

Structure Factor Check

3L70

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH TRIFLOXYSTROBIN BOU
 Date: 27-DEC-09
 PDB code: 3L70

Crystal

Cell parameters:

a: 169.61 Å b: 181.99 Å c: 240.54 Å
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 58.3 – 2.68 Å
 Reflections in file: 204662
 Unique reflections above 0: 204662
 above 1 σ : 197005
 above 3 σ : 125837

SF CHECK

Nominal resolution range: 58.3 – 2.75 Å
 \05max. from input data, min. from author\05
 Used reflections: 191524
 Reflections out of resolution: 13138
 Completeness: 99.3 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.063
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.5090 0.5016
 B_{overall} (by Patterson): 45. Å²
 Optical resolution: 2.05 Å
 Expected opt. resol. for complete data set: 2.05 Å
 Estimated minimal error: 0.069 Å

Model

32653 atoms (19 water molecules)

Number of chains: 51

Volume not occupied by model: 62.0 %

$\langle B \rangle$ (for atomic model): 65.6 Å²

$\sigma(B)$: 20.61 Å²

Matthews coefficient: 4.06

Corresponding solvent % : 69.47

Model vs. Structure Factors

R-factor for all reflections: 0.310
 Correlation factor: 0.861
 R-factor: 0.309
 for $F > 2.0 \sigma$
 nom. resolution range: 24.99 – 2.75 Å
 reflections used: 184829

Rfree: 0.332
 Nfree: 9231
 R-factor without free-refl.: 0.307
 Non free-reflections: 175598
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.491 Å
 Estimated maximal error: 0.300 Å
 DPI: 0.319 Å

Scaling

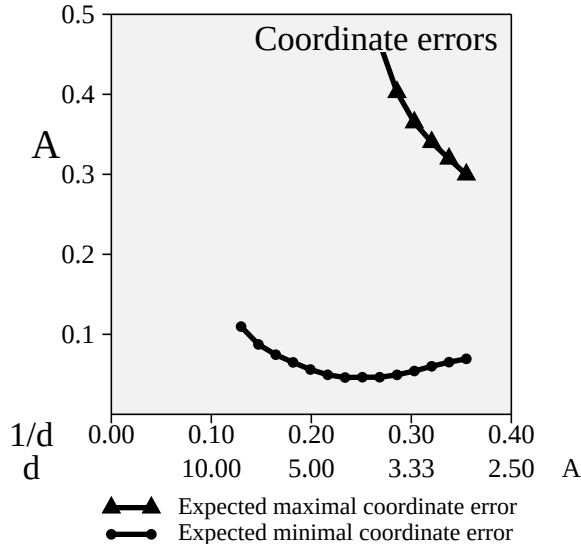
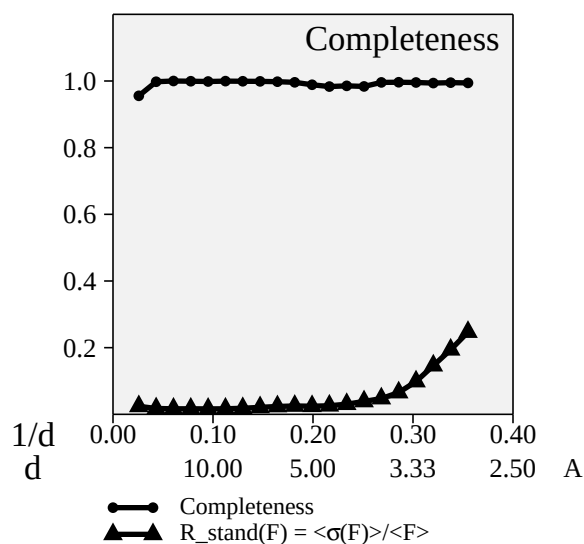
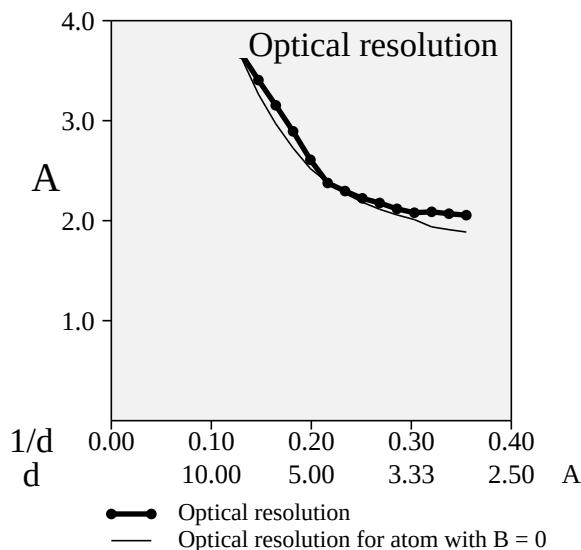
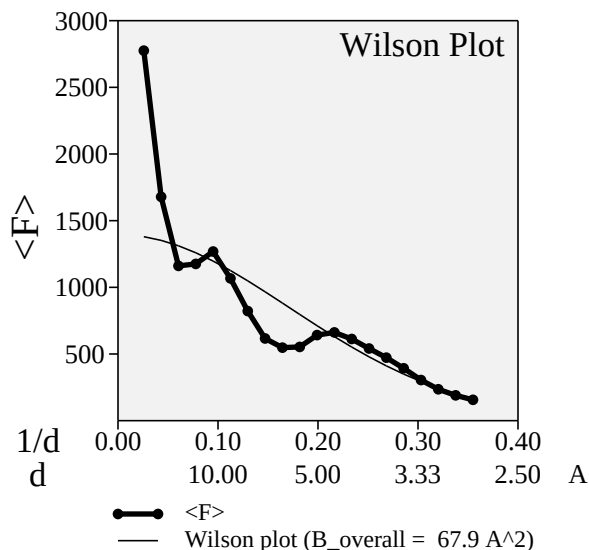
Scale: 0.474
 Bdiff: -8.04
 Anisothermal Scaling (Beta):
 9.6532 -2.3386 -2.0464 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.696 250.083

Refinement

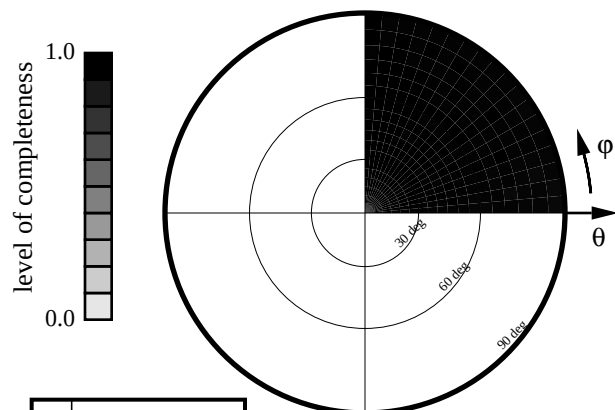
Program: CNS 1.1
 Nominal resolution range: 25.0 – 2.75 Å
 Reported R-factor: 0.267
 Number of reflections used: 191247
 Reported Rfree: 0.30
 Sigma cut-off: N.A.

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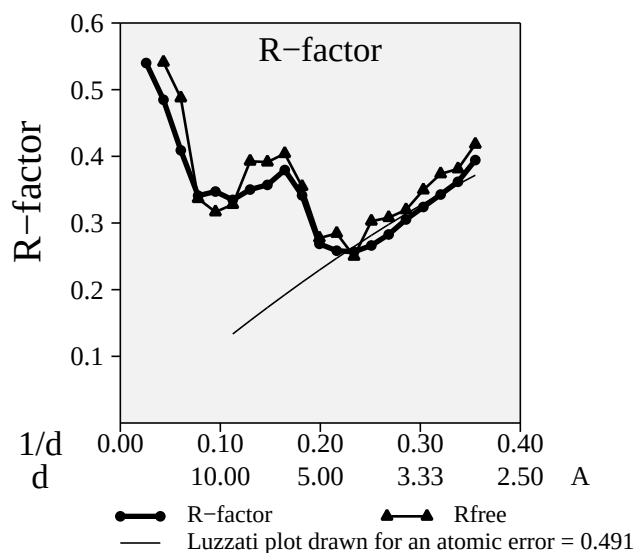


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

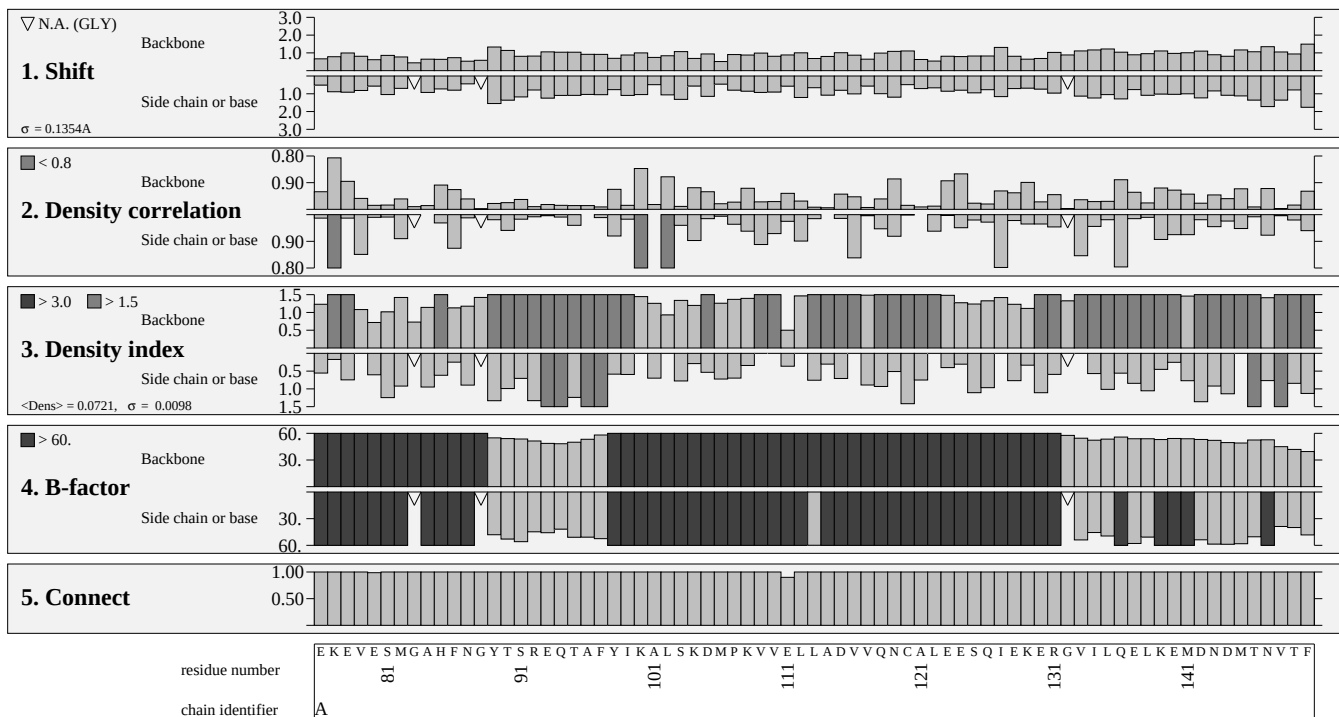
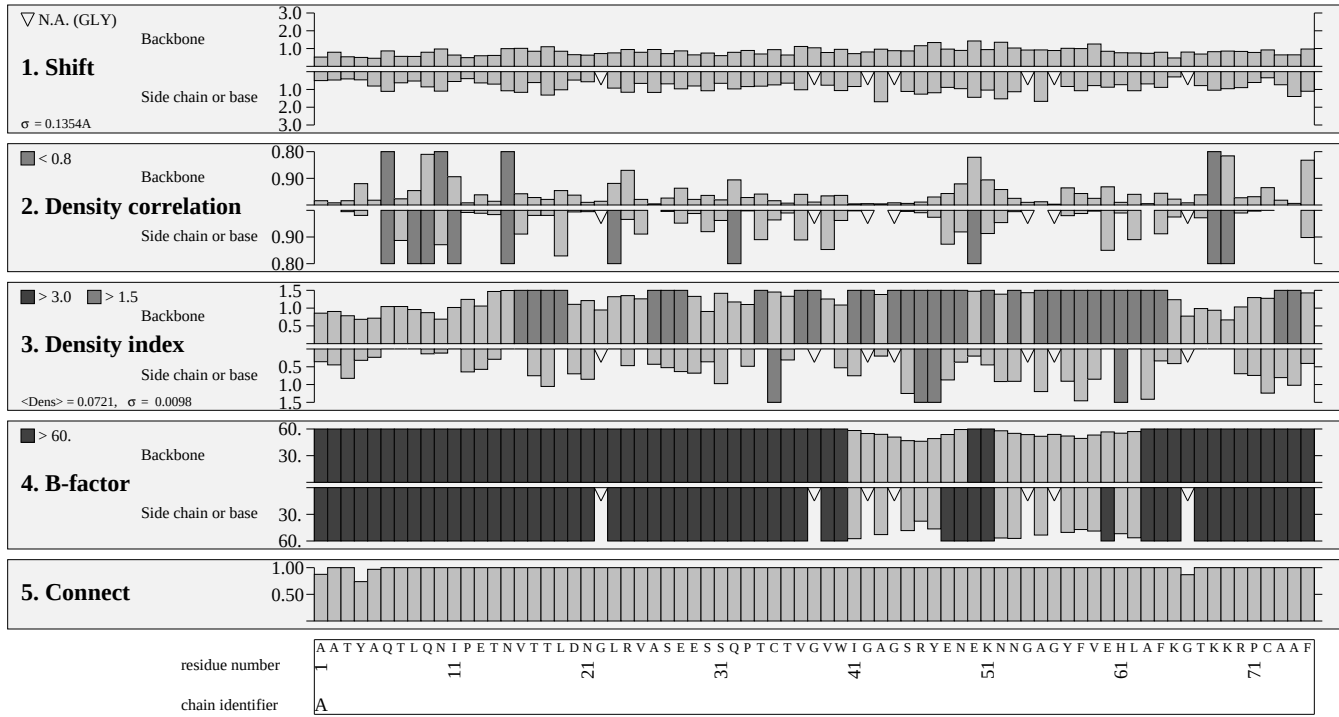
polar coordinates of the crystallographical axes



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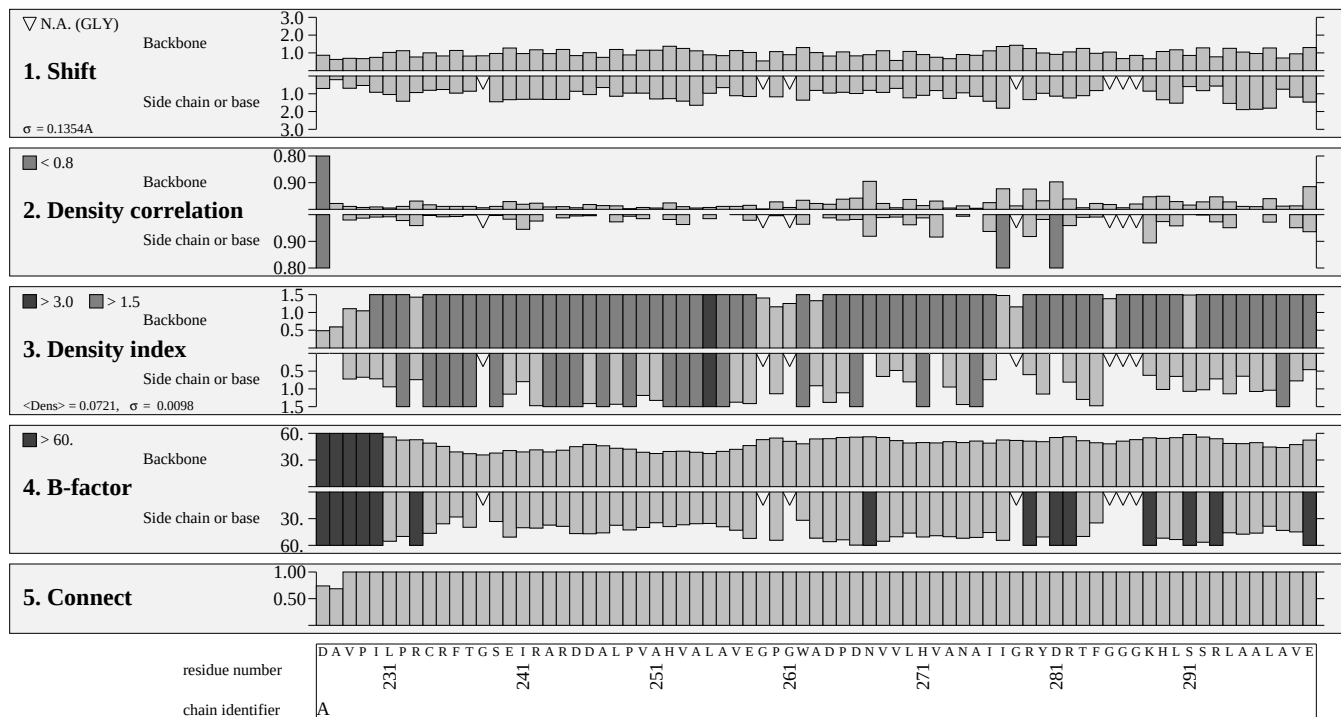
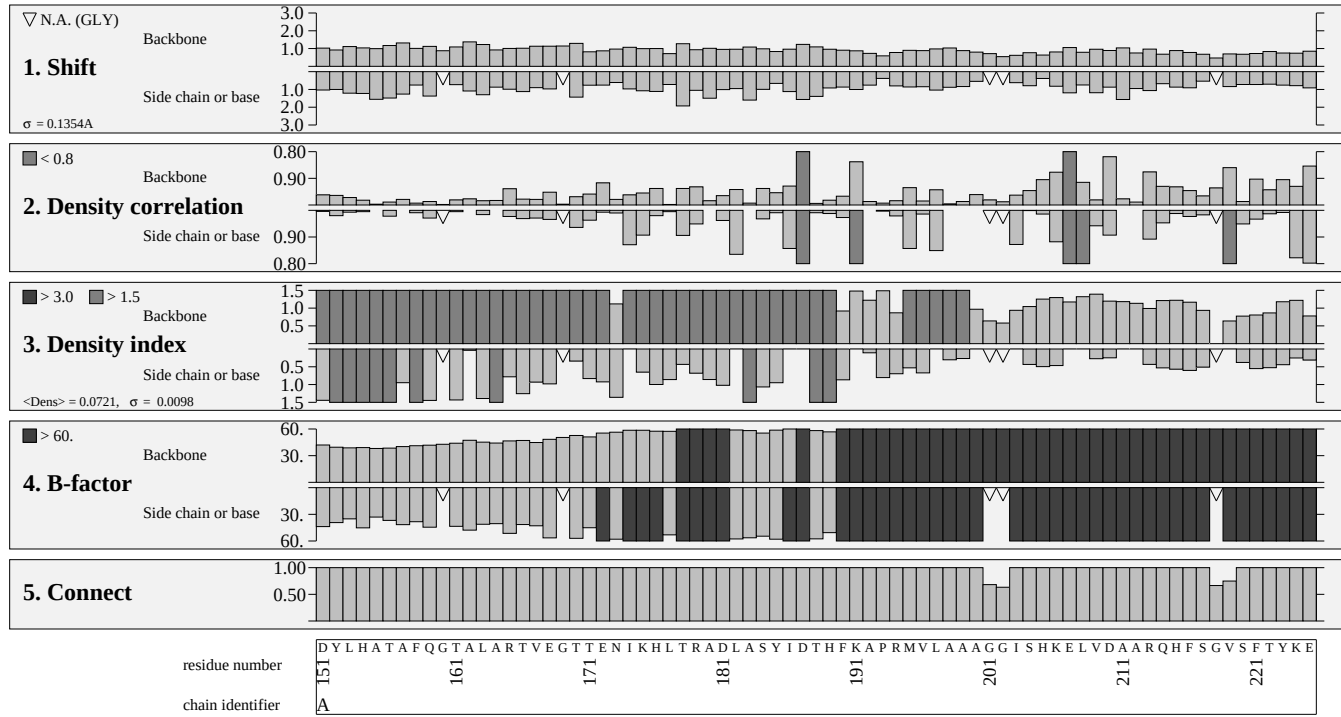
Local estimation



