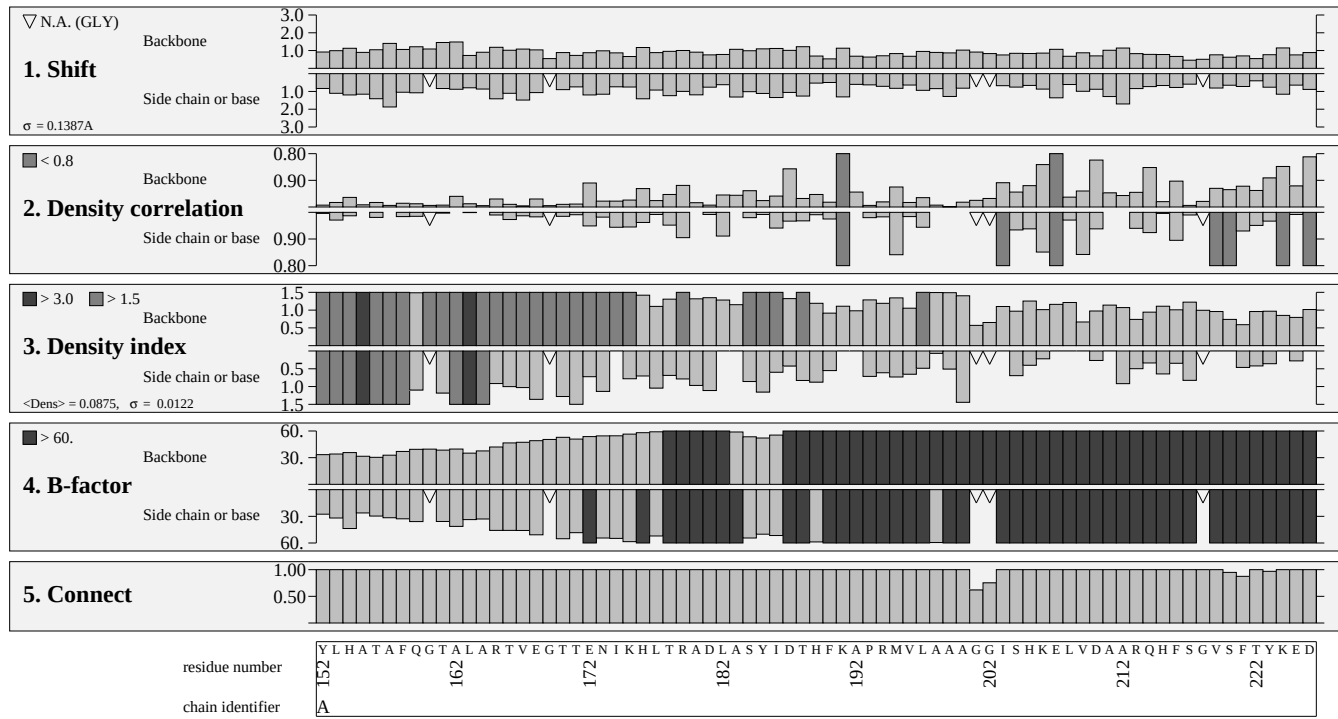
Local estimation



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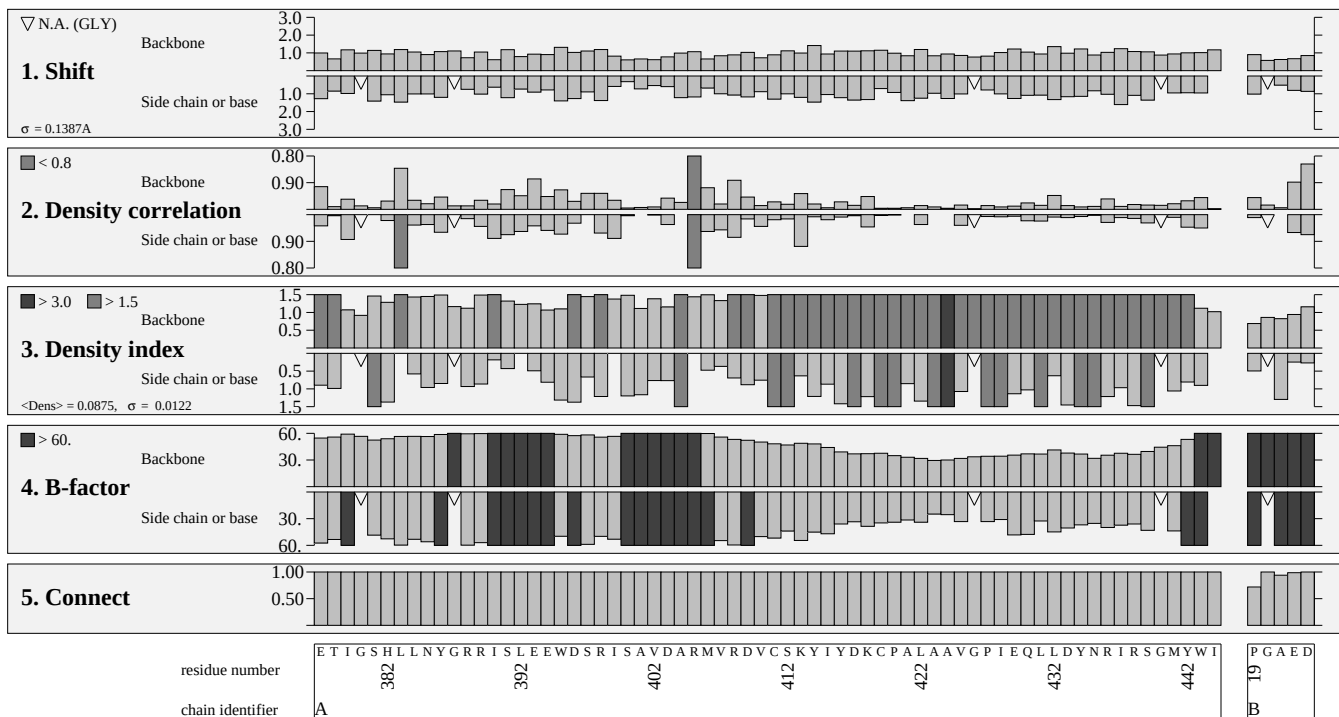
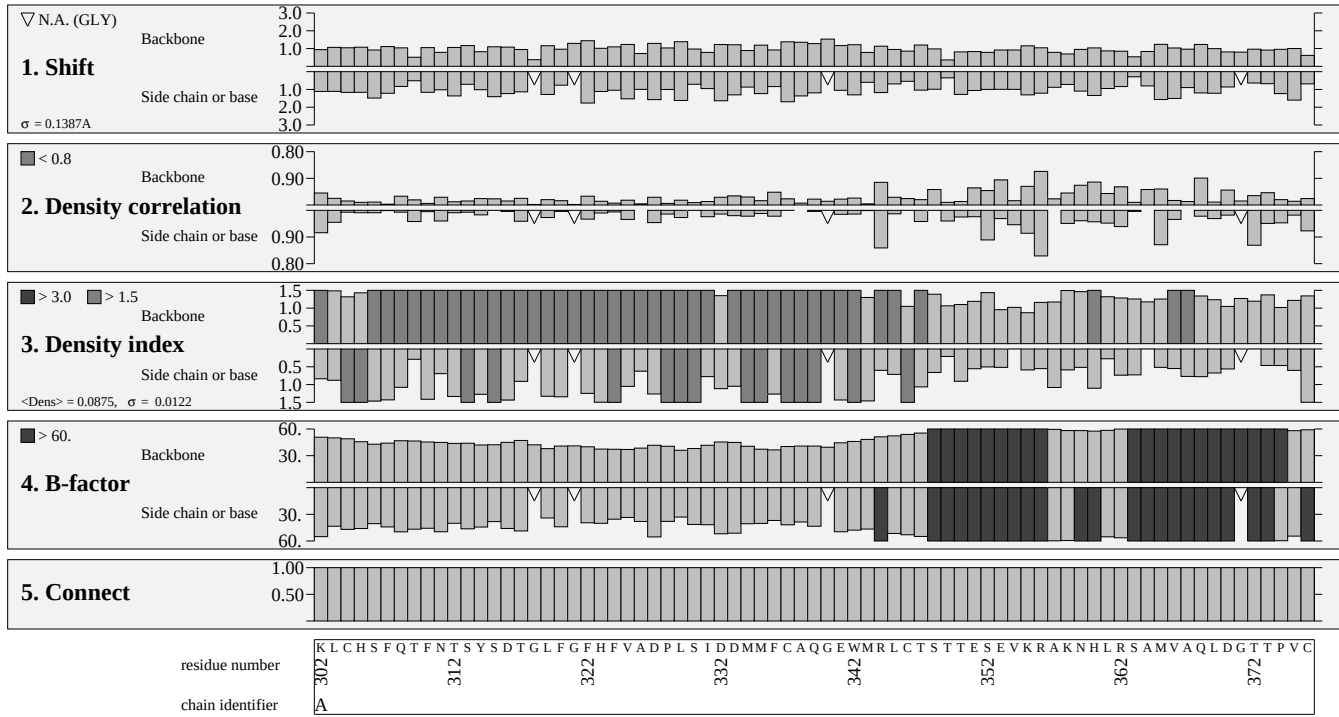
Local estimation (2)



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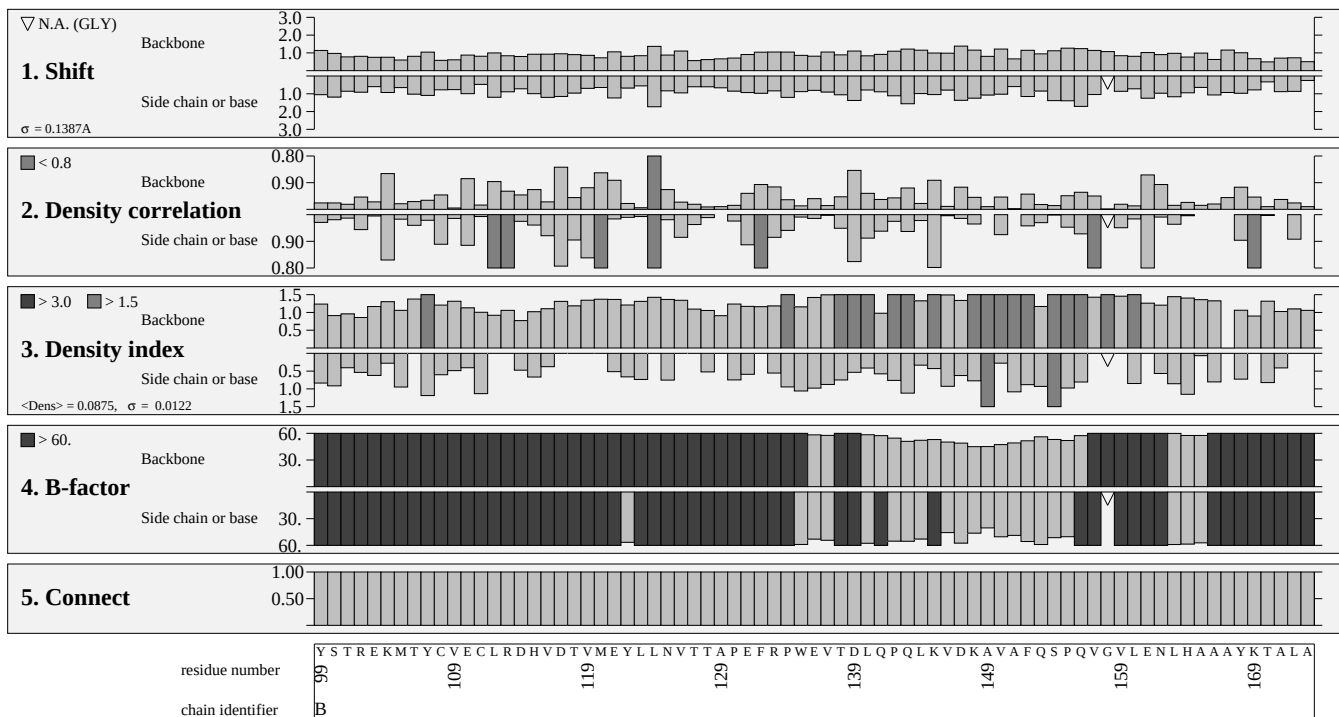
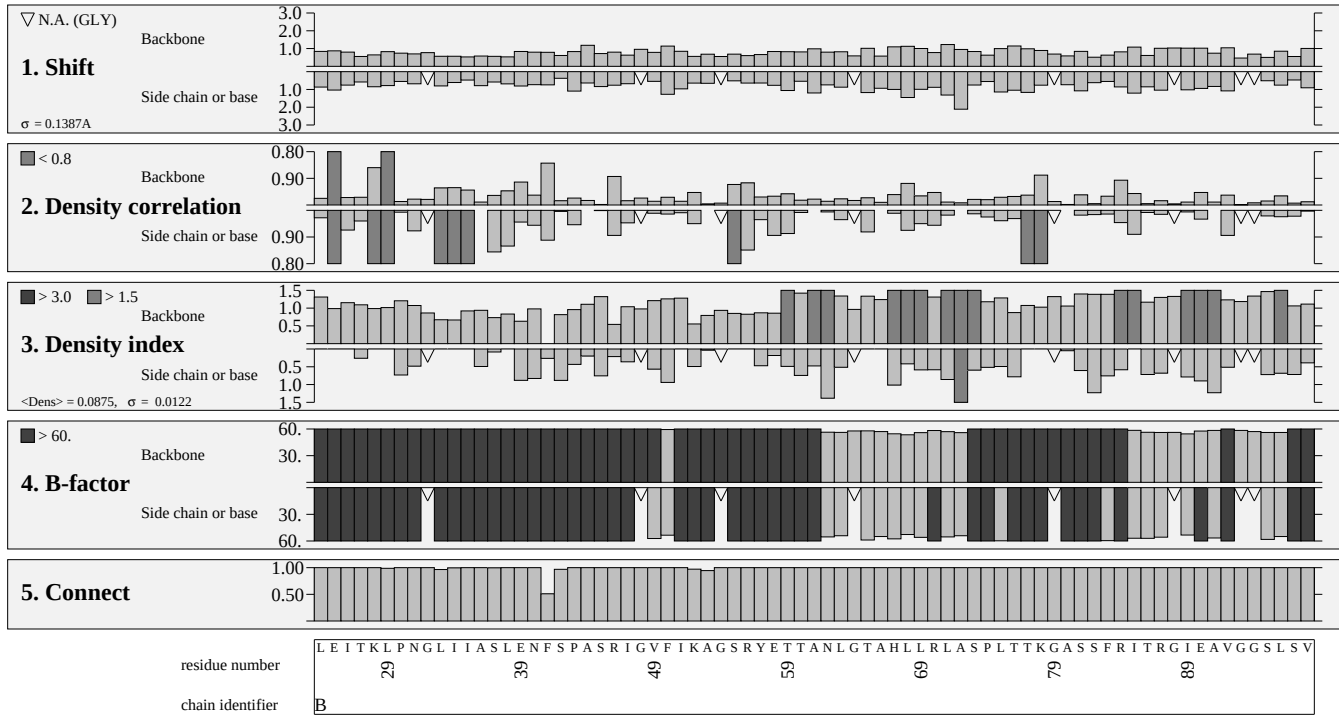
Local estimation (3)



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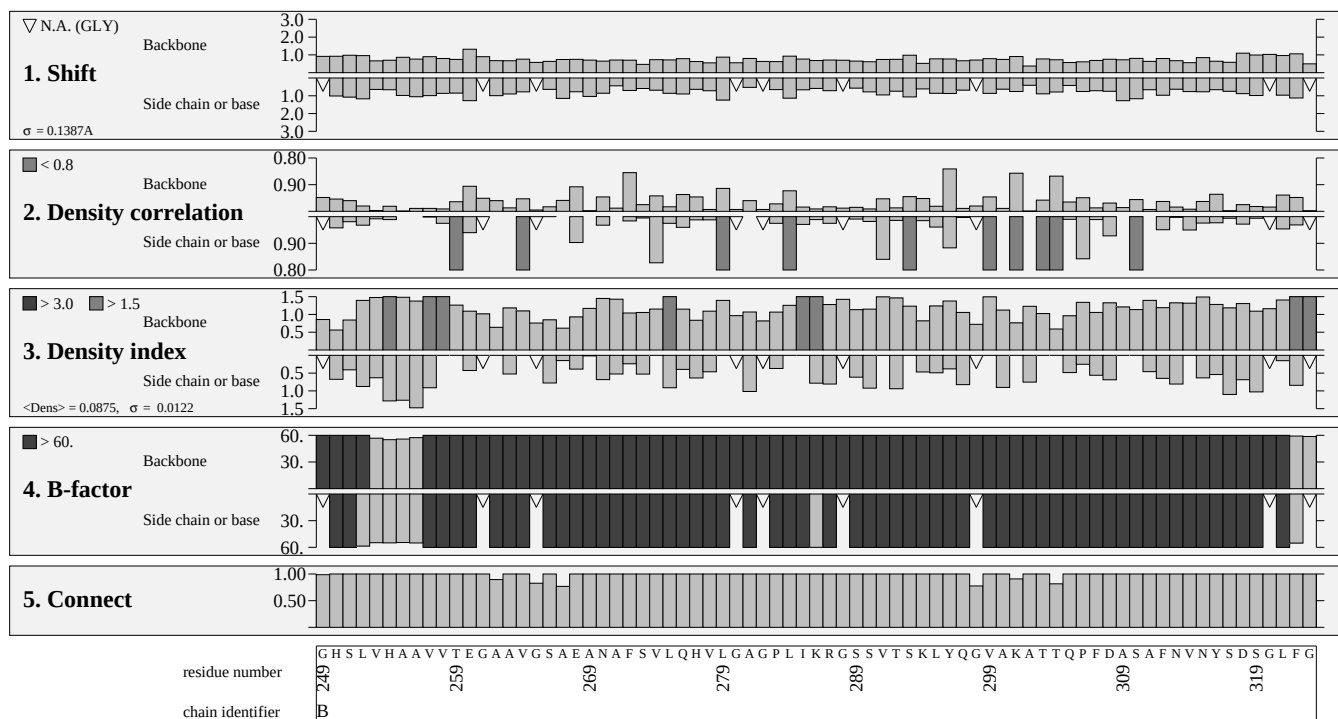
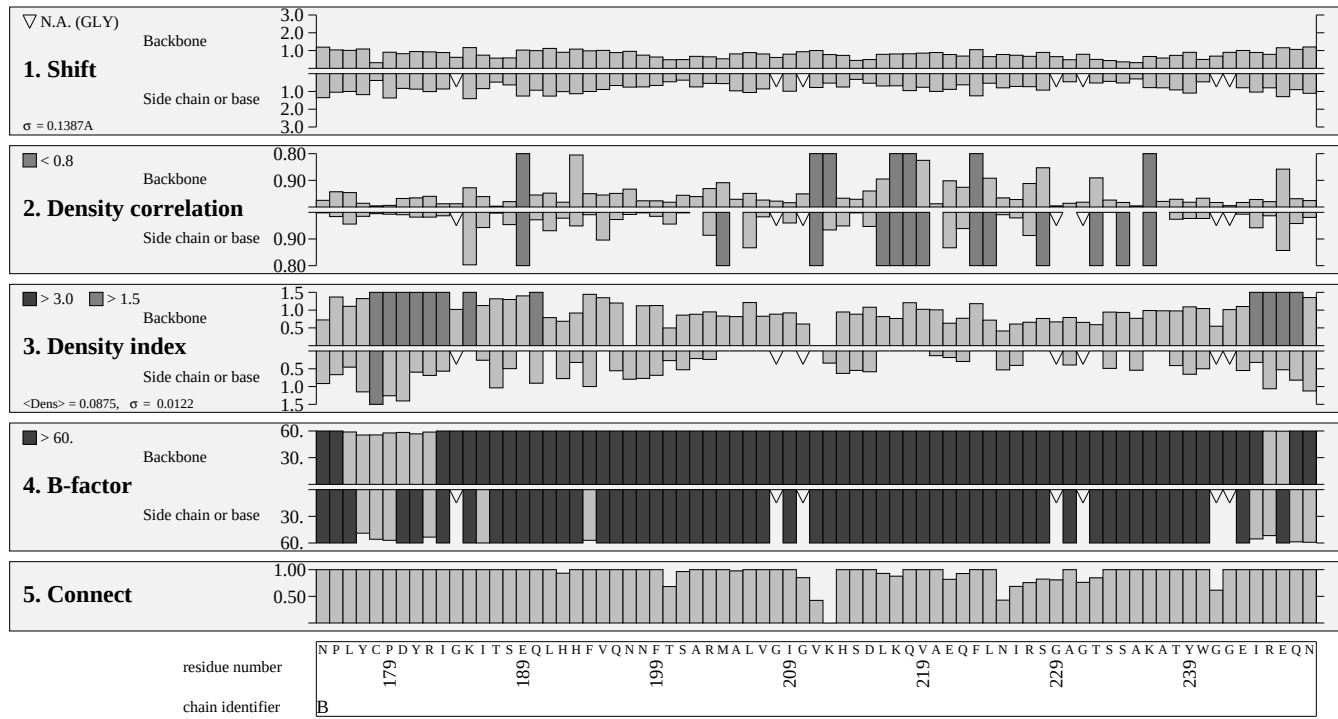
Local estimation (4)



