

Structure Factor Check

3L71

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH AZOXYSTROBIN BOUND
 Date: 27-DEC-09
 PDB code: 3L71

Crystal

Cell parameters:

a: 170.15 A b: 181.31 A c: 240.50 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 144.8 – 2.80 A
 Reflections in file: 170949
 Unique reflections above 0: 170949
 above 1 σ : 167603
 above 3 σ : 112140

SFCHECK

Nominal resolution range: 144.8 – 2.84 A
\05max. from input data, min. from author\05
 Used reflections: 165523
 Reflections out of resolution: 5426
 Completeness: 94.5 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.062
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.4725 0.4425
 B_{overall} (by Patterson): 49. A²
 Optical resolution: 2.13 A
 Expected opt. resol. for complete data set: 2.13 A
 Estimated minimal error: 0.067 A

Model

32655 atoms (19 water molecules)

Number of chains: 51
 Volume not occupied by model: 62.0 %
 $\langle B \rangle$ (for atomic model): 73.6 A²
 $\sigma(B)$: 18.83 A²
 Matthews coefficient: 4.06
 Corresponding solvent % : 69.45

Model vs. Structure Factors

R-factor for all reflections: 0.298
 Correlation factor: 0.865
 R-factor: 0.302
 for $F > 2.0\sigma$
 nom. resolution range: 24.94 – 2.84A
 reflections used: 162126

Rfree: 0.331
 Nfree: 3168
 R-factor without free-refl.: 0.301
 Non free-reflections: 158958
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.459 A
 Estimated maximal error: 0.353 A
 DPI: 0.350 A

Scaling

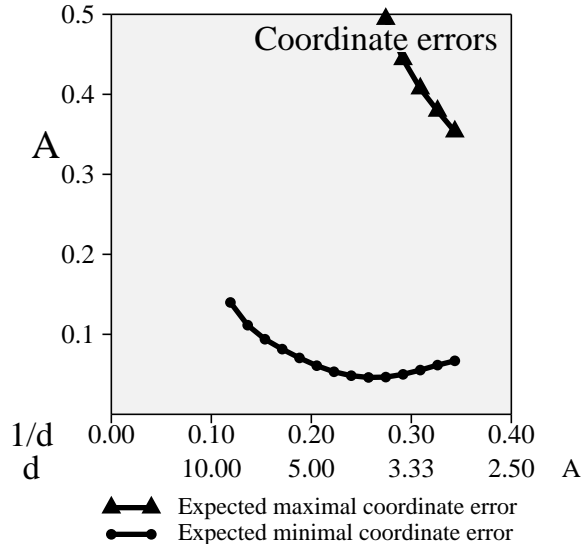
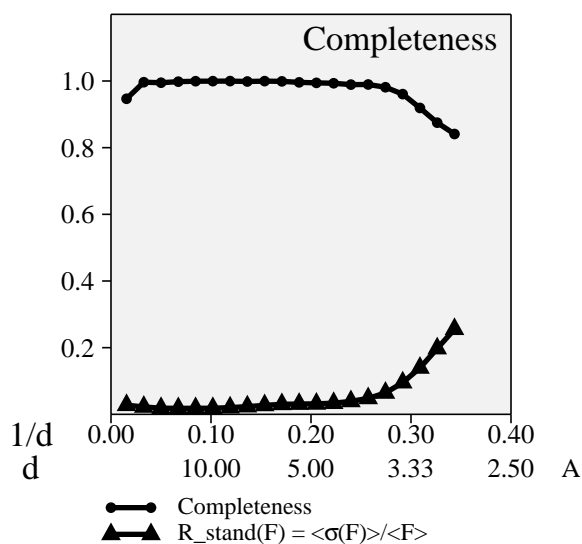
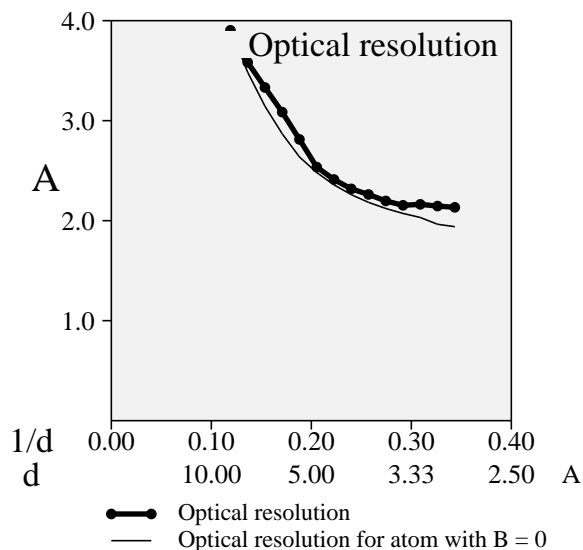
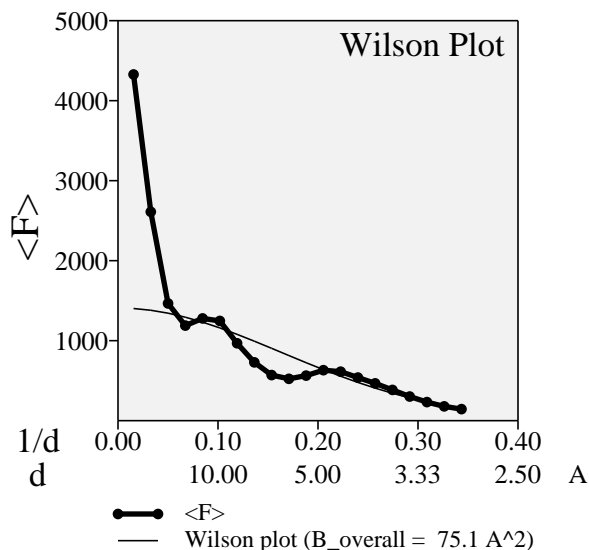
Scale: 0.476
 Bdiff: -9.70
 Anisothermal Scaling (Beta):
 10.9332 -1.7388 -2.6989 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.750 250.127

Refinement

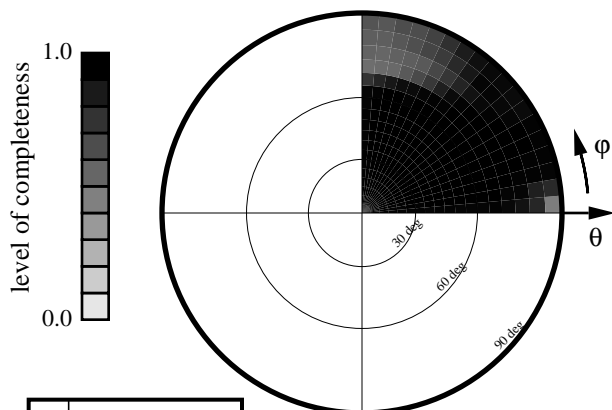
Program: CNS 1.1
 Nominal resolution range: 24.9 – 2.84 A
 Reported nominal resolution: 2.00 A
 Reported R-factor: 0.247
 Number of reflections used: 165215
 Reported Rfree: 0.28
 Sigma cut-off: N.A.

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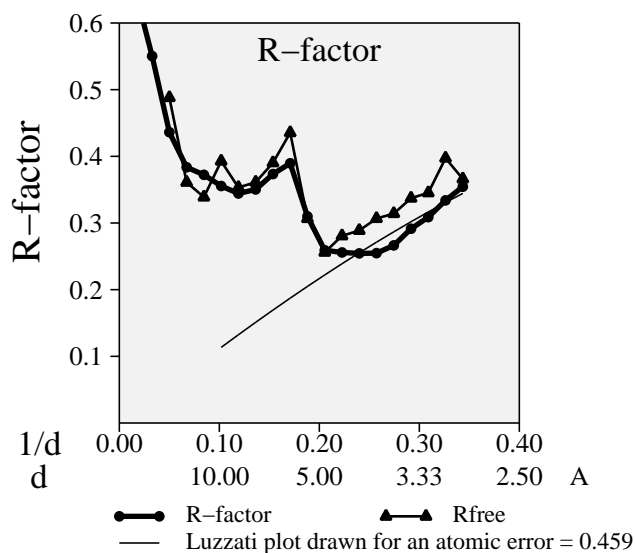


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

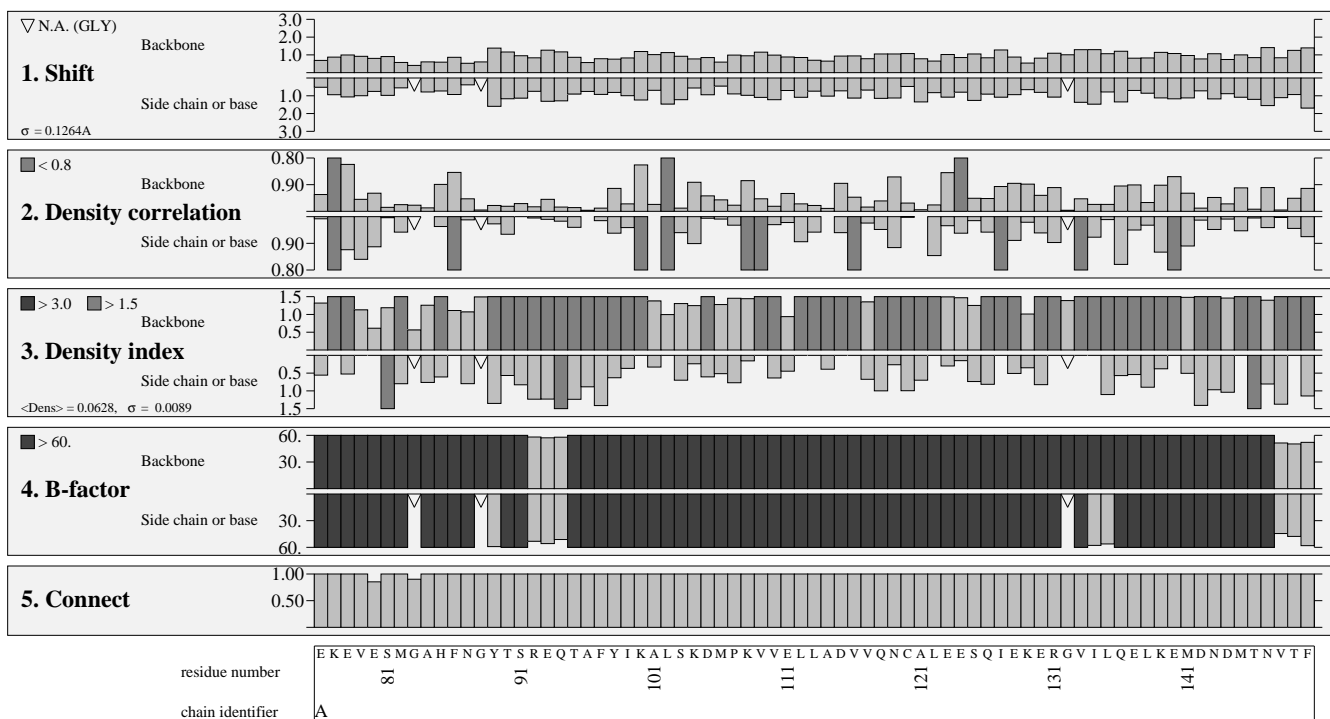
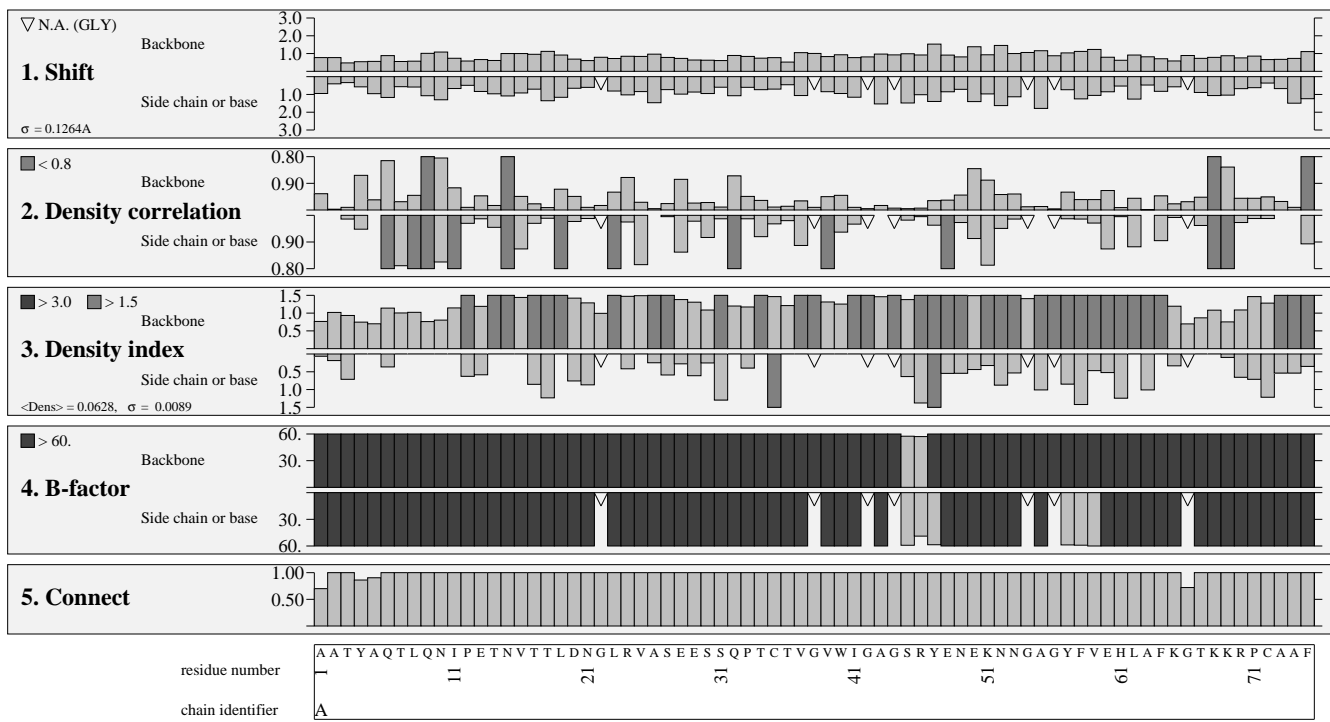
polar coordinates of the crystallographical axes



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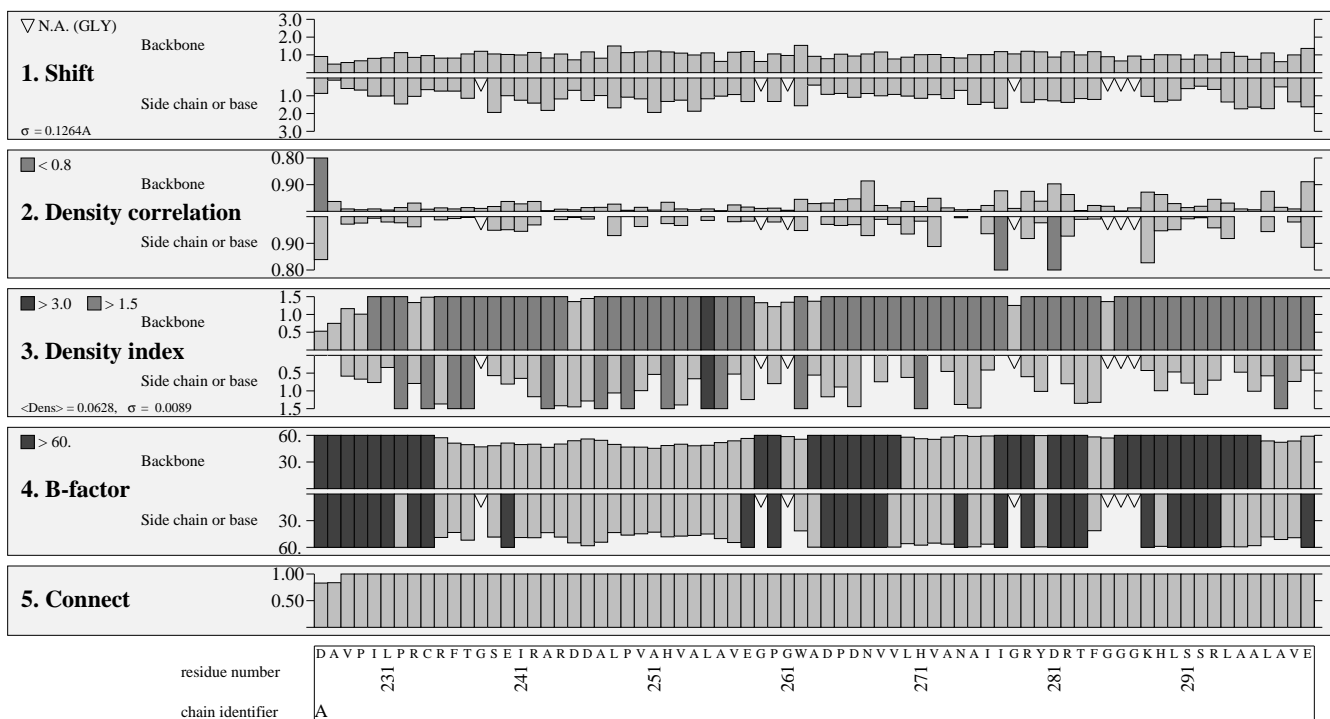
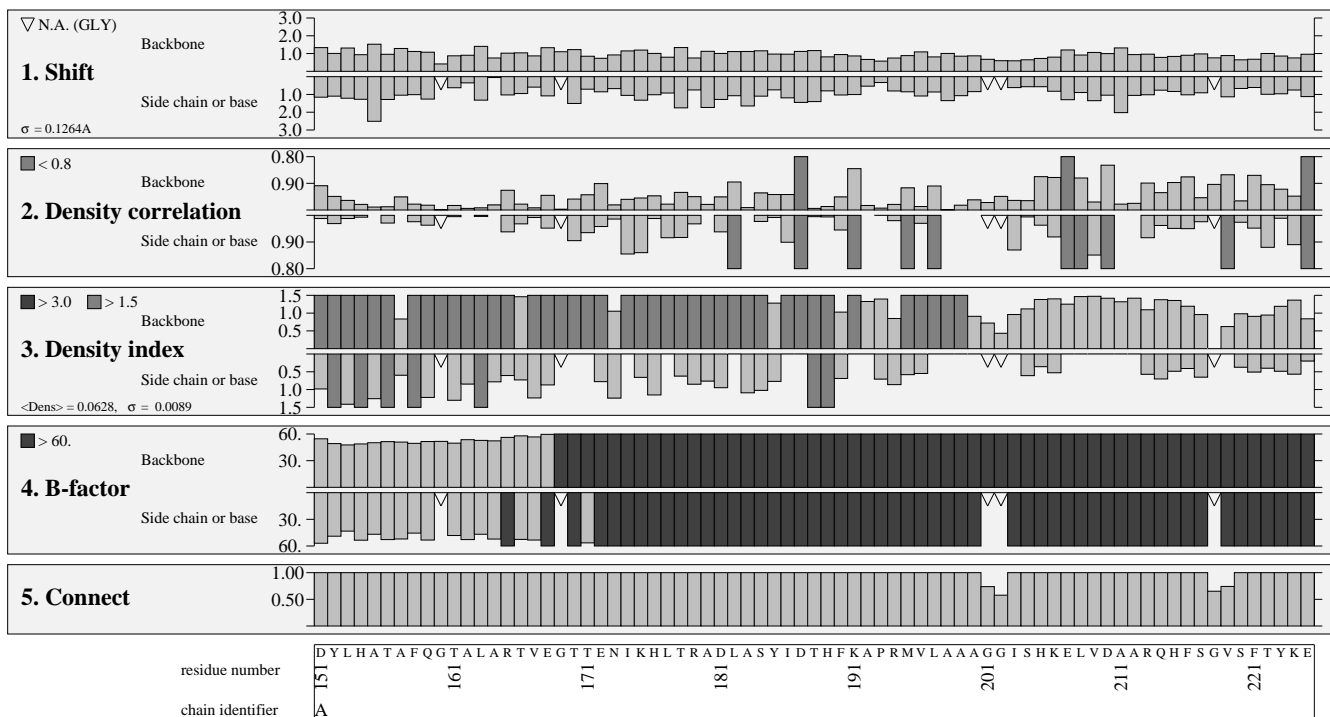
Local estimation