Structure Factor Check

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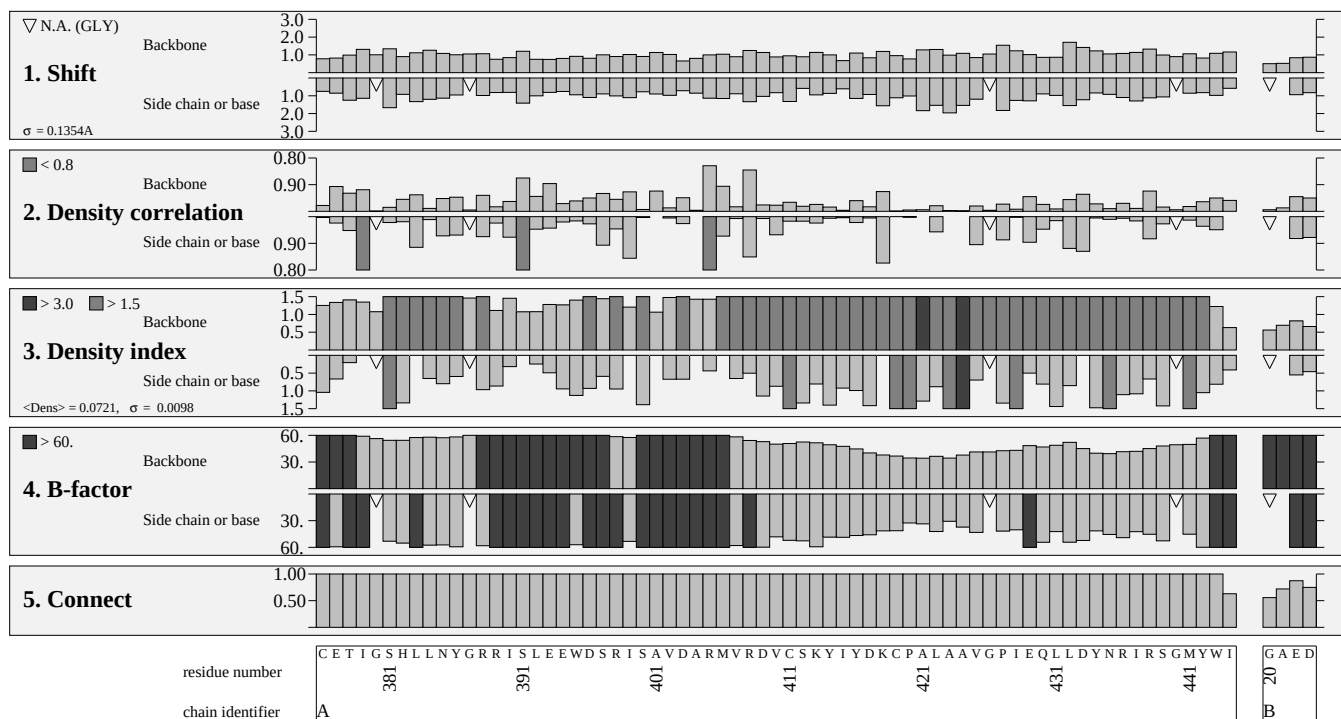
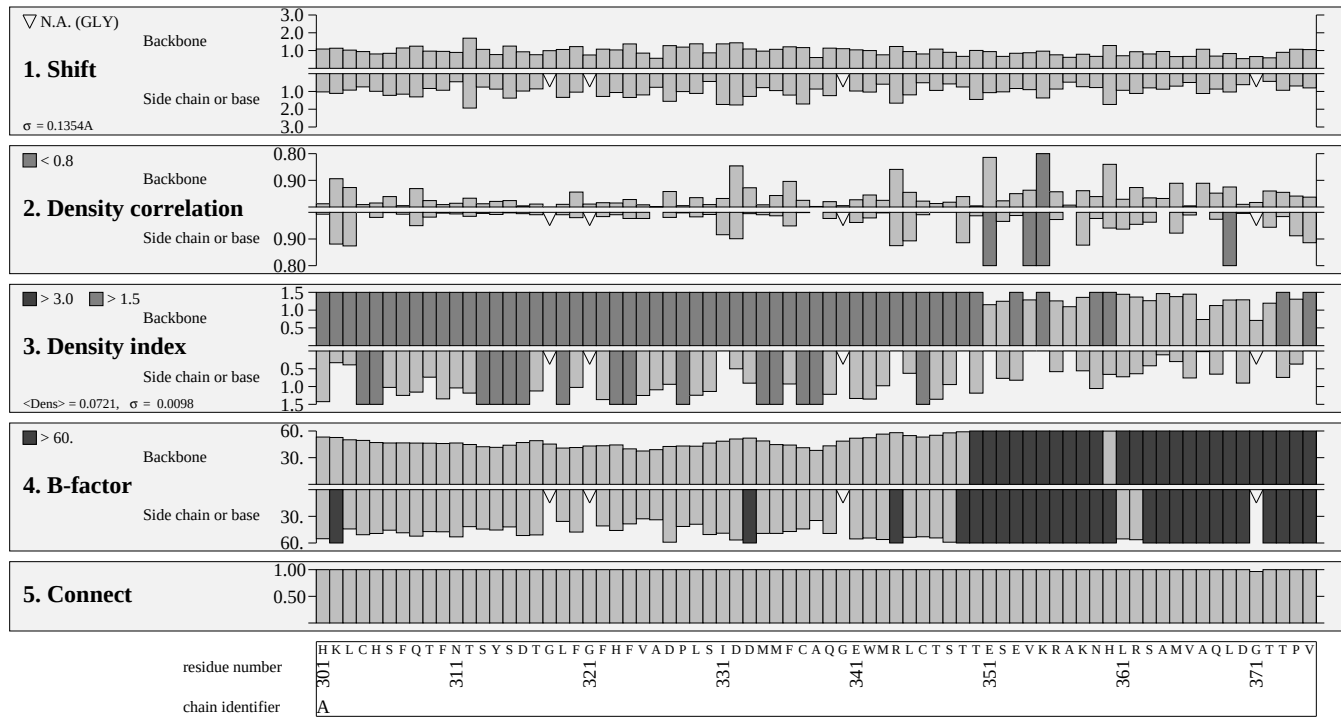
Local estimation (2)



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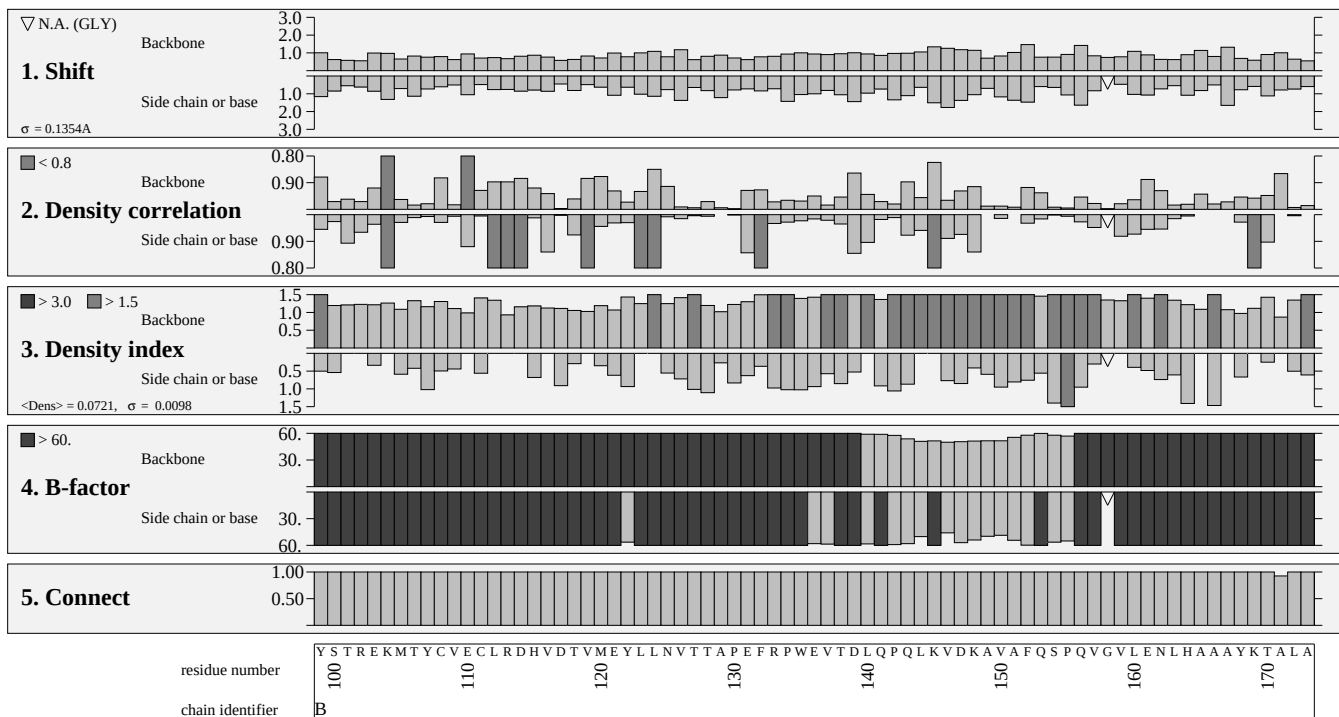
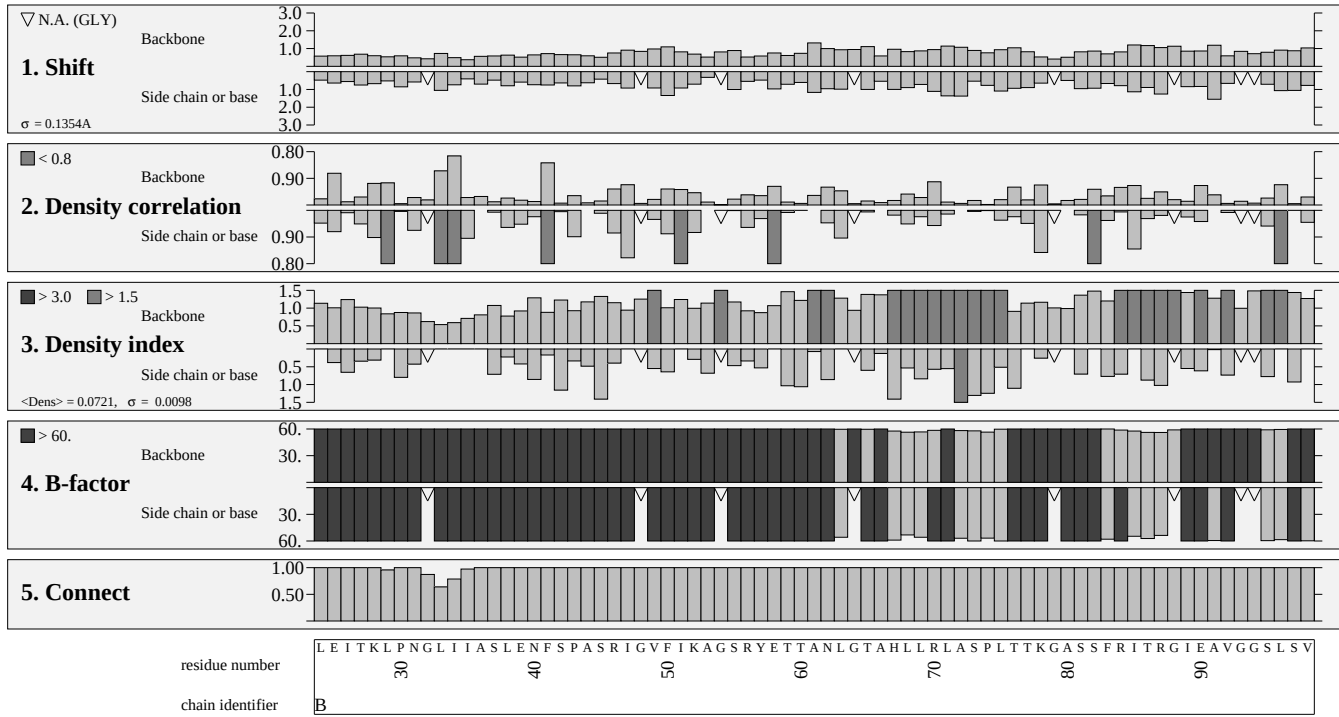
Local estimation (3)



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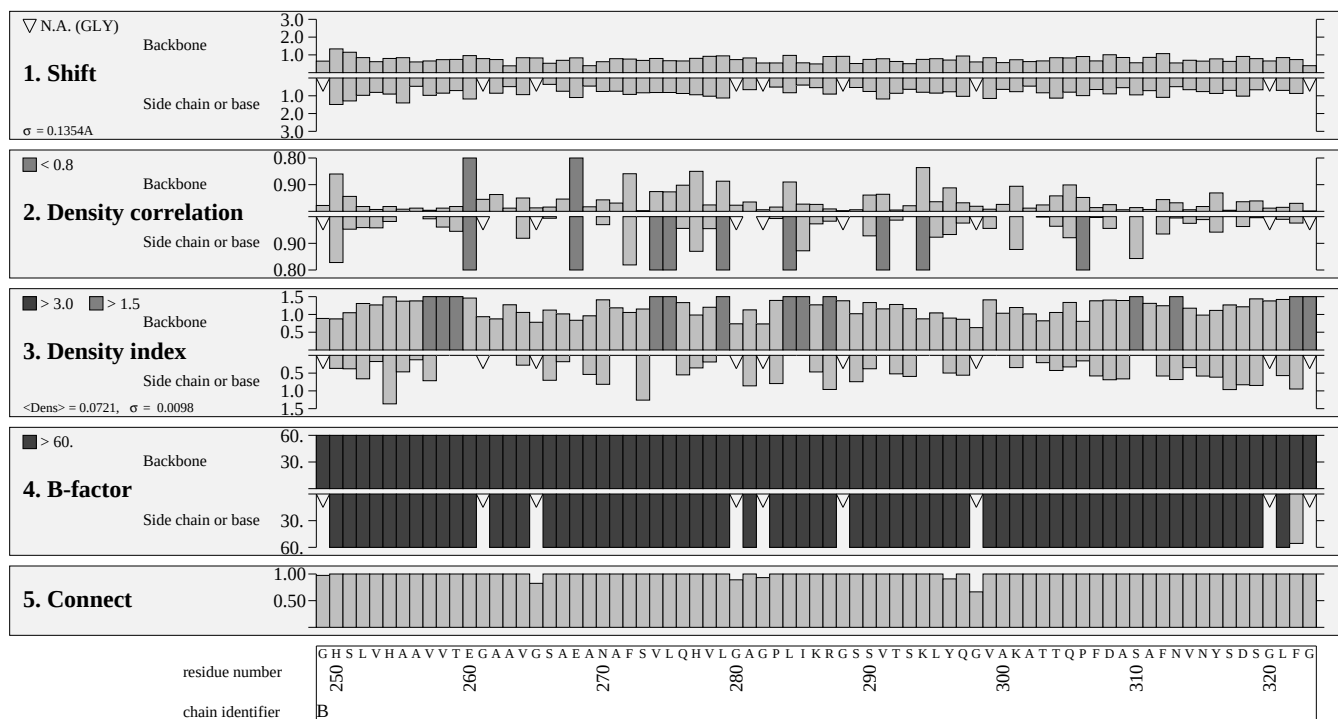
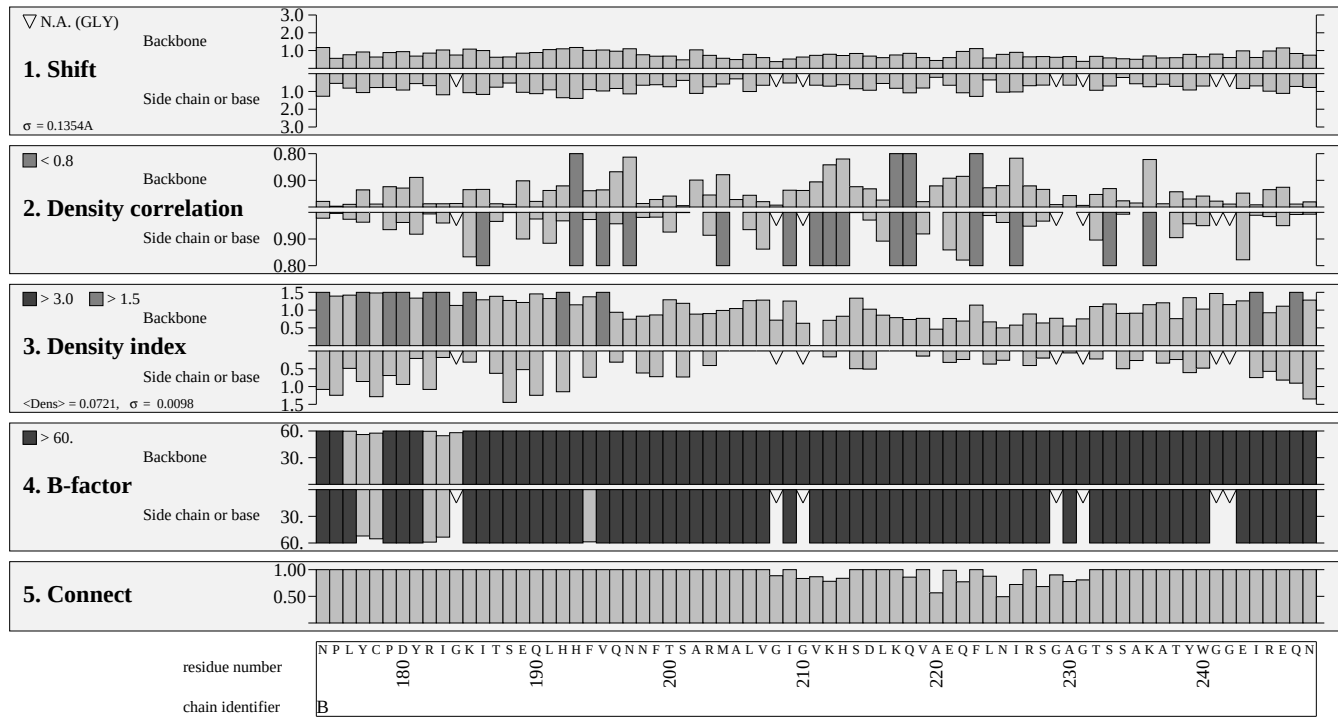
Local estimation (4)



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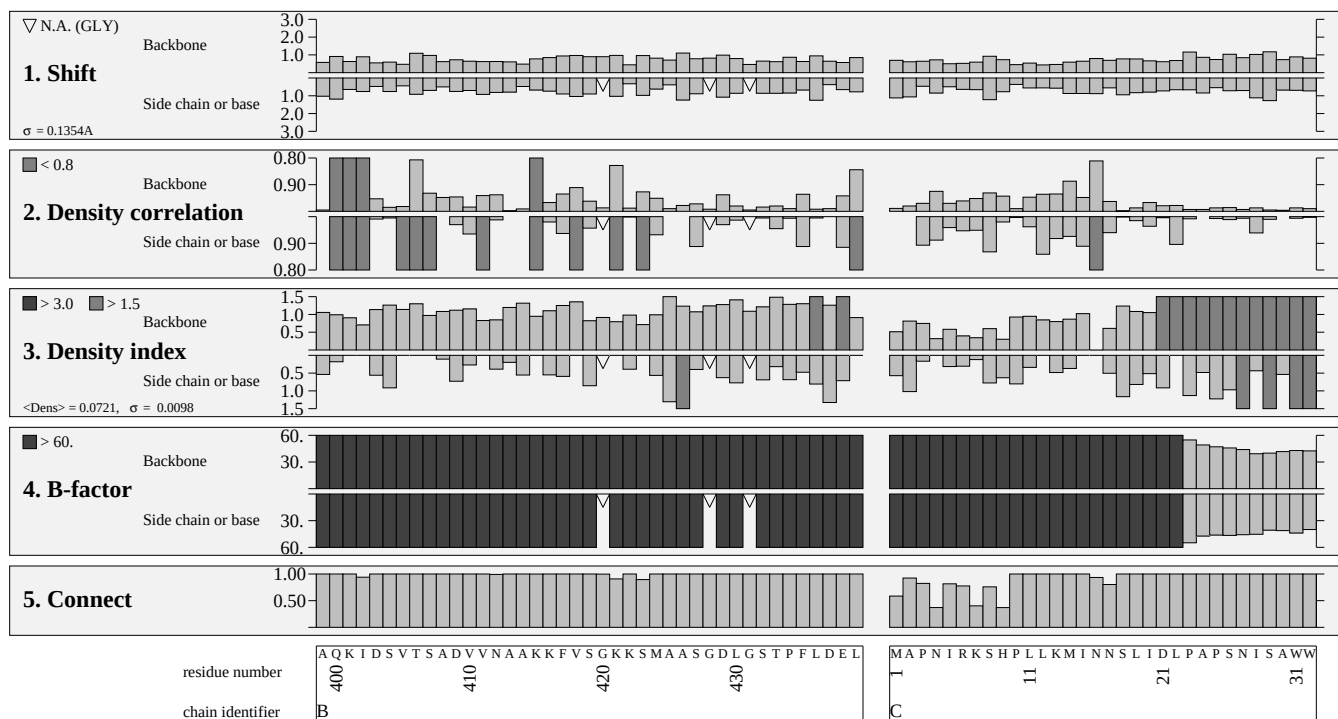
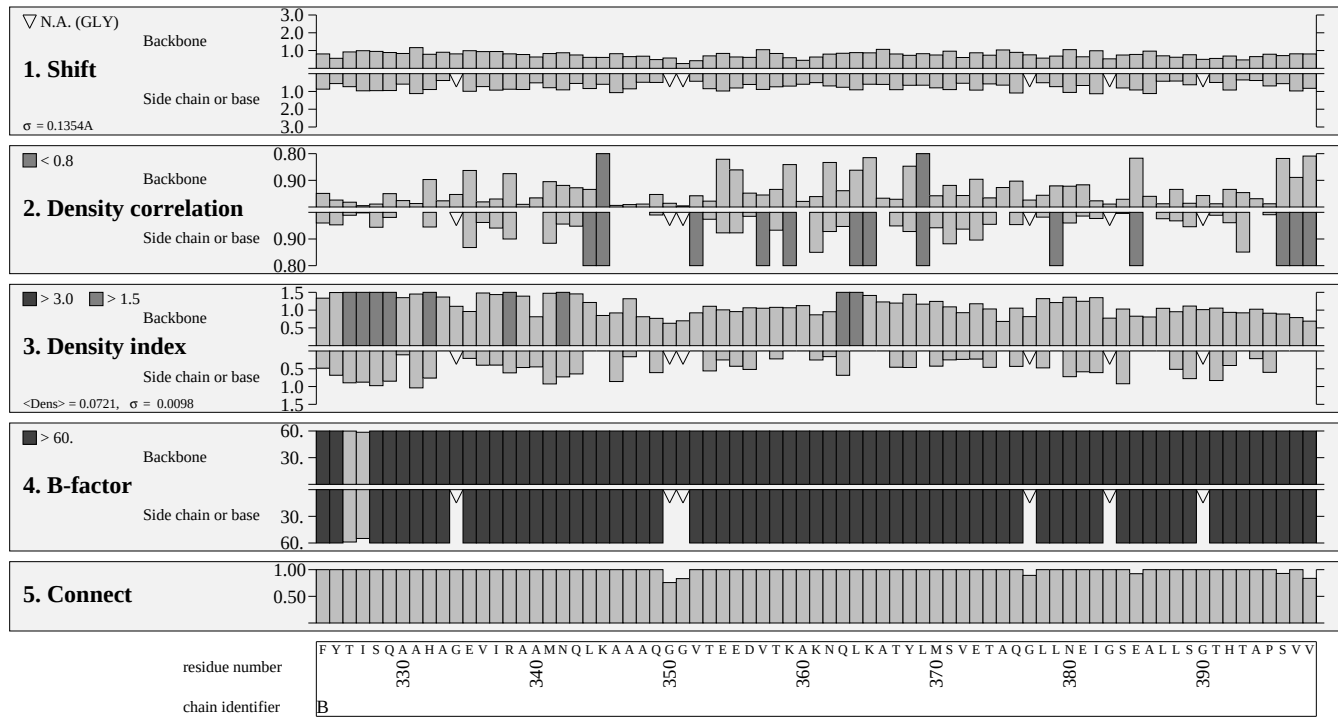
Local estimation (5)