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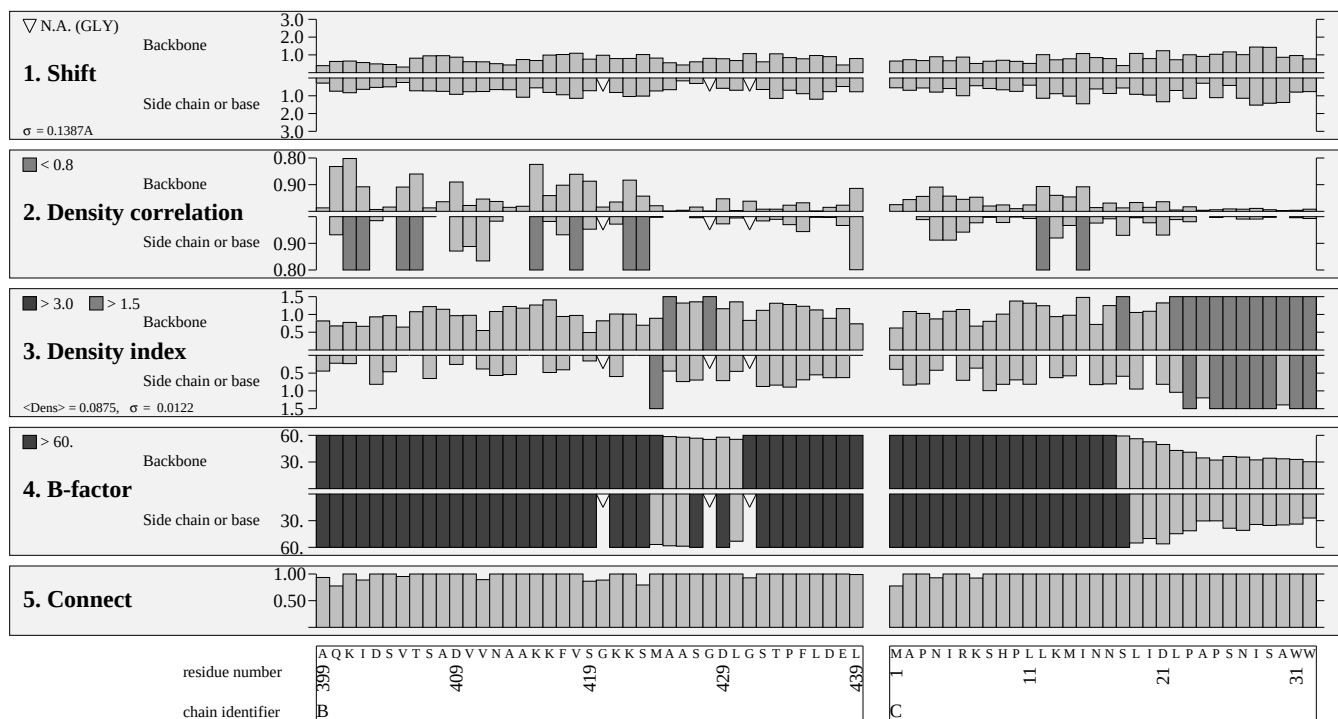
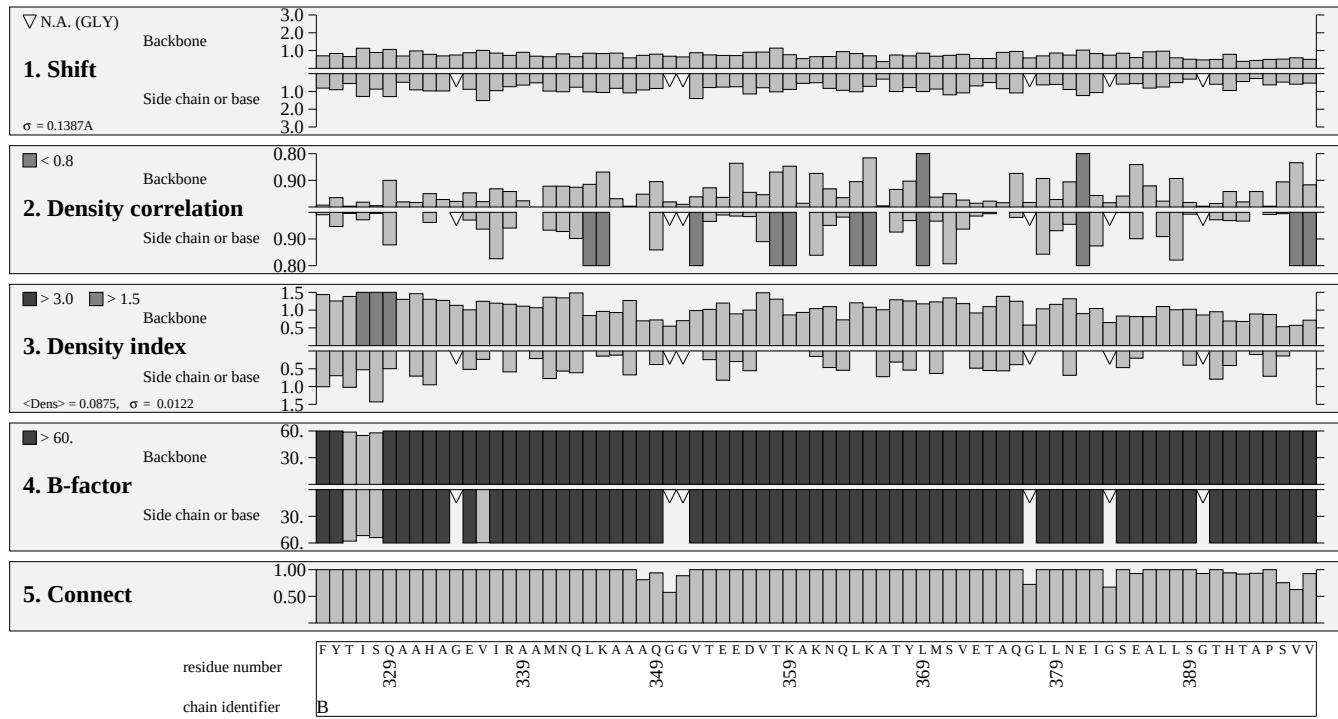
Local estimation (5)



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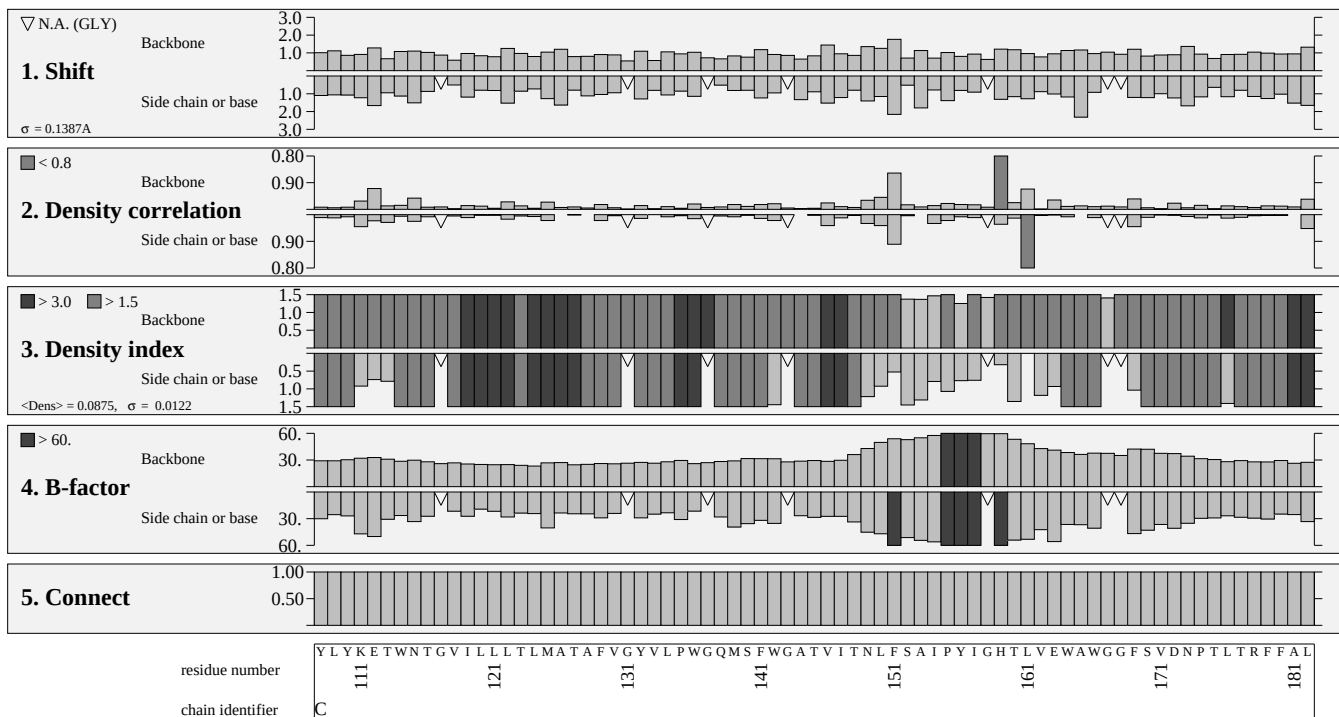
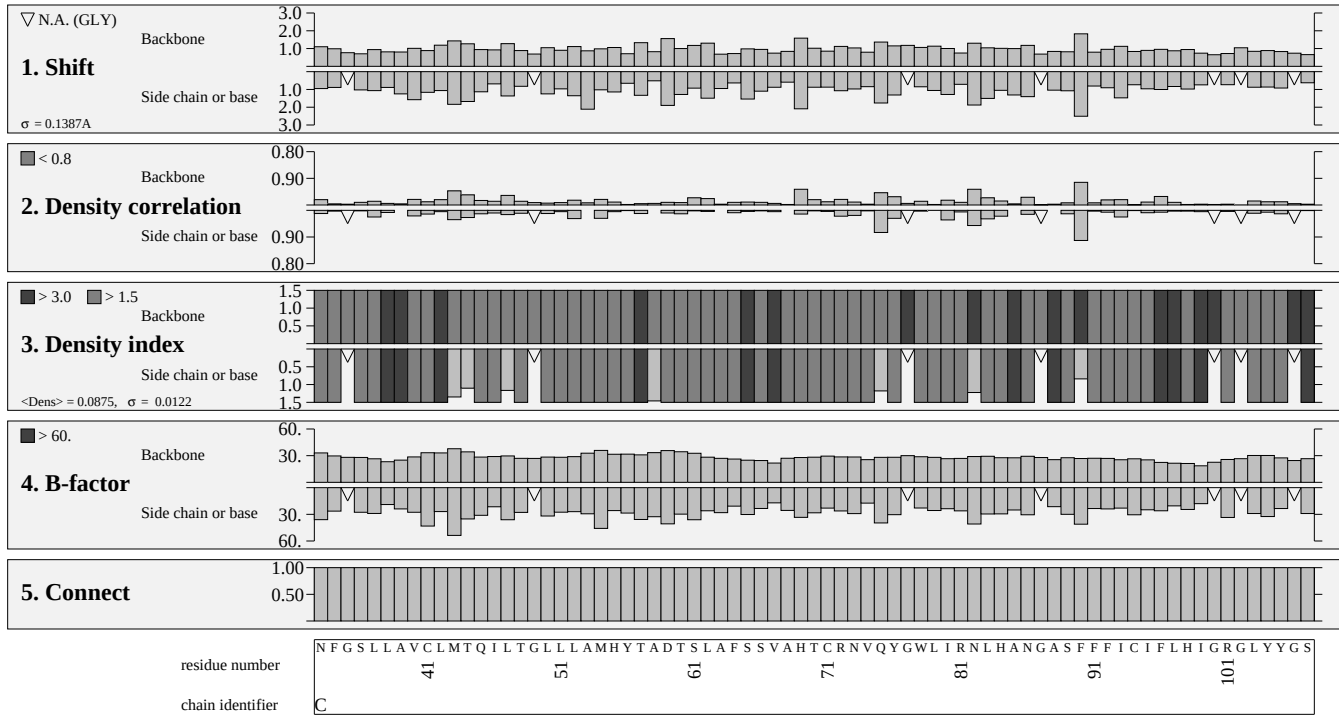
Local estimation (6)



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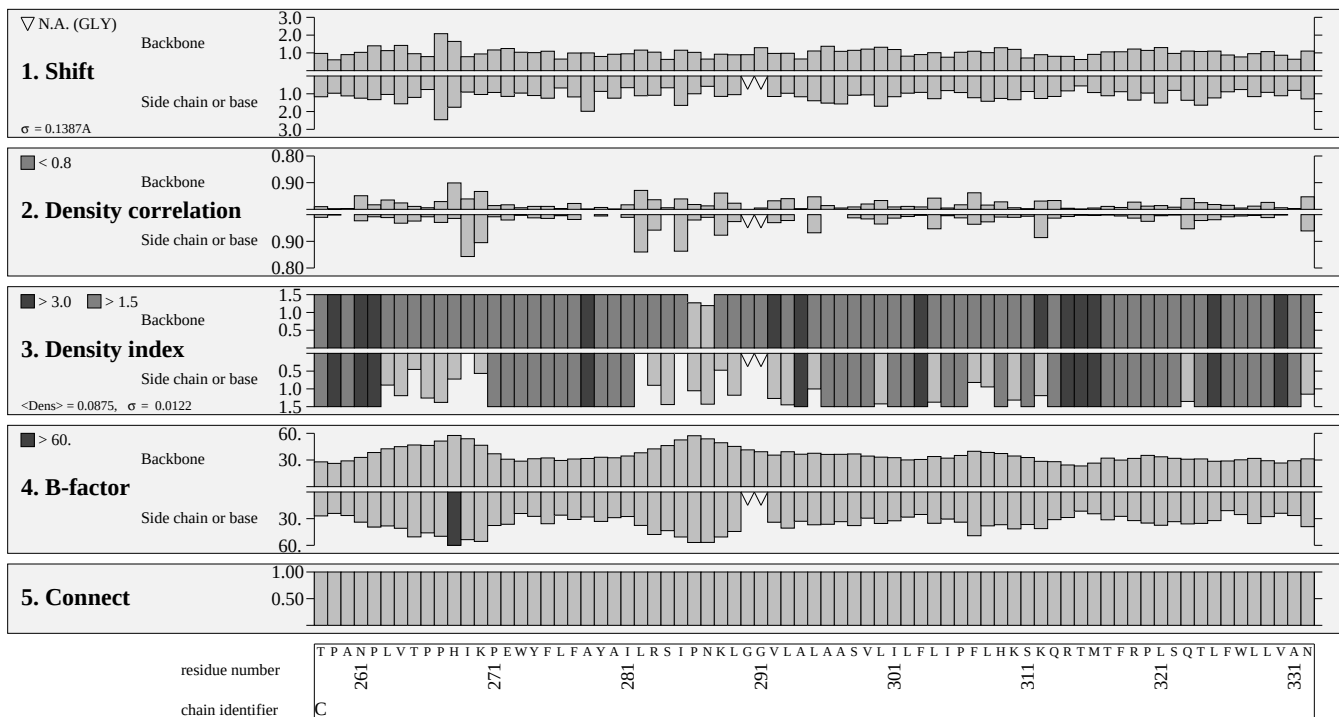
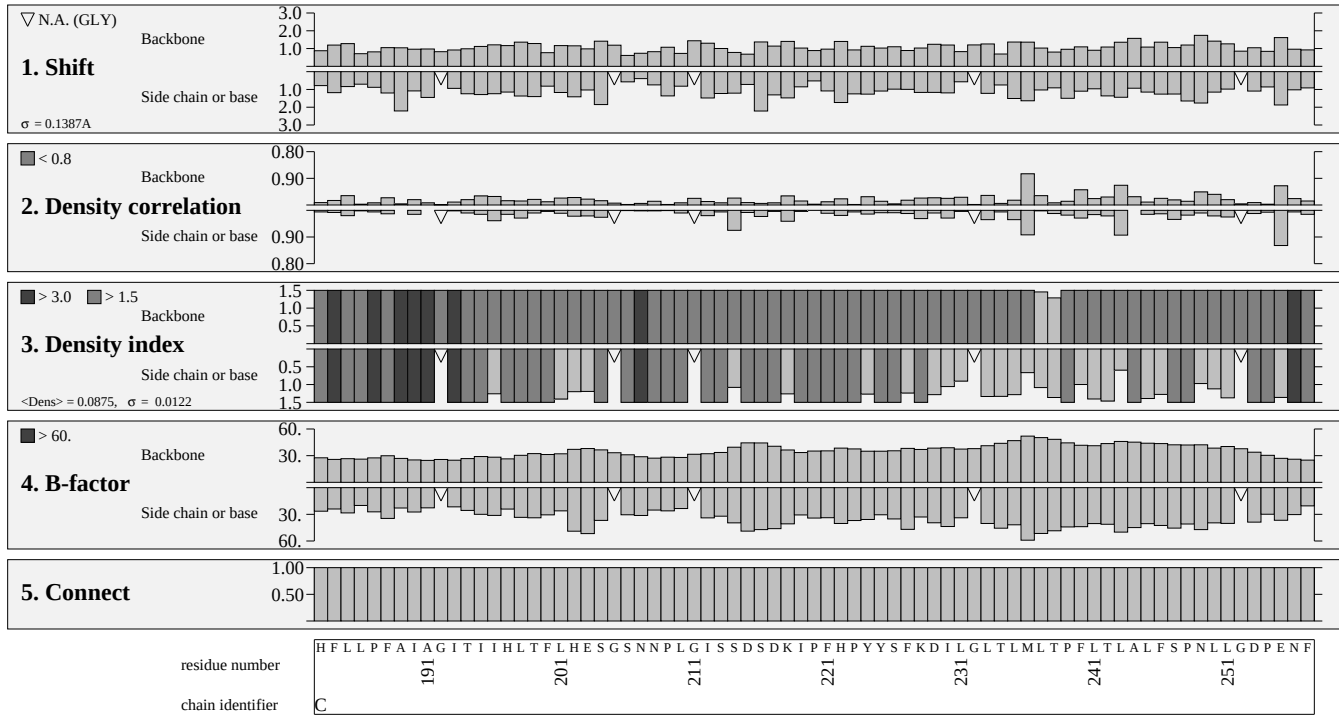
Local estimation (7)



