

Structure Factor Check

3L75

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH FENAMIDONE BOUND
 Date: 28-DEC-09
 PDB code: 3L75

Crystal

Cell parameters:

a: 172.29 A b: 182.14 A c: 241.20 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 58.8 – 2.79 A
 Reflections in file: 183994
 Unique reflections above 0: 183994
 above 1 σ : 178823
 above 3 σ : 120410

SF CHECK

Nominal resolution range: 58.8 – 2.79 A
 \05max. from input data, min. from author\05
 Used reflections: 183854
 Reflections out of resolution: 140
 Completeness: 97.6 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.070
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.6055 0.6856
 B_{overall} (by Patterson): 47. A²
 Optical resolution: 2.09 A
 Expected opt. resol. for complete data set: 2.09 A
 Estimated minimal error: 0.069 A

Model

32691 atoms (28 water molecules)

Number of chains: 51

Volume not occupied by model: 62.6 %

$\langle B \rangle$ (for atomic model): 66.7 A²

$\sigma(B)$: 20.63 A²

Matthews coefficient: 4.13

Corresponding solvent % : 70.02

Model vs. Structure Factors

R-factor for all reflections: 0.287
 Correlation factor: 0.865
 R-factor: 0.291
 for $F > 2.0 \sigma$

nom. resolution range: 58.78 – 2.79 A
 reflections used: 178861

Rfree: 0.313
 Nfree: 3500
 R-factor without free-refl.: 0.291
 Non free-reflections: 175361
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.448 A
 Estimated maximal error: 0.246 A
 DPI: 0.325 A

Scaling

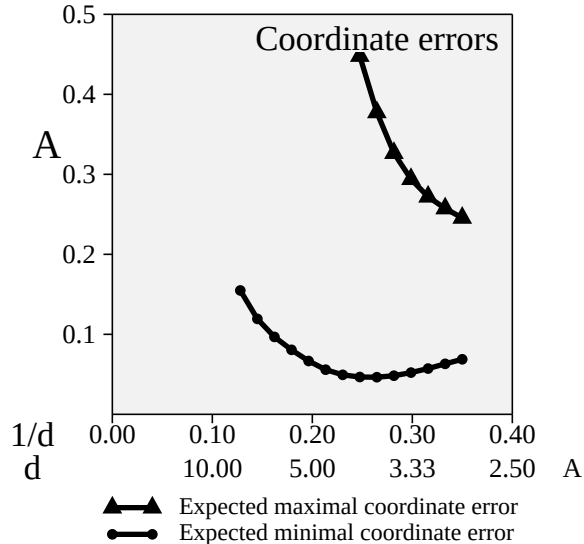
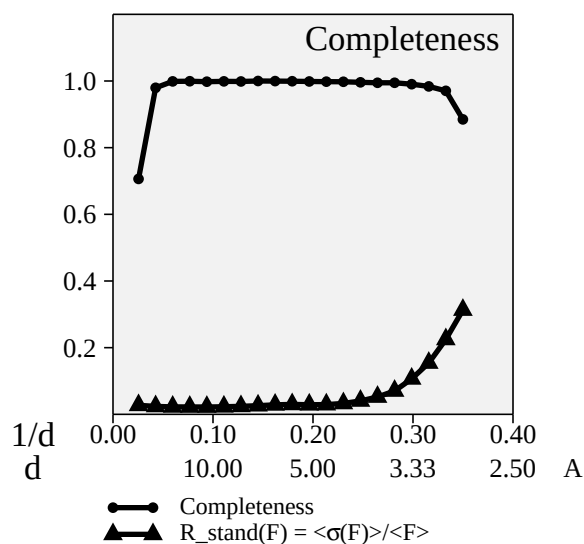
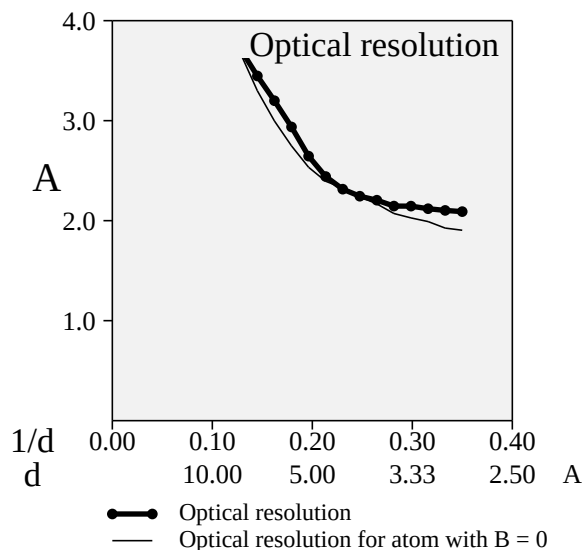
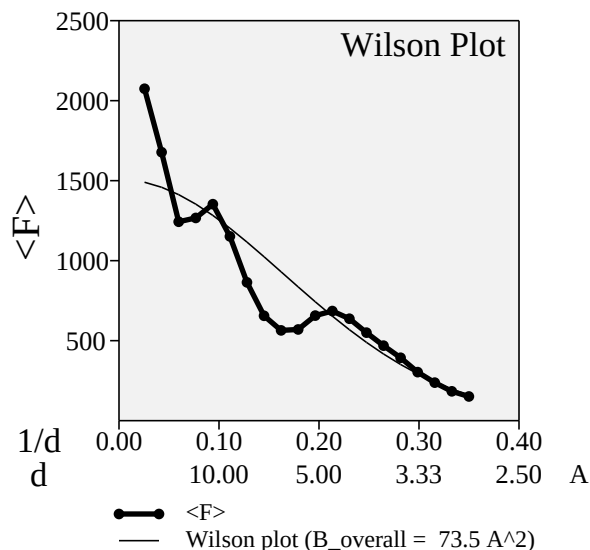
Scale: 0.490
 Bdiff: -6.57
 Anisothermal Scaling (Beta):
 6.4751 -2.1813 0.6422 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.675 250.084

Refinement

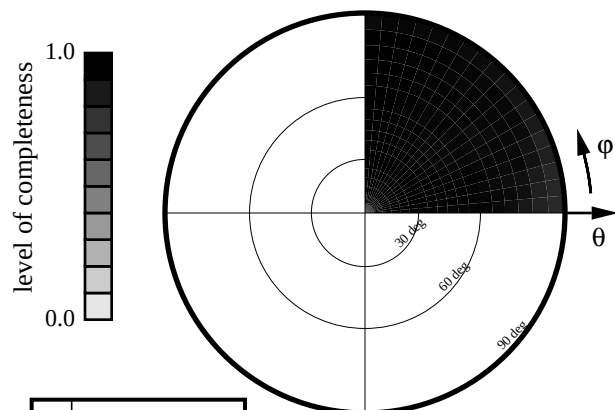
Program: CNS 1.1
 Nominal resolution range: 58.8 – 2.79 A
 Reported R-factor: 0.248
 Number of reflections used: 183854
 Reported Rfree: 0.28
 Sigma cut-off: N.A.

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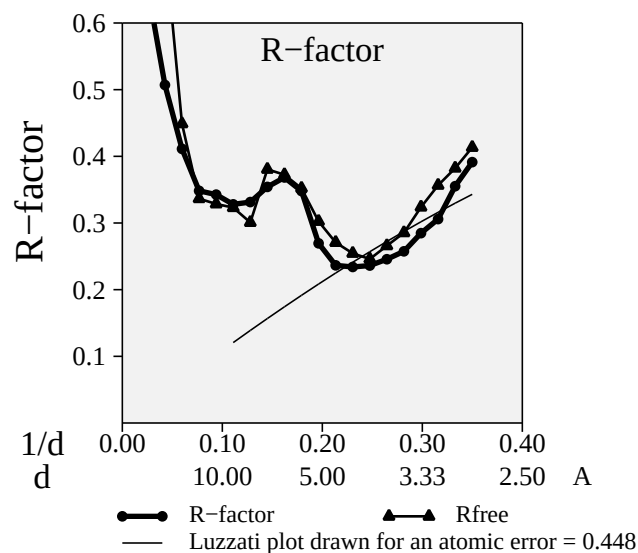


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

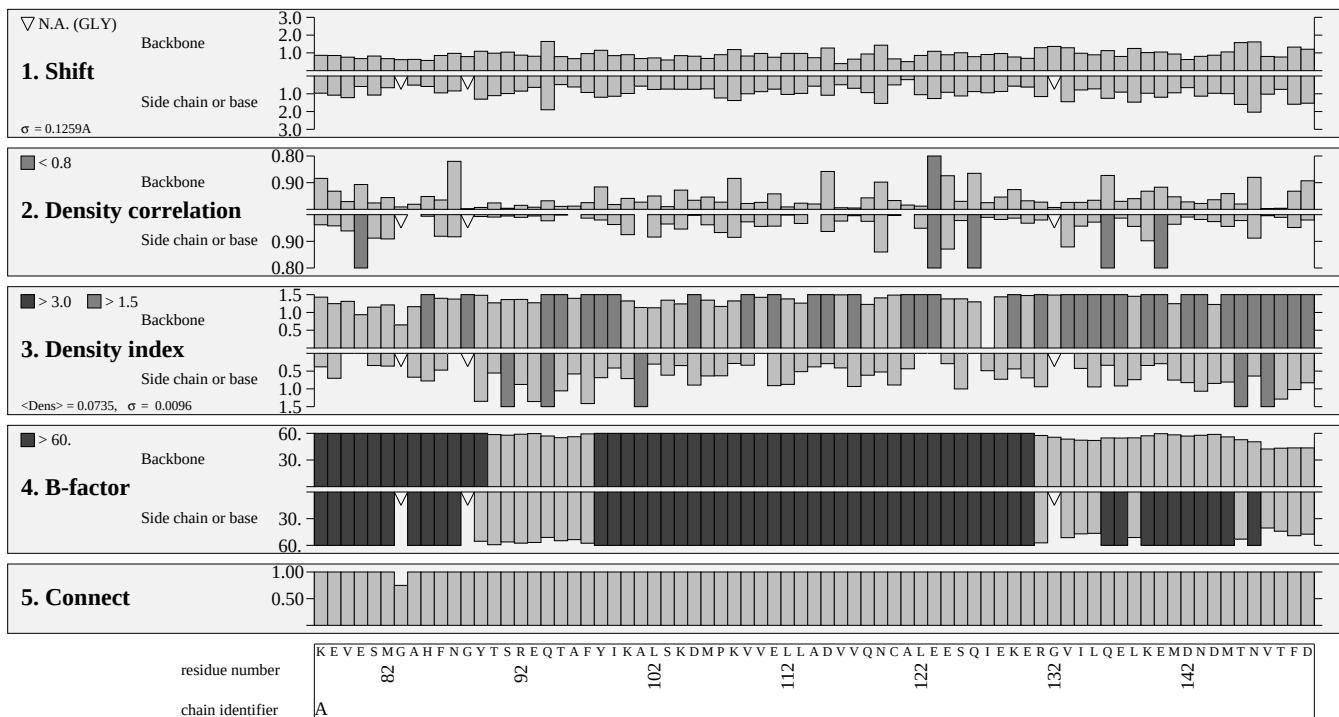
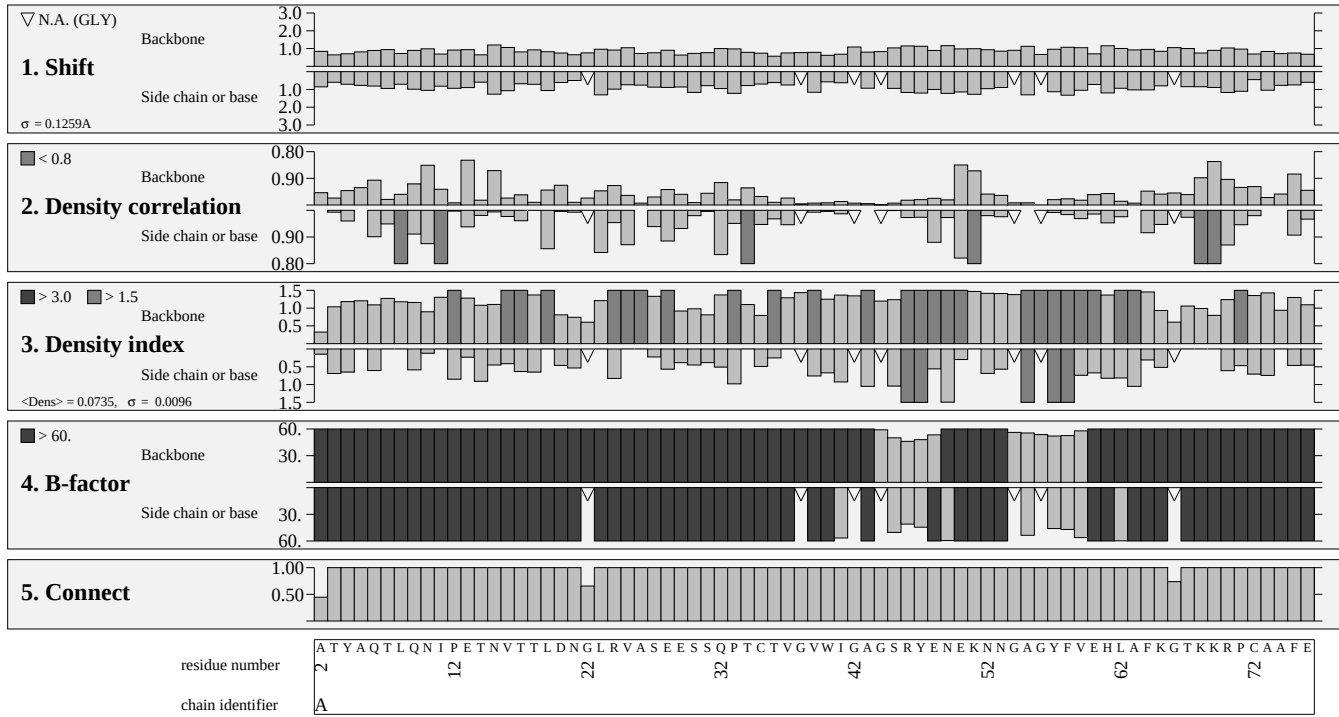
polar coordinates of the crystallographical axes



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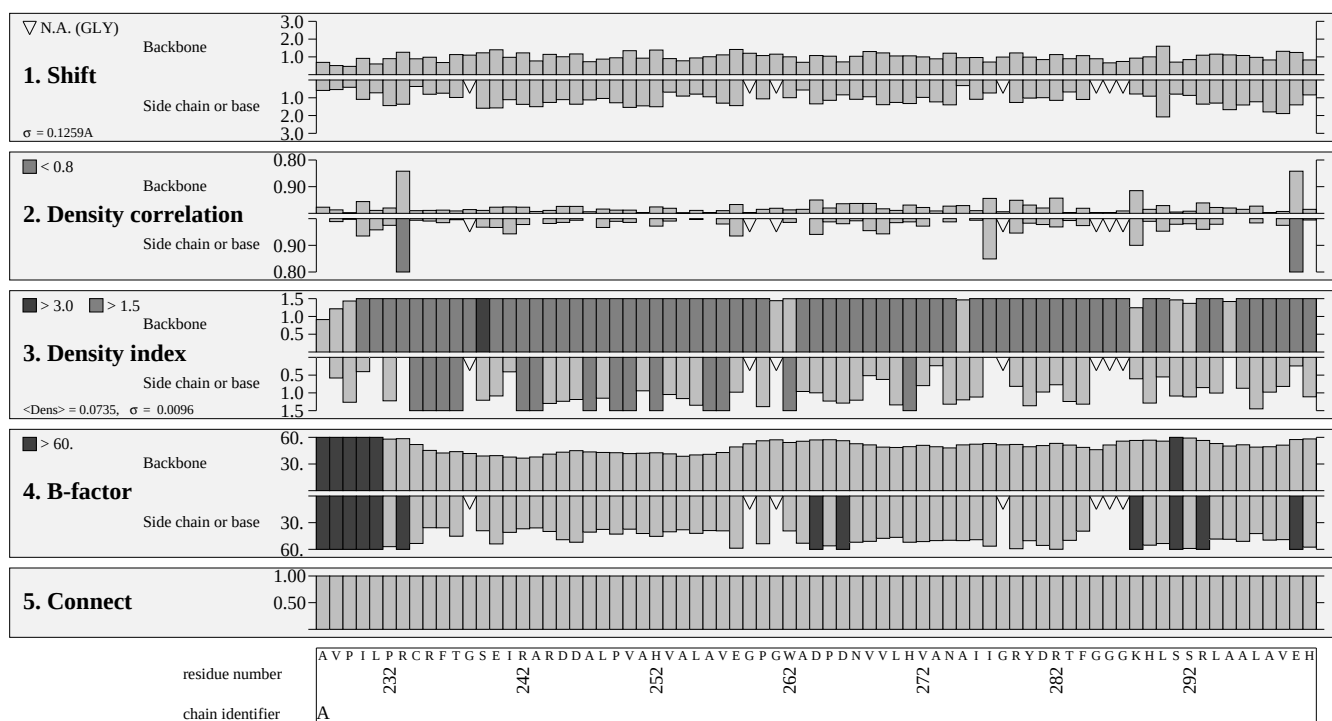
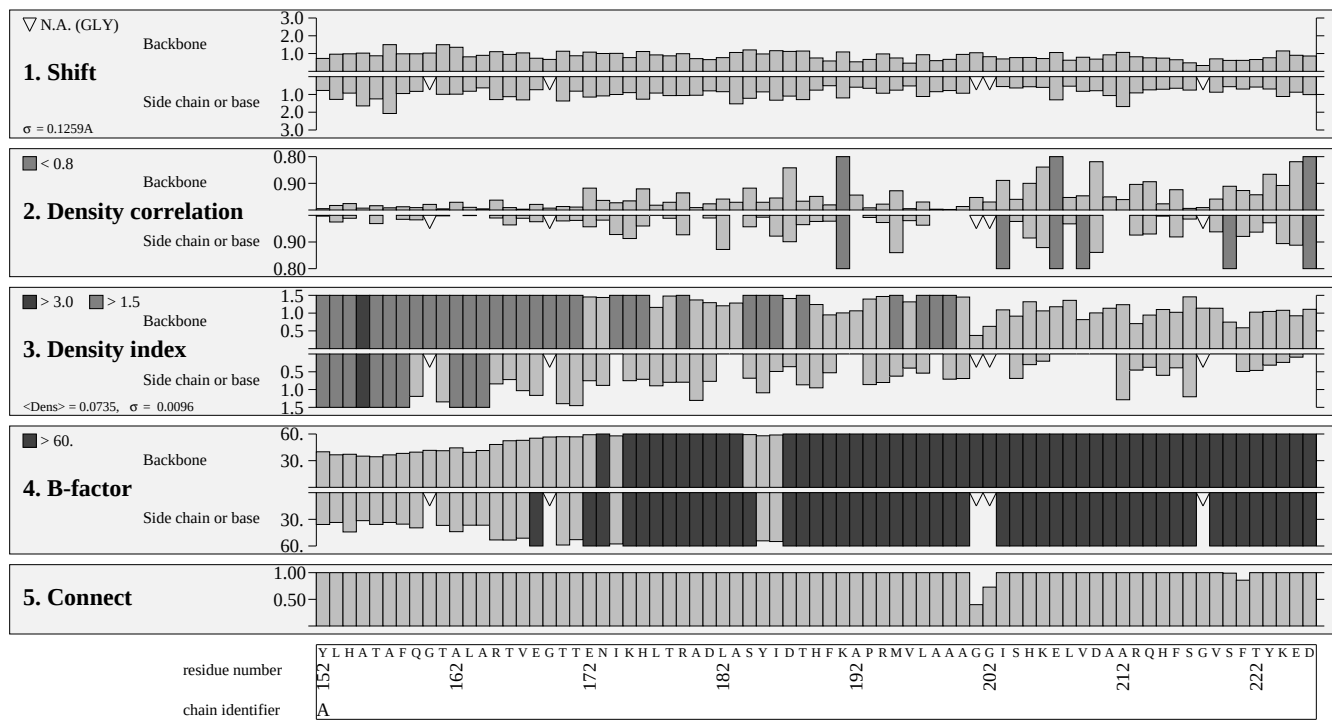
Local estimation