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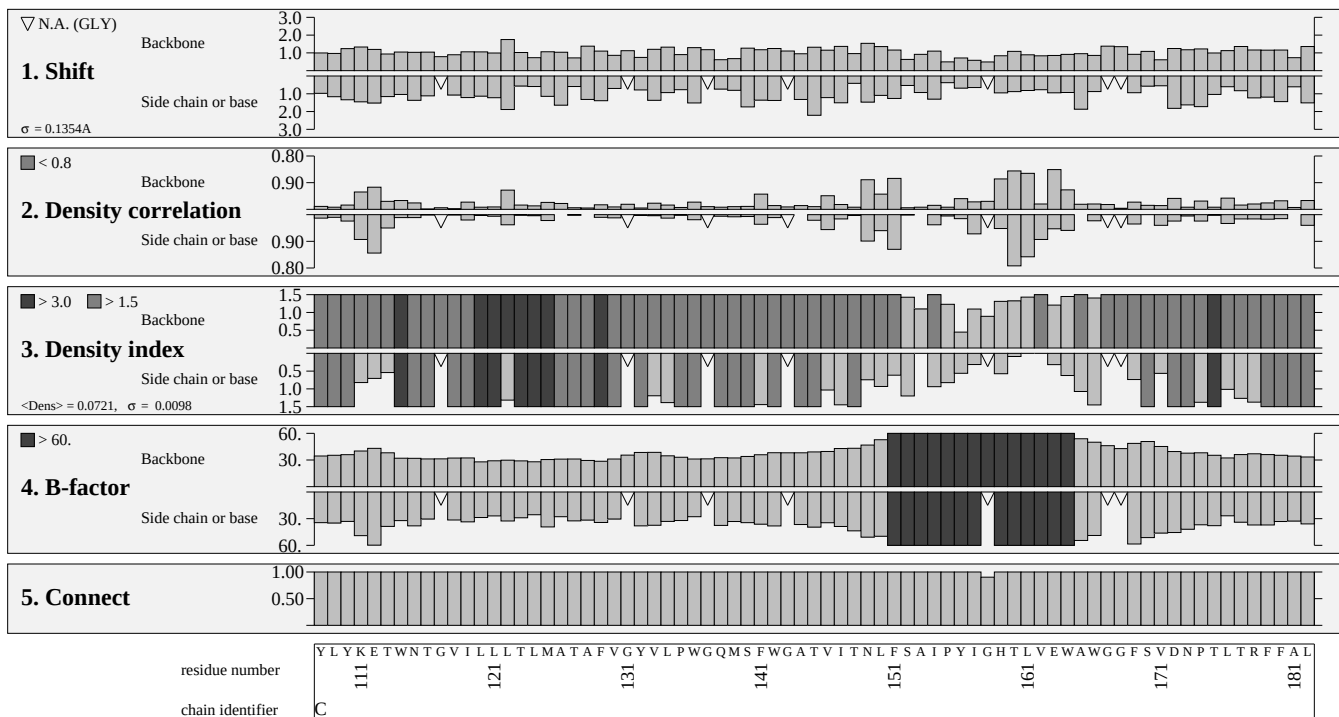
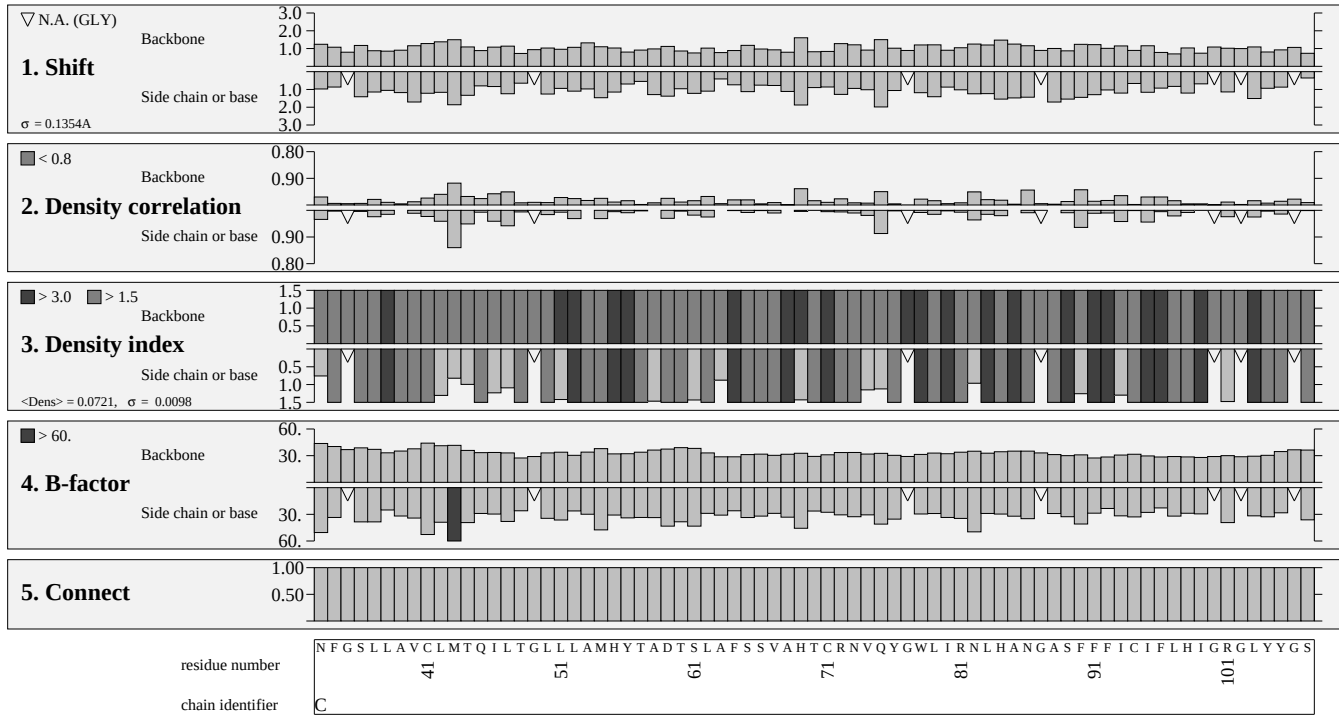
Local estimation (6)



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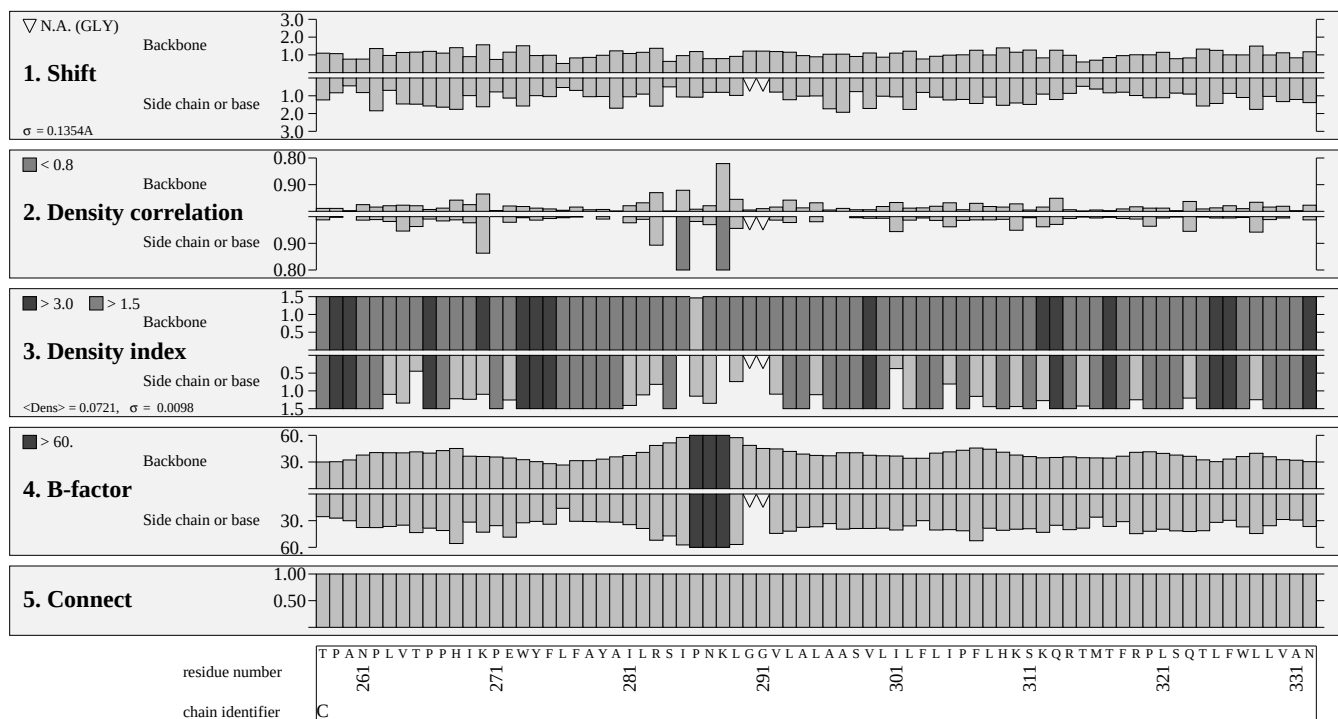
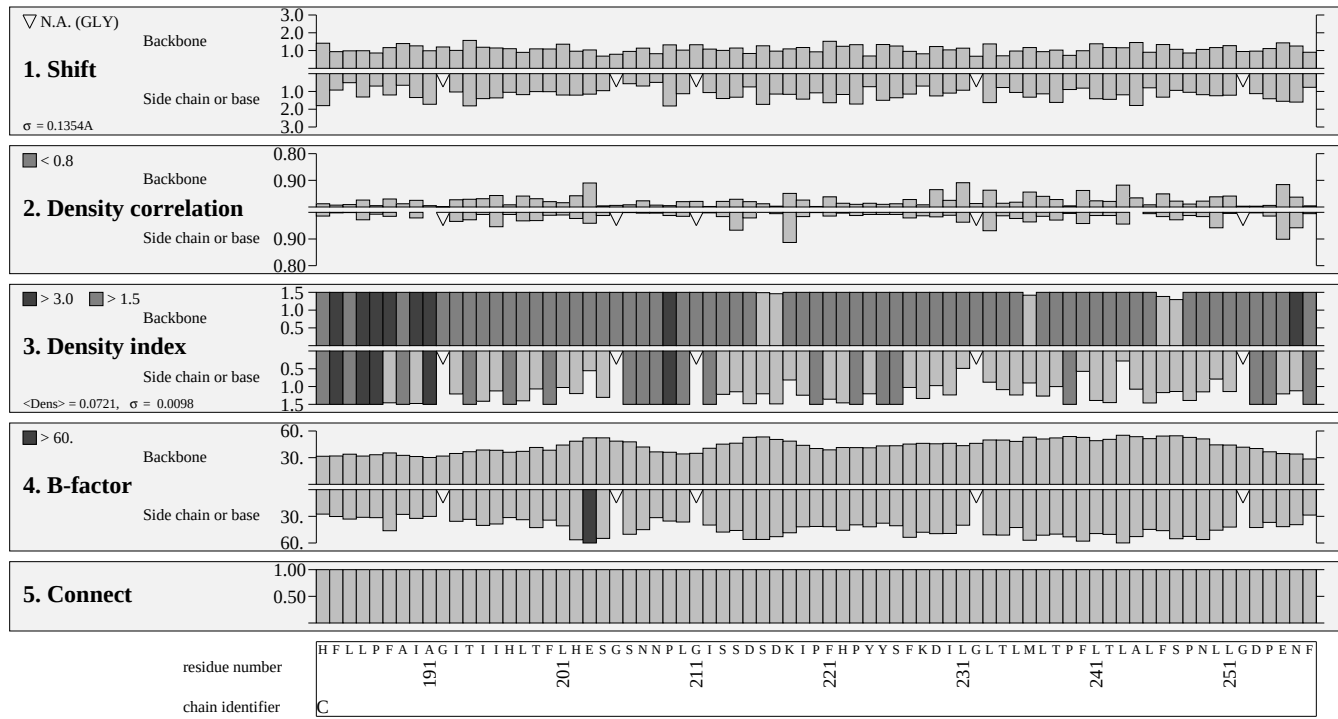
Local estimation (7)



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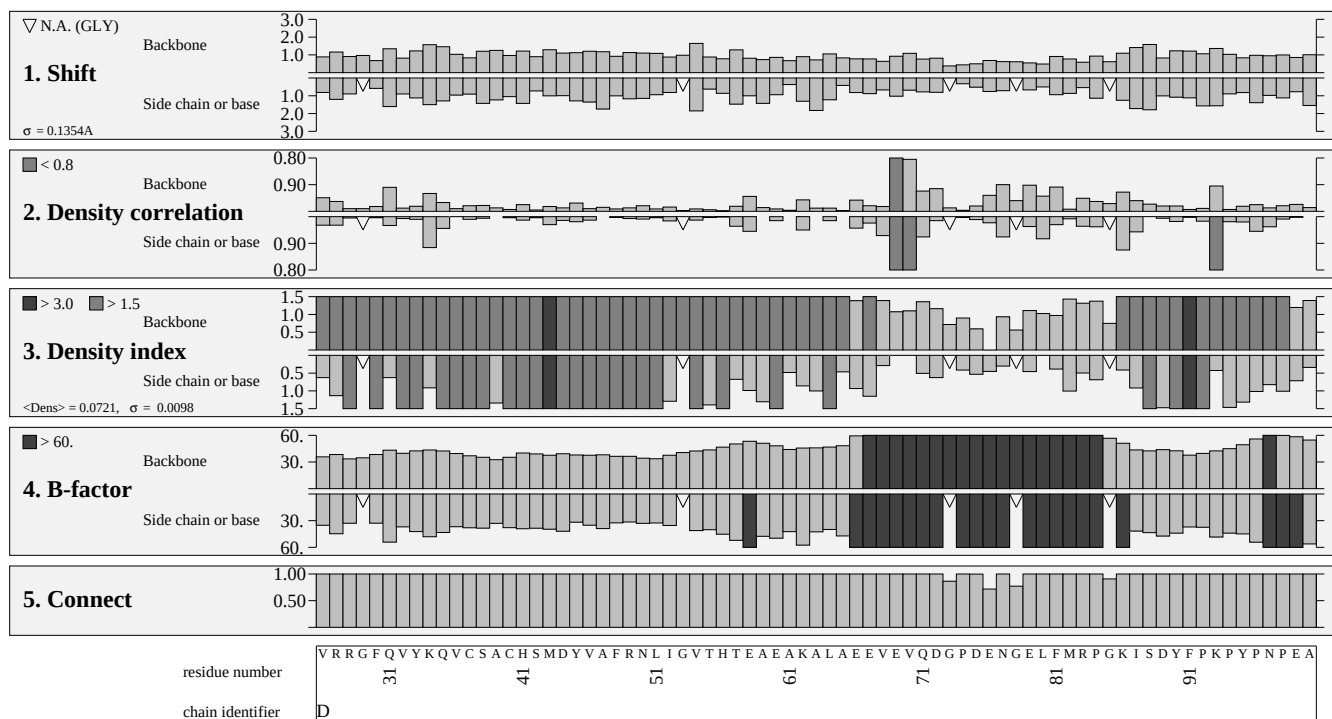
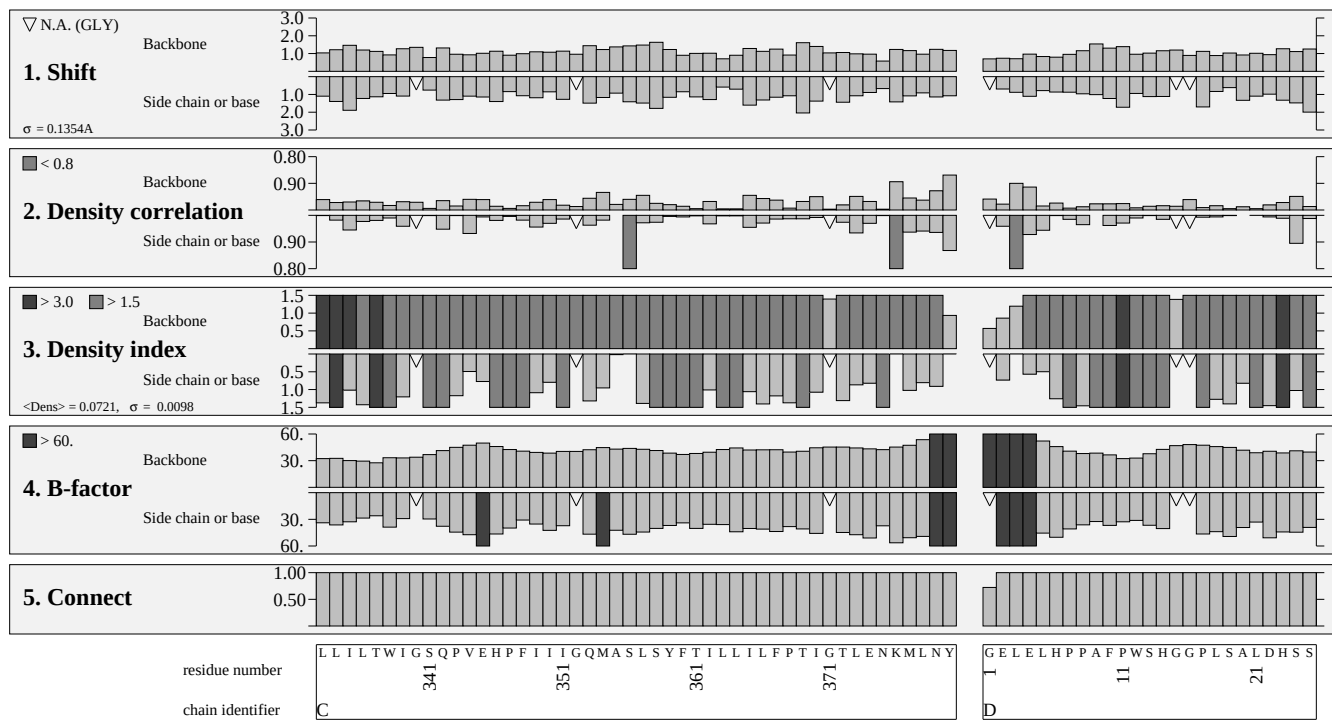
Local estimation (8)



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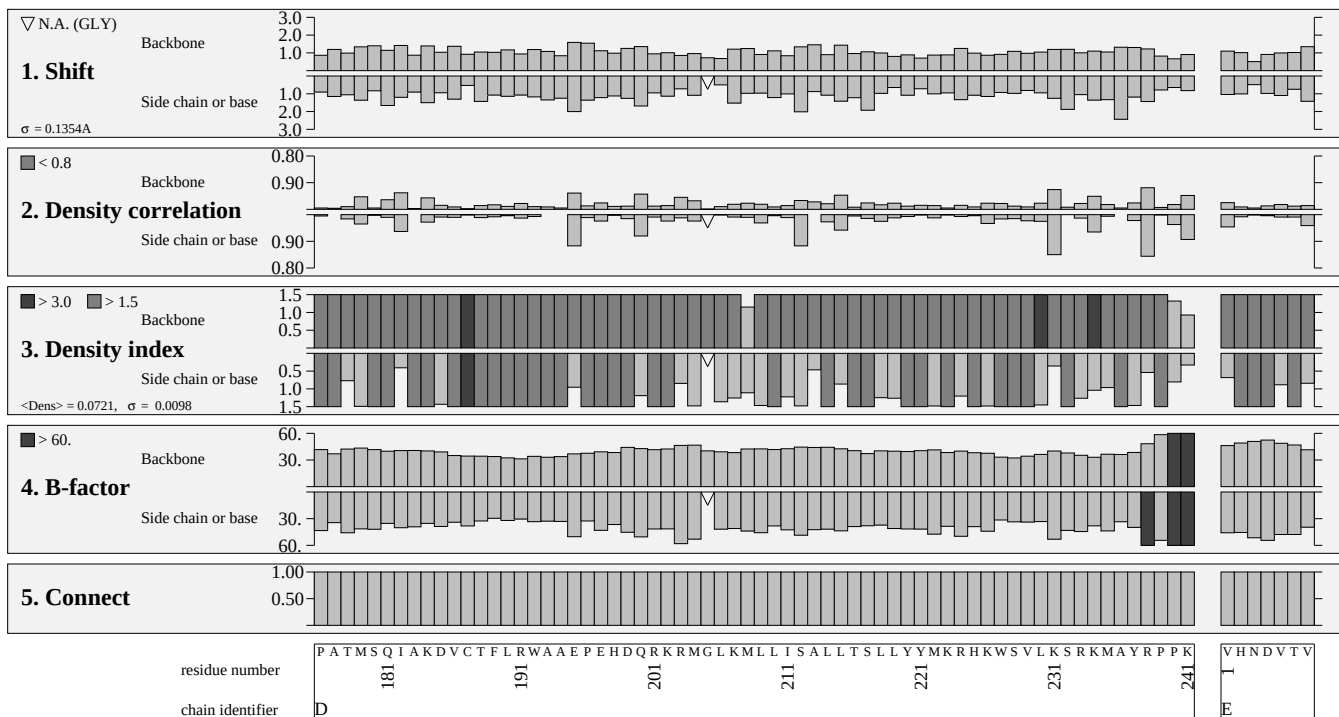
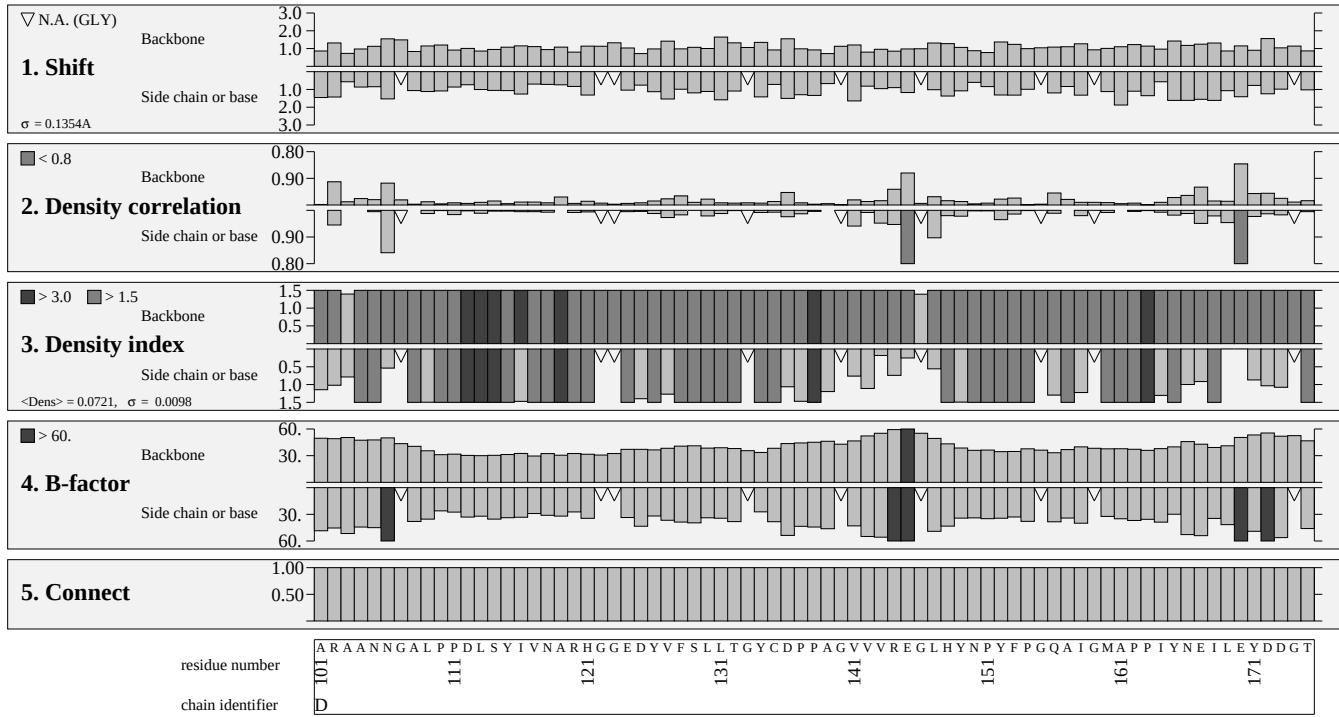
Local estimation (9)