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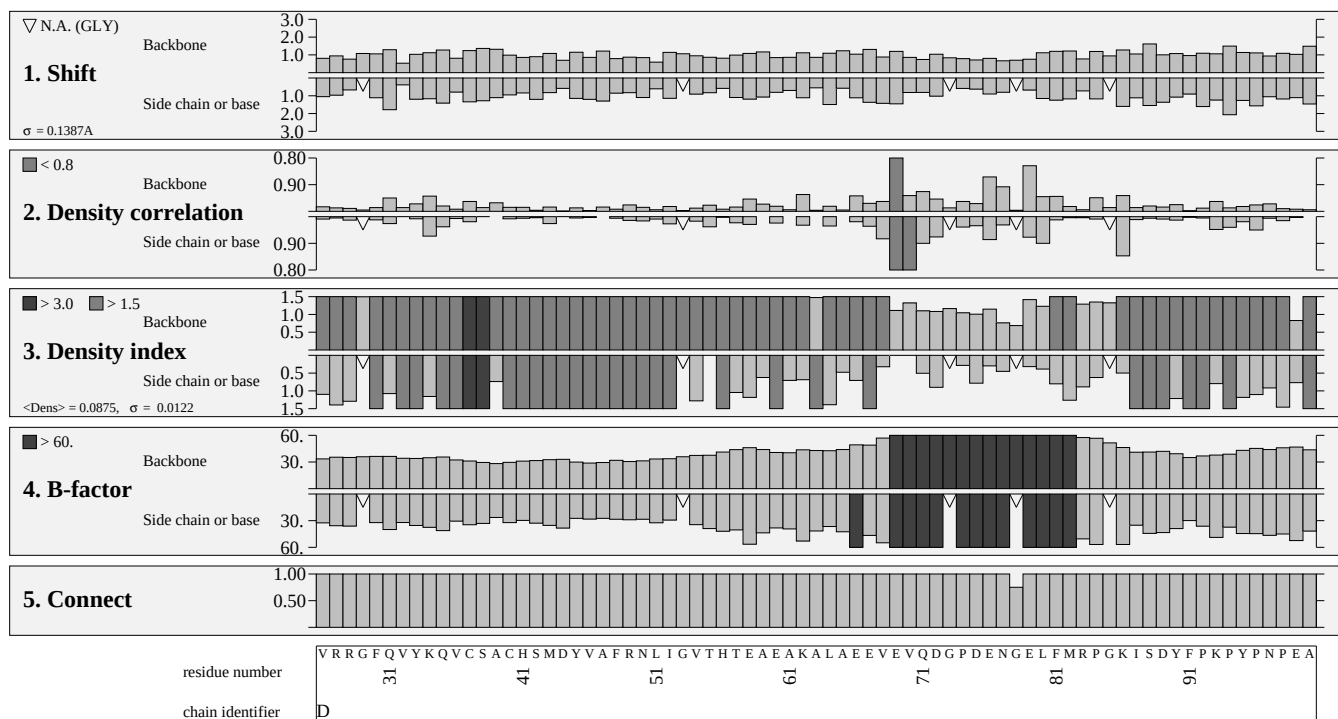
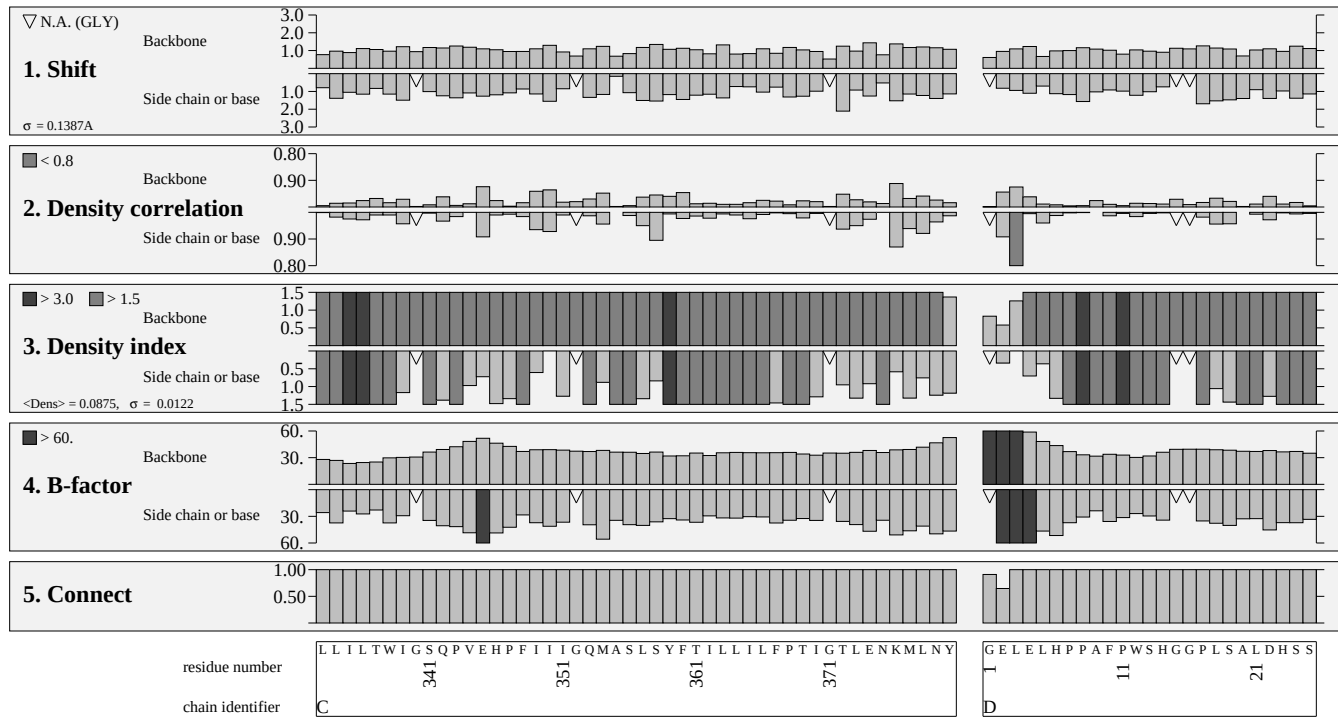
Local estimation (8)



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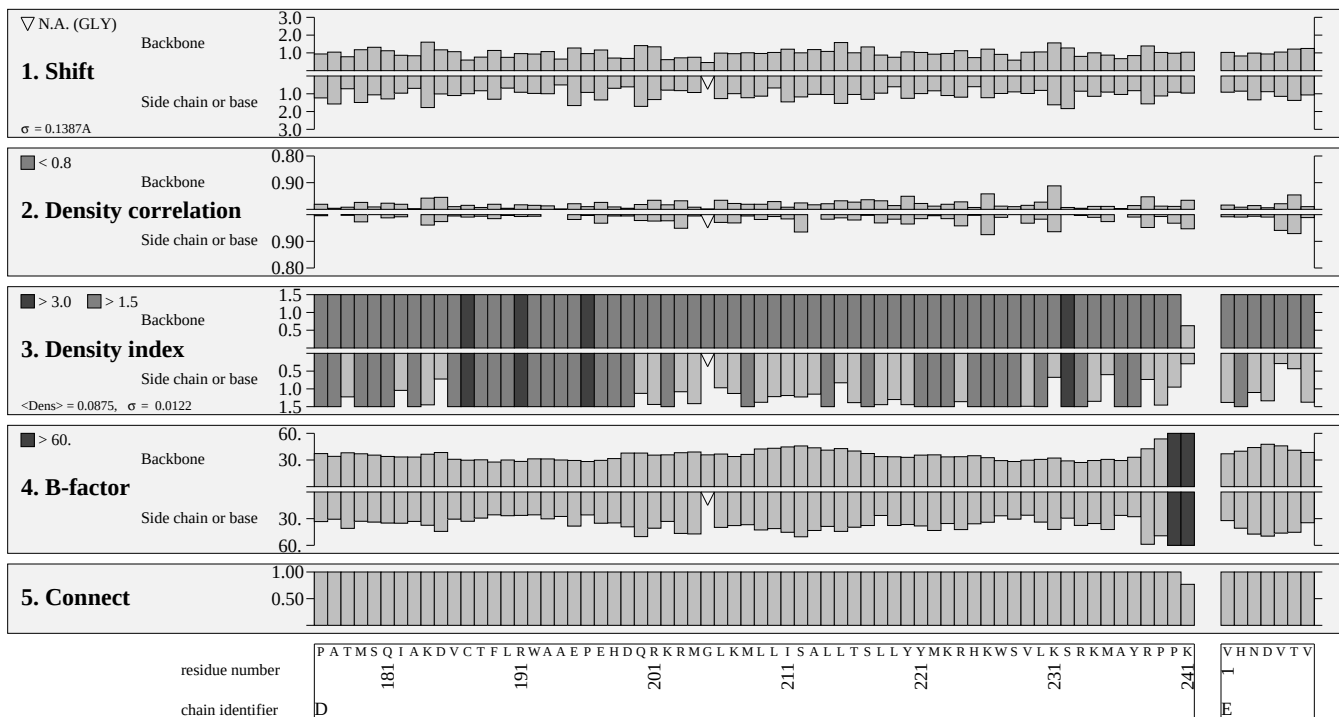
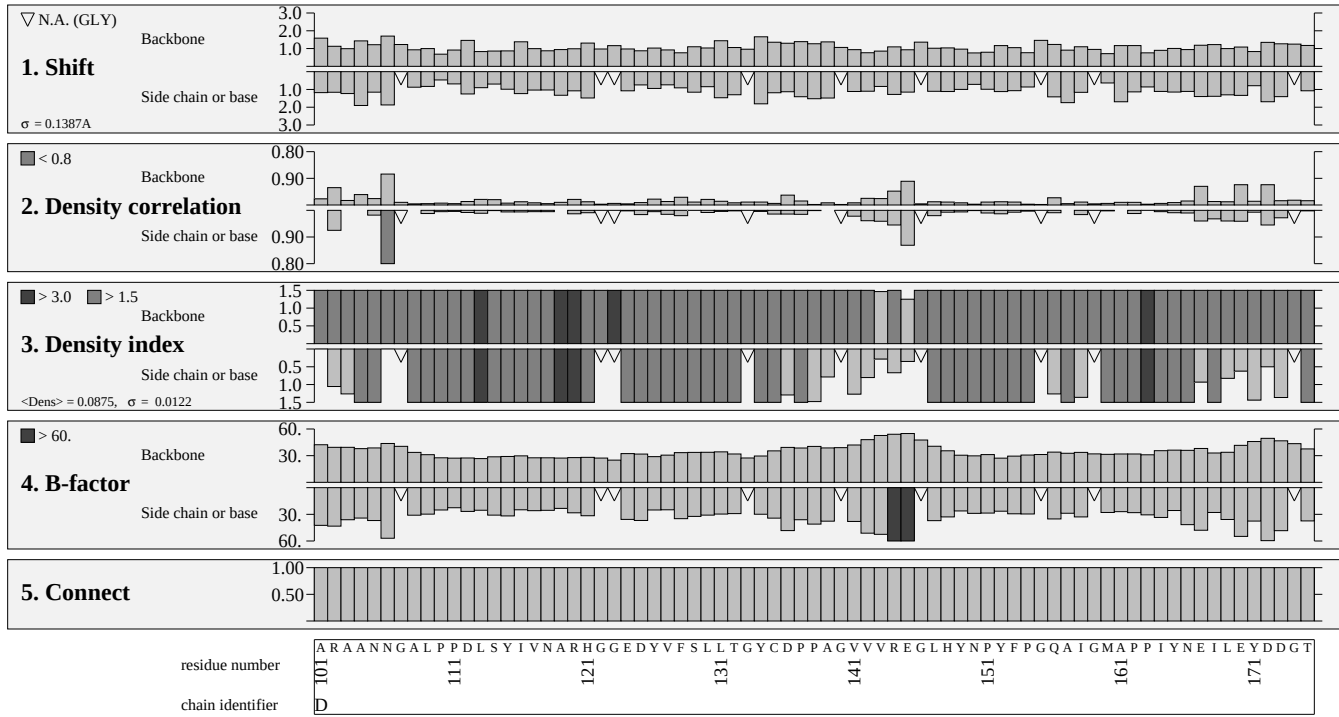
Local estimation (9)



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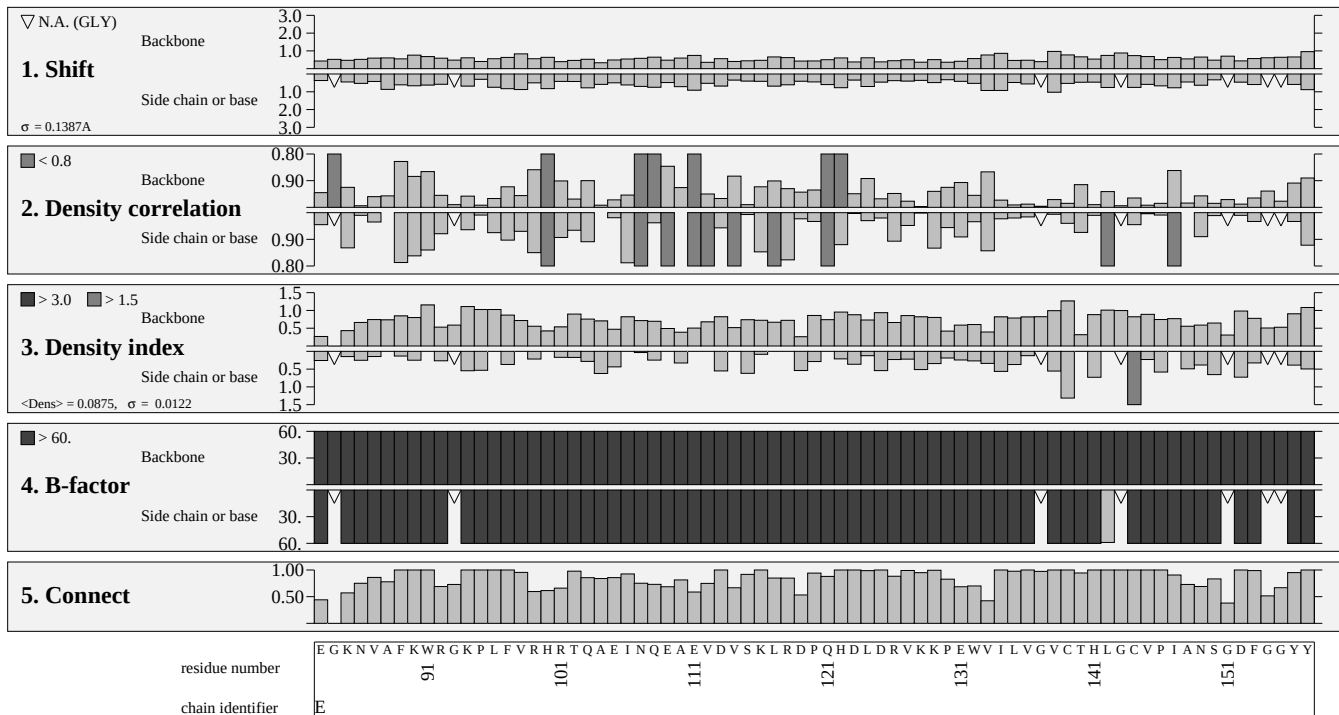
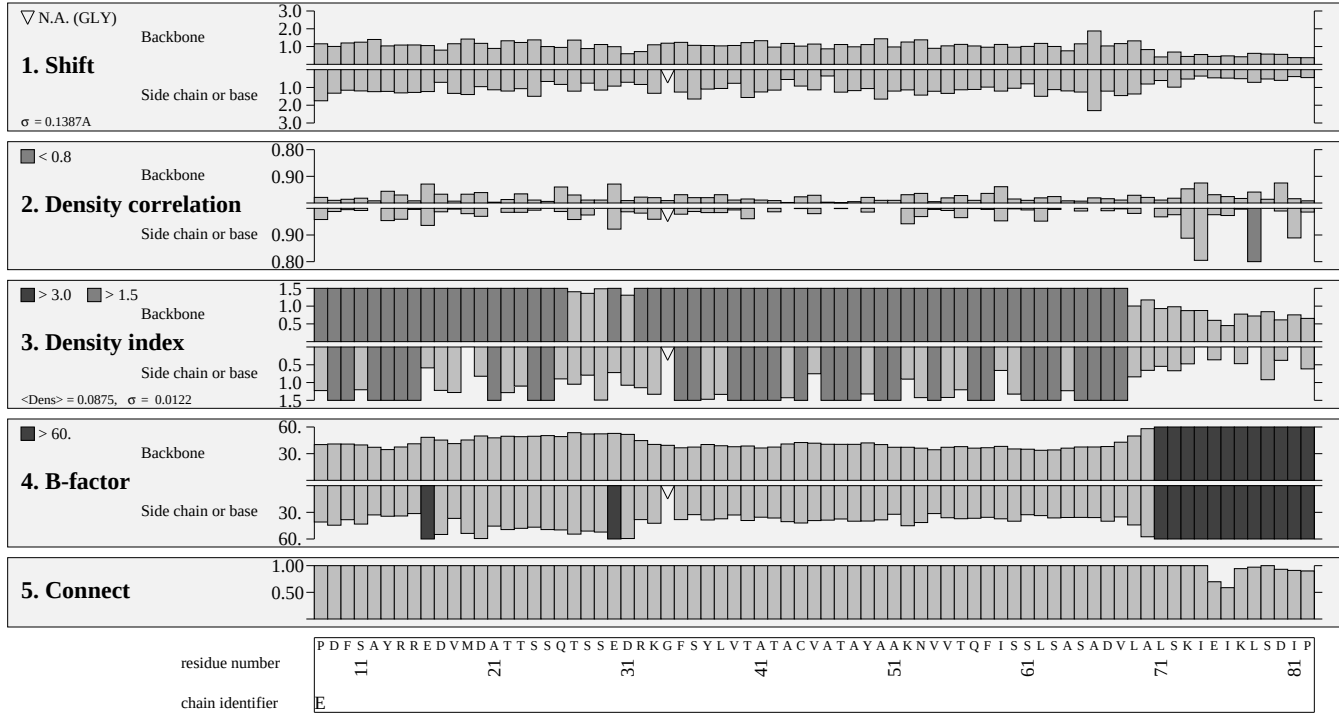
Local estimation (10)



