

Structure Factor Check

3L73

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH TRIAZOLONE INHIBITO
 Date: 27-DEC-09
 PDB code: 3L73

Crystal

Cell parameters:

a: 171.50 A b: 182.93 A c: 241.03 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 25.0 – 2.90 A
 Reflections in file: 166720
 Unique reflections above 0: 166720
 above 1 σ : 161882
 above 3 σ : 96414

SF CHECK

Nominal resolution range: 25.0 – 3.04 A
 \05max. from input data, min. from author\05
 Used reflections: 145117
 Reflections out of resolution: 21603
 Completeness: 99.7 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.073
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.4474 0.4507
 B_{overall} (by Patterson): 53. A²
 Optical resolution: 2.25 A
 Expected opt. resol. for complete data set: 2.25 A
 Estimated minimal error: 0.093 A

Model

32645 atoms (19 water molecules)

Number of chains: 51

Volume not occupied by model: 62.4 %

$\langle B \rangle$ (for atomic model): 79.6 A²

$\sigma(B)$: 18.27 A²

Matthews coefficient: 4.14

Corresponding solvent % : 70.03

Model vs. Structure Factors

R-factor for all reflections: 0.306
 Correlation factor: 0.851
 R-factor: 0.307
 for $F > 2.0 \sigma$
 nom. resolution range: 24.97 – 3.04 A
 reflections used: 141487

Rfree: 0.335
 Nfree: 2775
 R-factor without free-refl.: 0.307
 Non free-reflections: 138712
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.604 A
 Estimated maximal error: 0.414 A
 DPI: 0.376 A

Scaling

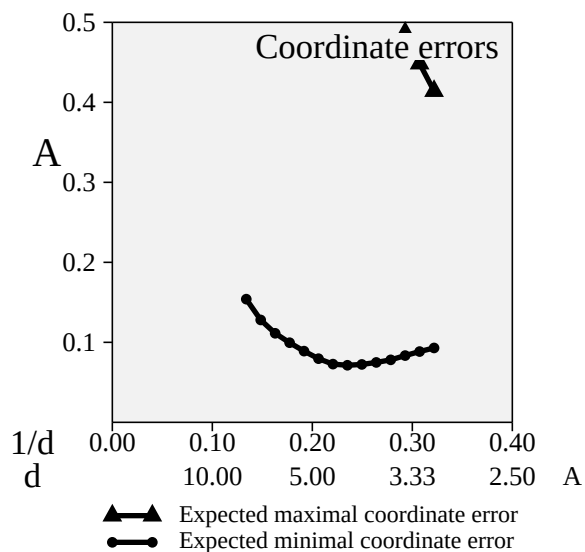
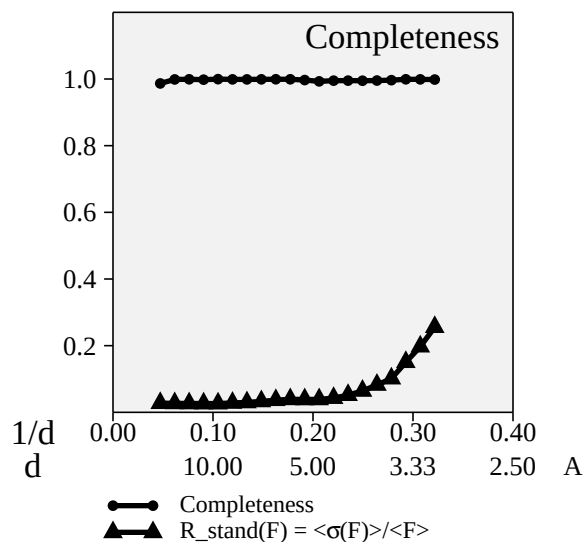
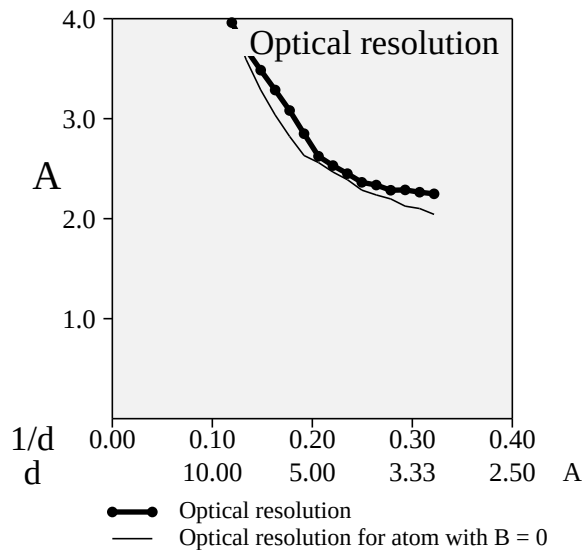
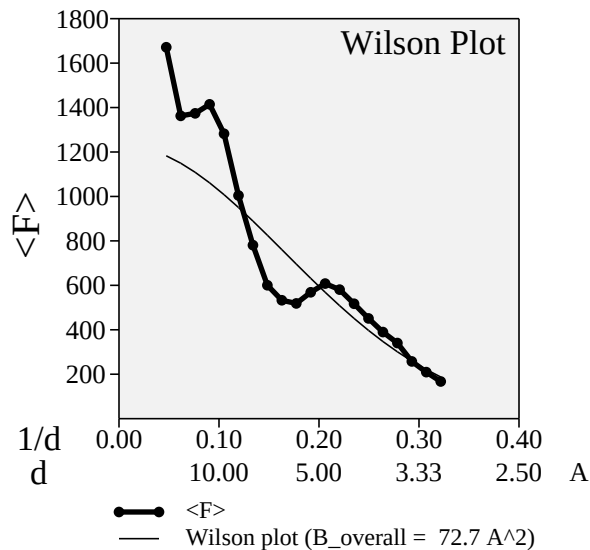
Scale: 0.483
 Bdiff: -9.31
 Anisothermal Scaling (Beta):
 12.5073 -4.4573 -3.7911 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.416 250.040

Refinement

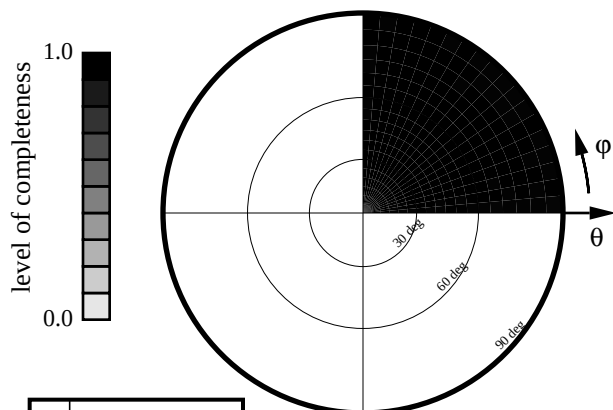
Program: CNS 1.1
 Nominal resolution range: 25.0 – 3.04 A
 Reported R-factor: 0.259
 Number of reflections used: 145117
 Reported Rfree: 0.29
 Sigma cut-off: N.A.

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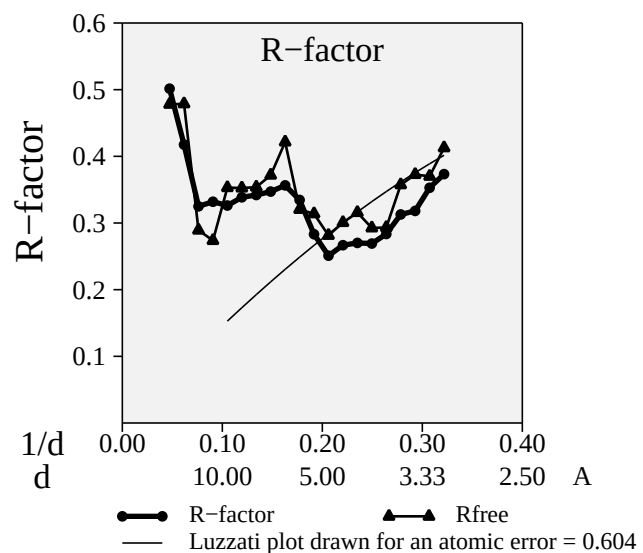


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

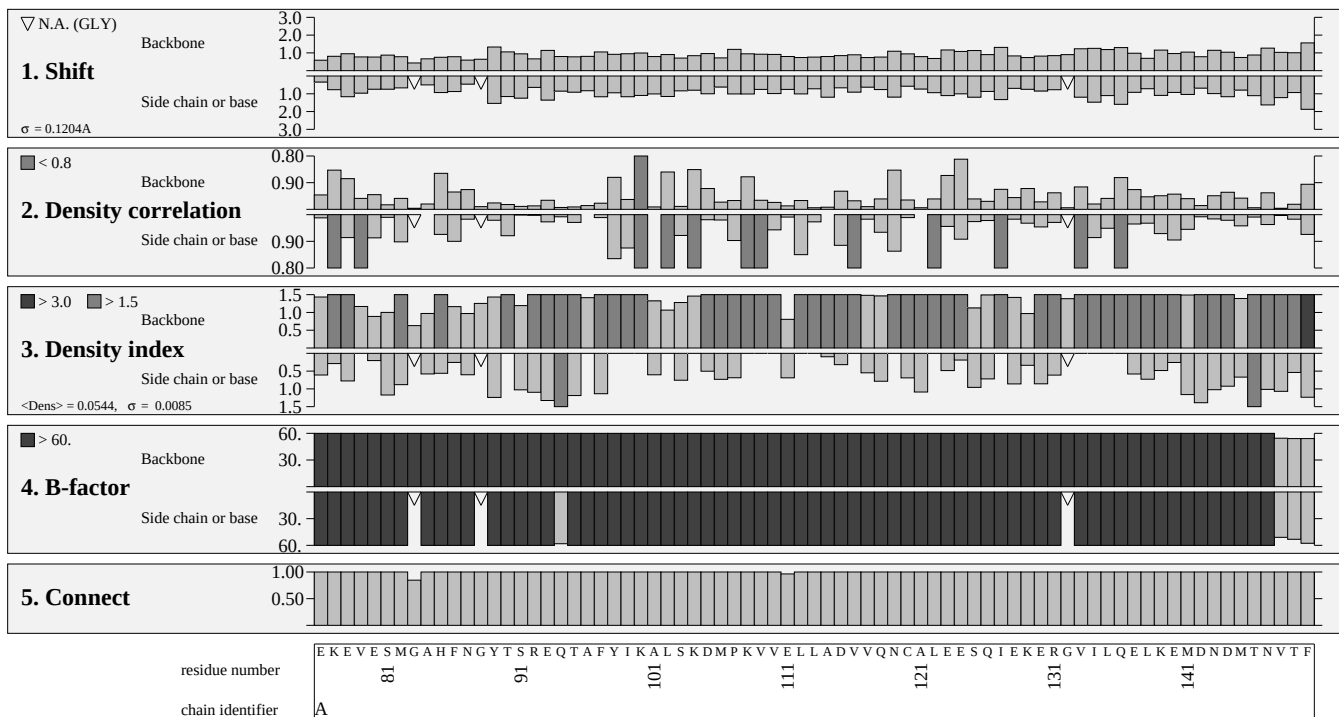
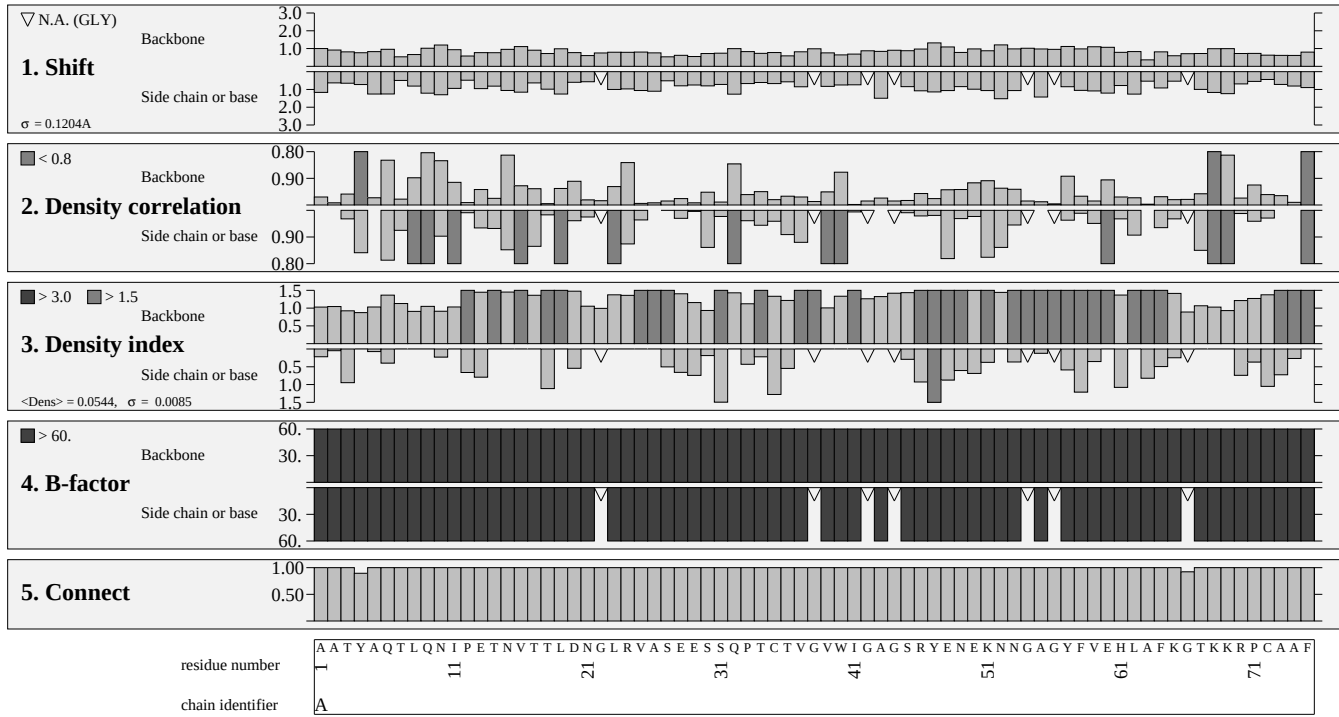
polar coordinates of the crystallographical axes



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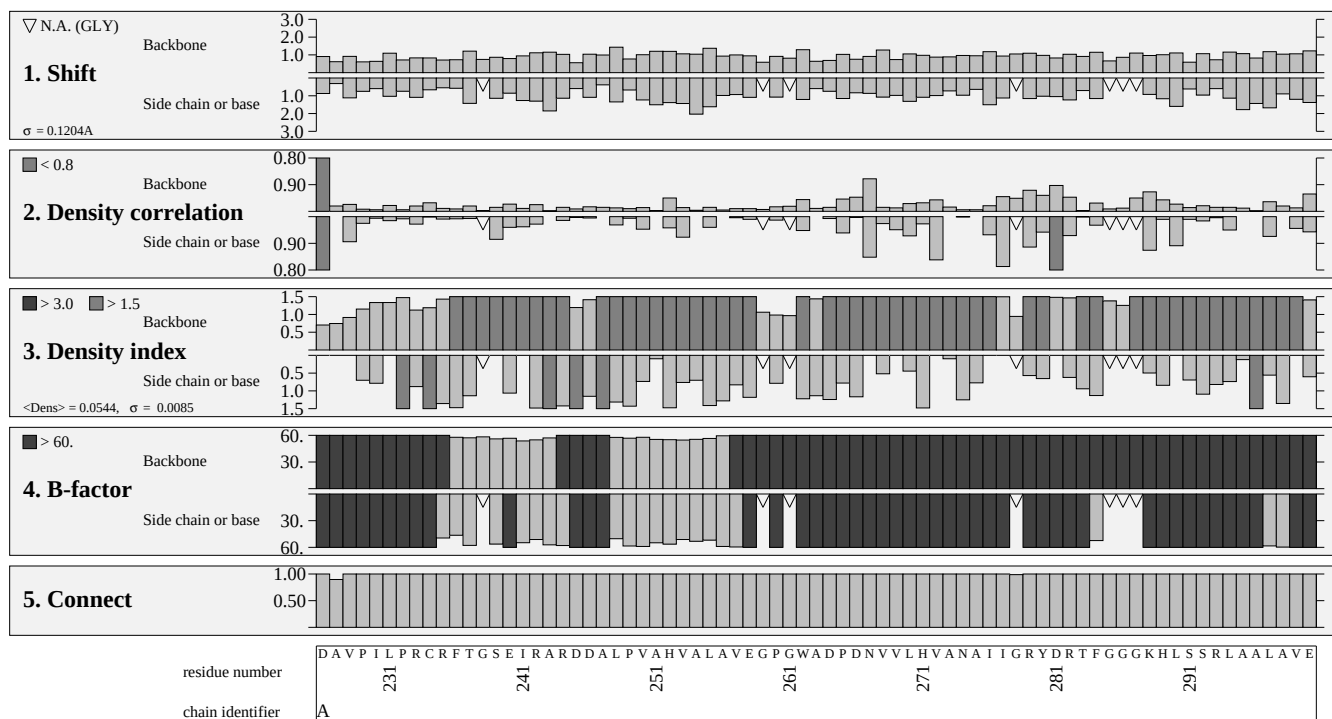
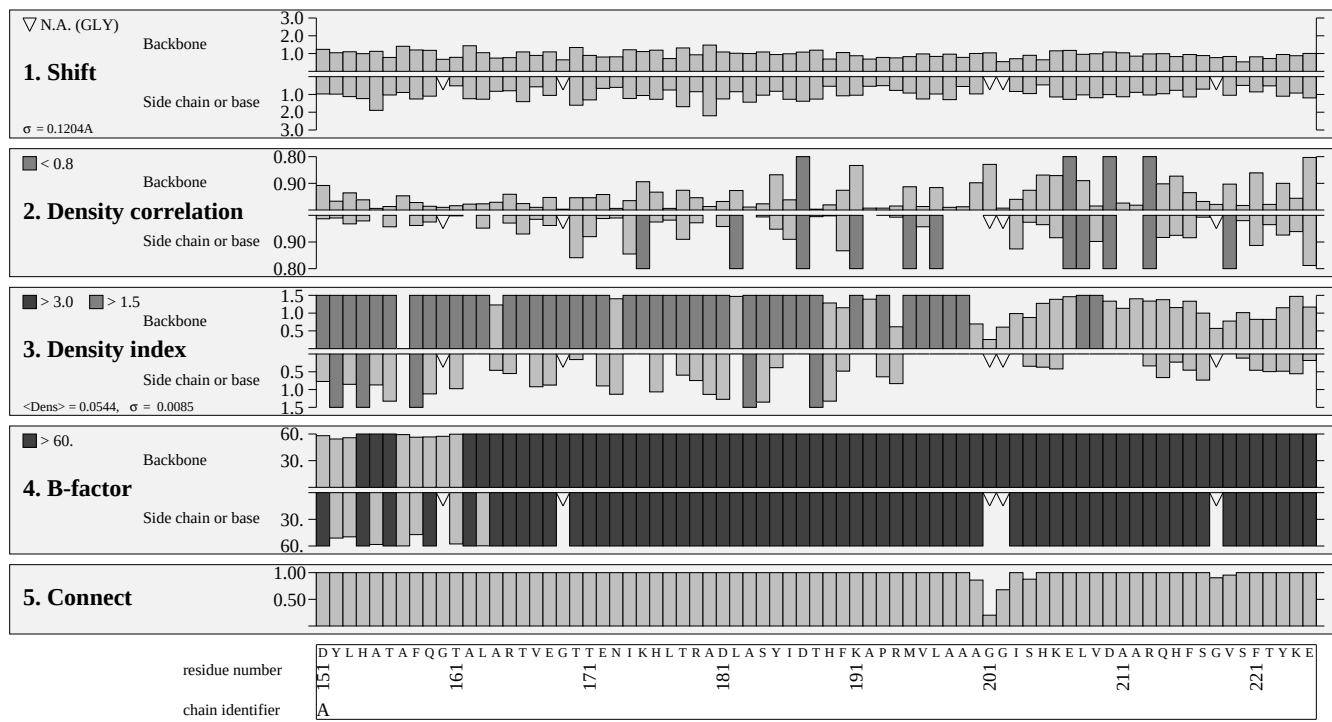
Local estimation