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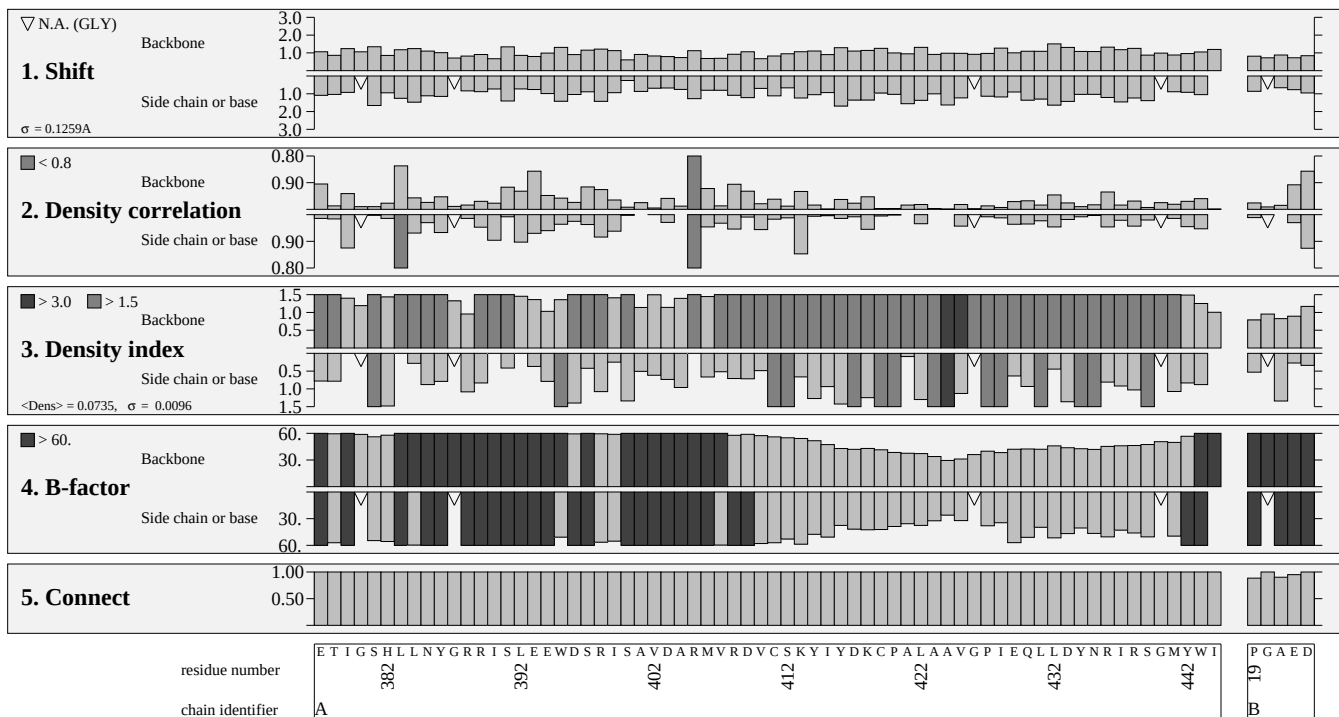
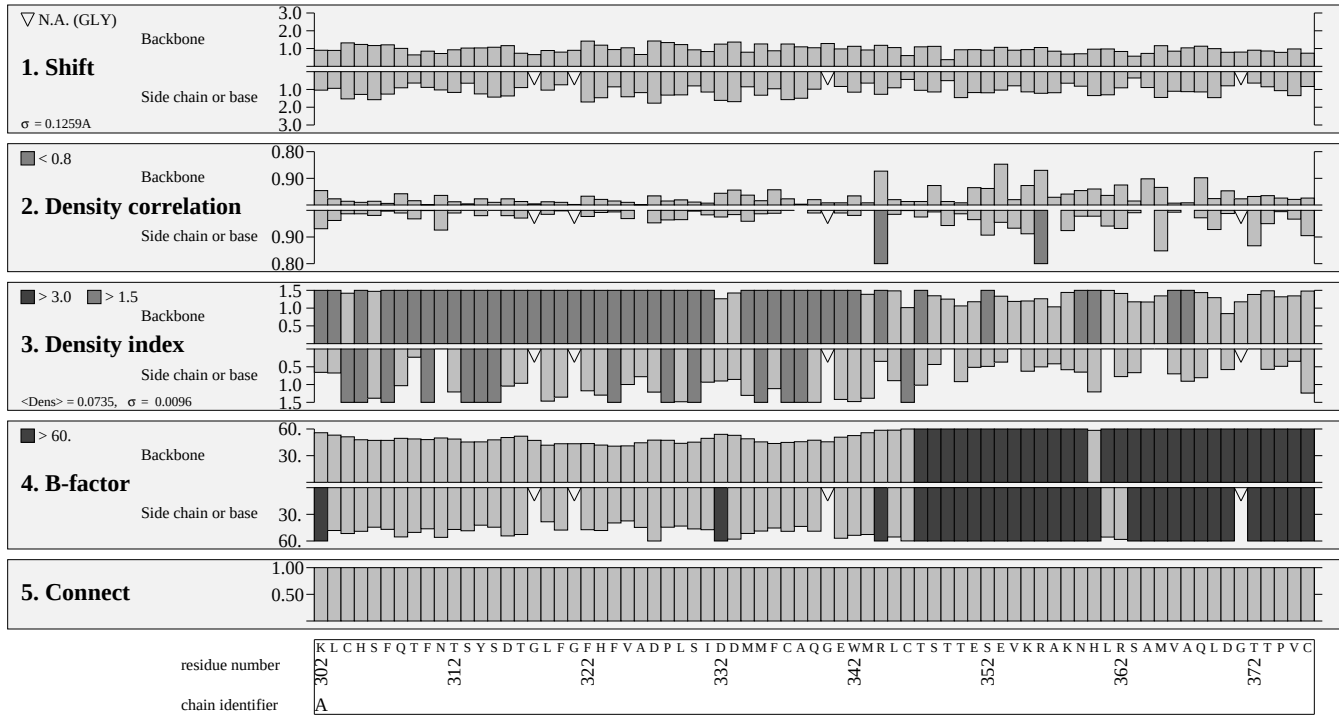
Local estimation (2)



Structure Factor Check

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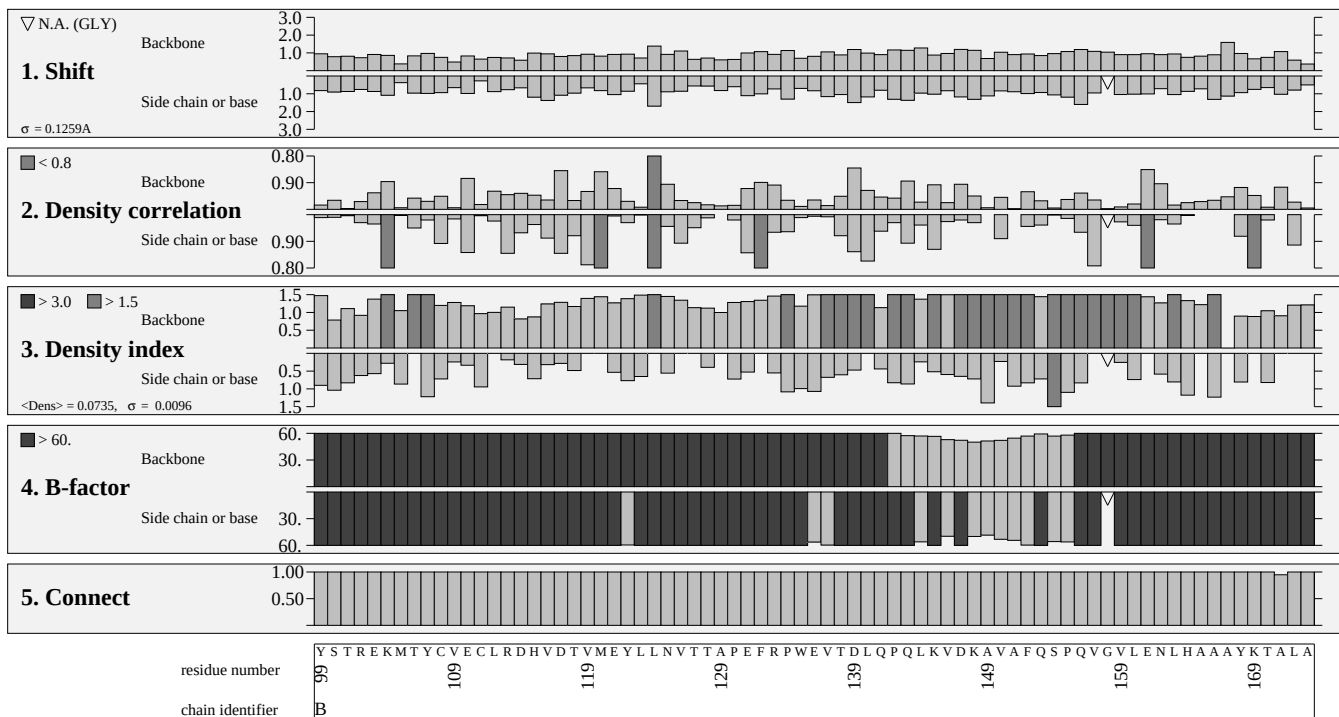
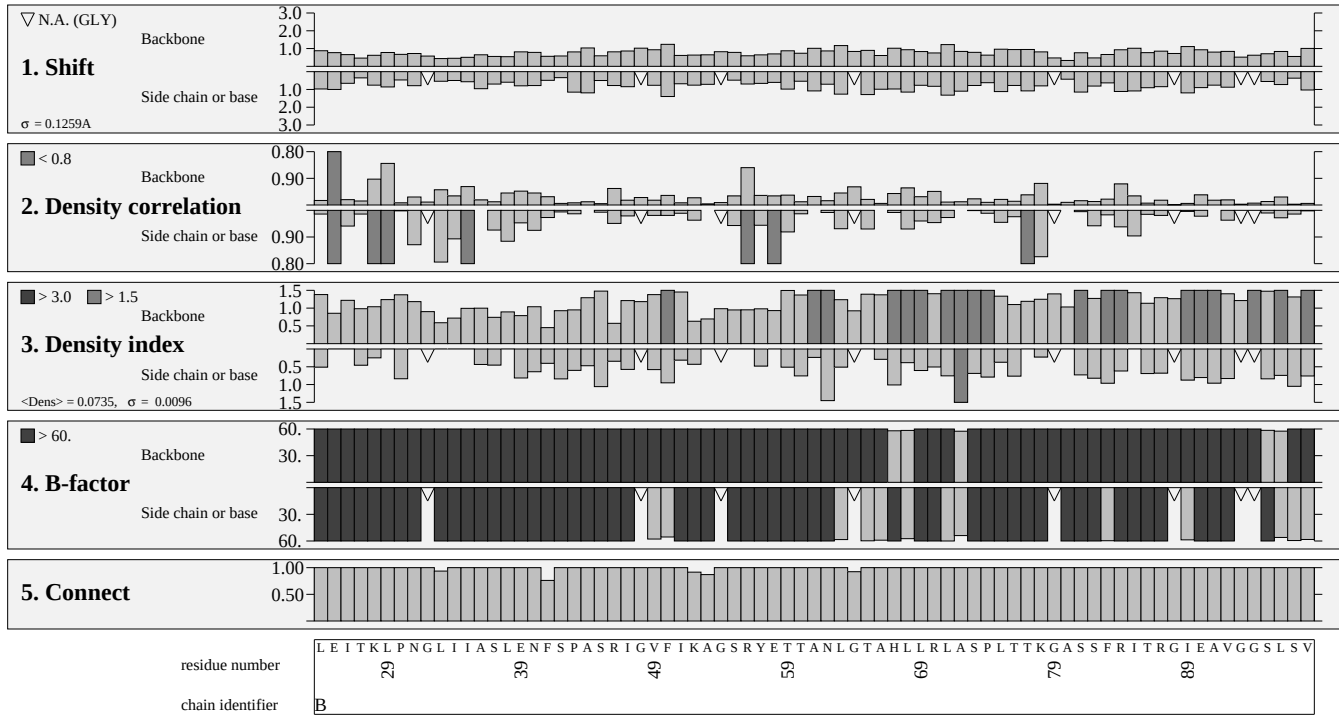
Local estimation (3)



Structure Factor Check

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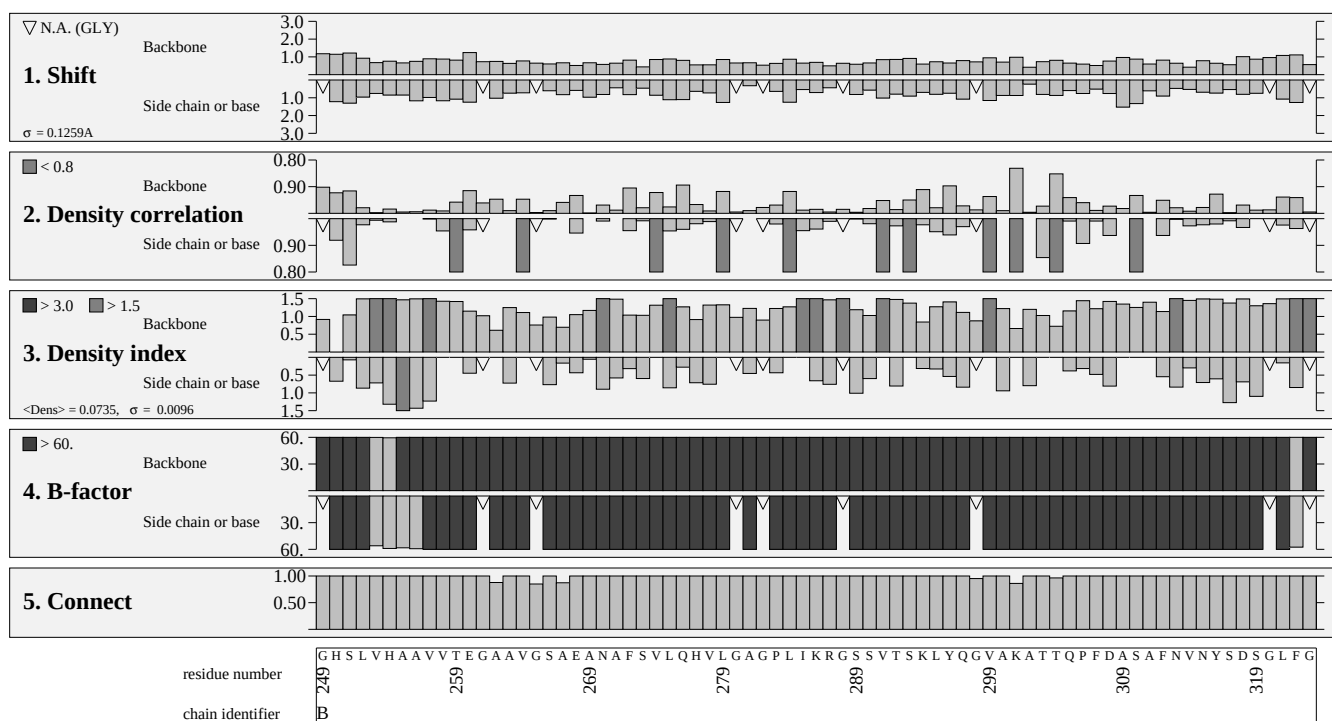
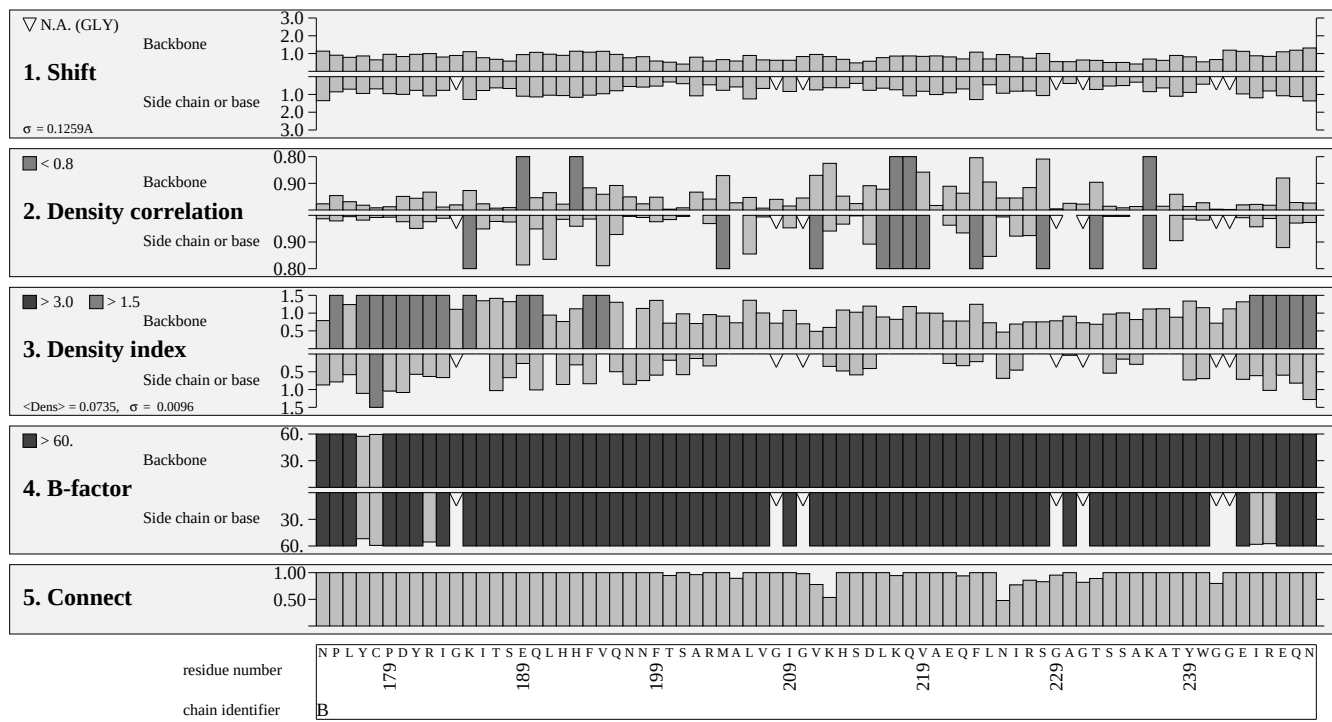
Local estimation (4)



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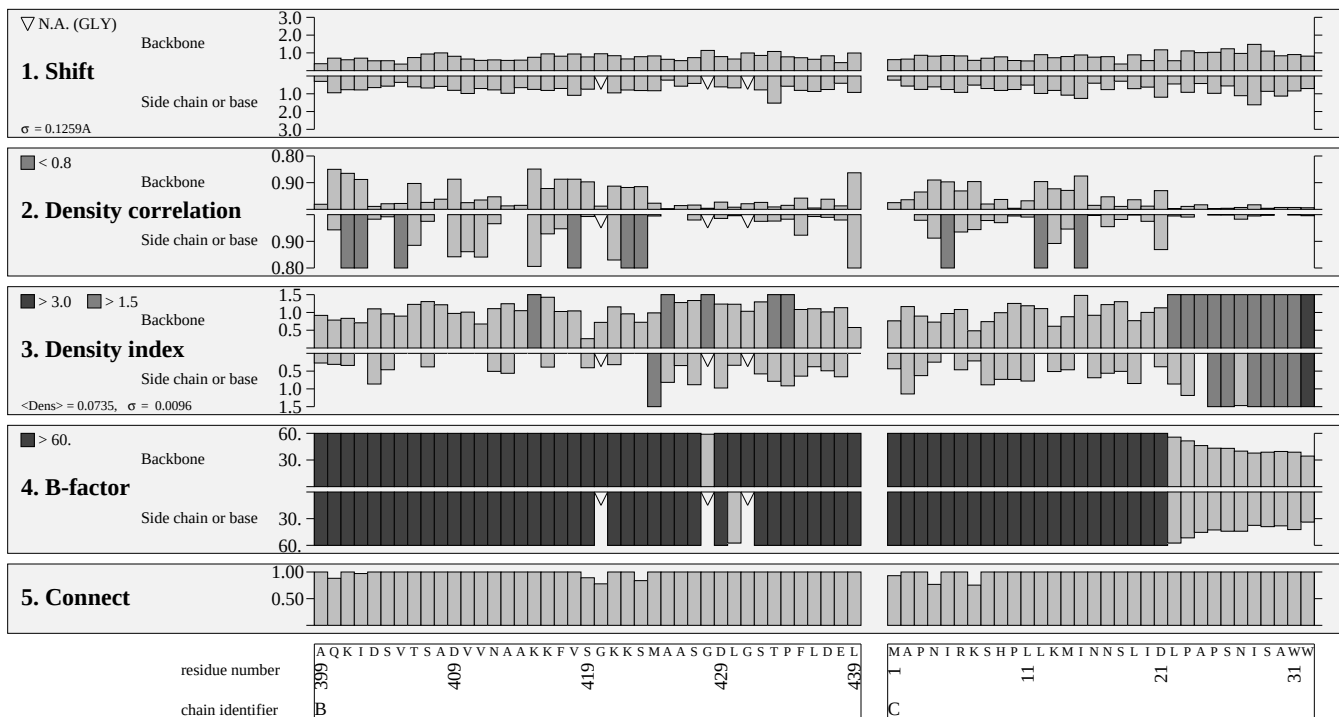
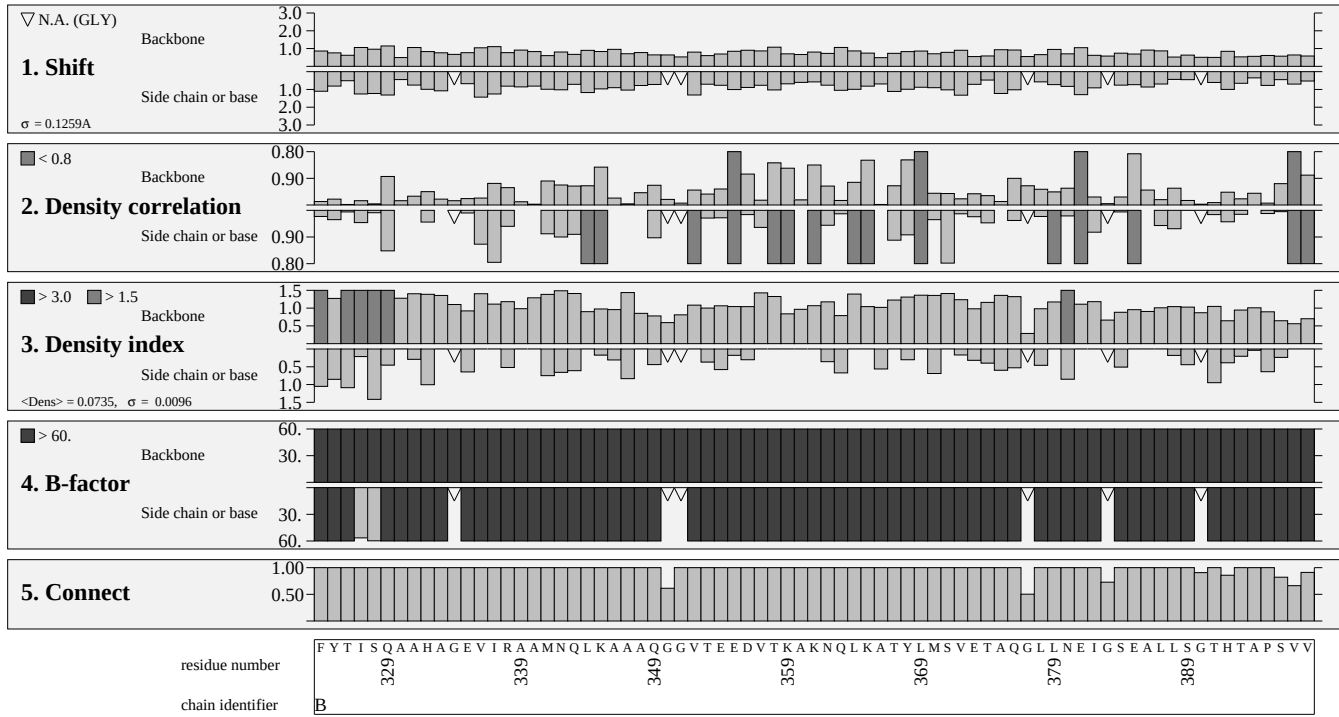
Local estimation (5)