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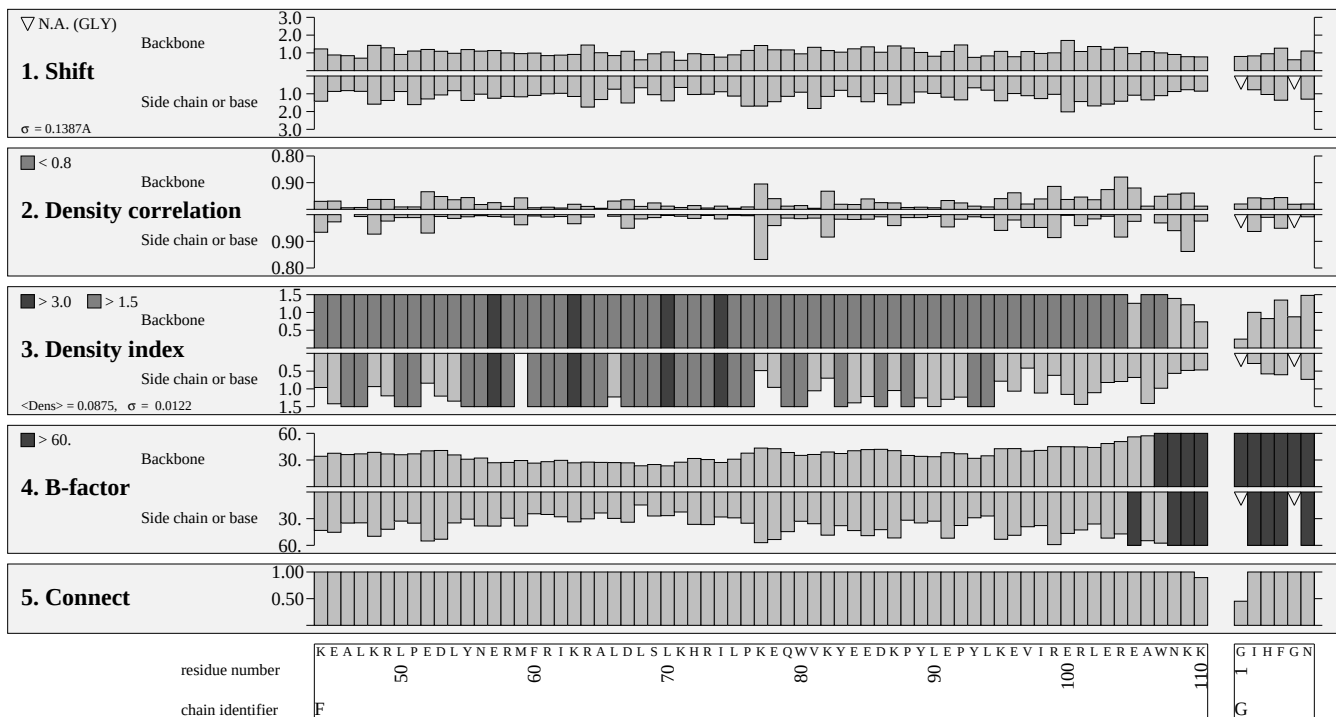
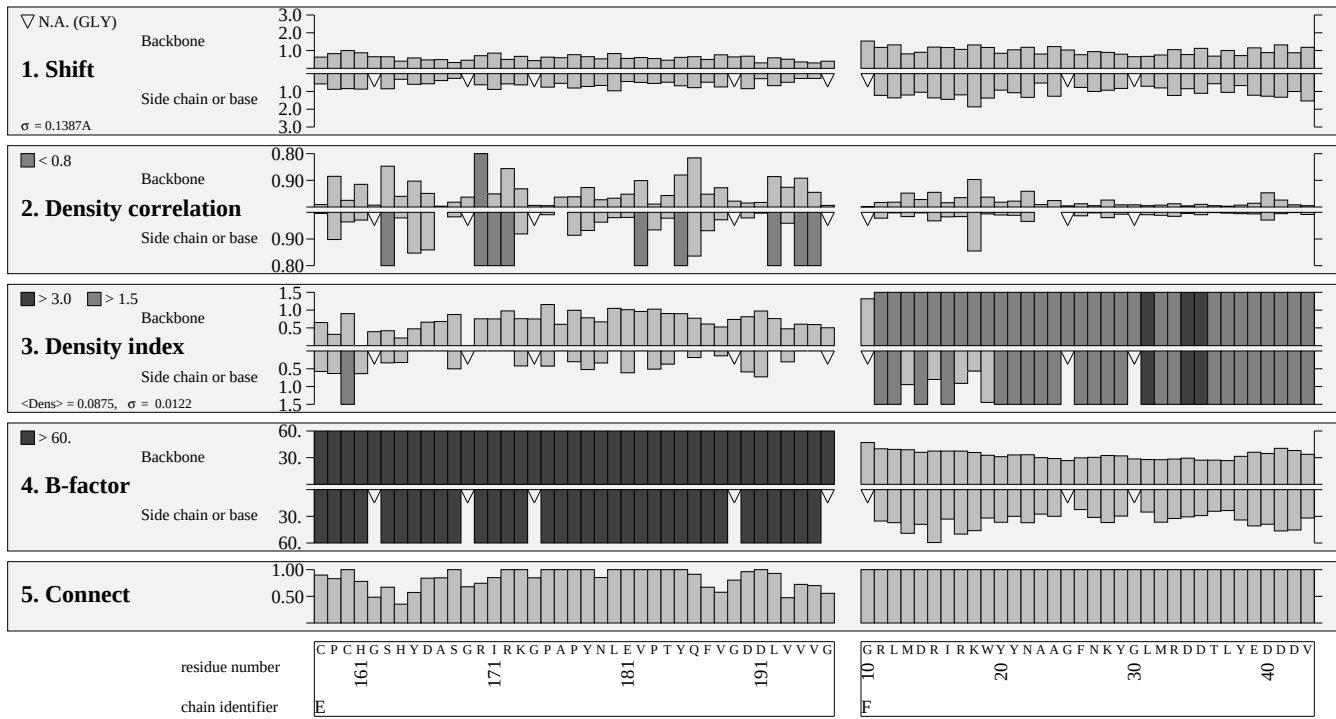
Local estimation (11)



Structure Factor Check

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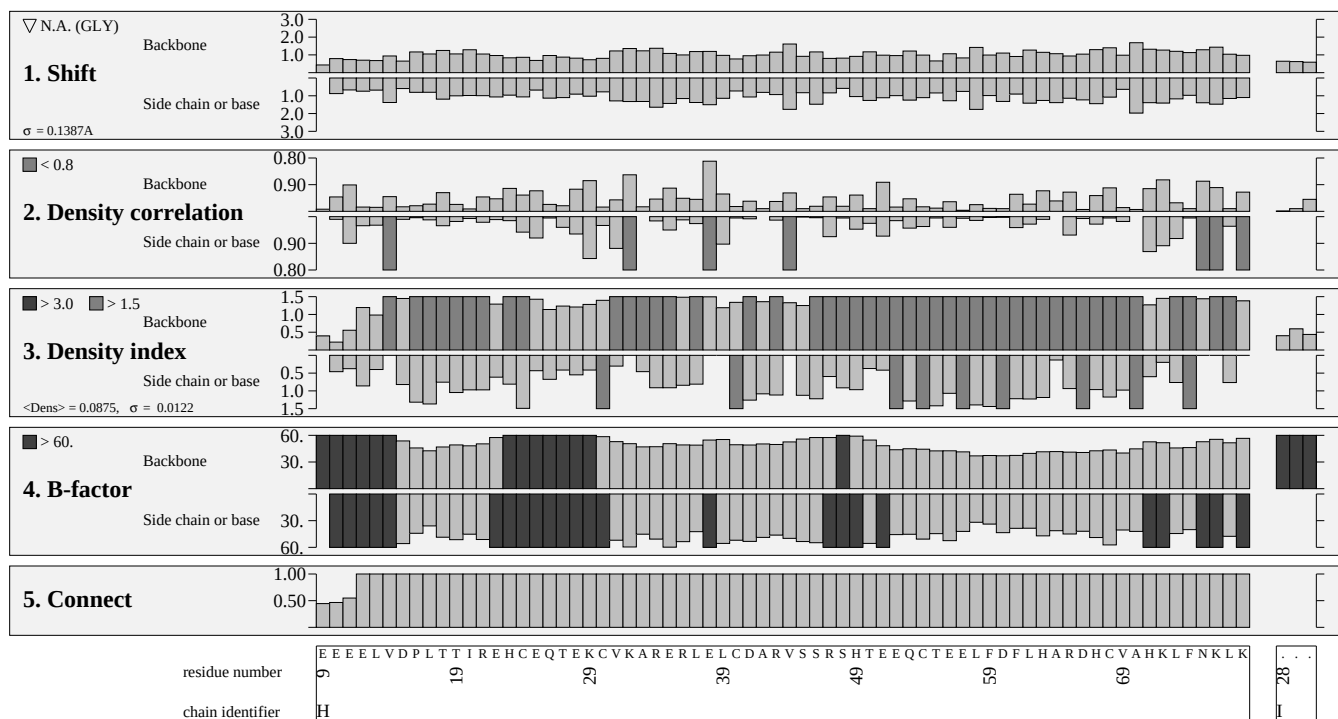
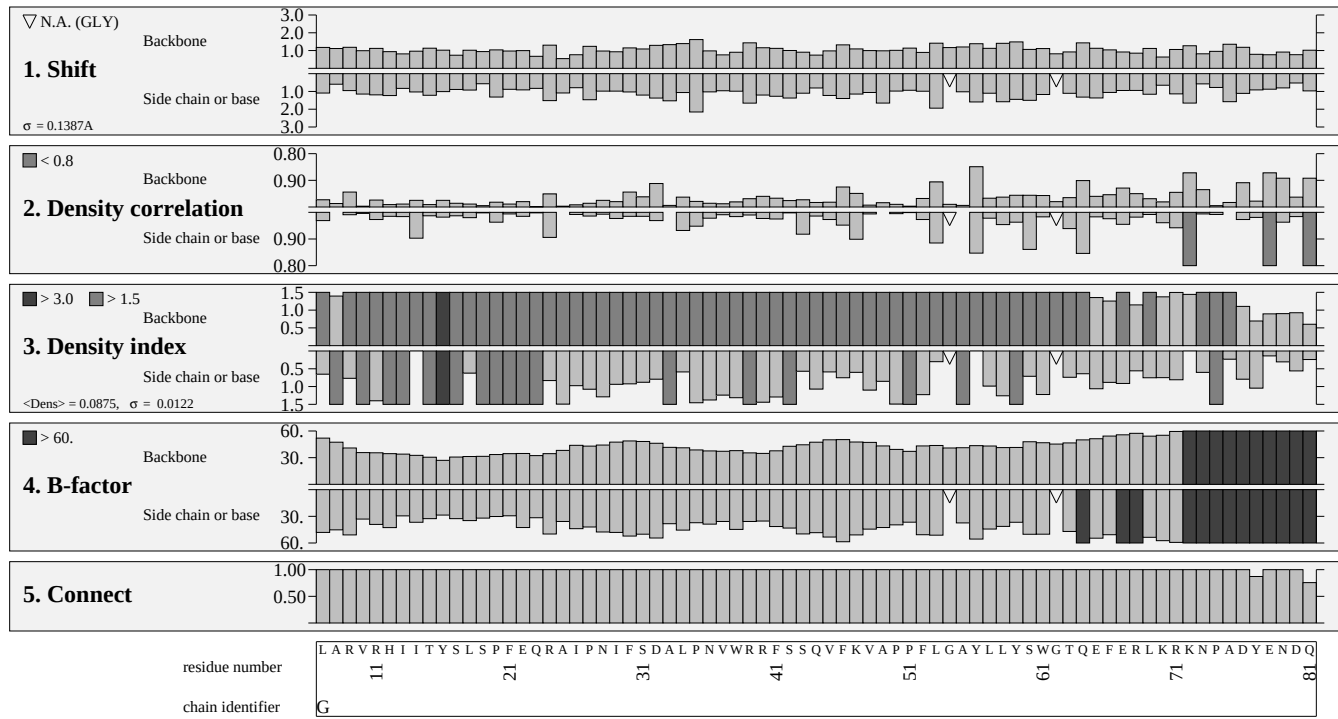
Local estimation (12)



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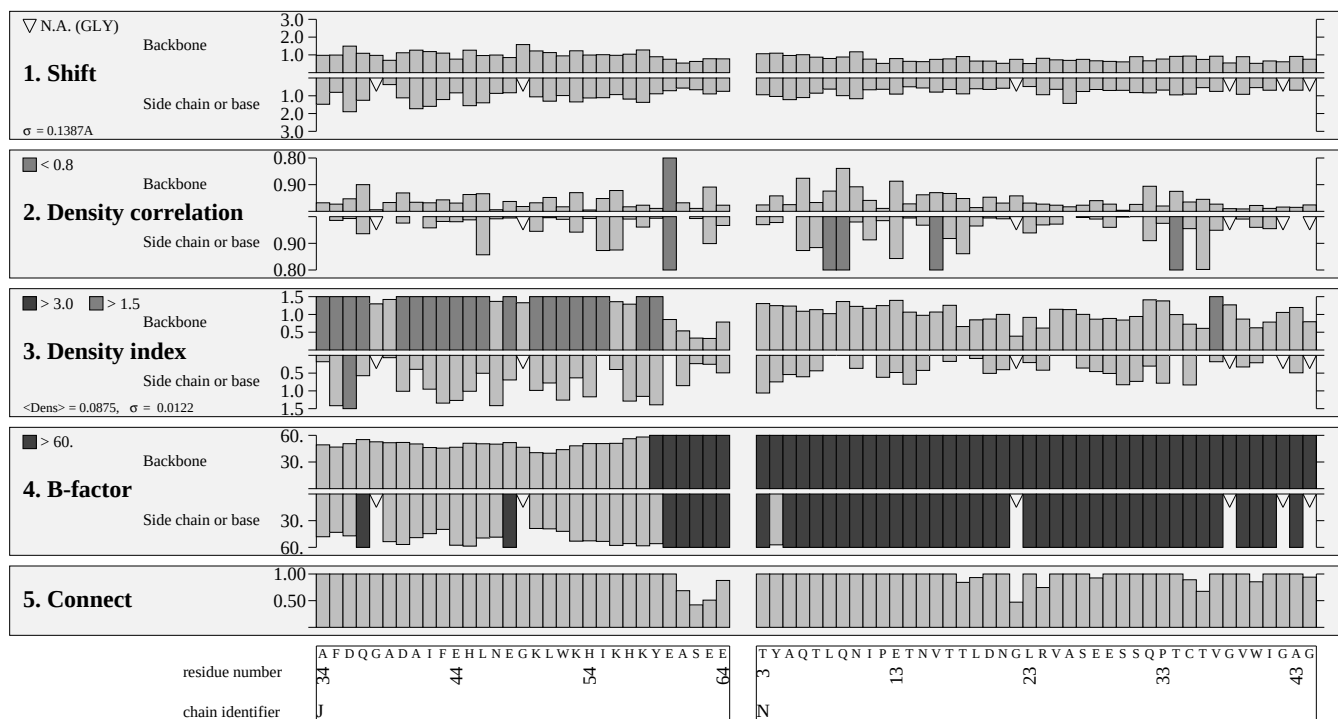
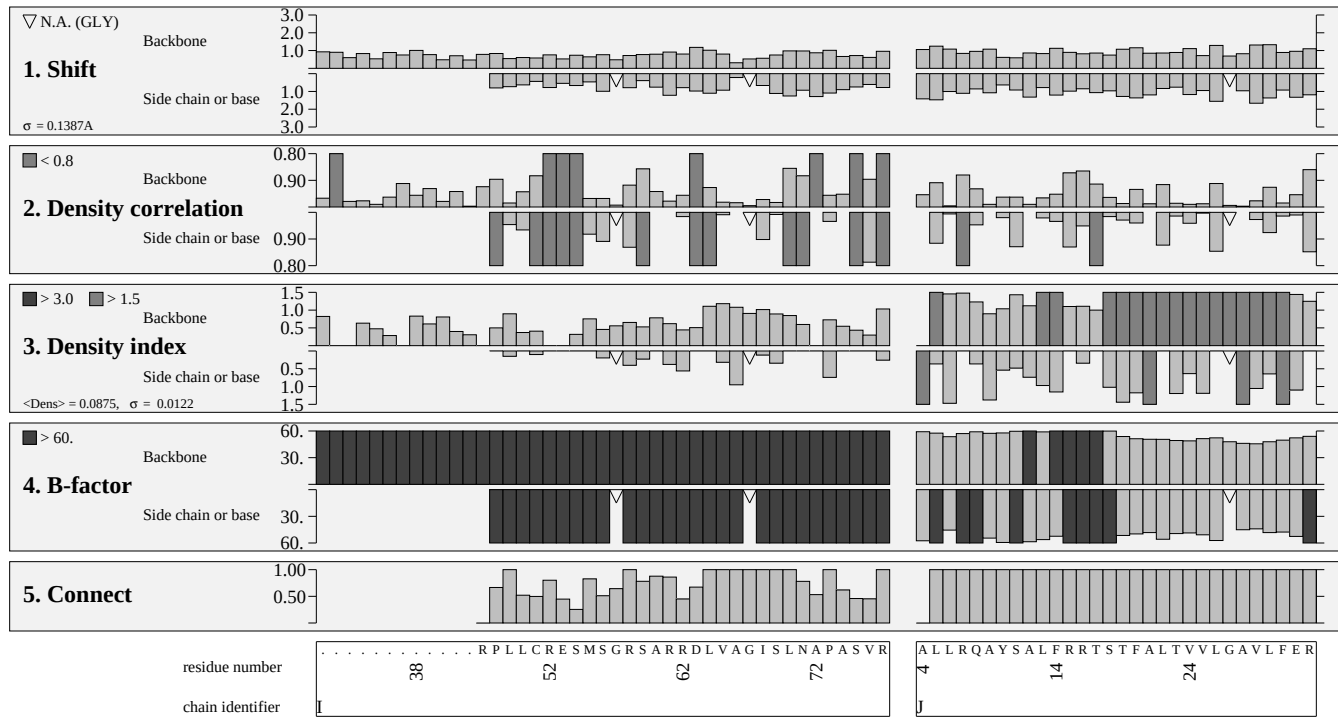
Local estimation (13)



Structure Factor Check

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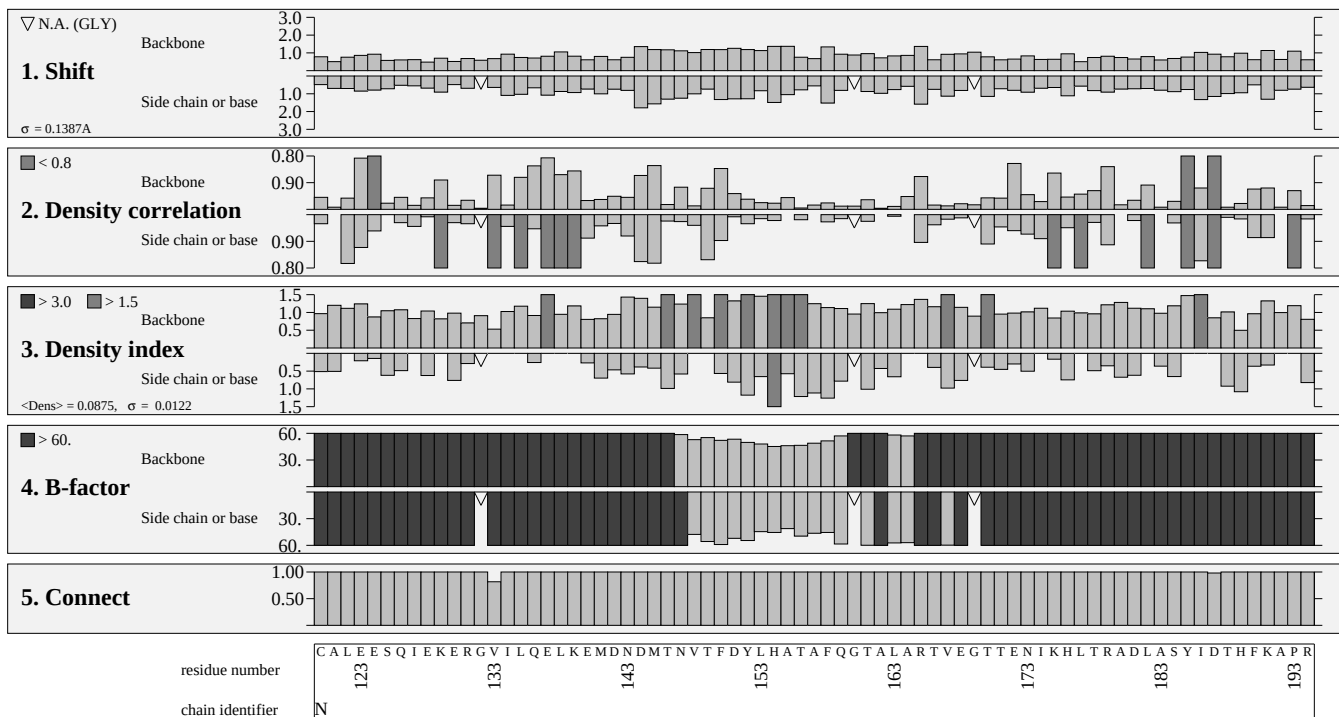
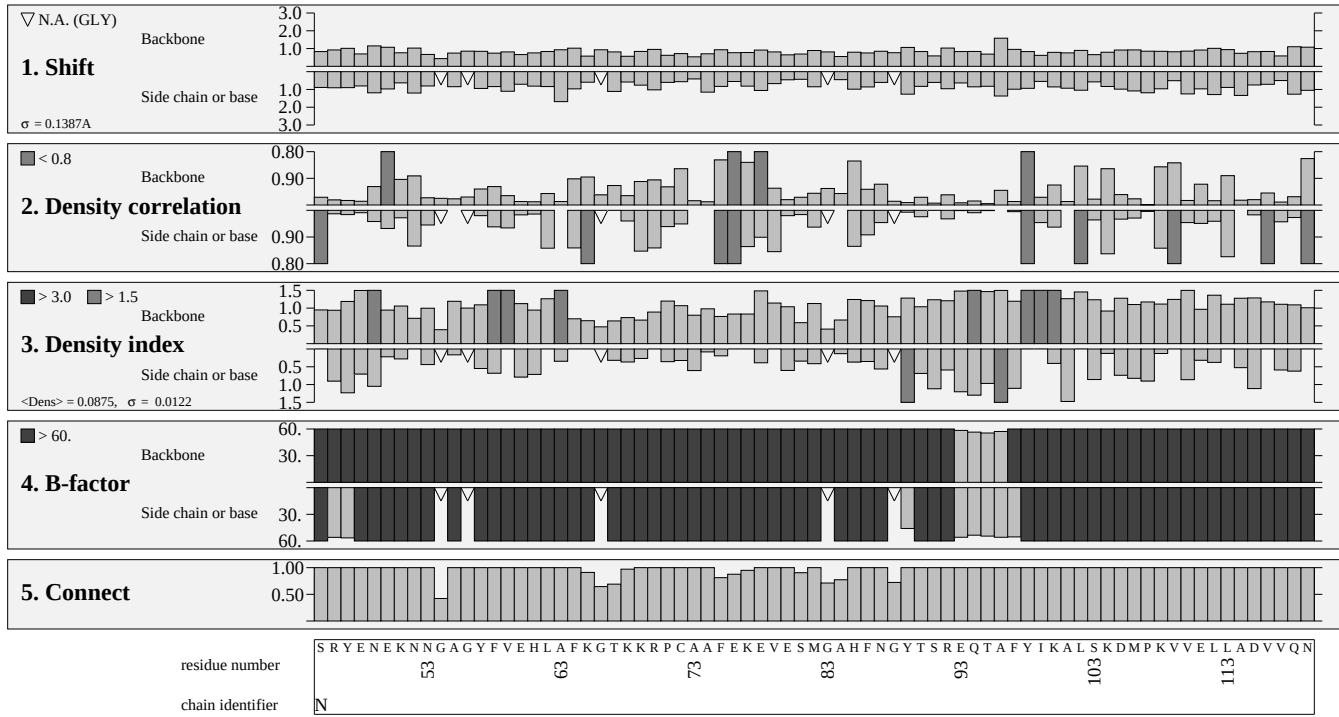
Local estimation (14)