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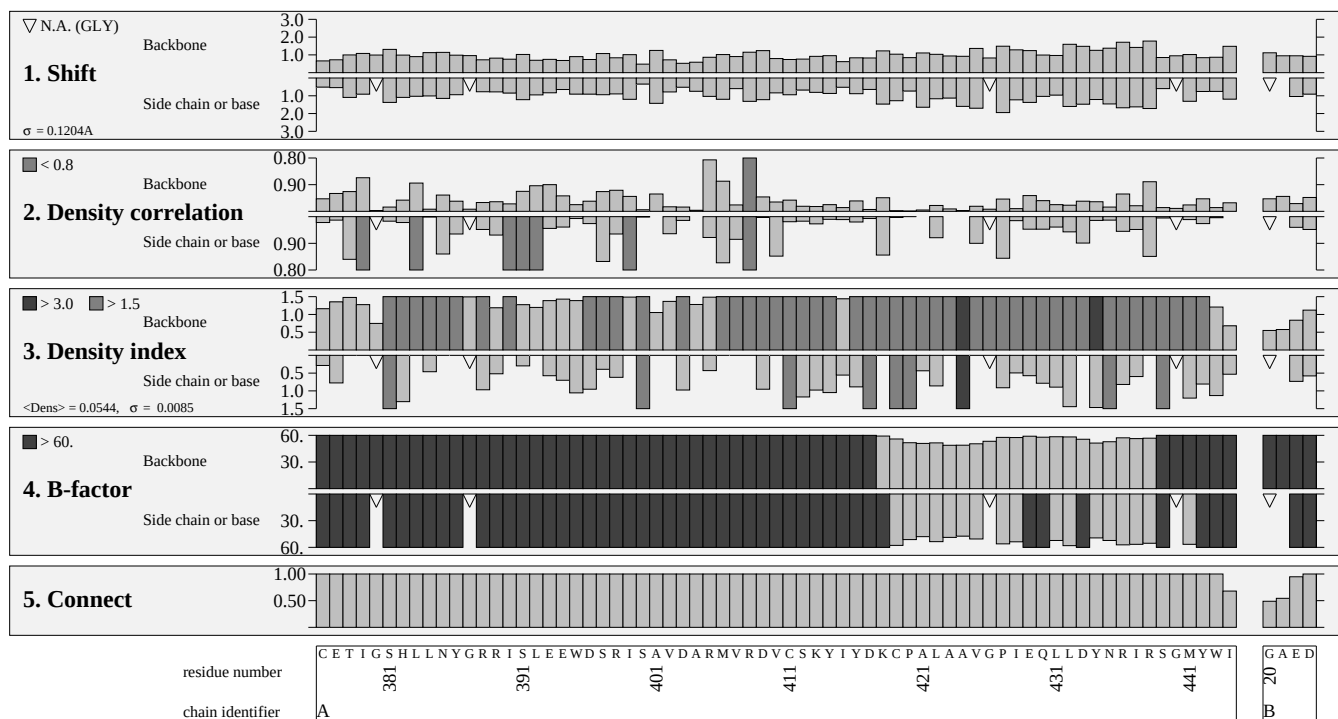
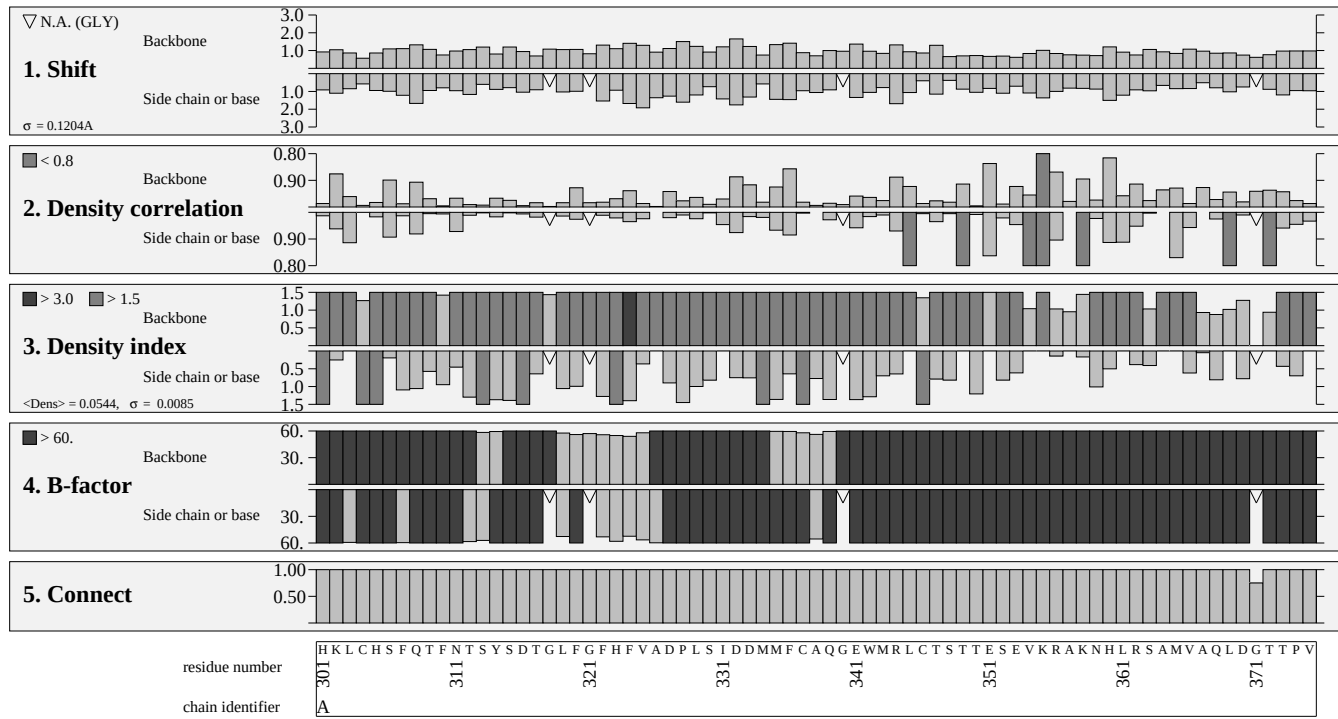
Local estimation (2)



Structure Factor Check

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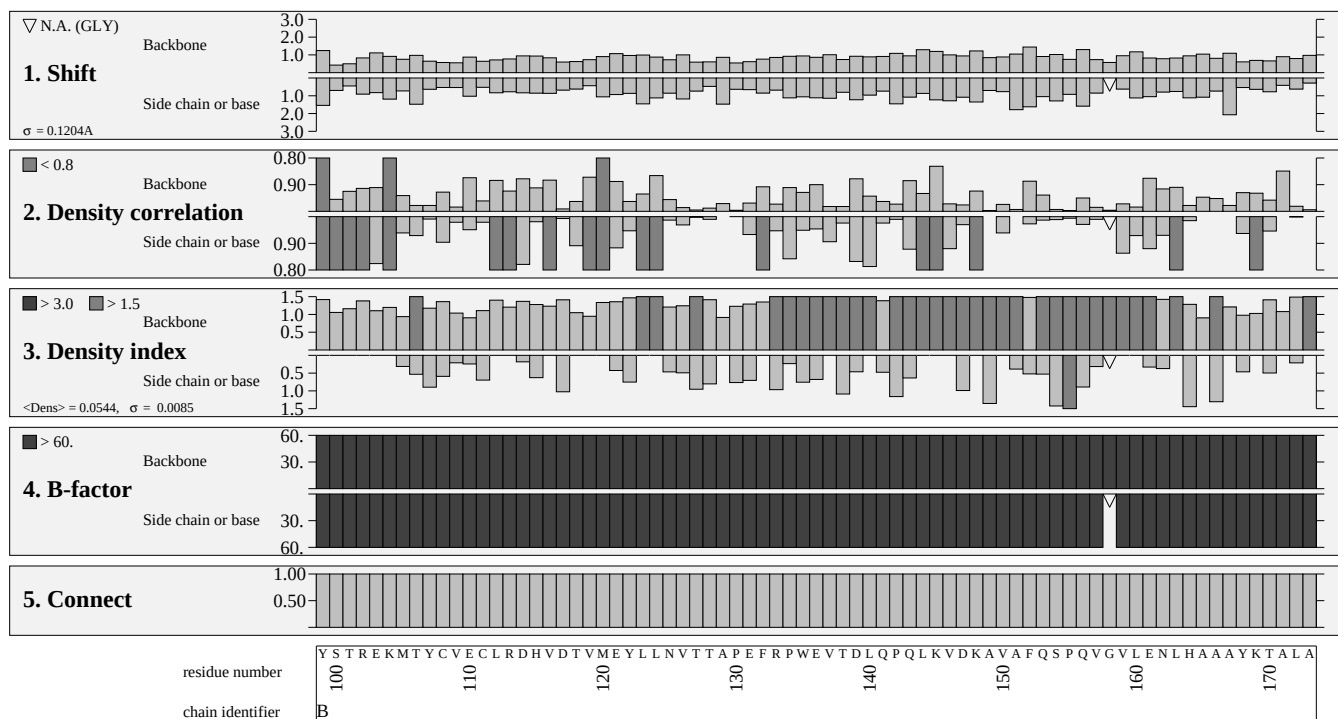
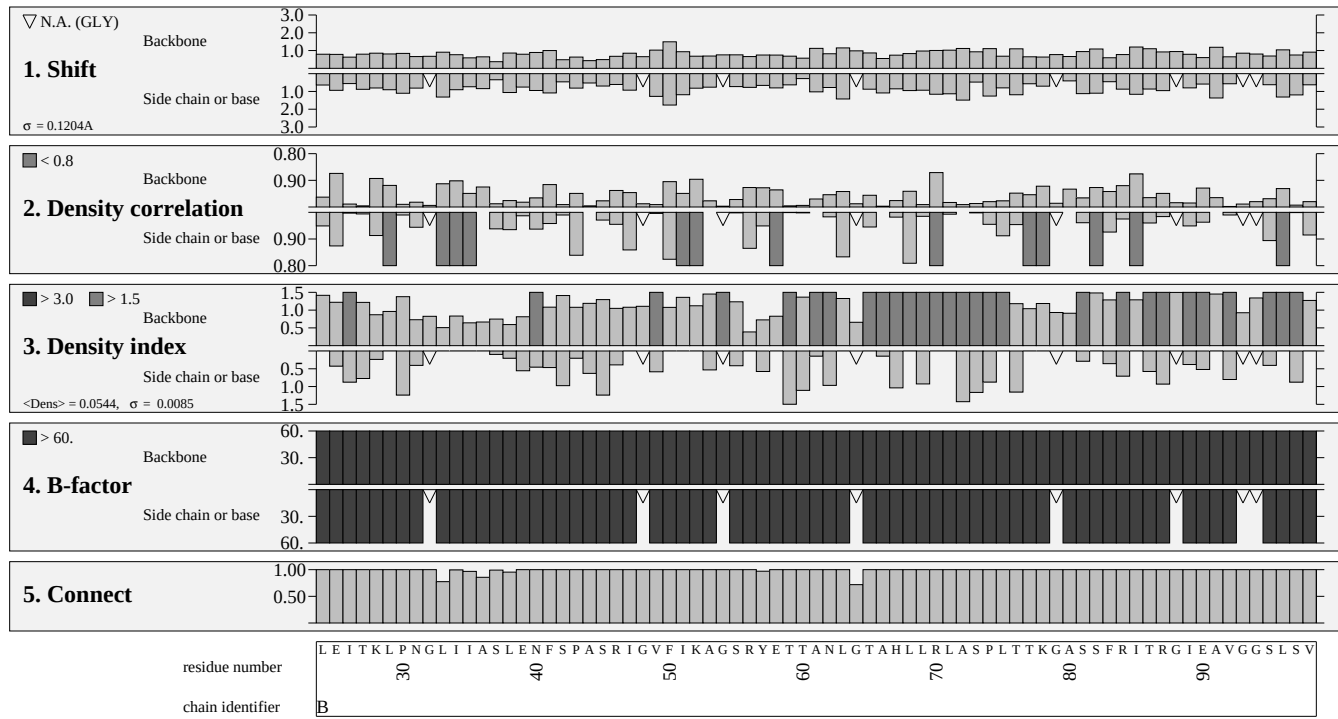
Local estimation (3)



Structure Factor Check

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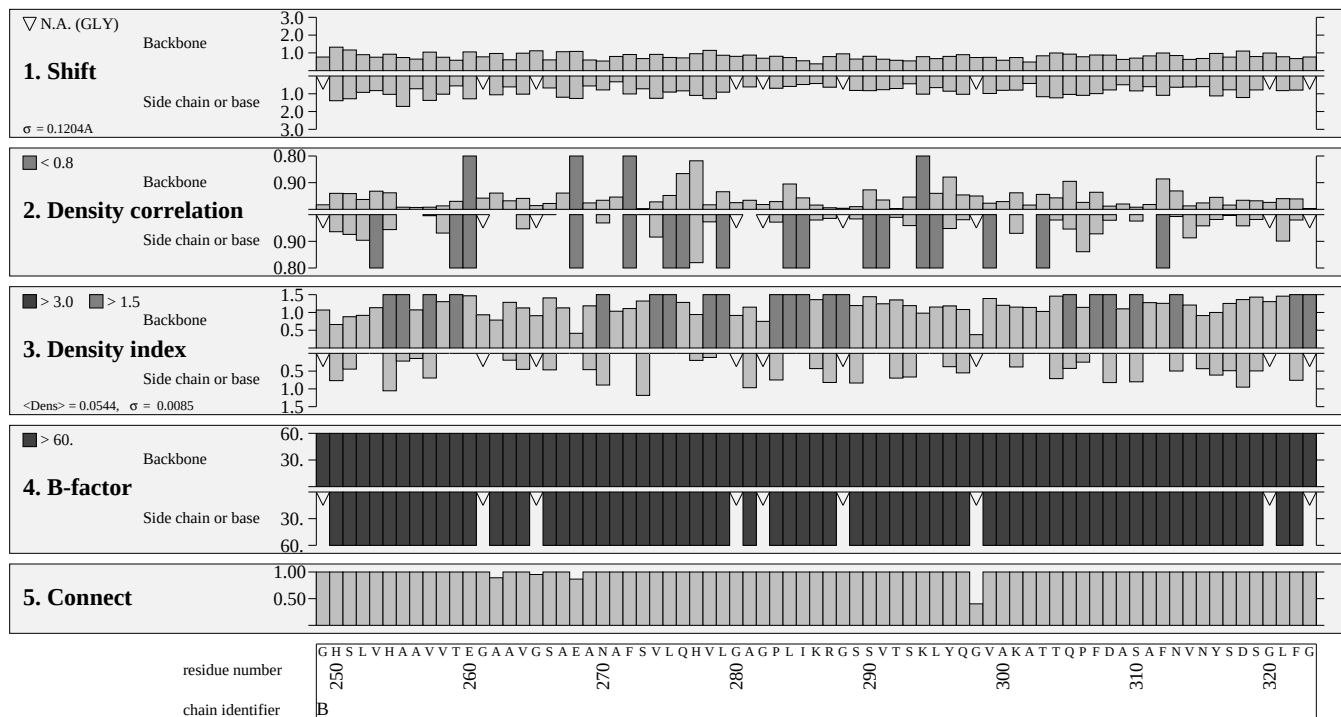
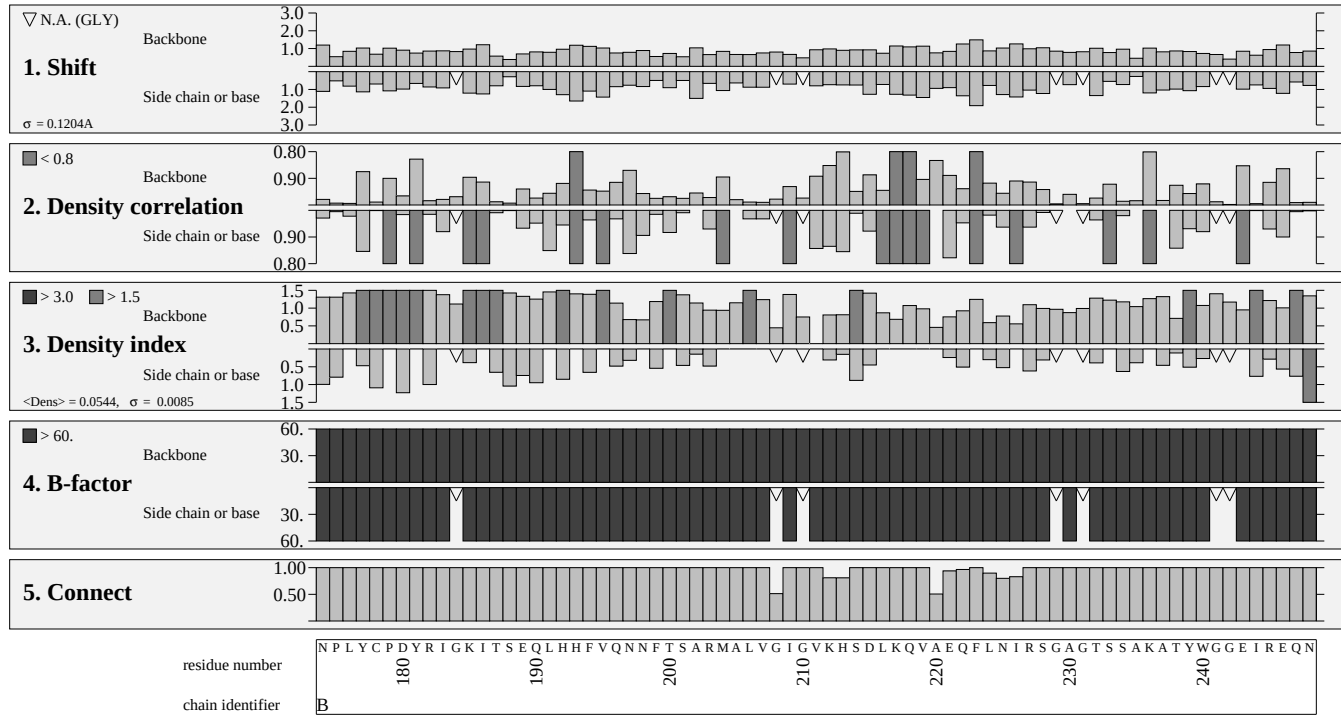
Local estimation (4)



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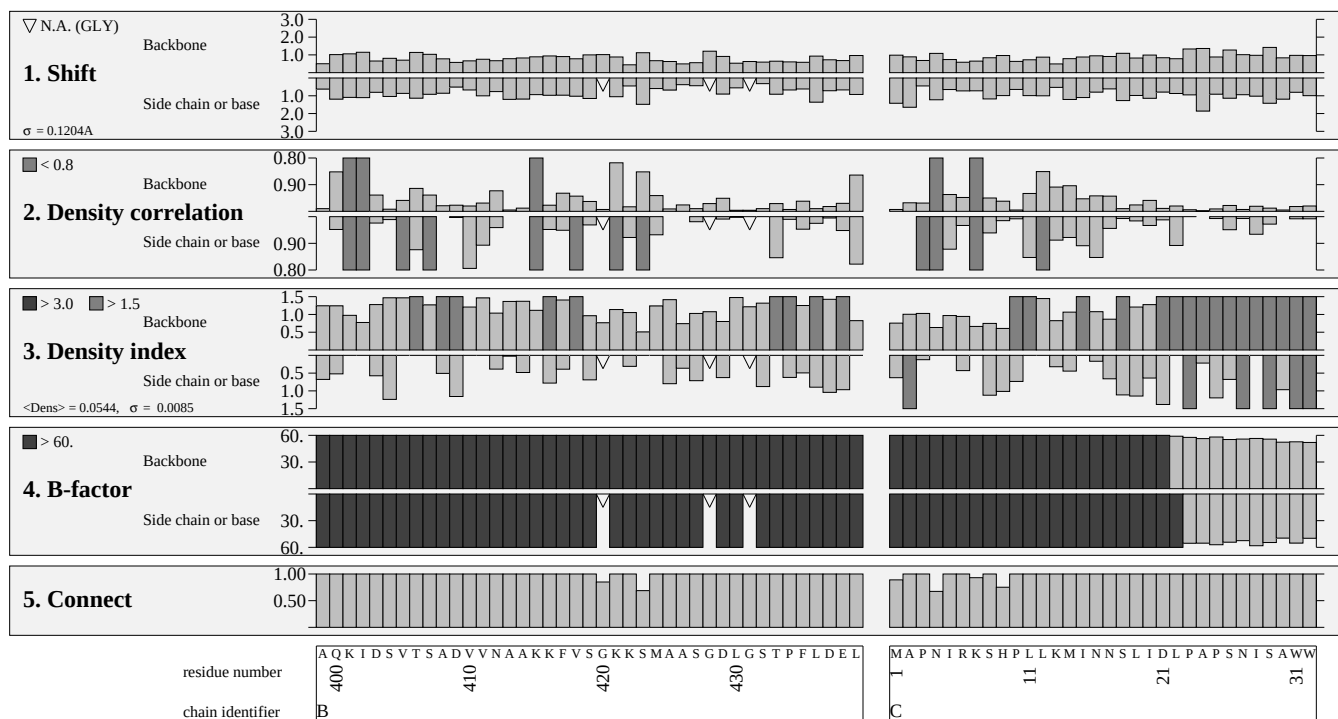
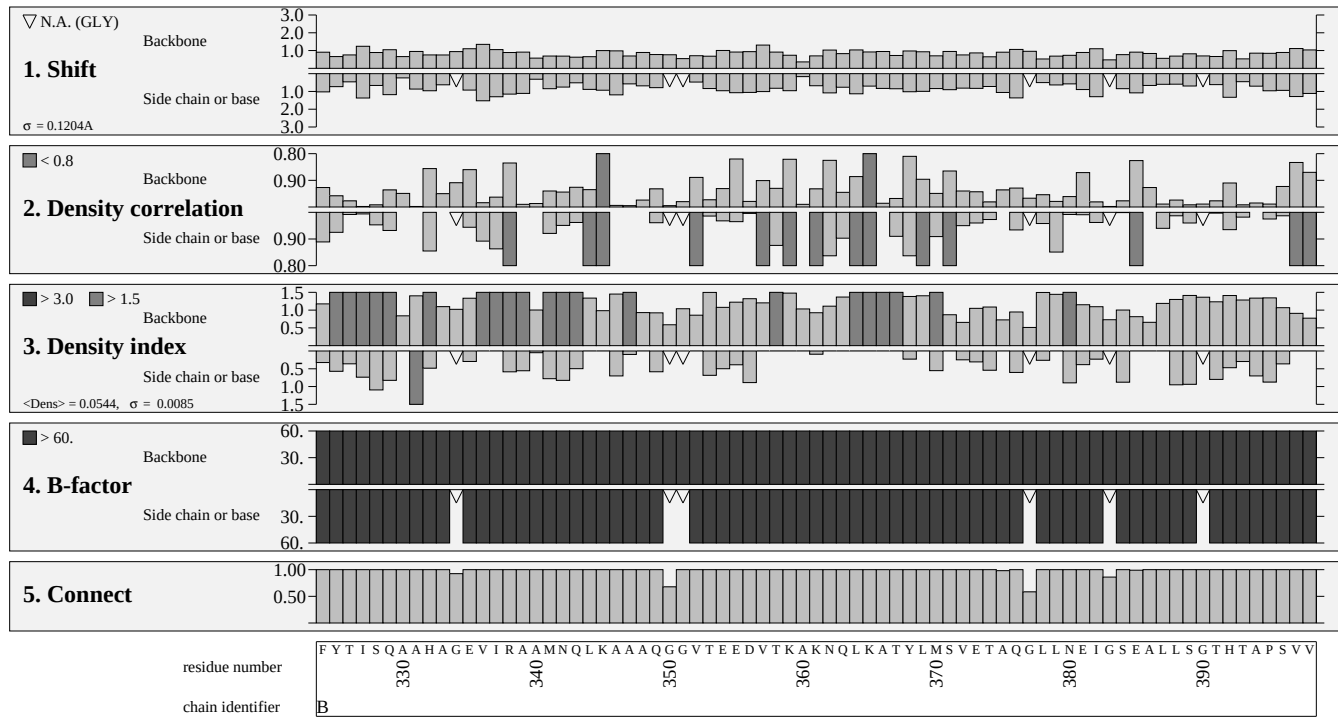
Local estimation (5)