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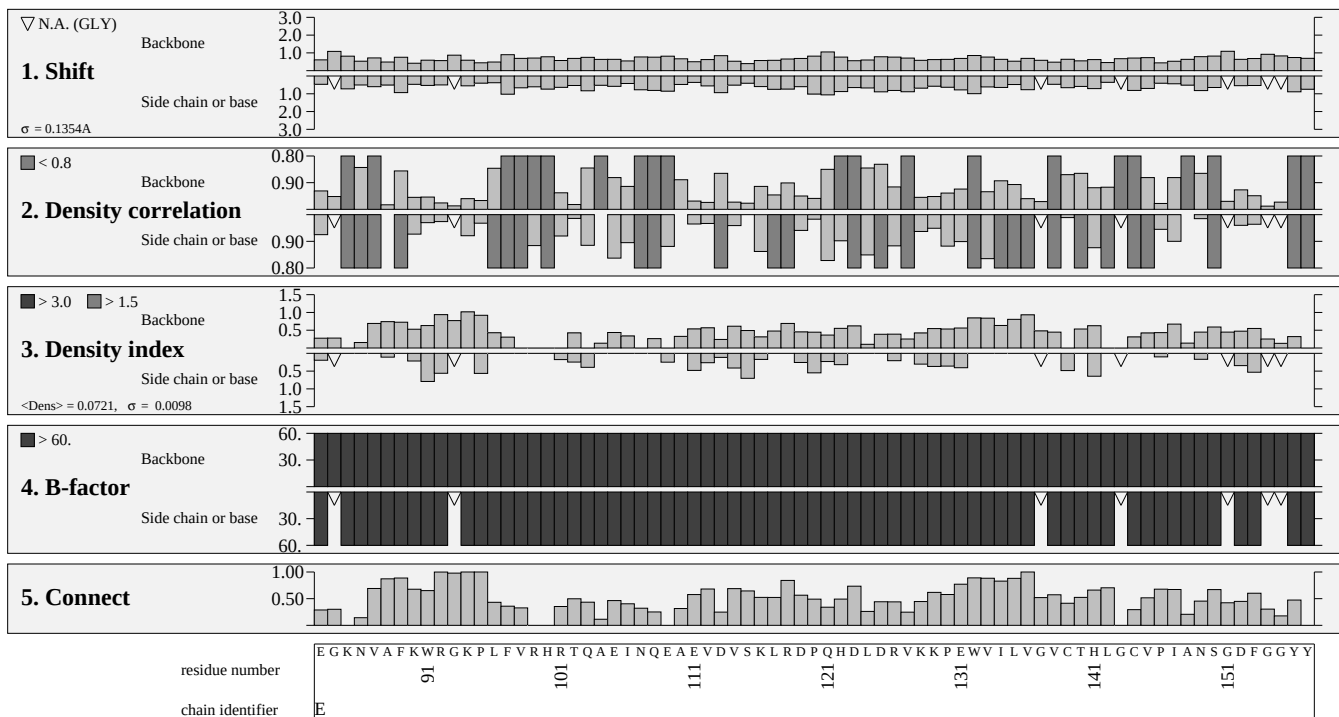
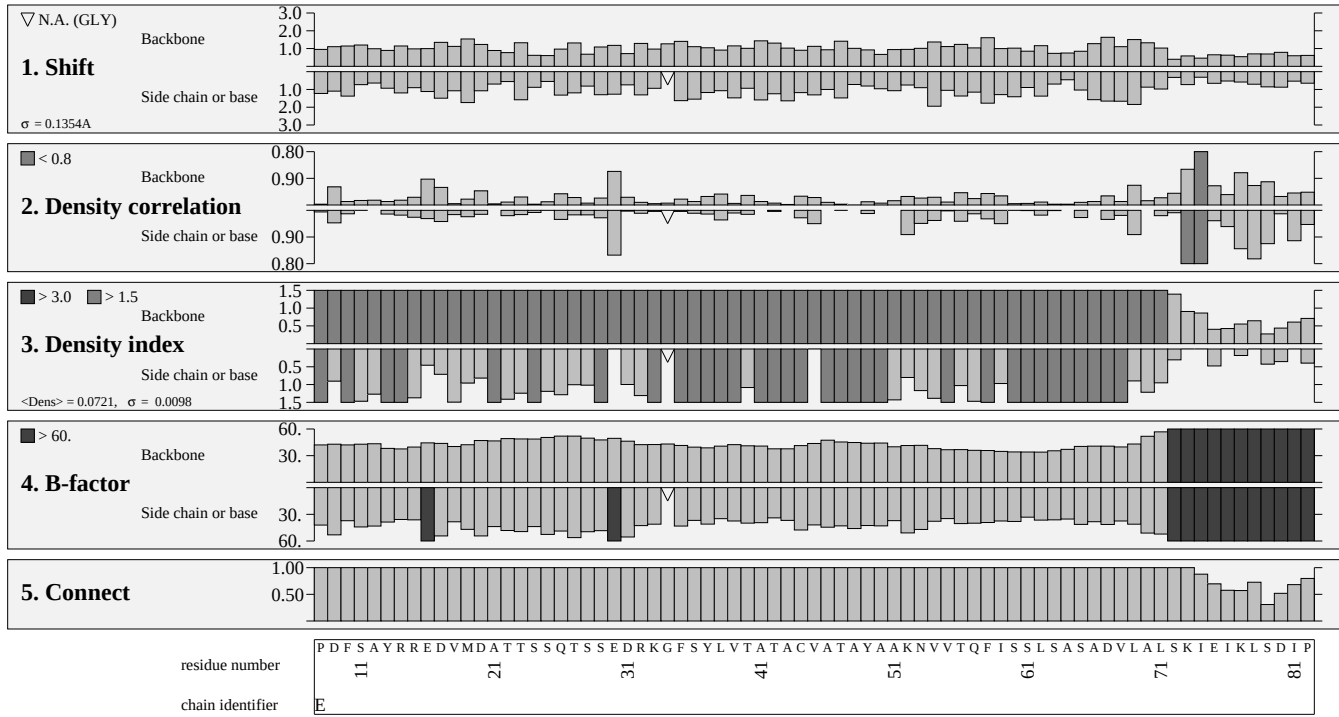
Local estimation (10)



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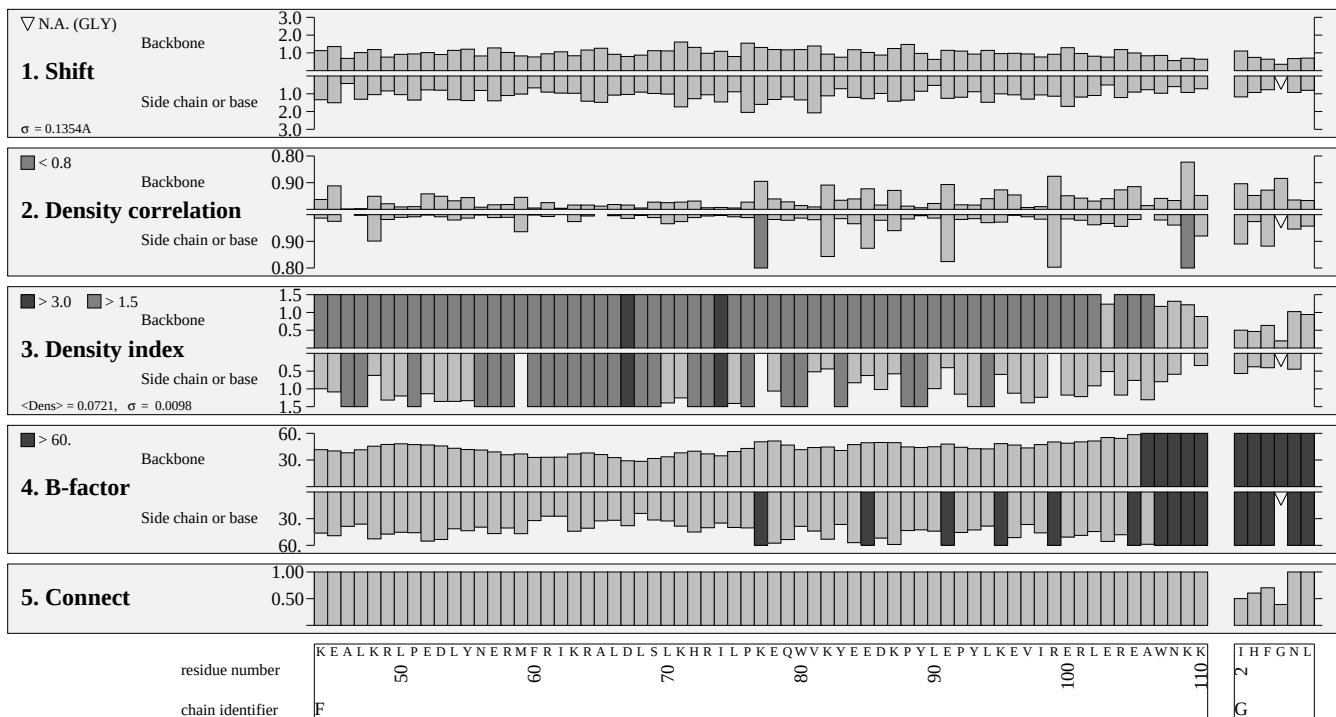
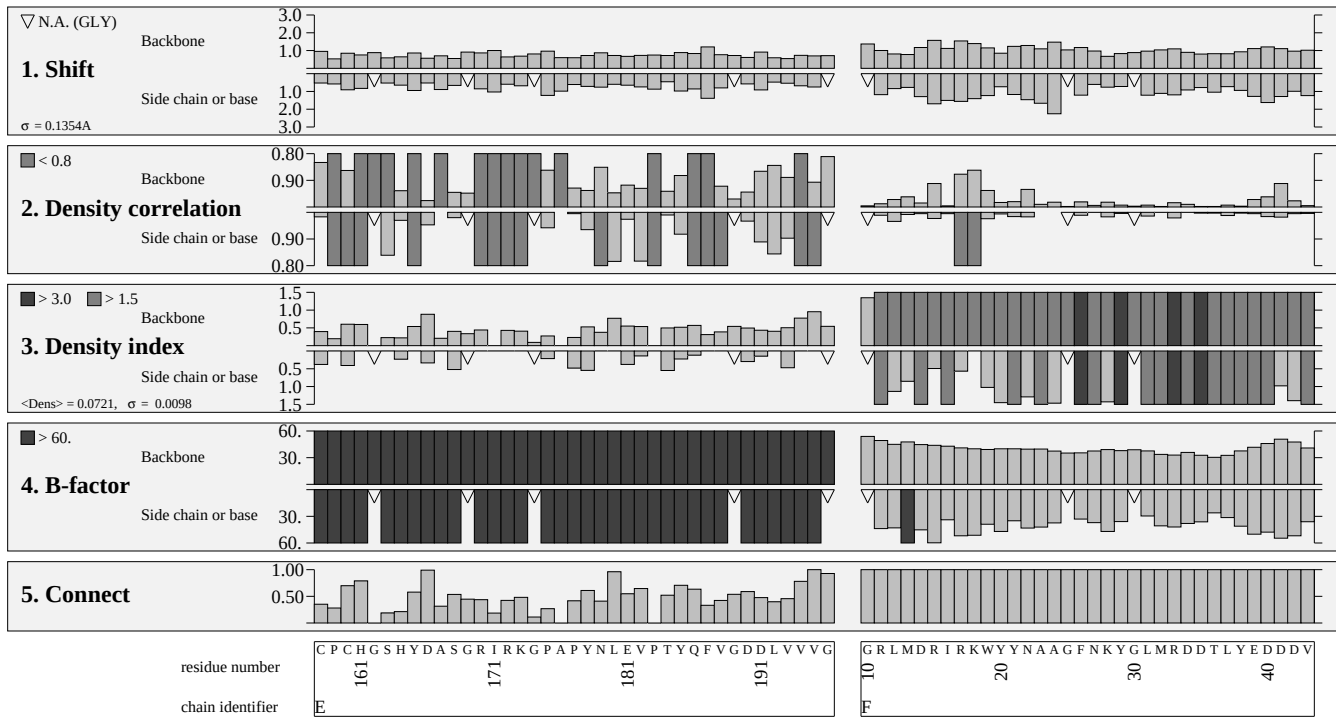
Local estimation (11)



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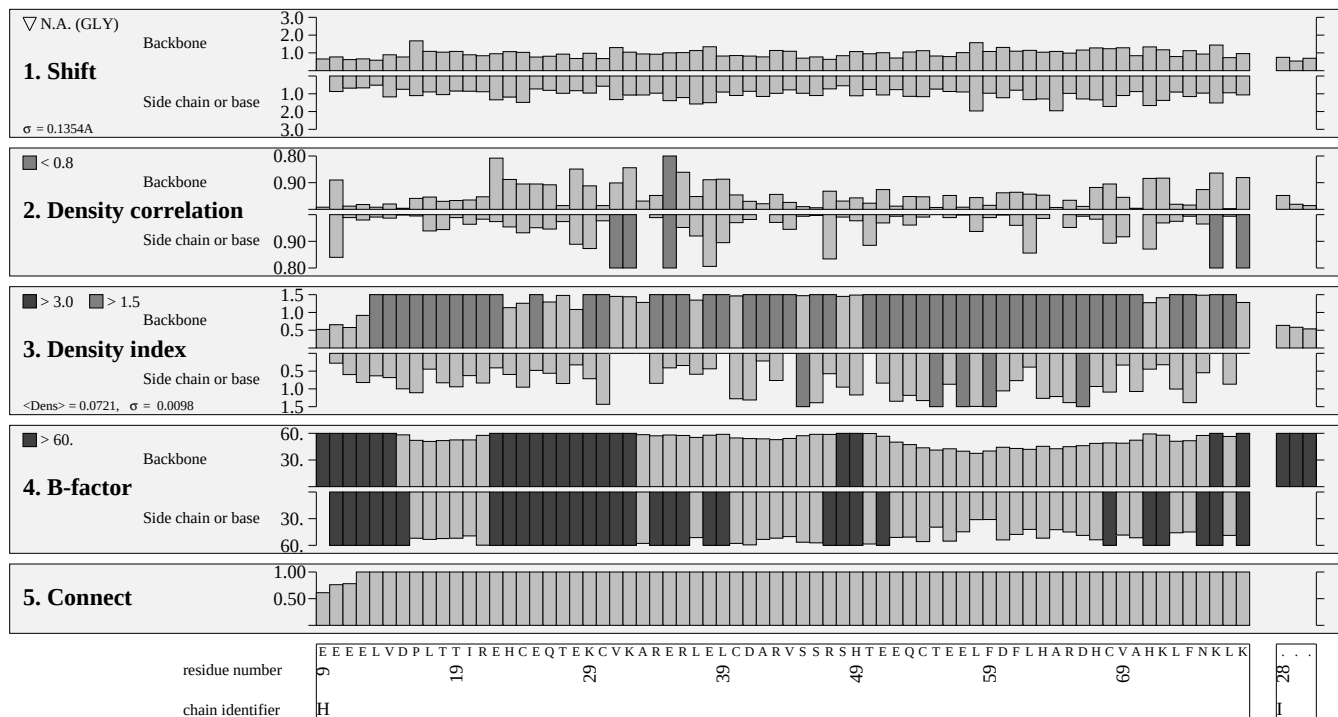
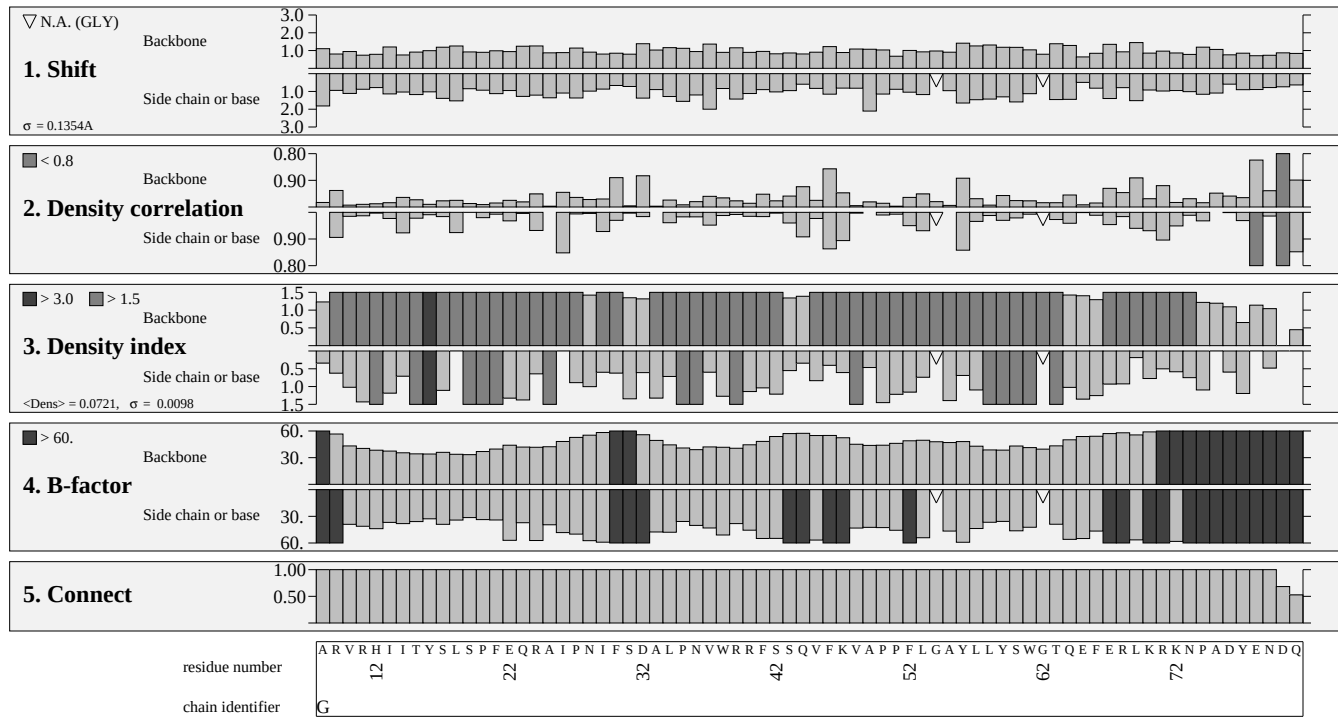
Local estimation (12)



Structure Factor Check

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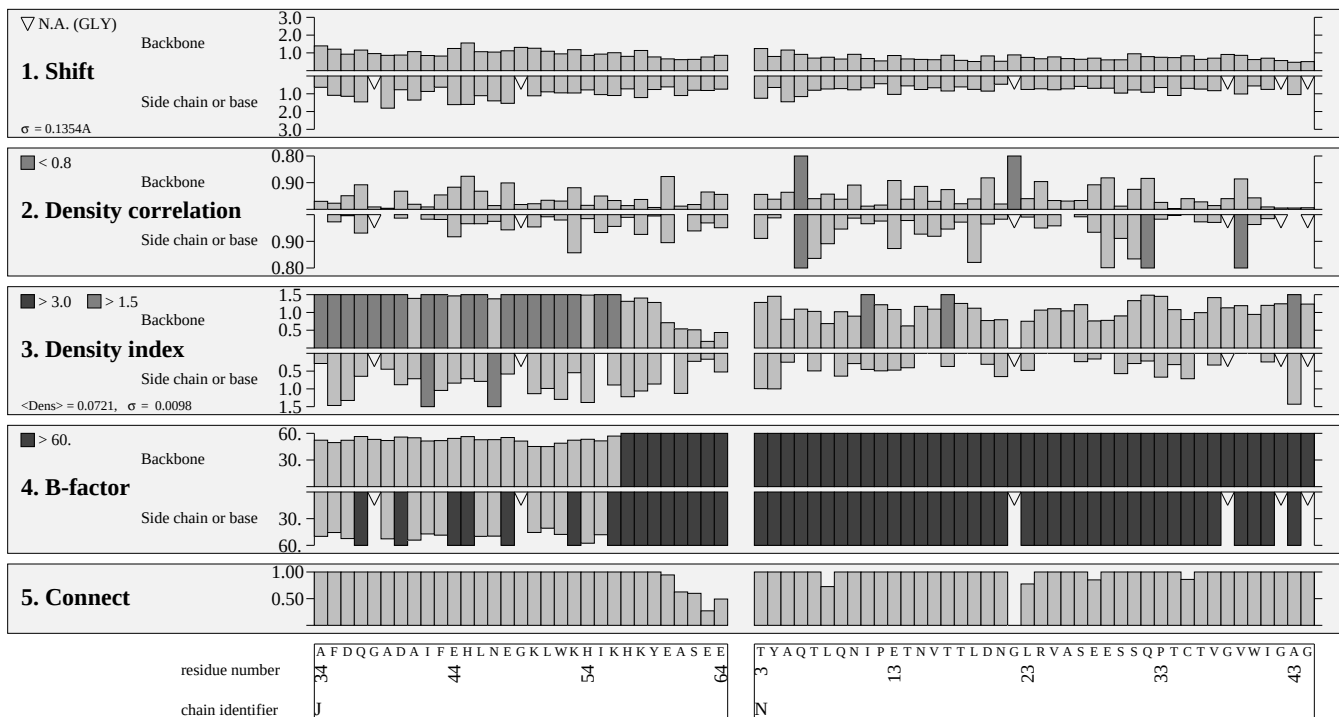
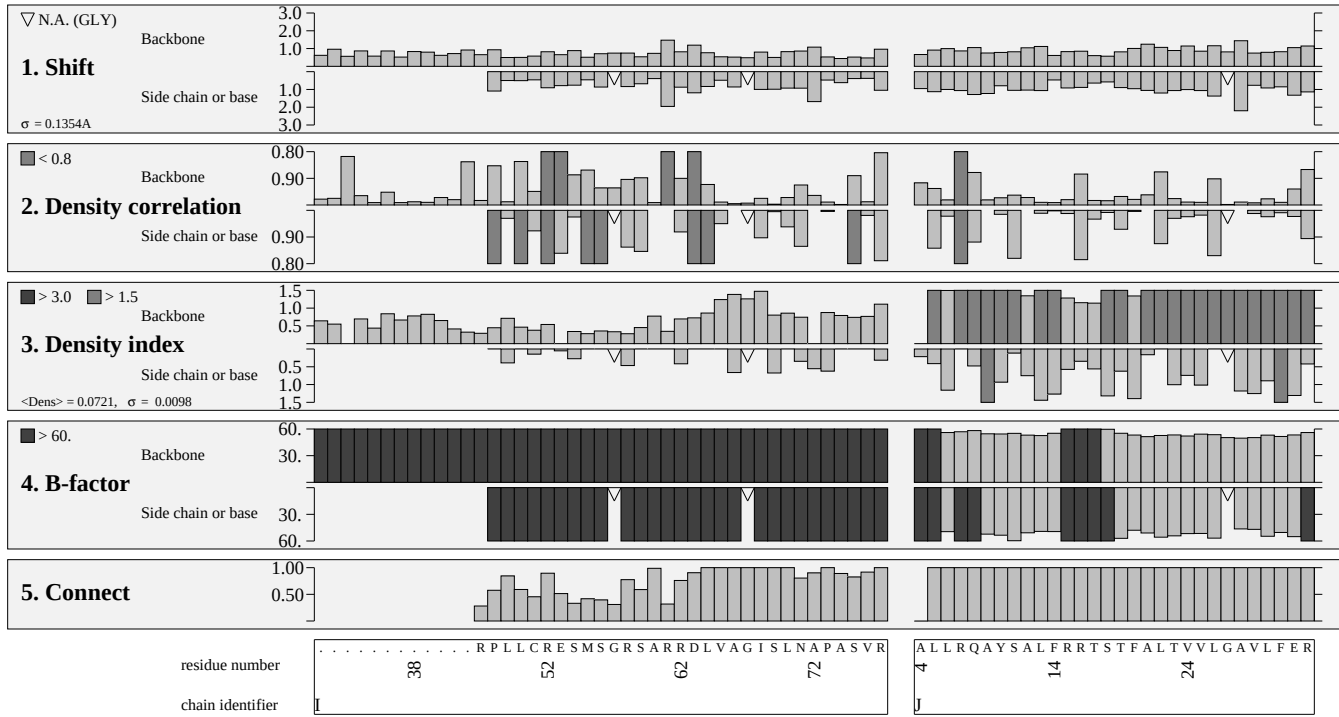
Local estimation (13)