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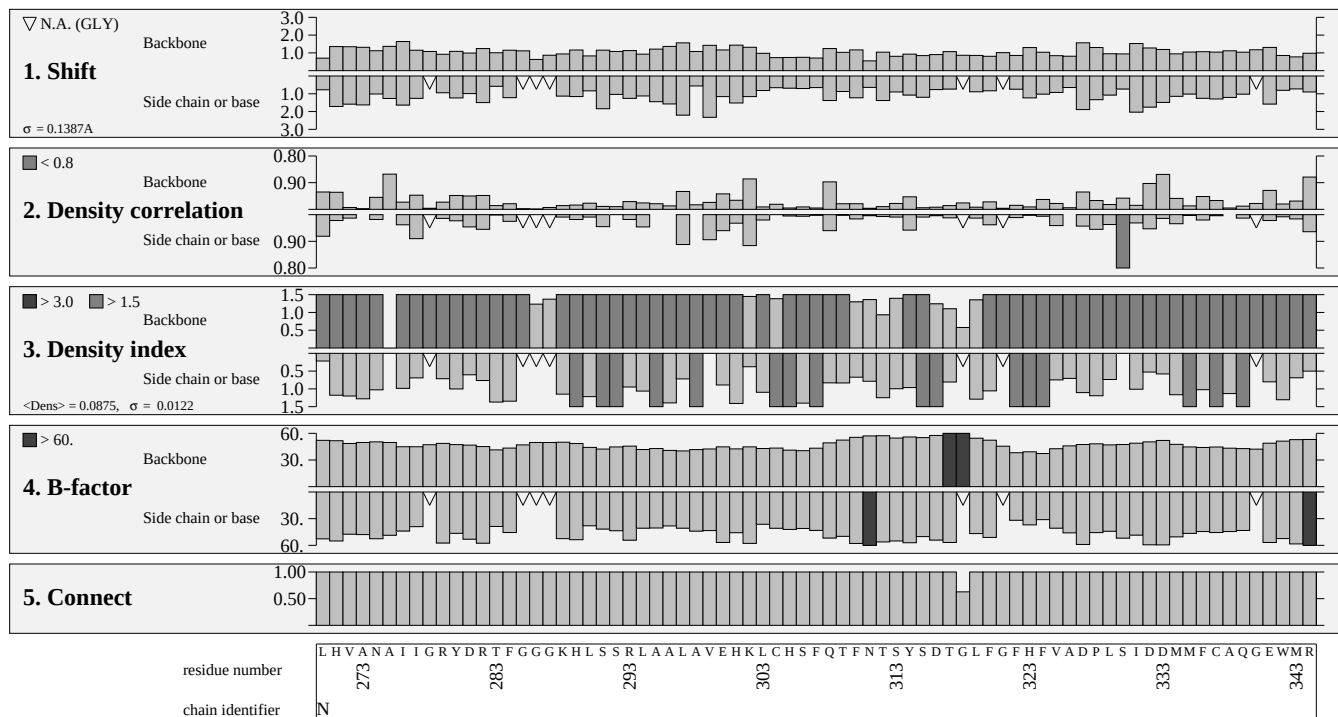
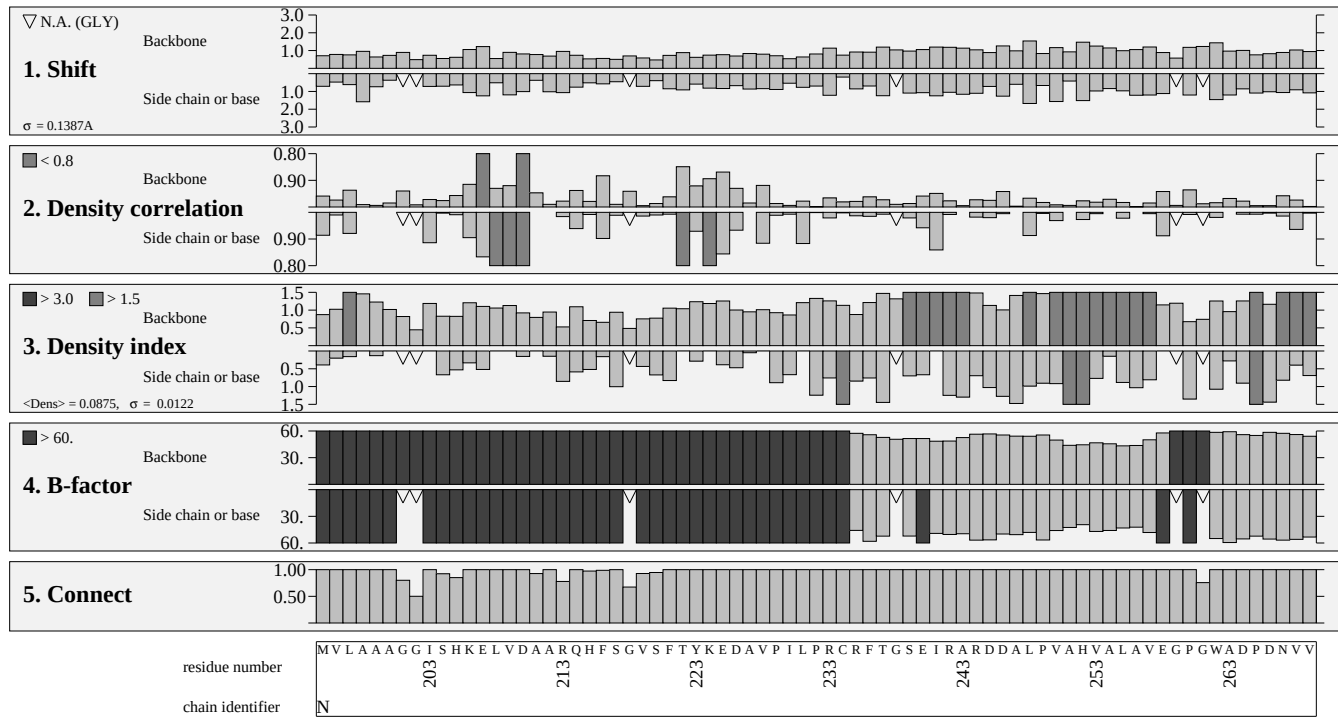
Local estimation (15)



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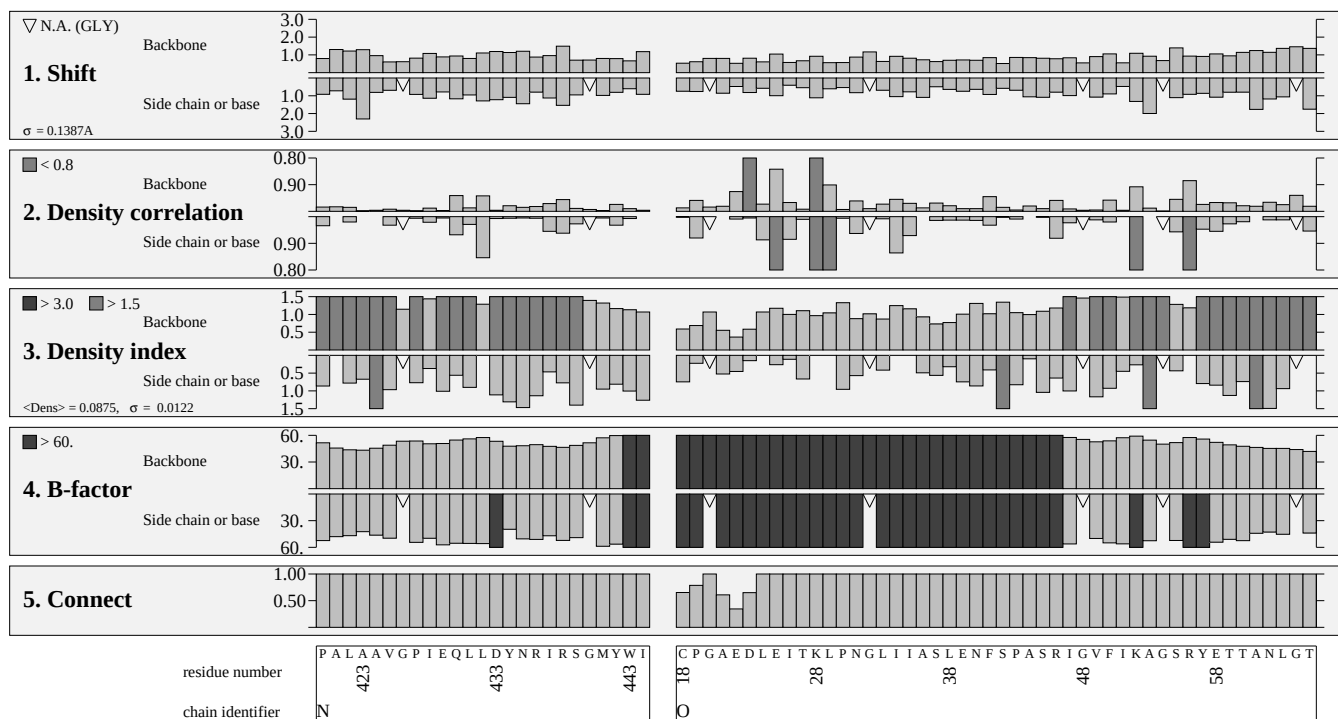
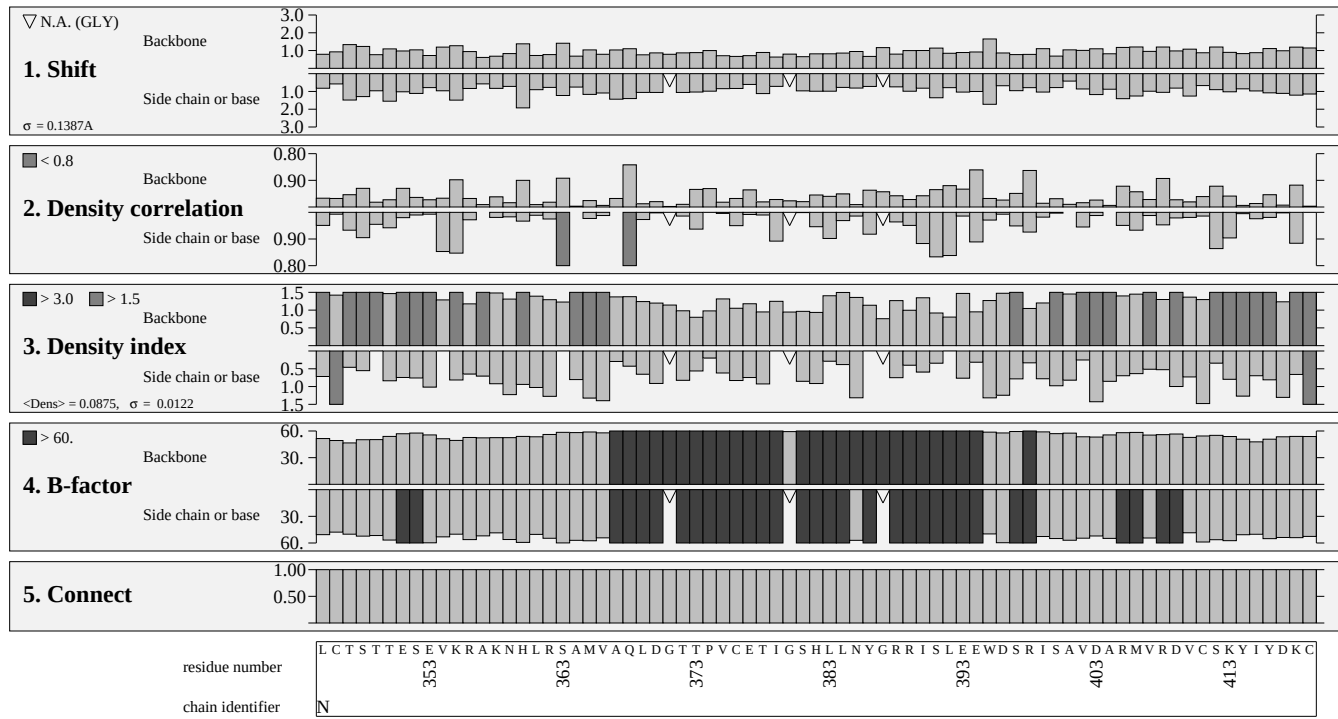
Local estimation (16)



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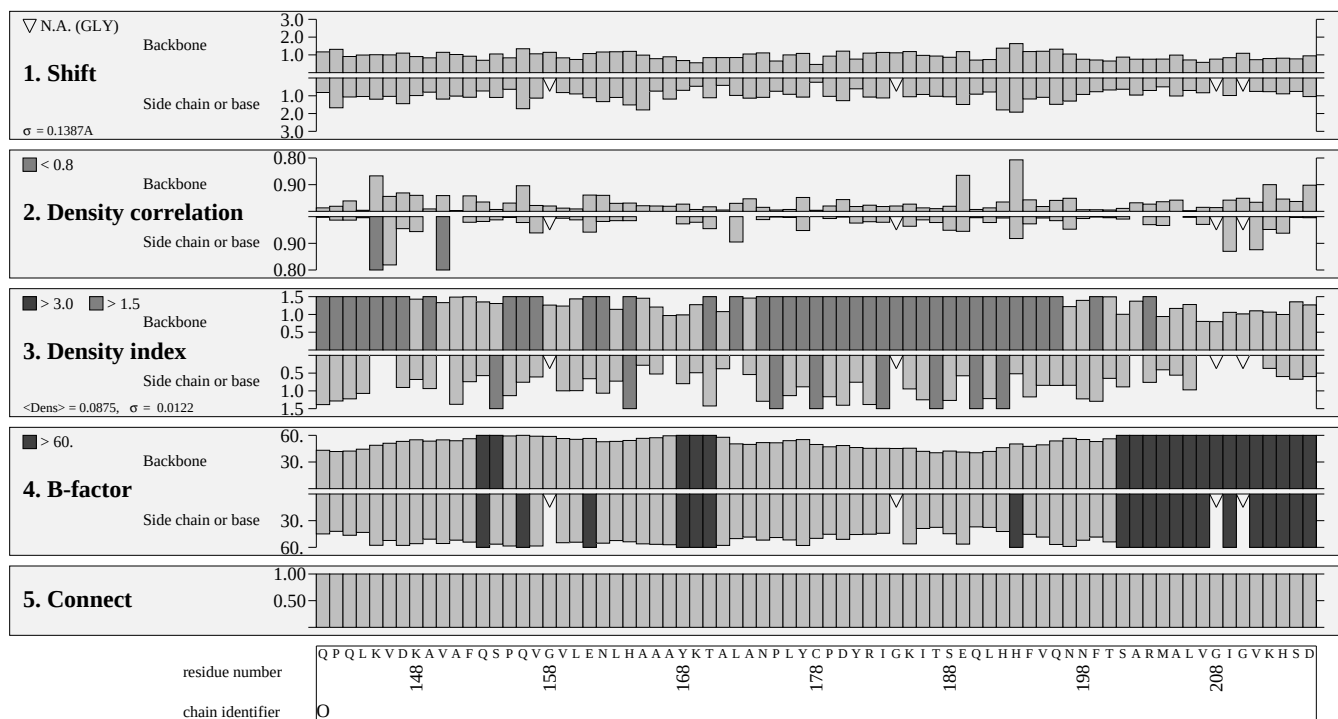
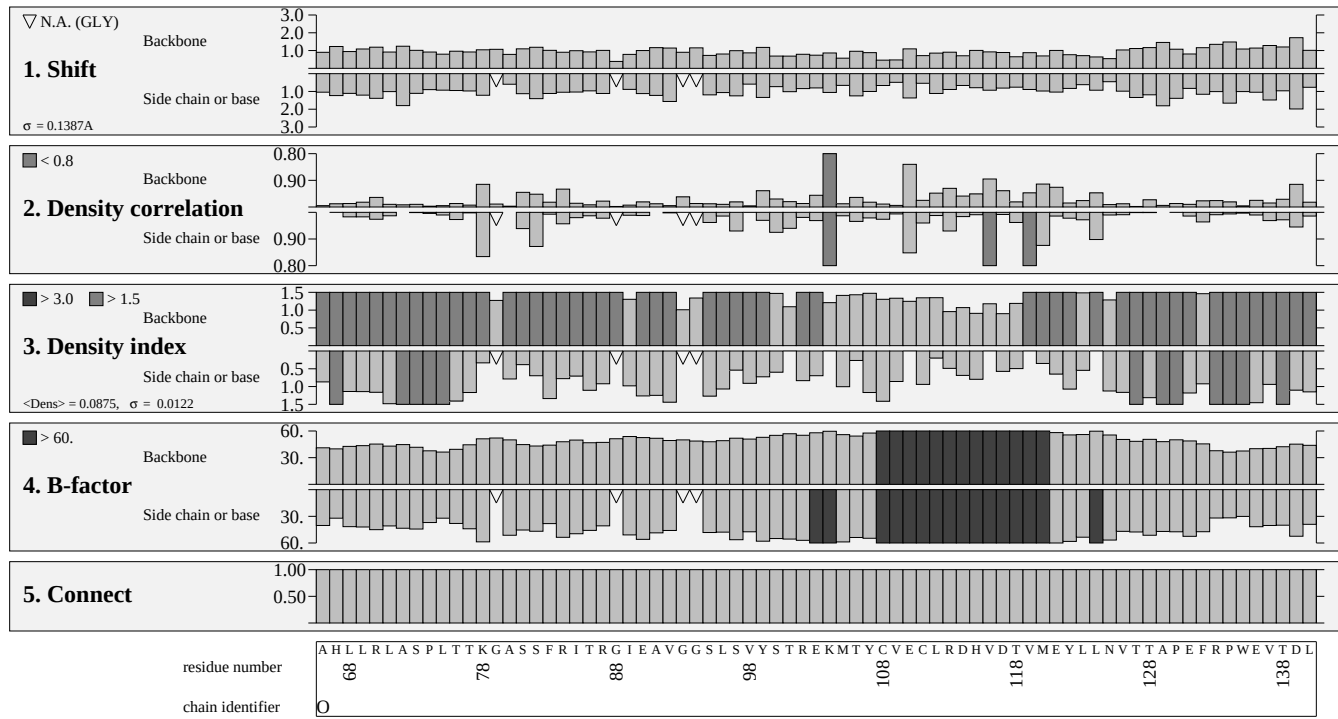
Local estimation (17)