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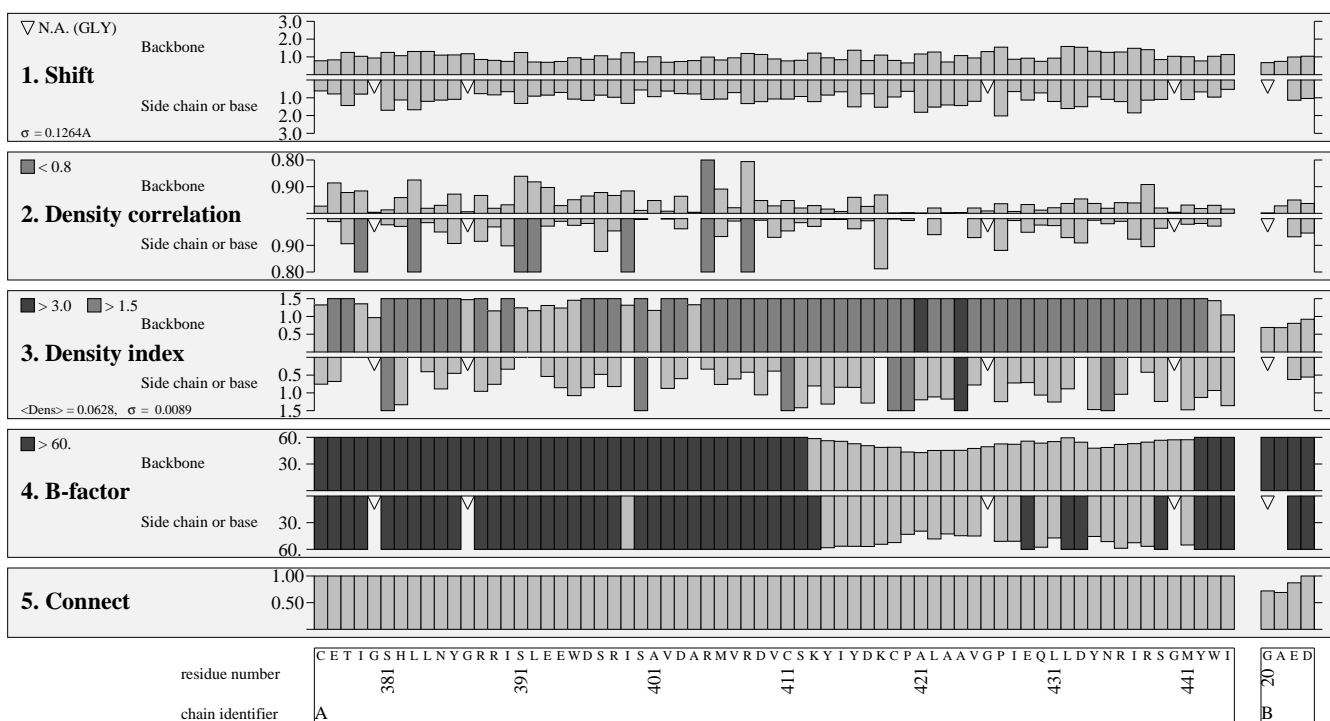
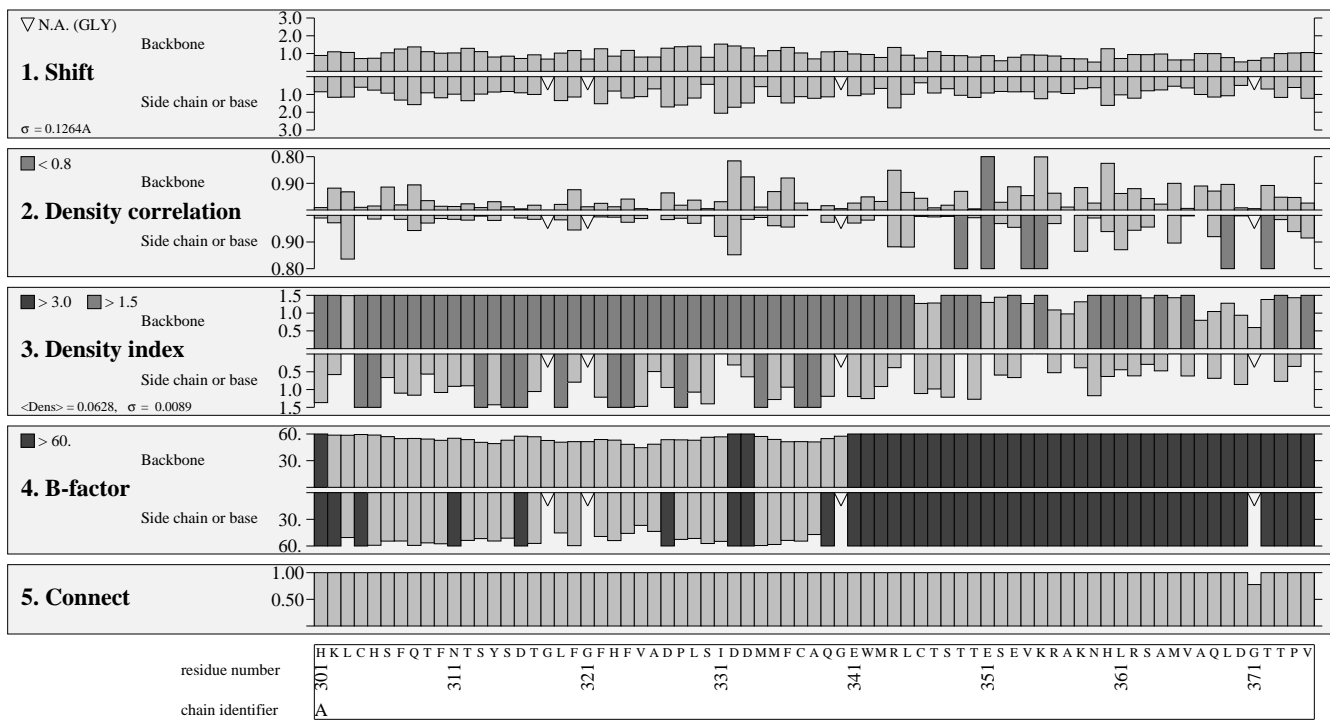
Local estimation (2)



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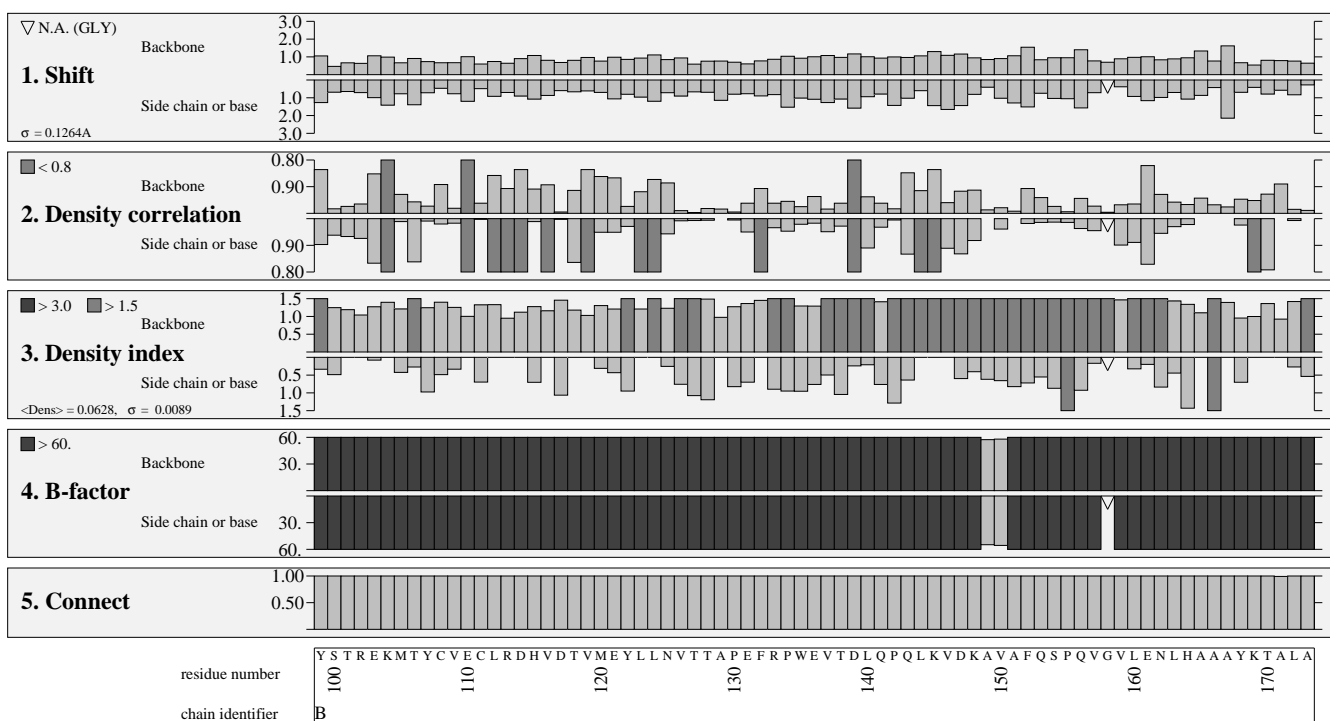
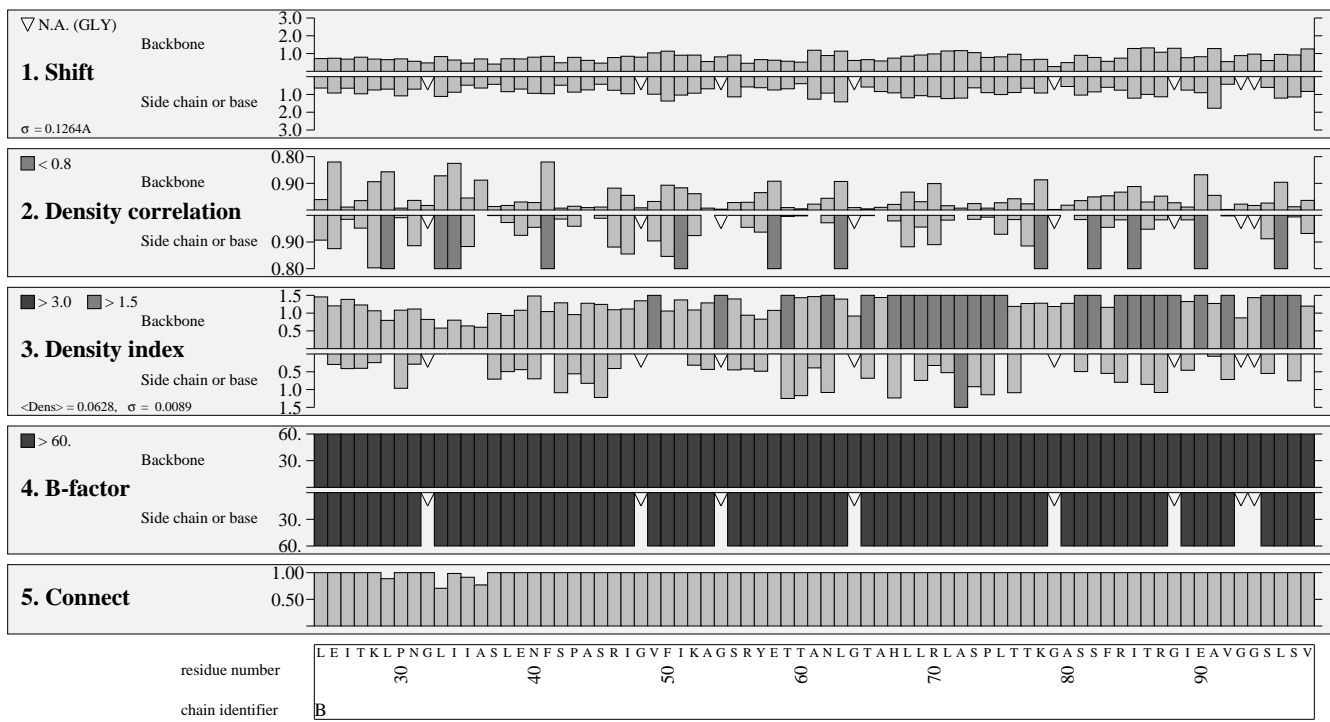
Local estimation (3)



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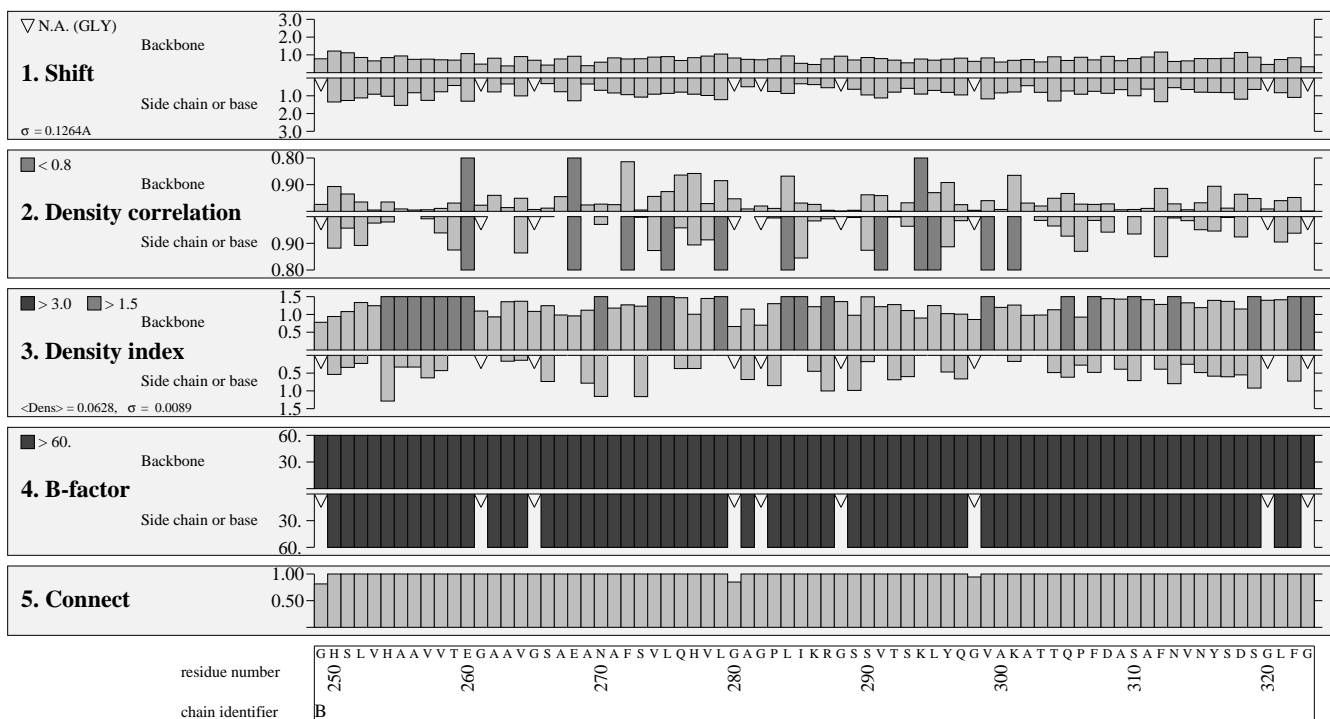
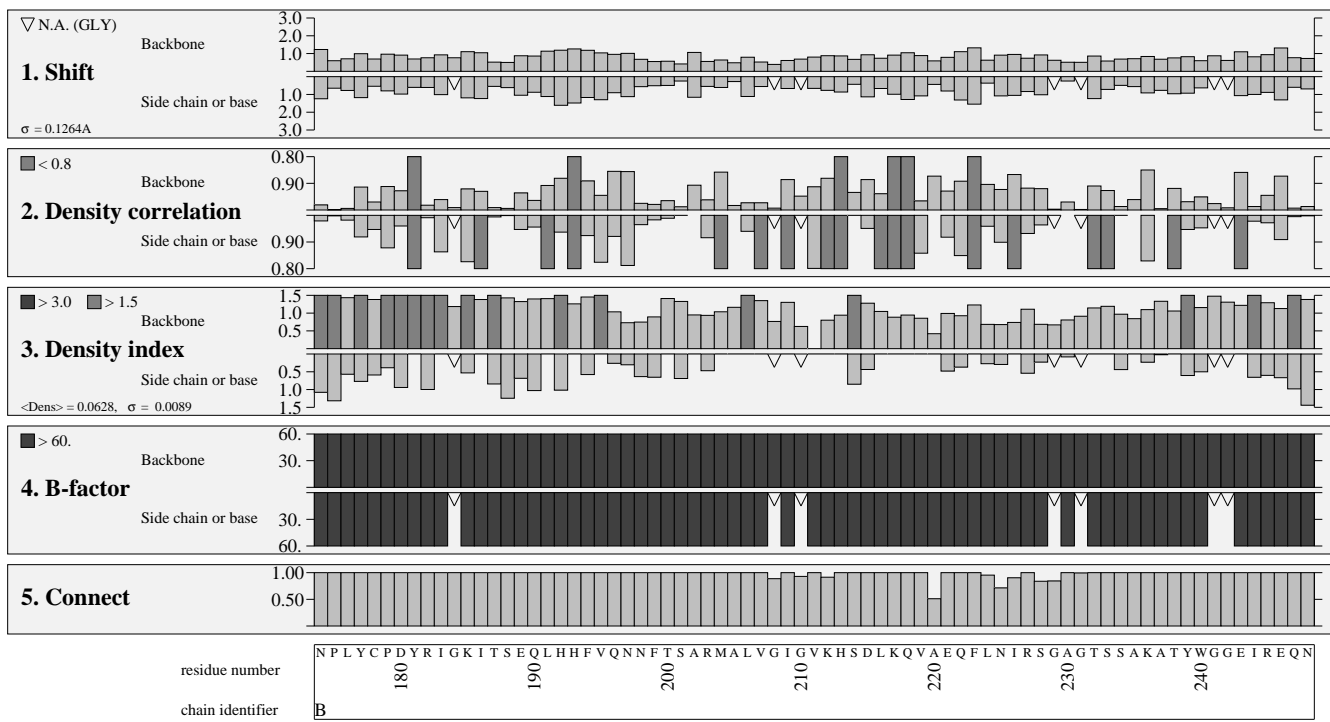
Local estimation (4)



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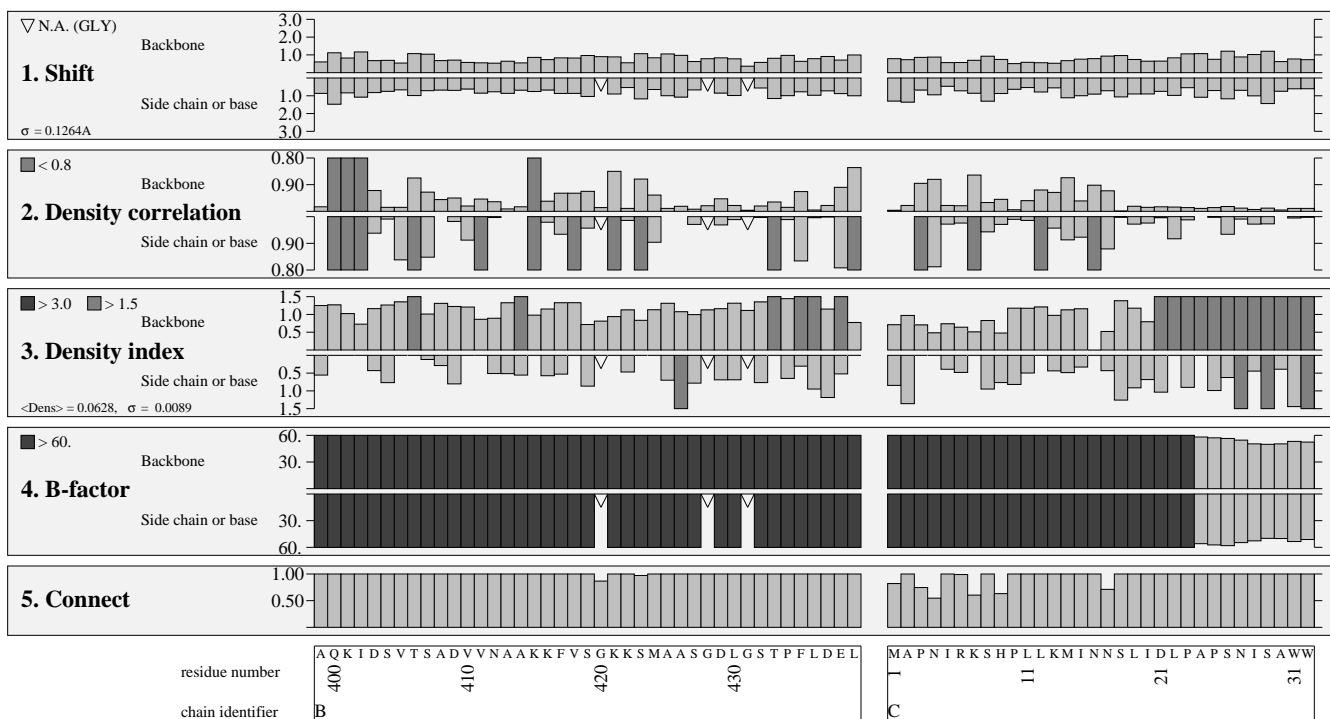
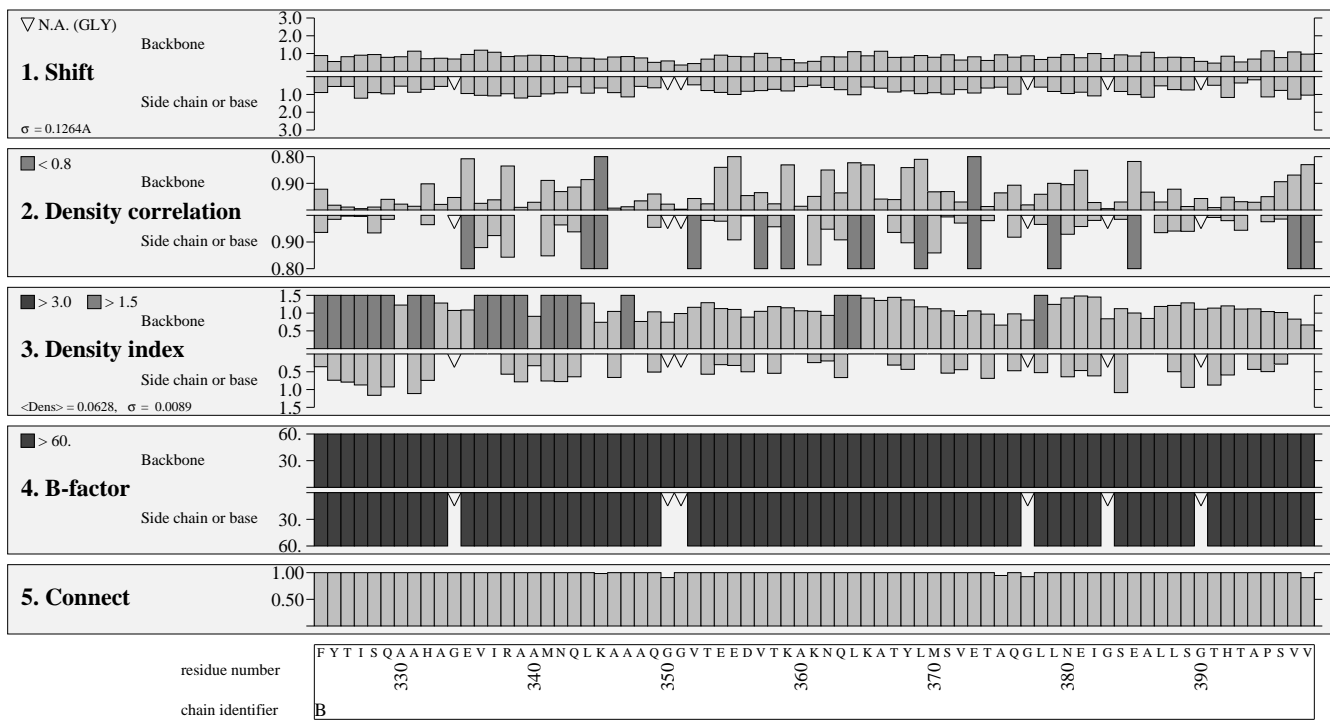
Local estimation (5)



