

Structure Factor Check

2A06

Title: BOVINE CYTOCHROME BC1 COMPLEX WITH STIGMATELLIN BOUND
 Date: 16-JUN-05
 PDB code: 2A06

Crystal

Cell parameters:

a: 128.25 Å b: 168.80 Å c: 230.82 Å
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Number of NCS-operators: 1
 NC-symmetry only for information

Structure Factors

Input

Nominal resolution range: 37.9 – 2.00 Å
 Reflections in file: 308086
 Unique reflections above 0: 308086
 above 1 σ : 300977
 above 3 σ : 180169

SF CHECK

Nominal resolution range: 37.9 – 2.10 Å
 \05max. from input data, min. from author\05
 Used reflections: 276806
 Reflections out of resolution: 31280
 Completeness: 95.3 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.057
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.9620 1.0000 0.8986
 B_{overall} (by Patterson): 37.Å²
 Optical resolution: 1.73 Å
 Expected opt. resol. for complete data set: 1.73 Å
 Estimated minimal error: 0.033 Å

Model

33890 atoms (1612 water molecules)
 Number of chains: 51
 Volume not occupied by model: 42.2 %
 $\langle B \rangle$ (for atomic model): 48.1 Å²
 $\sigma(B)$: 16.67 Å²
 Matthews coefficient: 2.63
 Corresponding solvent % : 52.92

Model vs. Structure Factors

R-factor for all reflections: 0.238
 Correlation factor: 0.933
 R-factor: 0.243
 for $F > 2.0\sigma$
 nom. resolution range: 37.87 – 2.10 Å
 reflections used: 271225

Rfree: 0.282
 Nfree: 13479
 R-factor without free-refl.: 0.241
 Non free-reflections: 257746
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.300 Å
 Estimated maximal error: 0.084 Å
 DPI: 0.174 Å