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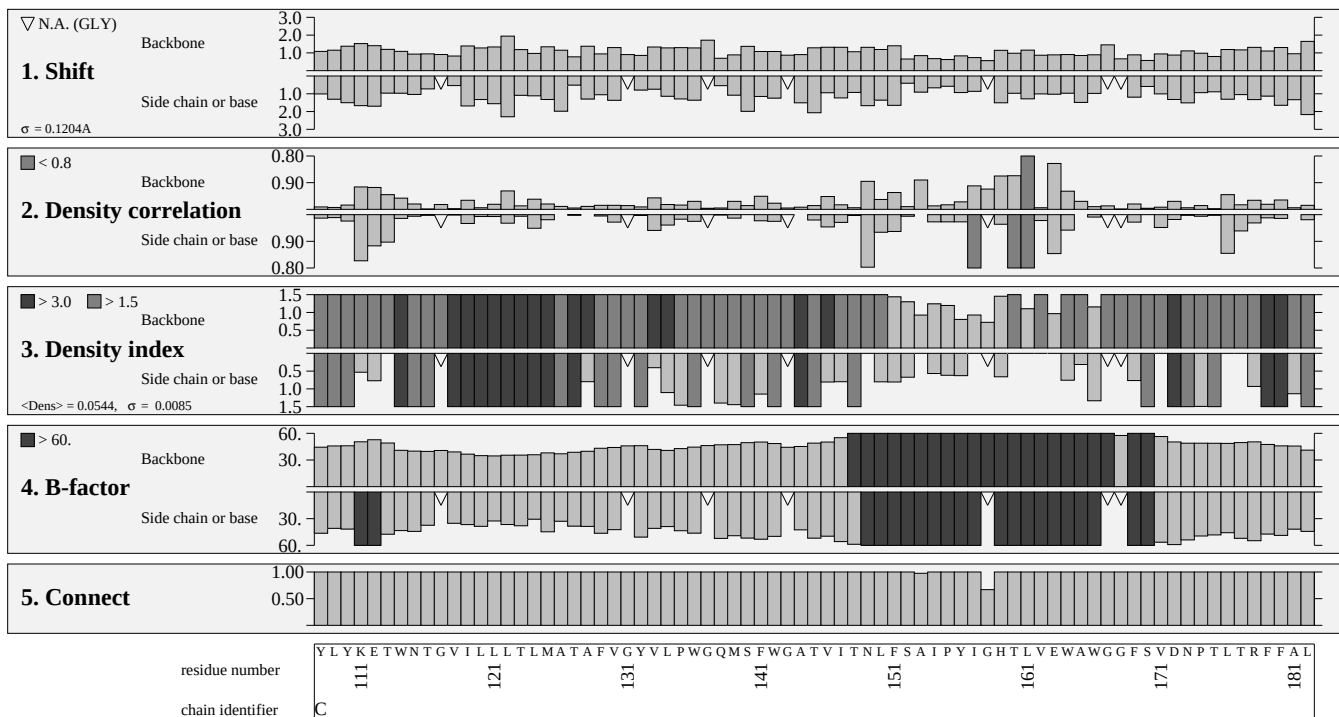
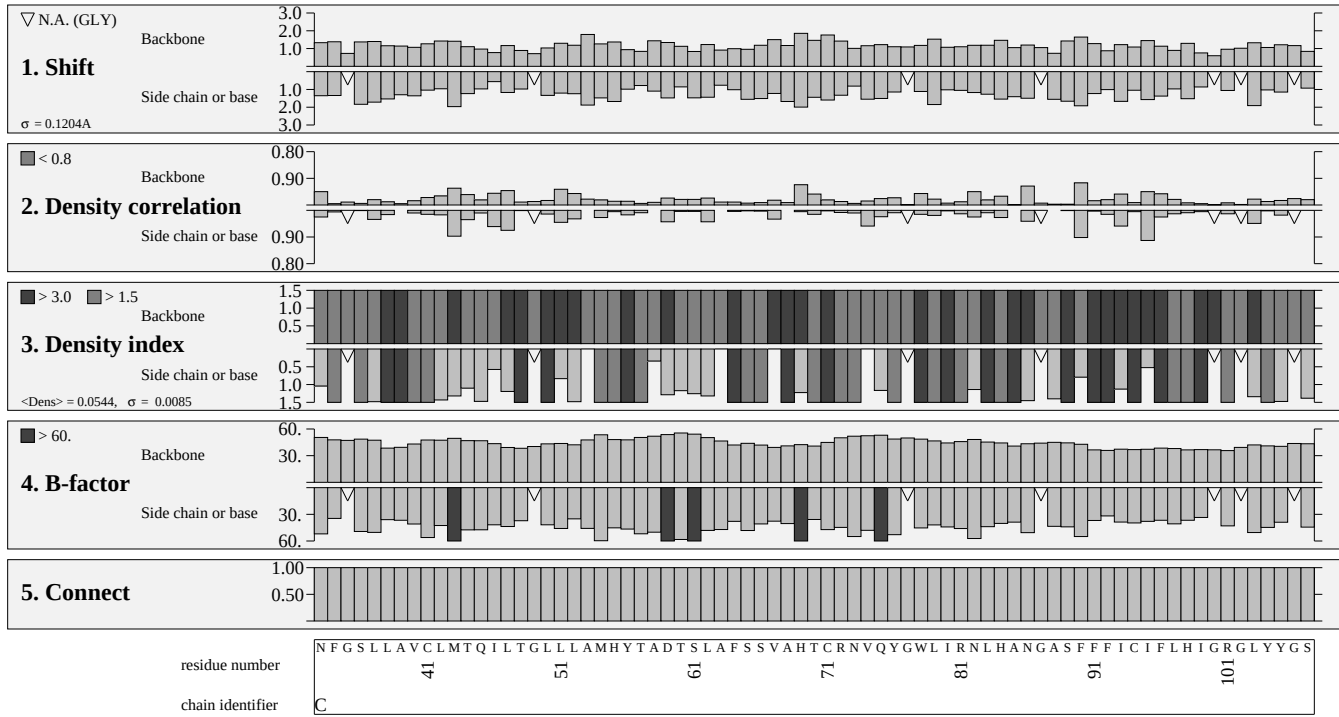
Local estimation (6)



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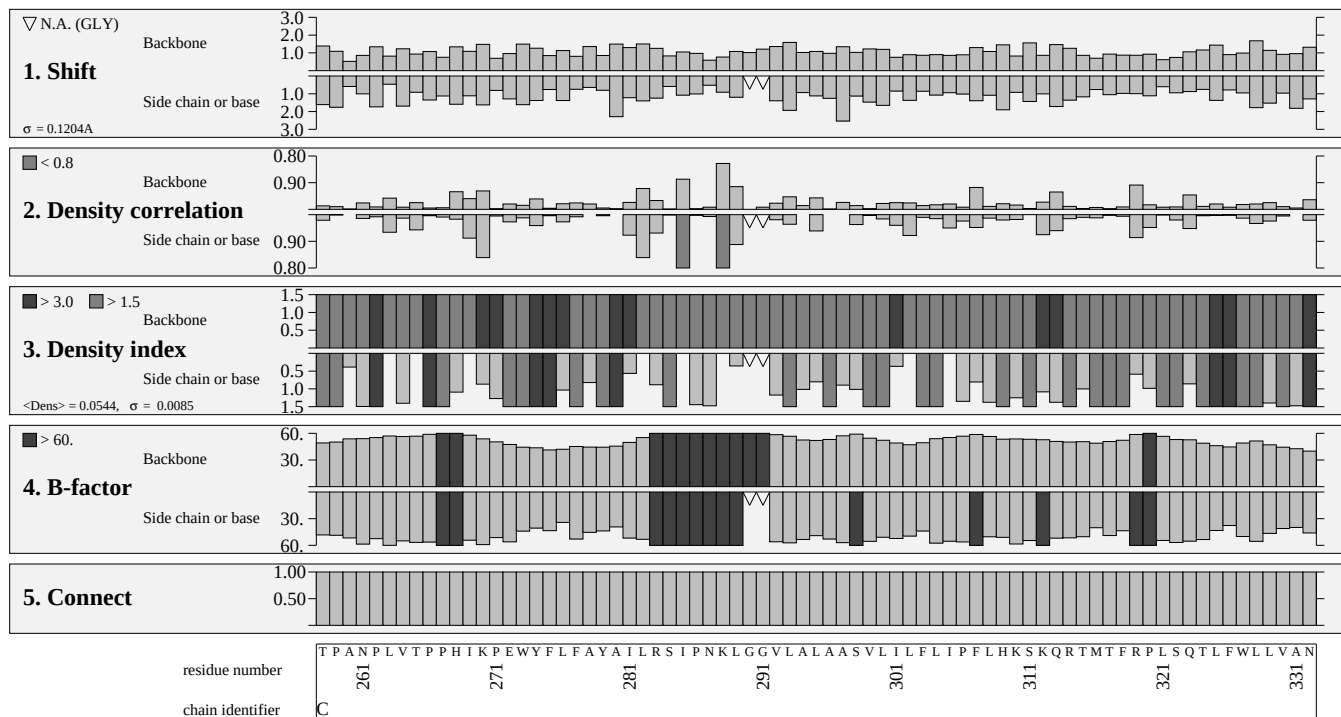
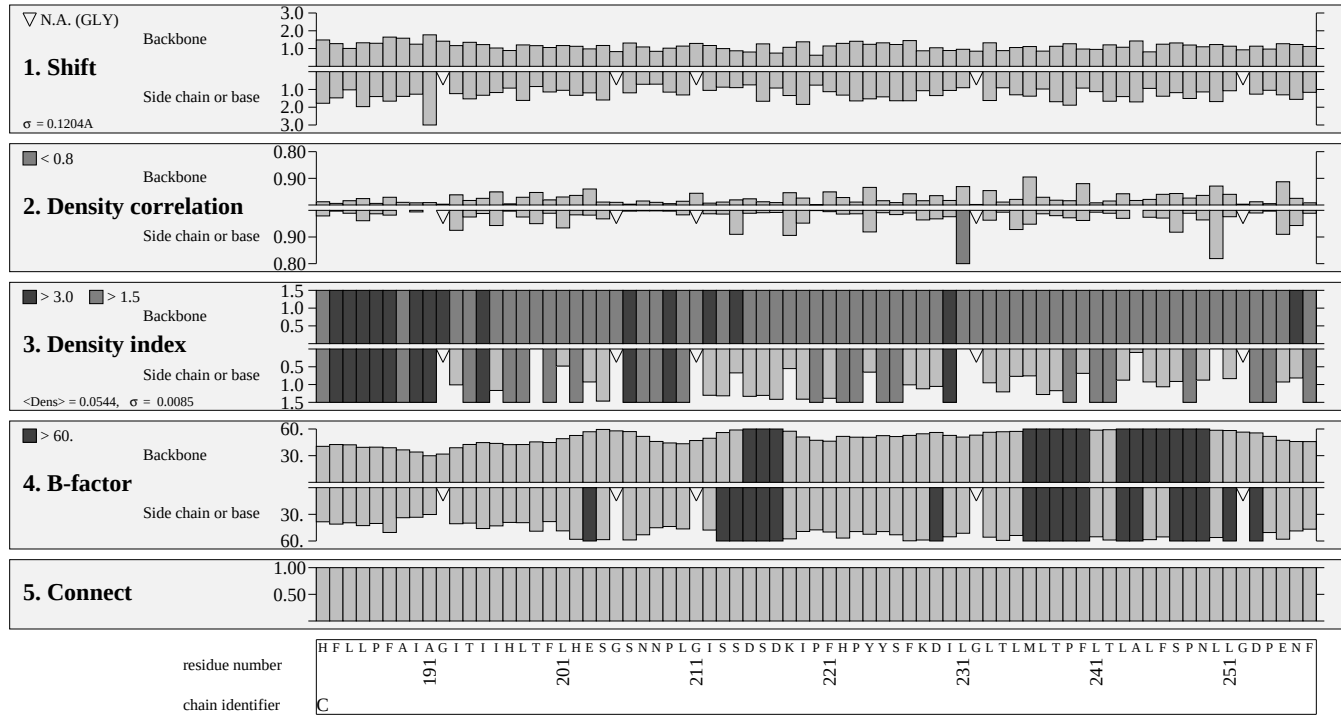
Local estimation (7)



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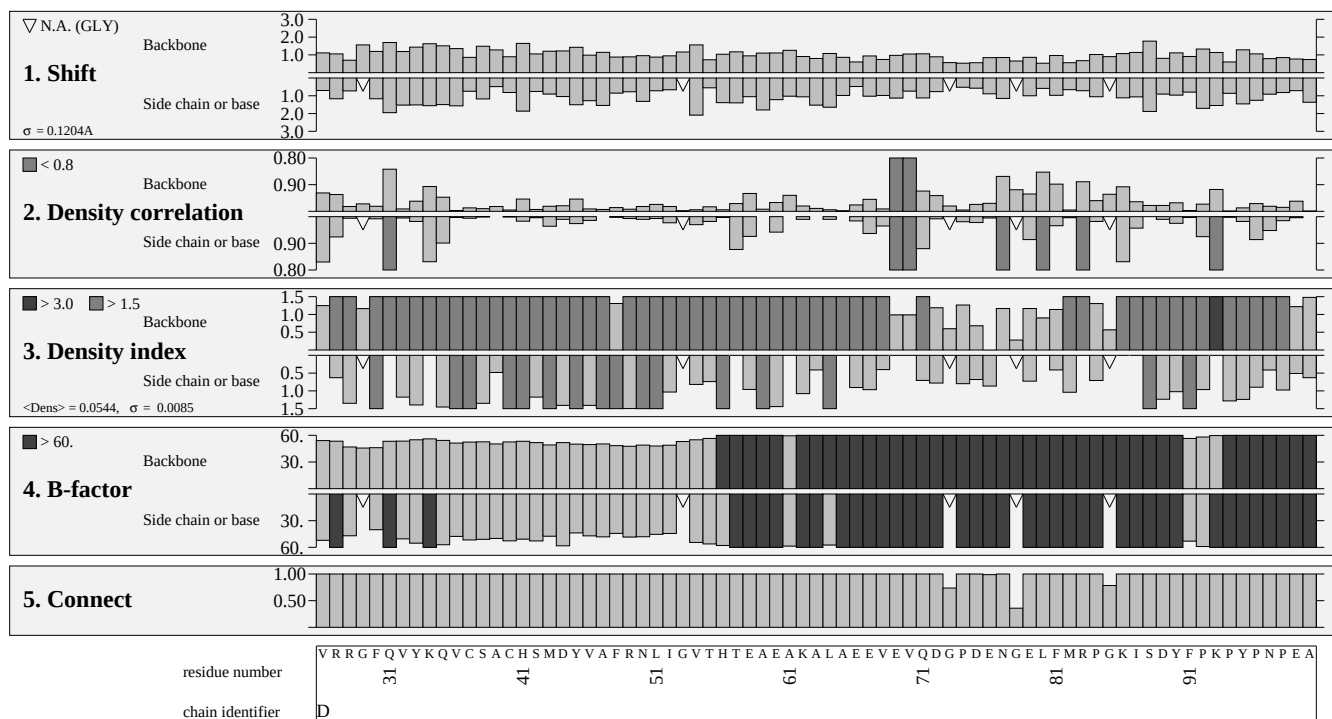
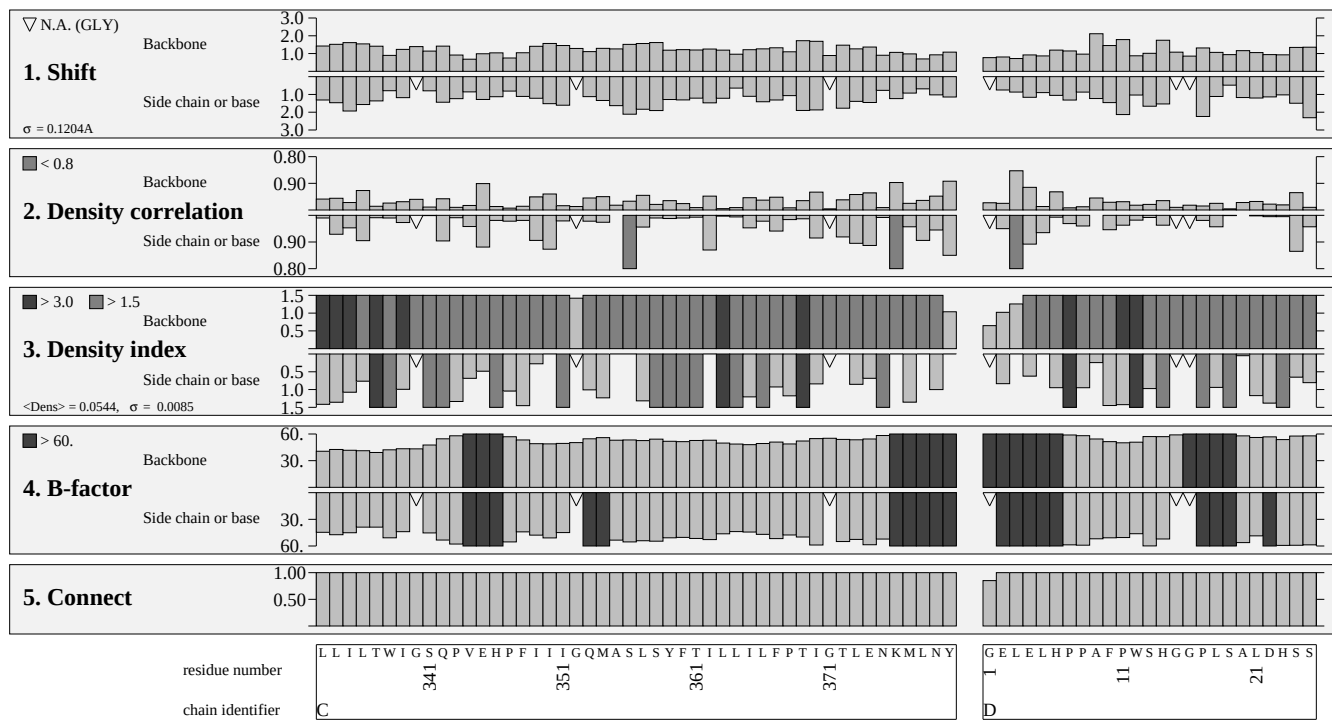
Local estimation (8)



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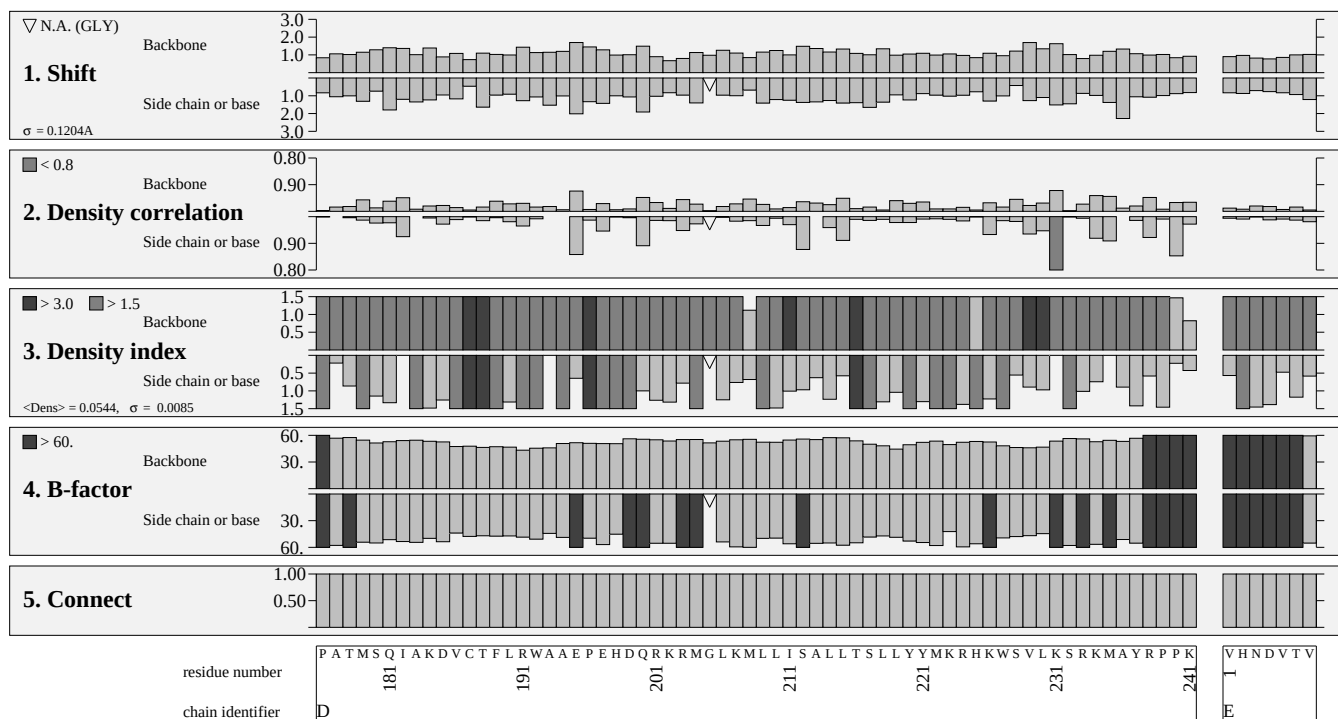
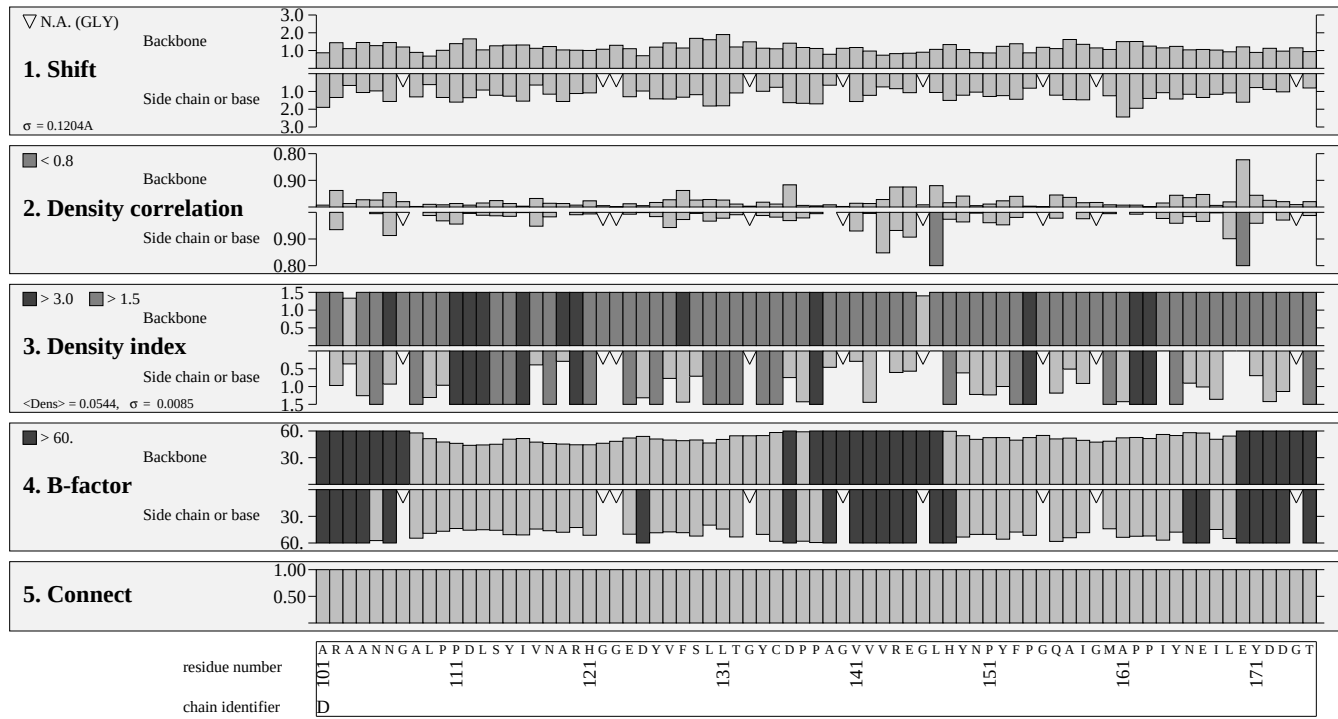
Local estimation (9)