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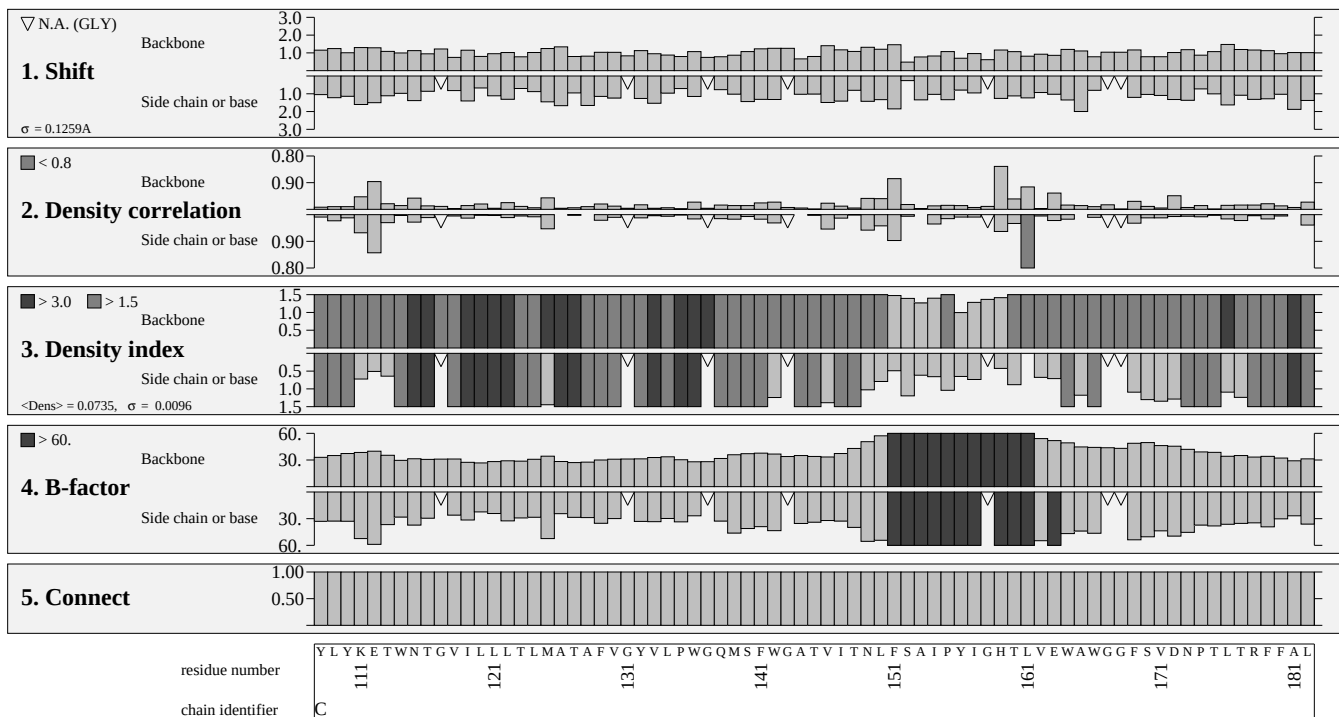
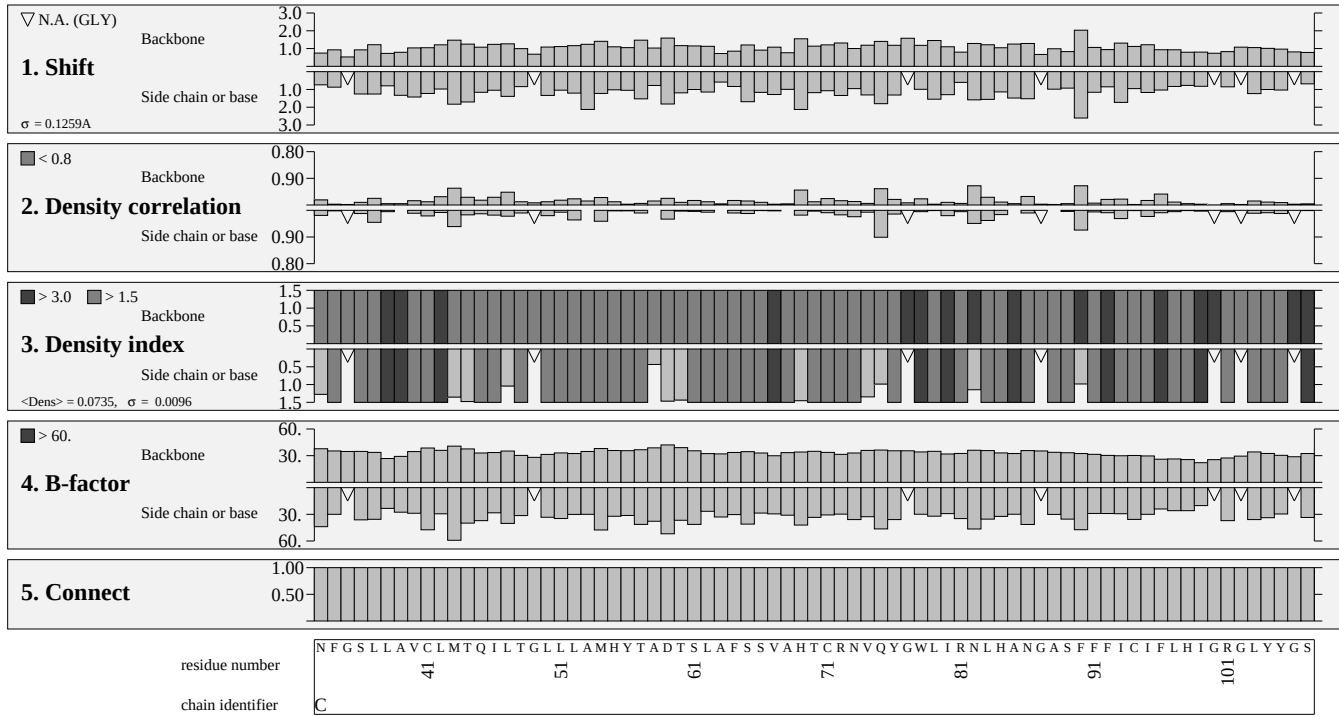
Local estimation (6)



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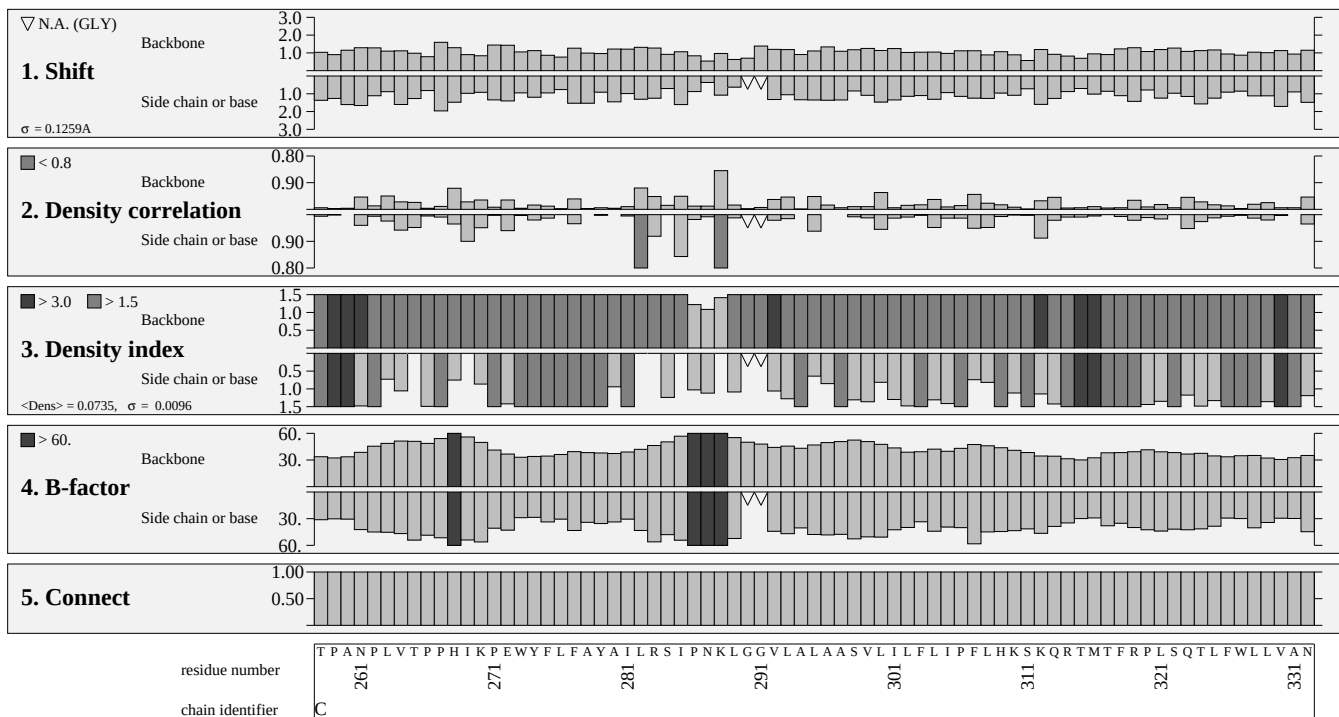
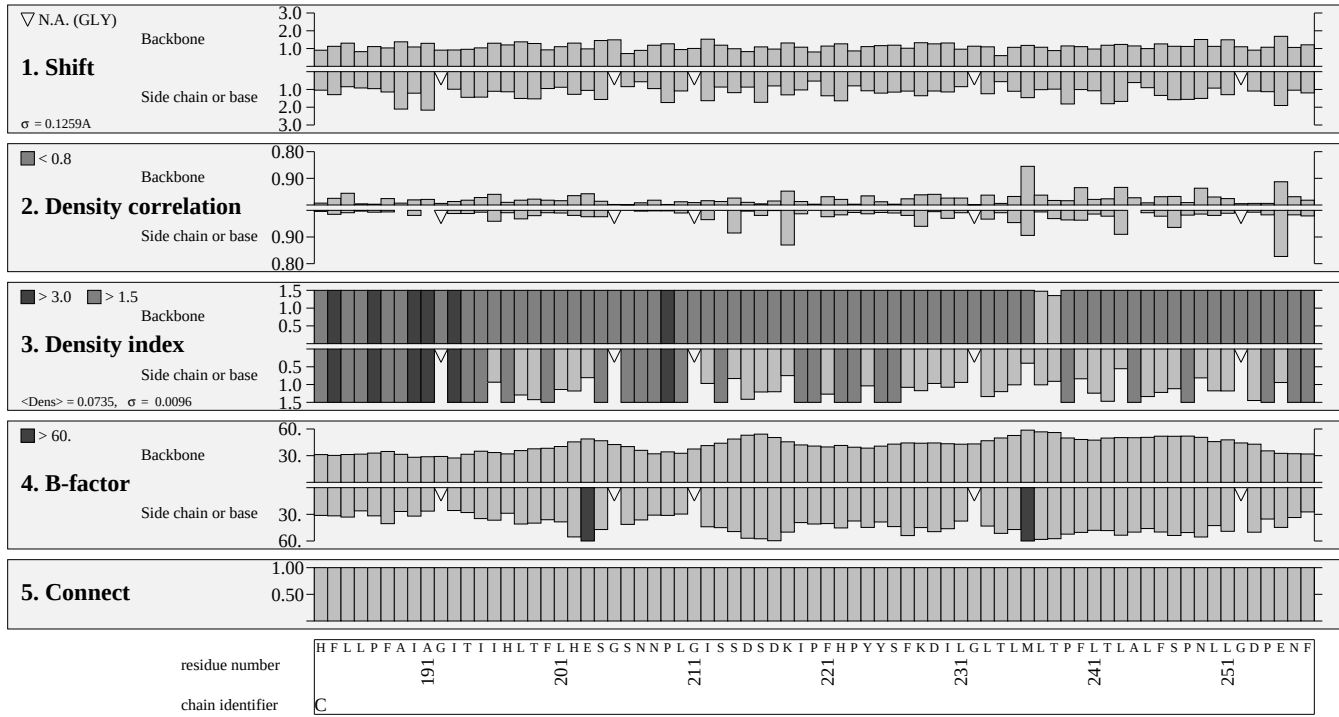
Local estimation (7)



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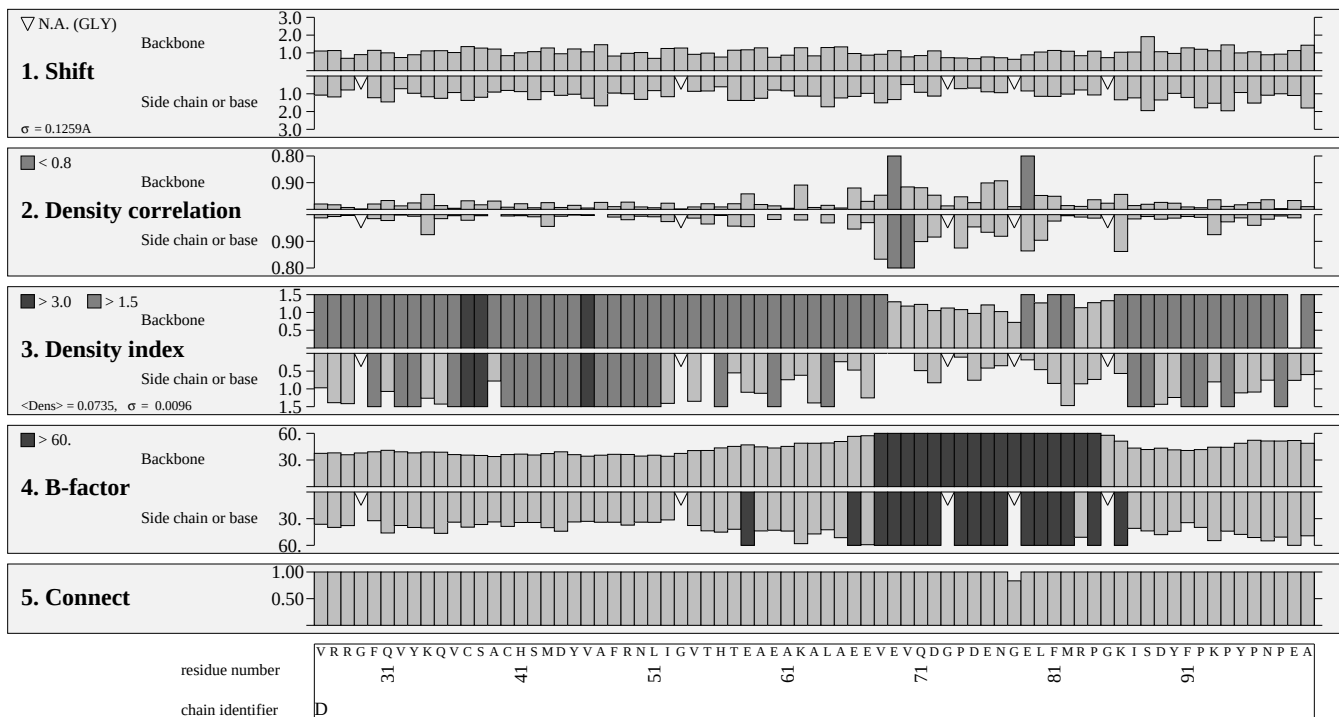
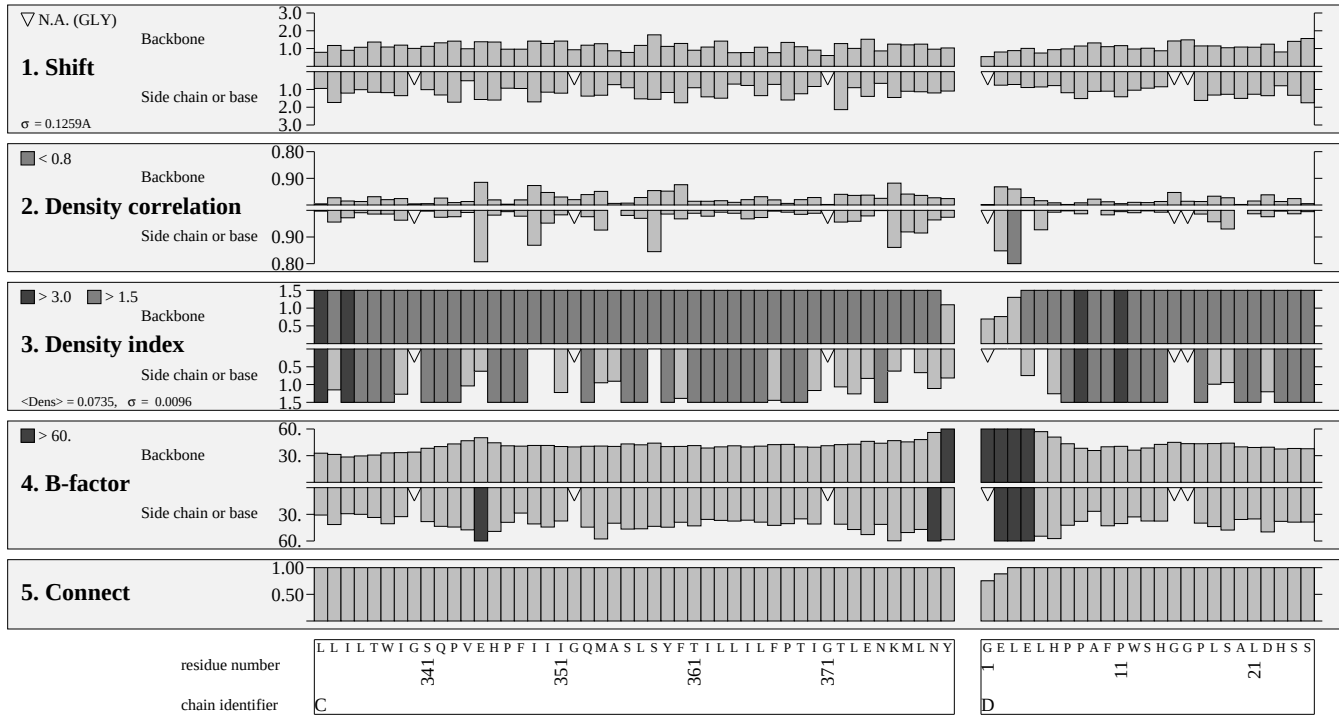
Local estimation (8)



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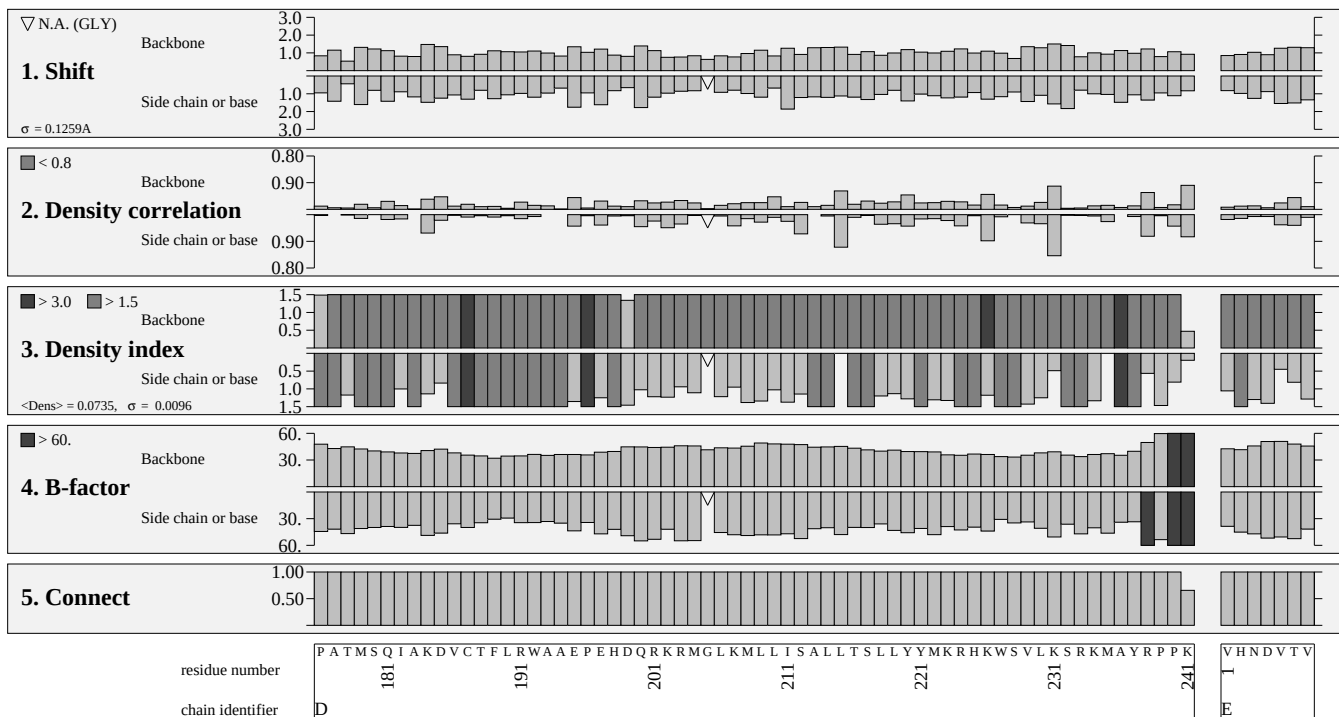
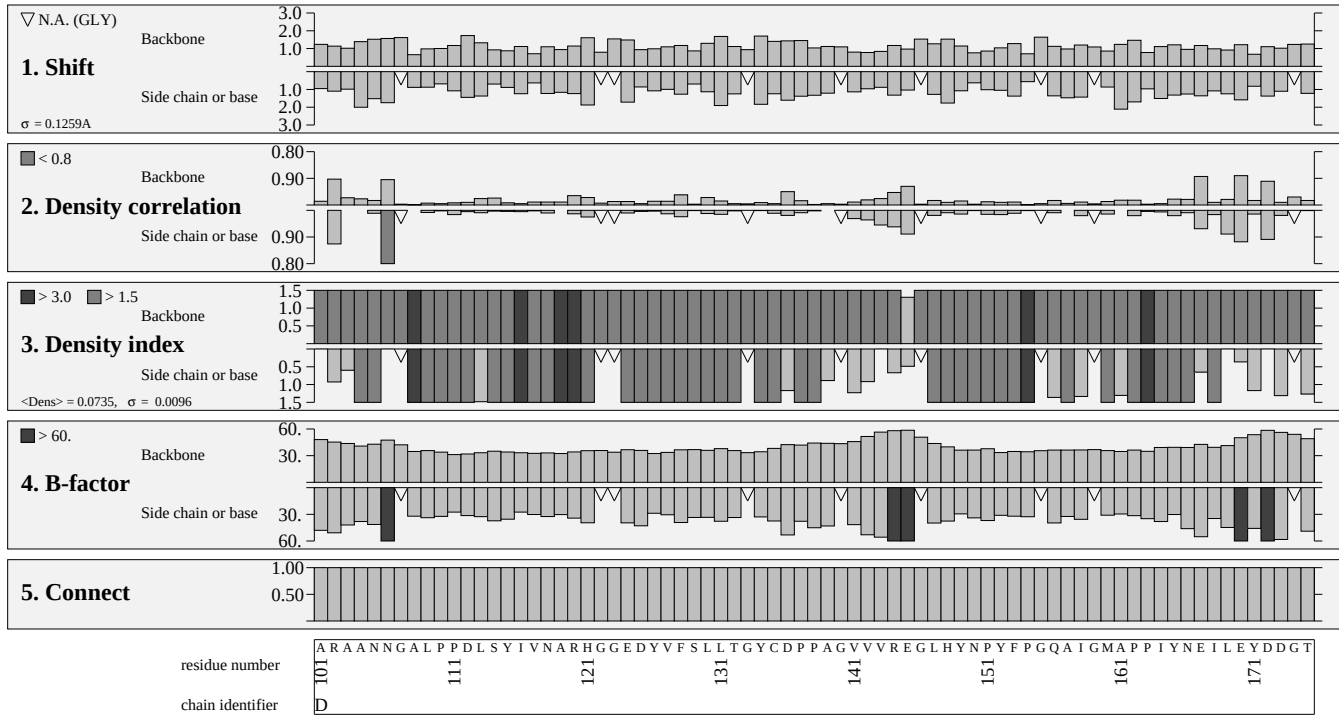
Local estimation (9)