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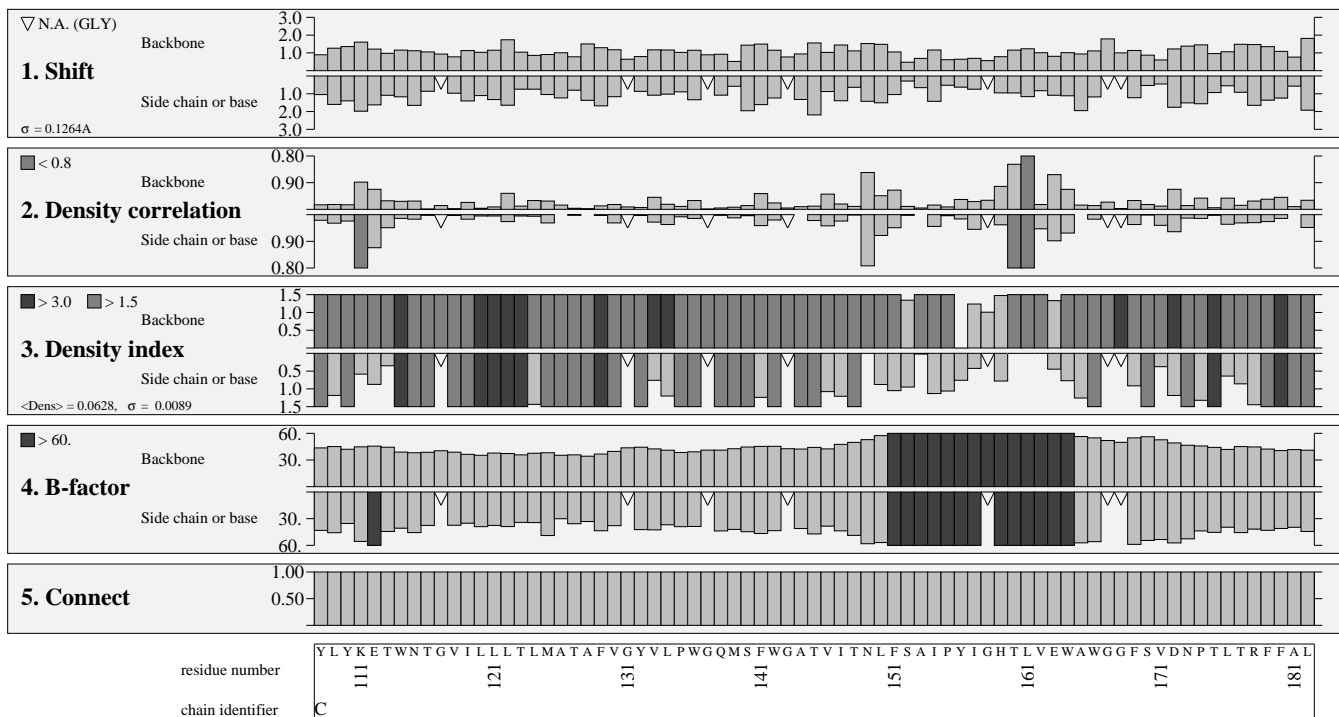
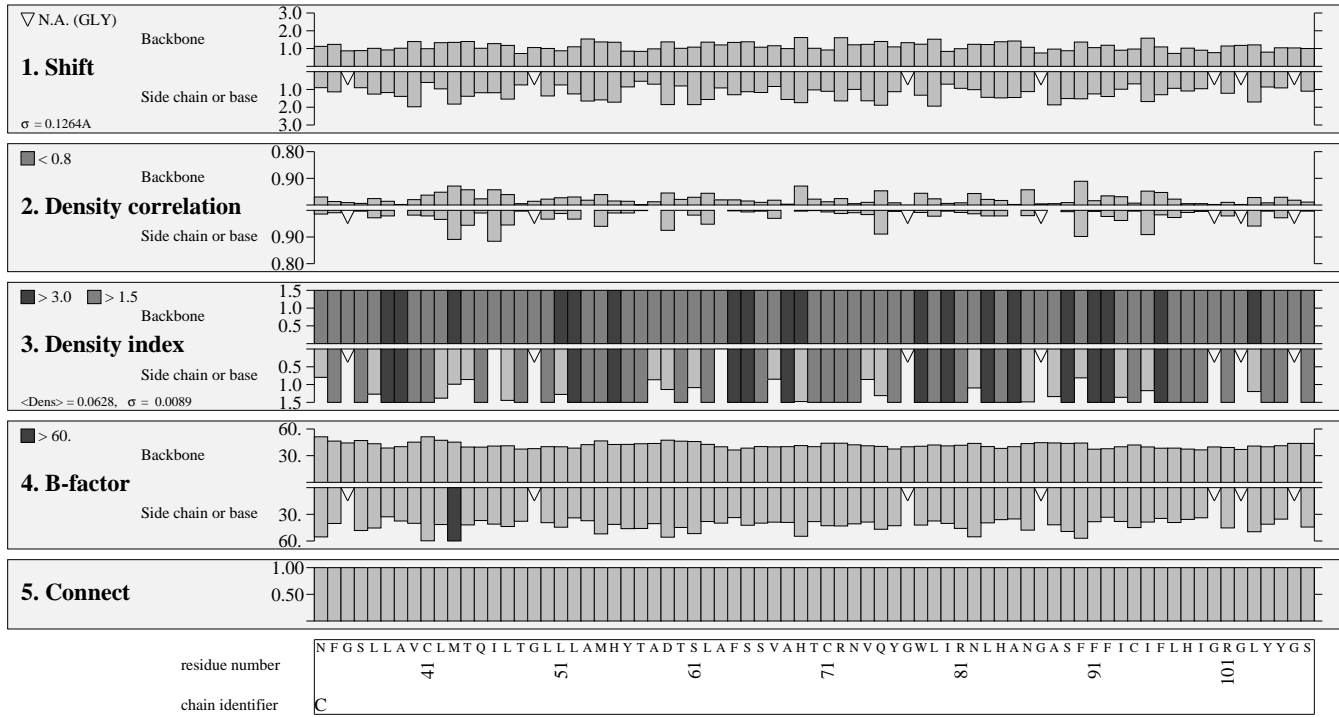
Local estimation (6)



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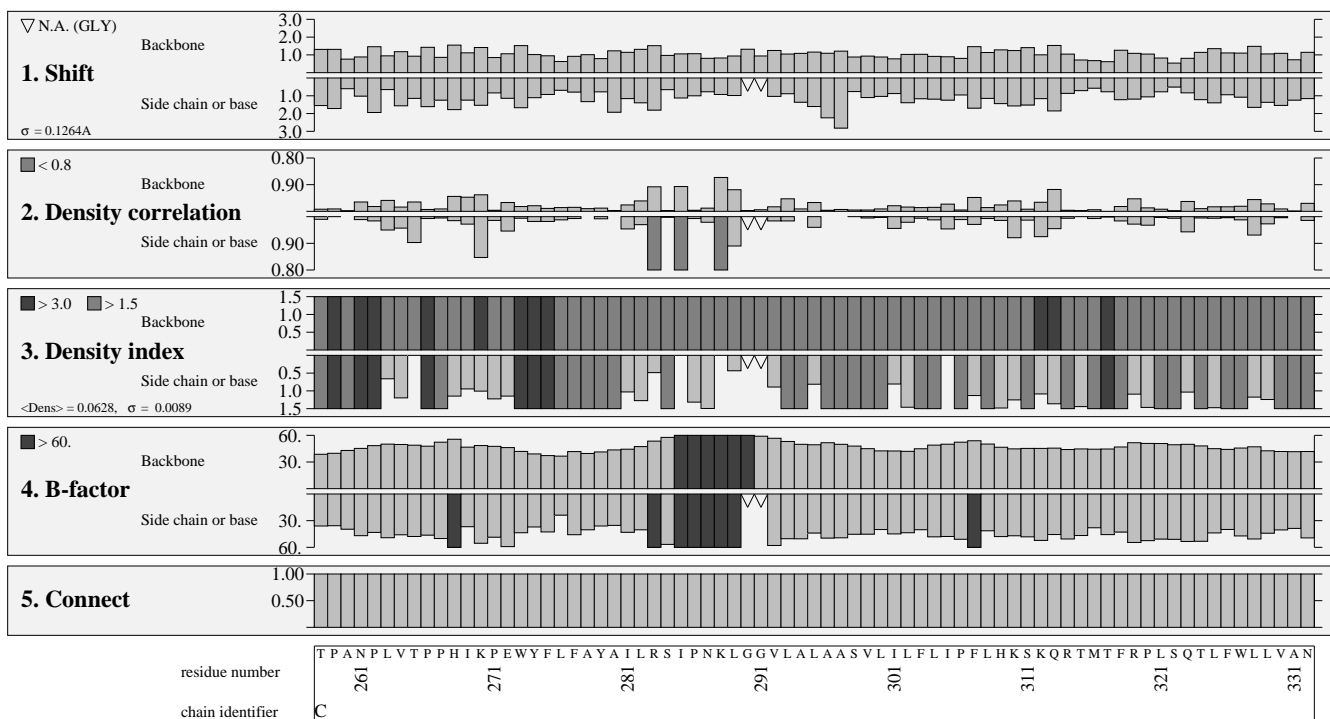
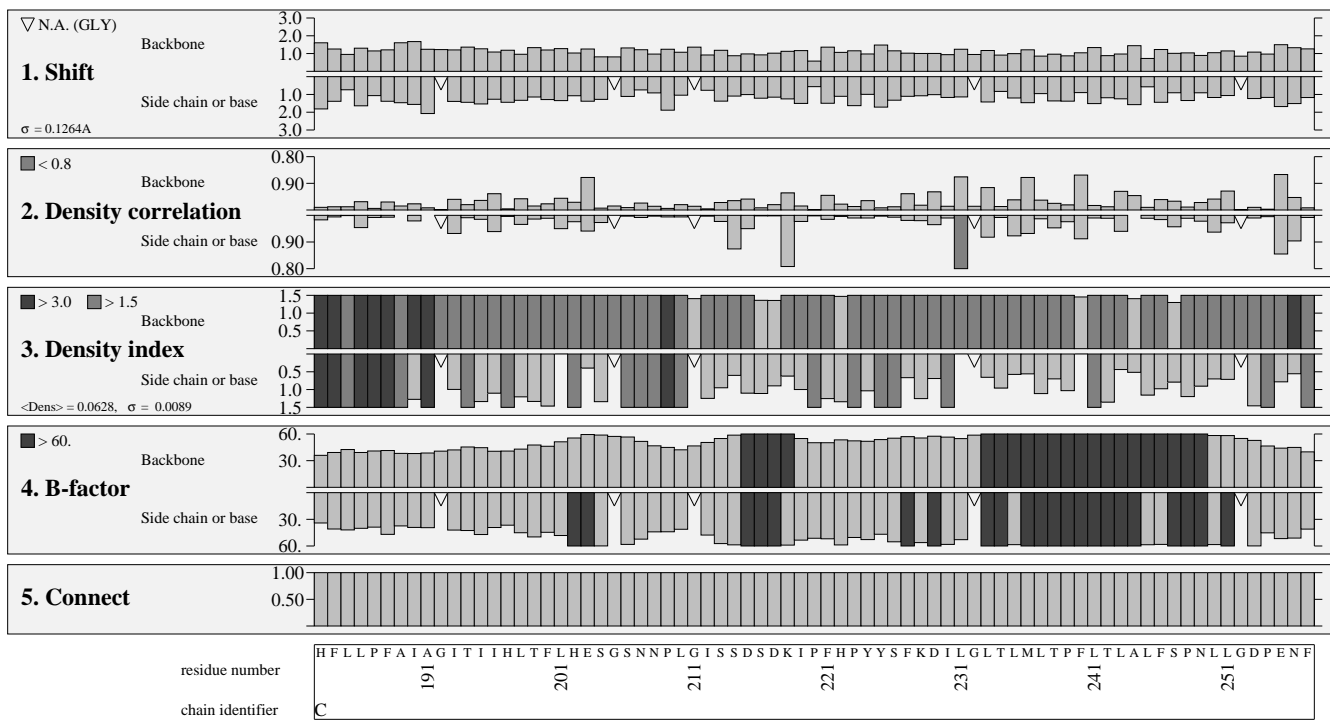
Local estimation (7)



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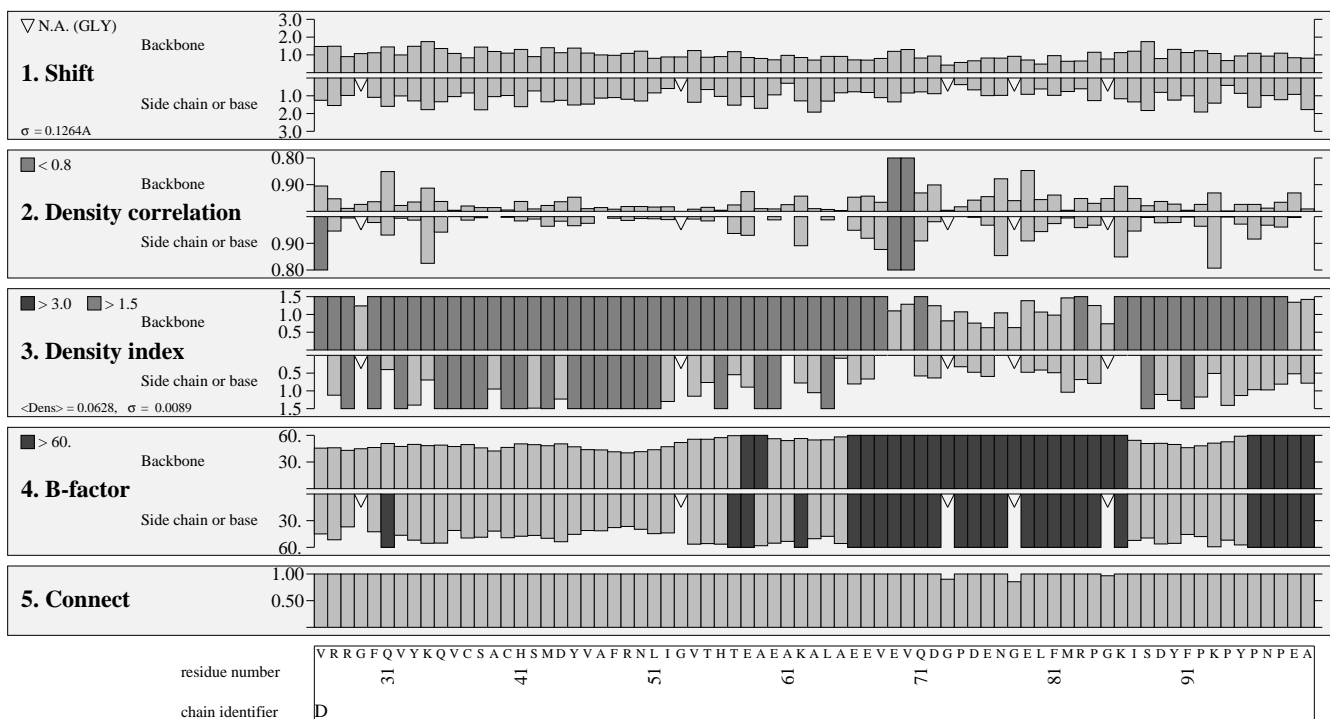
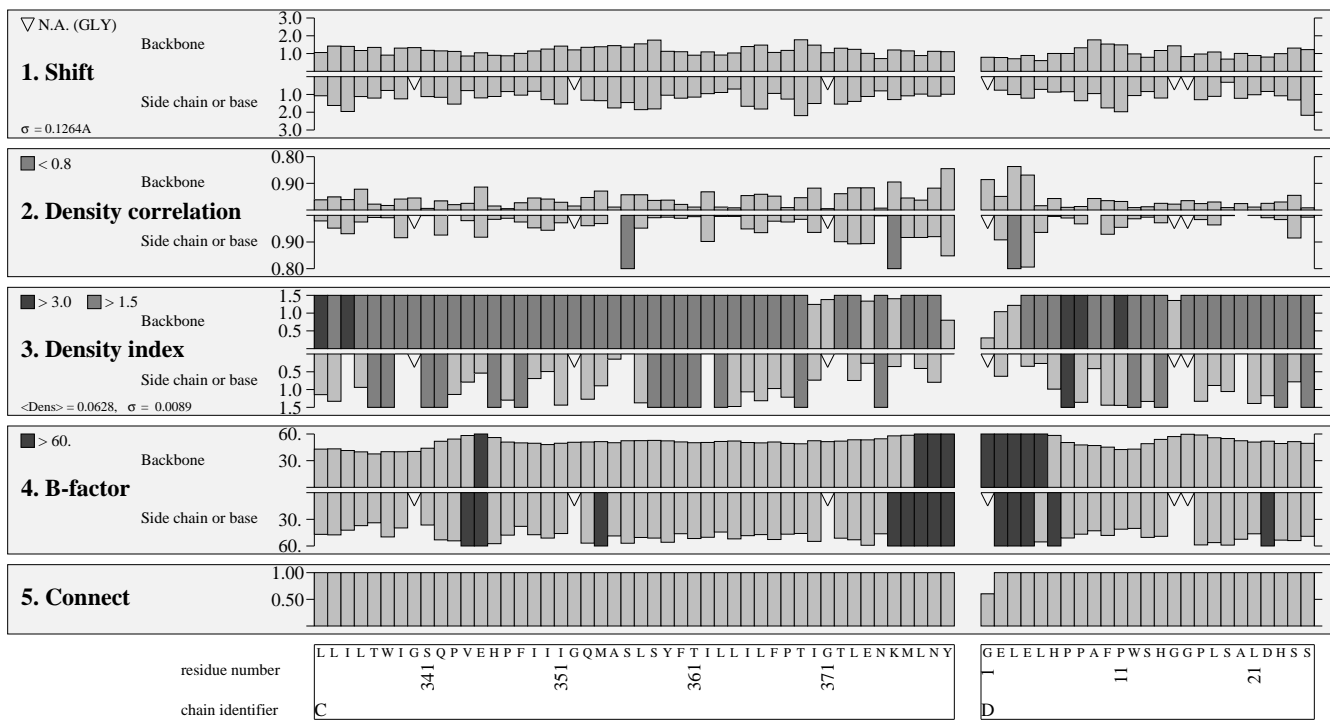
Local estimation (8)



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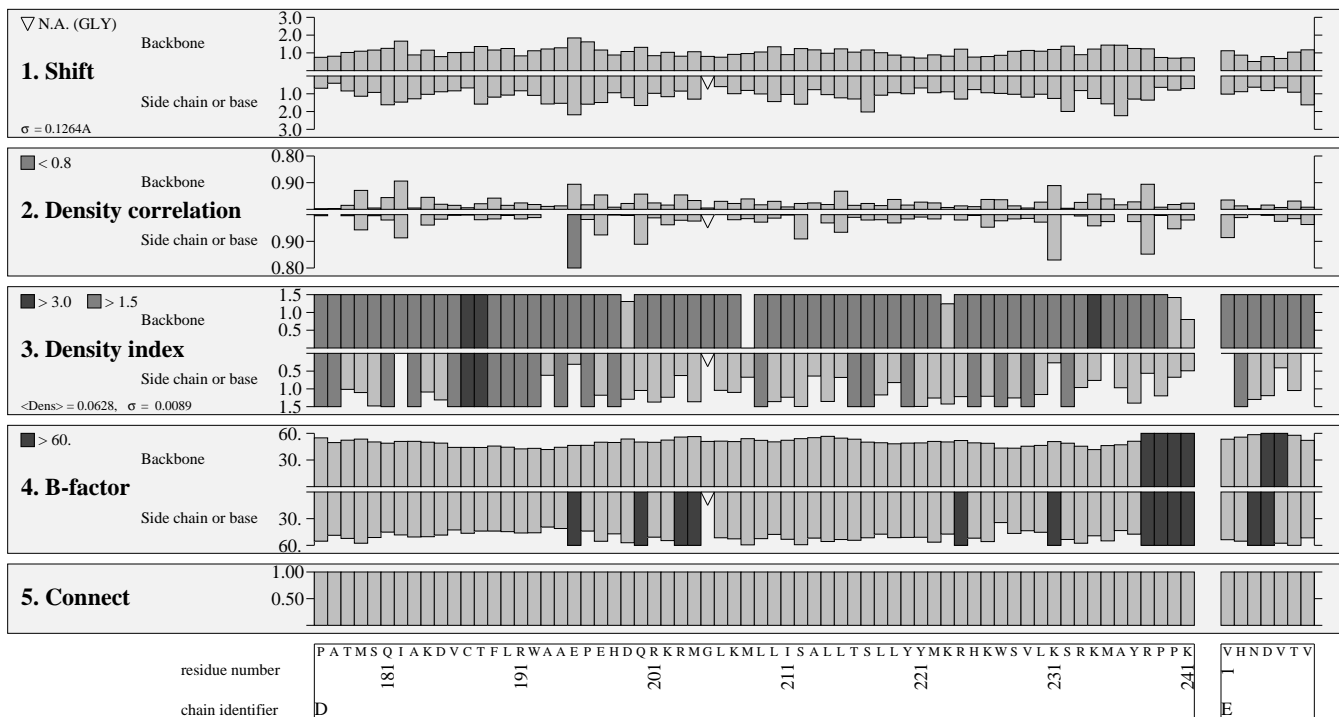
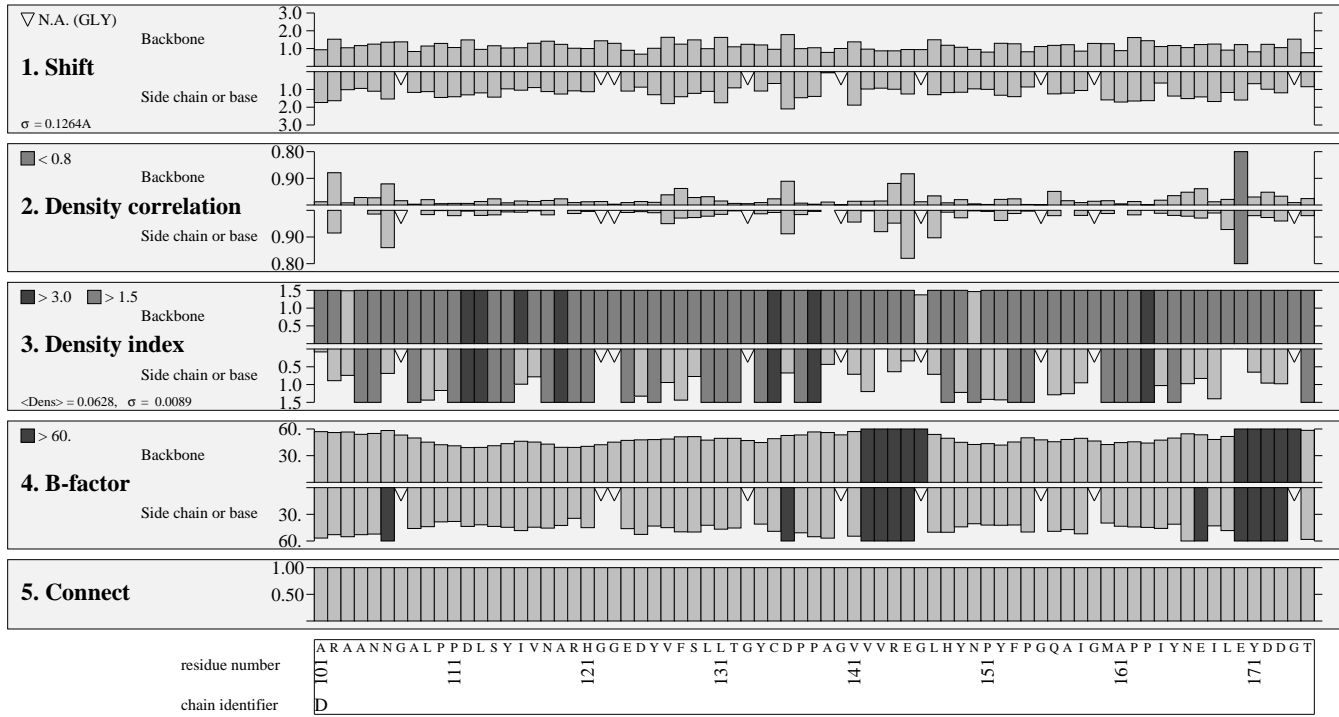
Local estimation (9)