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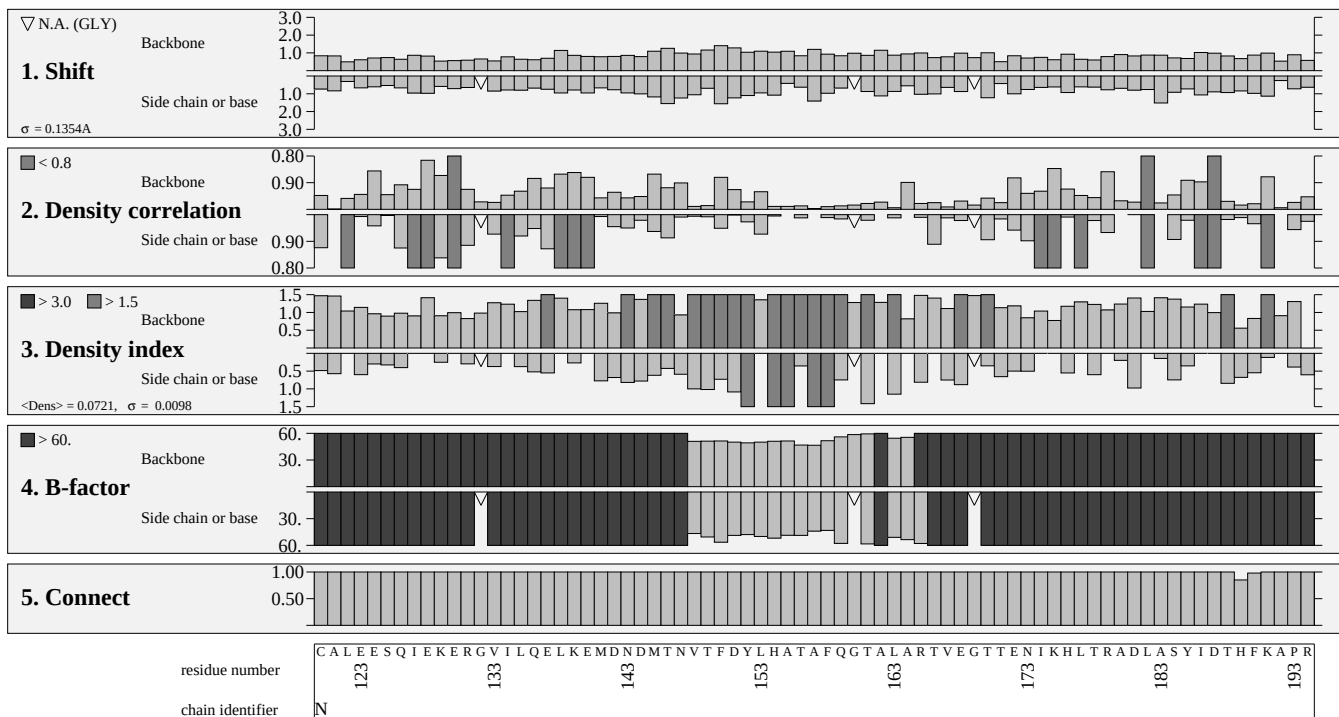
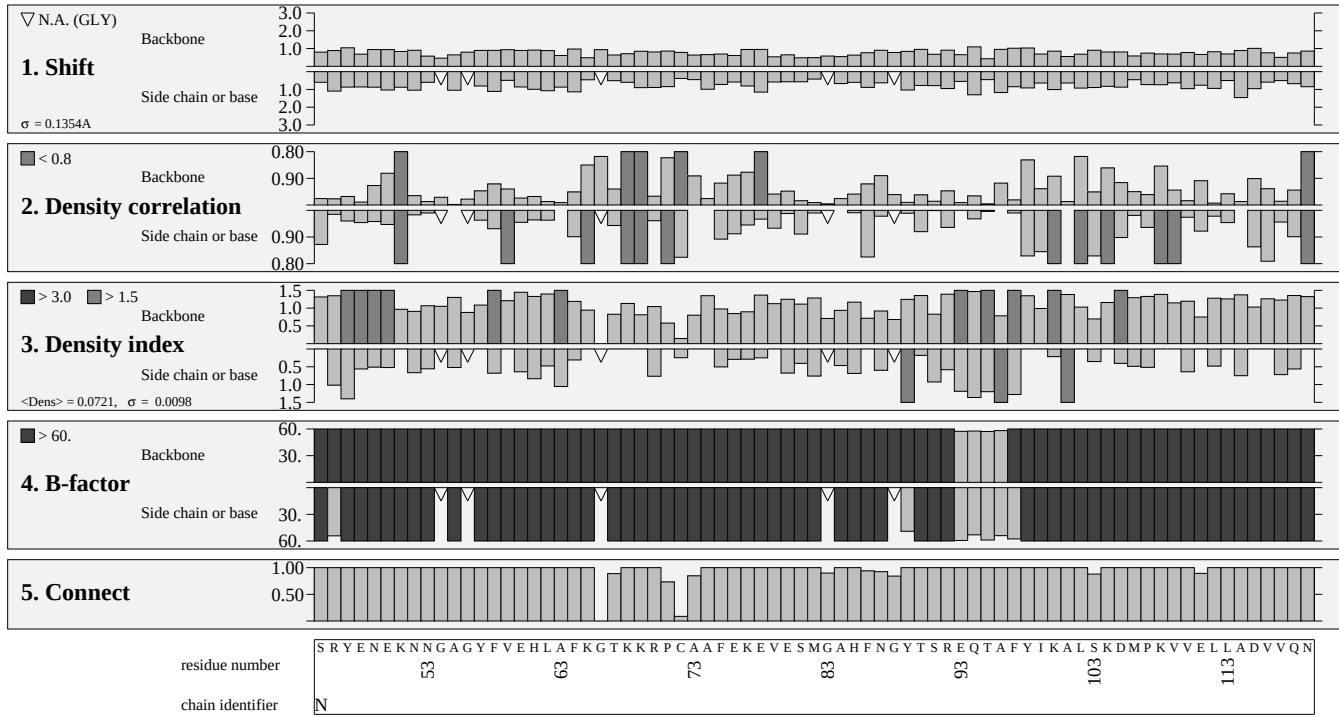
Local estimation (14)



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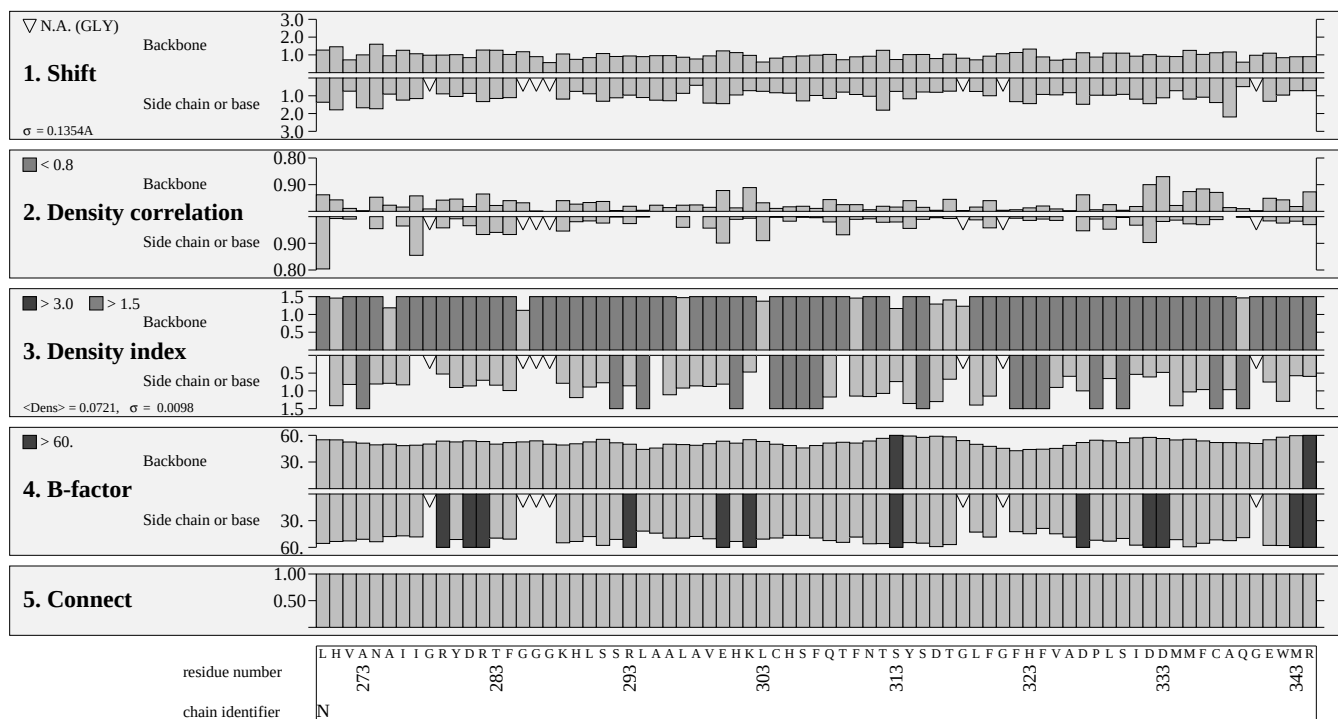
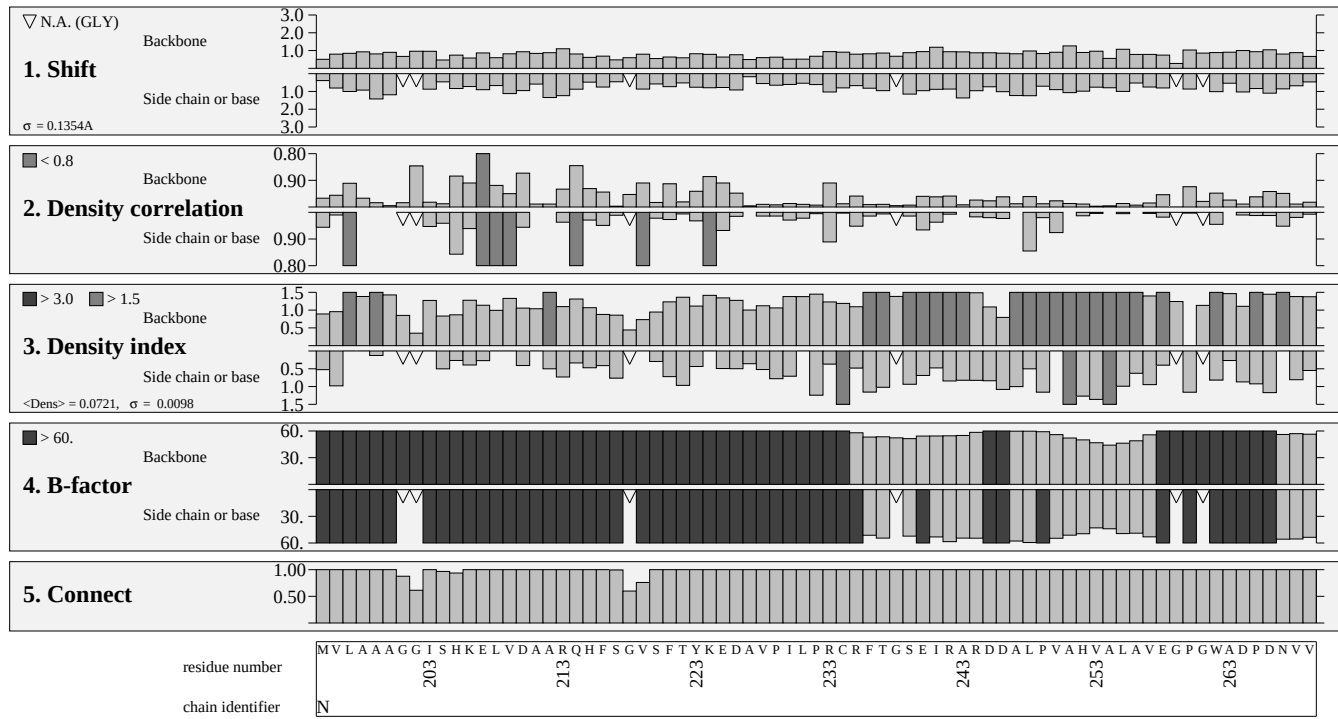
Local estimation (15)



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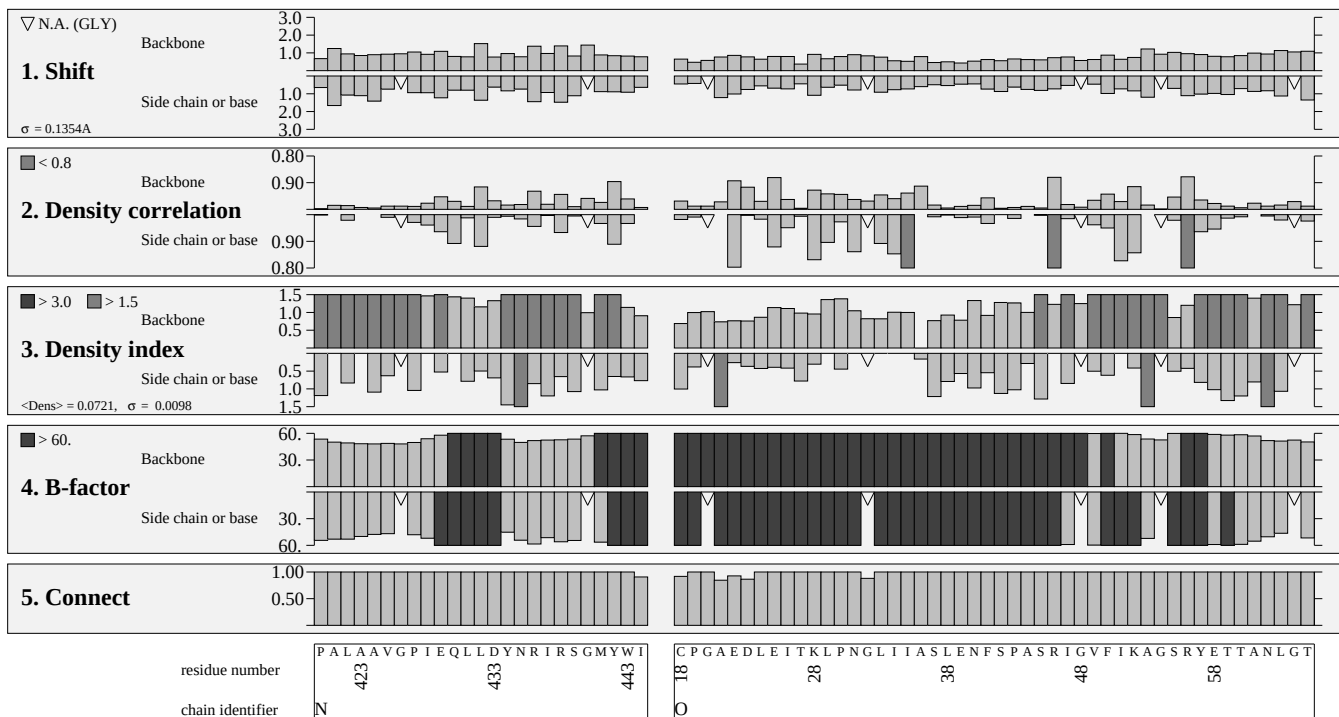
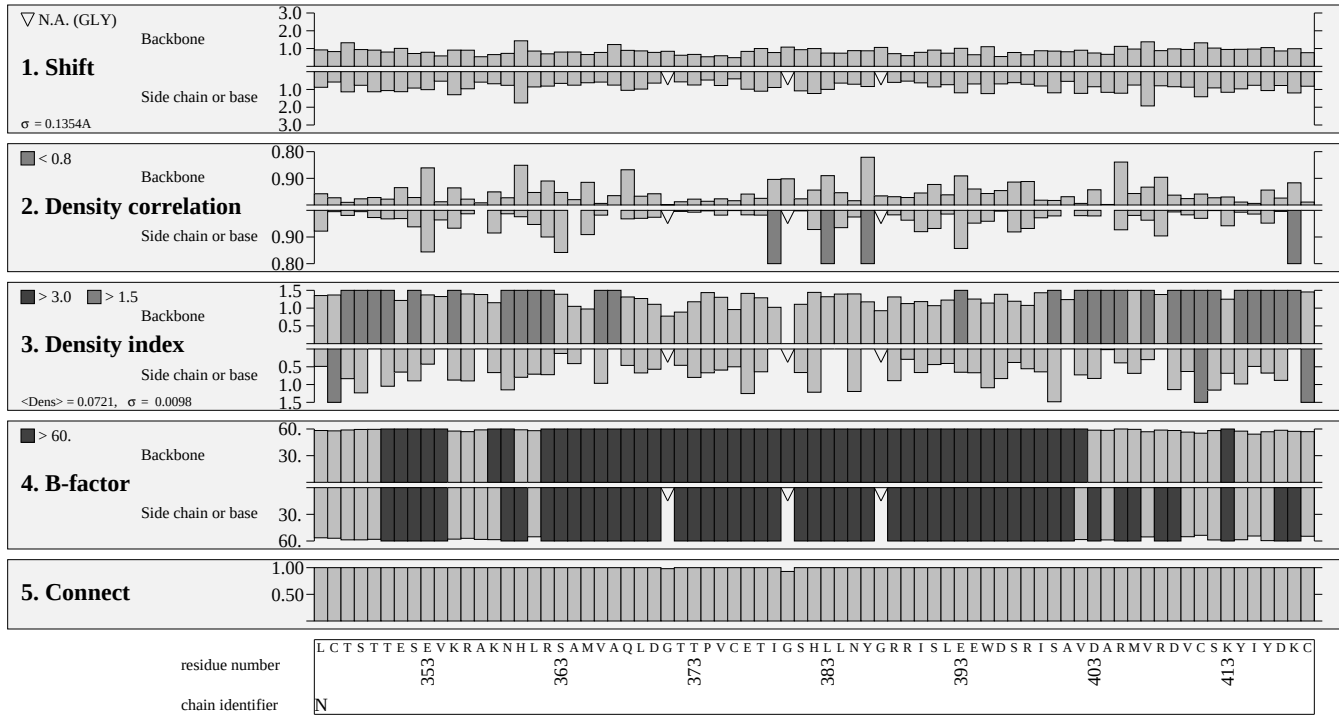
Local estimation (16)