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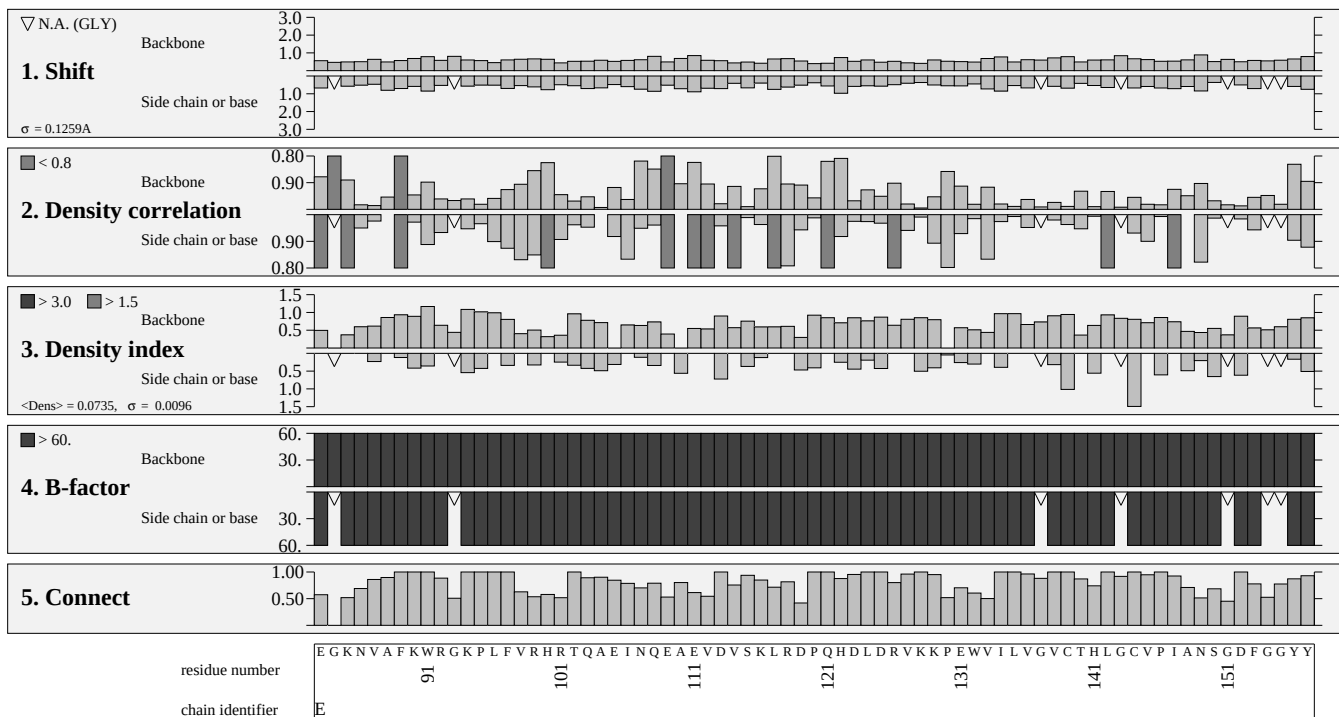
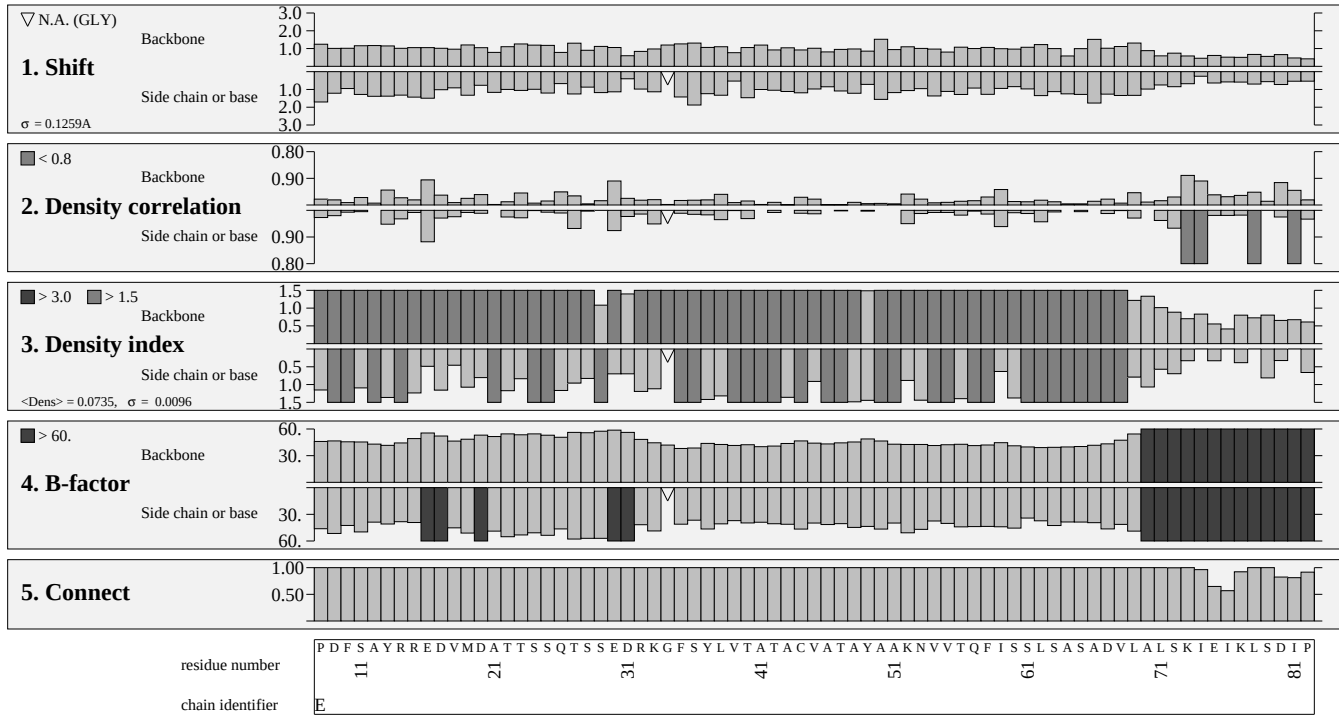
Local estimation (10)



Structure Factor Check

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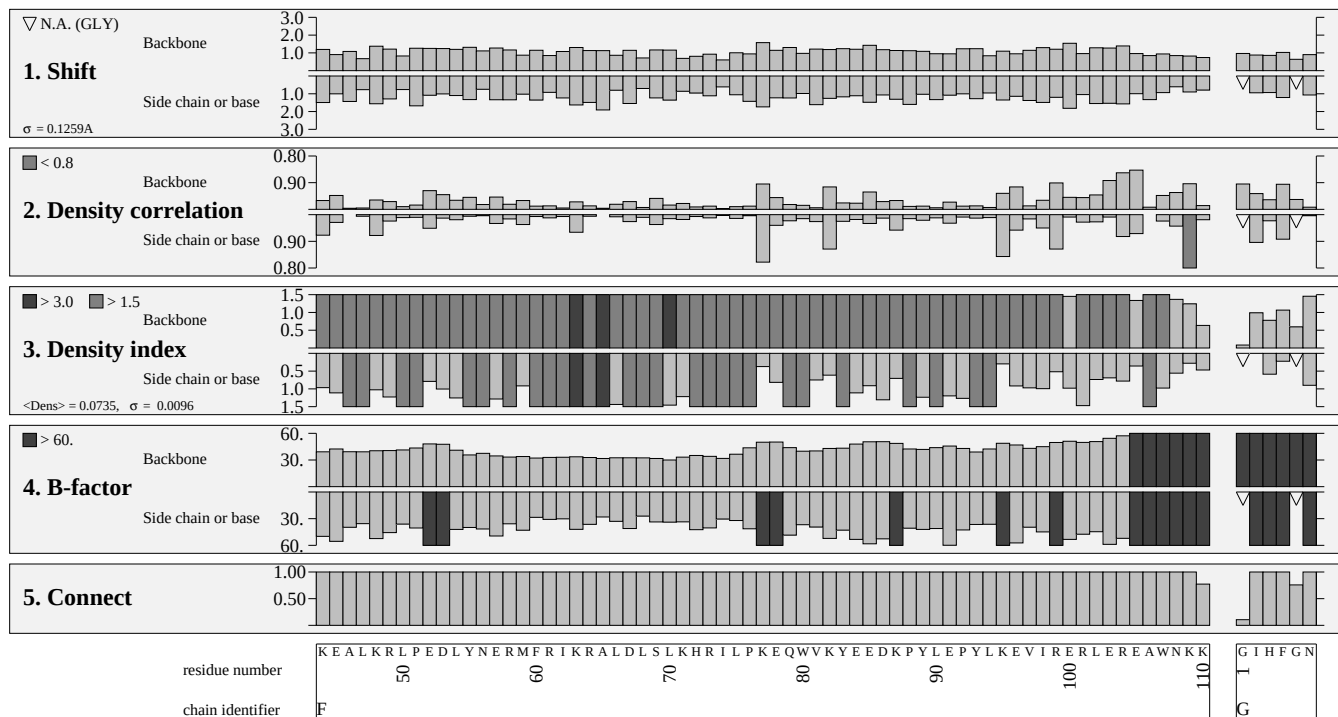
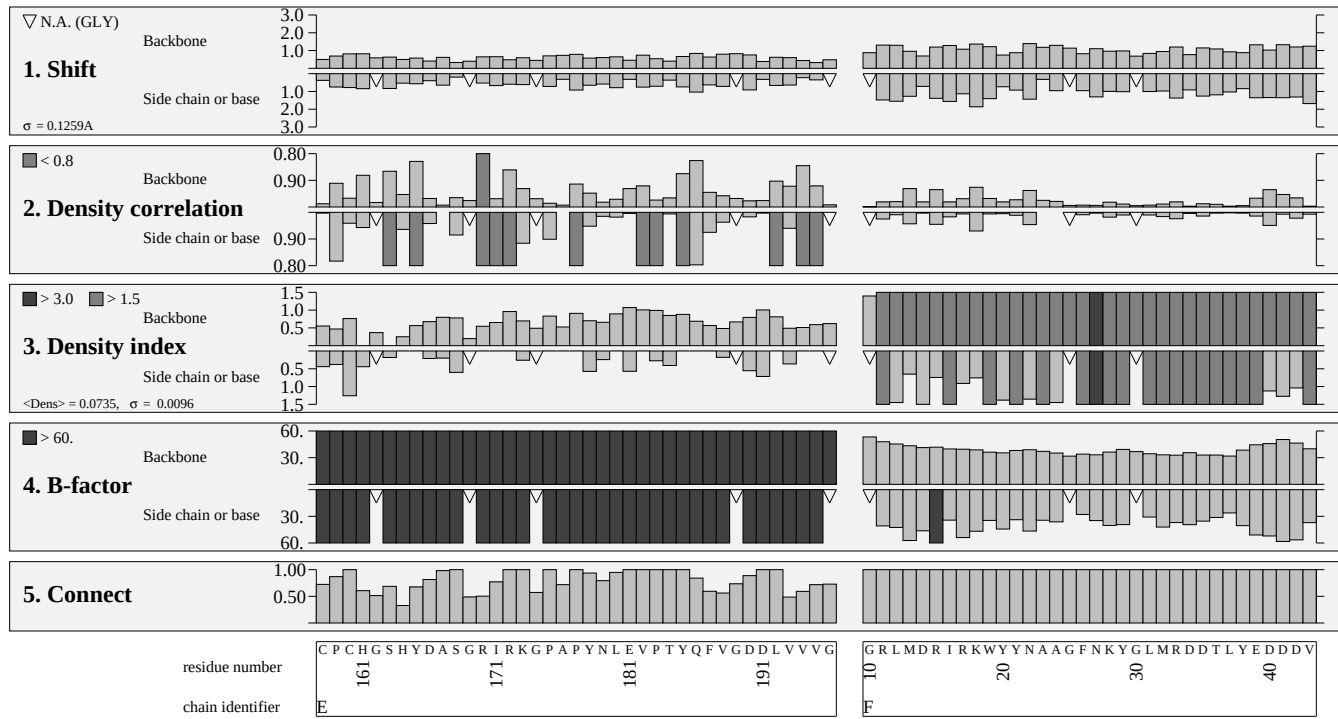
Local estimation (11)



Structure Factor Check

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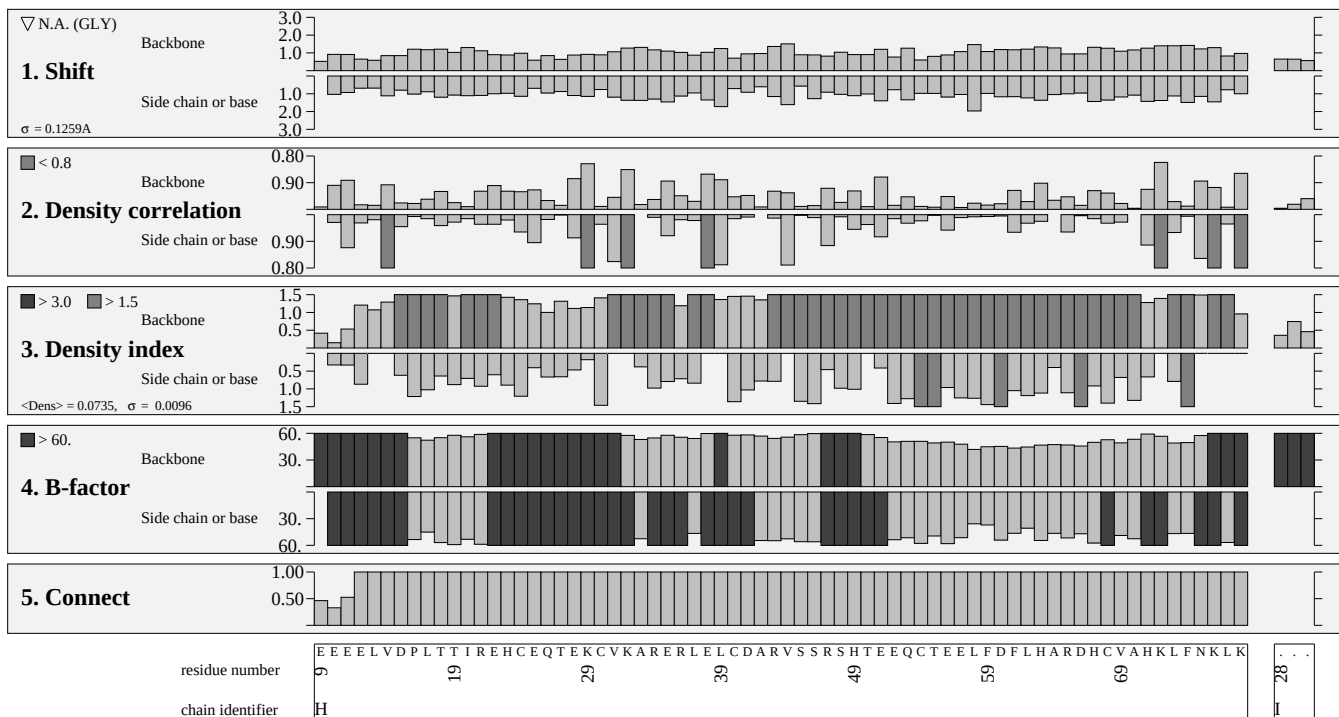
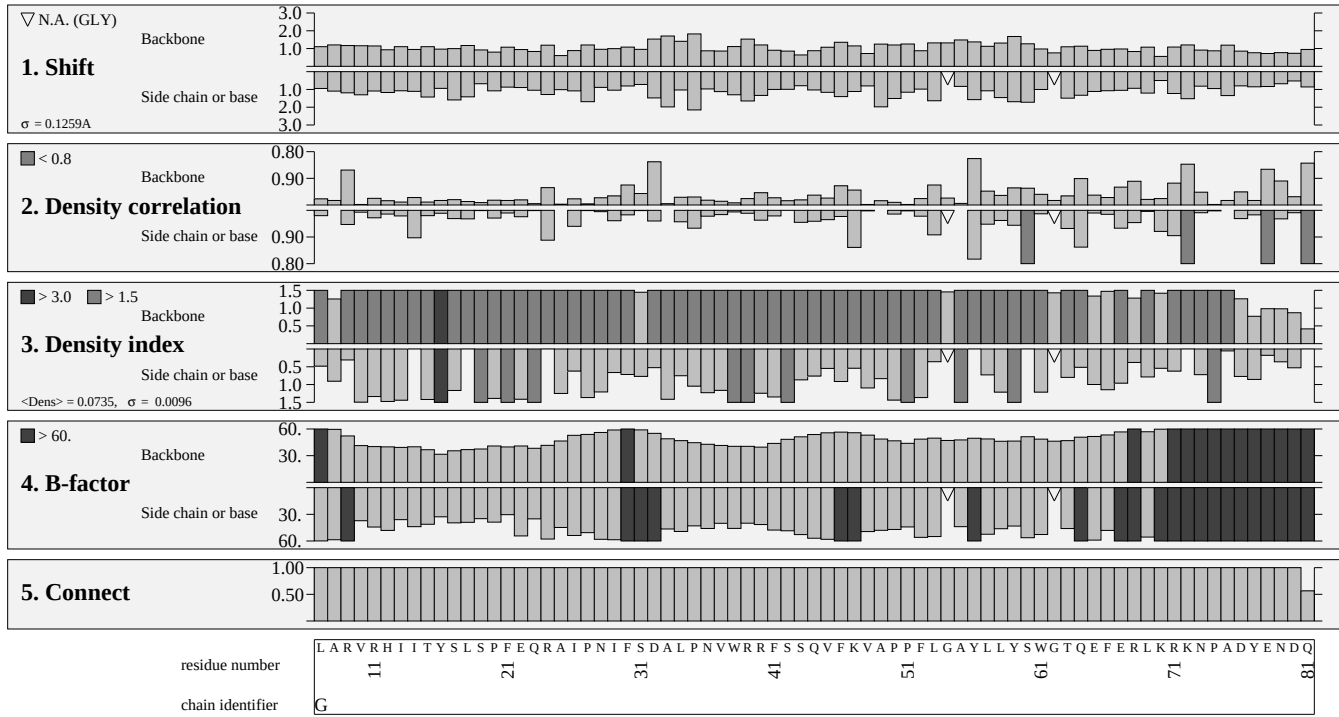
Local estimation (12)