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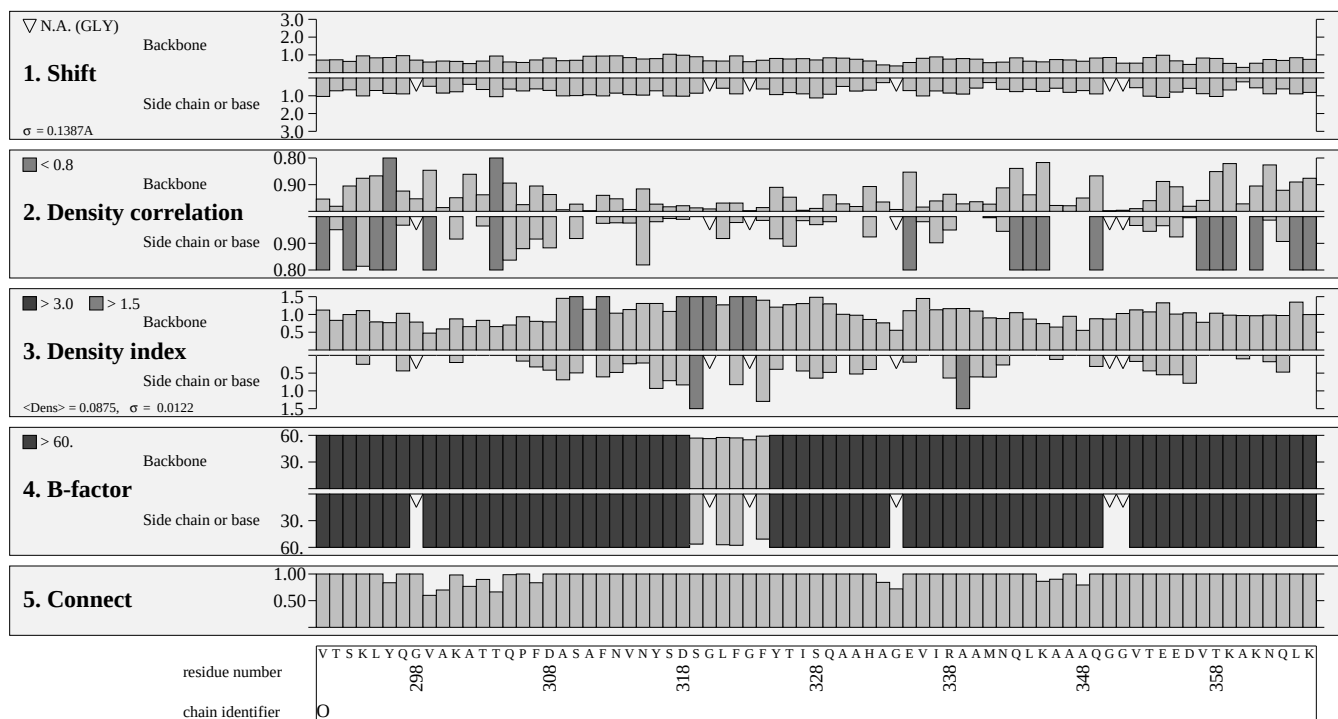
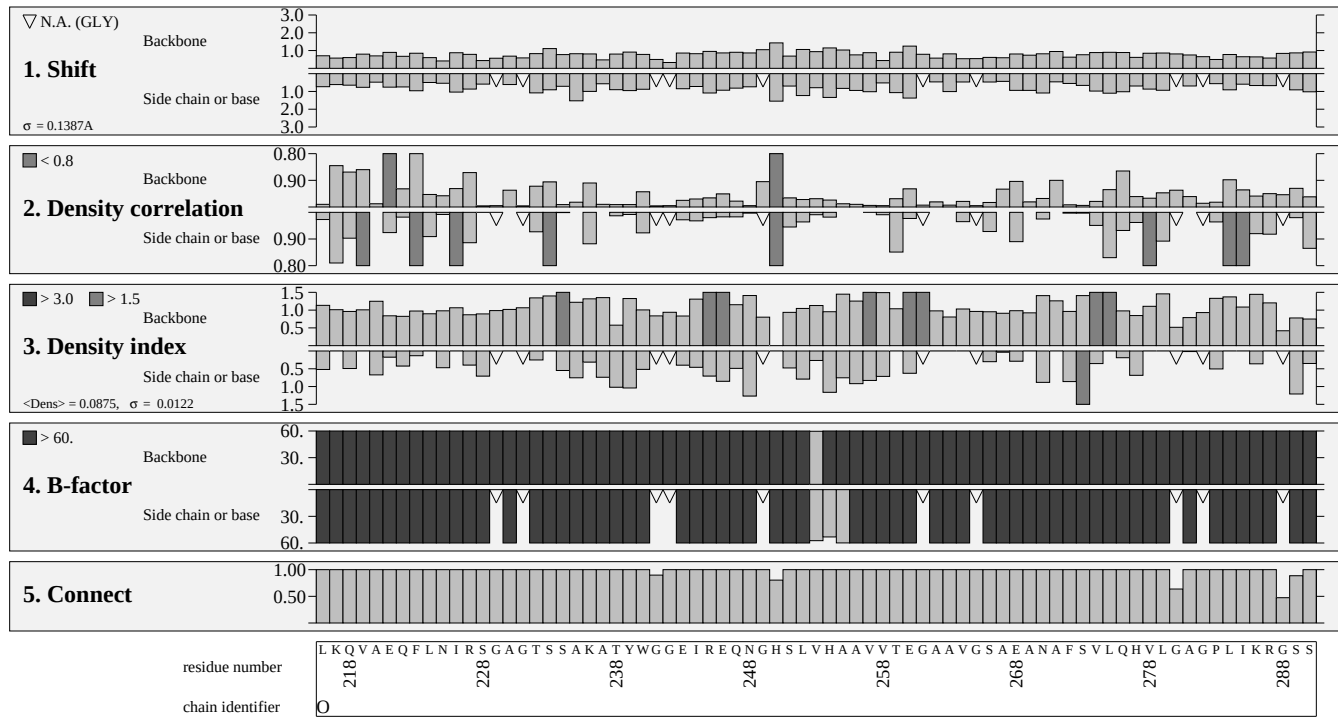
Local estimation (18)



Structure Factor Check

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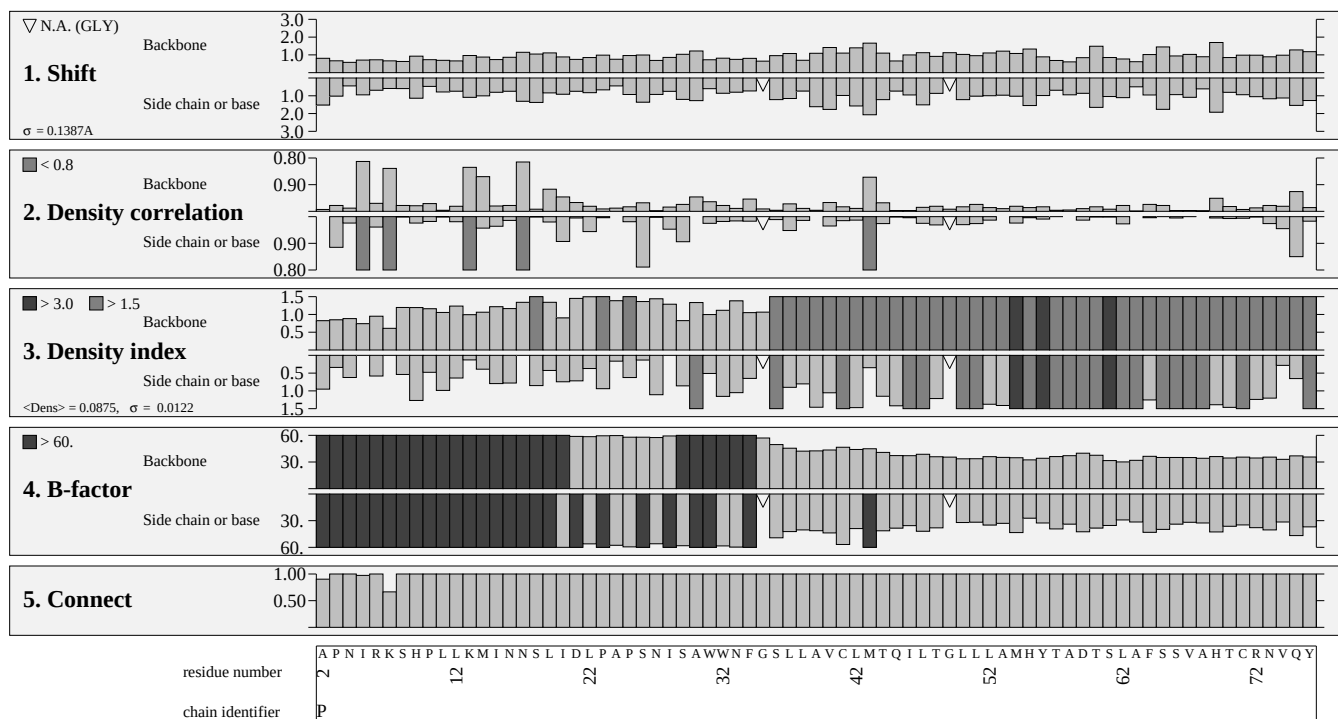
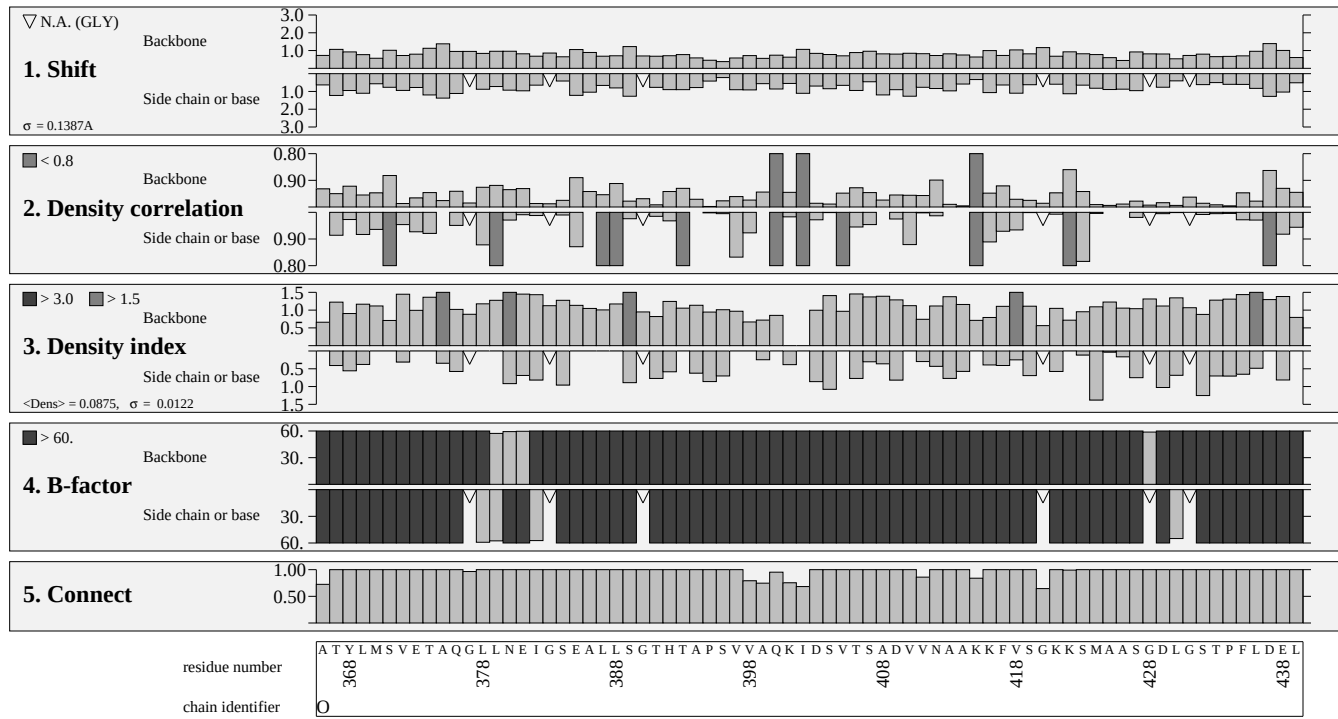
Local estimation (19)



Structure Factor Check

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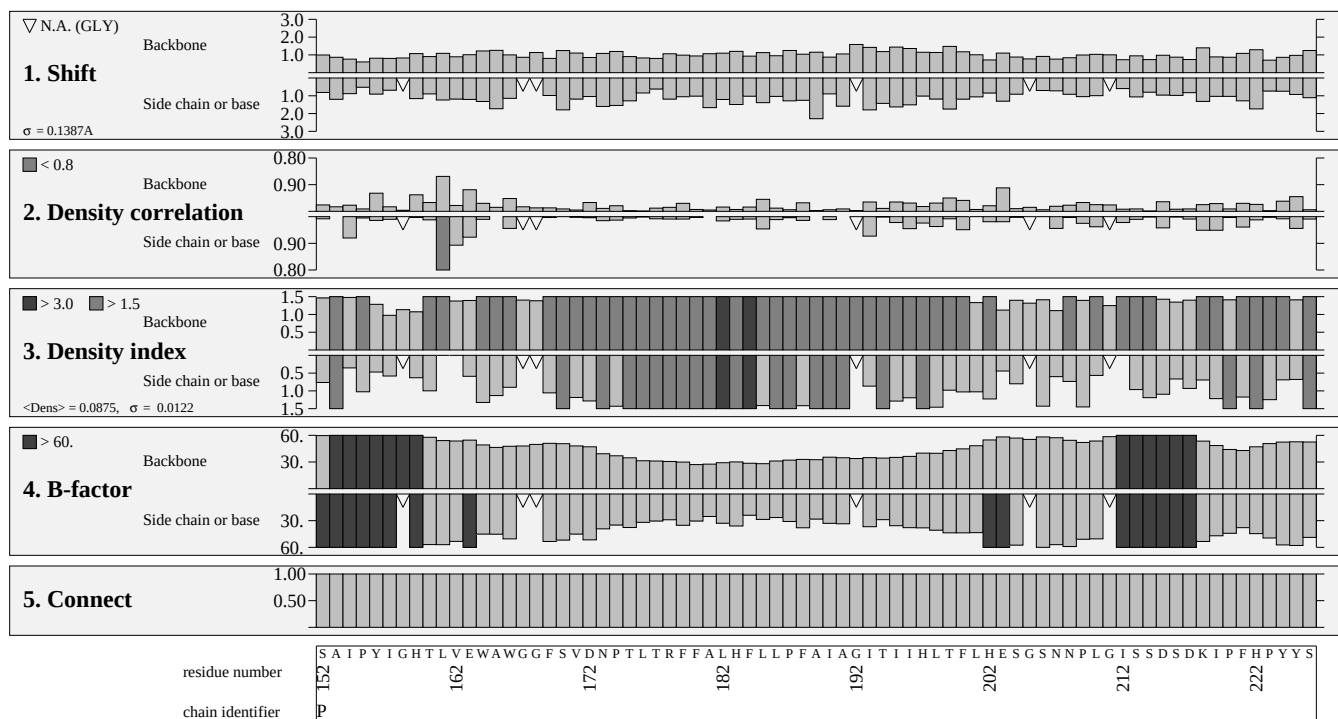
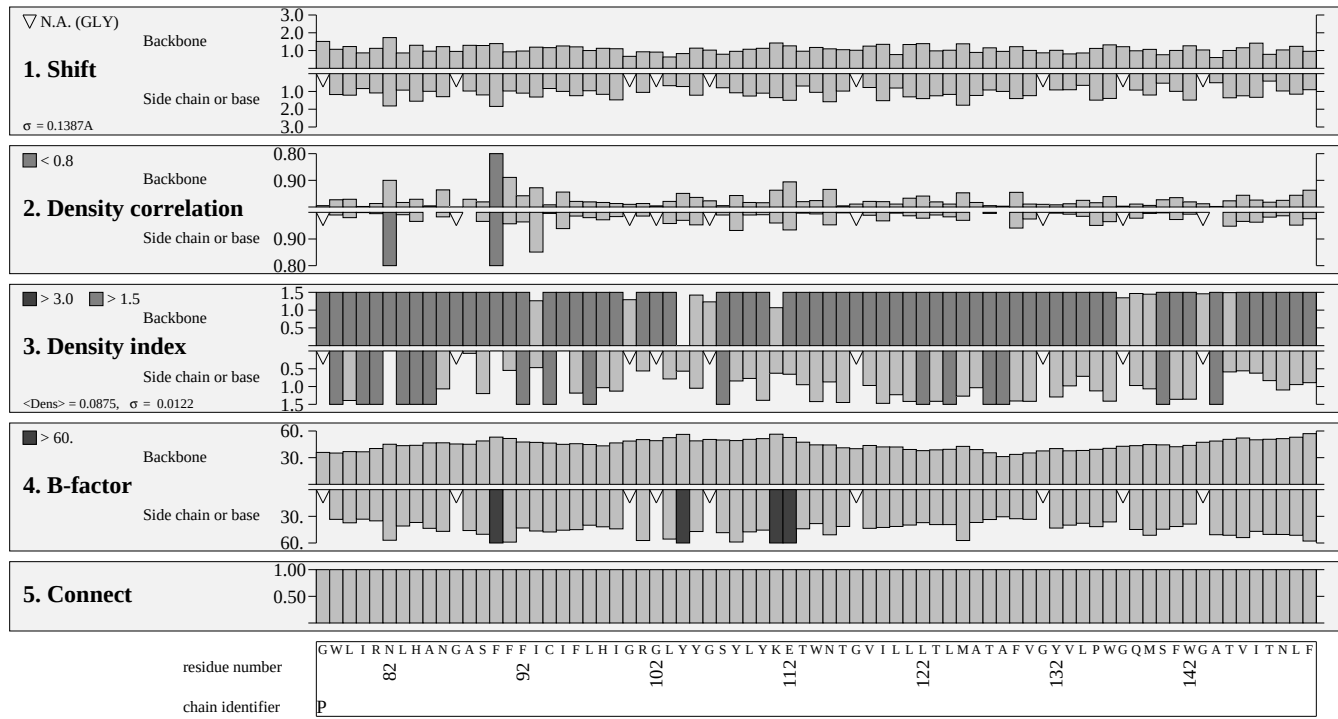
Local estimation (20)