Scaling

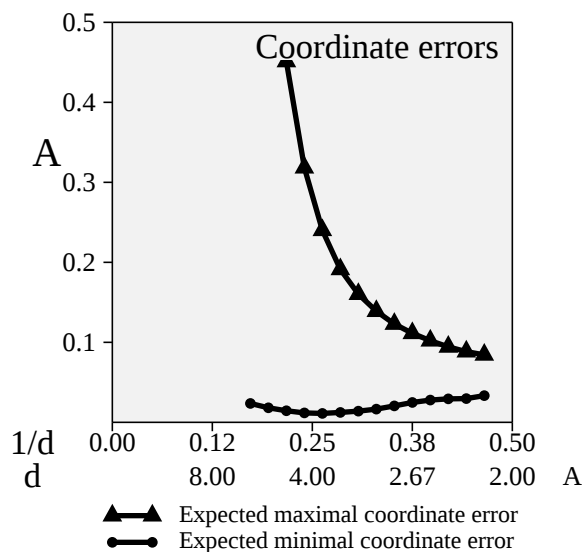
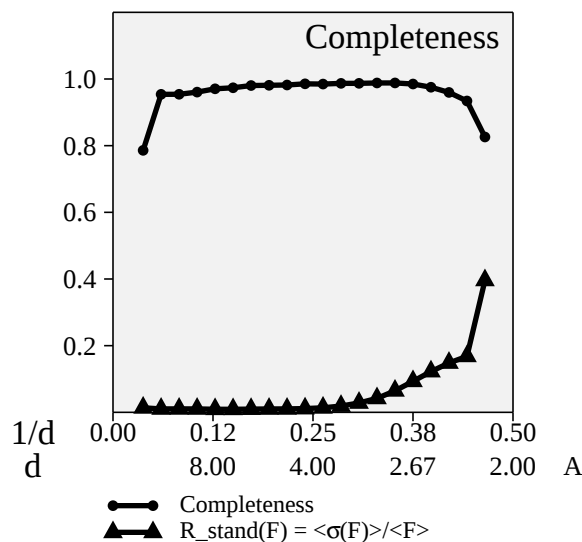
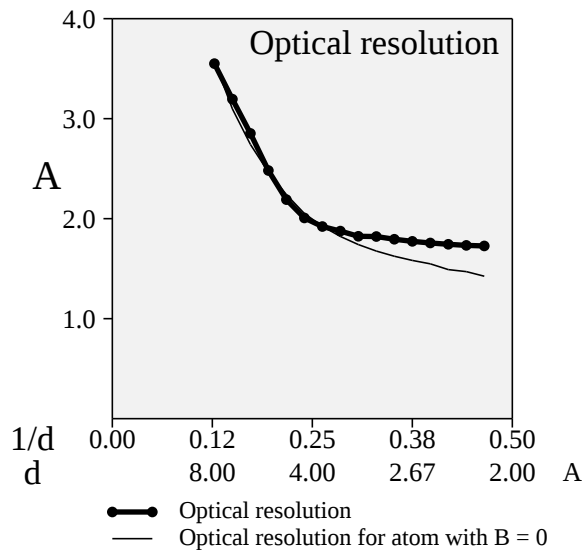
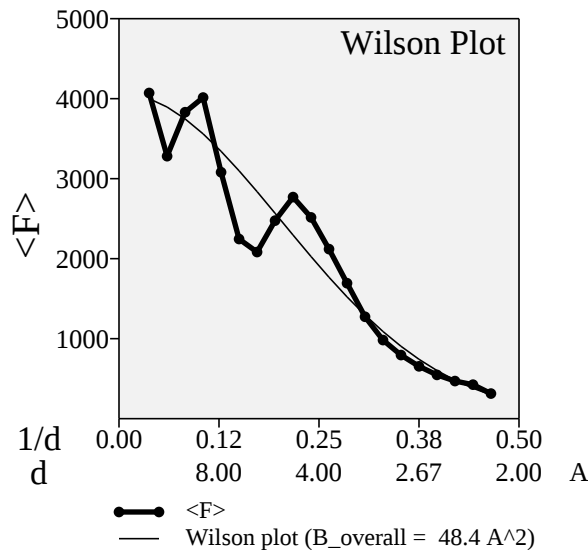
Scale: 1.718
 B_{diff} : -4.66
 Anisothermal Scaling (Beta):
 1.9764 2.2039 0.7640 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.832 250.036

Refinement

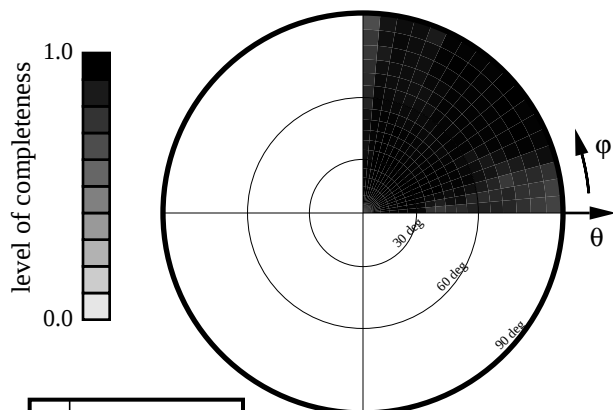
Program: CNS 1.1
 Nominal resolution range: 37.9 – 2.10 Å
 Reported R-factor: 0.222
 Number of reflections used: 276810
 Reported Rfree: 0.26
 Sigma cut-off: N.A.