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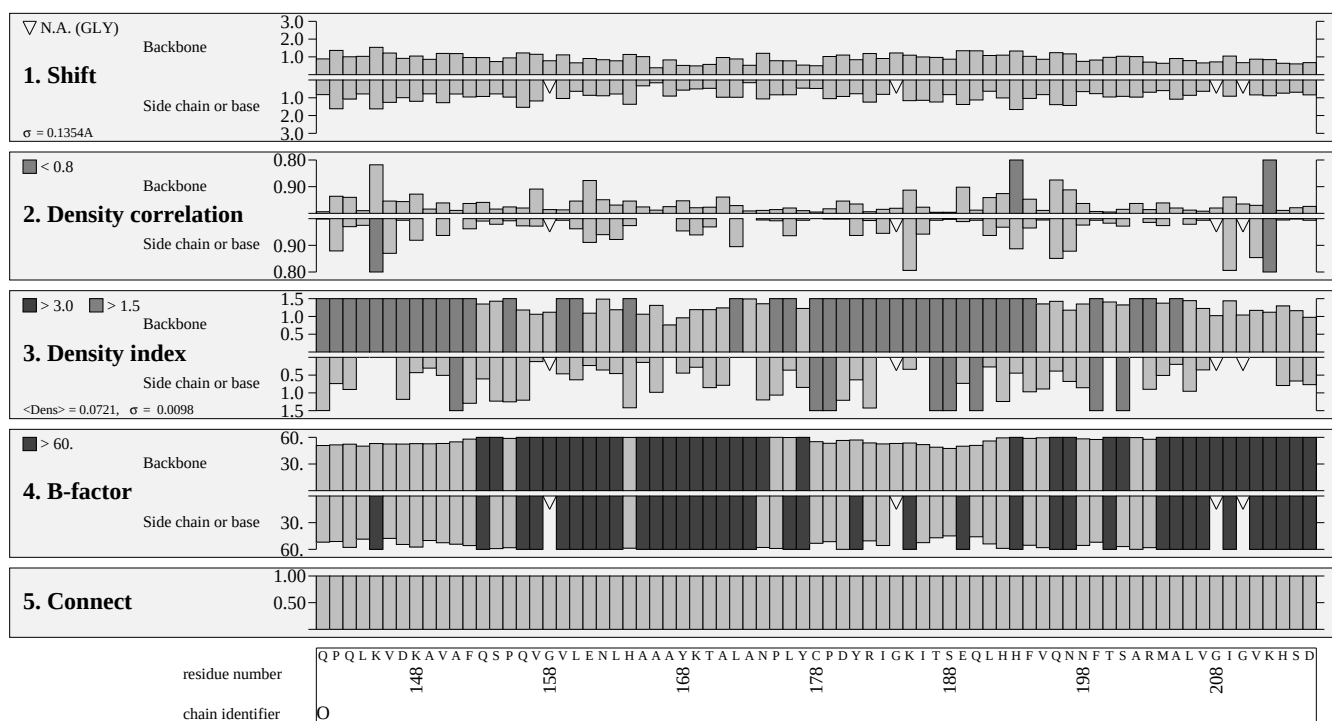
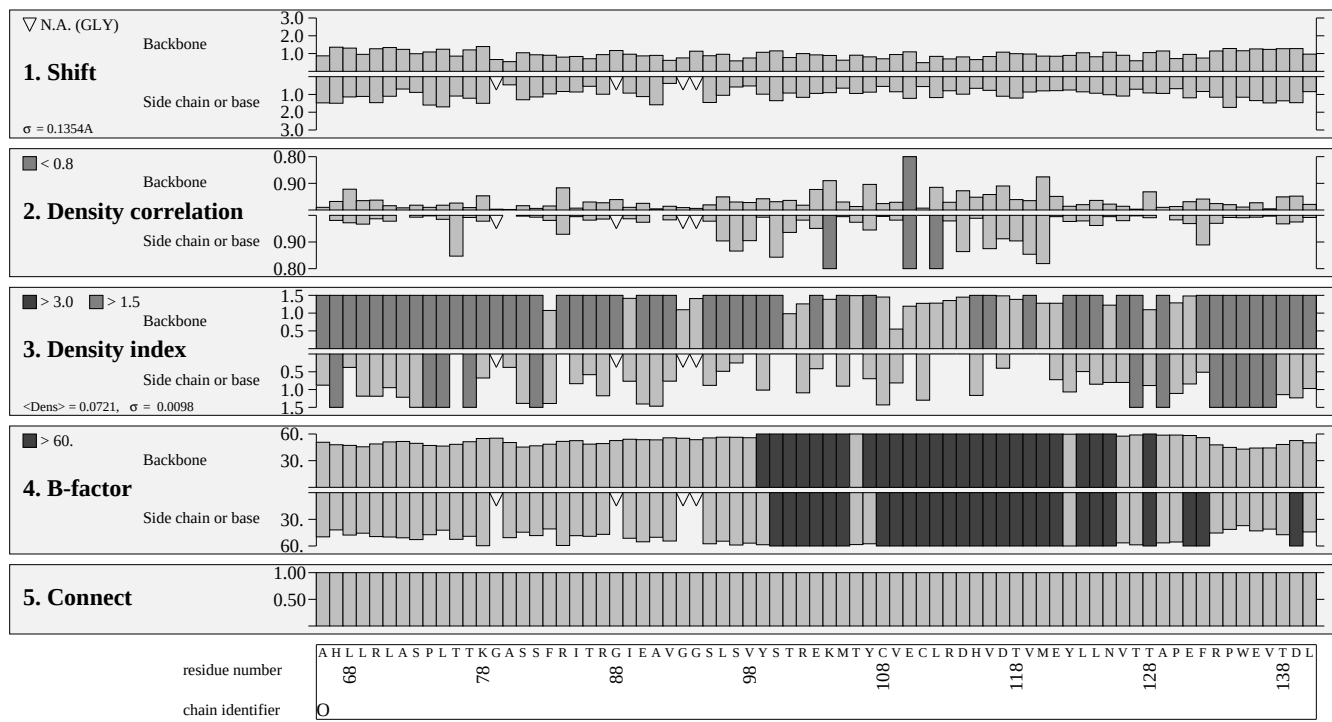
Local estimation (17)



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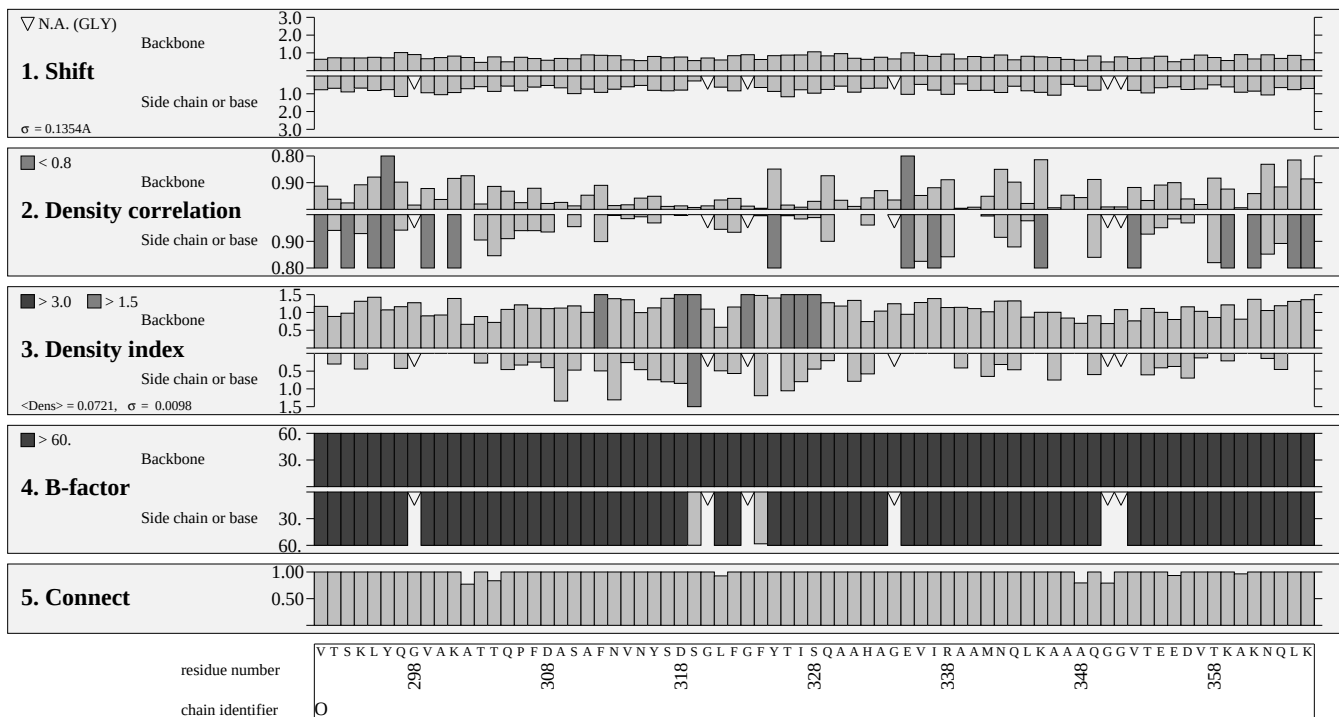
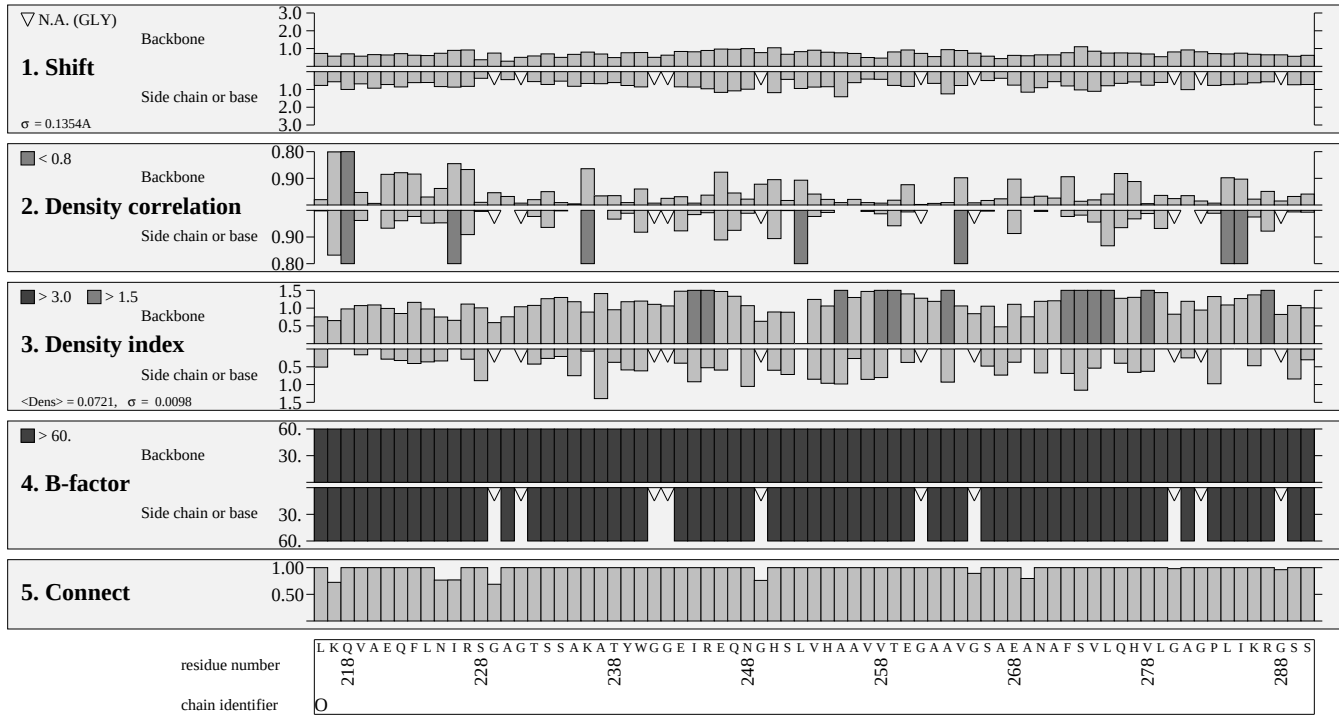
Local estimation (18)



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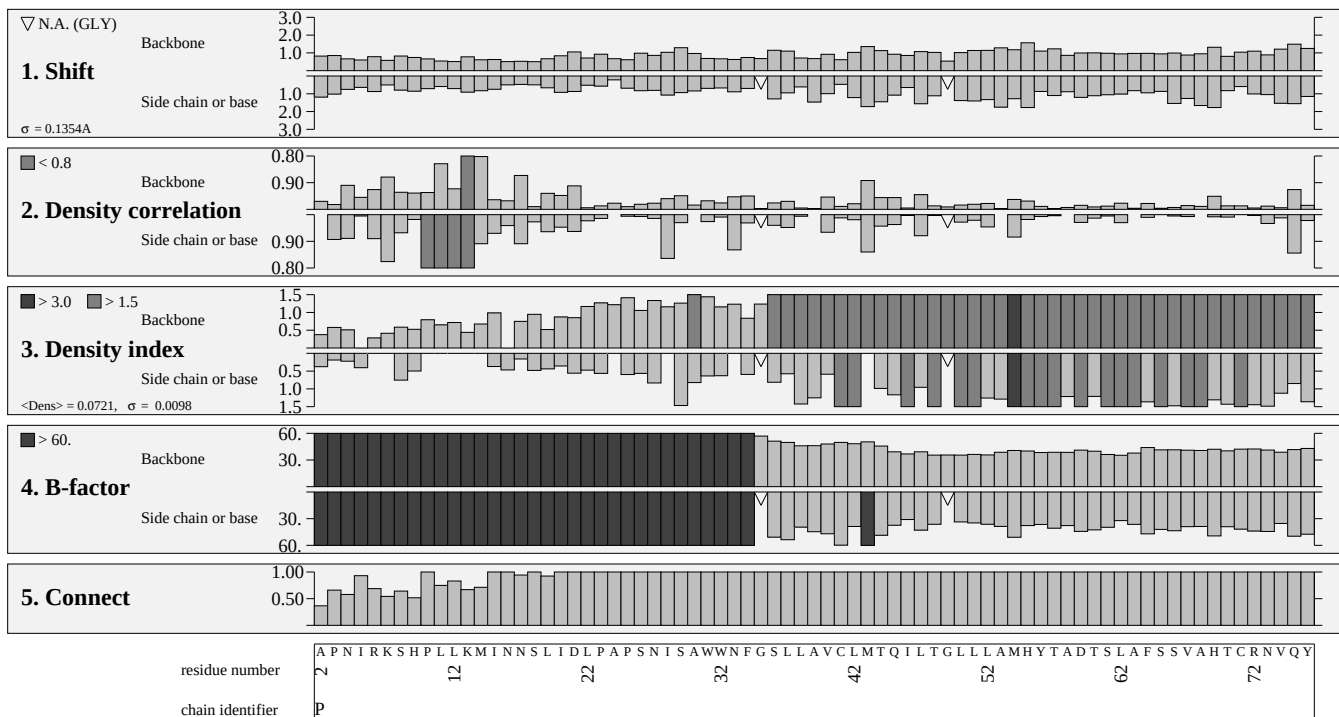
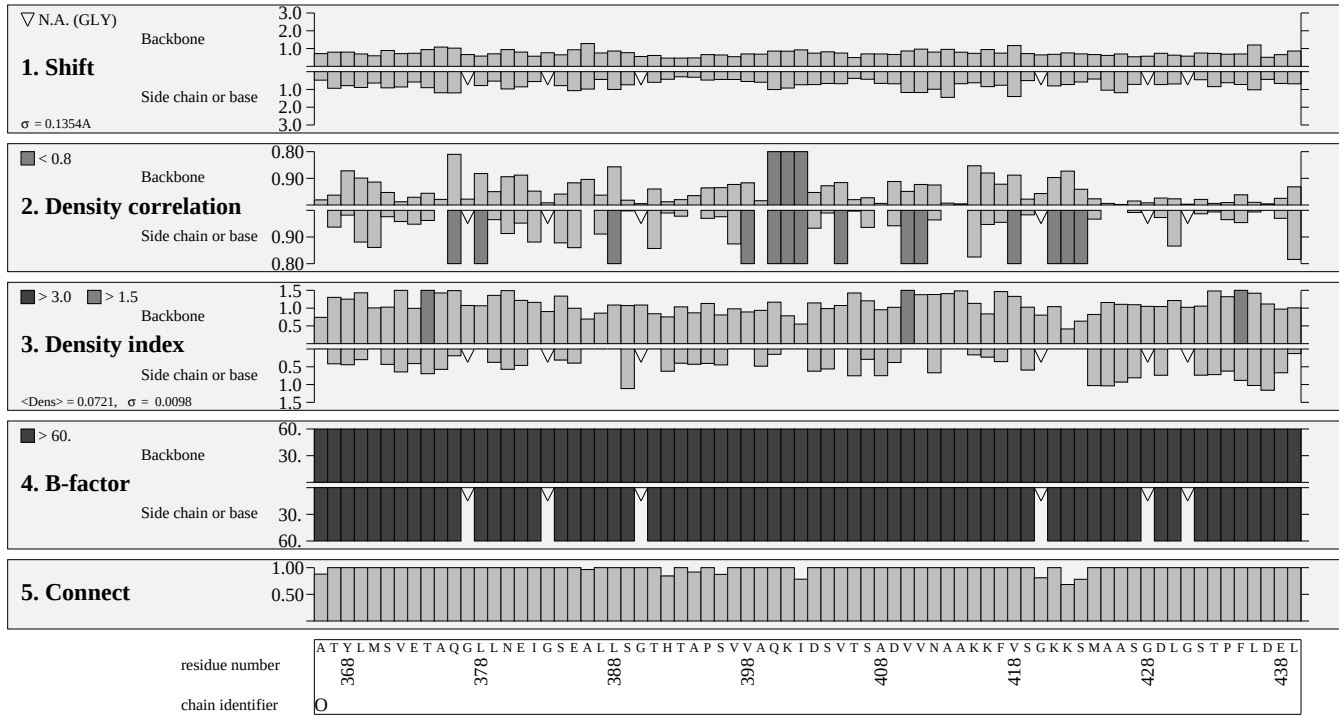
Local estimation (19)



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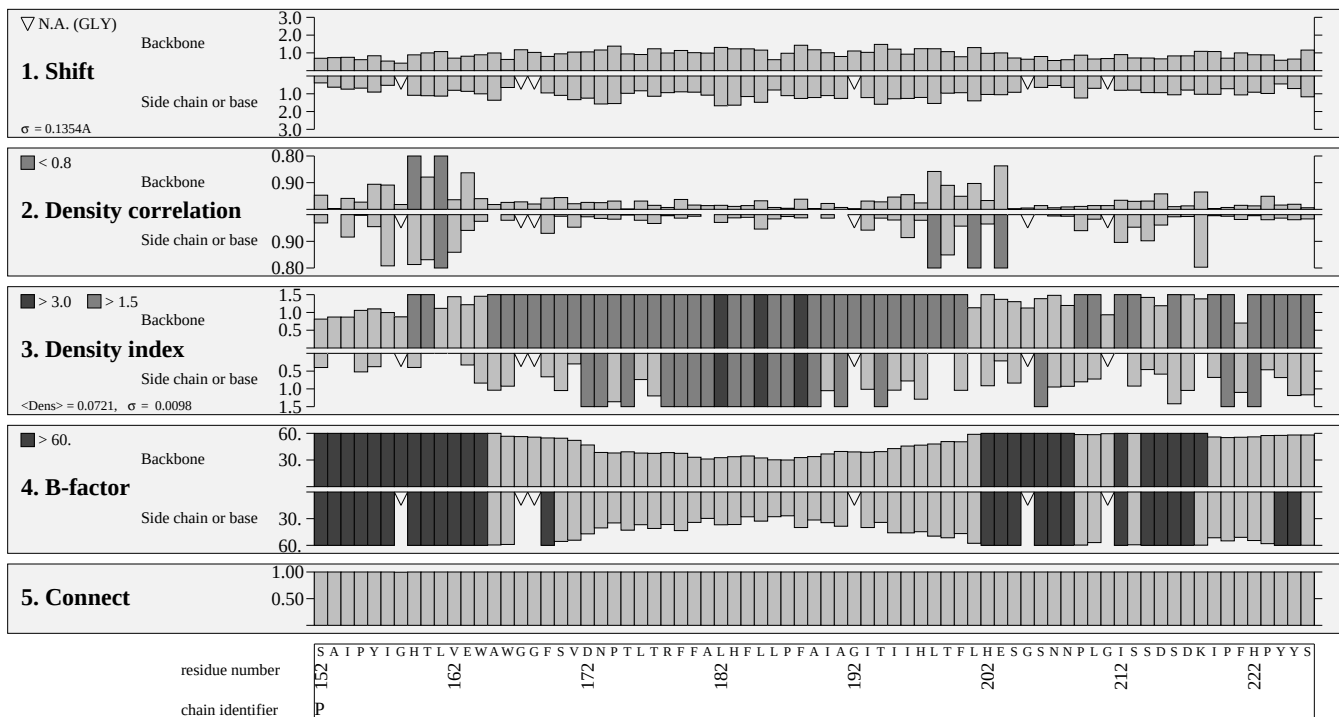
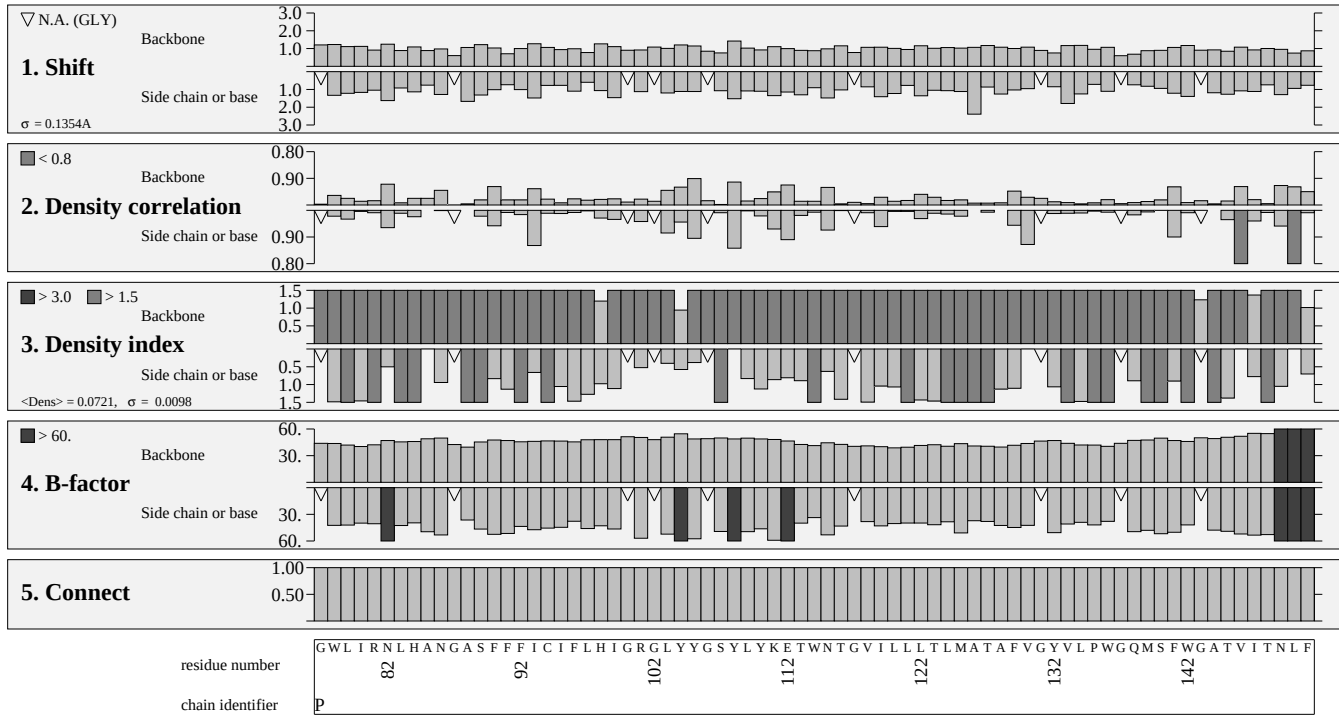
Local estimation (20)