Structure Factor Check

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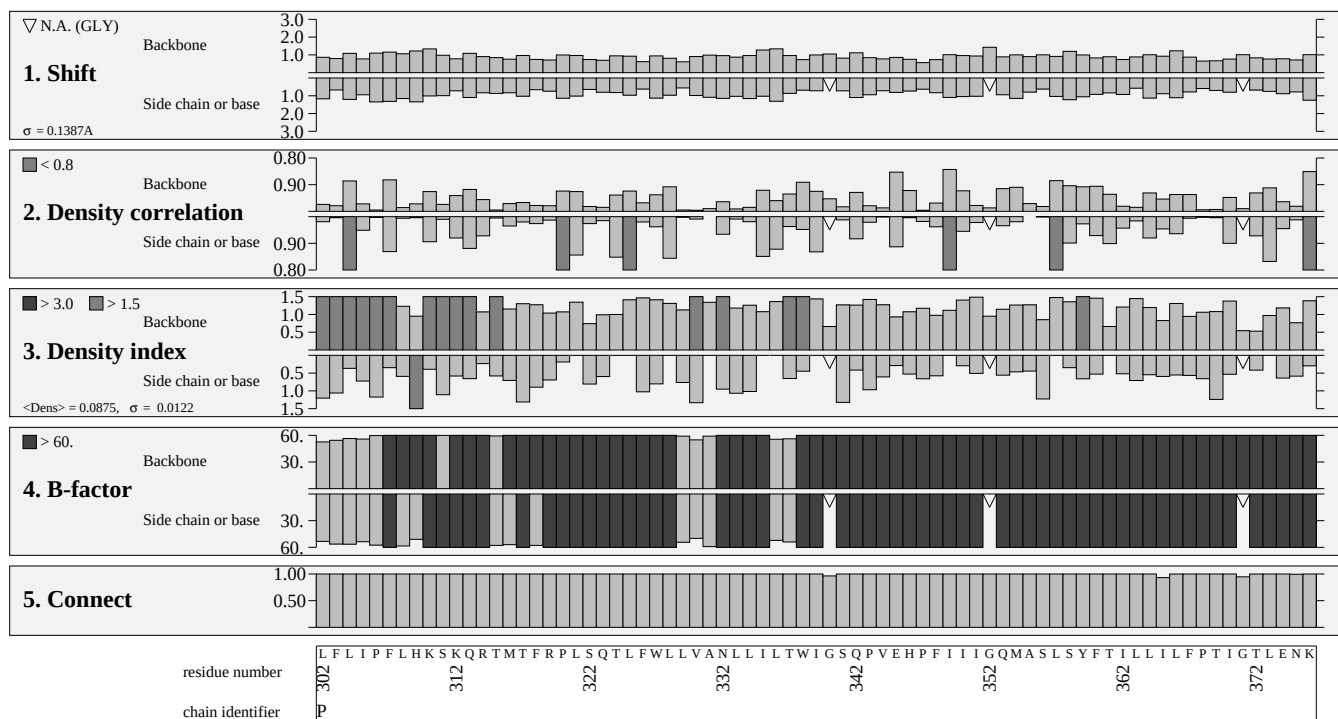
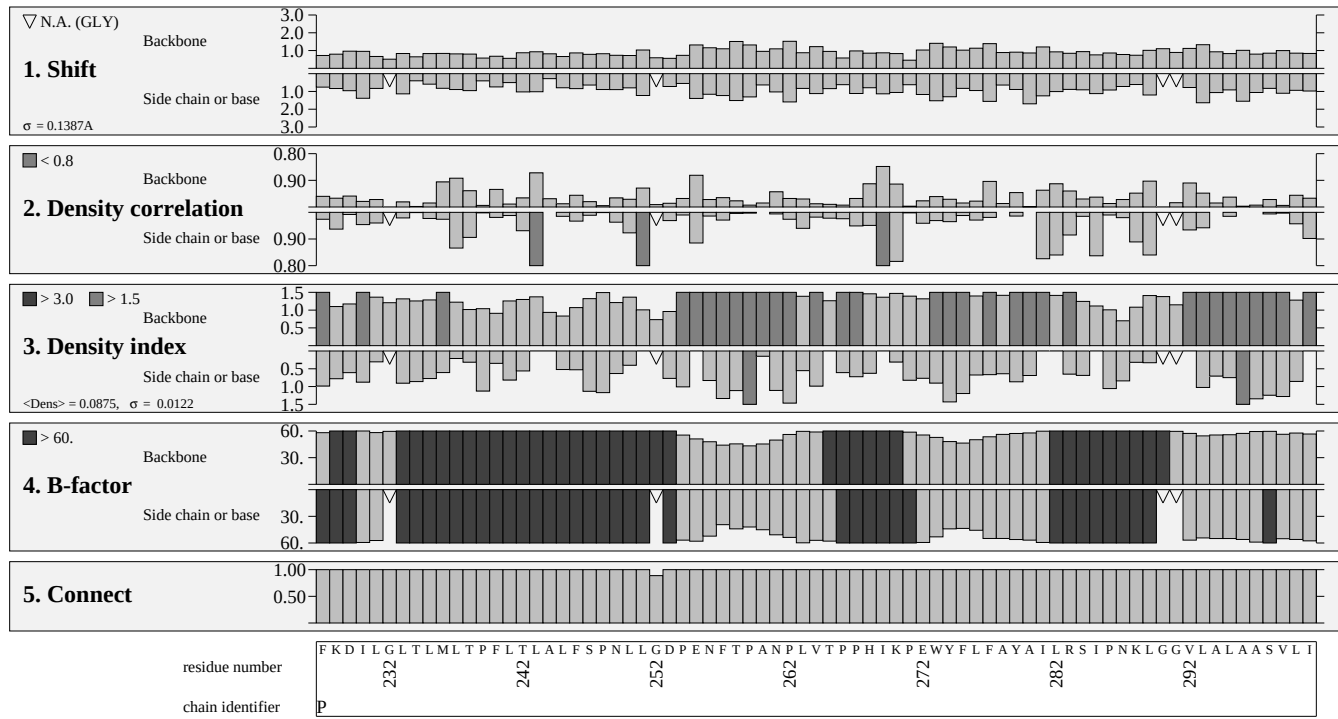
Local estimation (21)



Structure Factor Check

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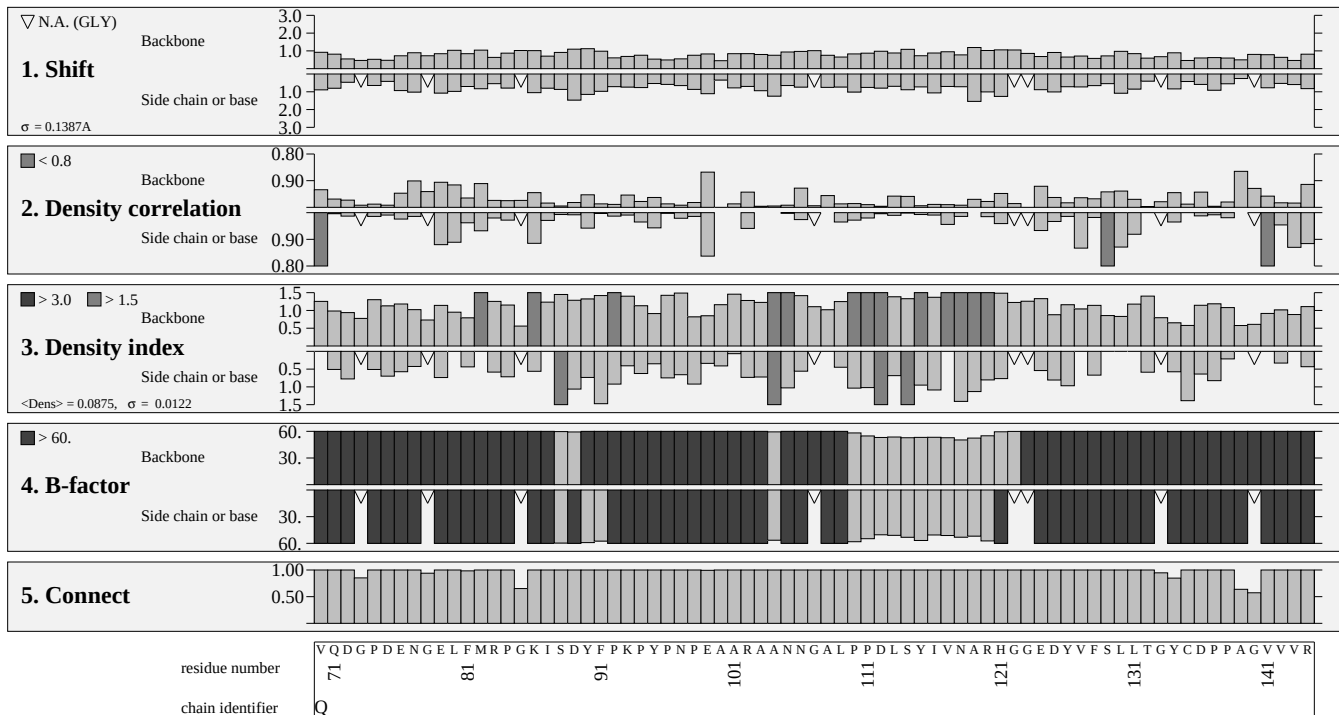
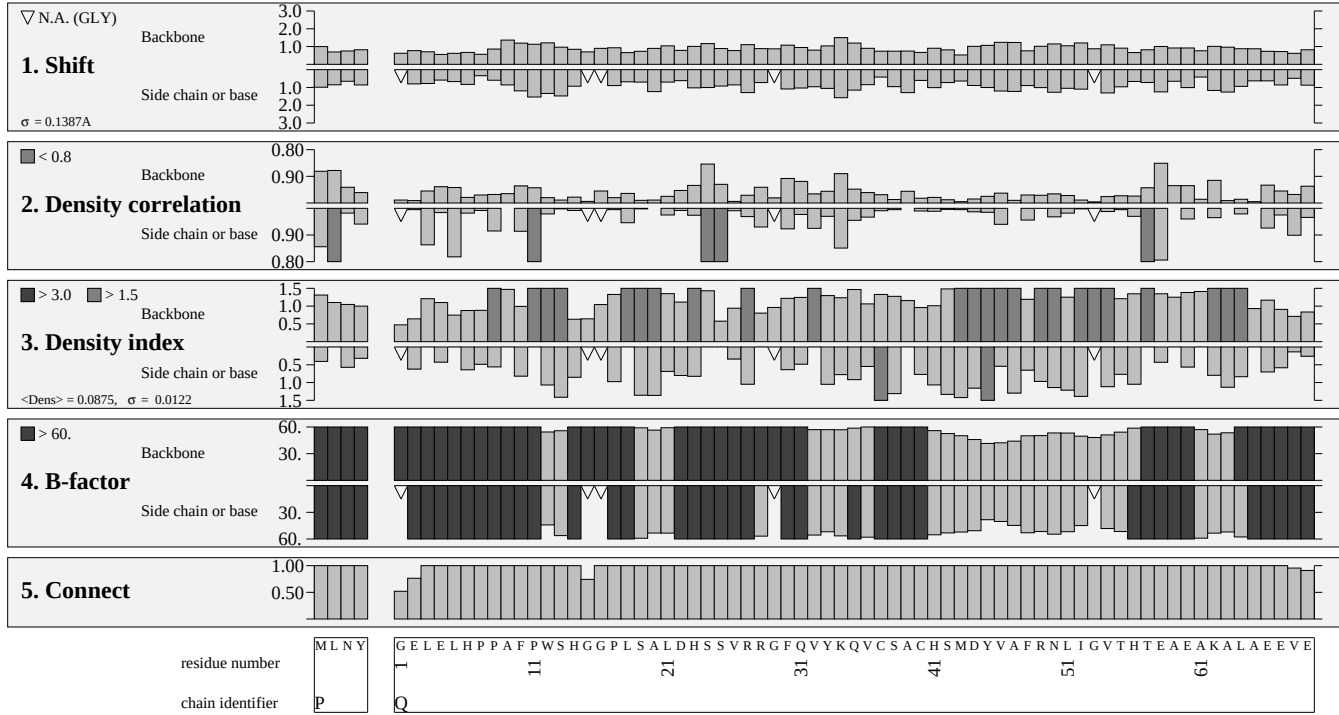
Local estimation (22)



Structure Factor Check

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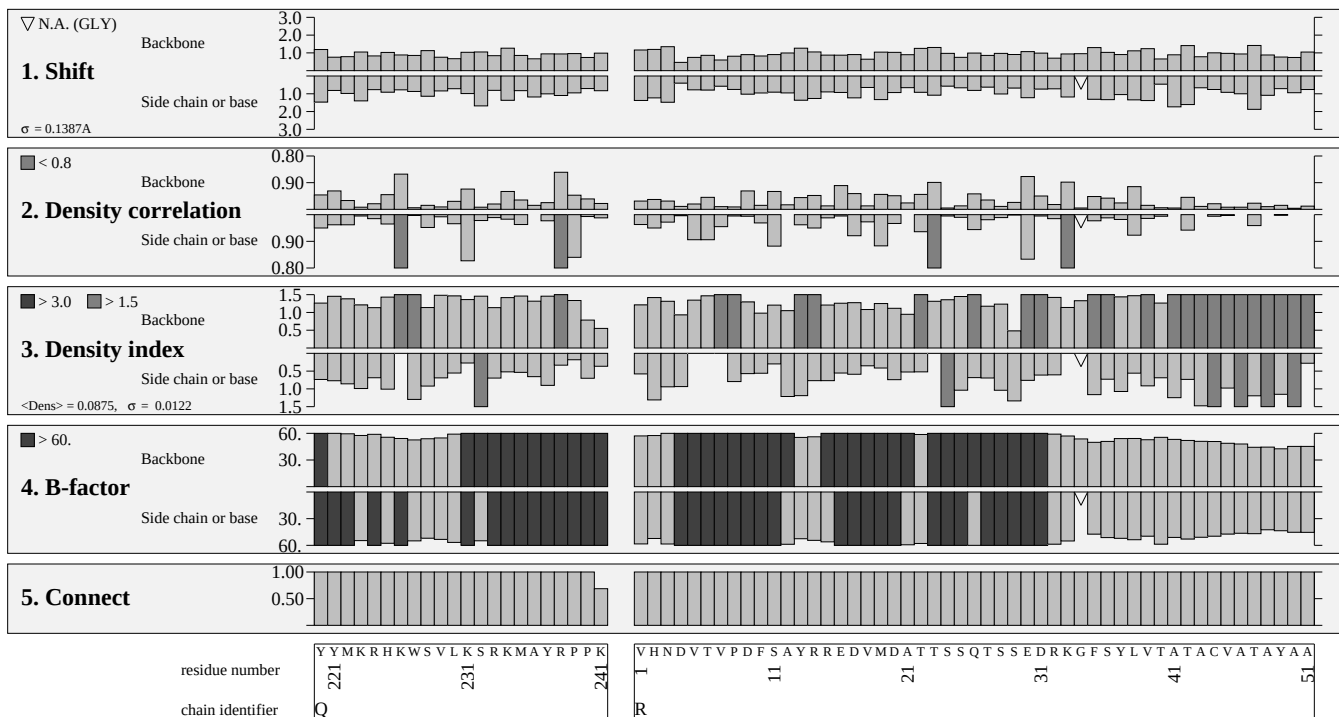
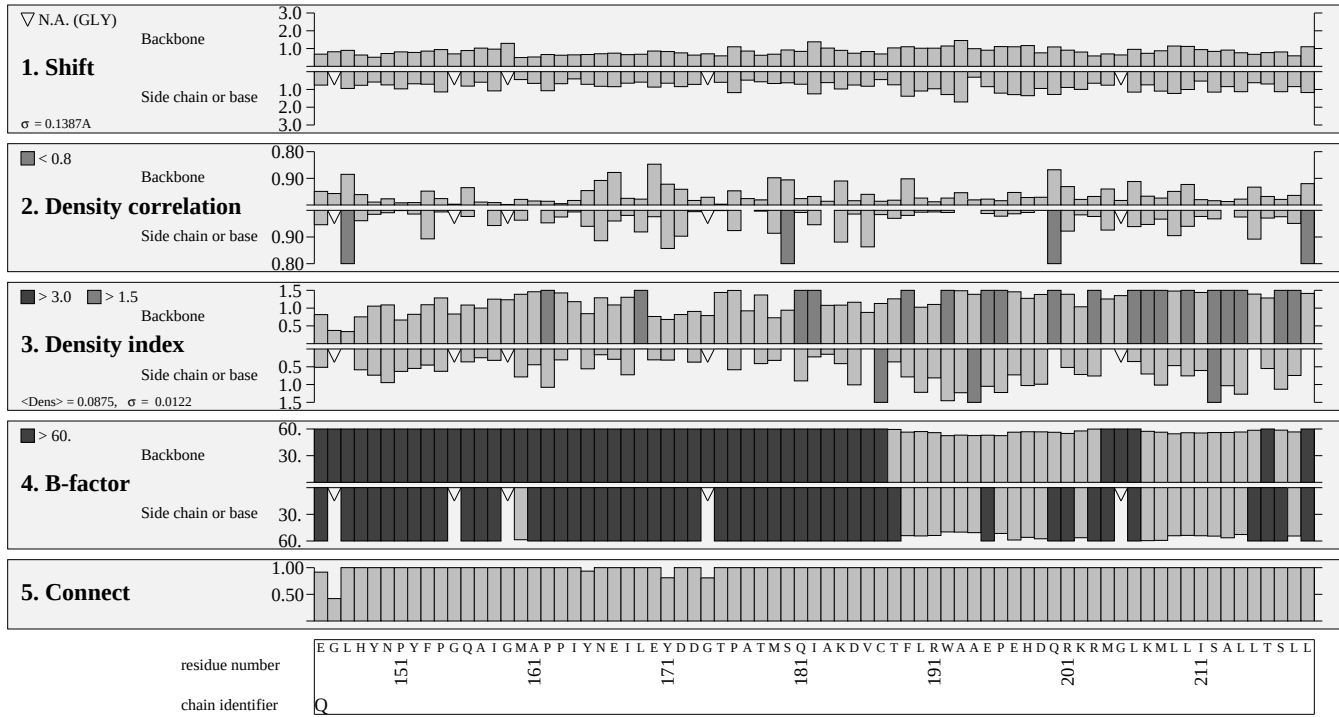
Local estimation (23)



Structure Factor Check

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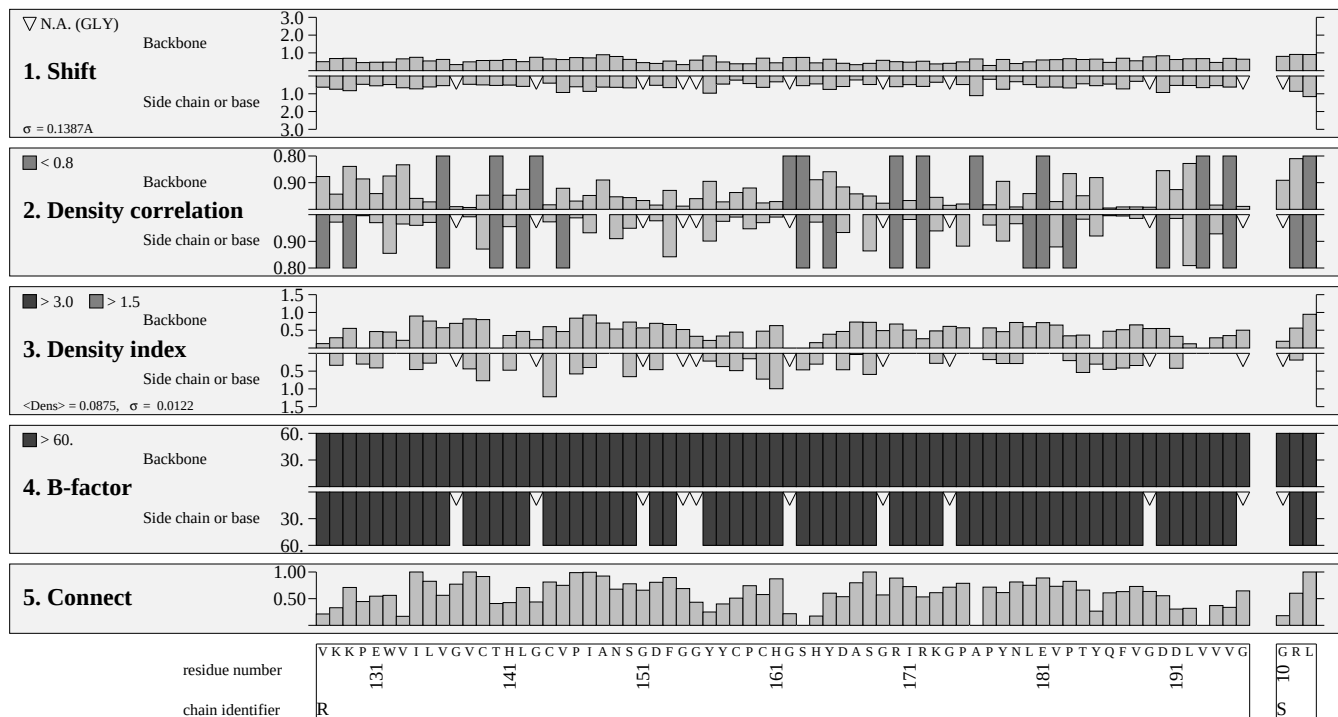
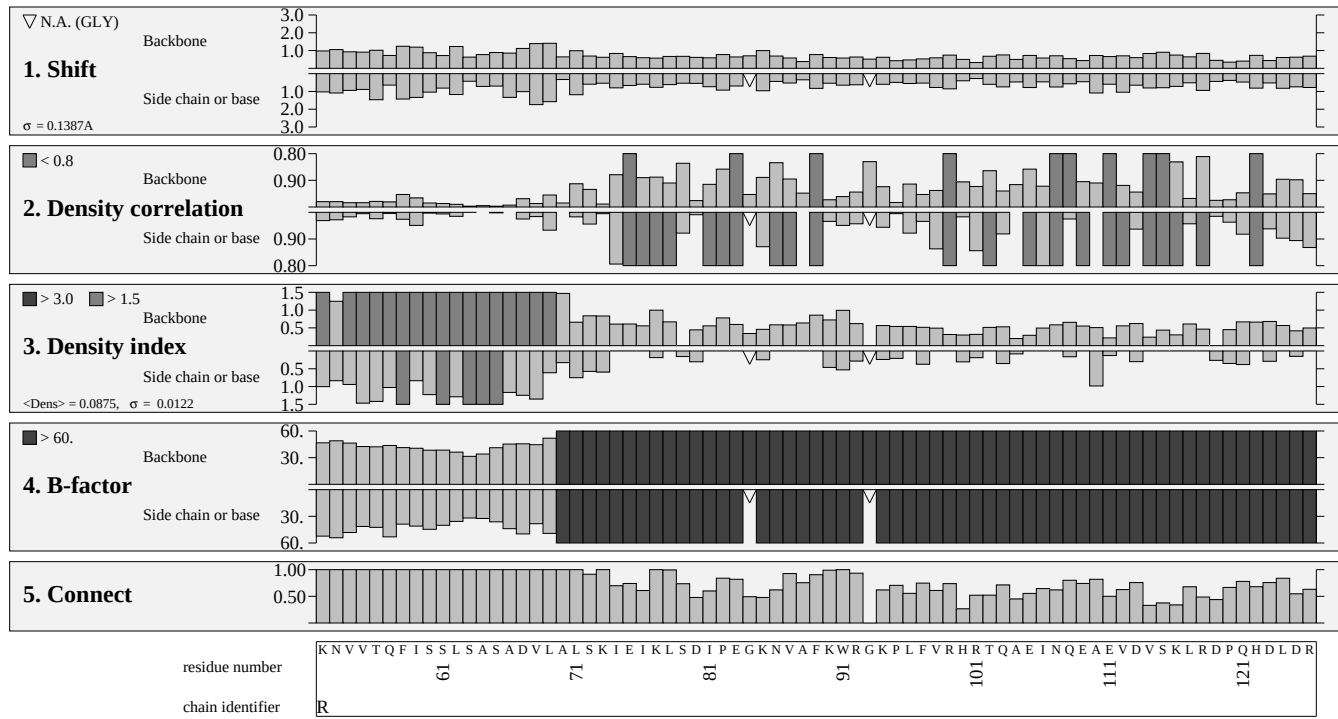
Local estimation (24)