Structure Factor Check

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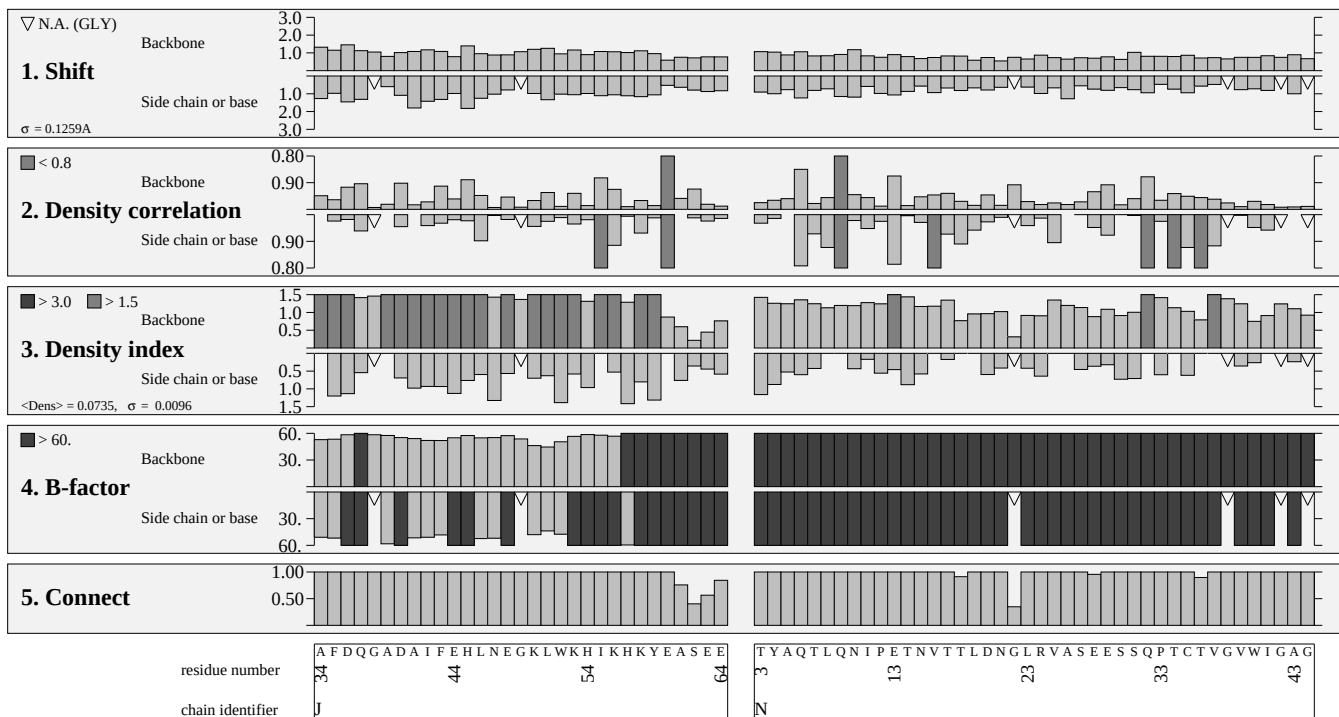
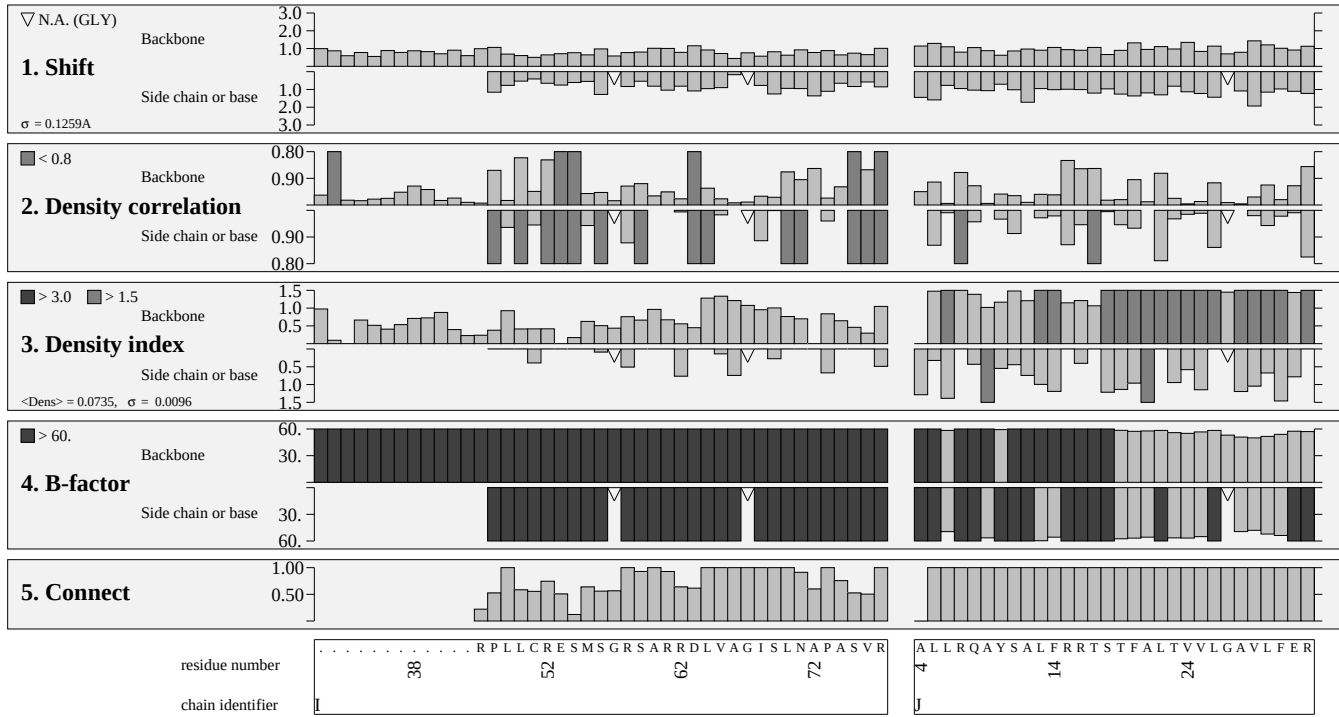
Local estimation (13)



Structure Factor Check

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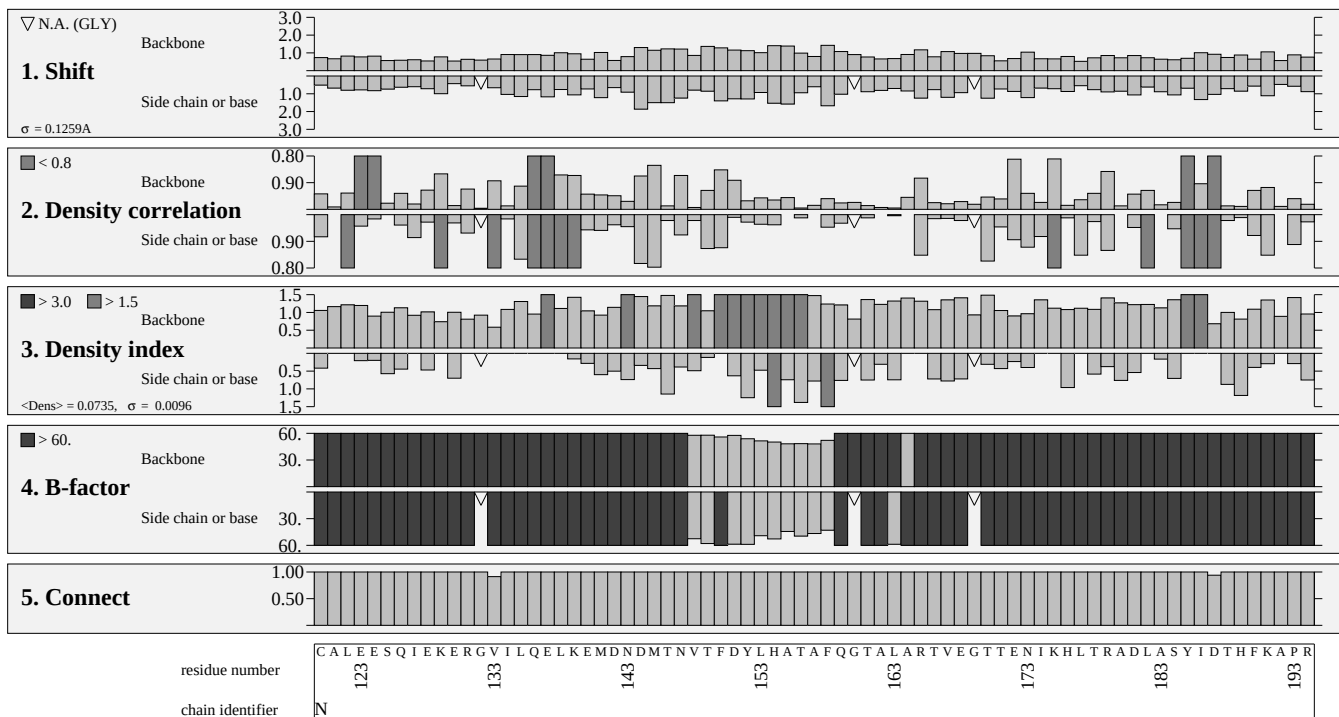
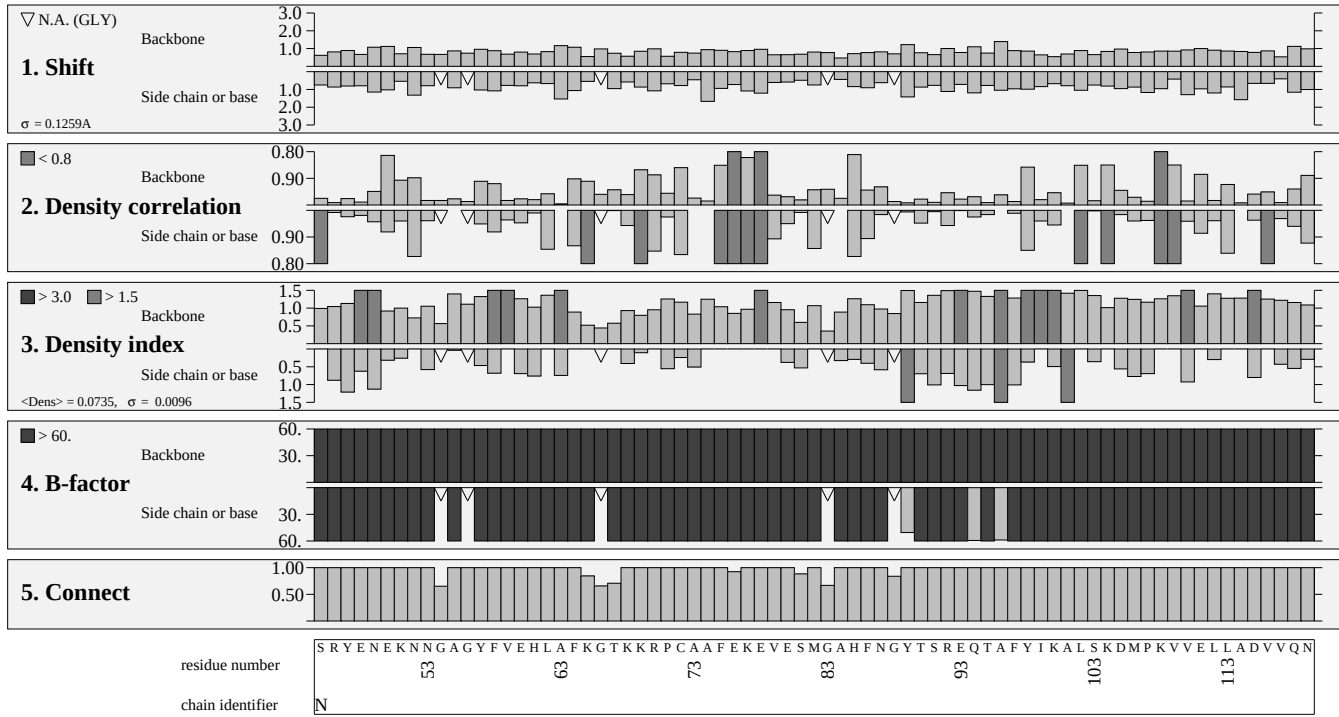
Local estimation (14)



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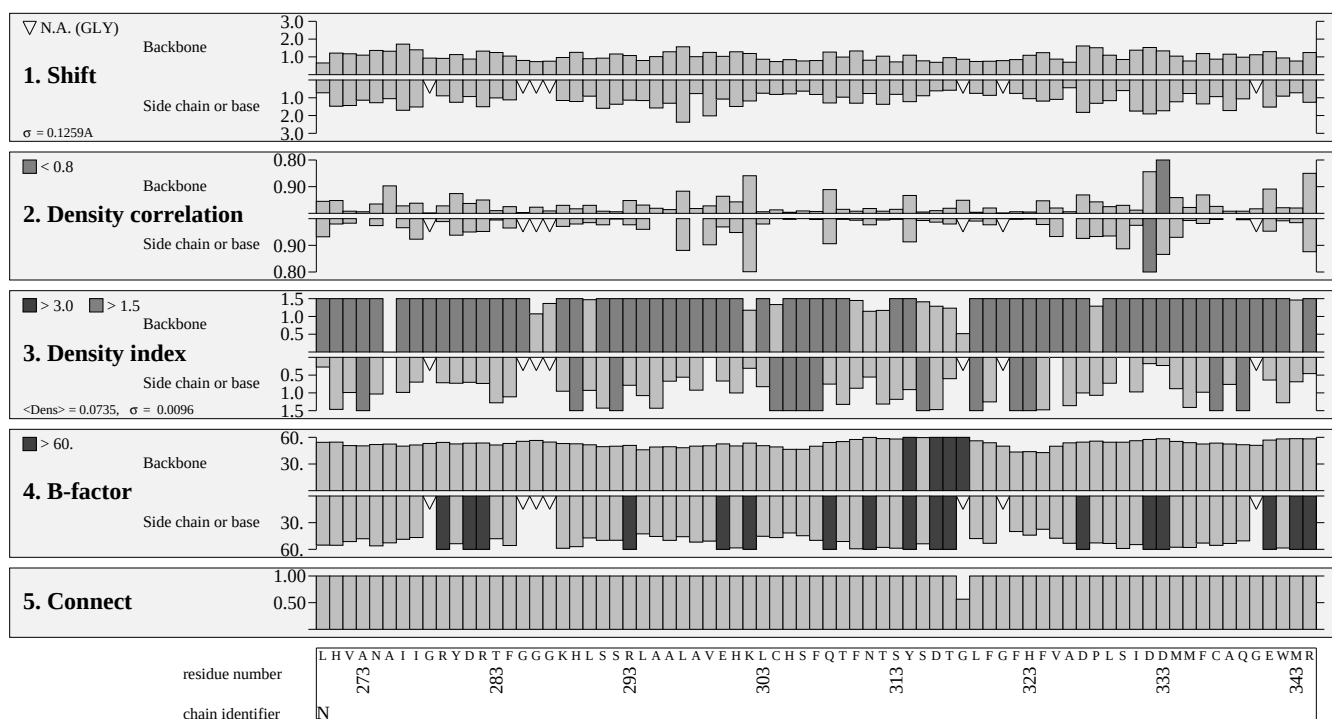
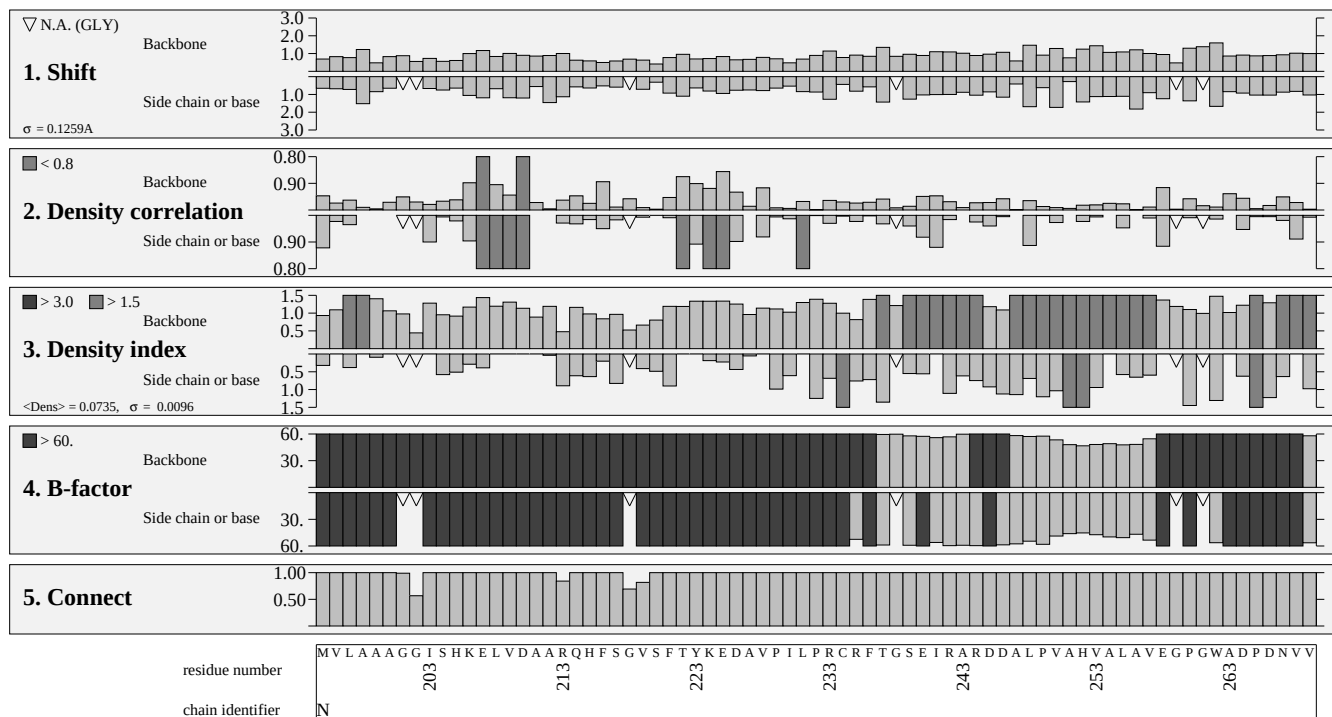
Local estimation (15)



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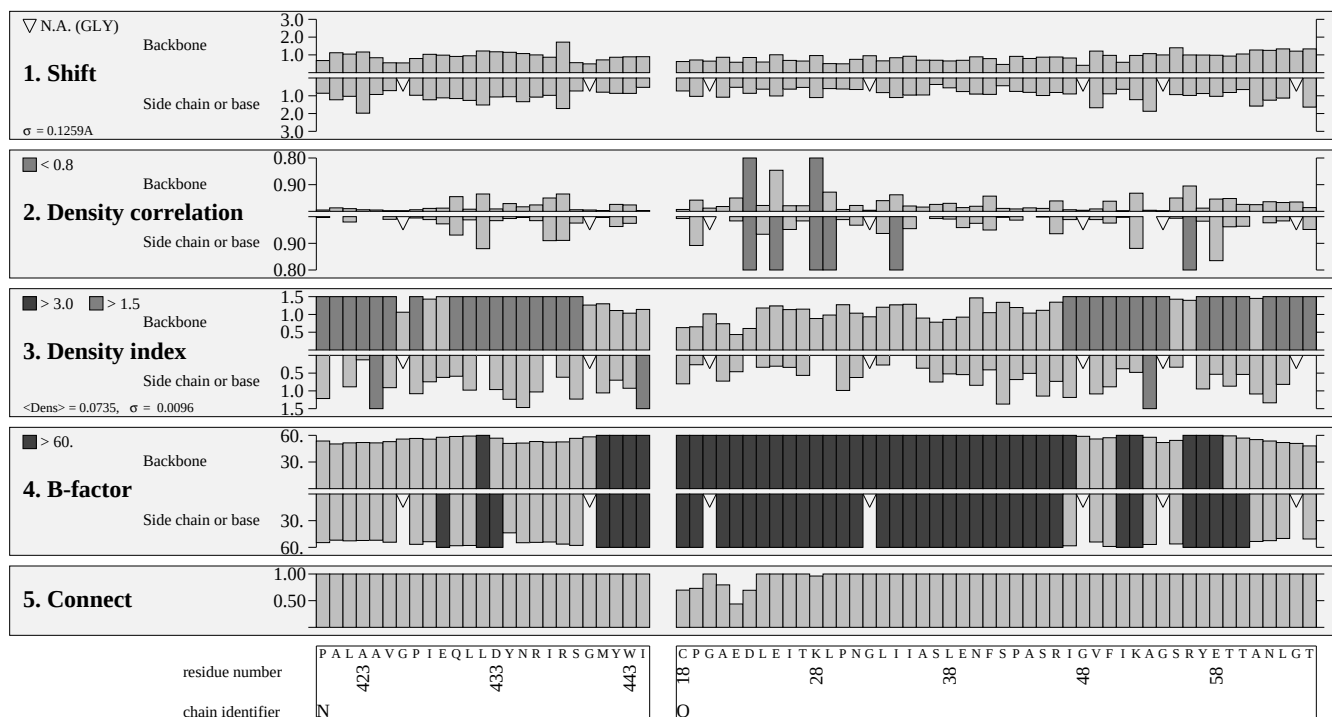
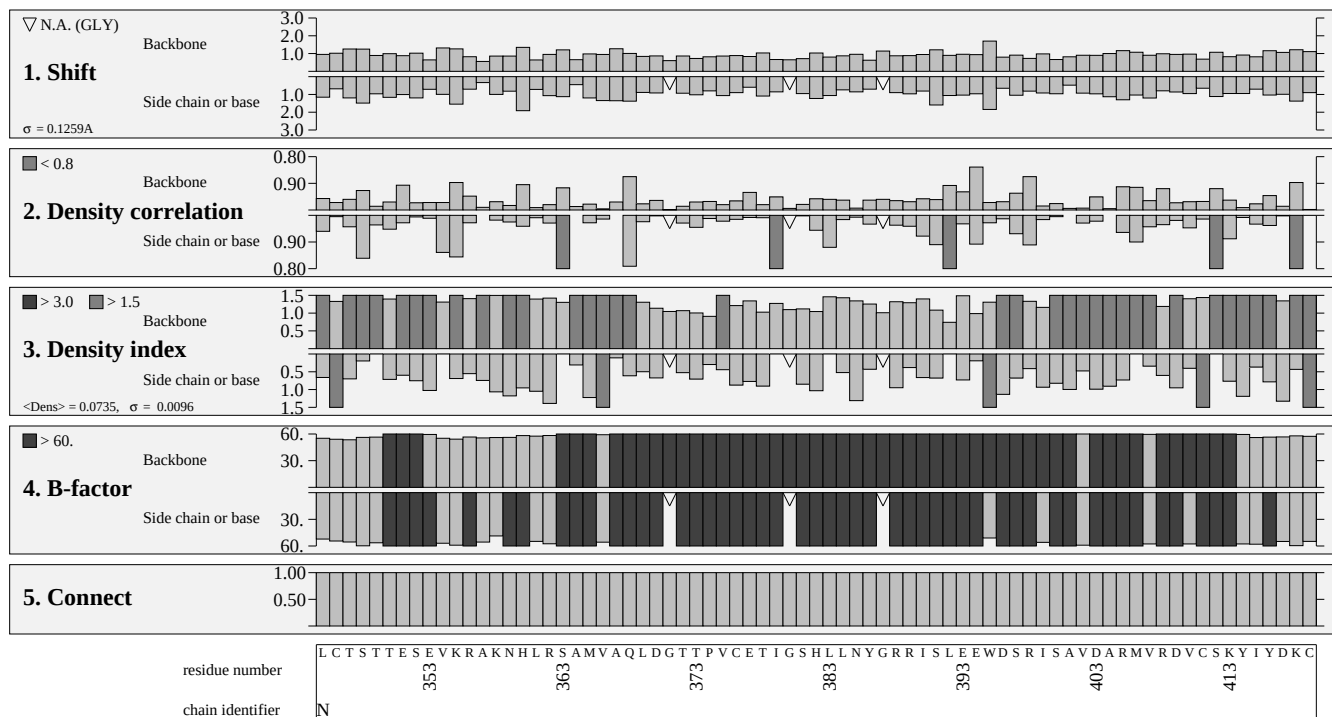
Local estimation (16)