Structure Factor Check

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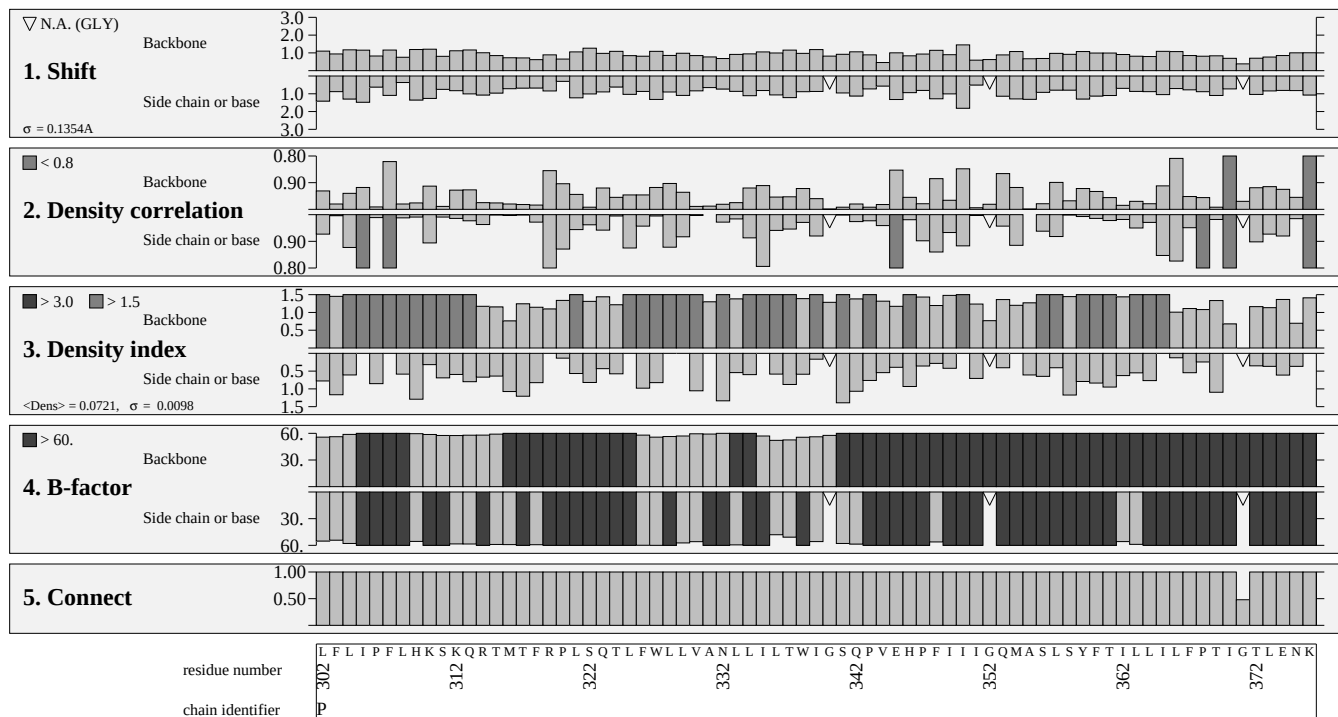
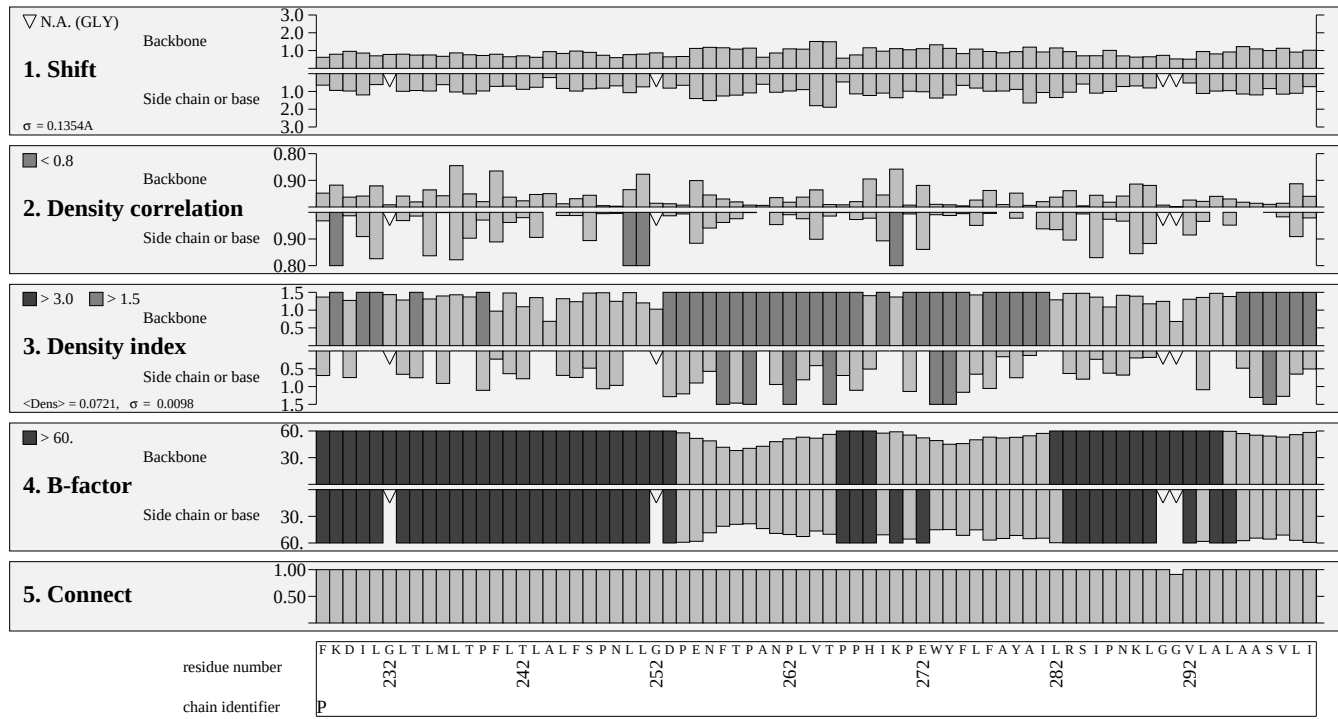
Local estimation (21)



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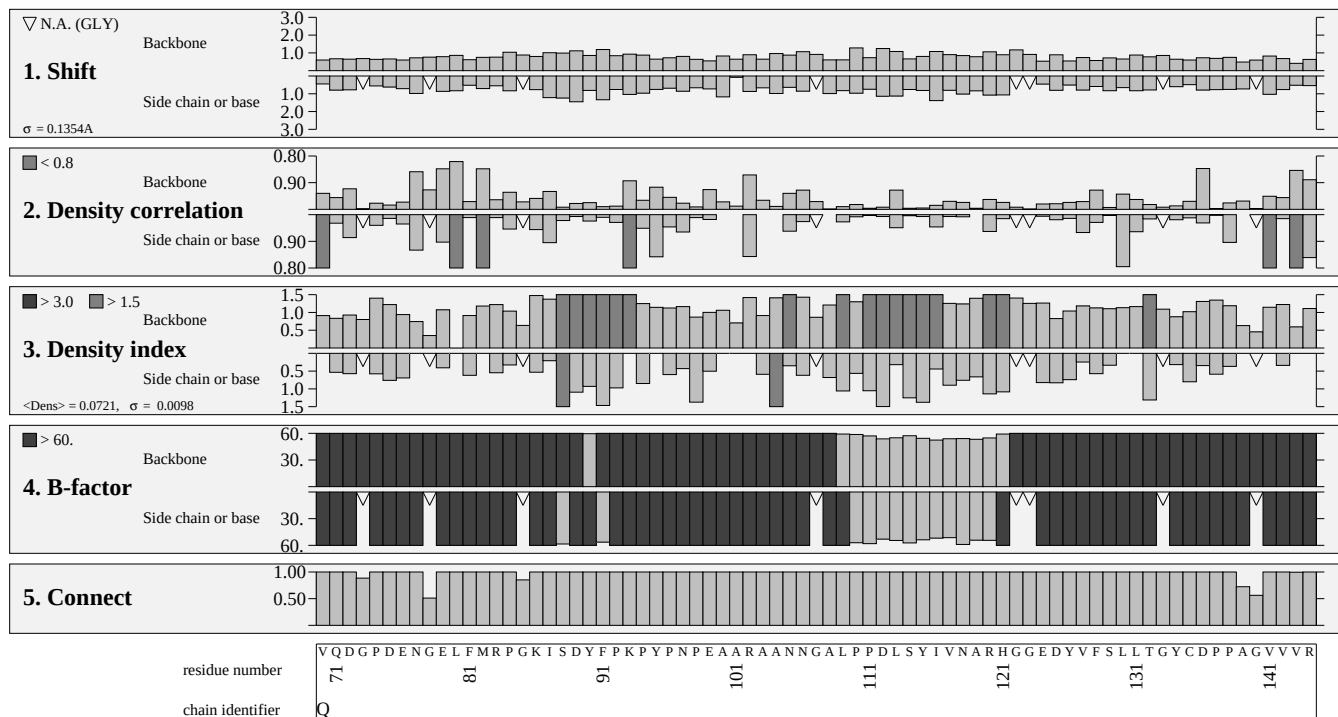
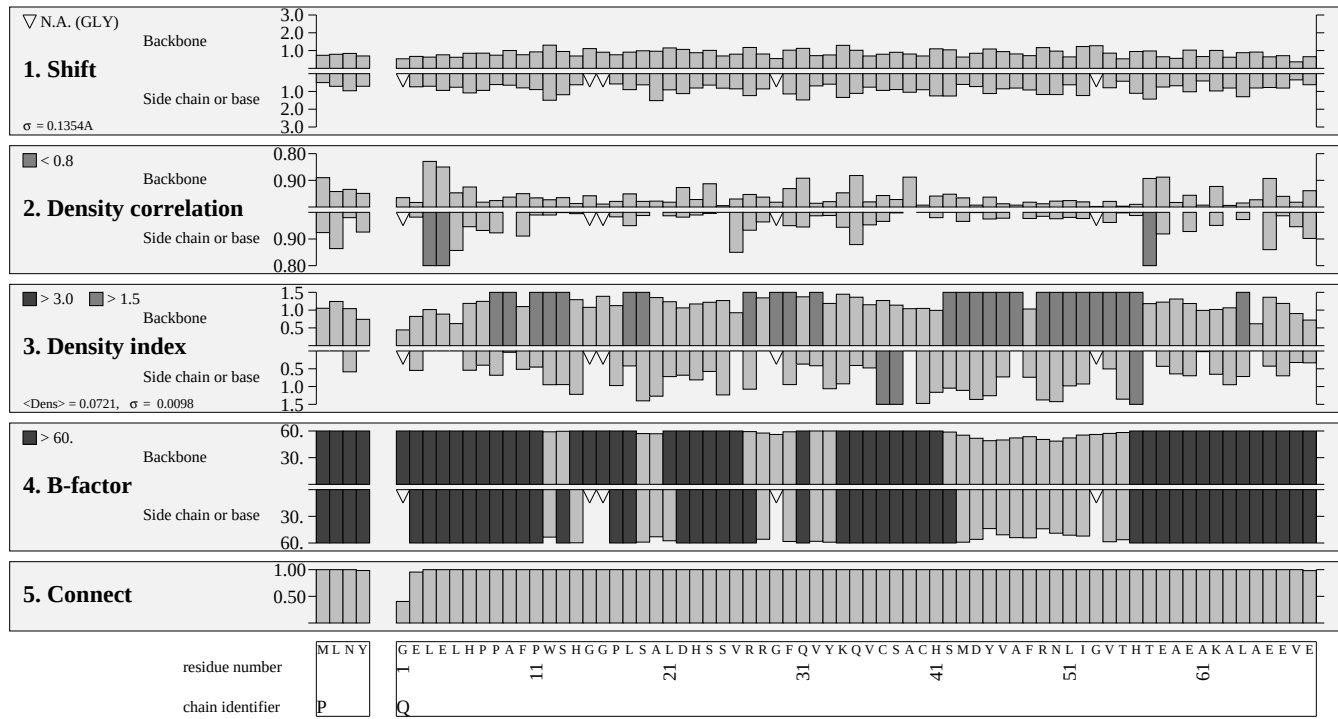
Local estimation (22)



Structure Factor Check

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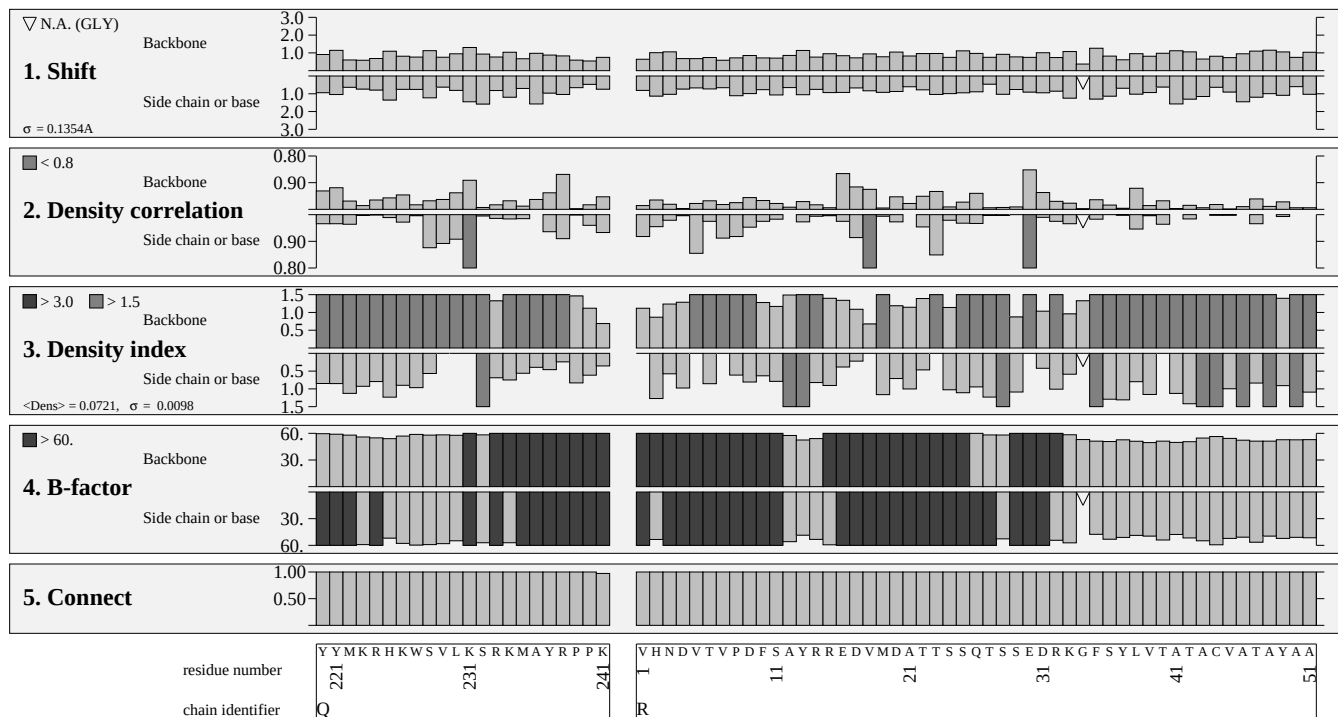
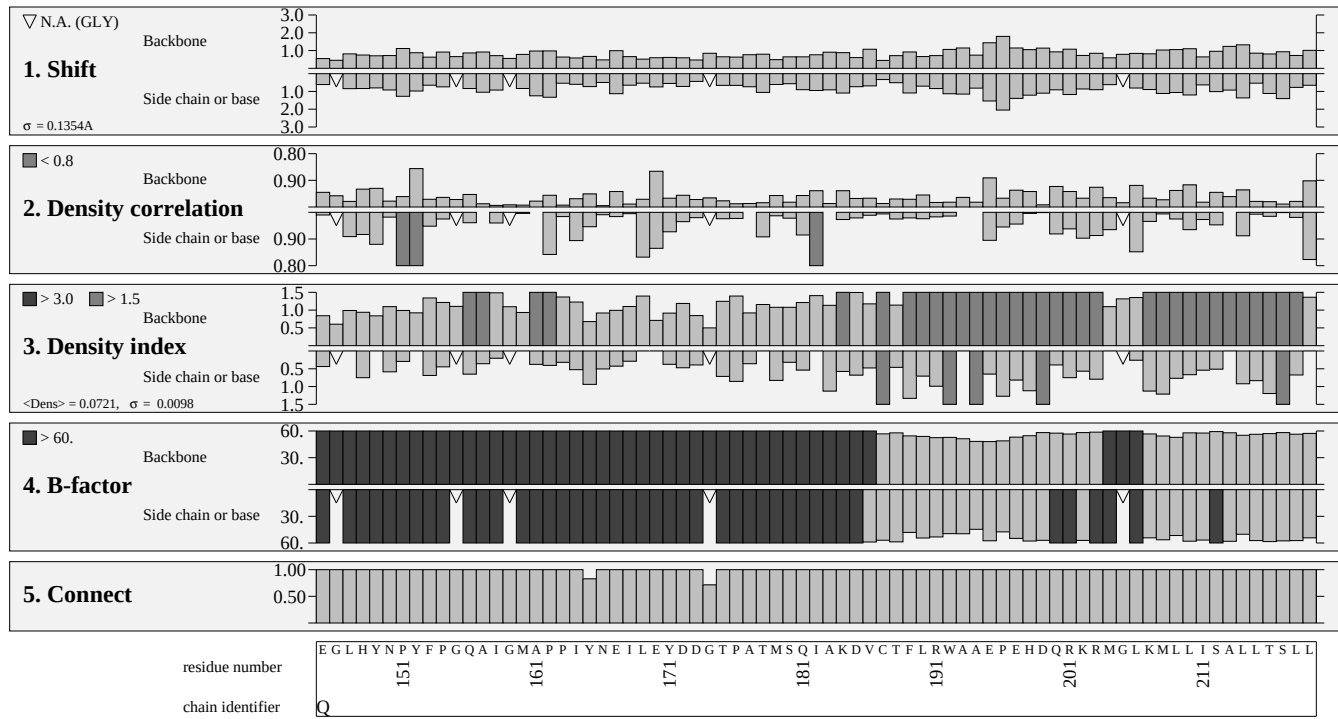
Local estimation (23)



Structure Factor Check

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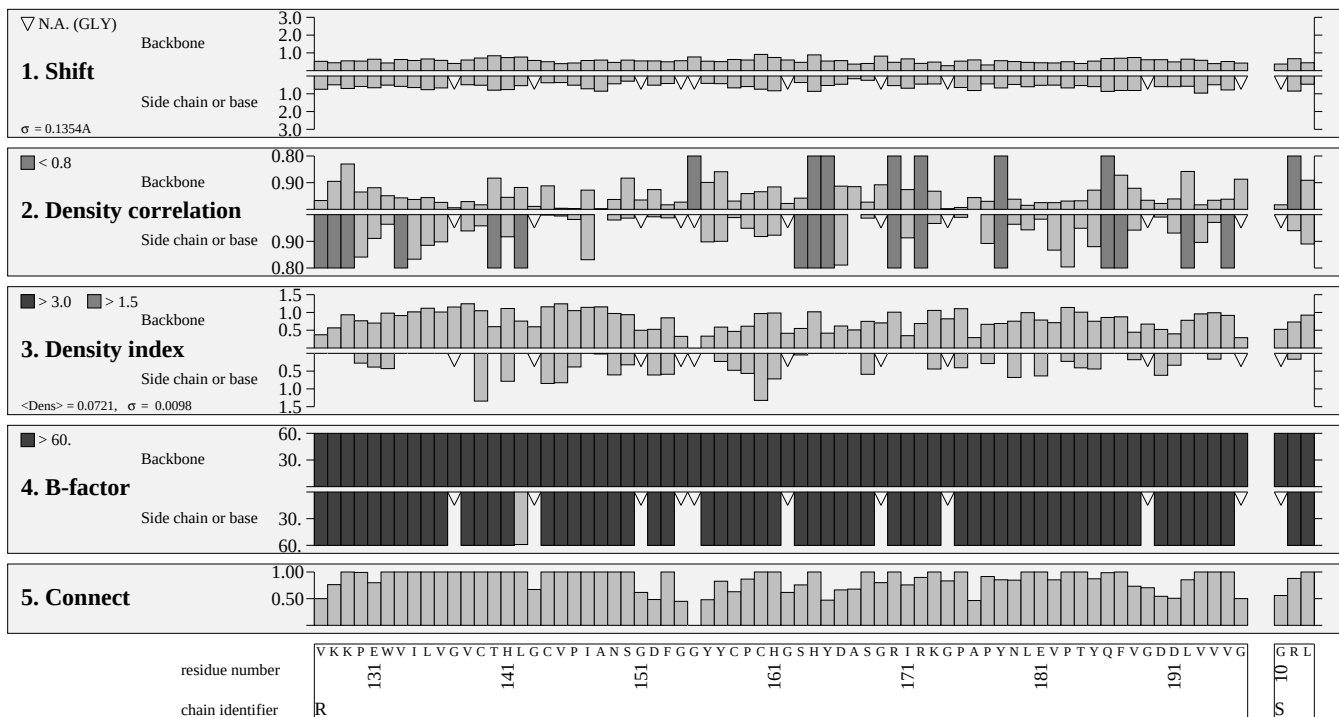
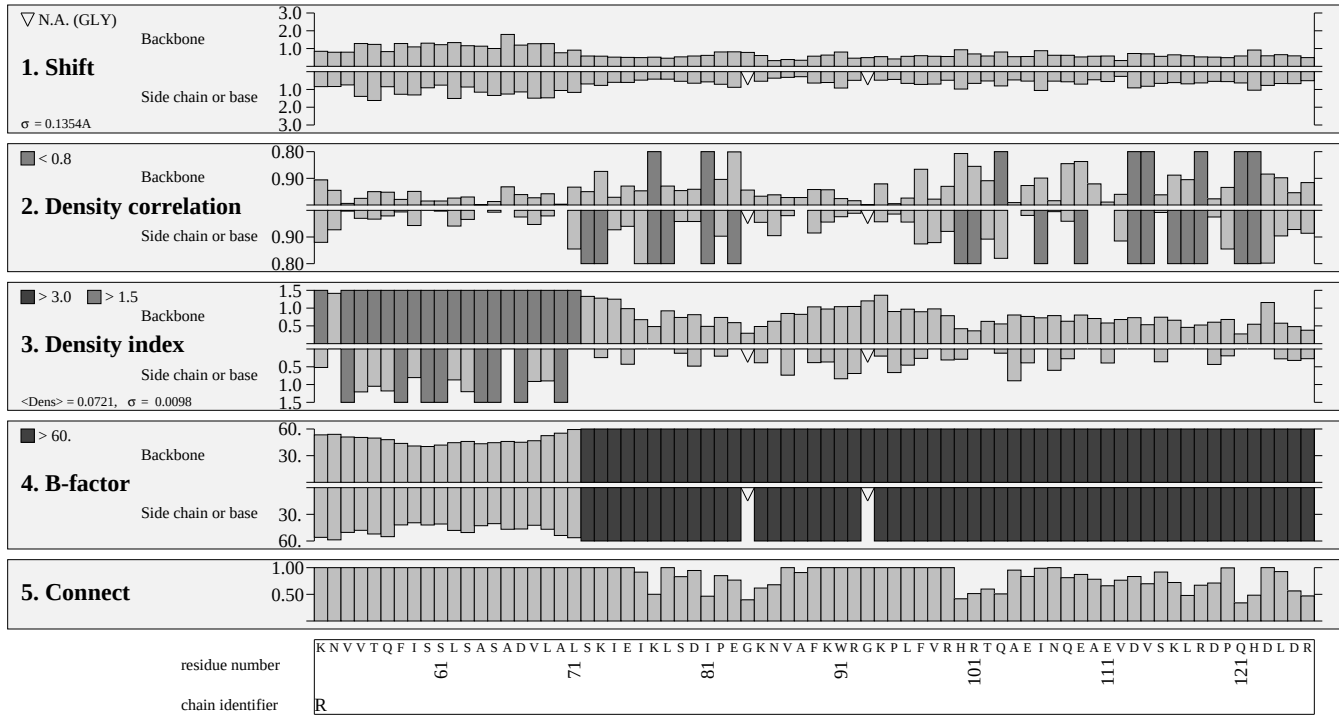
Local estimation (24)