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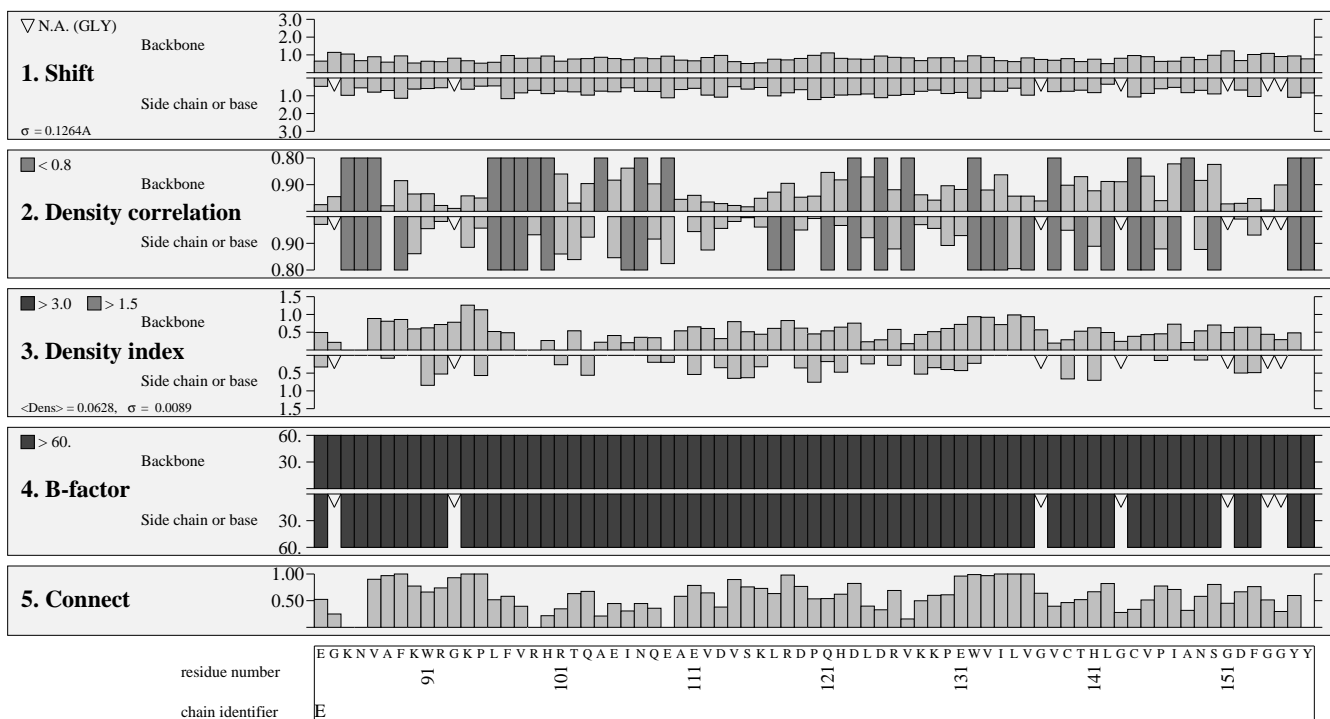
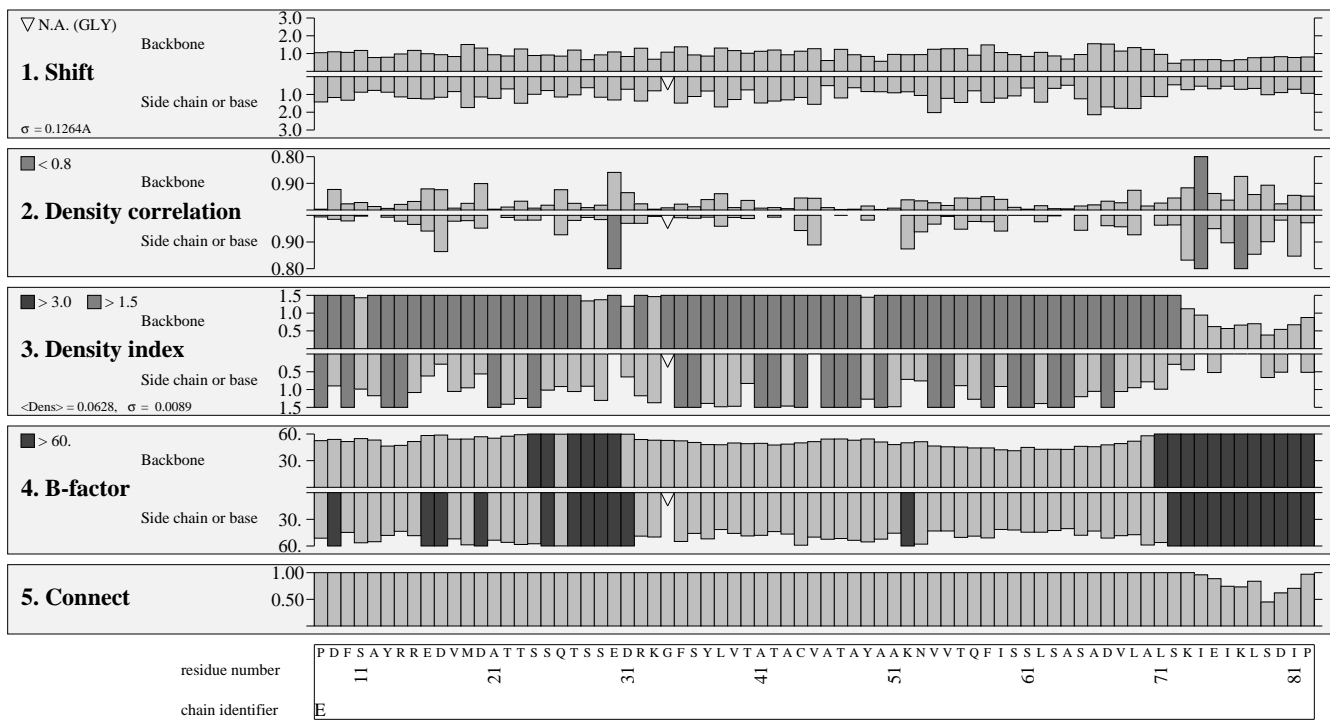
Local estimation (10)



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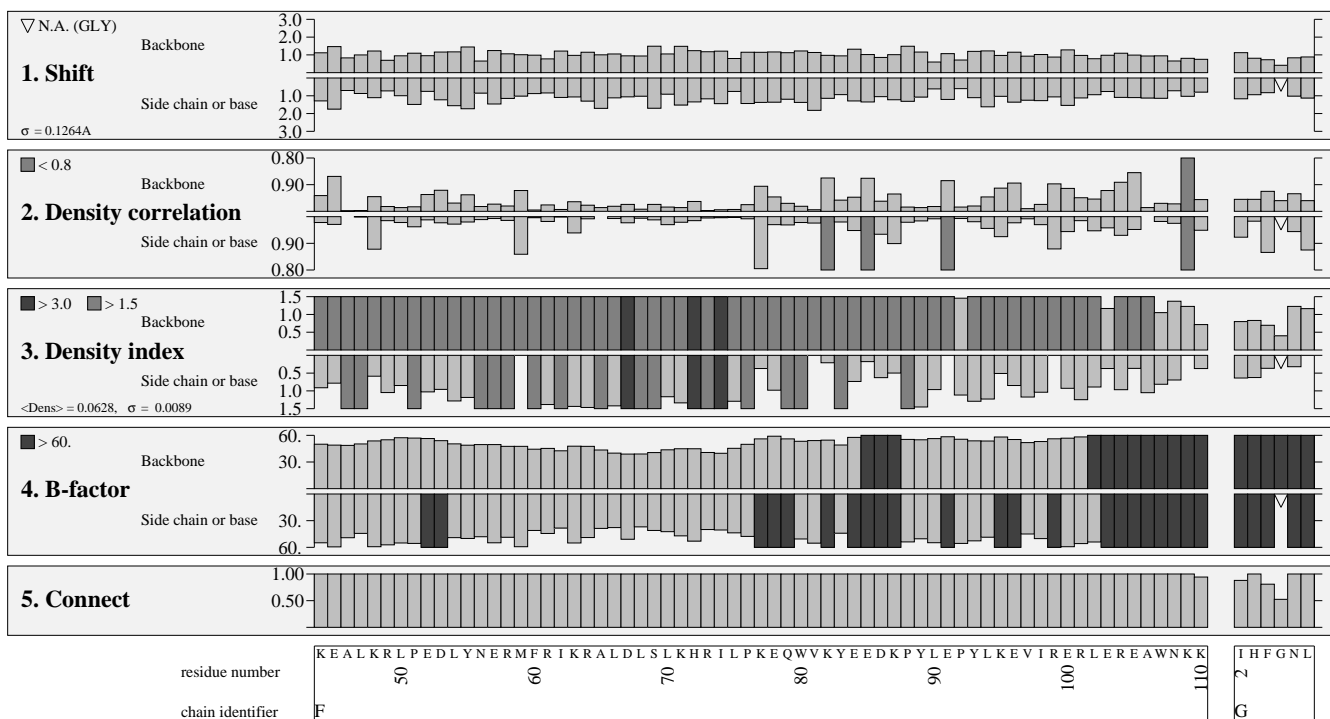
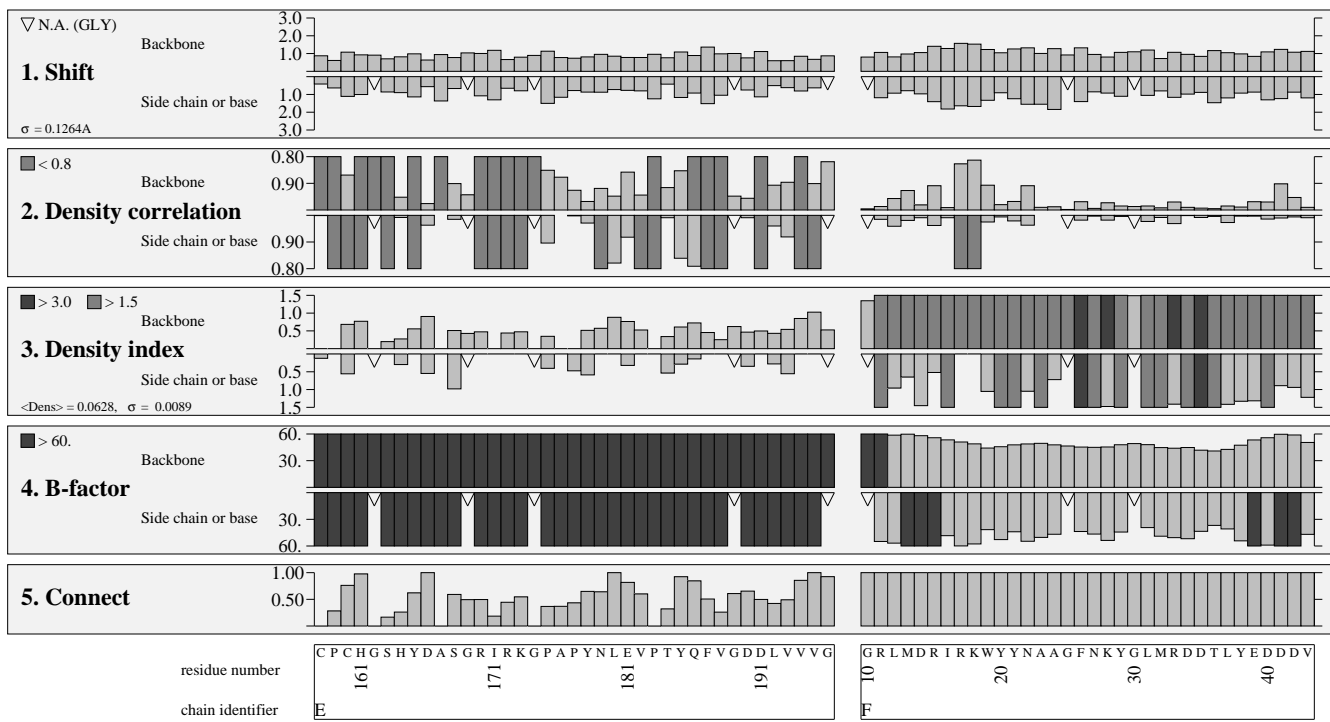
Local estimation (11)



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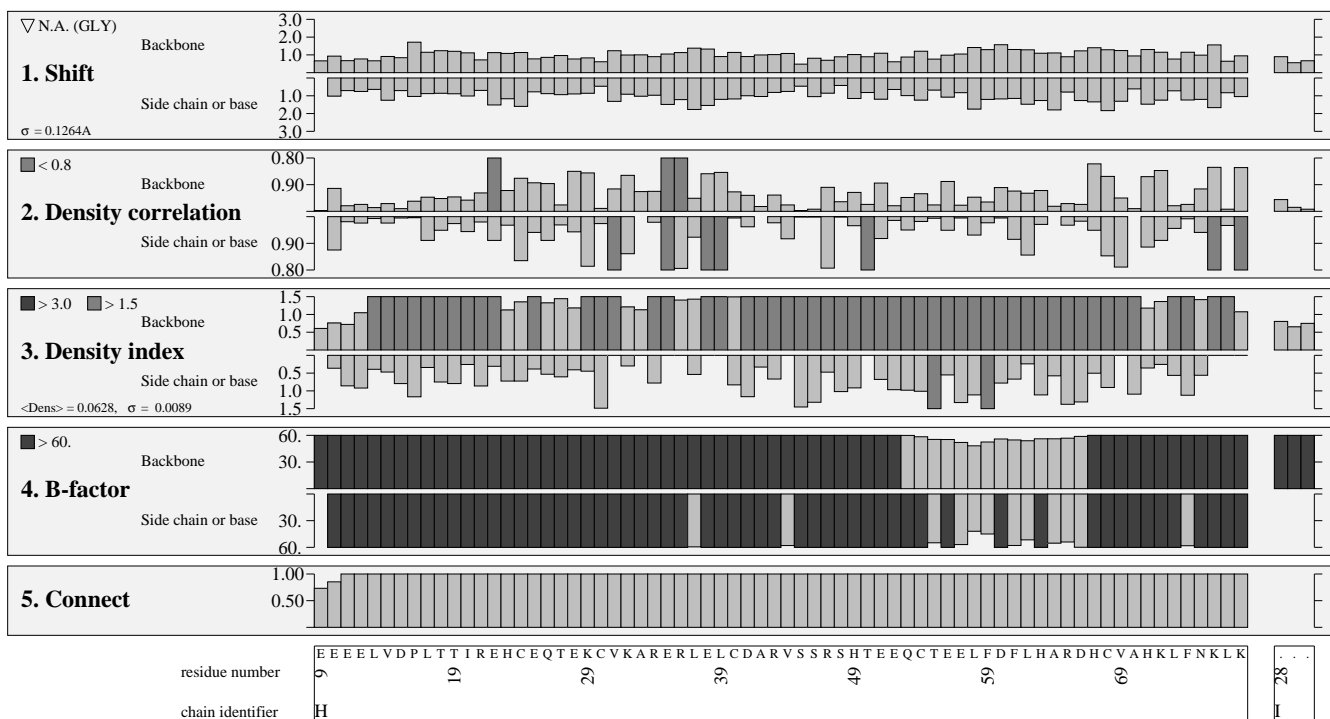
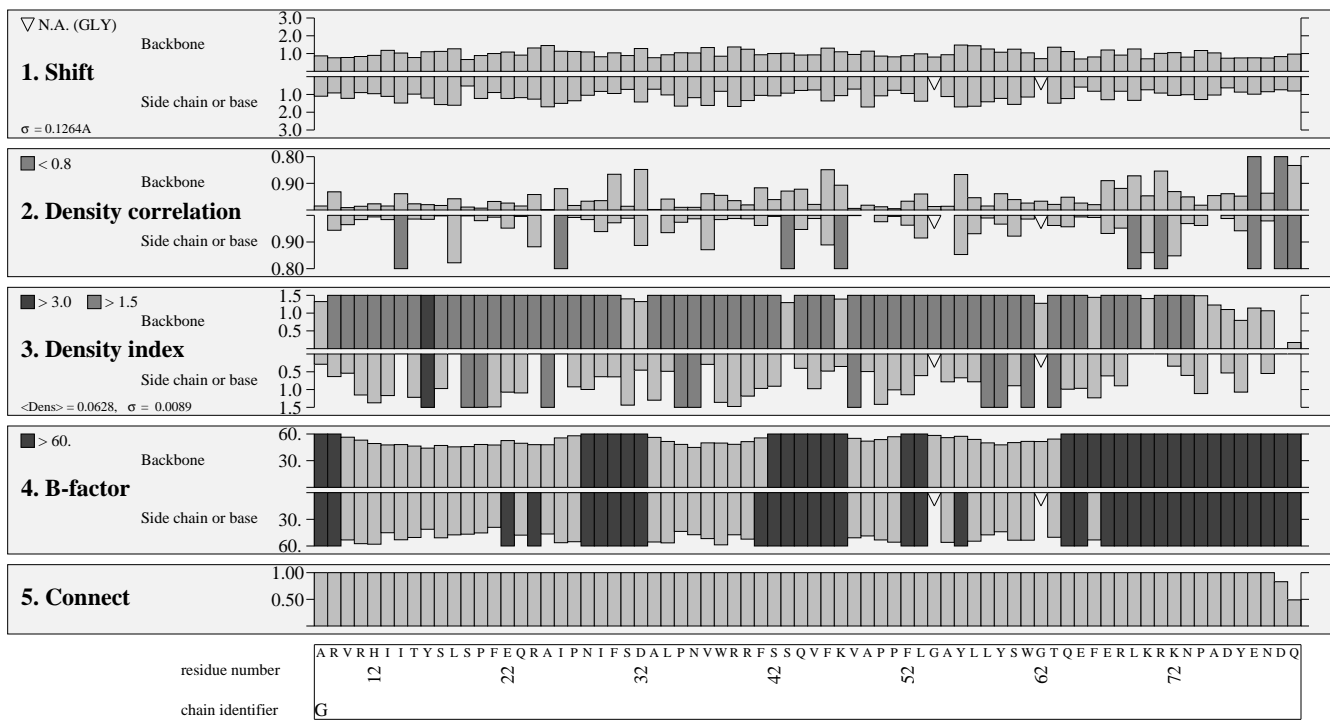
Local estimation (12)