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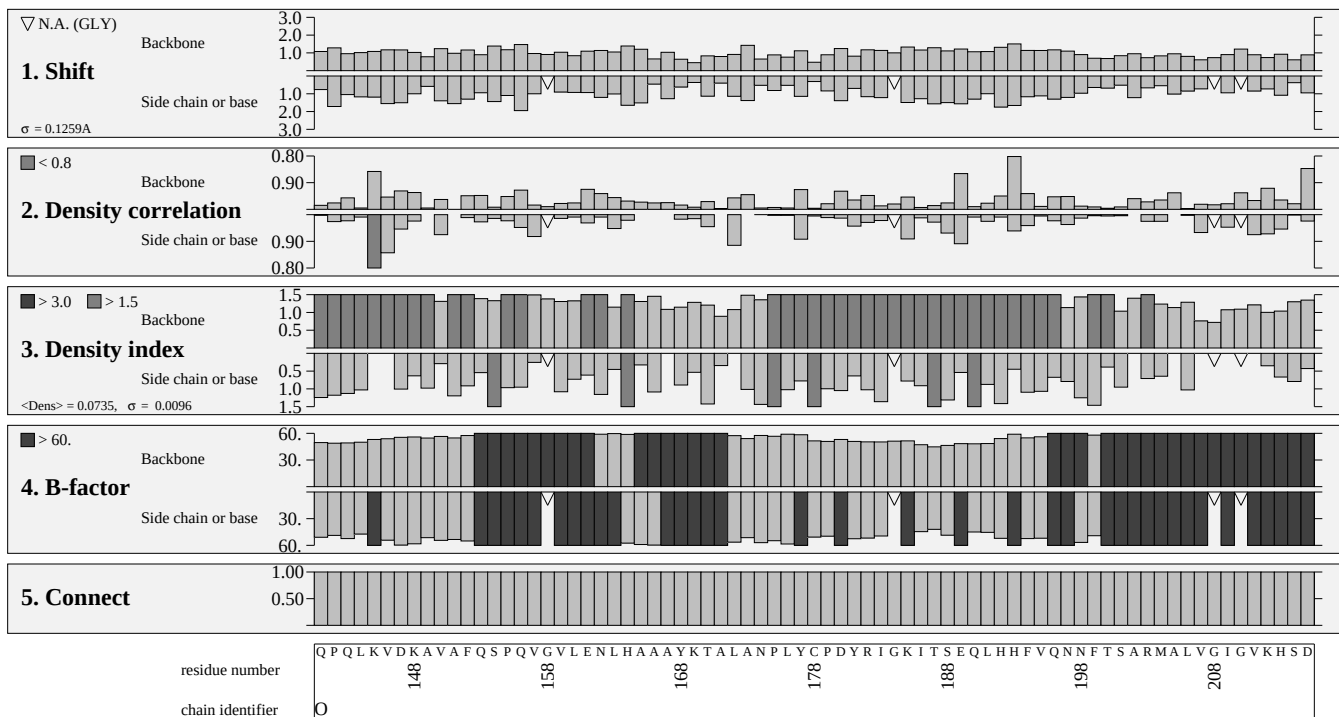
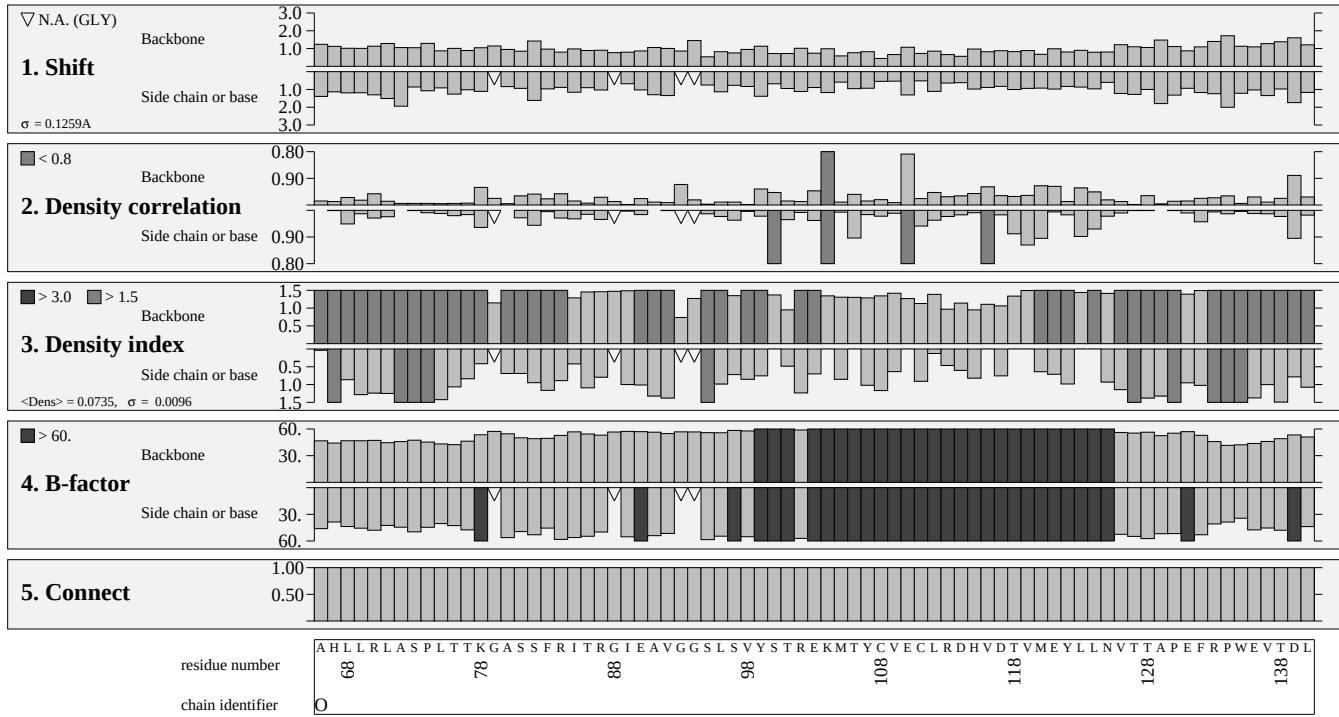
Local estimation (17)



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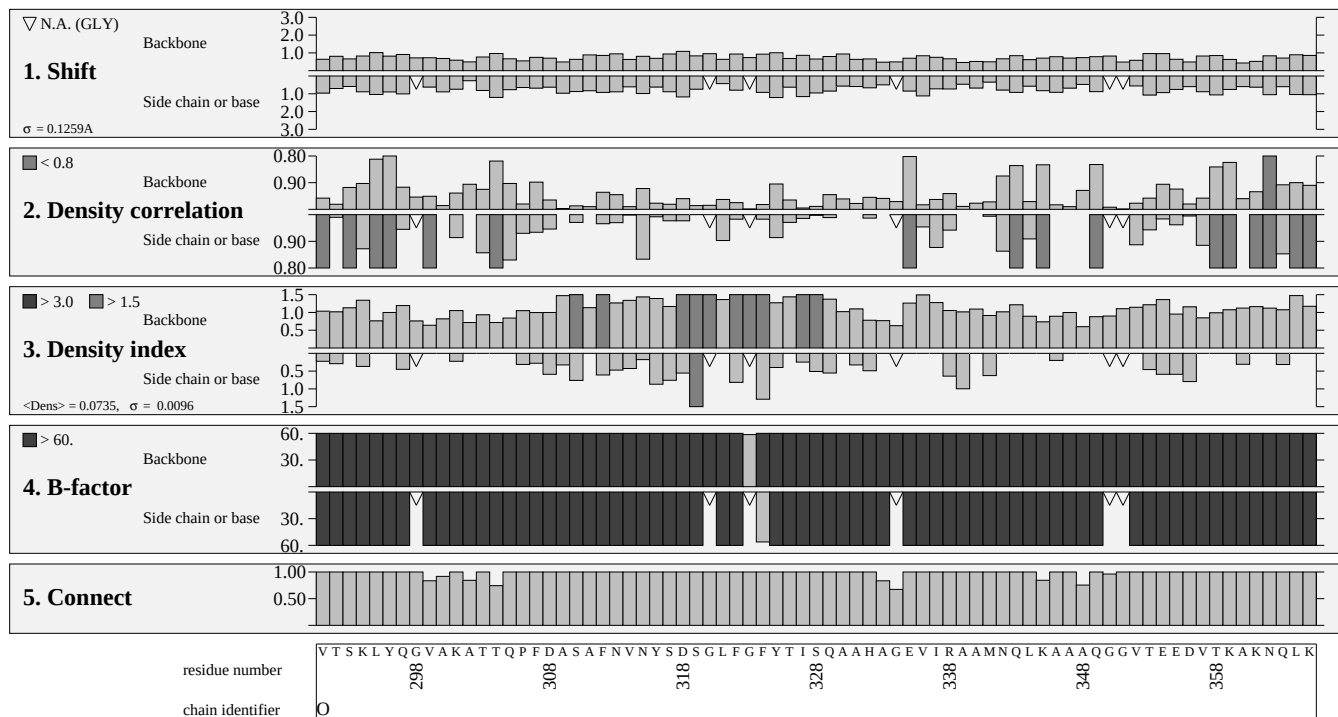
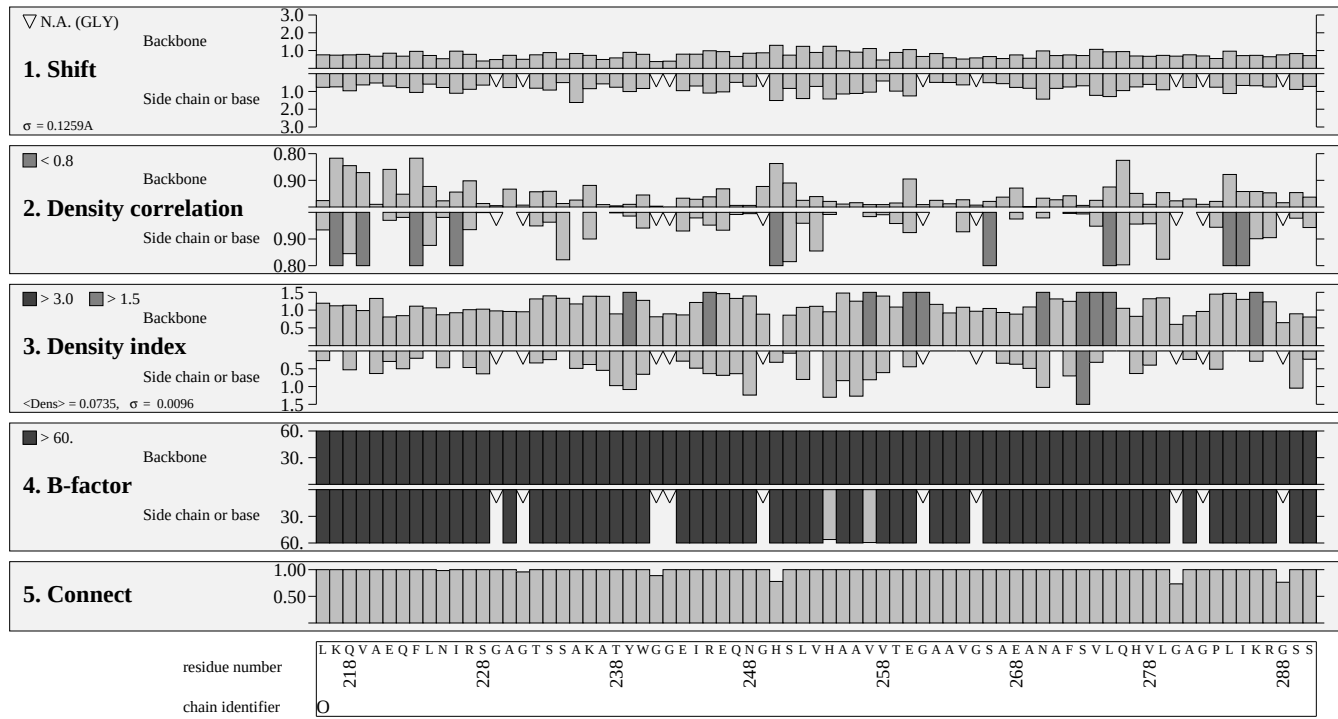
Local estimation (18)



Structure Factor Check

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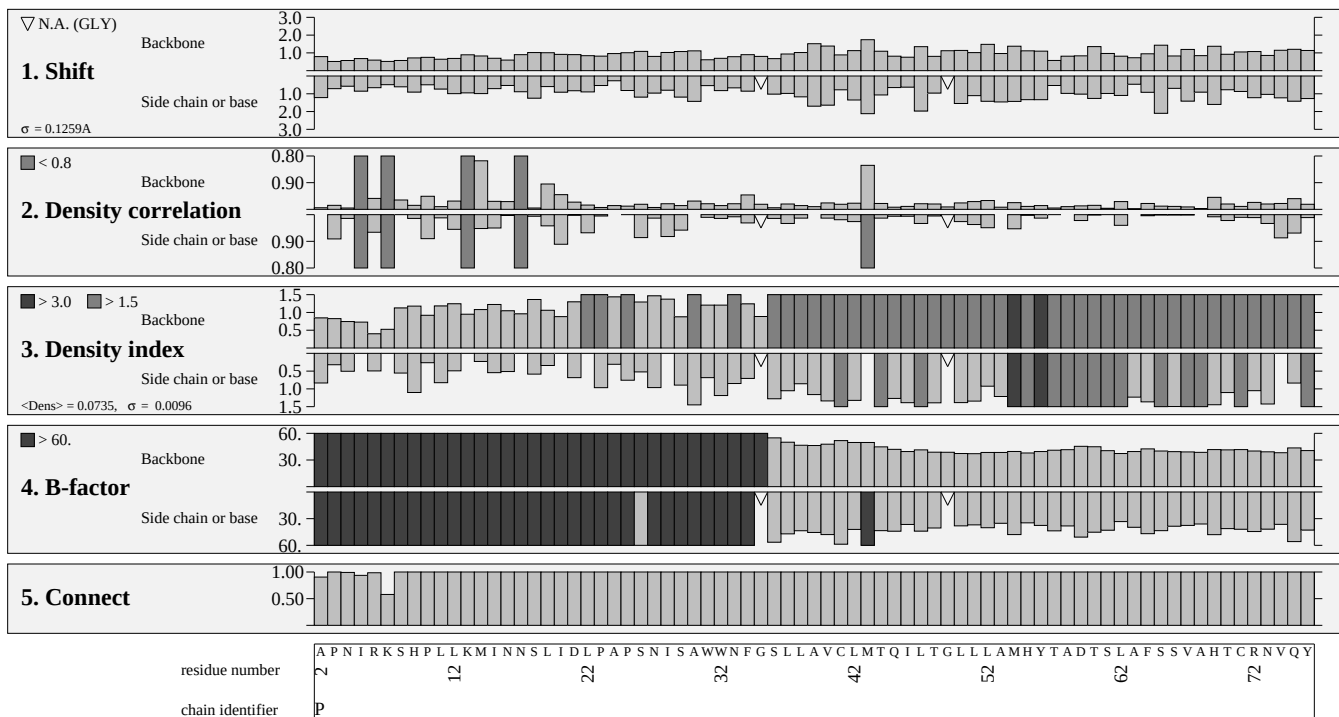
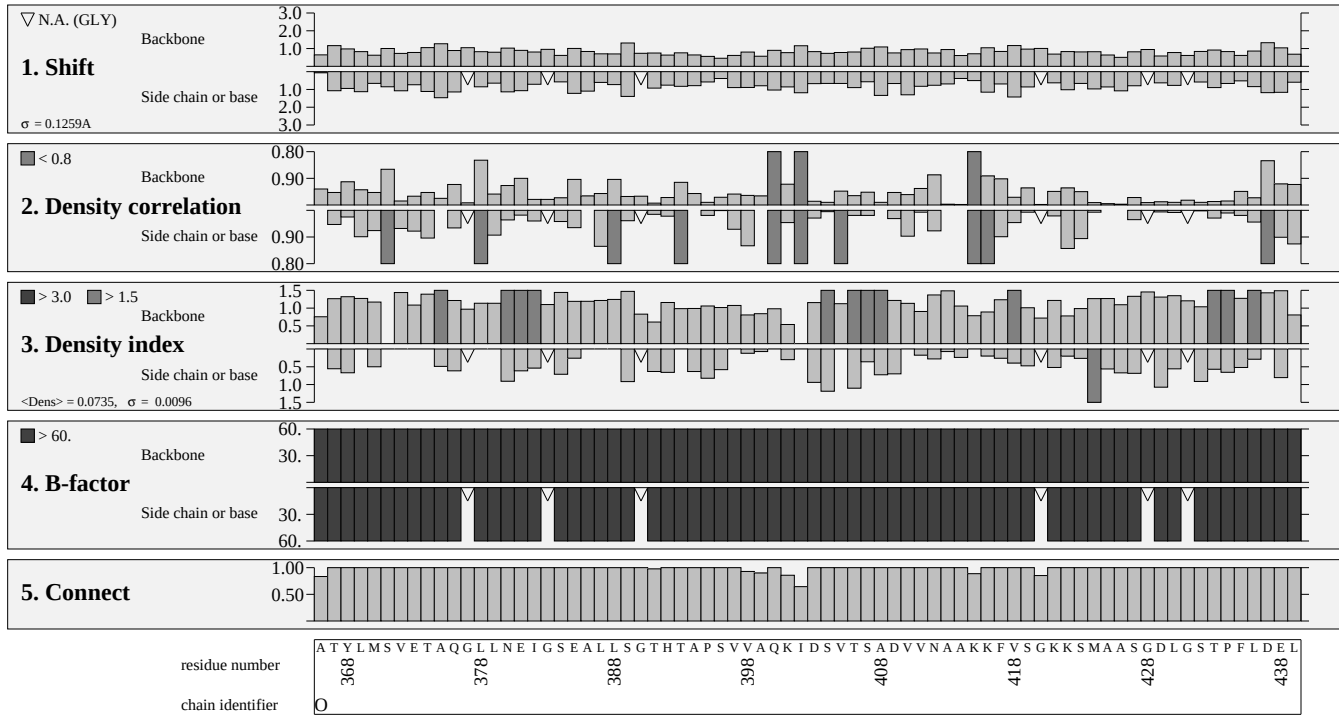
Local estimation (19)



Structure Factor Check

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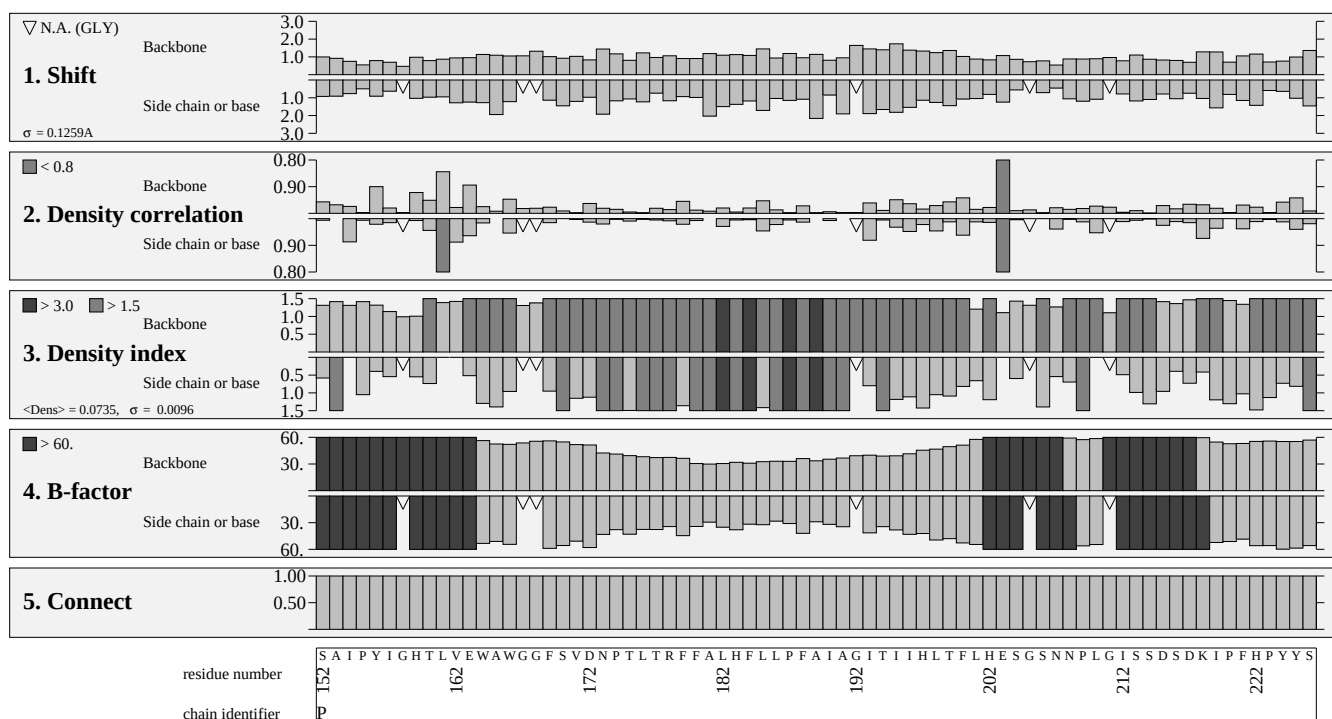
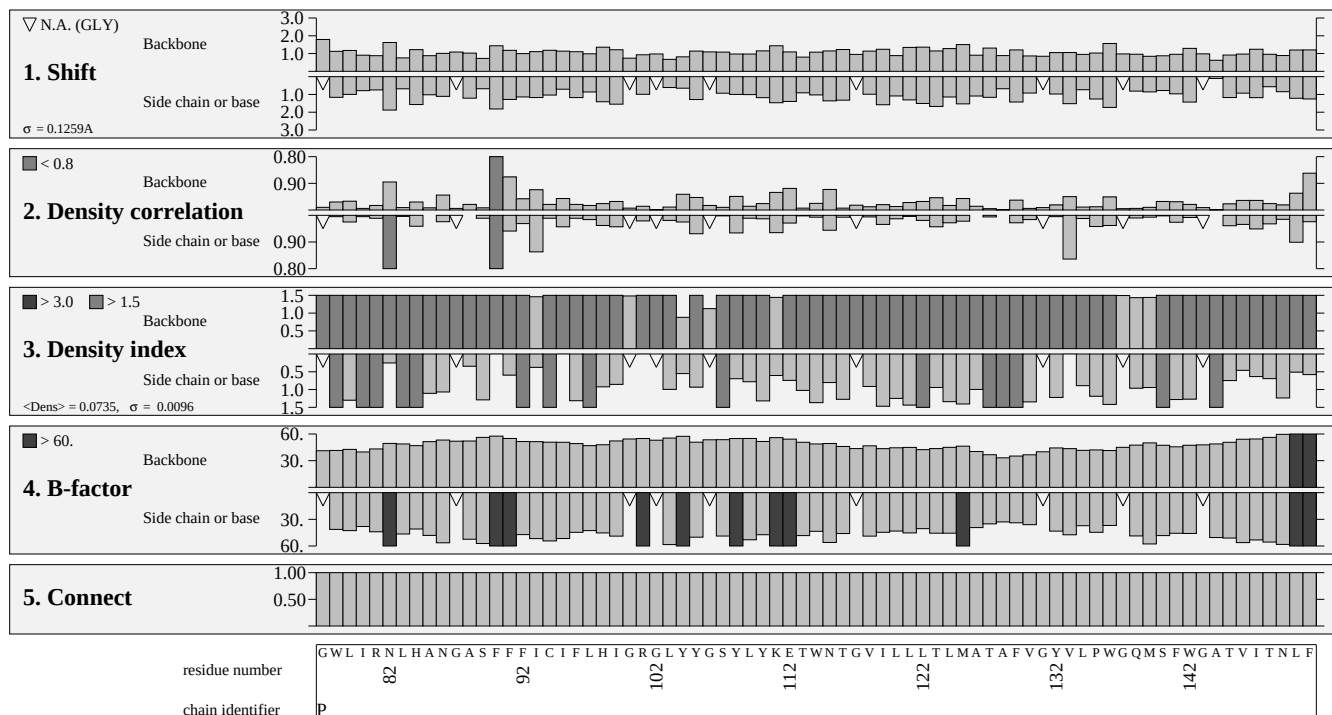
Local estimation (20)