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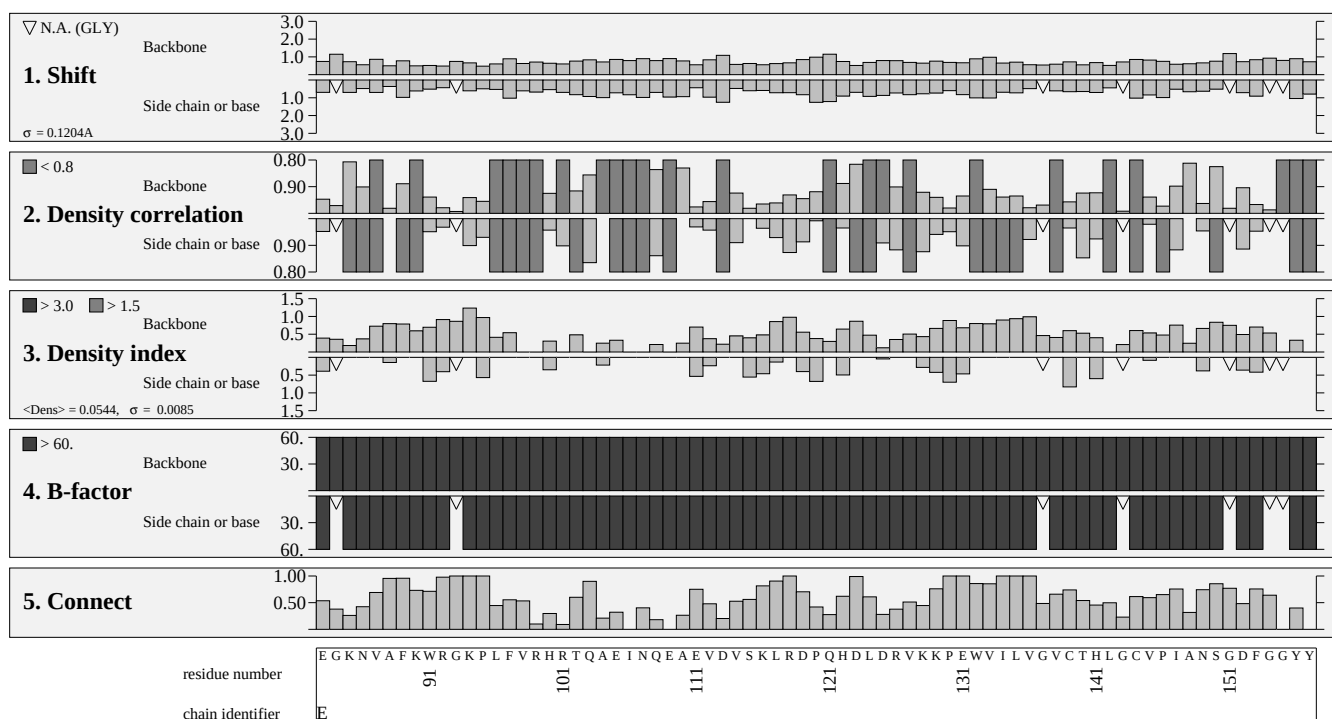
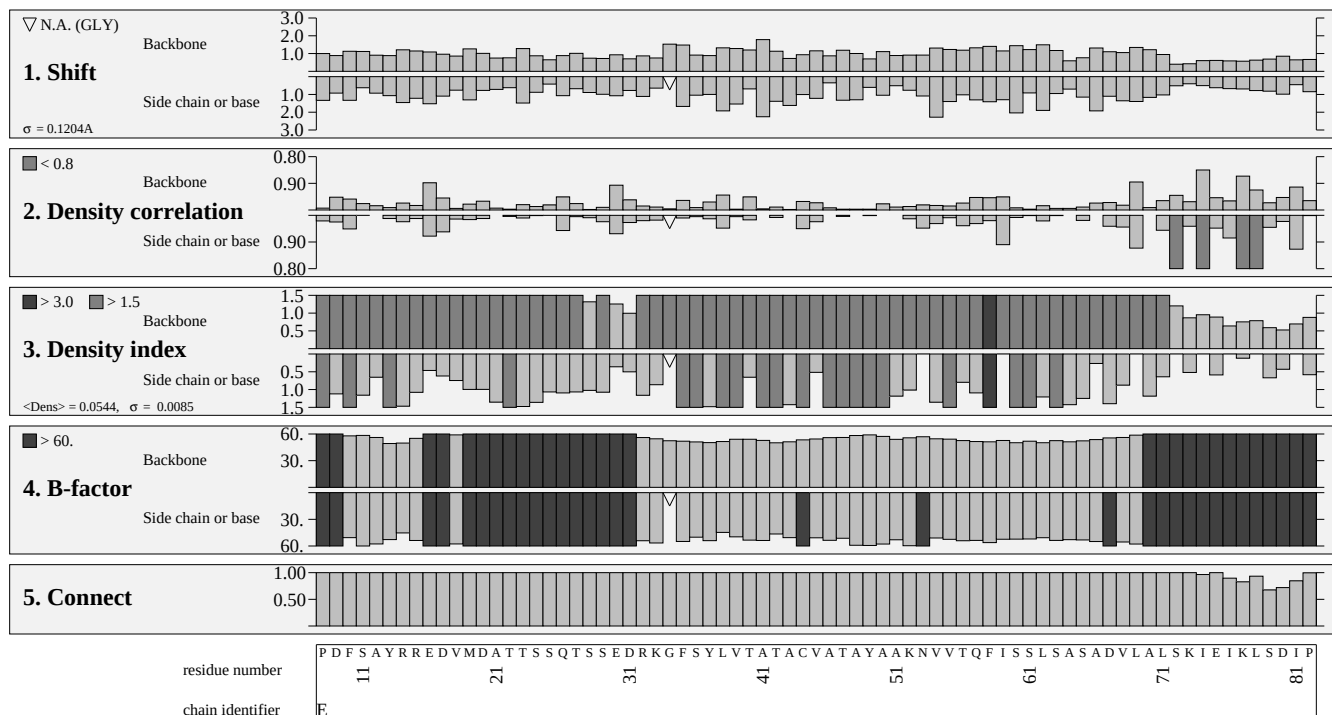
Local estimation (10)



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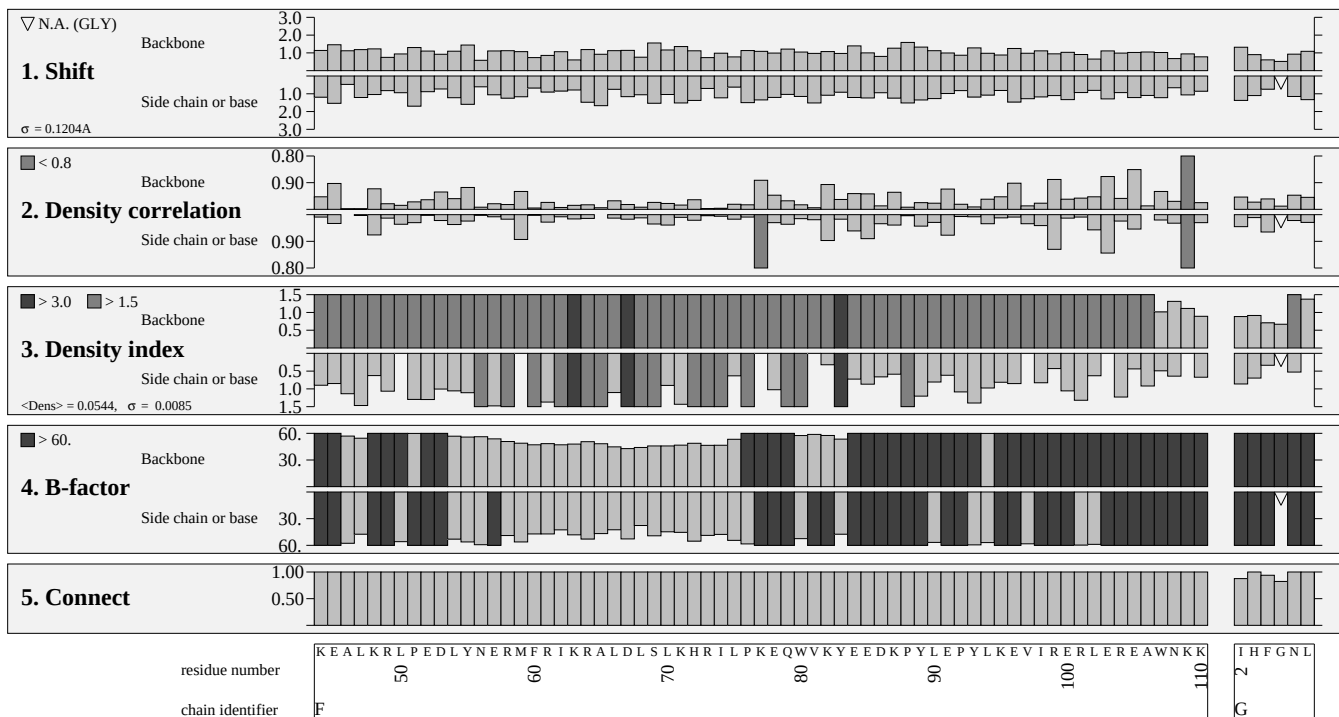
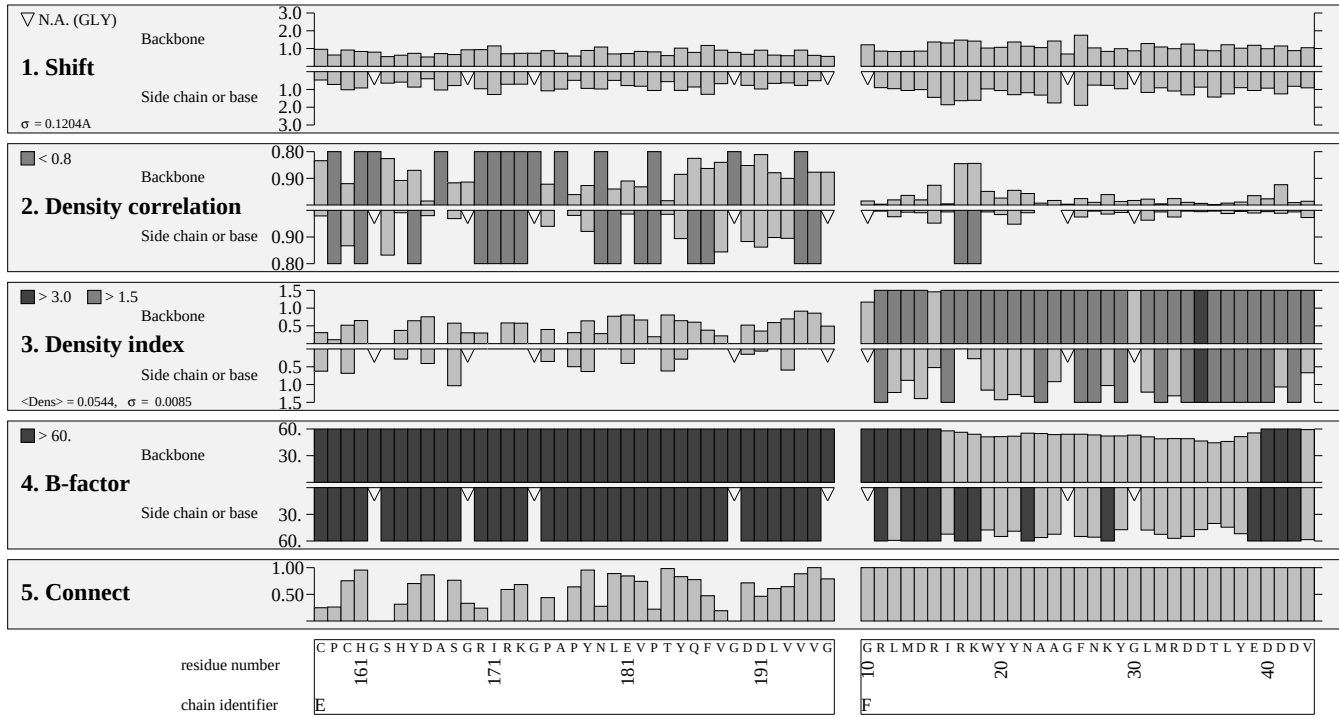
Local estimation (11)



Structure Factor Check

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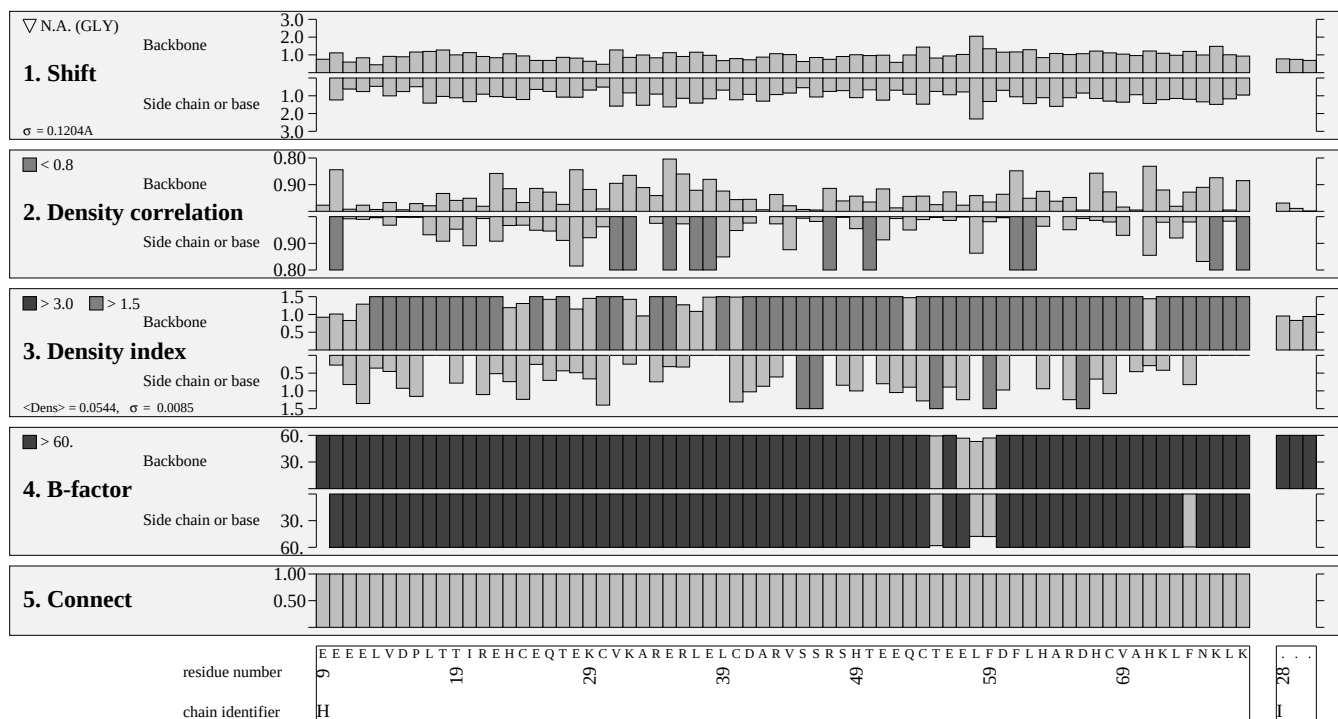
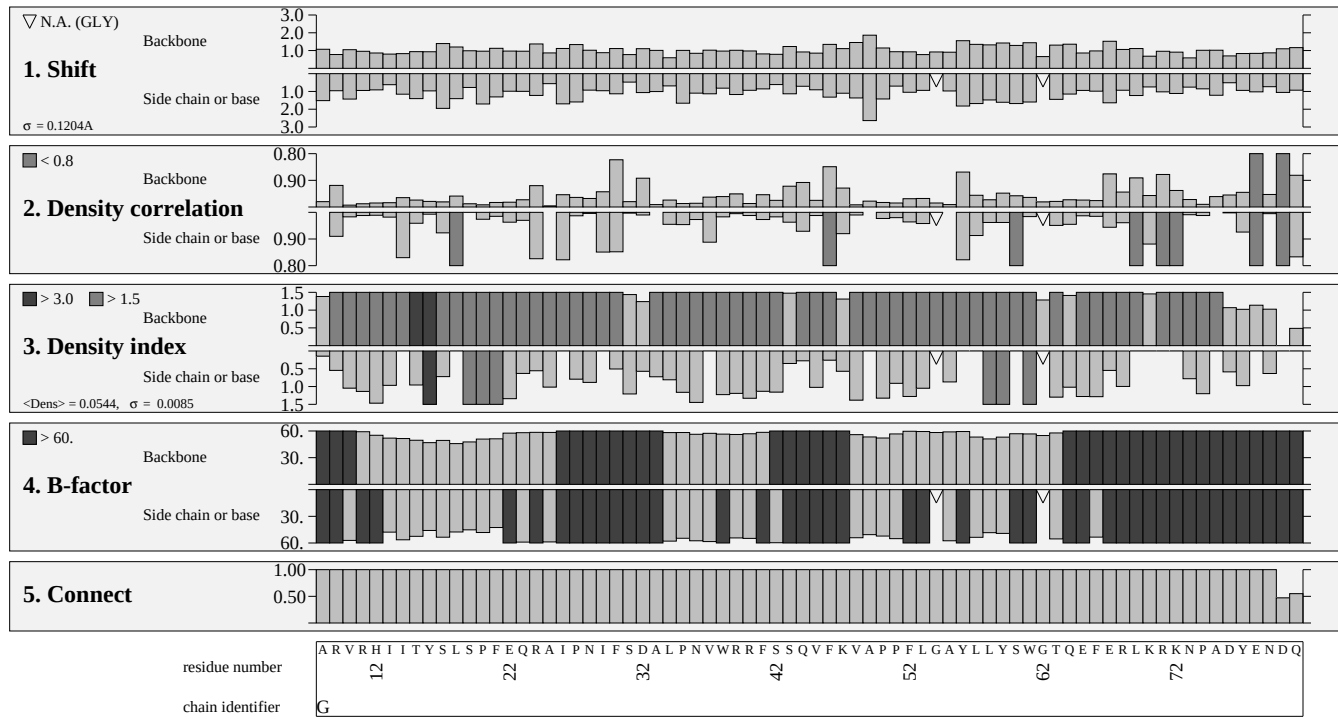
Local estimation (12)



Structure Factor Check

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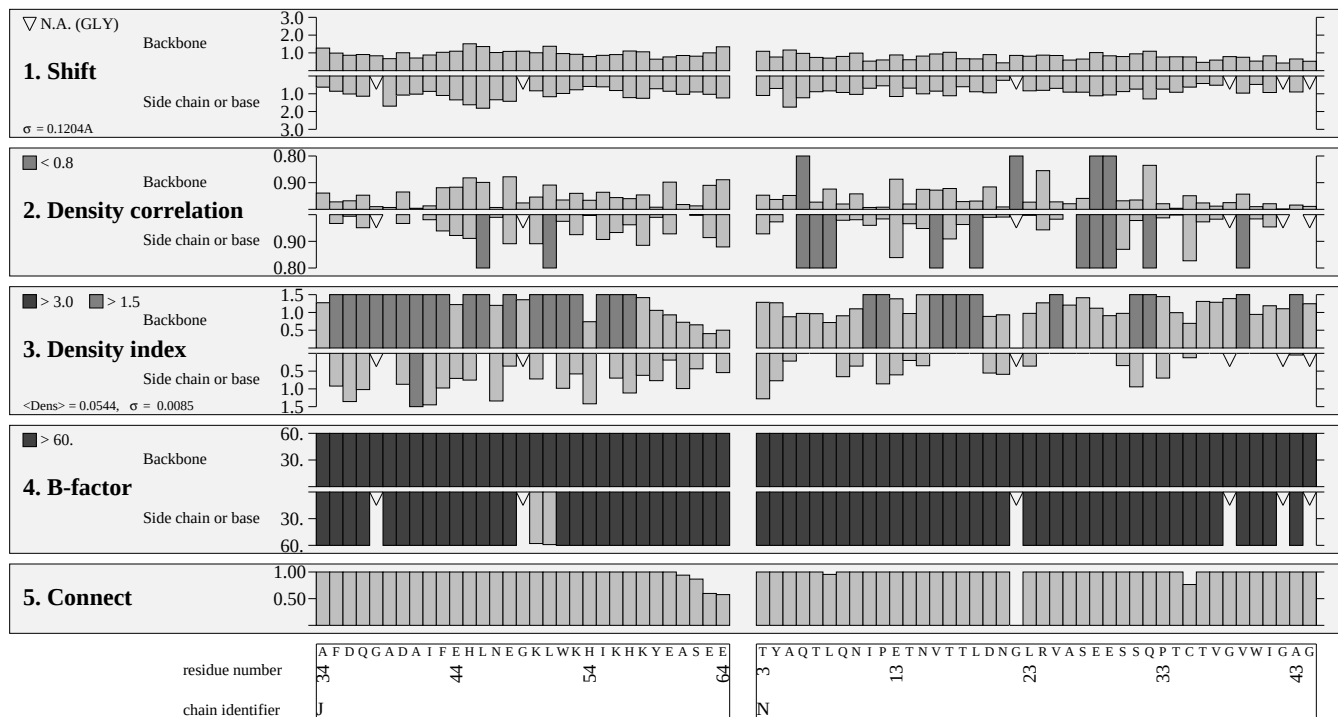
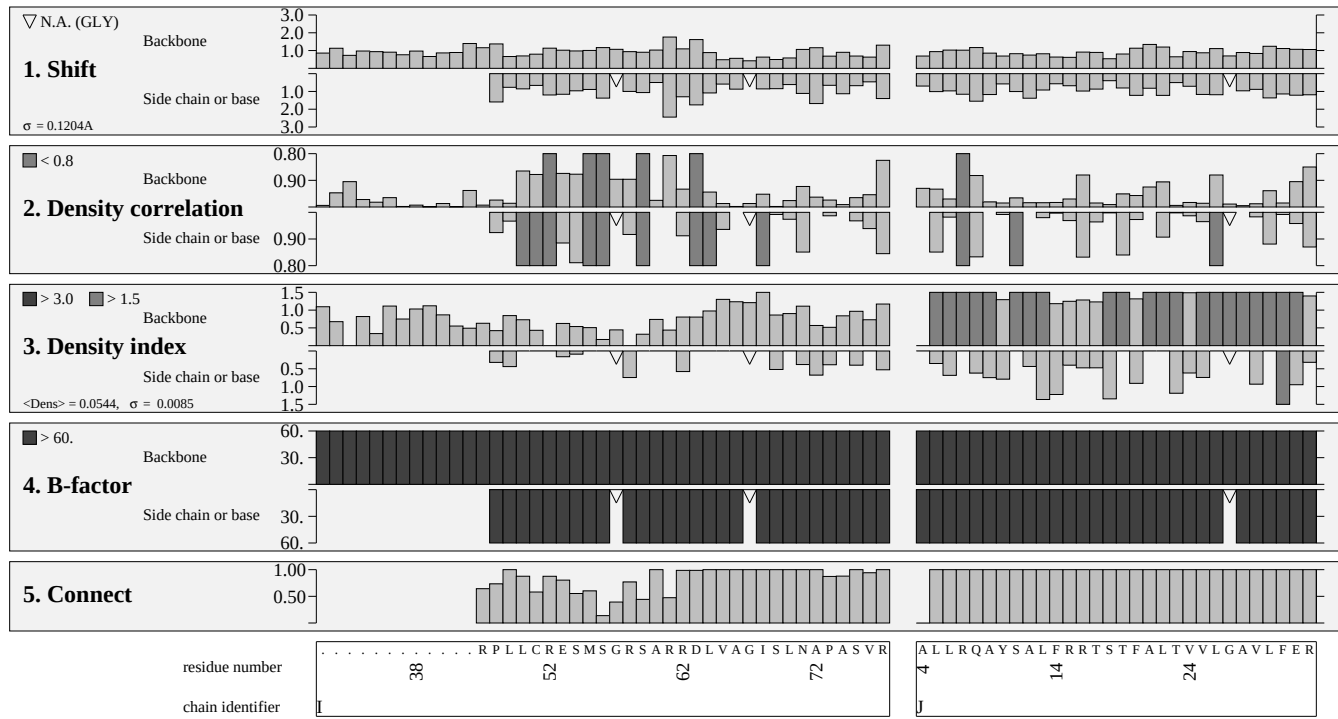
Local estimation (13)