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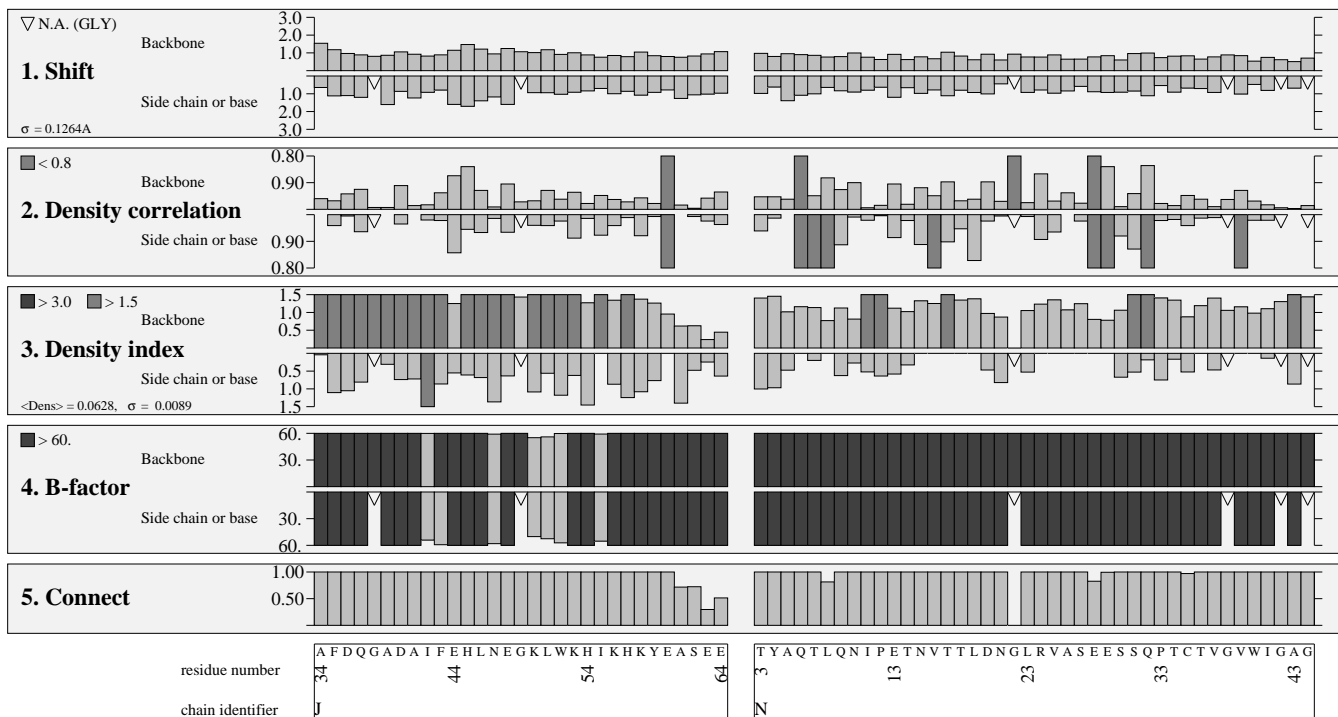
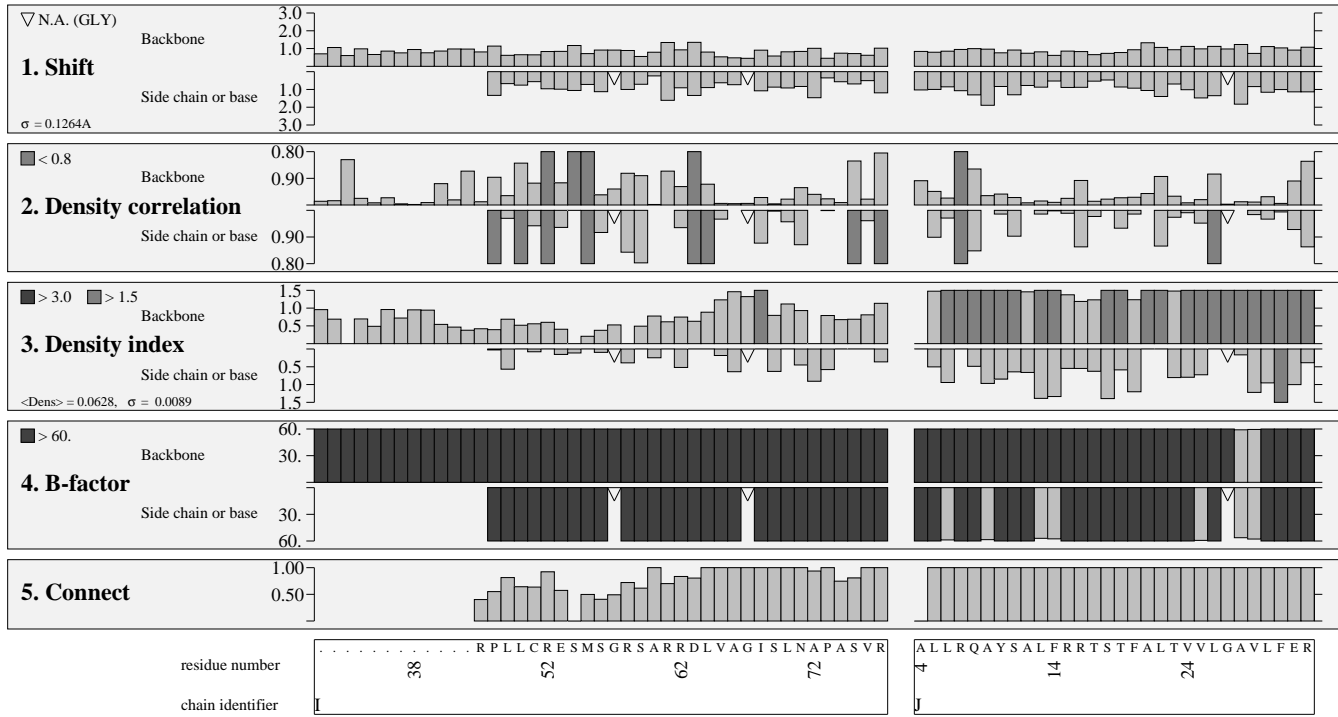
Local estimation (13)



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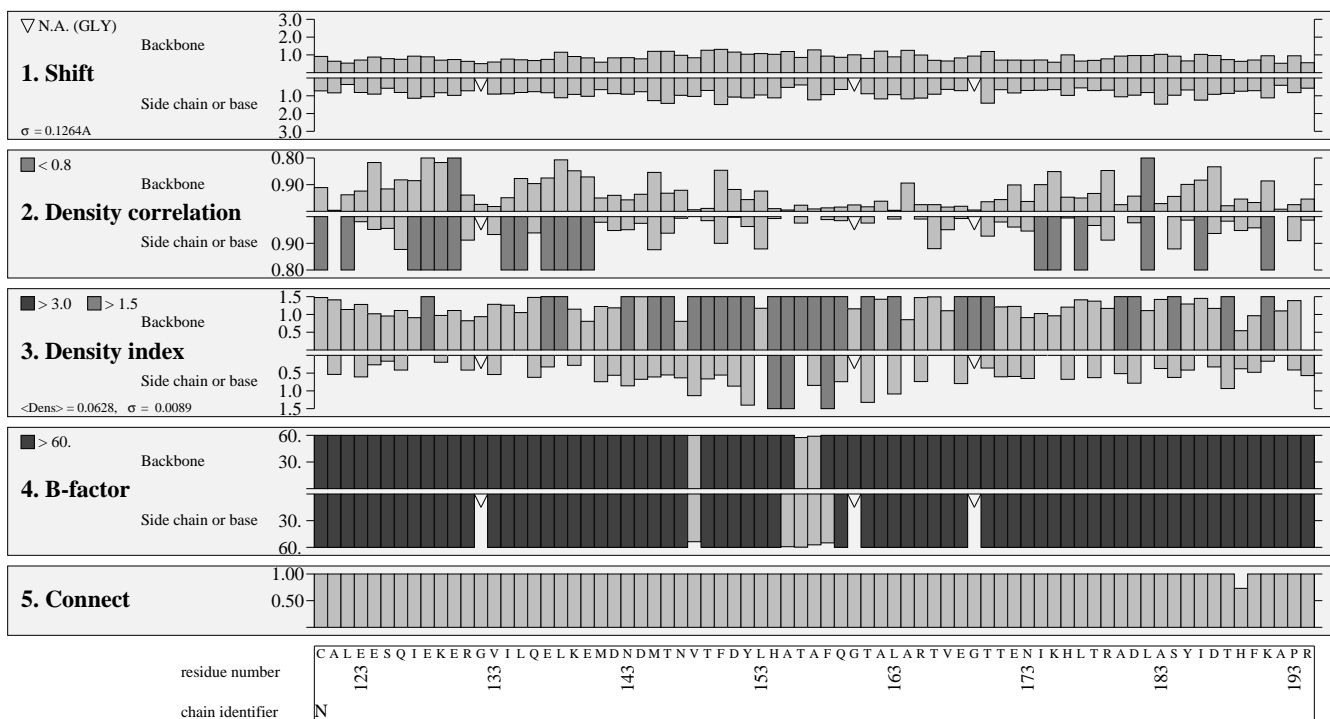
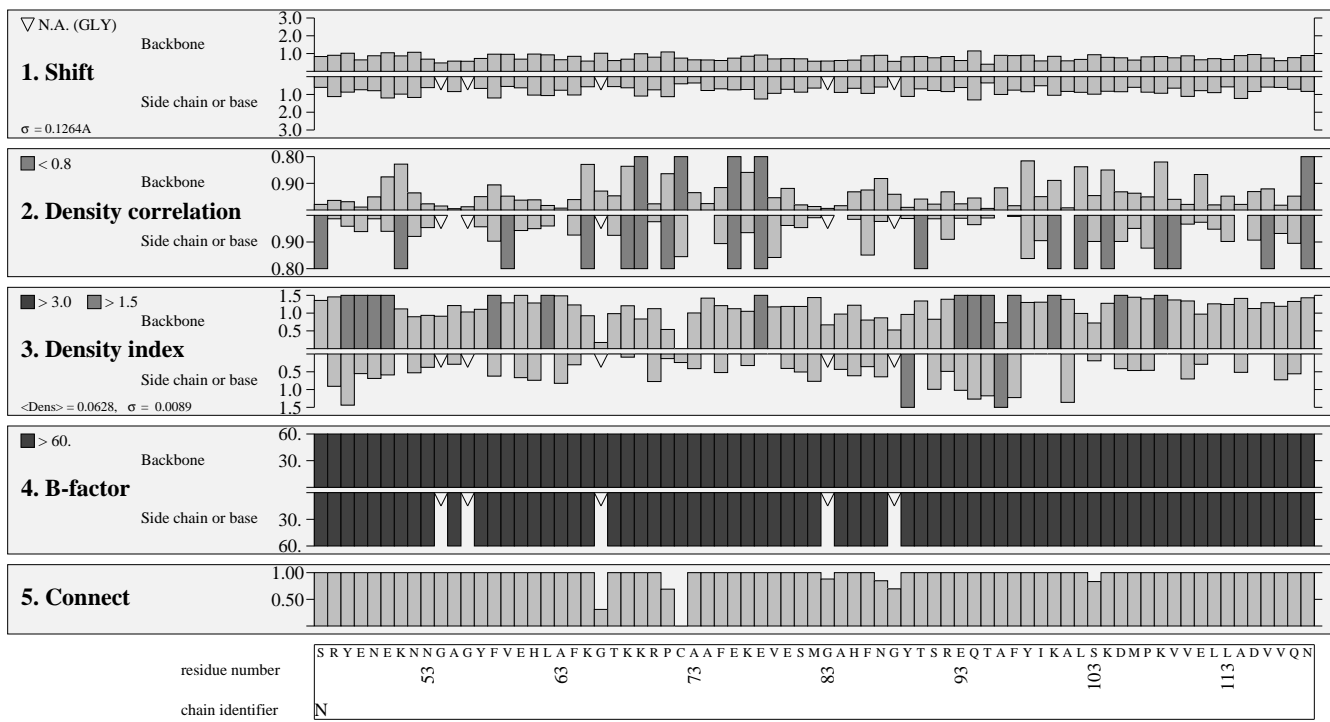
Local estimation (14)



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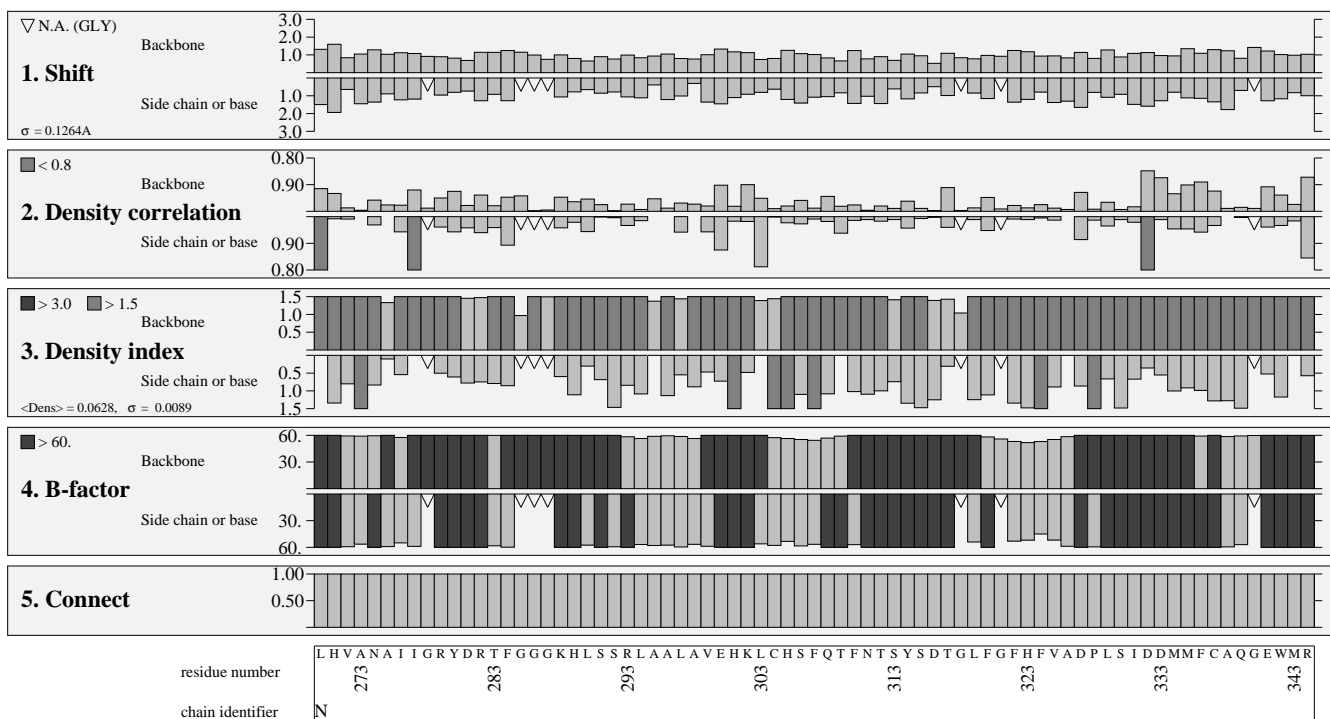
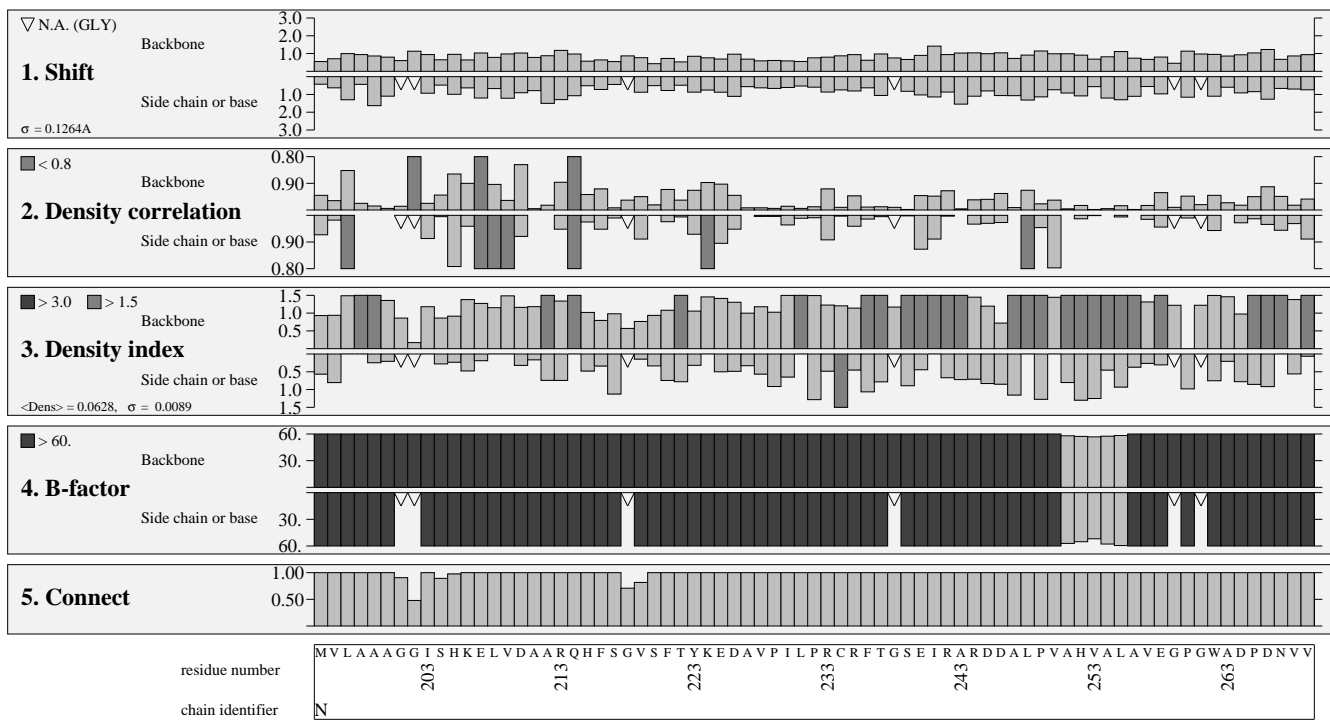
Local estimation (15)



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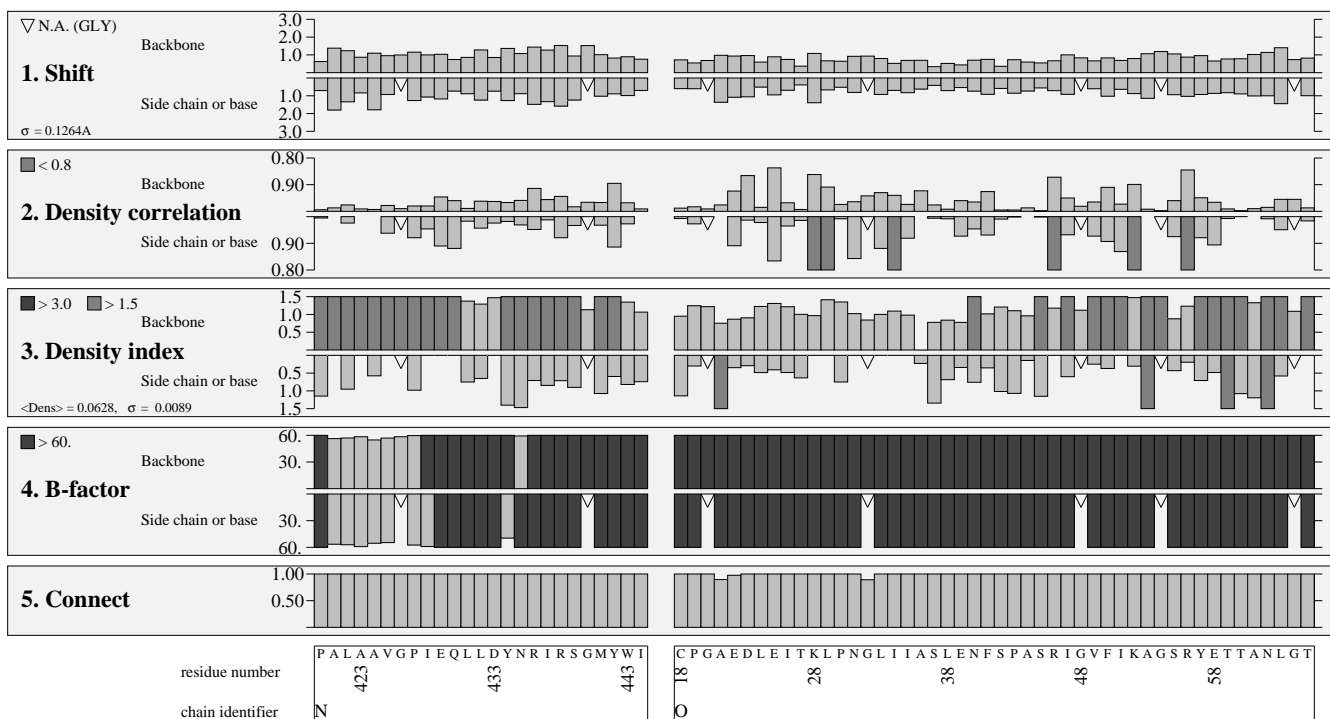
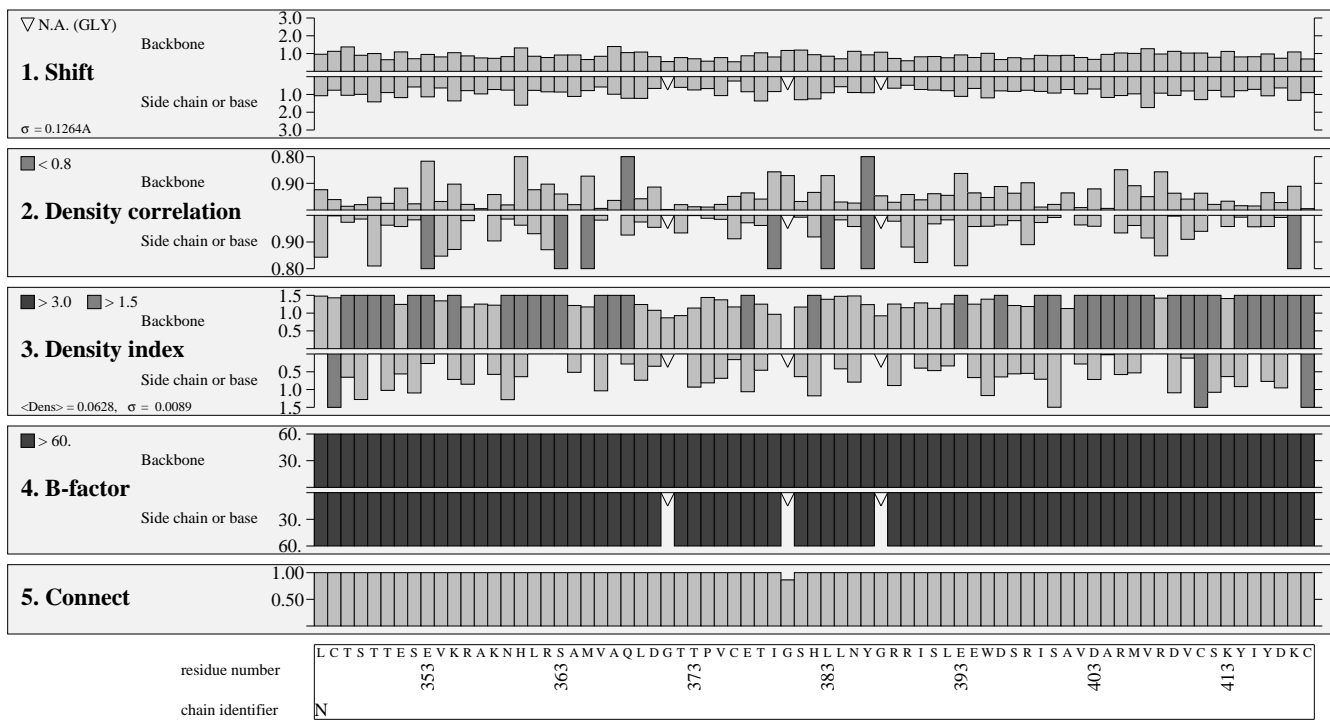
Local estimation (16)