Structure Factor Check

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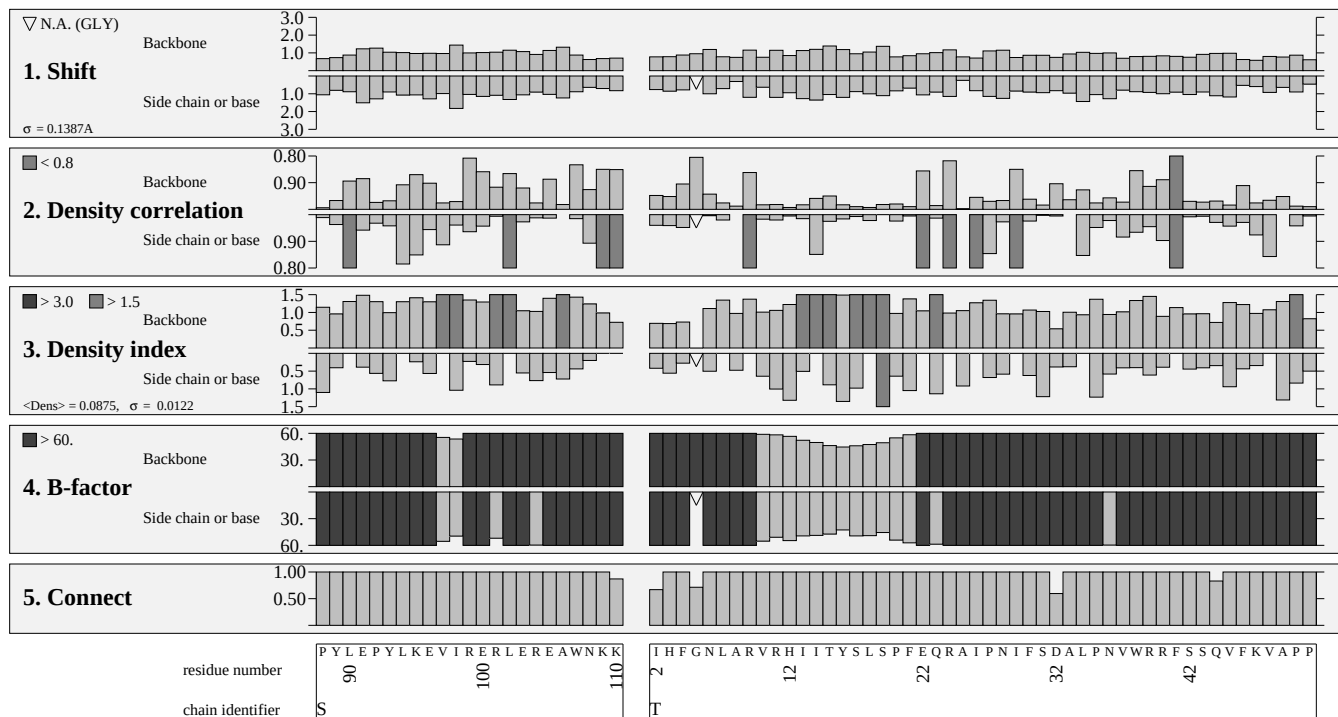
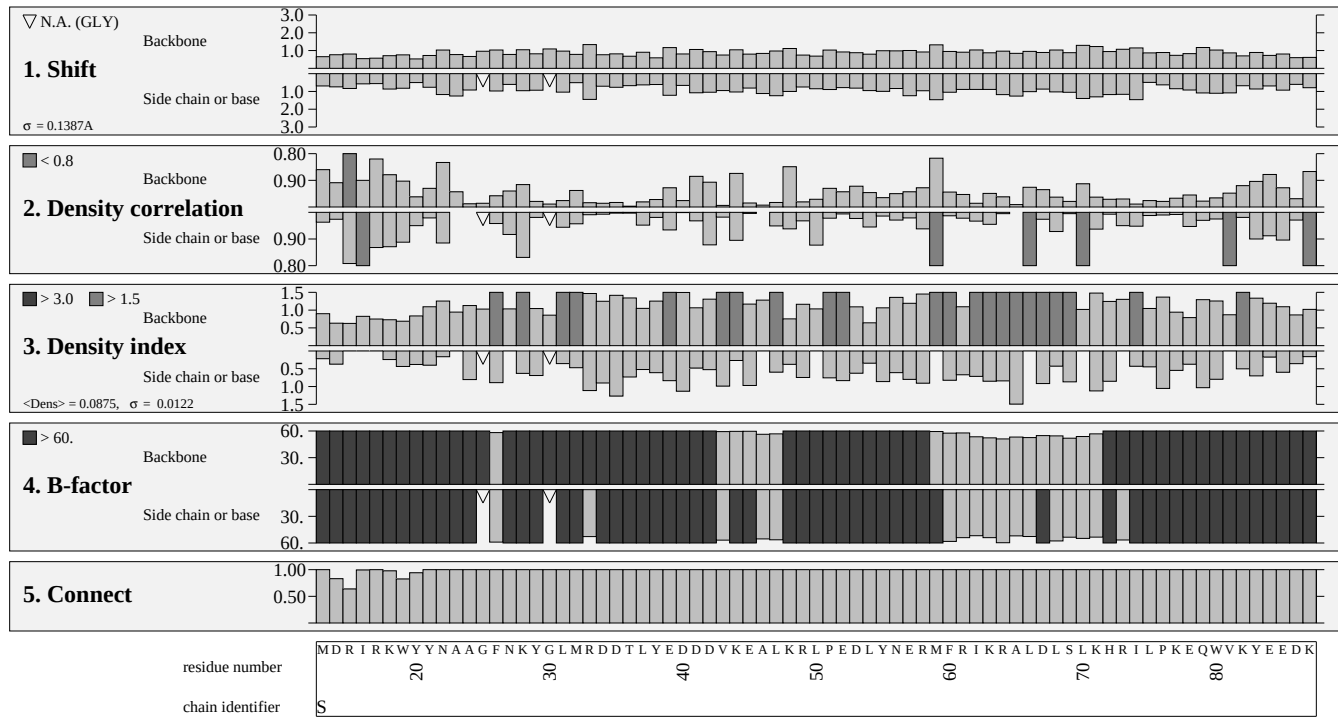
Local estimation (25)



Structure Factor Check

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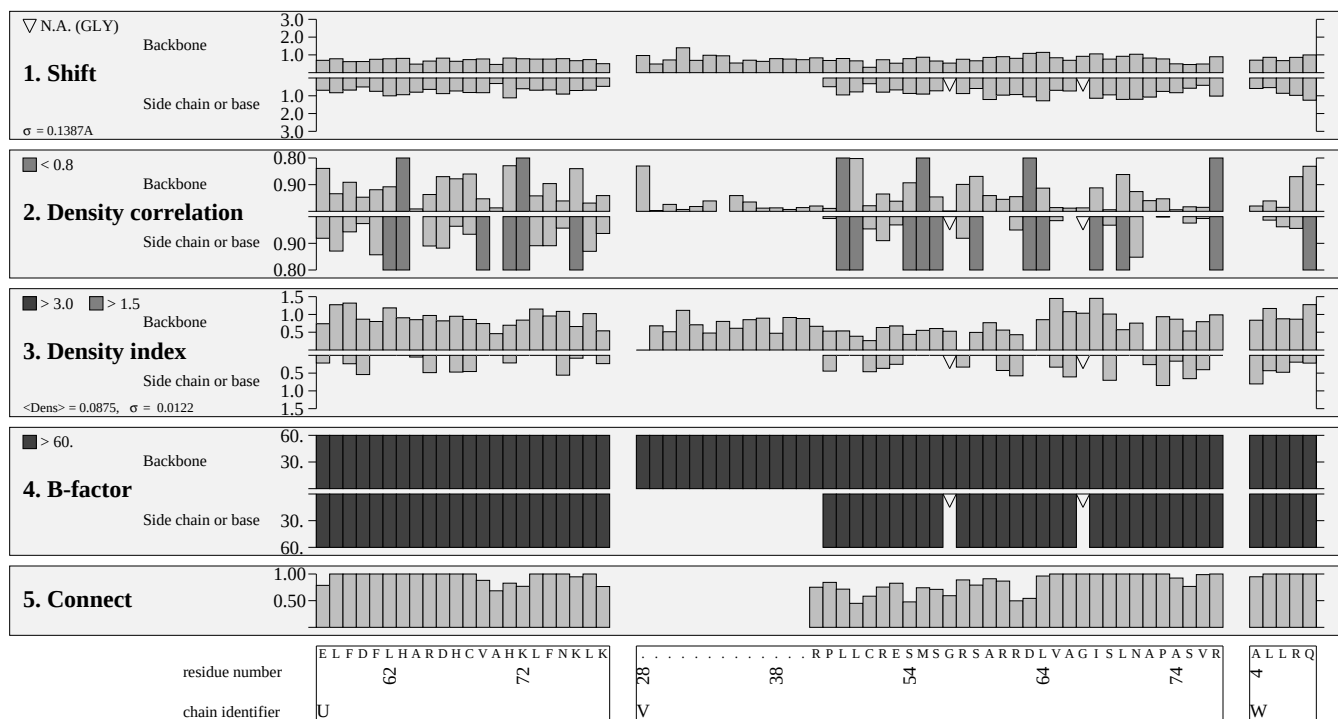
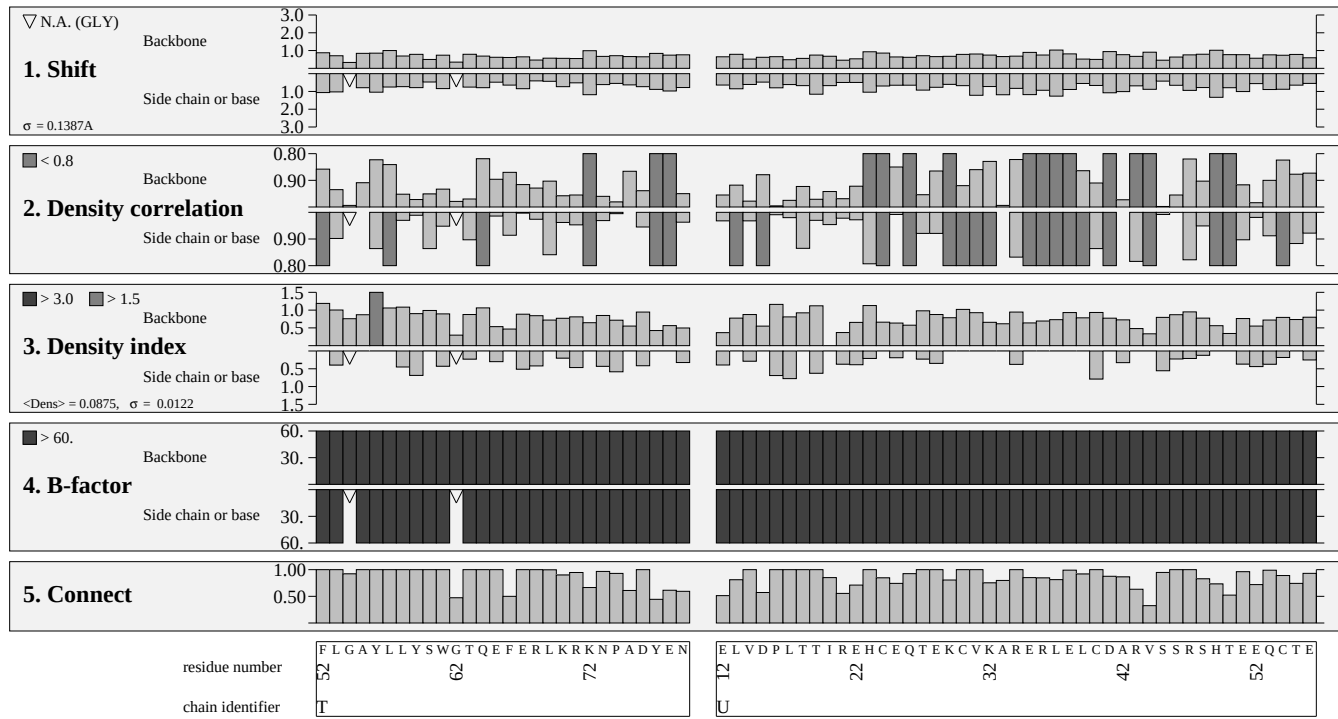
Local estimation (26)



Structure Factor Check

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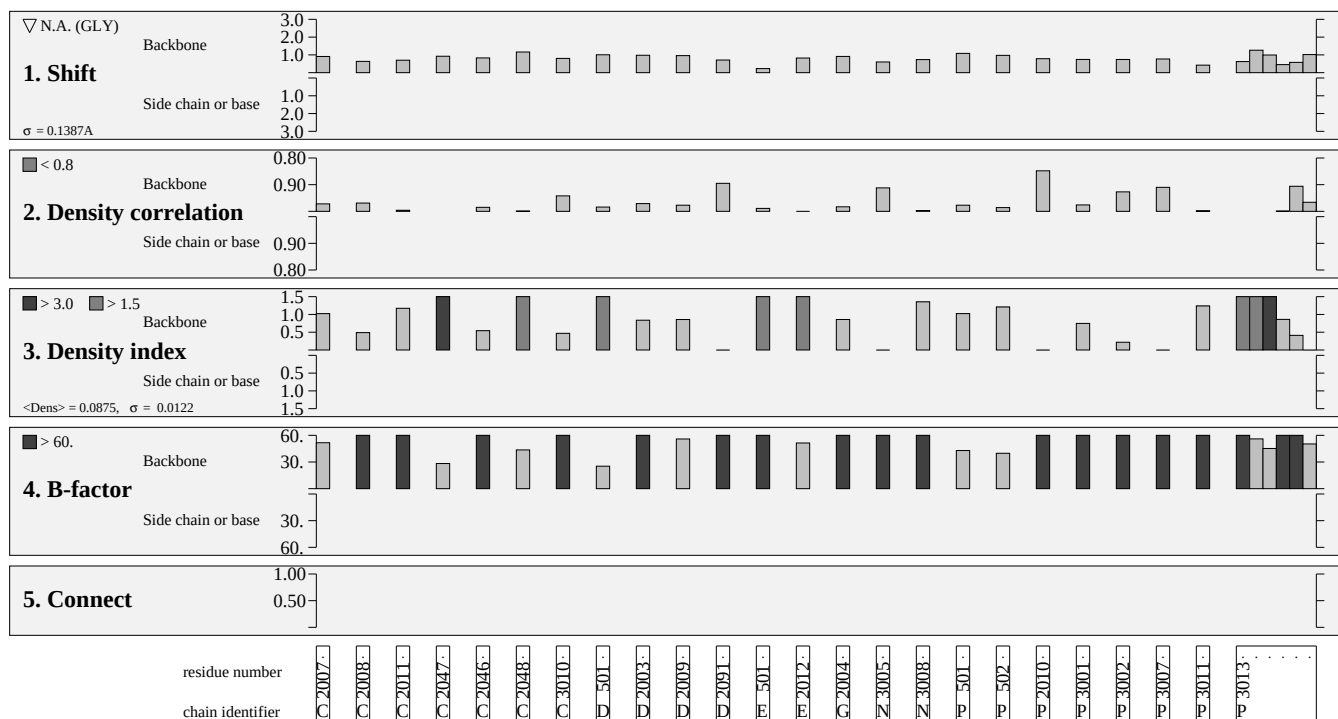
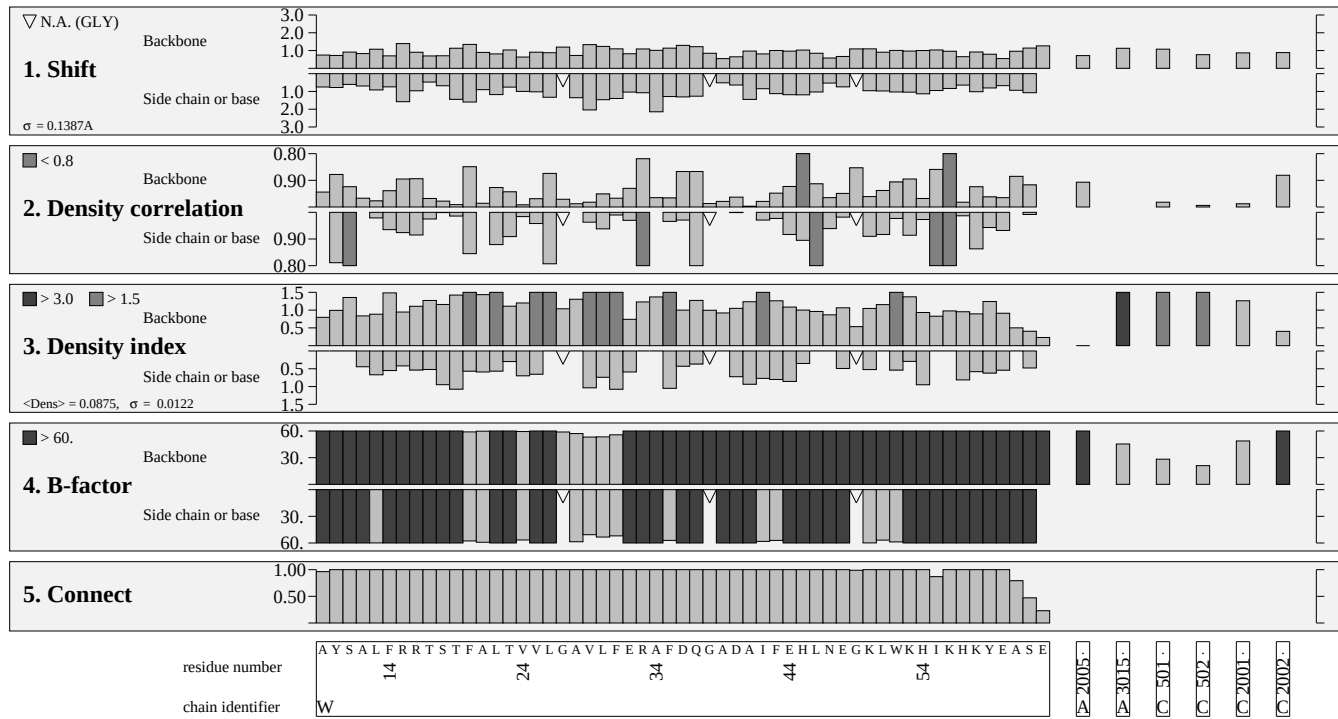
Local estimation (27)



Structure Factor Check

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Local estimation (28)



Local estimation (29)