Structure Factor Check

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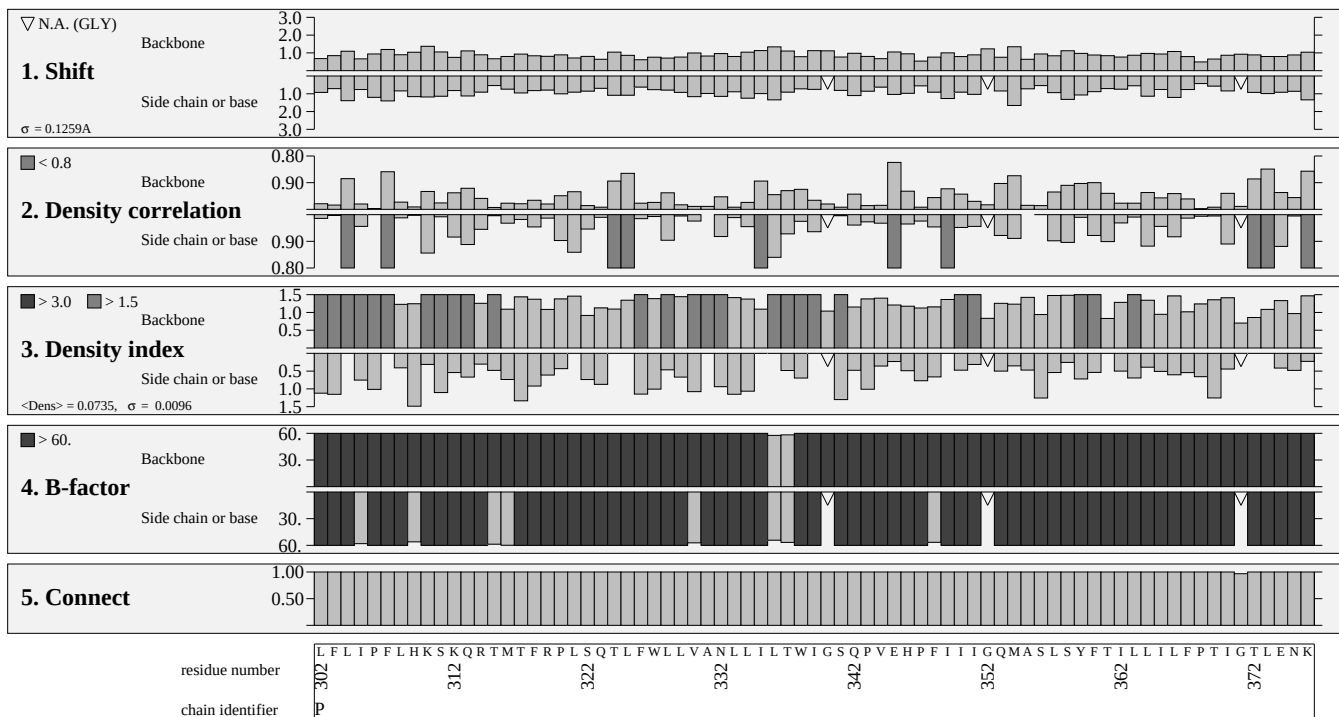
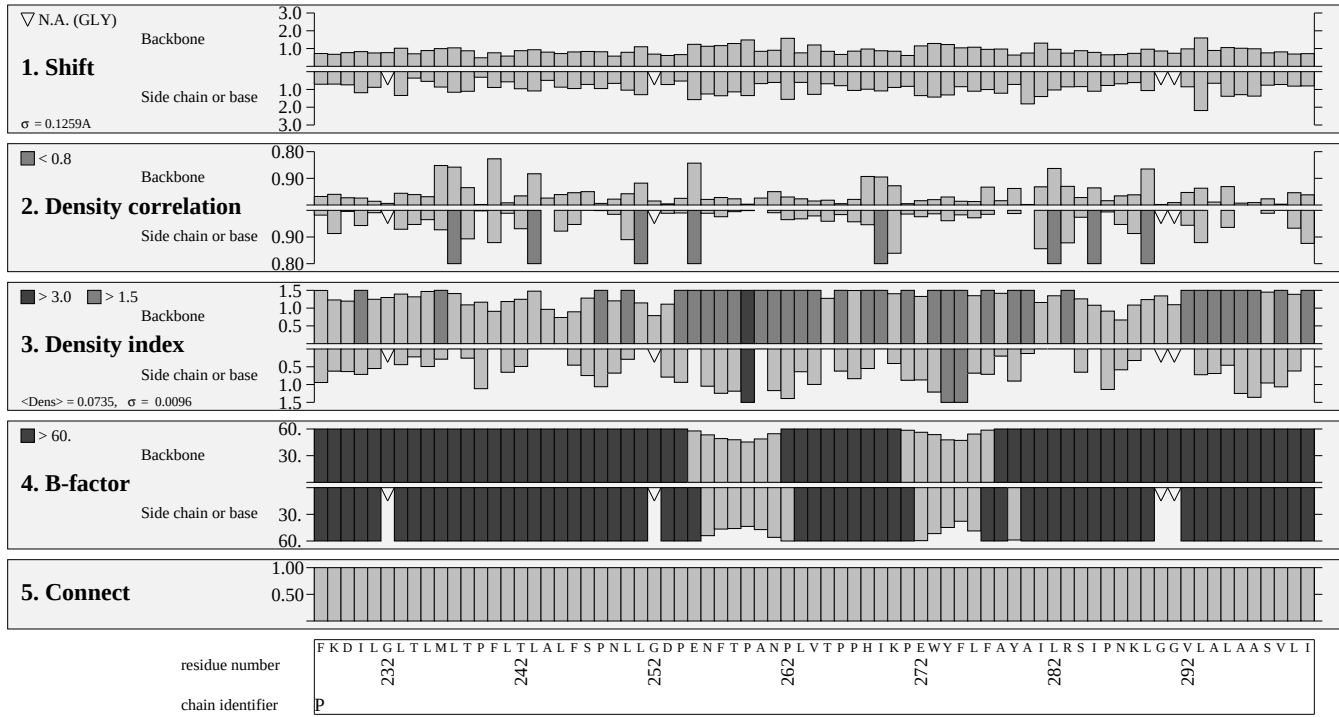
Local estimation (21)



Structure Factor Check

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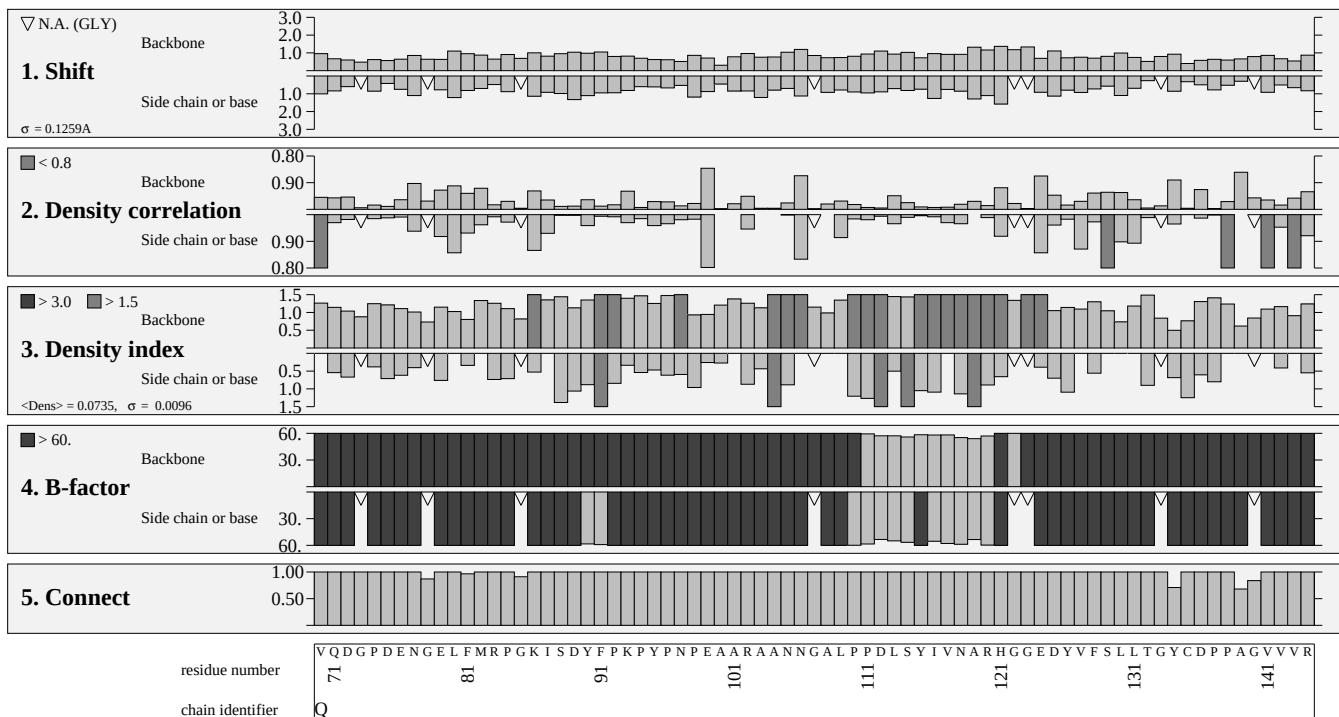
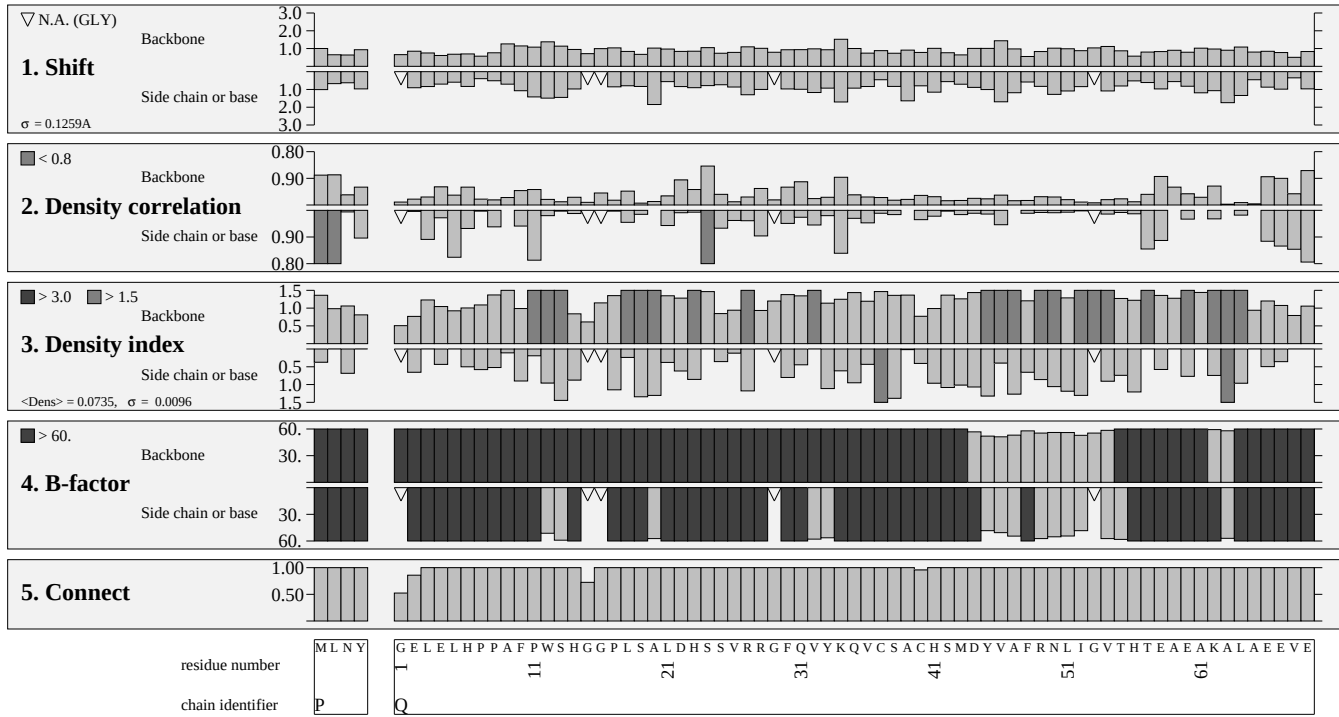
Local estimation (22)



Structure Factor Check

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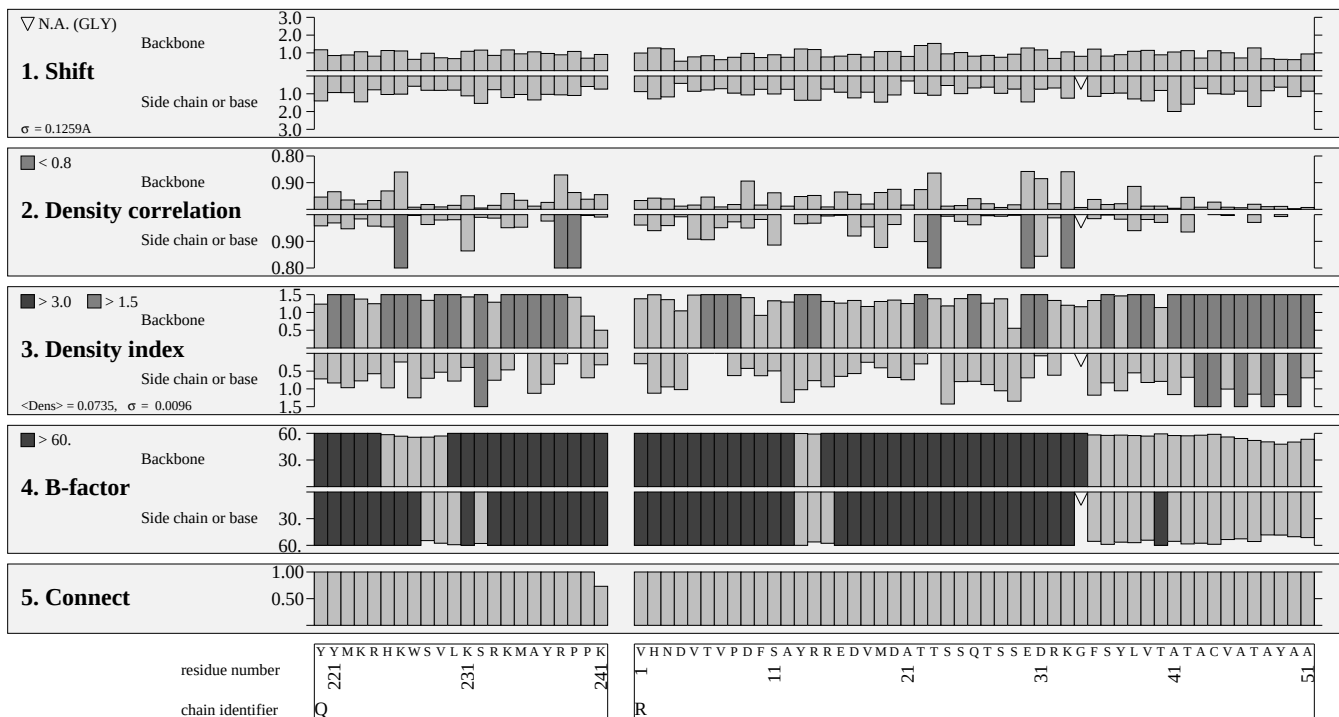
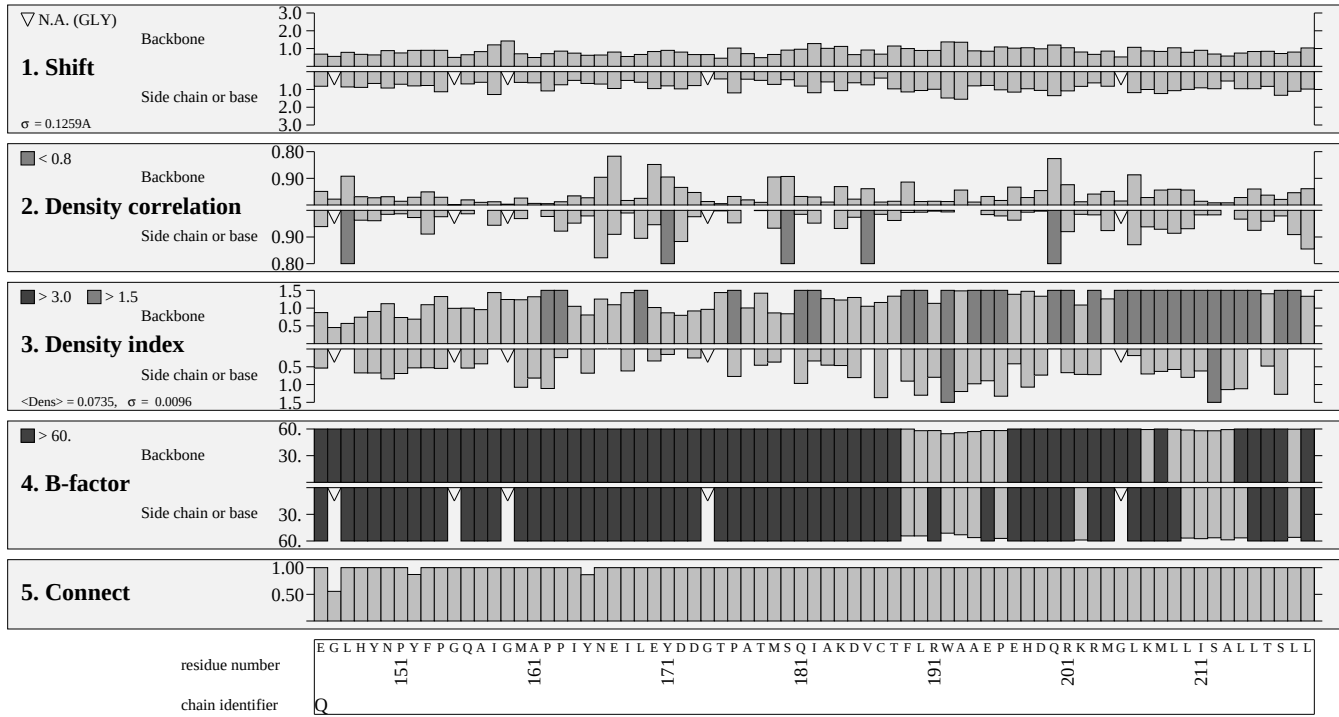
Local estimation (23)