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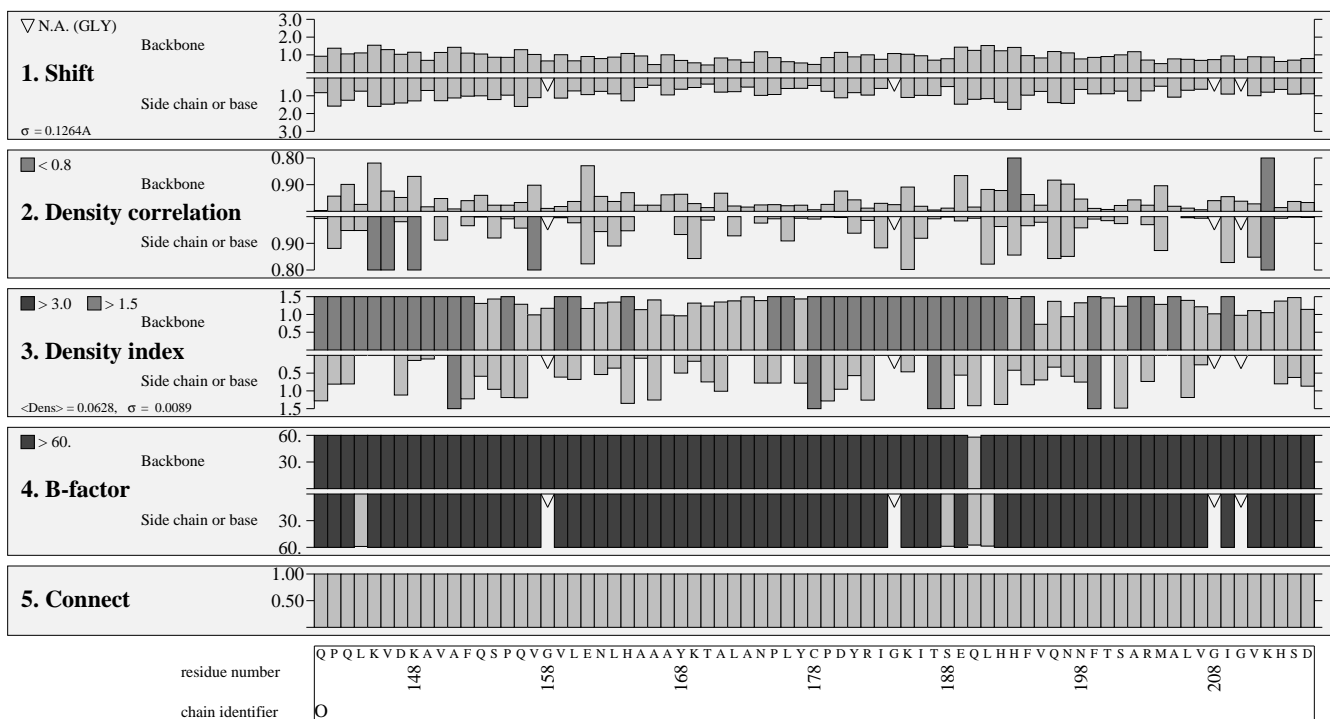
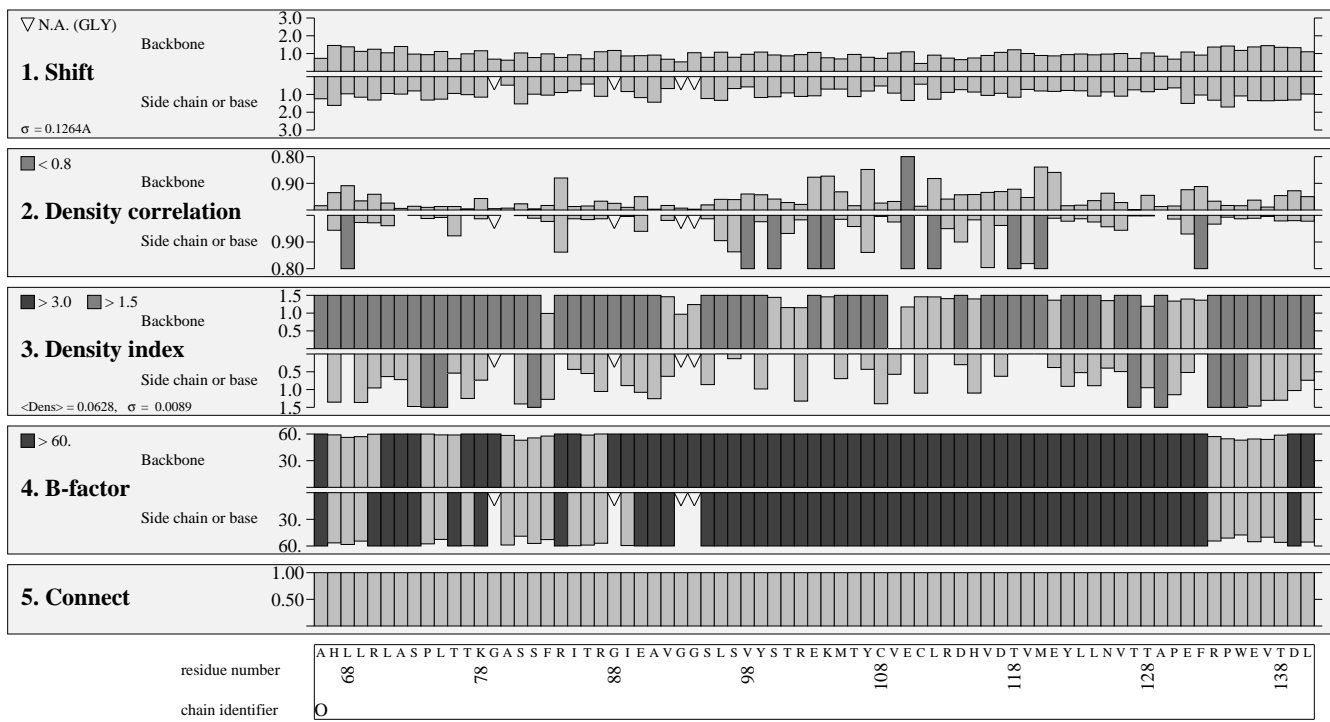
Local estimation (17)



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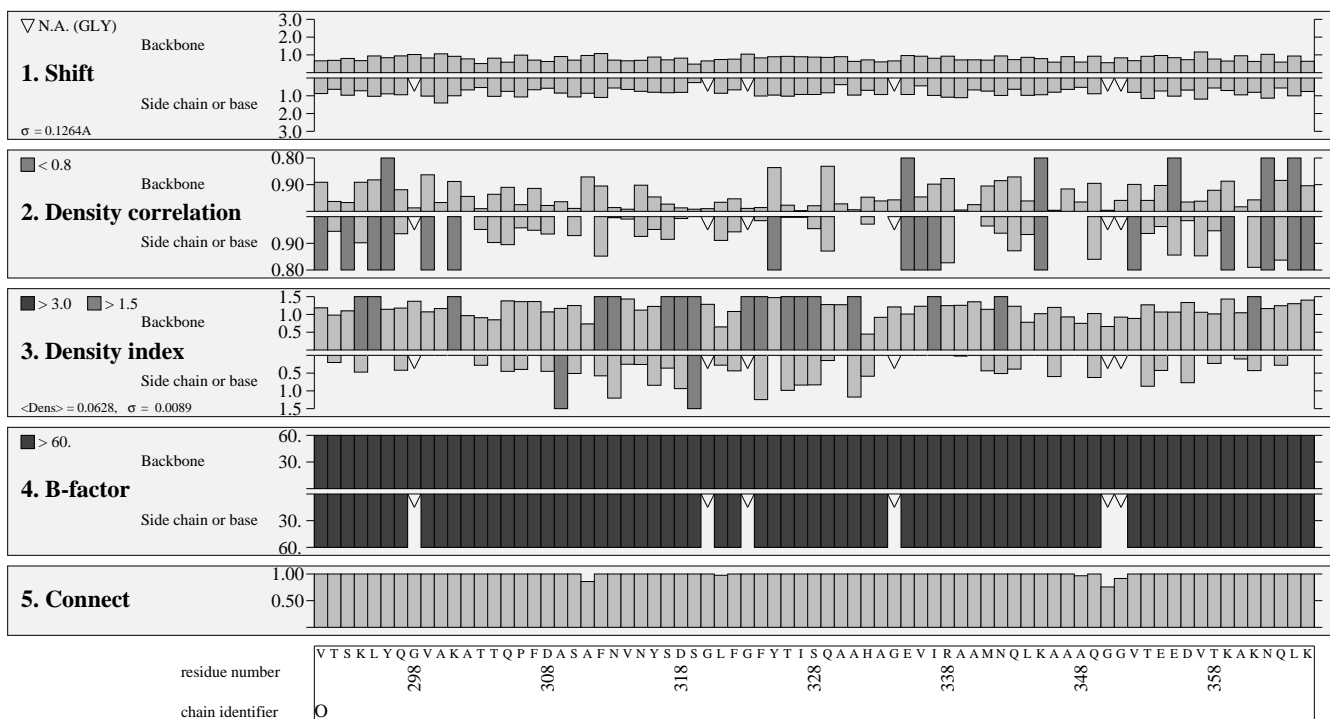
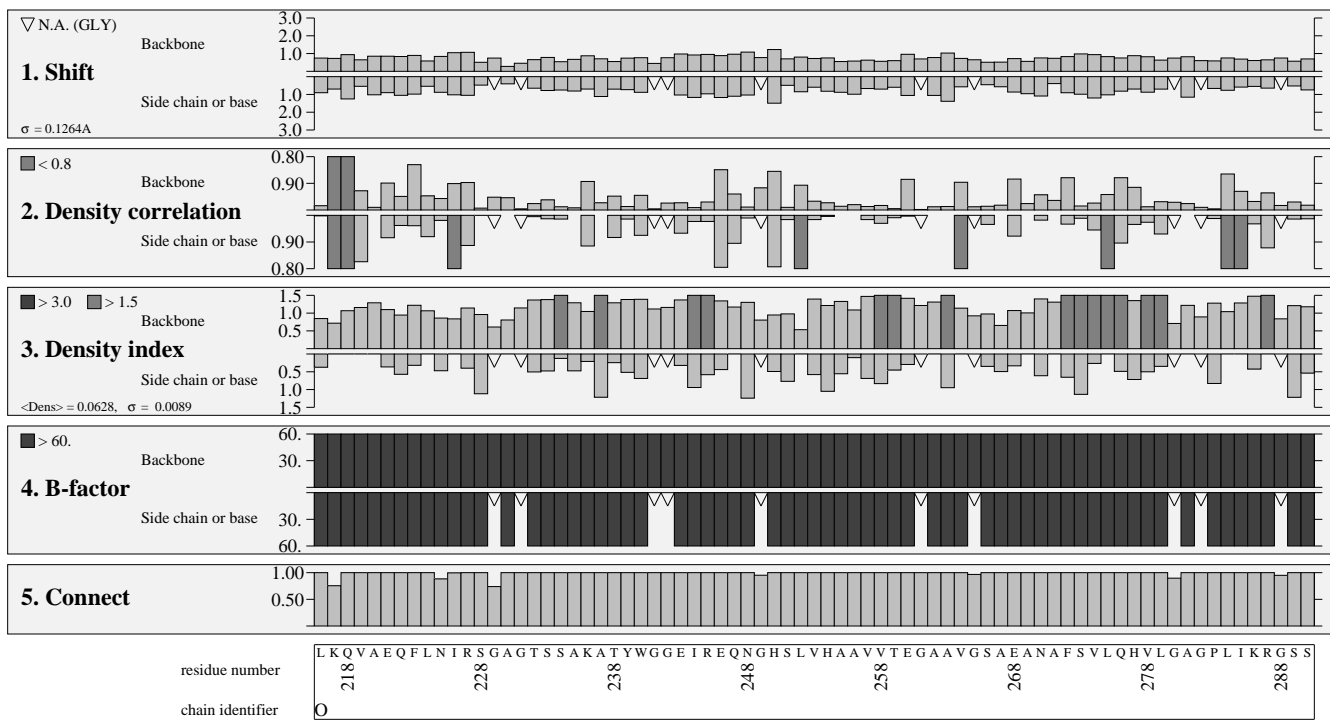
Local estimation (18)



Structure Factor Check

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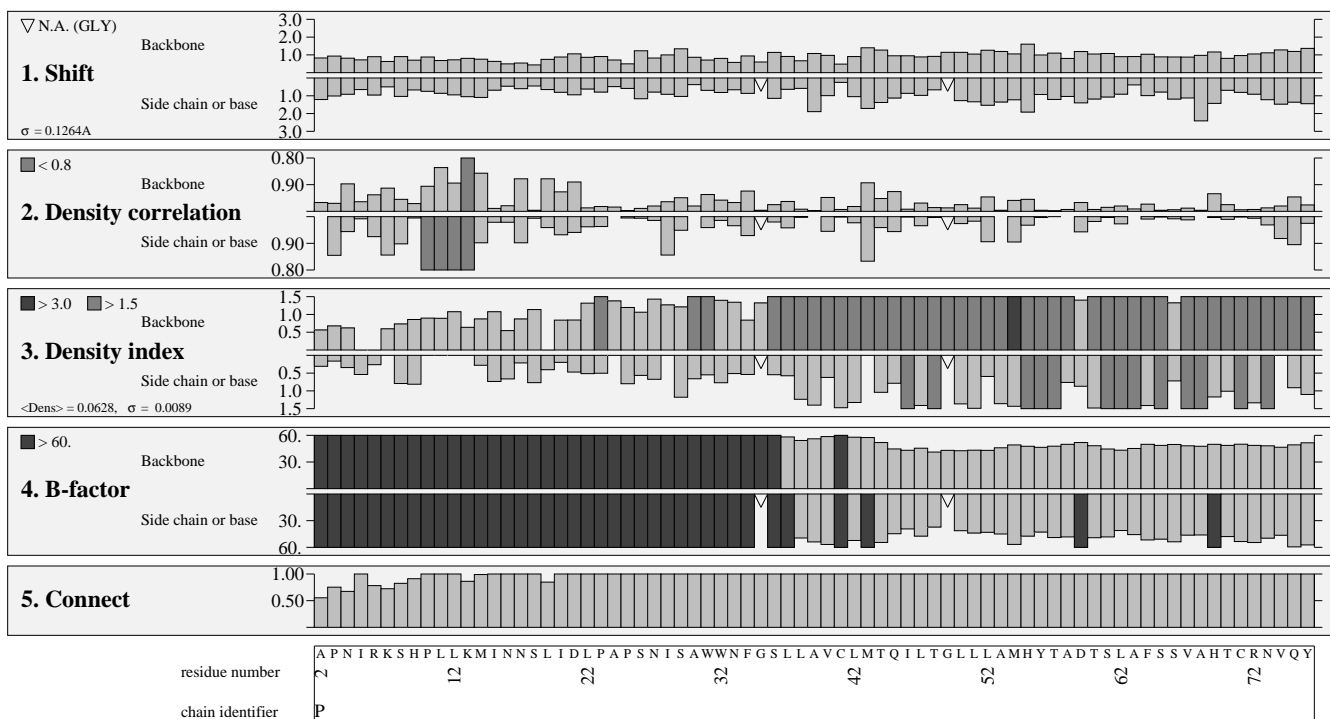
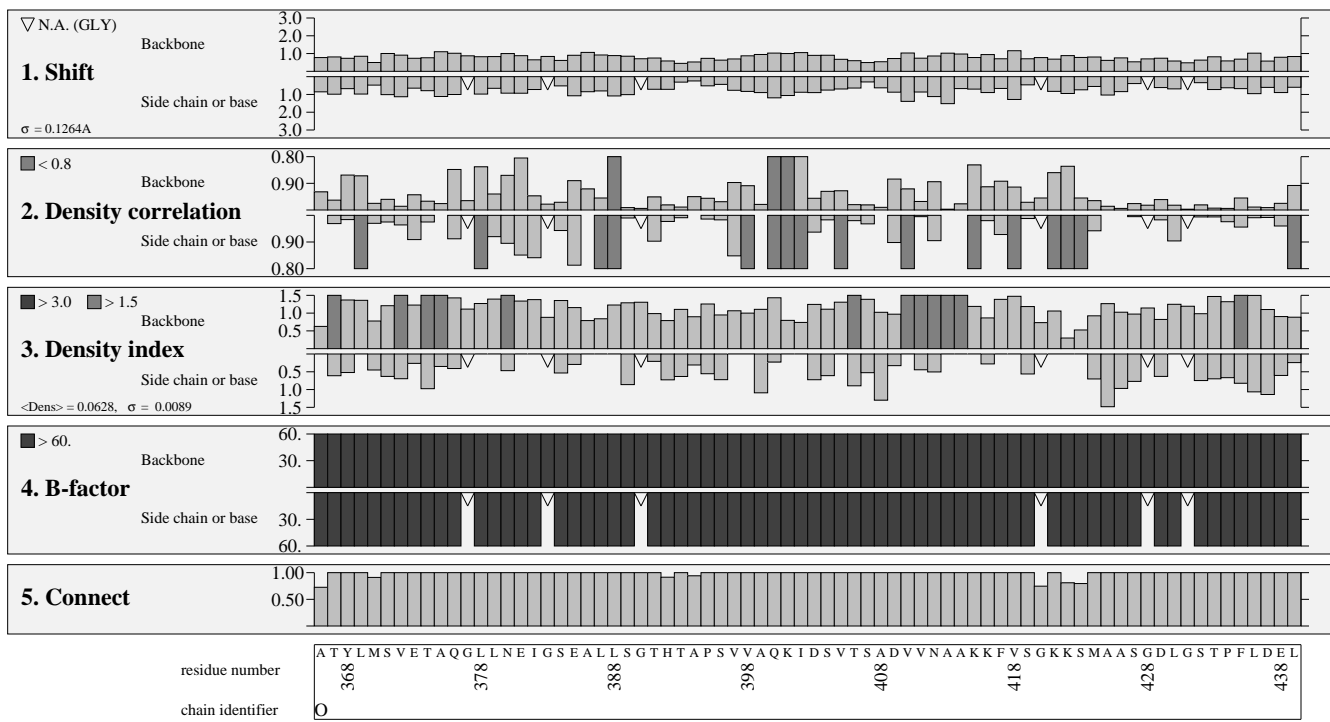
Local estimation (19)



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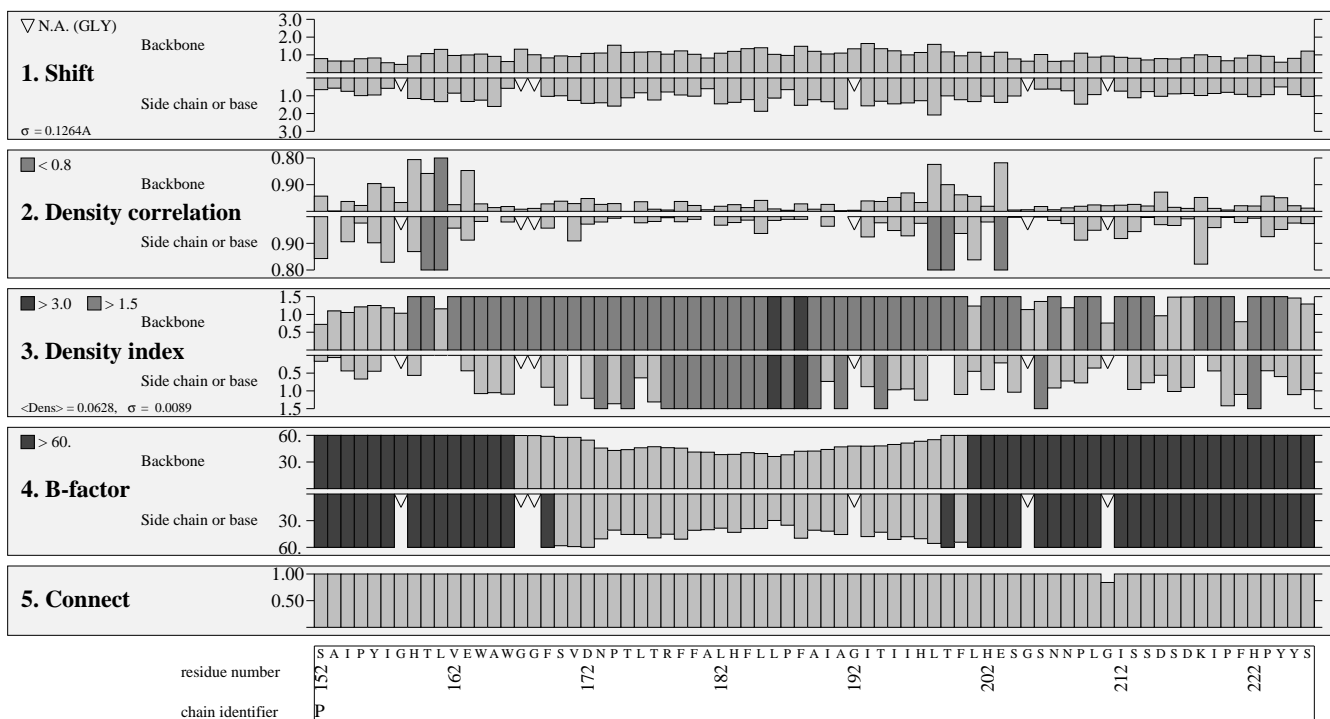
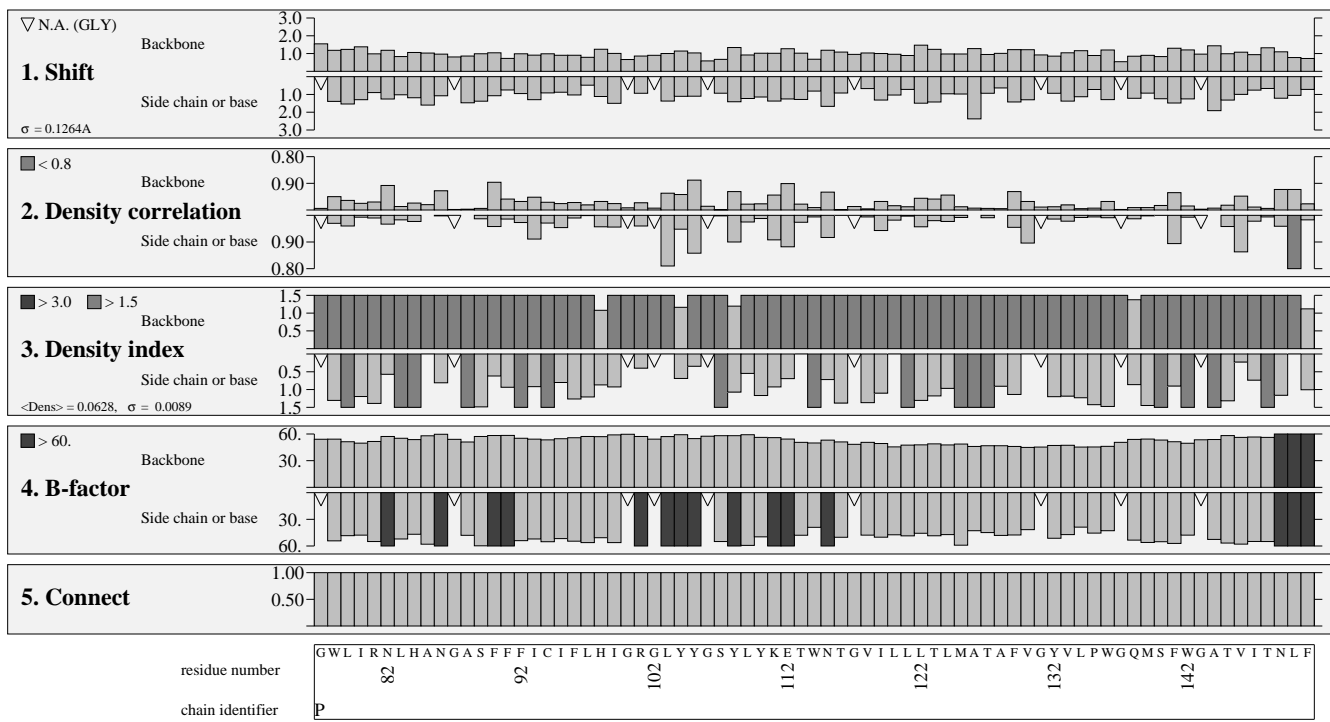
Local estimation (20)