Structure Factor Check

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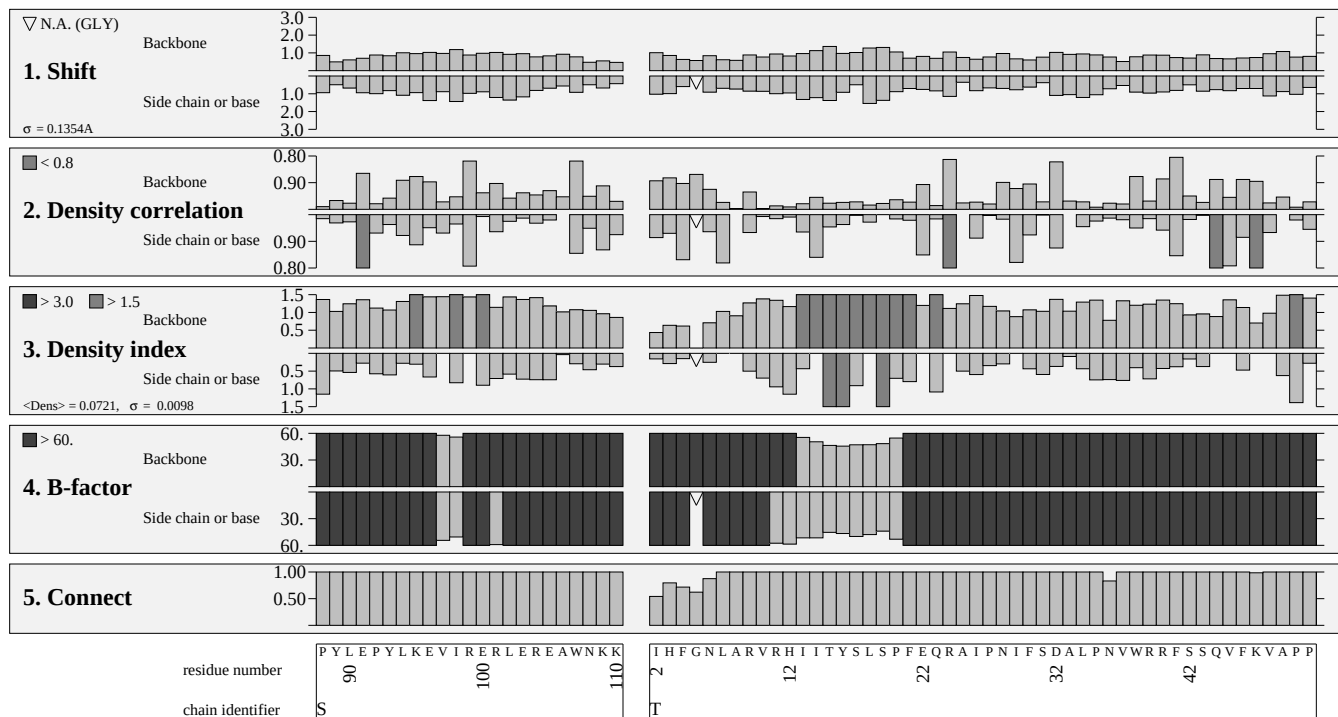
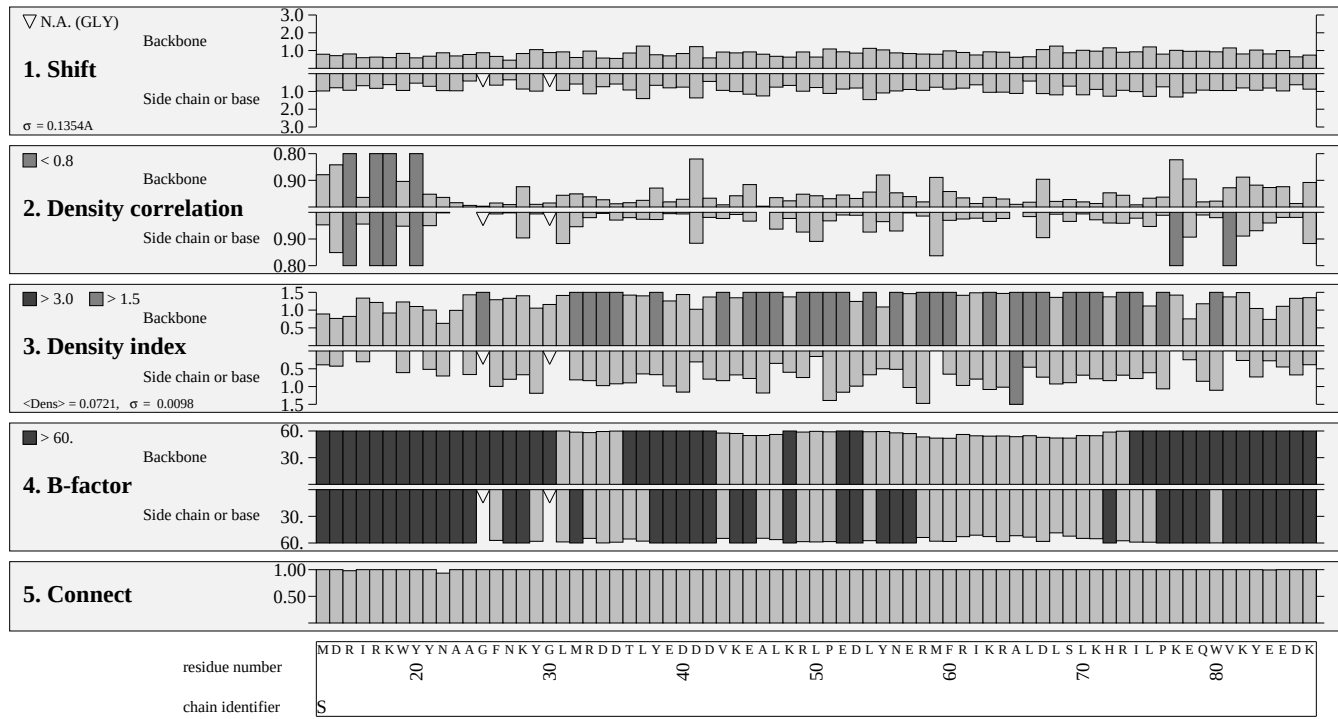
Local estimation (25)



Structure Factor Check

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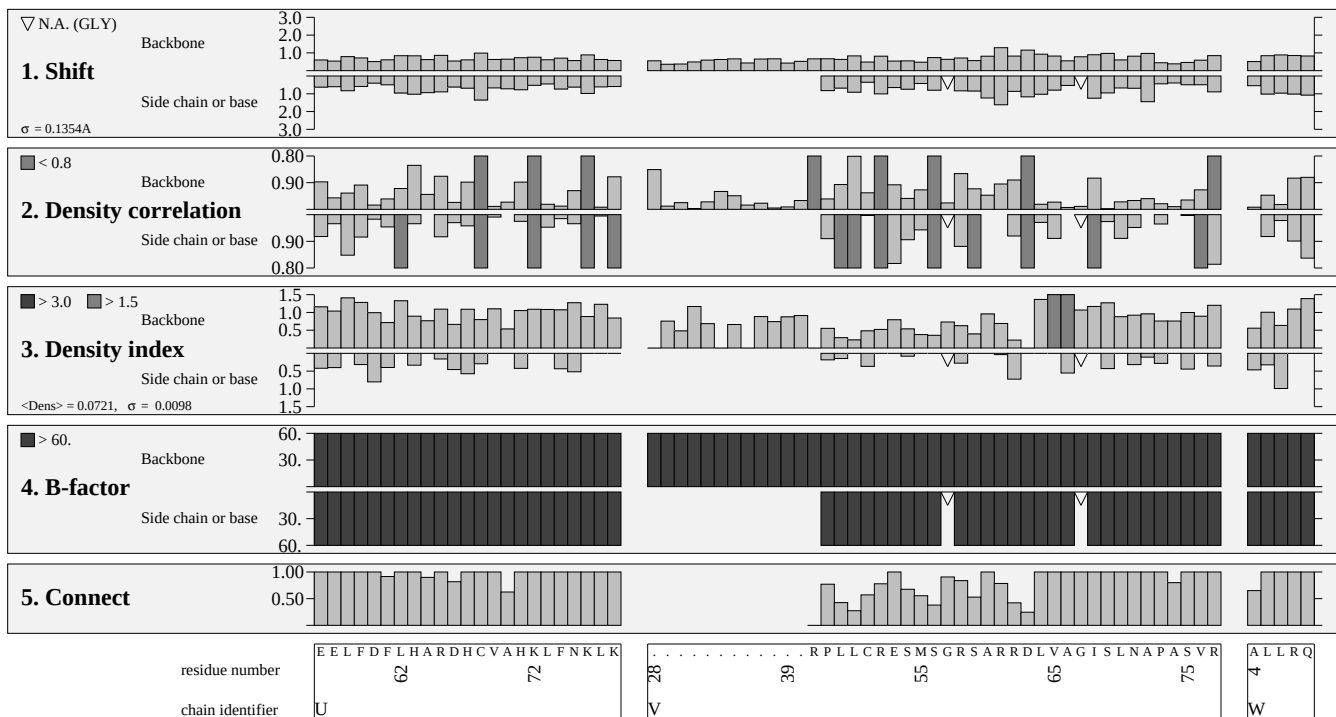
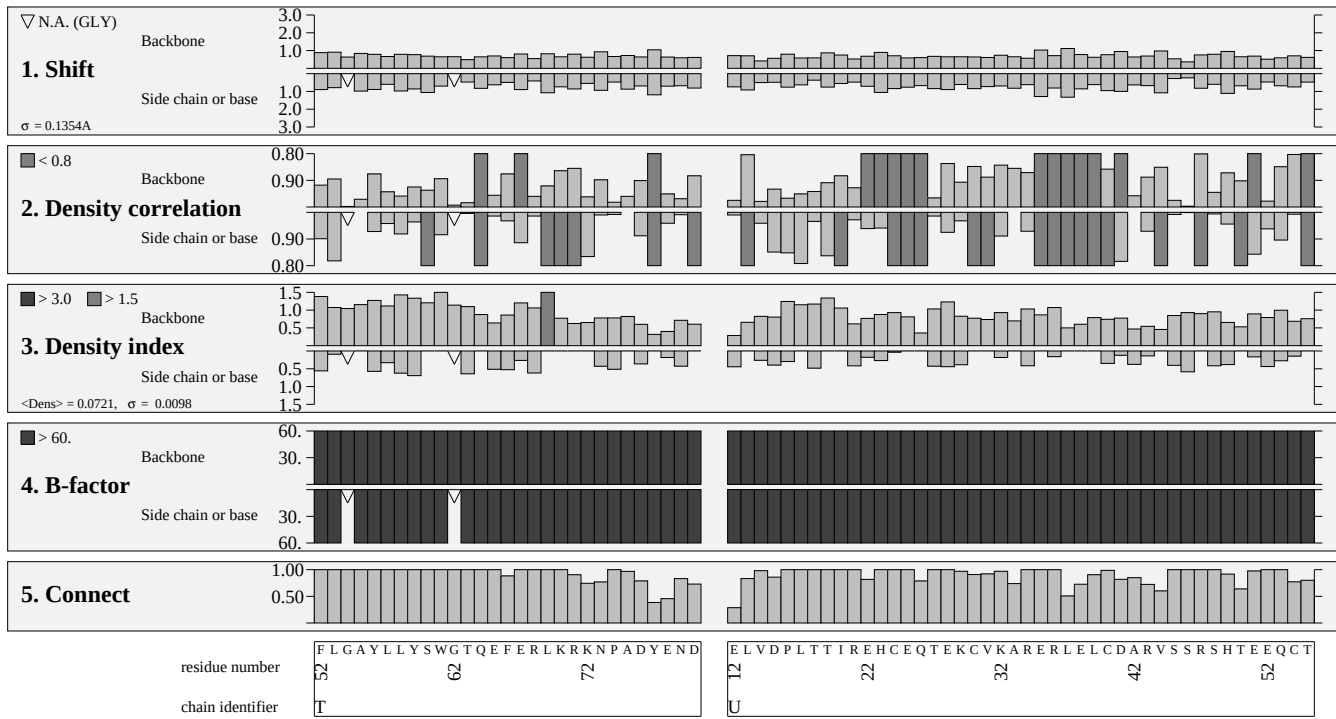
Local estimation (26)



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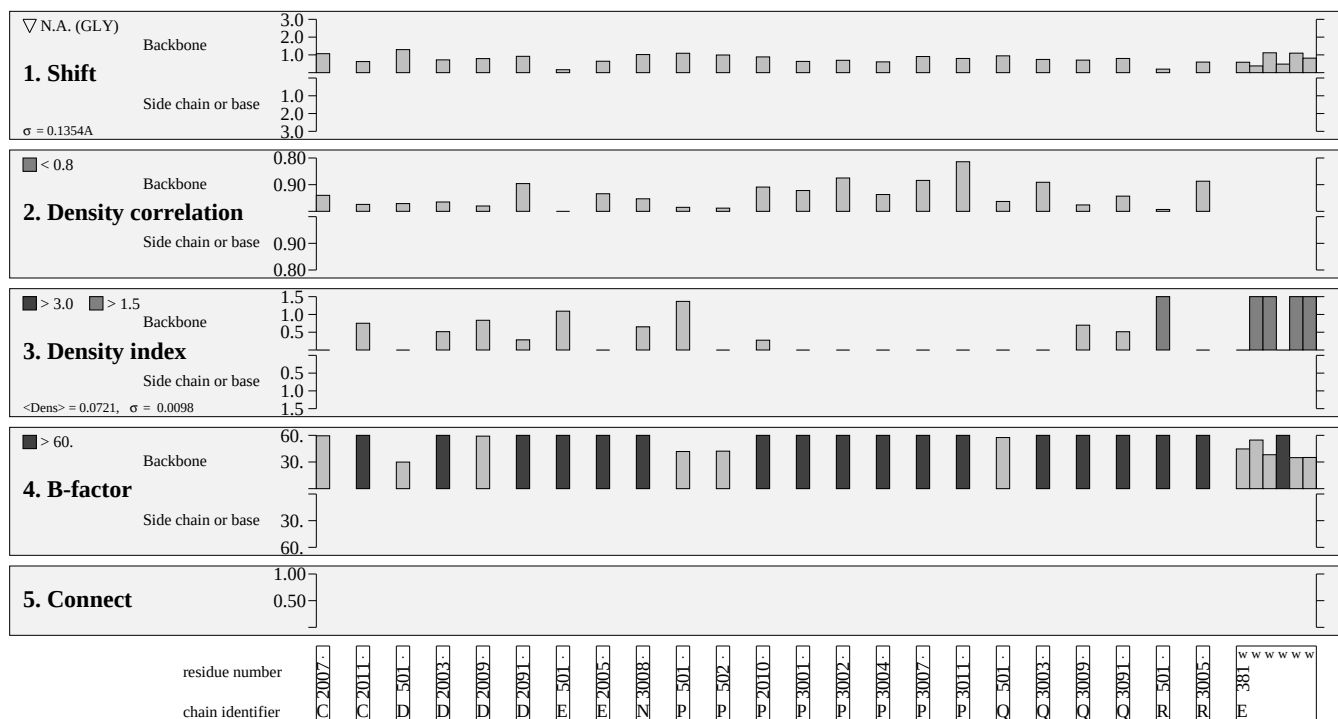
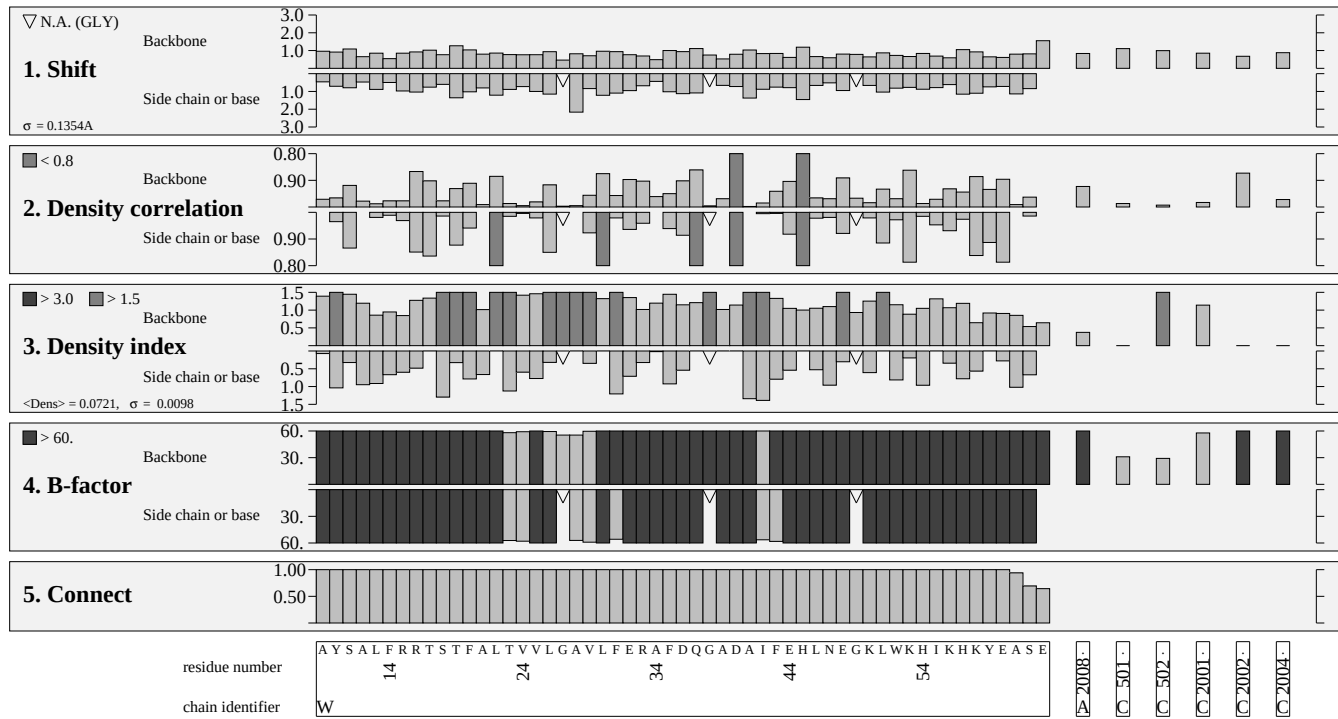
Local estimation (27)



Structure Factor Check

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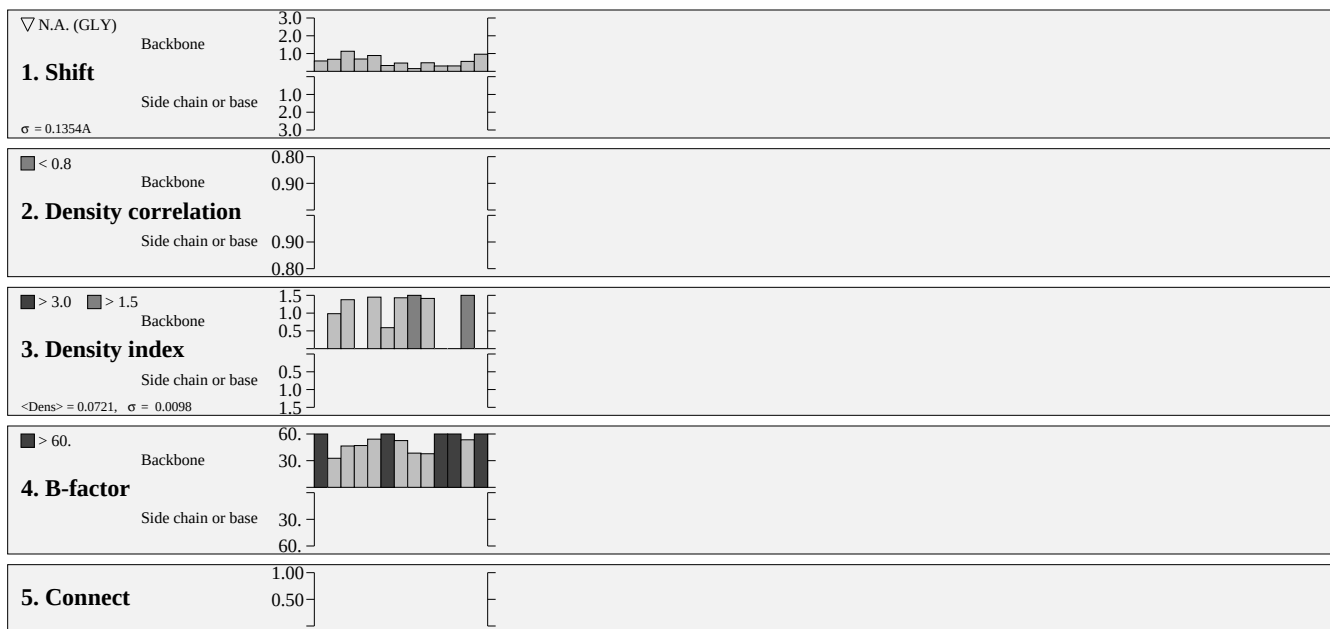
Local estimation (28)



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Local estimation (29)



residue number

chain identifier

382
E