Structure Factor Check

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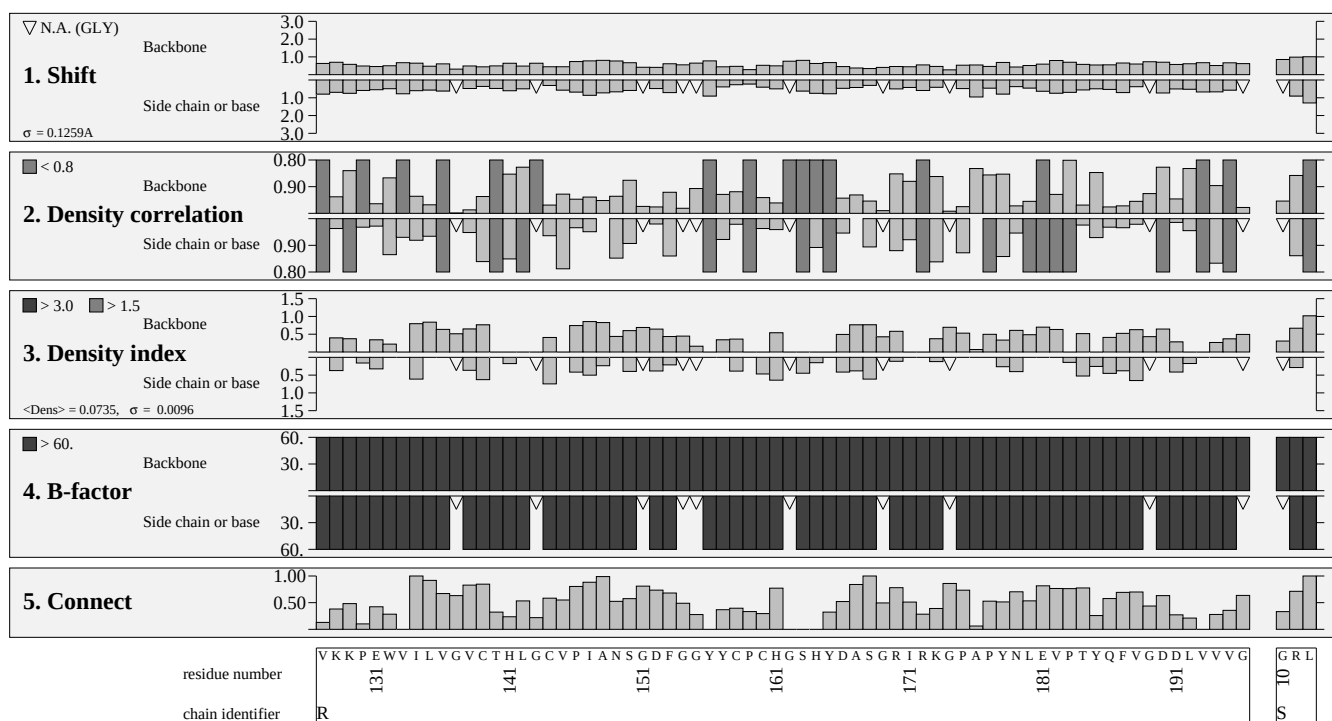
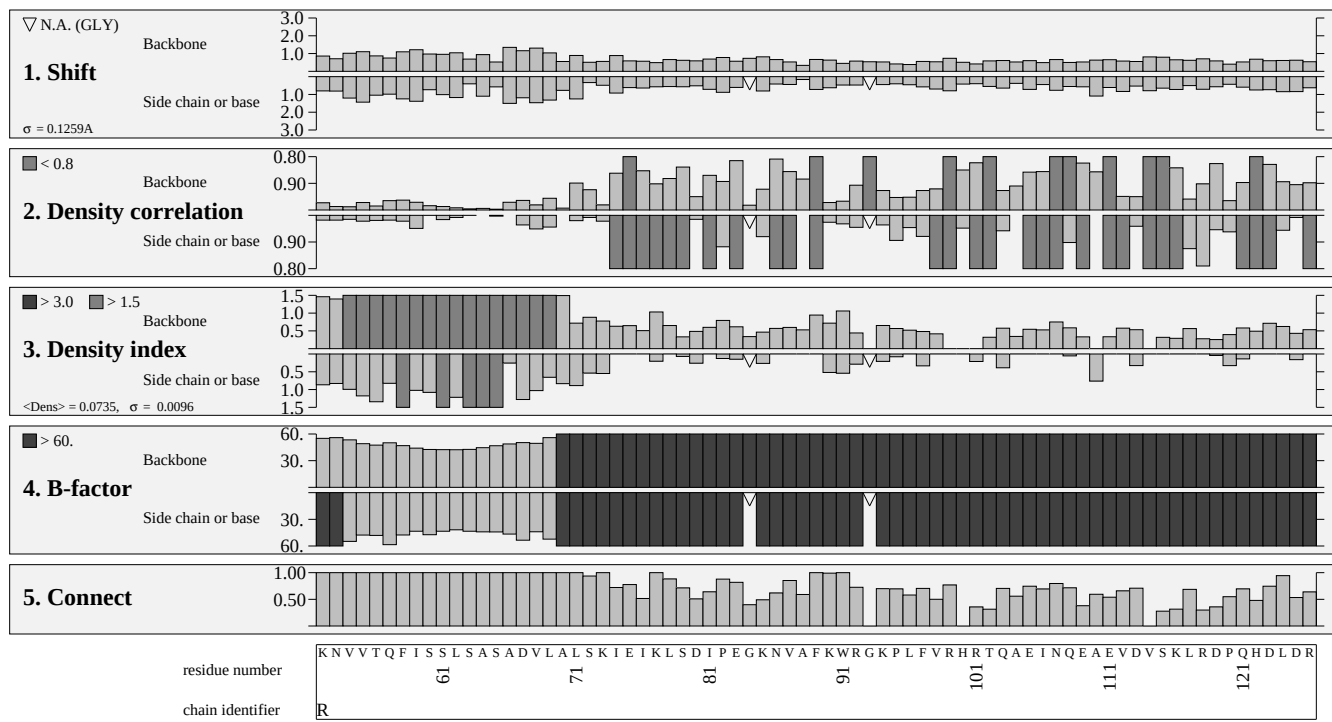
Local estimation (24)



Structure Factor Check

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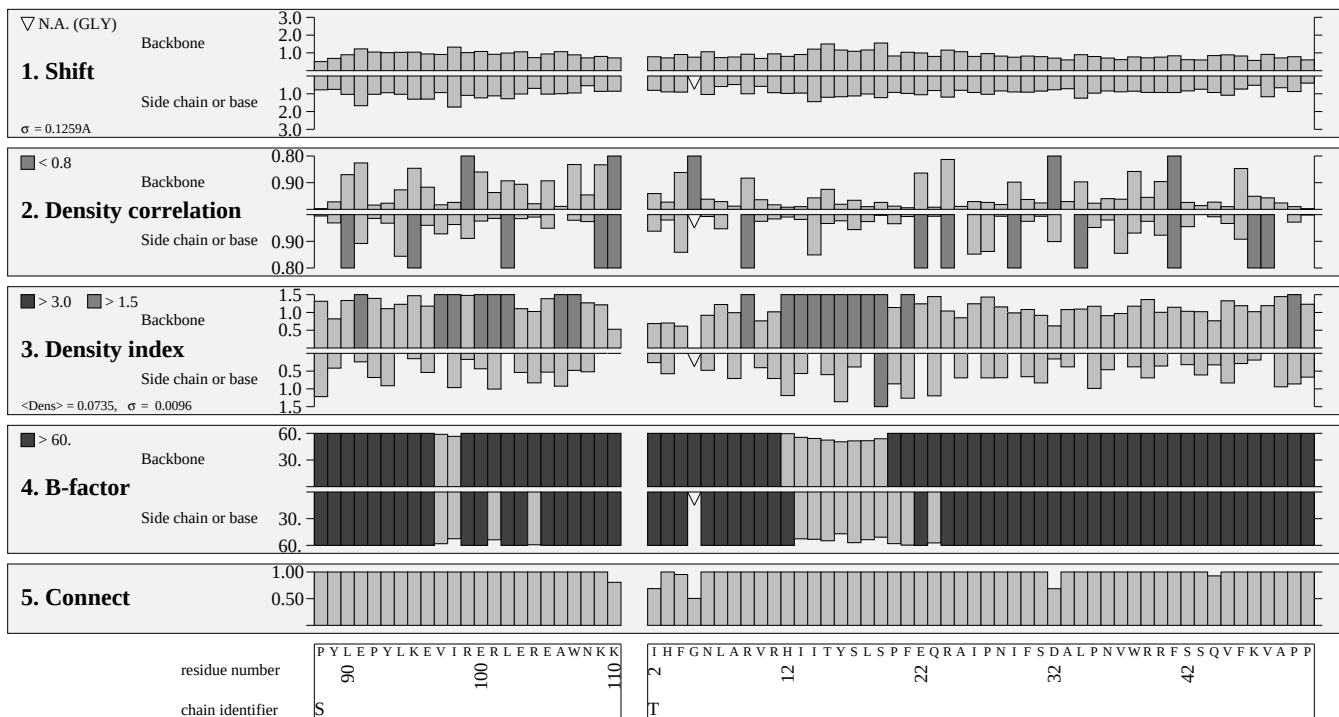
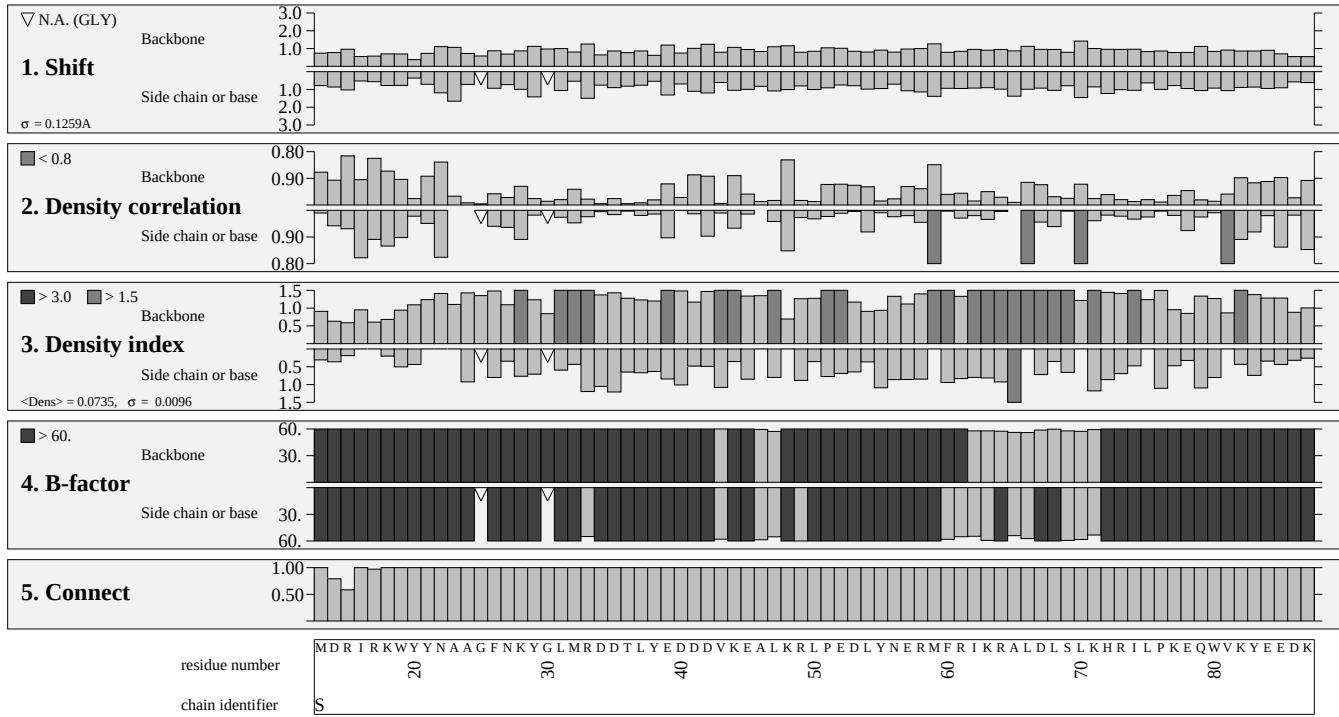
Local estimation (25)



Structure Factor Check

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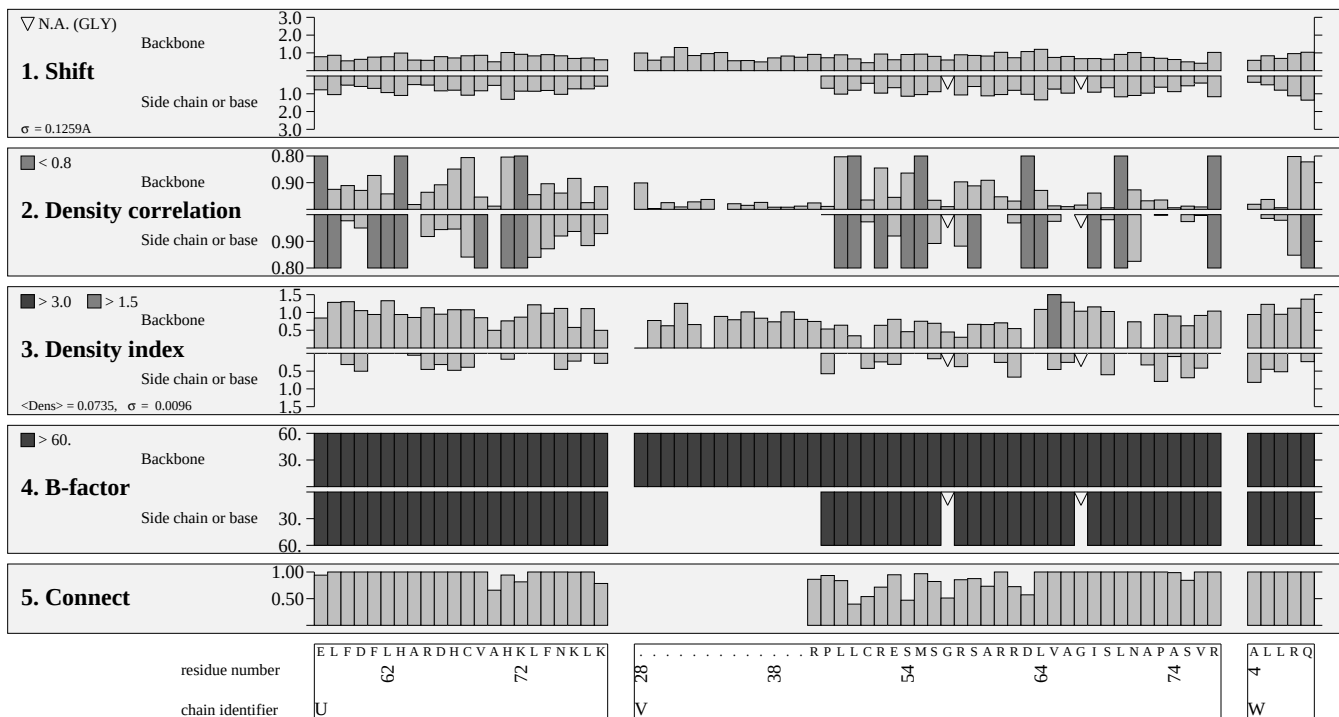
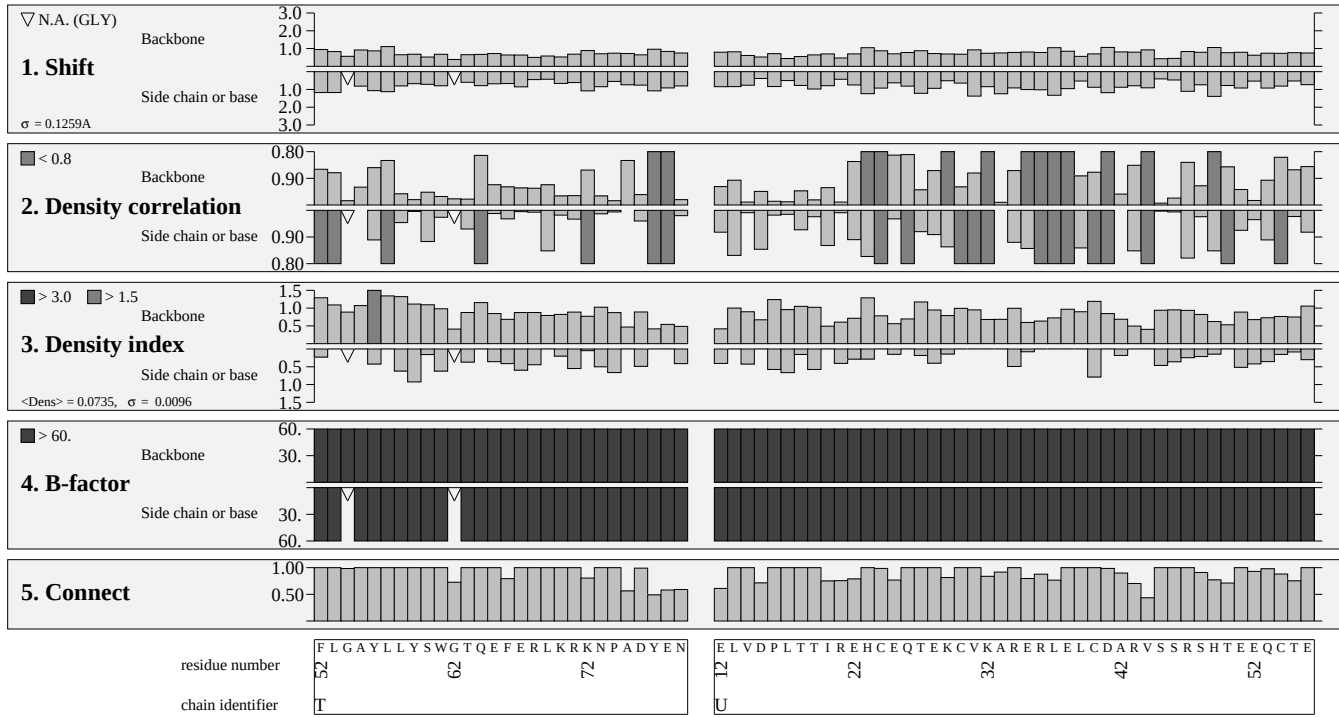
Local estimation (26)



Structure Factor Check

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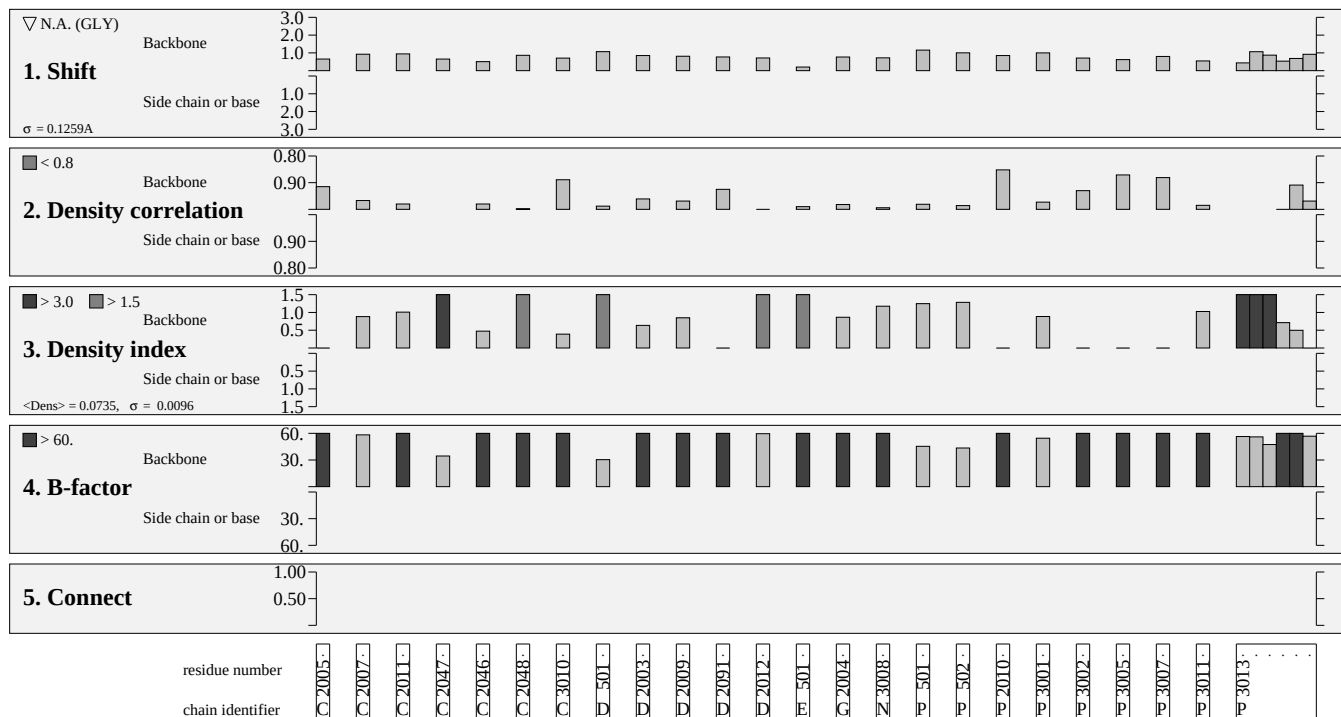
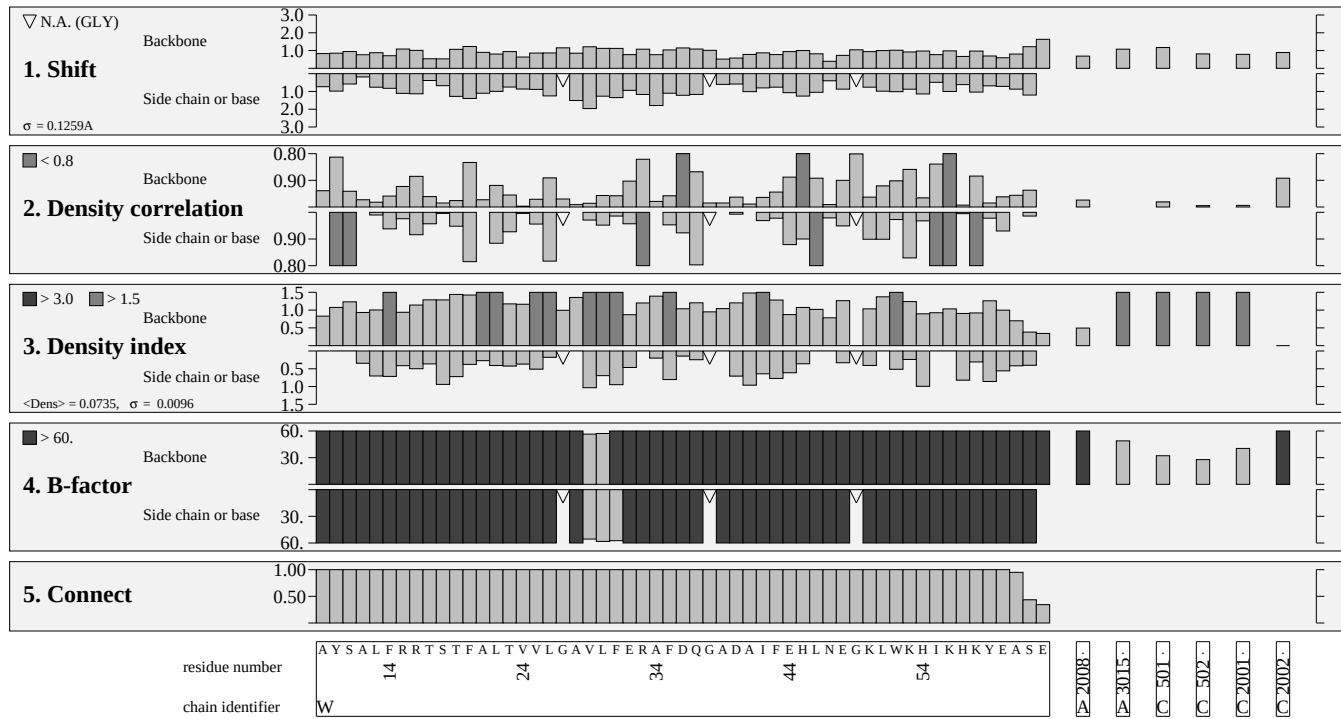
Local estimation (27)



Structure Factor Check

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Local estimation (28)



Local estimation (29)