Structure Factor Check

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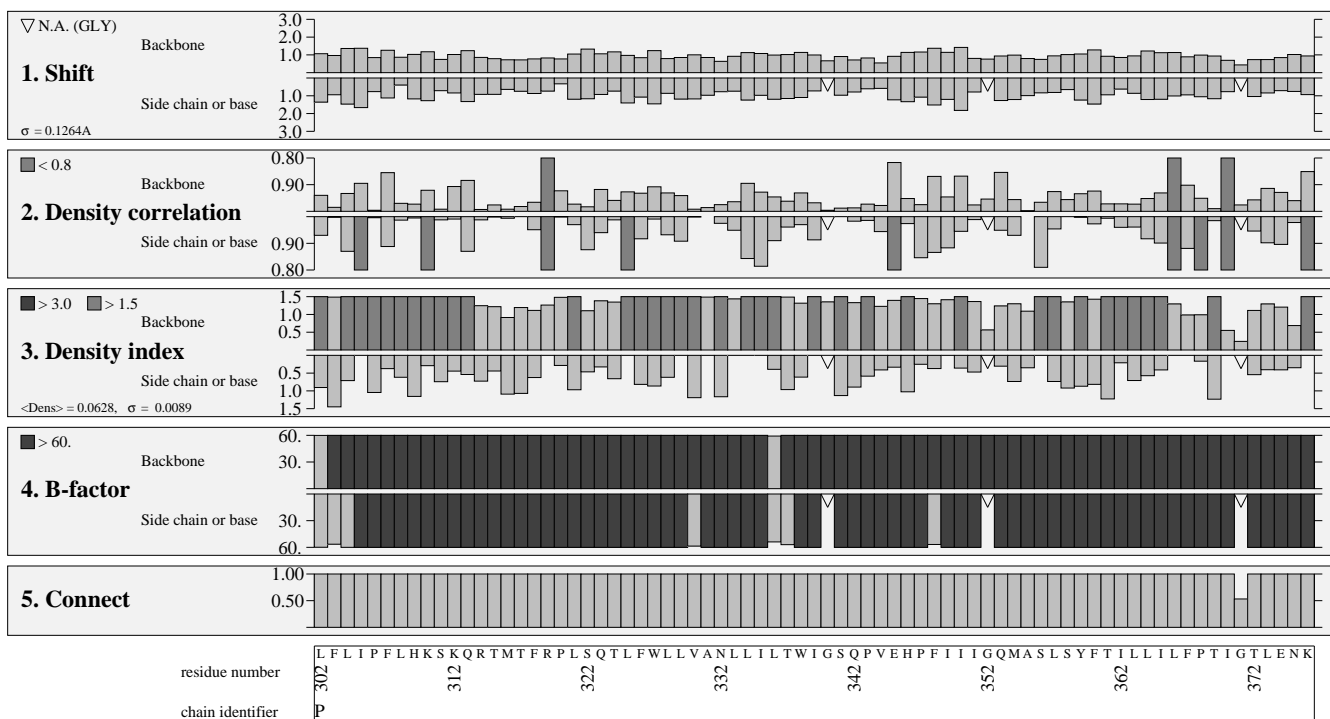
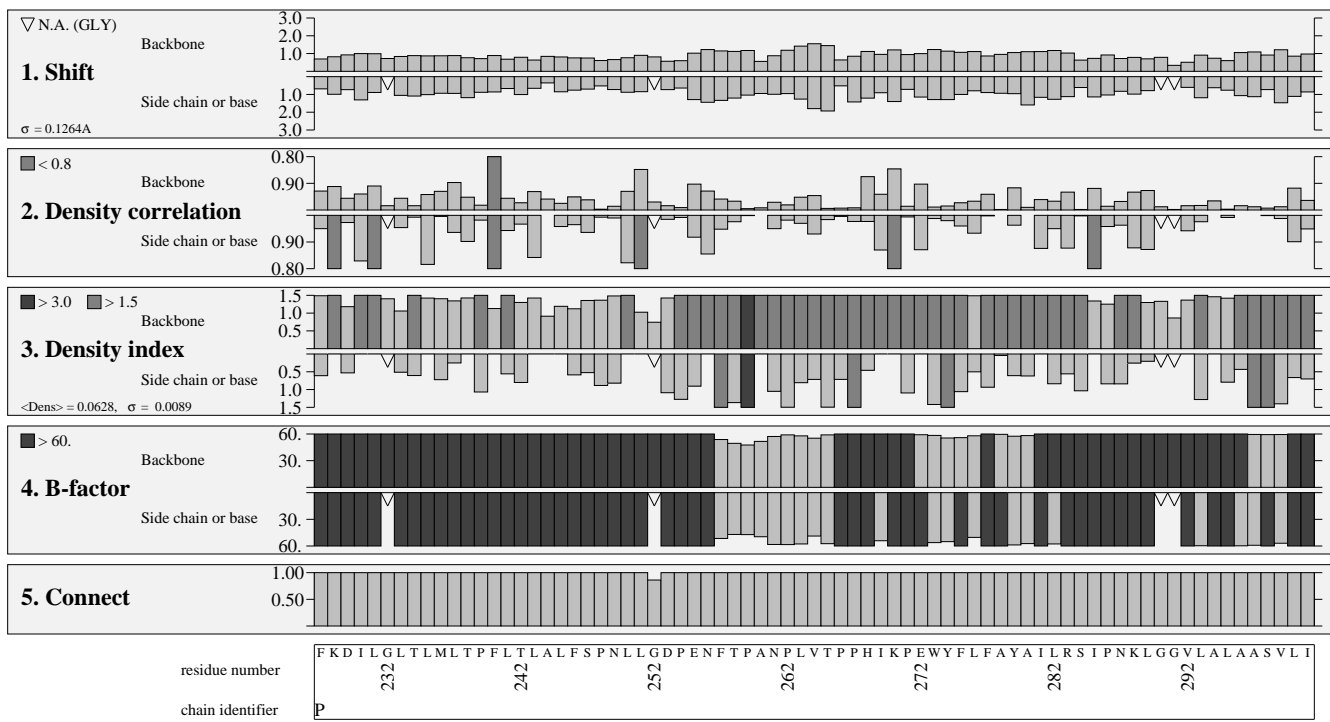
Local estimation (21)



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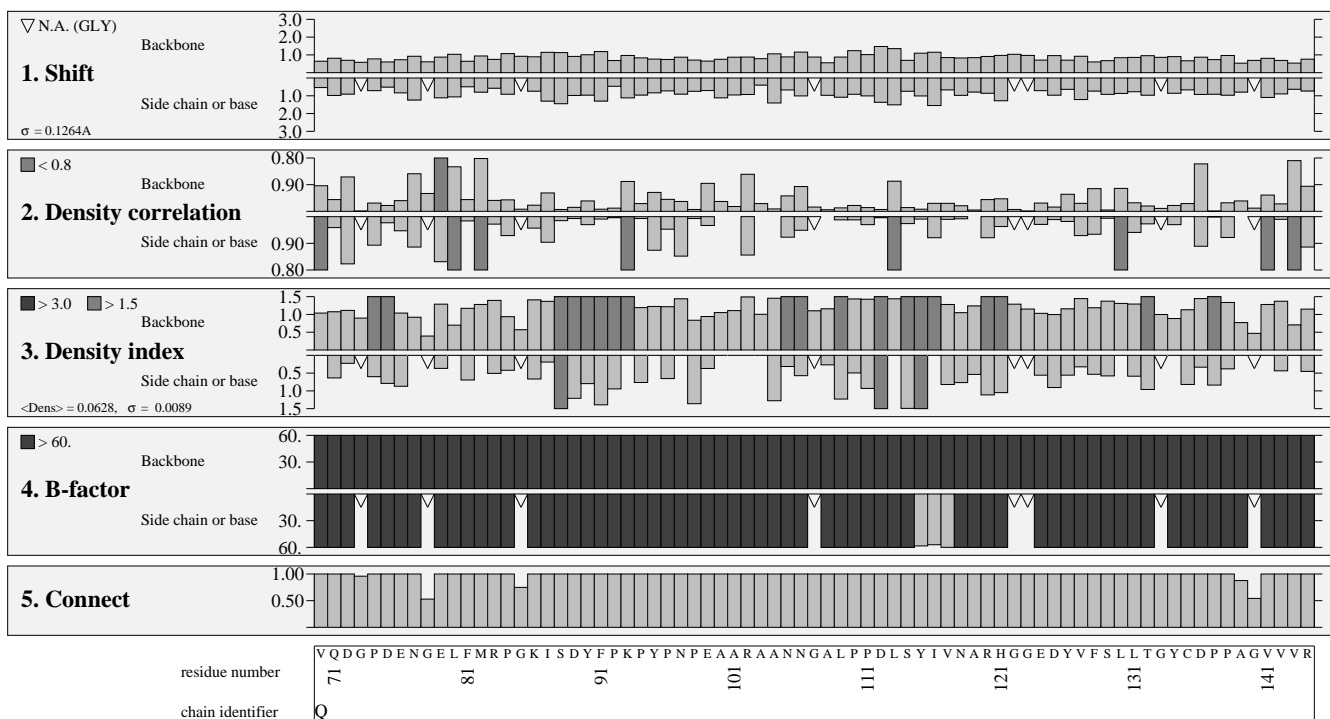
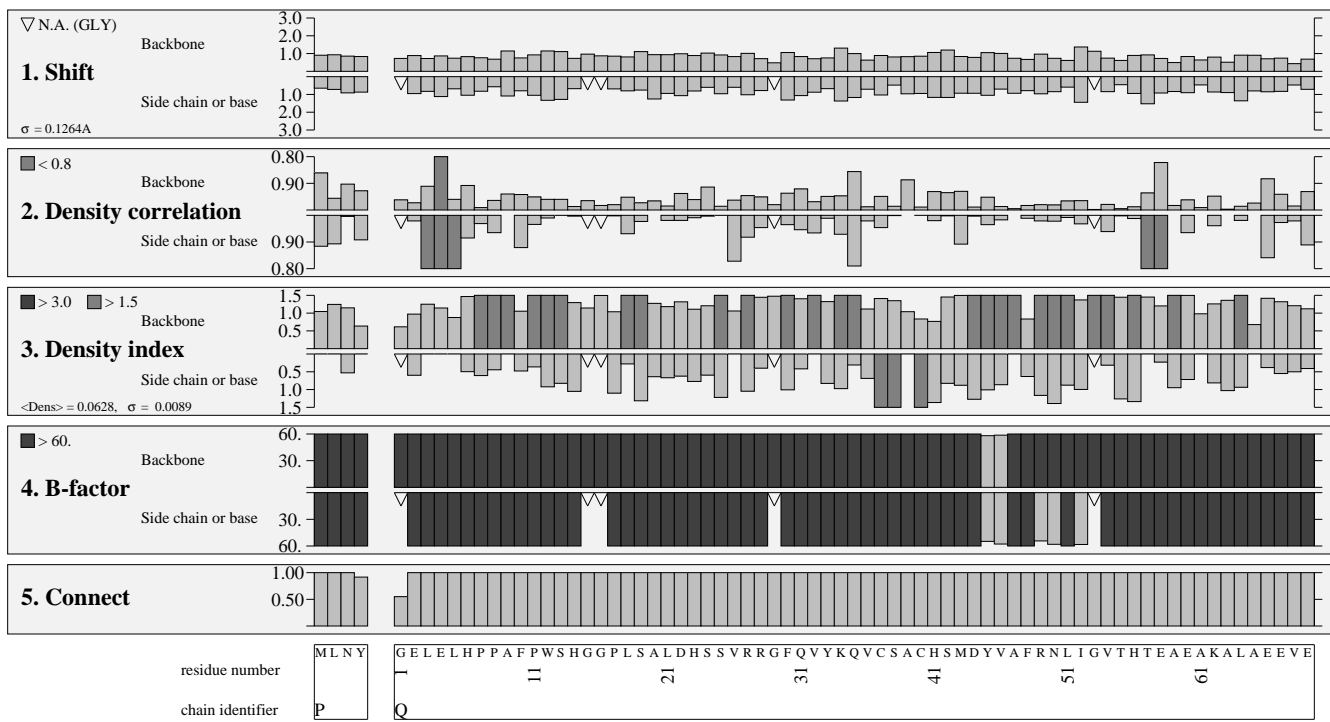
Local estimation (22)



Structure Factor Check

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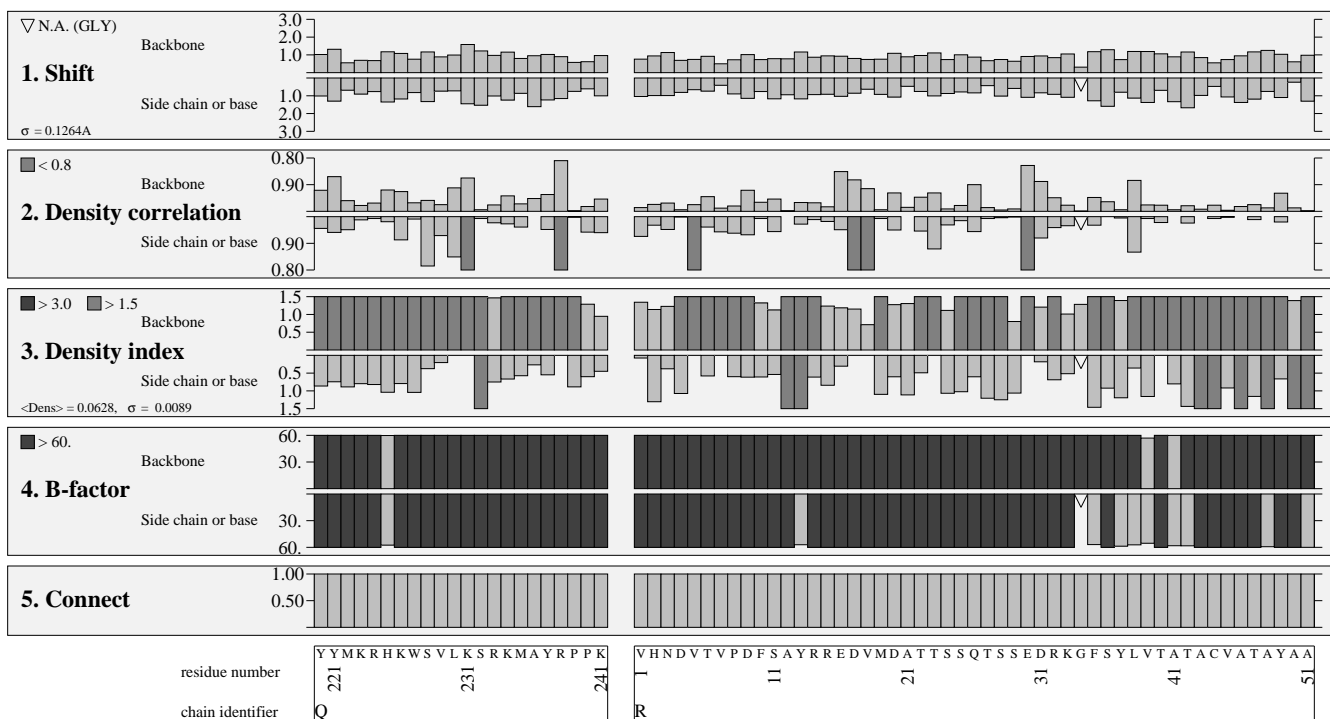
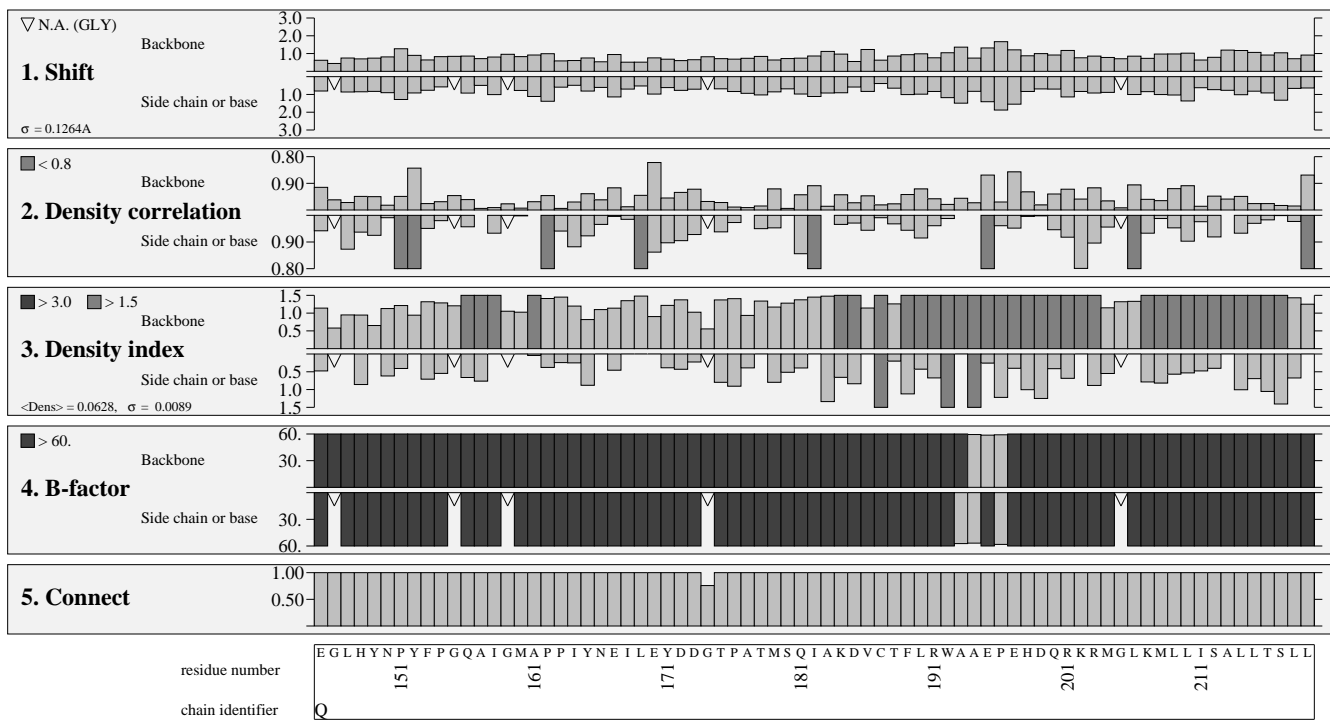
Local estimation (23)