Structure Factor Check

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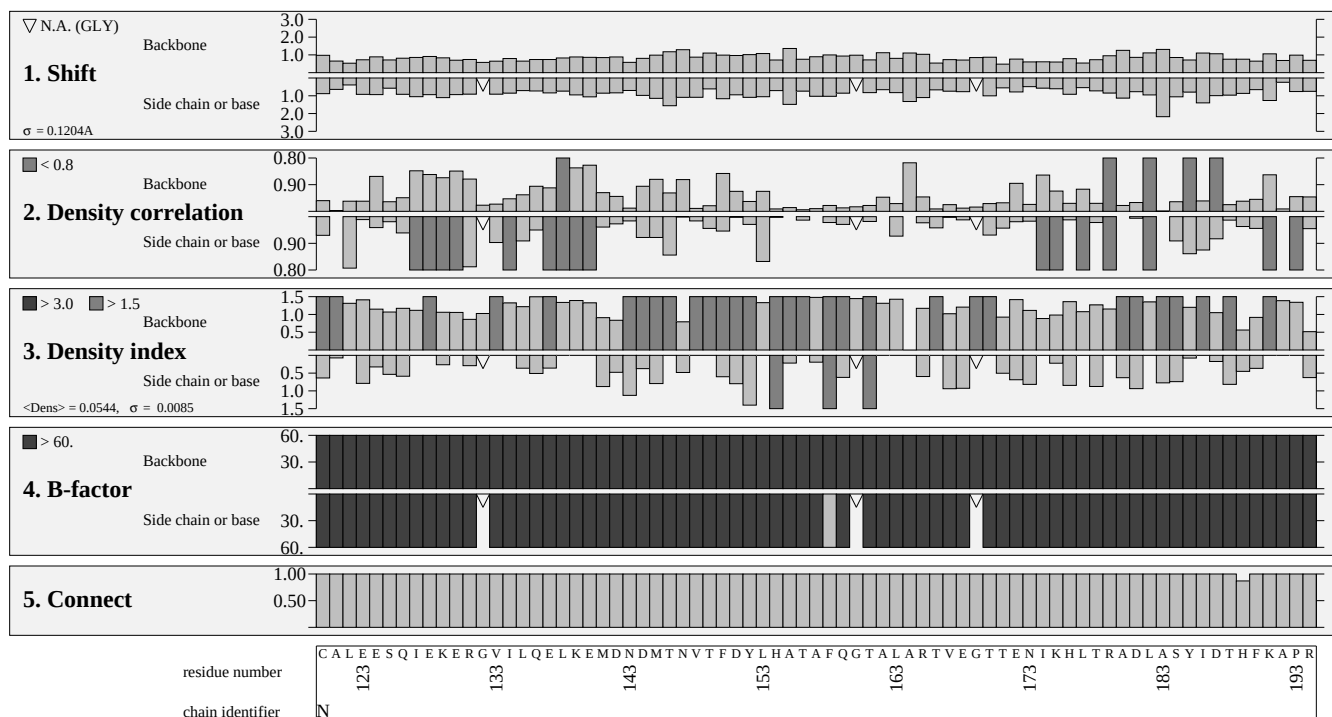
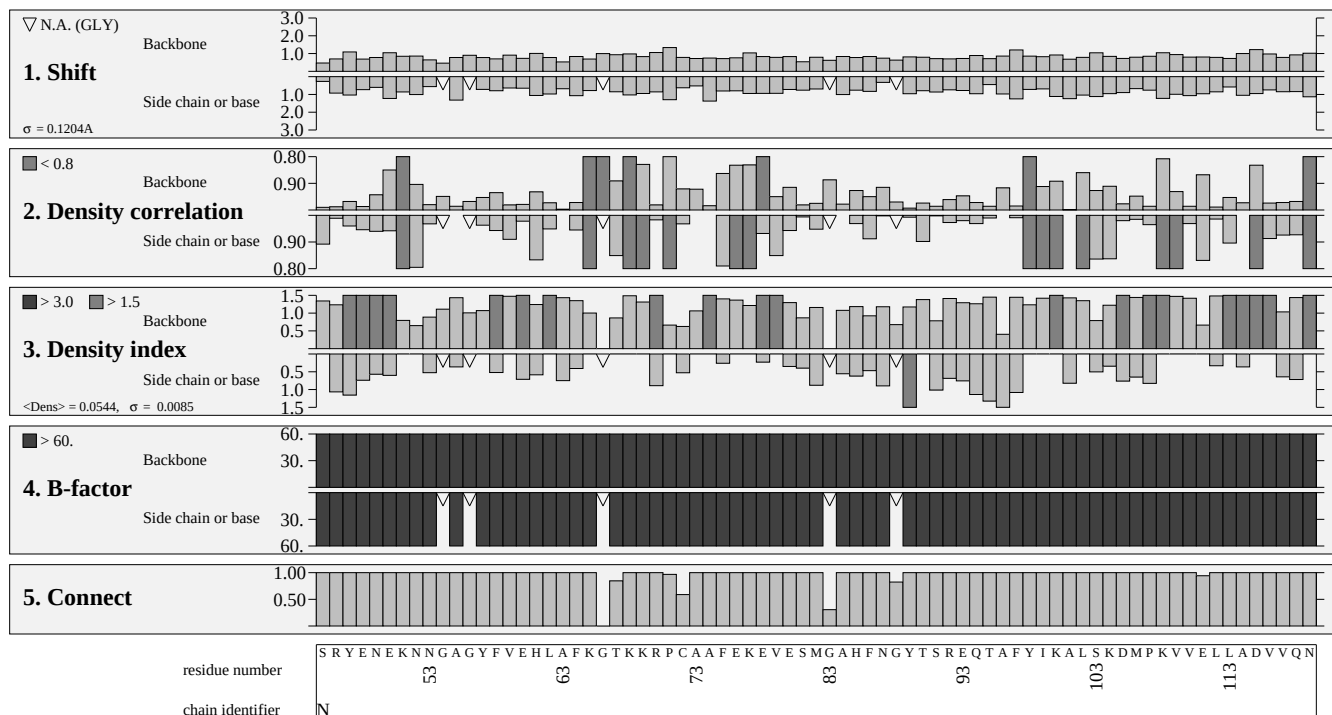
Local estimation (14)



Structure Factor Check

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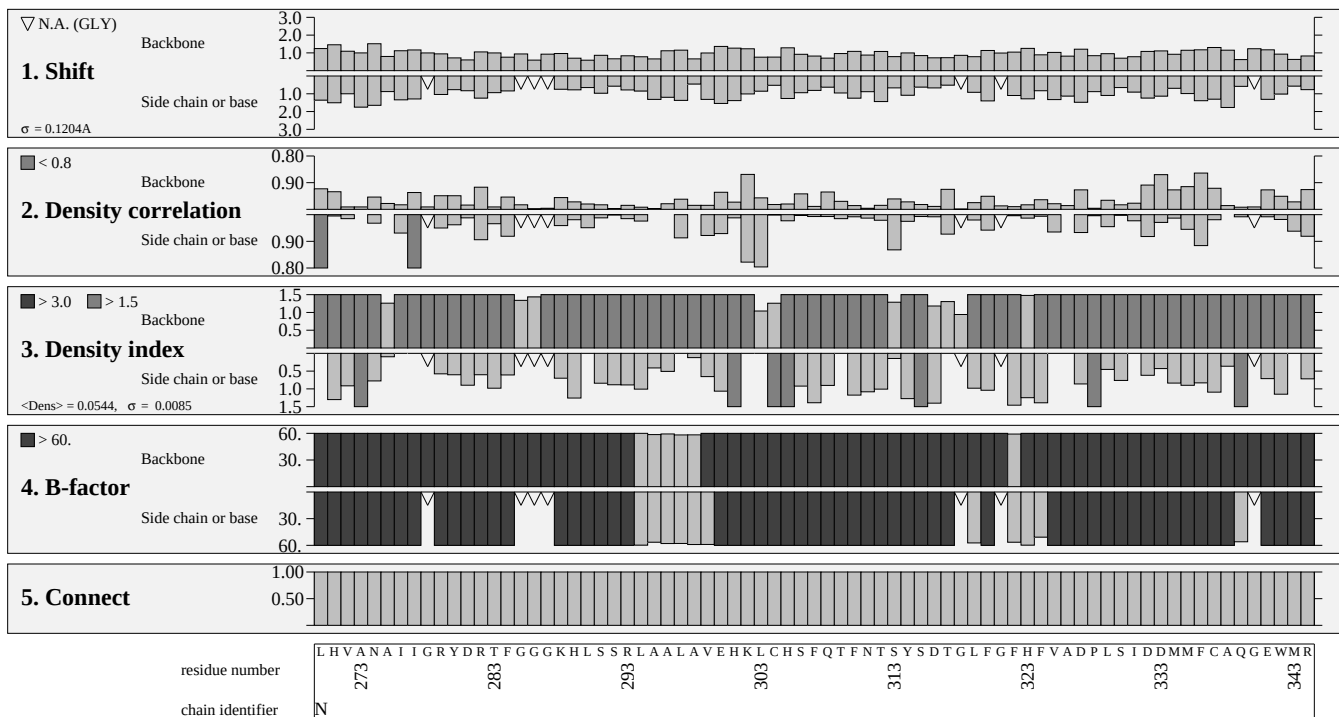
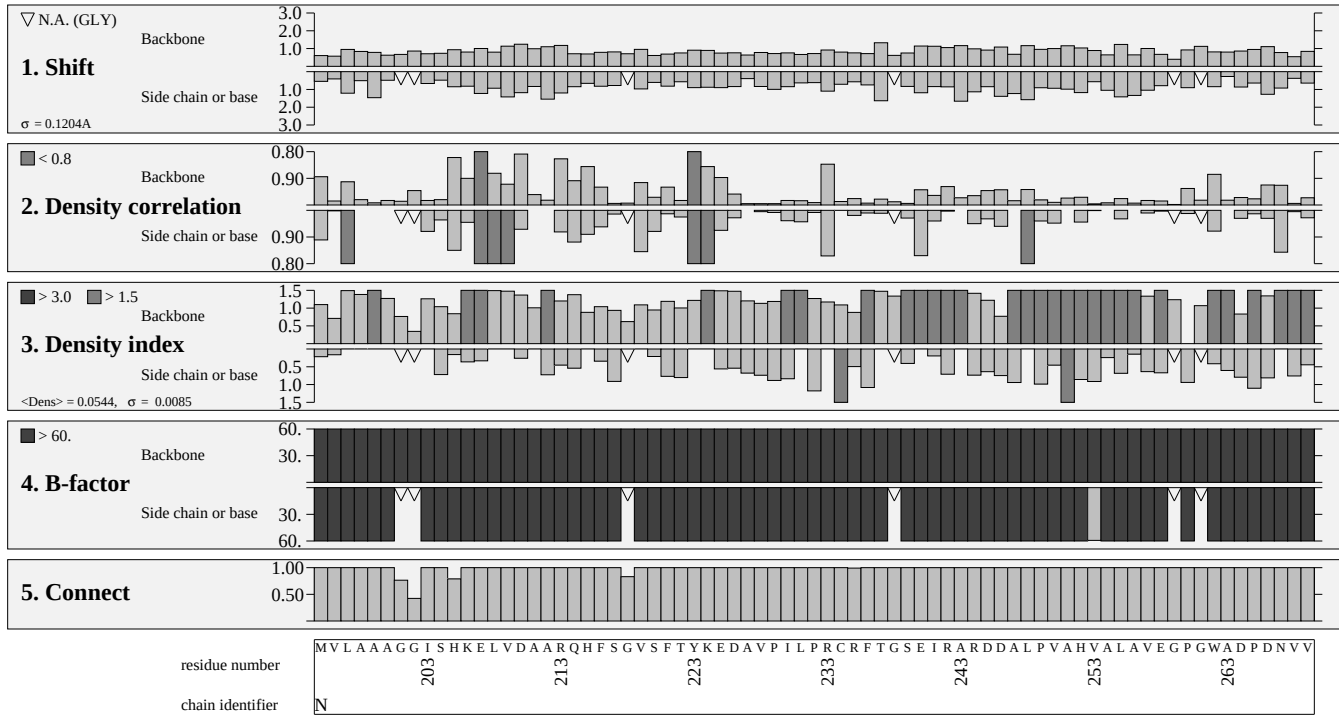
Local estimation (15)



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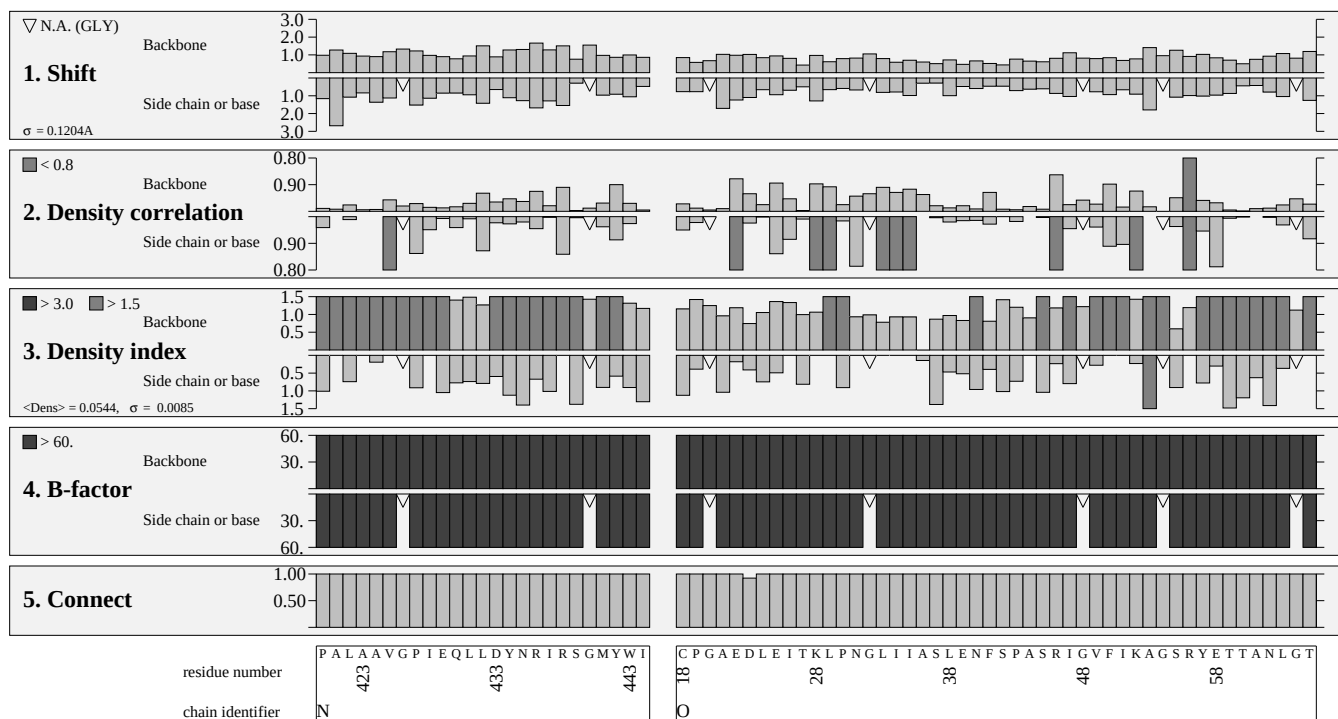
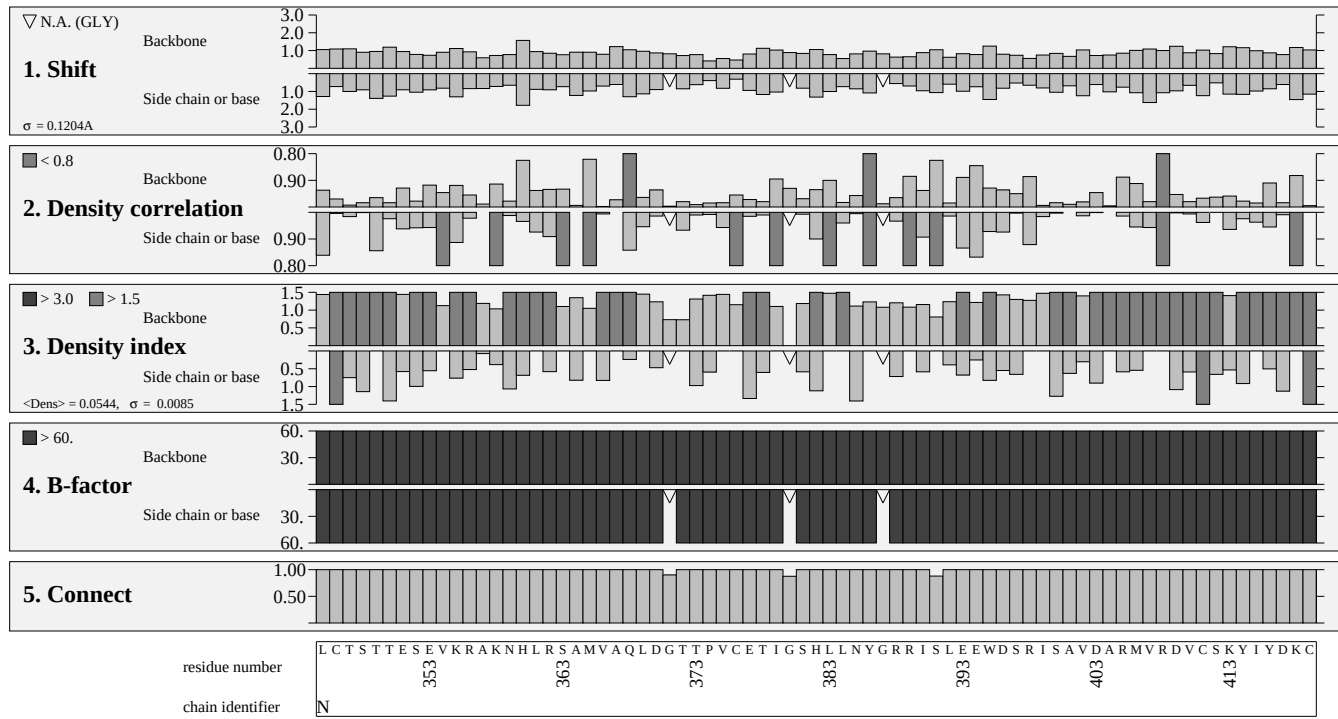
Local estimation (16)