Structure Factor Check

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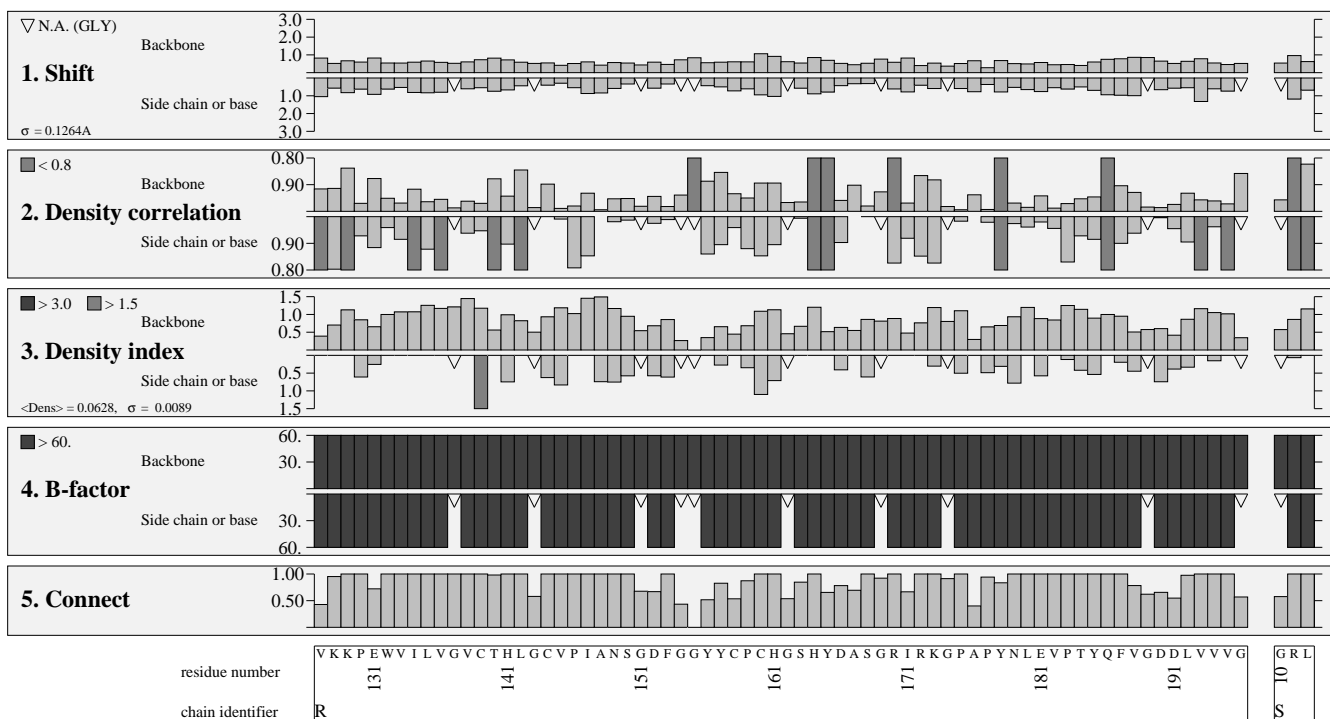
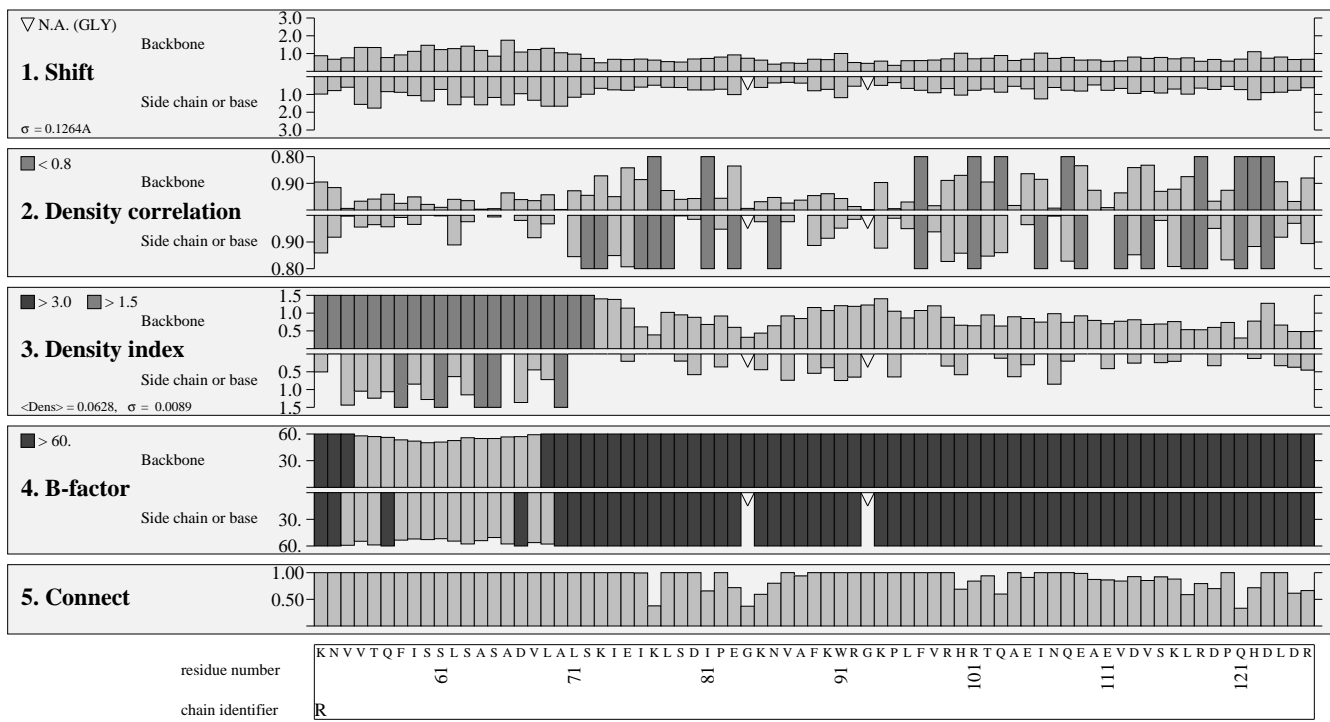
Local estimation (24)



Structure Factor Check

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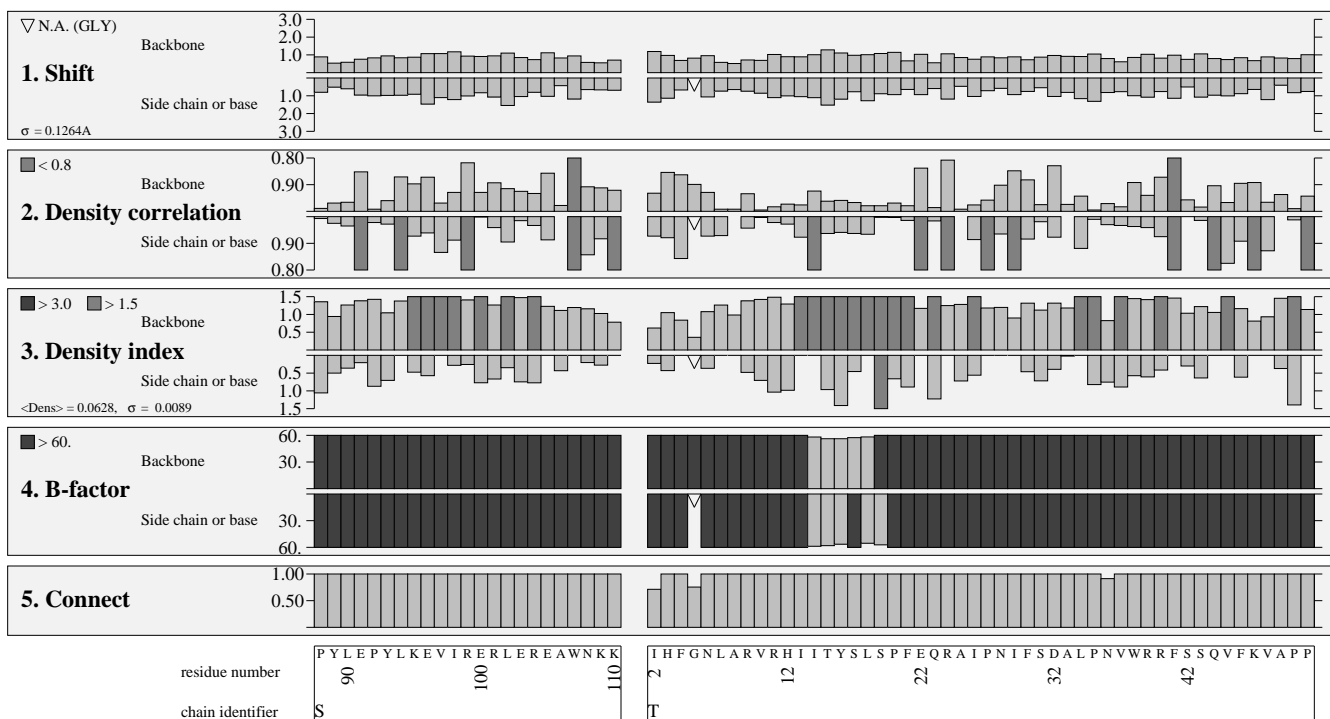
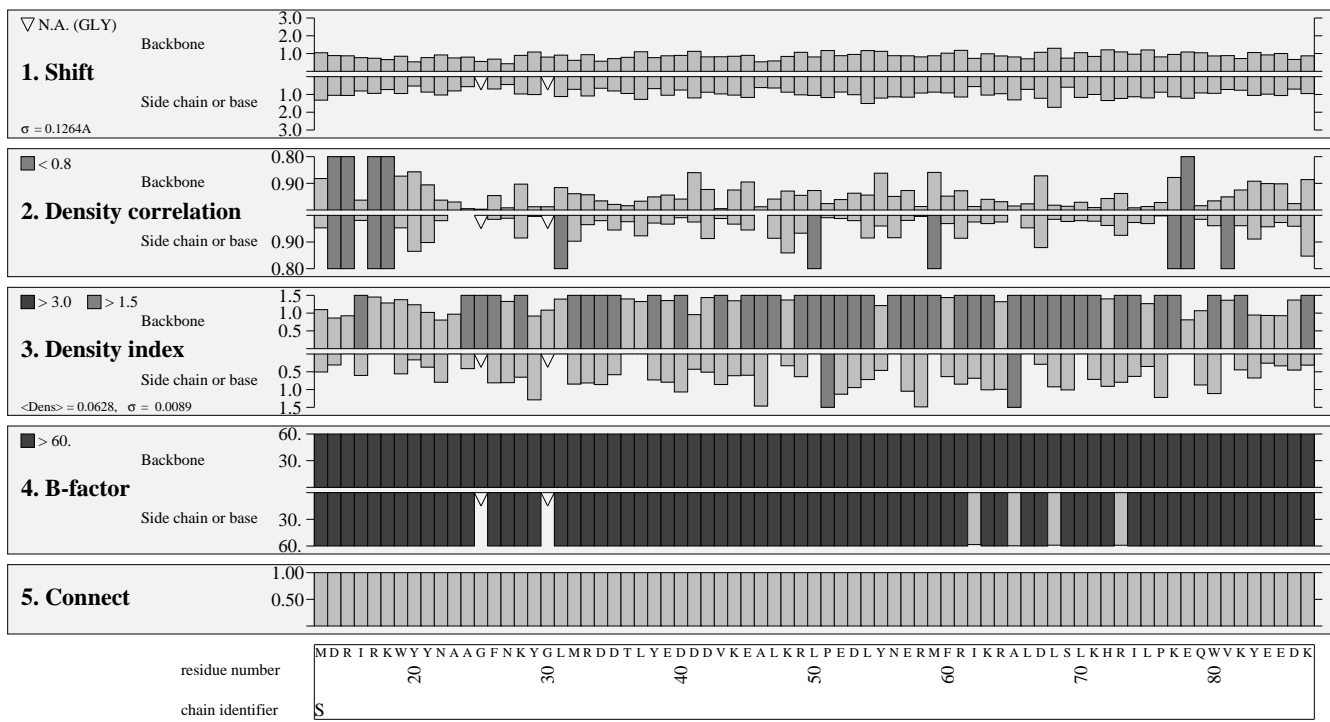
Local estimation (25)



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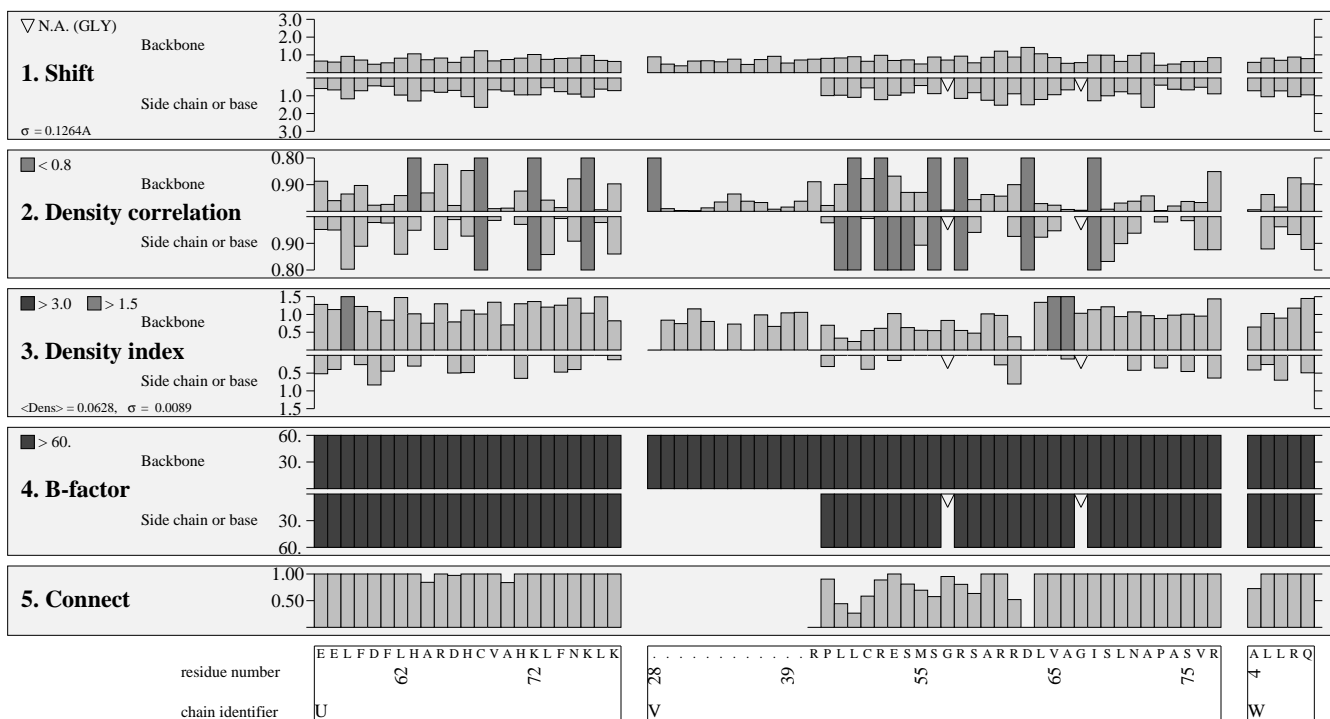
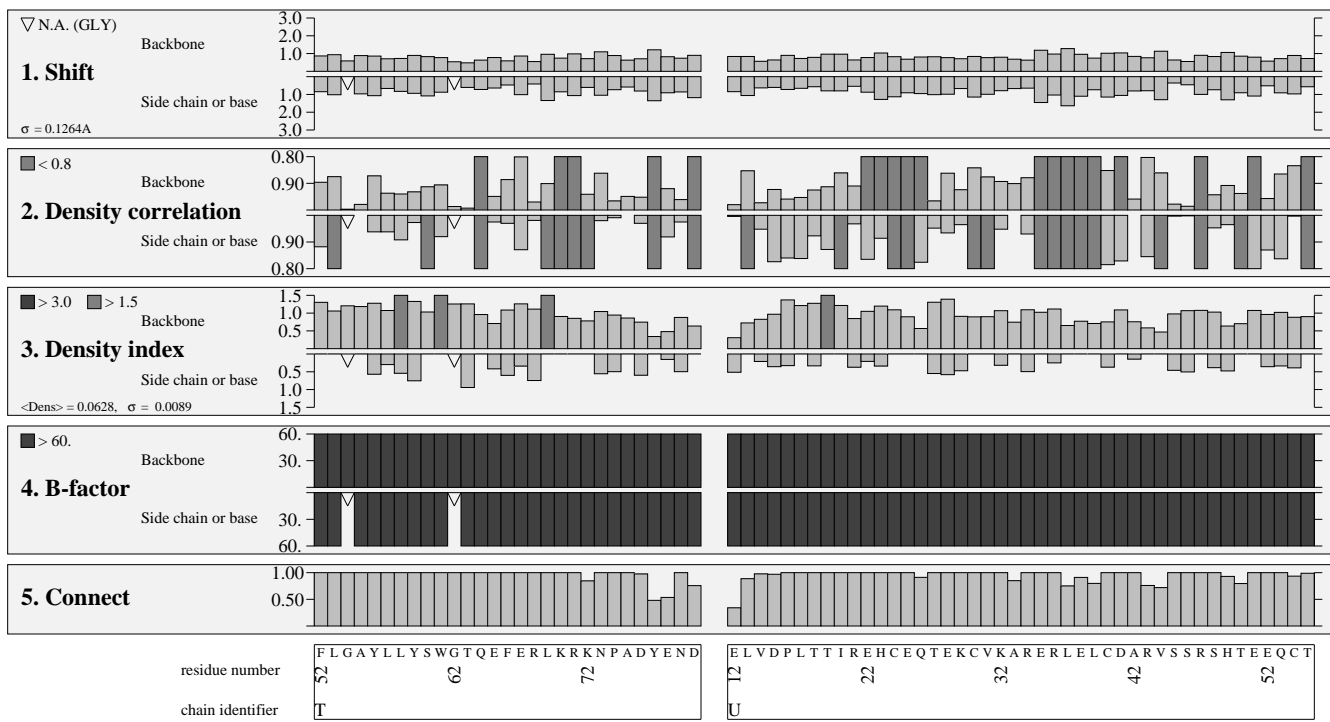
Local estimation (26)



Structure Factor Check

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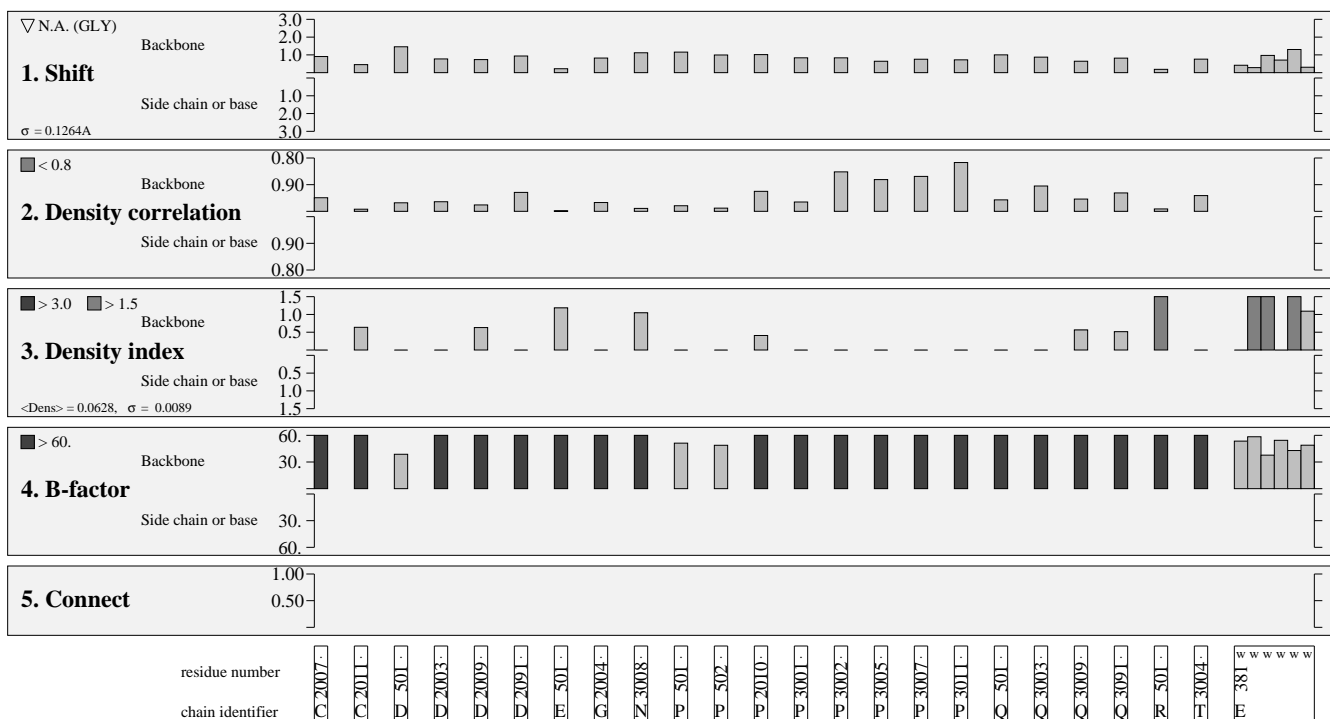
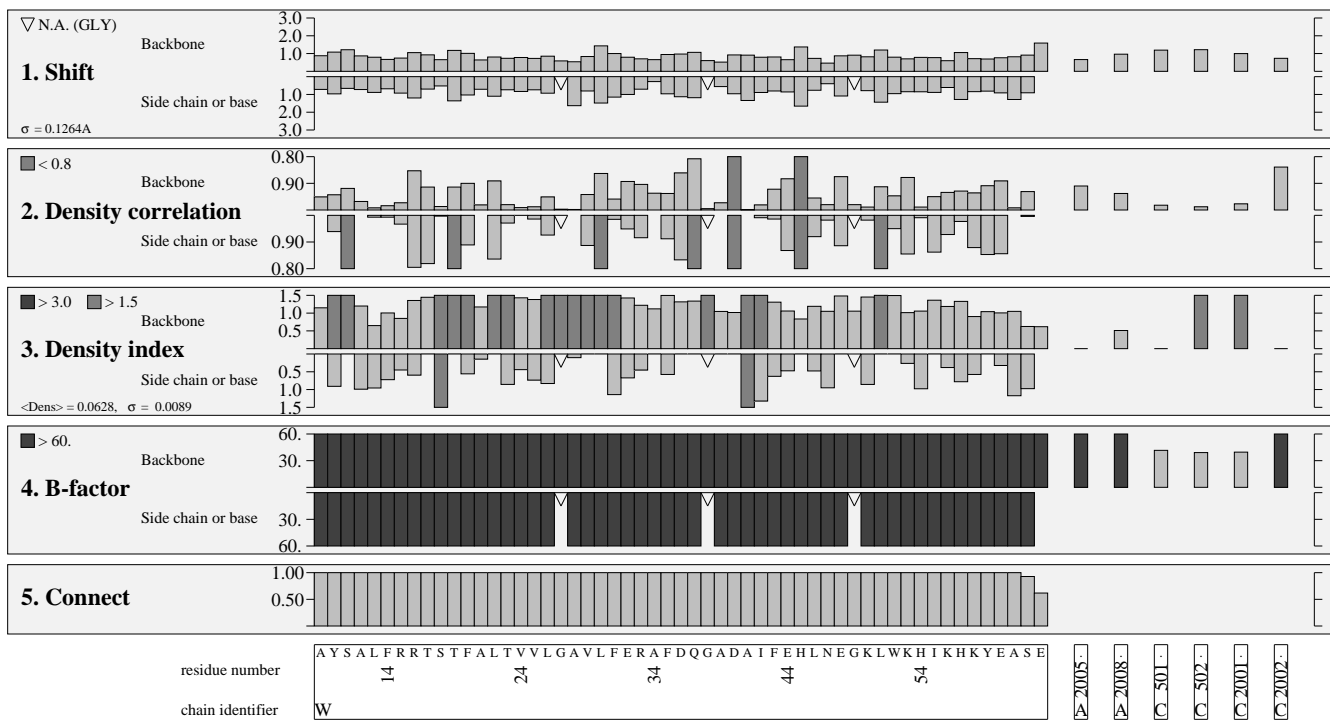
Local estimation (27)



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Local estimation (28)



Structure Factor Check

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Local estimation (29)



residue number

chain identifier

wwwwwwwww
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