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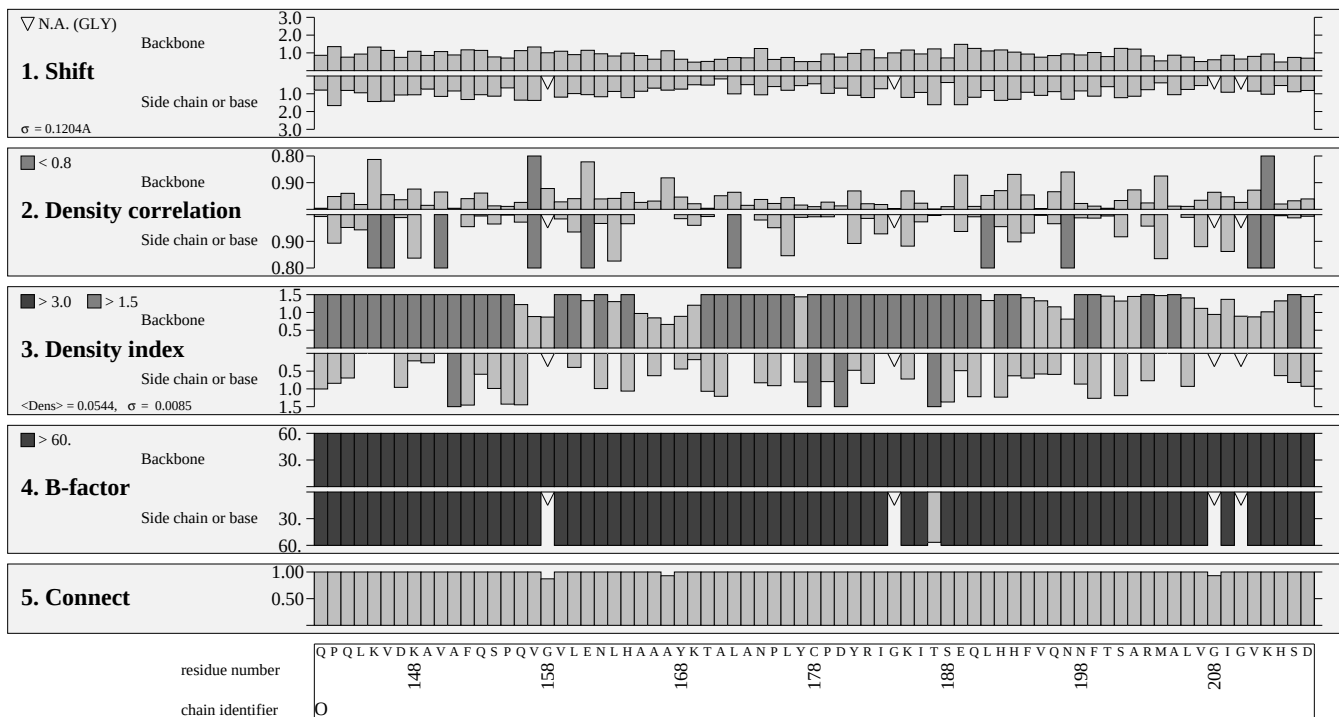
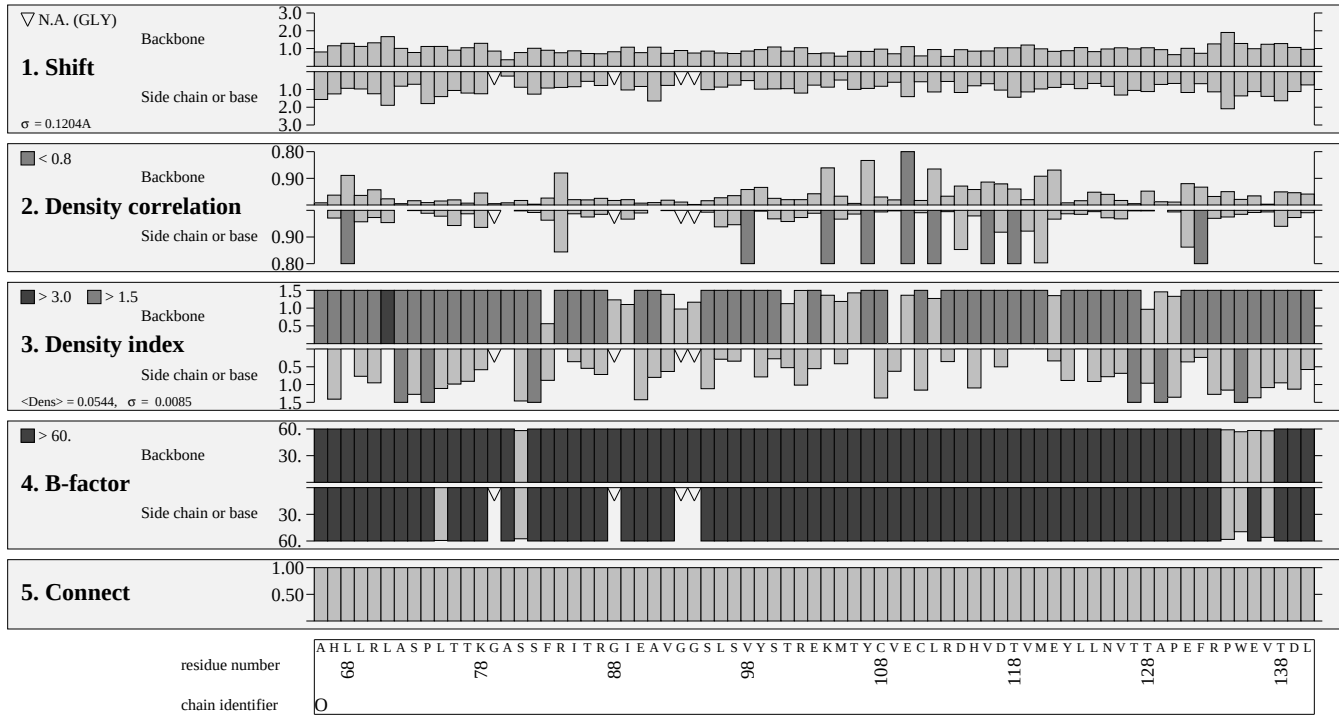
Local estimation (17)



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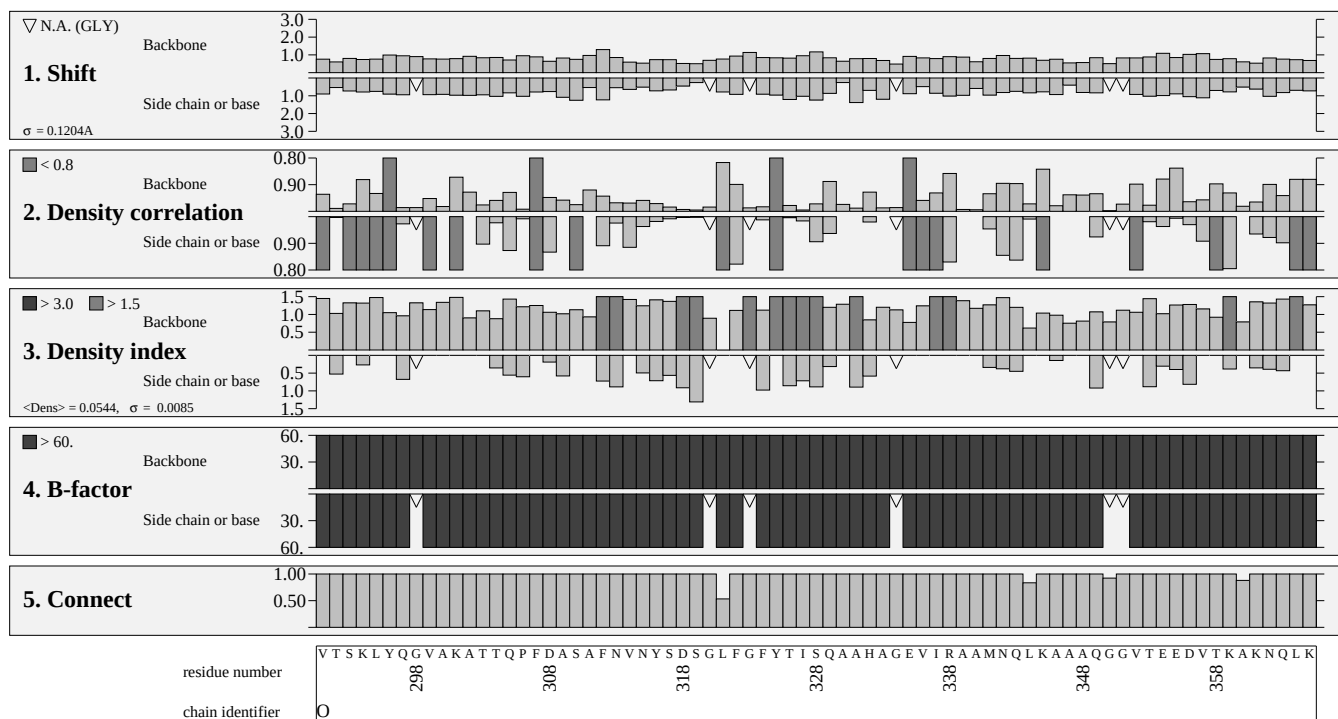
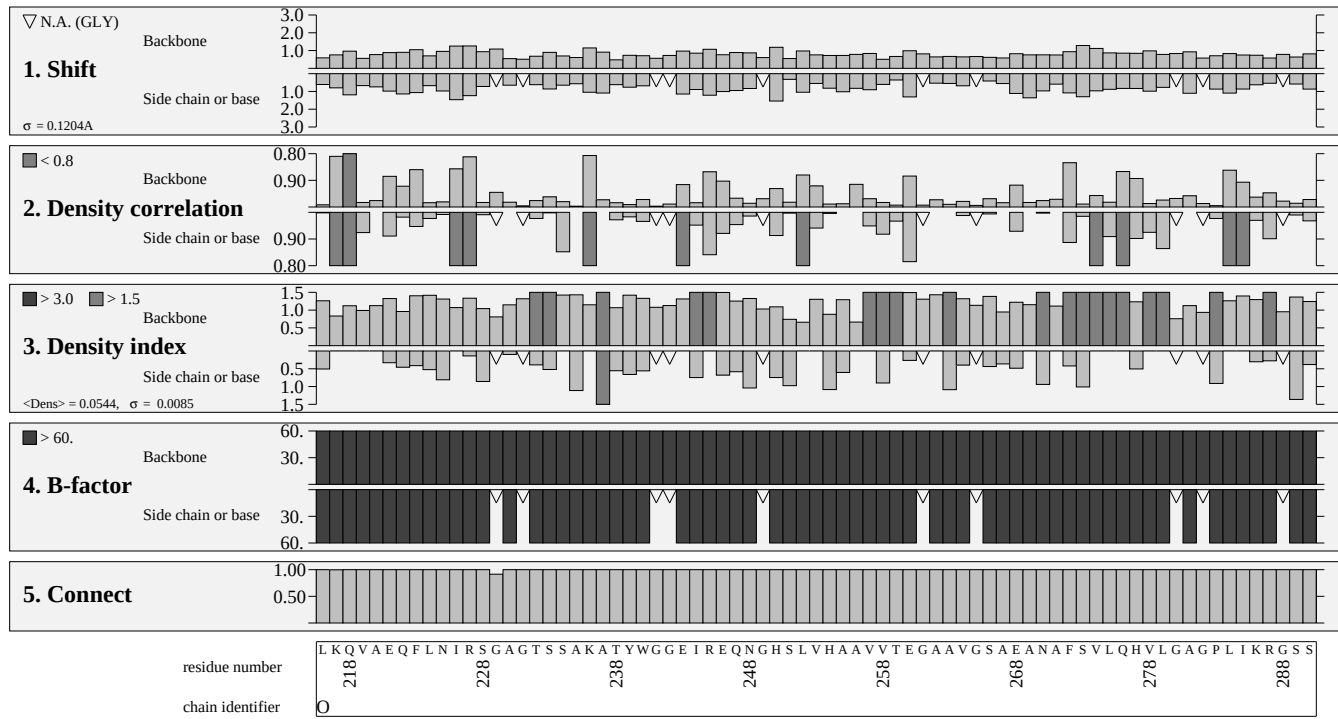
Local estimation (18)



Structure Factor Check

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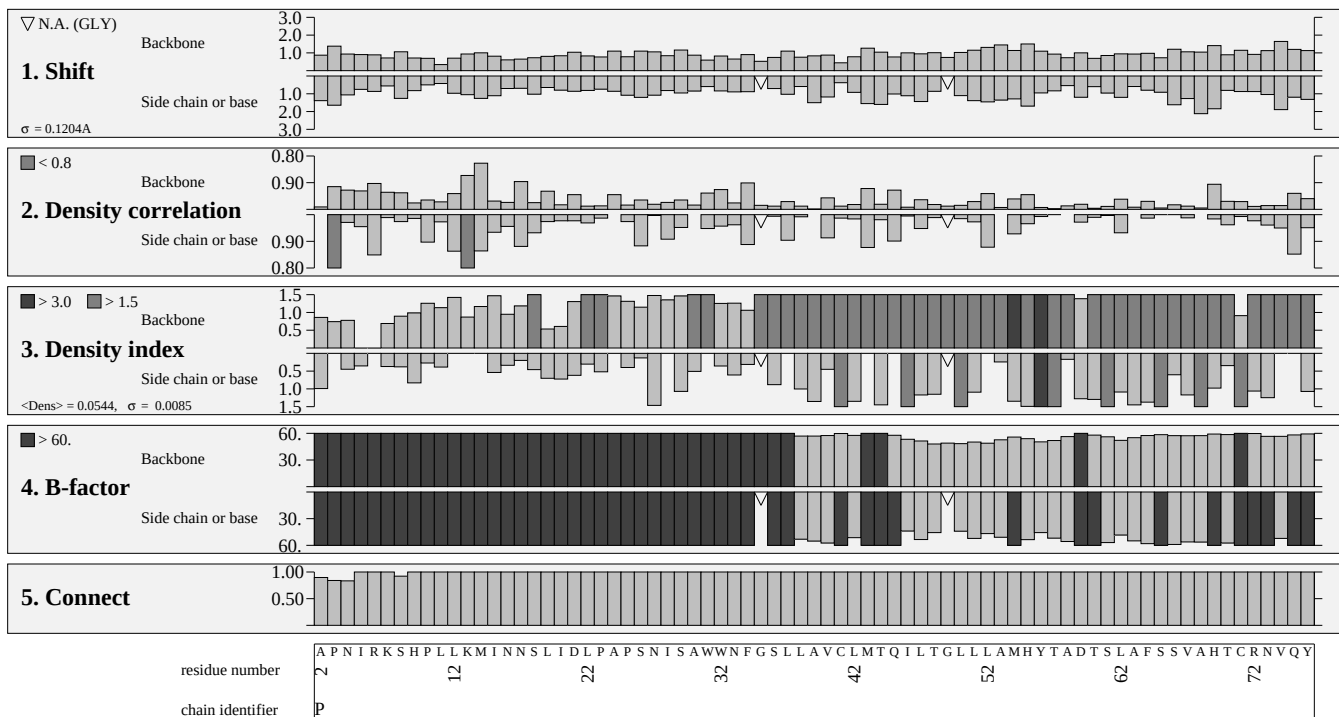
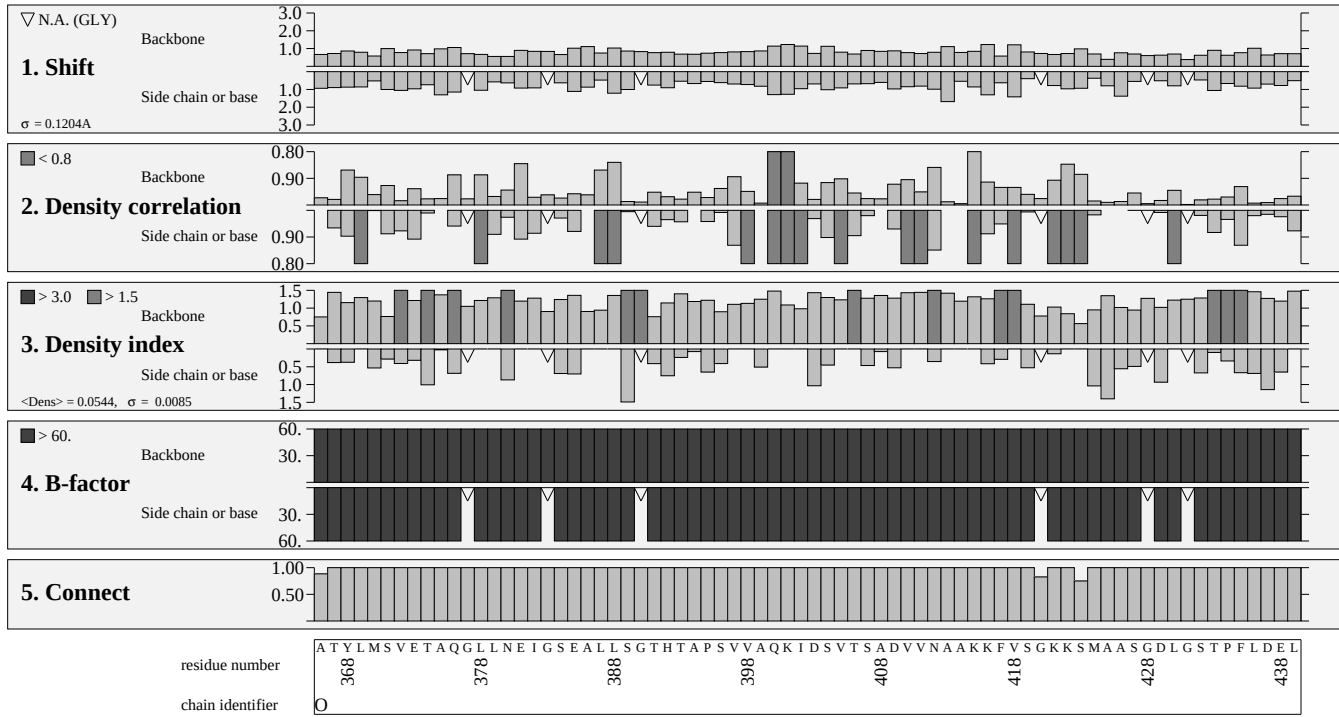
Local estimation (19)



Structure Factor Check

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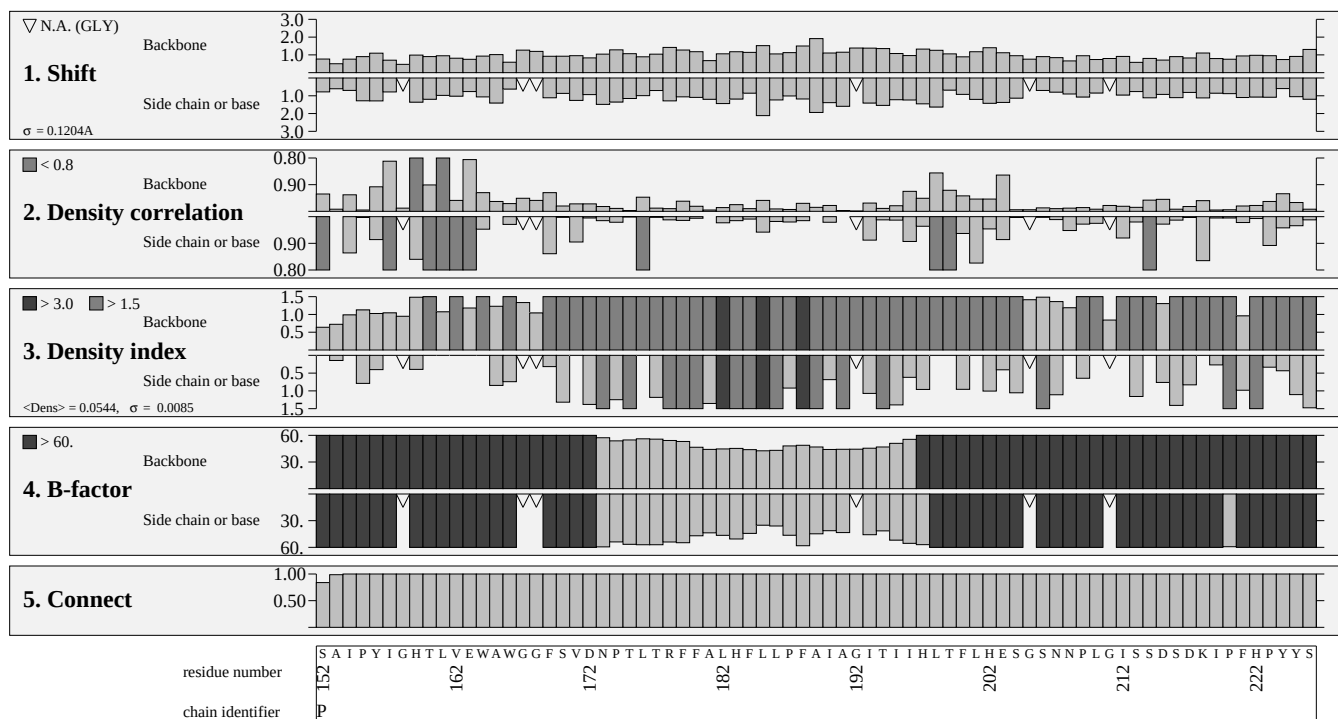
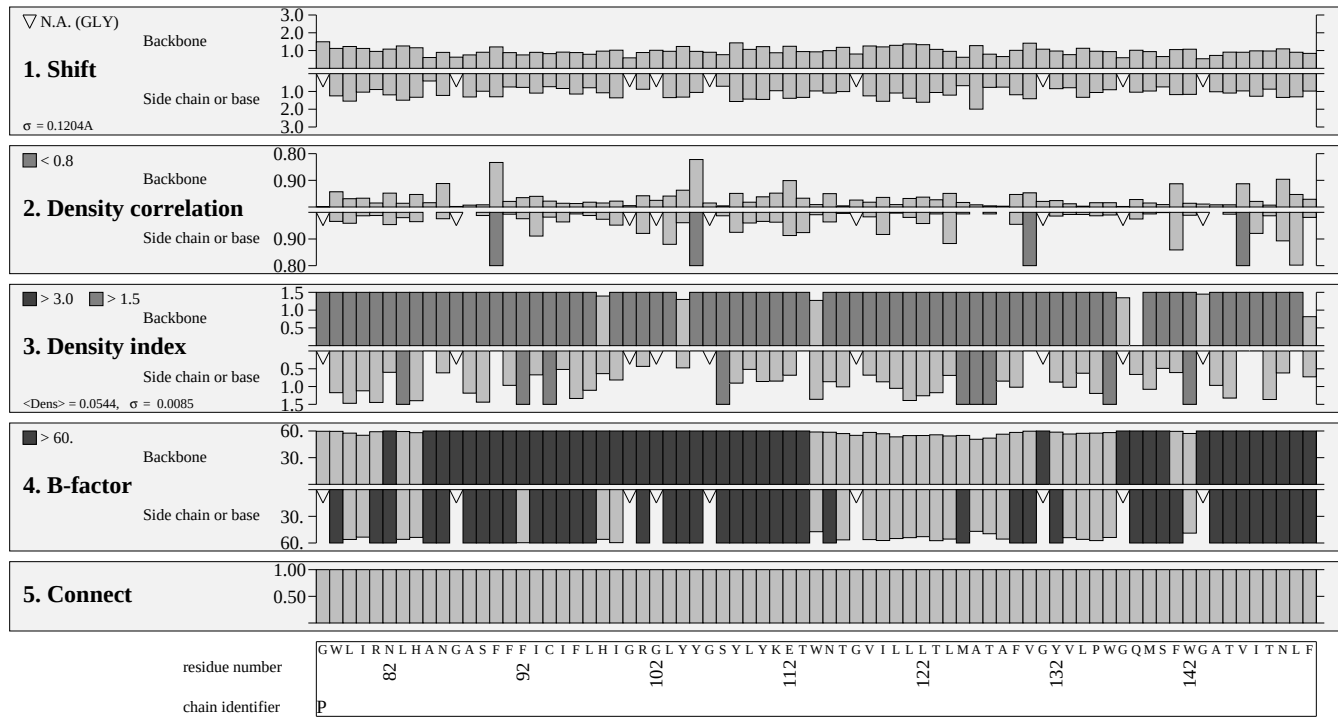
Local estimation (20)



Structure Factor Check

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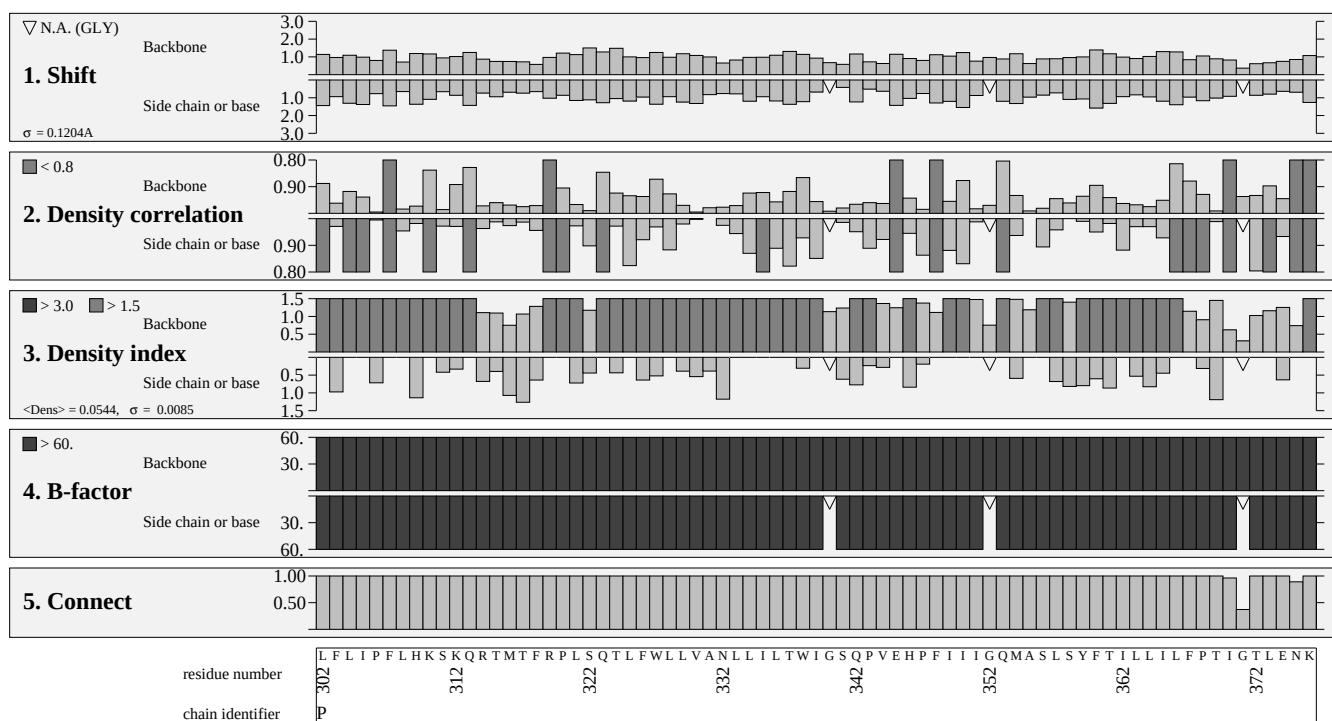
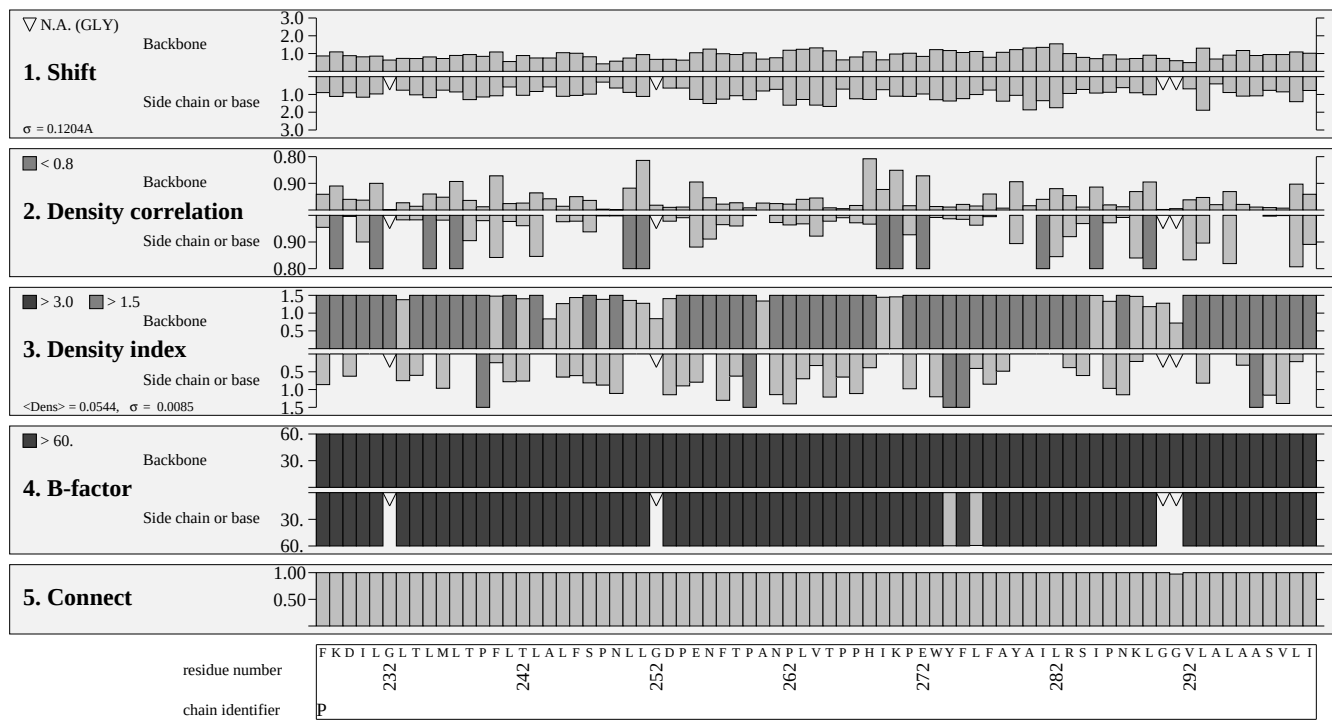
Local estimation (21)



Structure Factor Check

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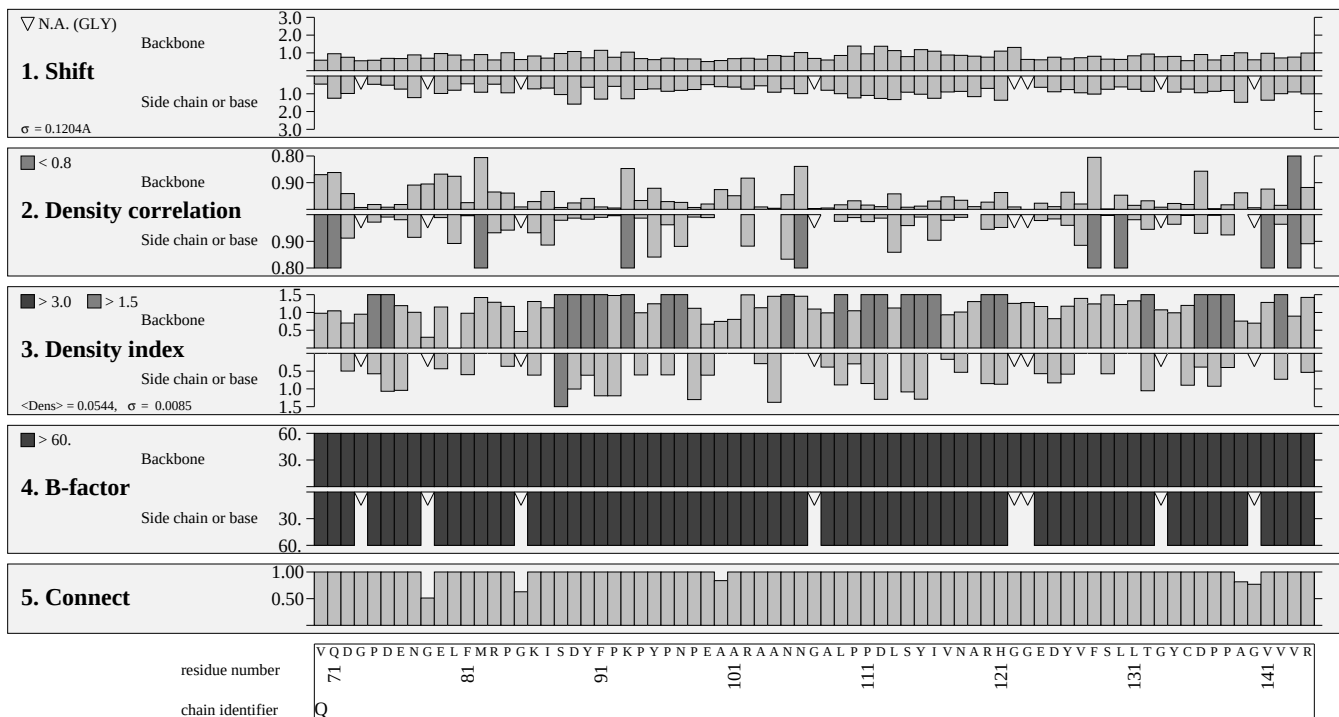
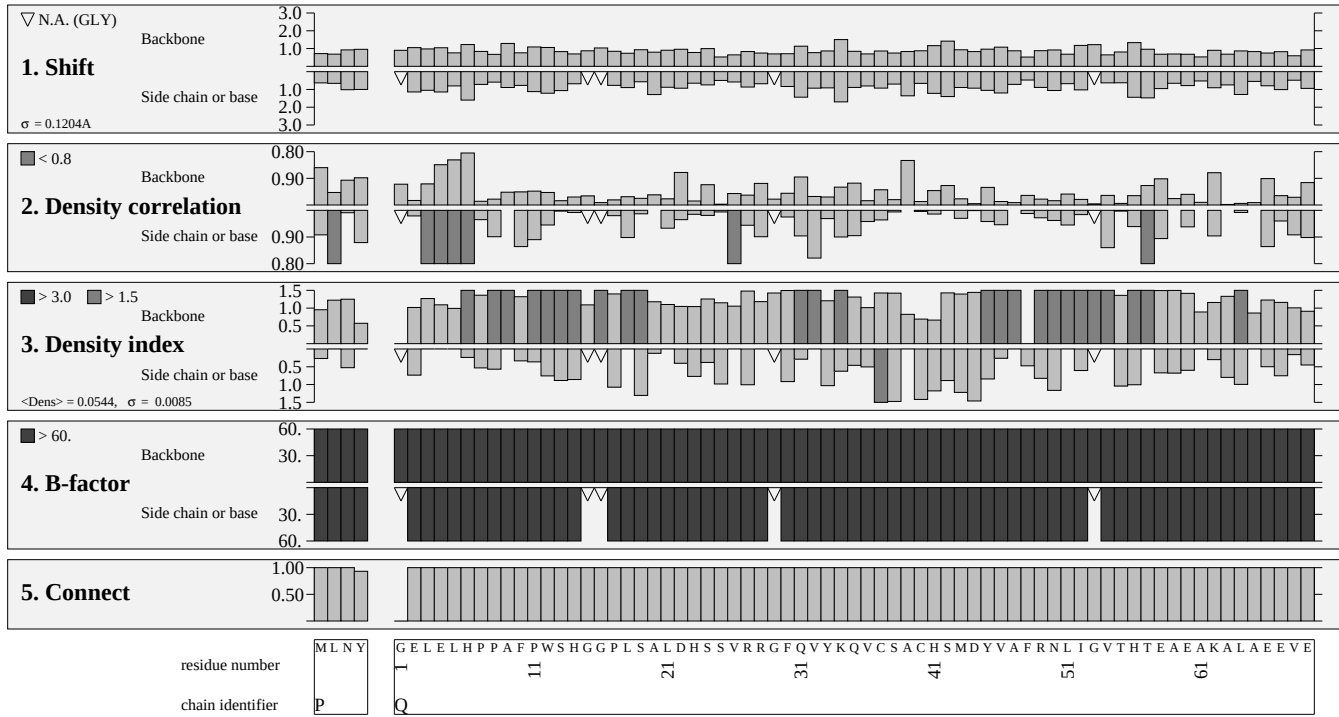
Local estimation (22)



Structure Factor Check

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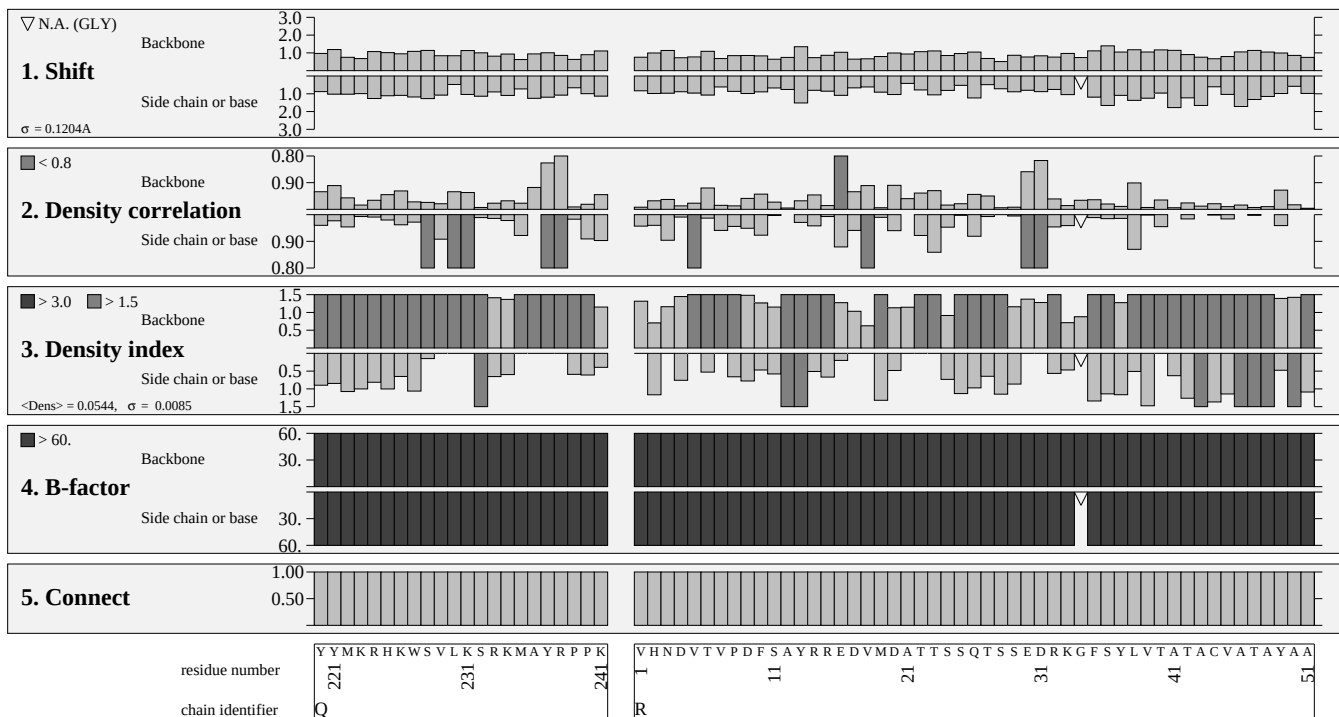
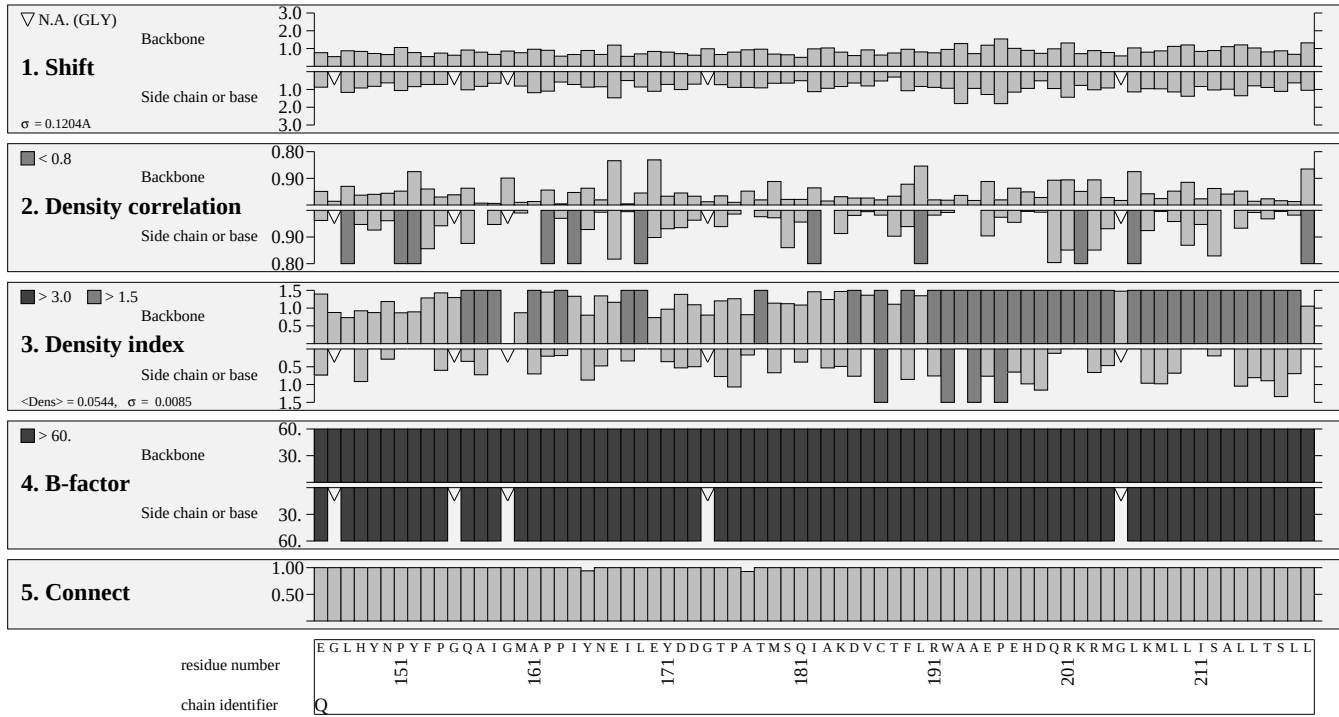
Local estimation (23)



Structure Factor Check

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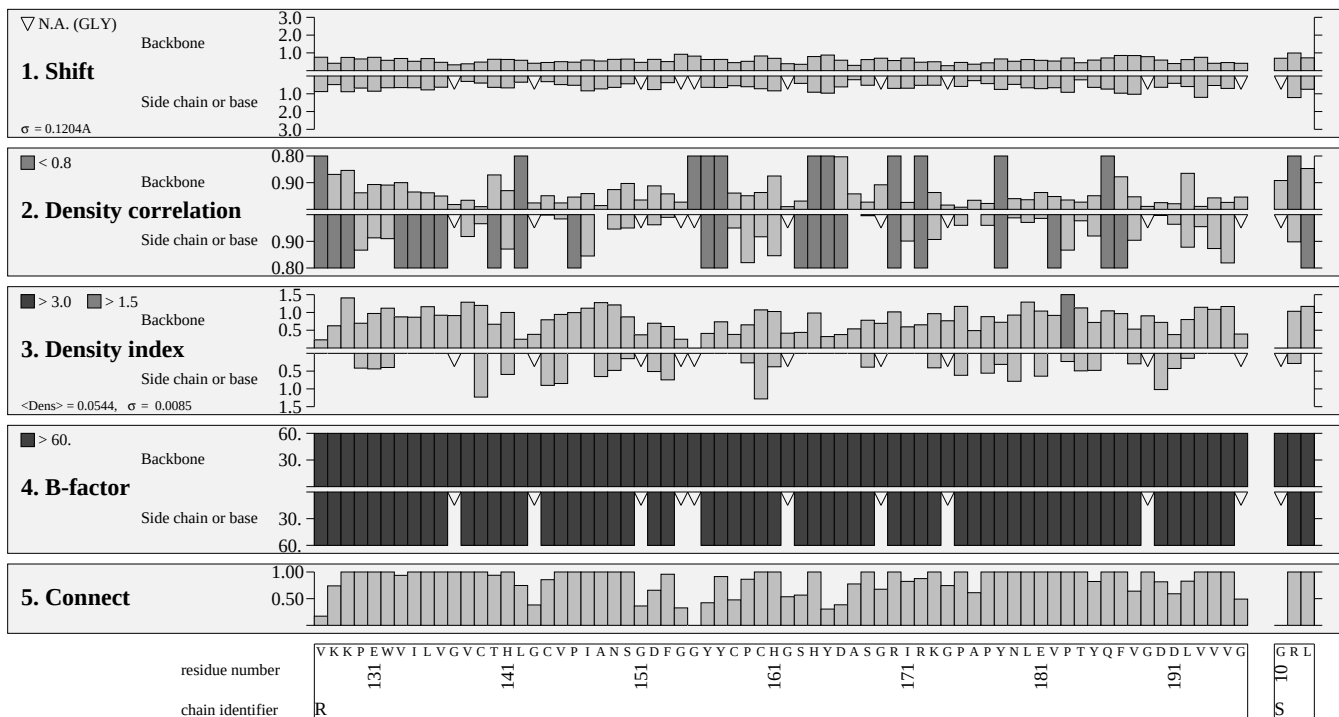
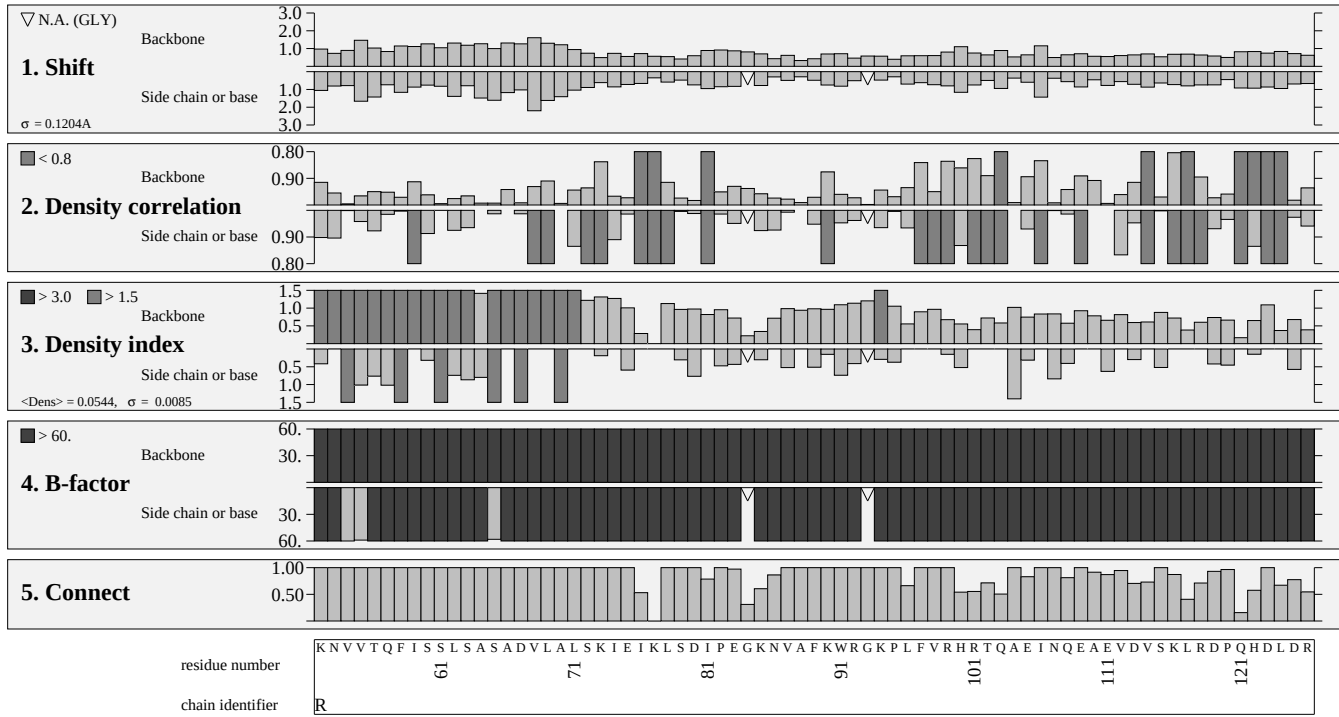
Local estimation (24)



Structure Factor Check

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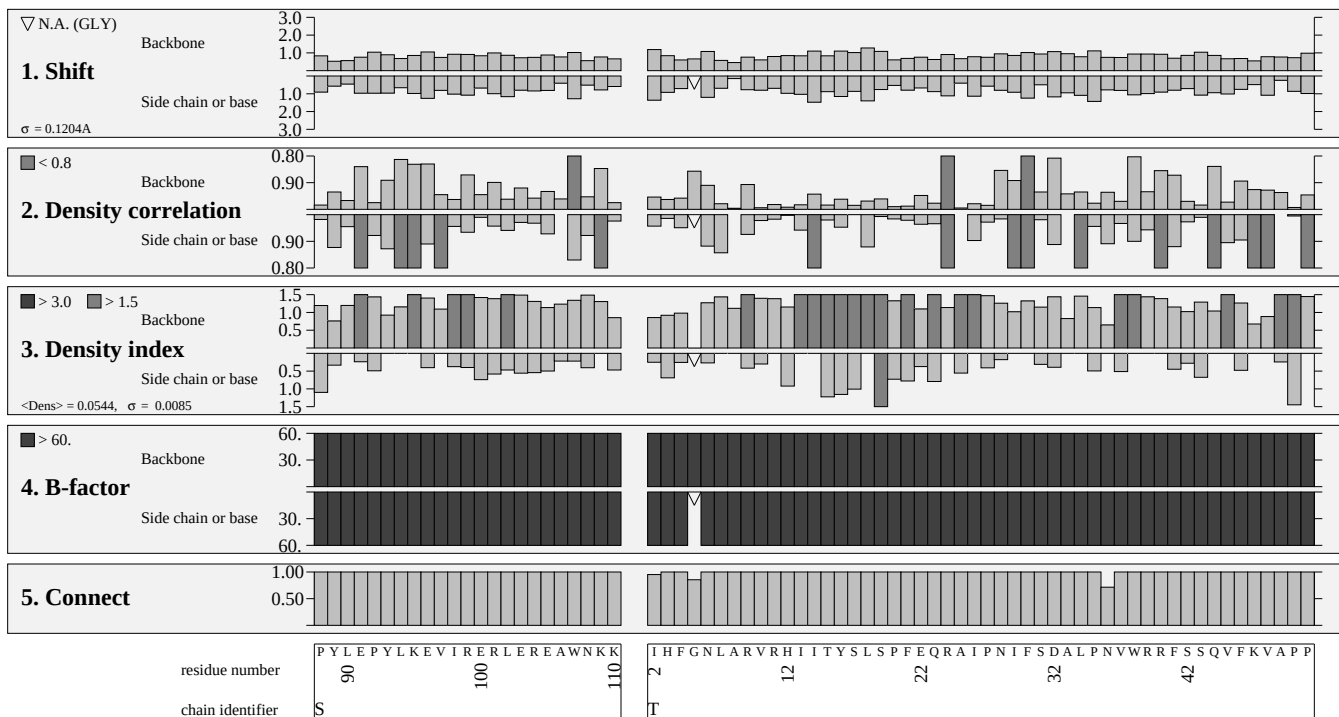
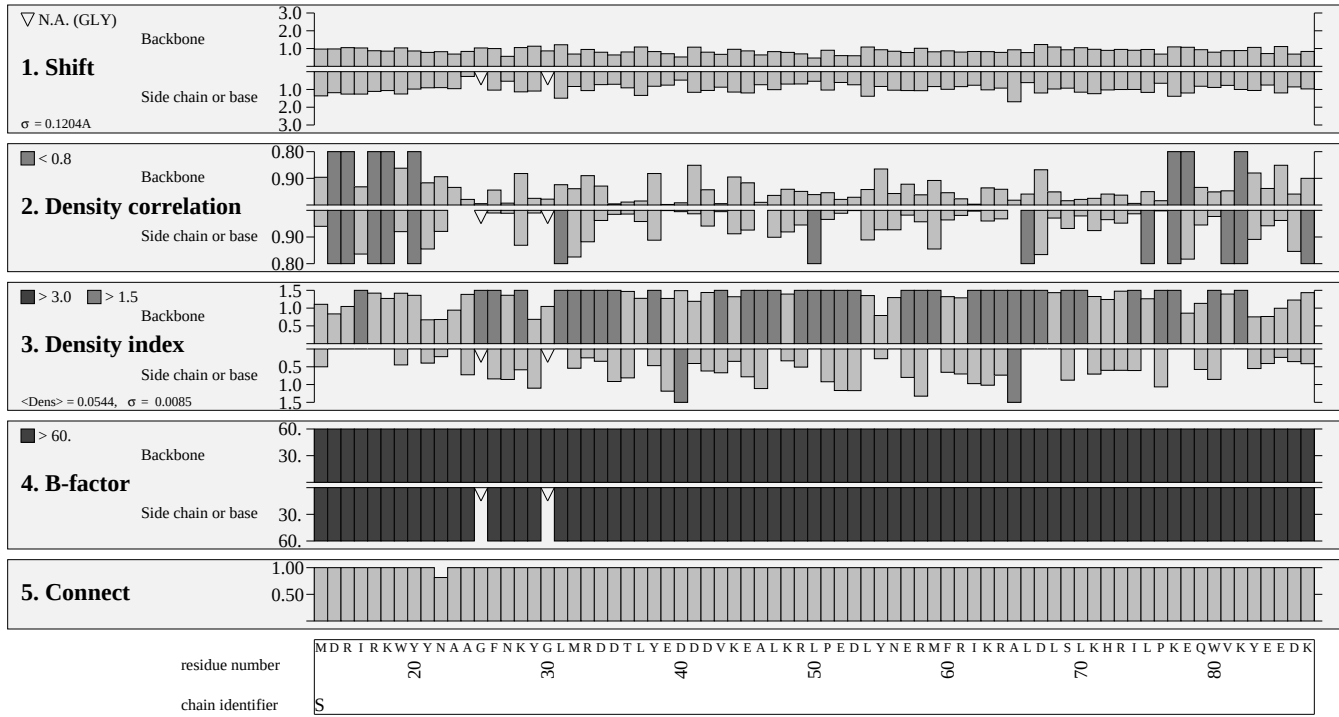
Local estimation (25)



Structure Factor Check

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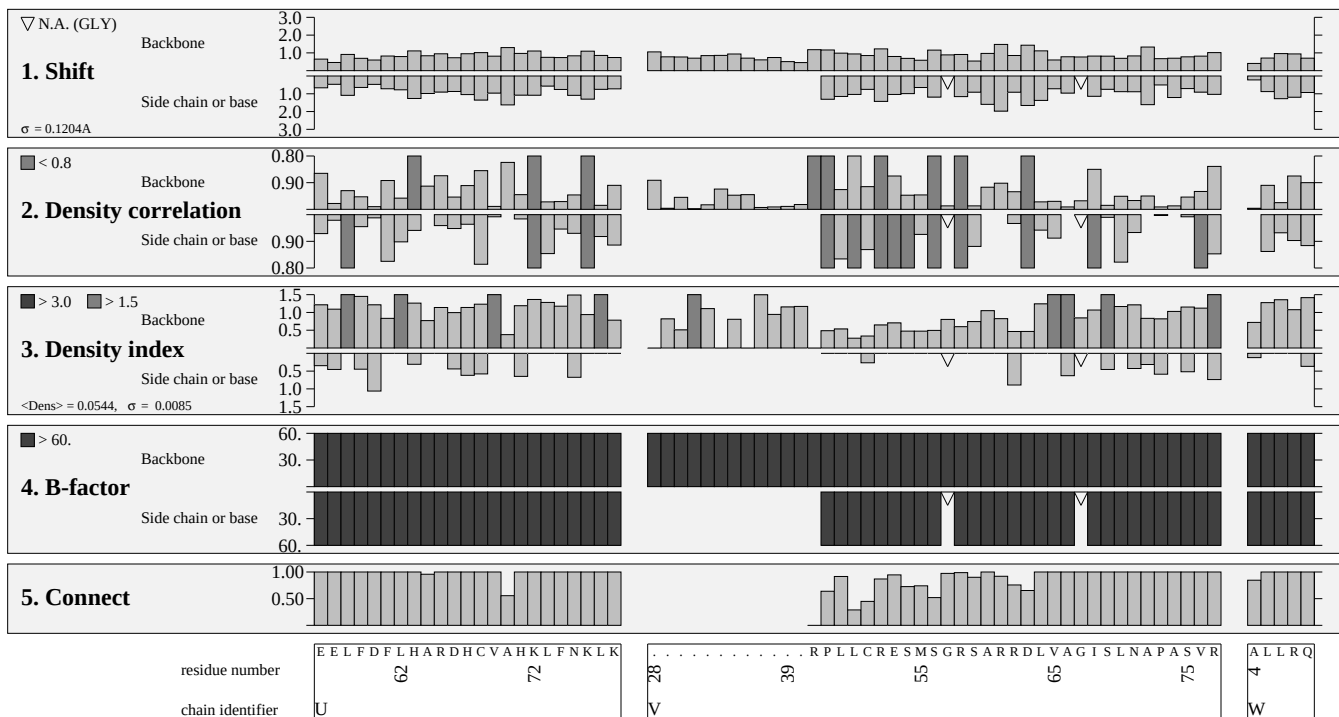
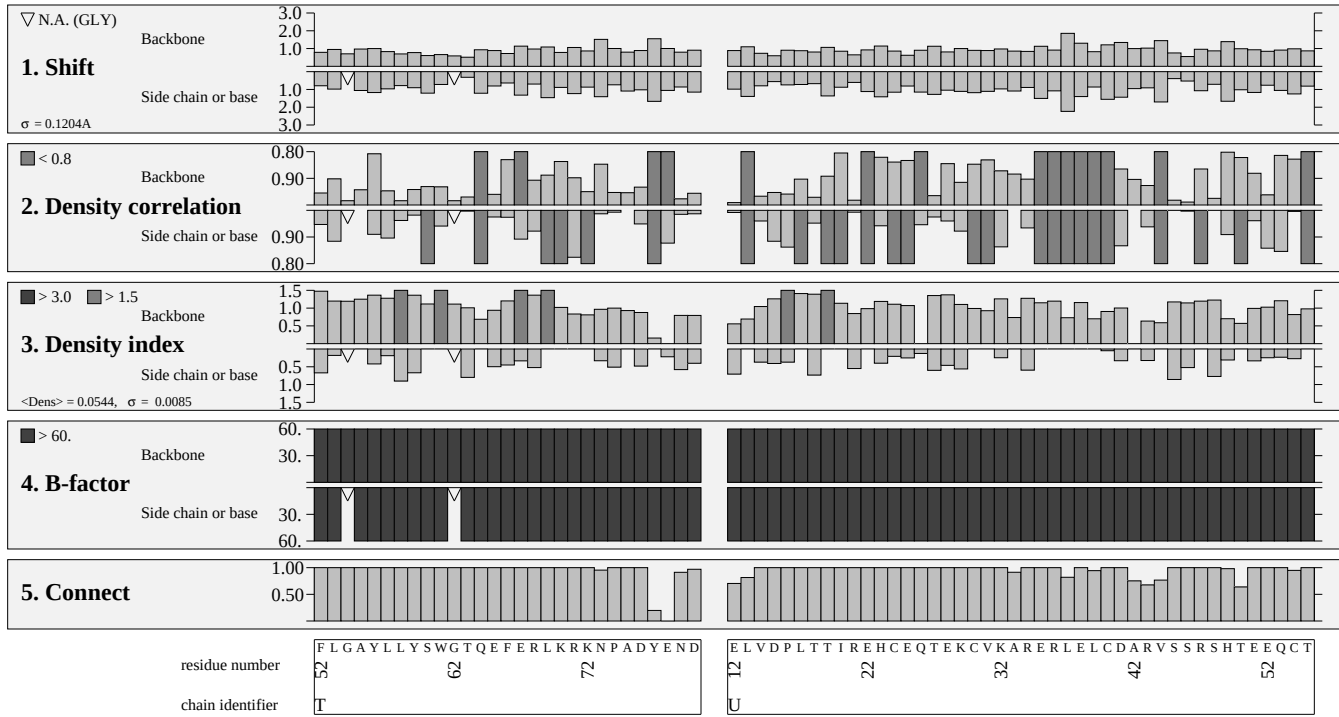
Local estimation (26)



Structure Factor Check

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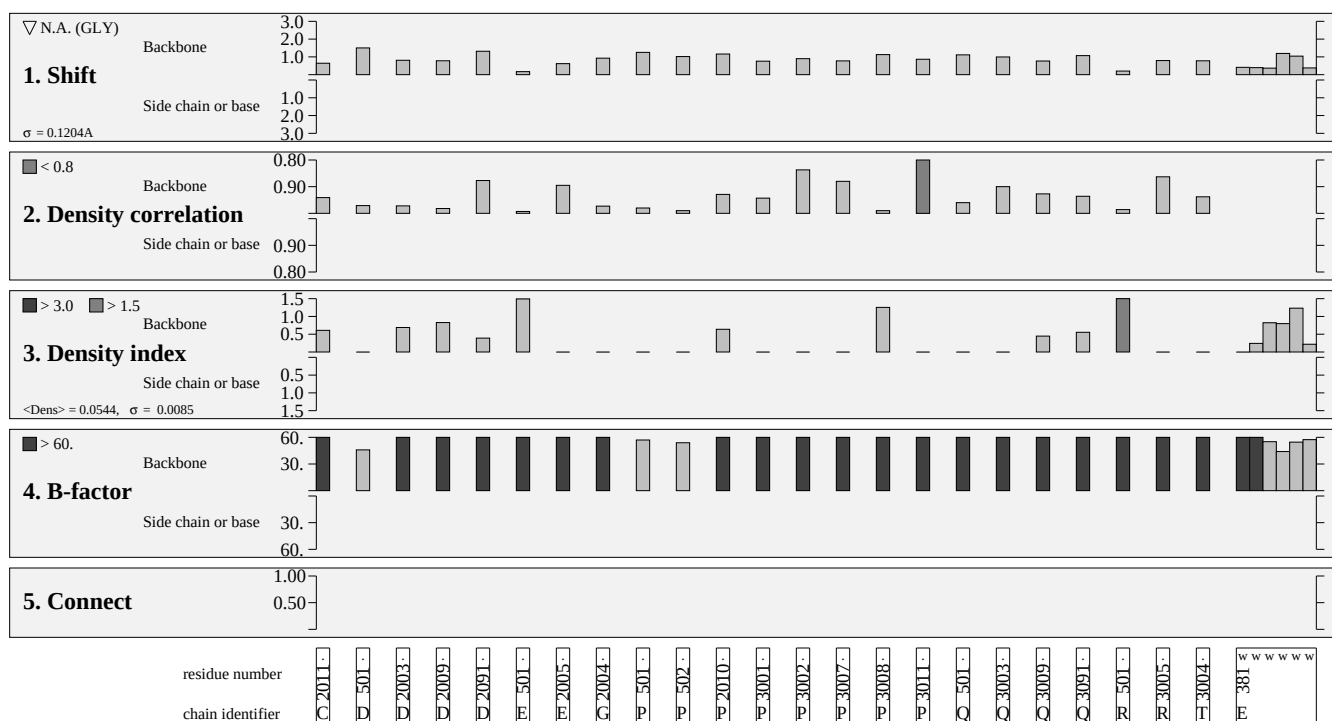
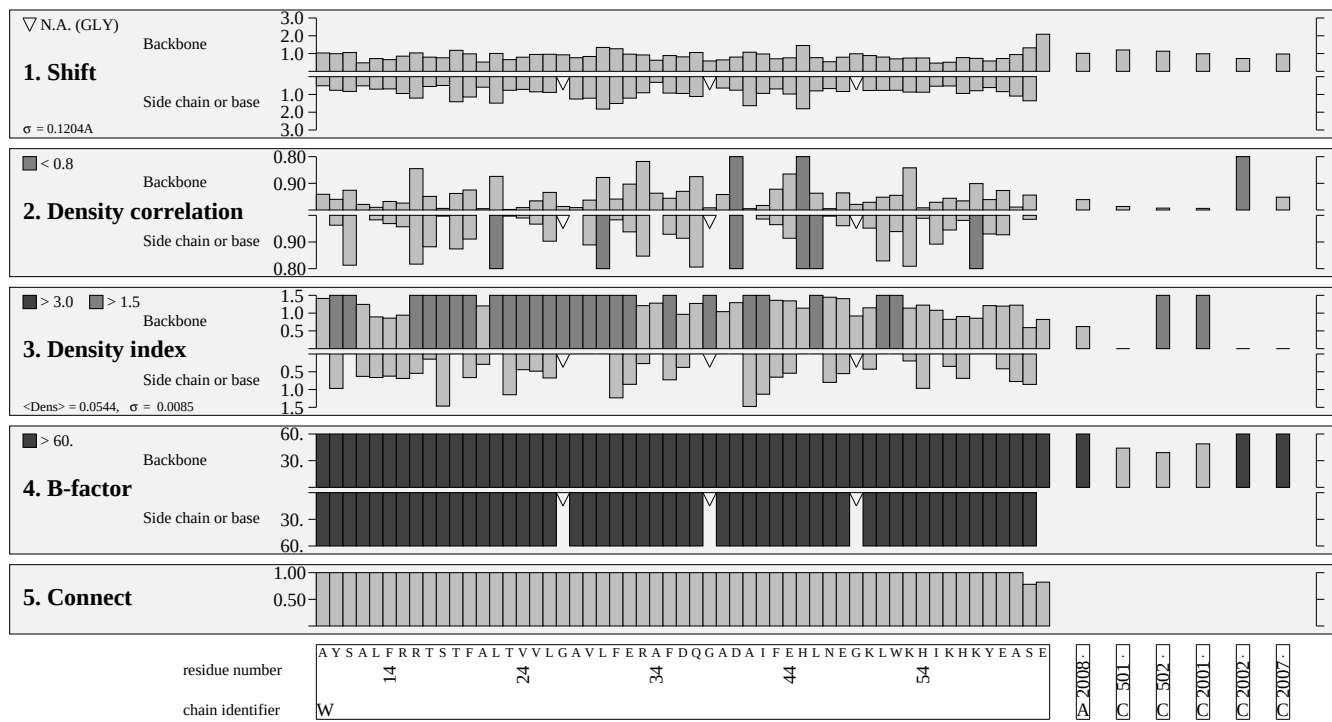
Local estimation (27)



Structure Factor Check

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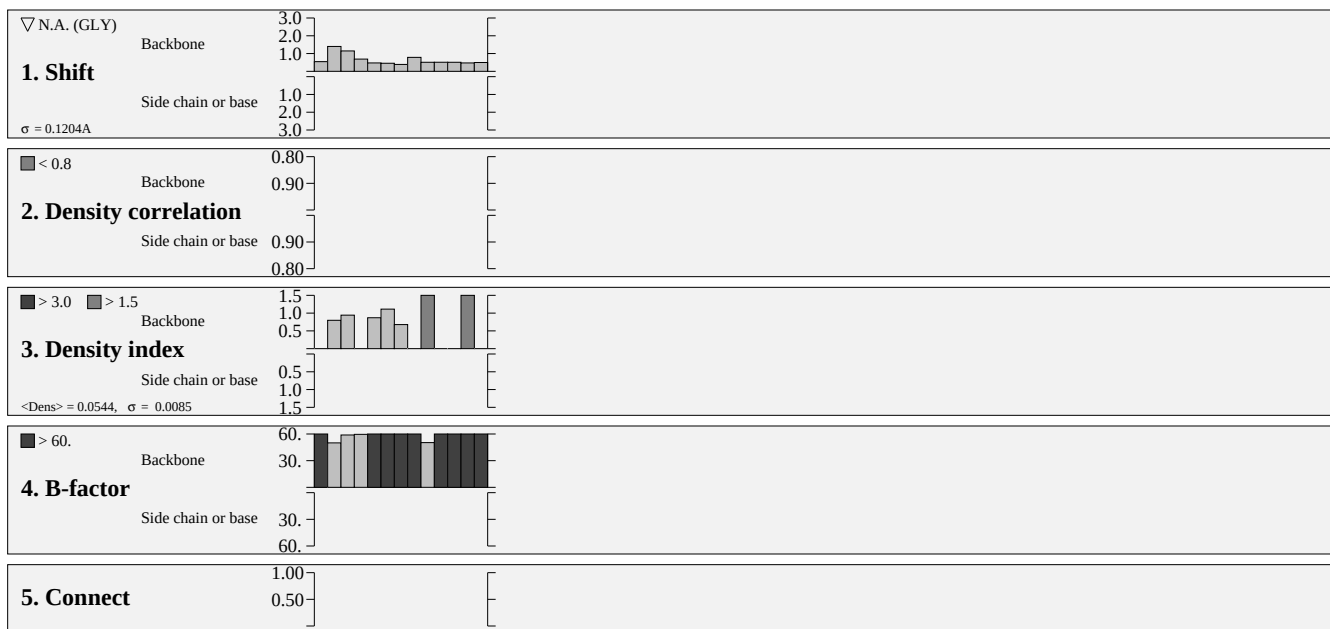
Local estimation (28)



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Local estimation (29)



residue number

chain identifier

382
E