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2A06

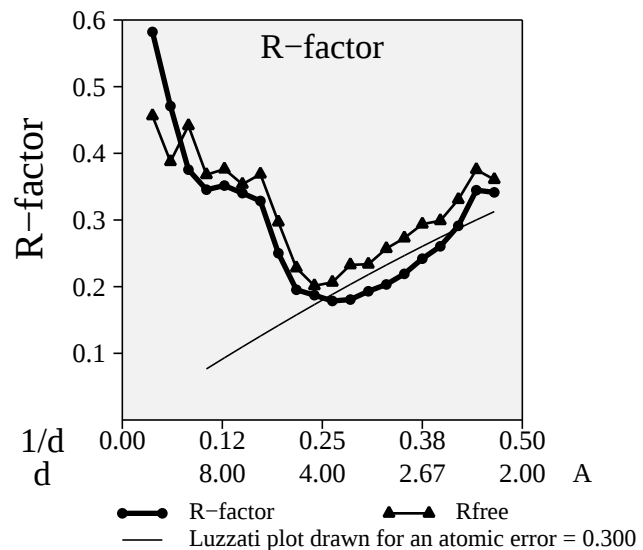


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

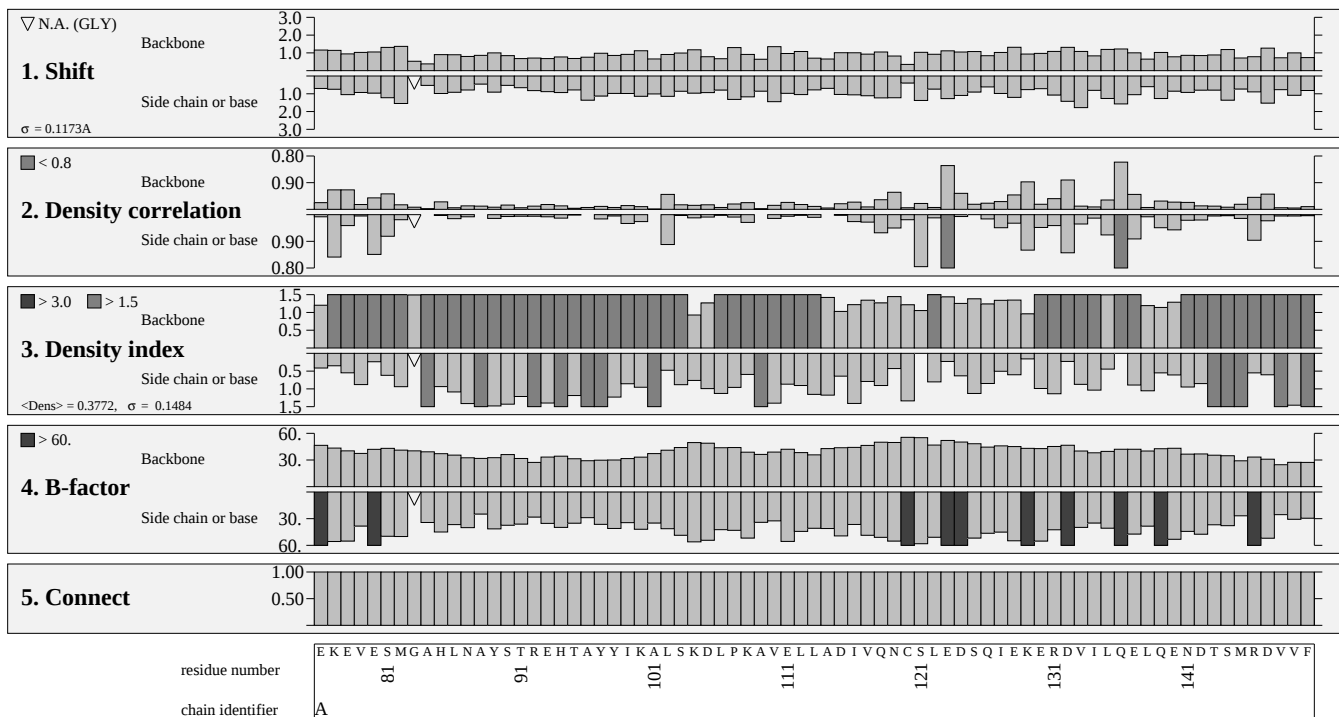
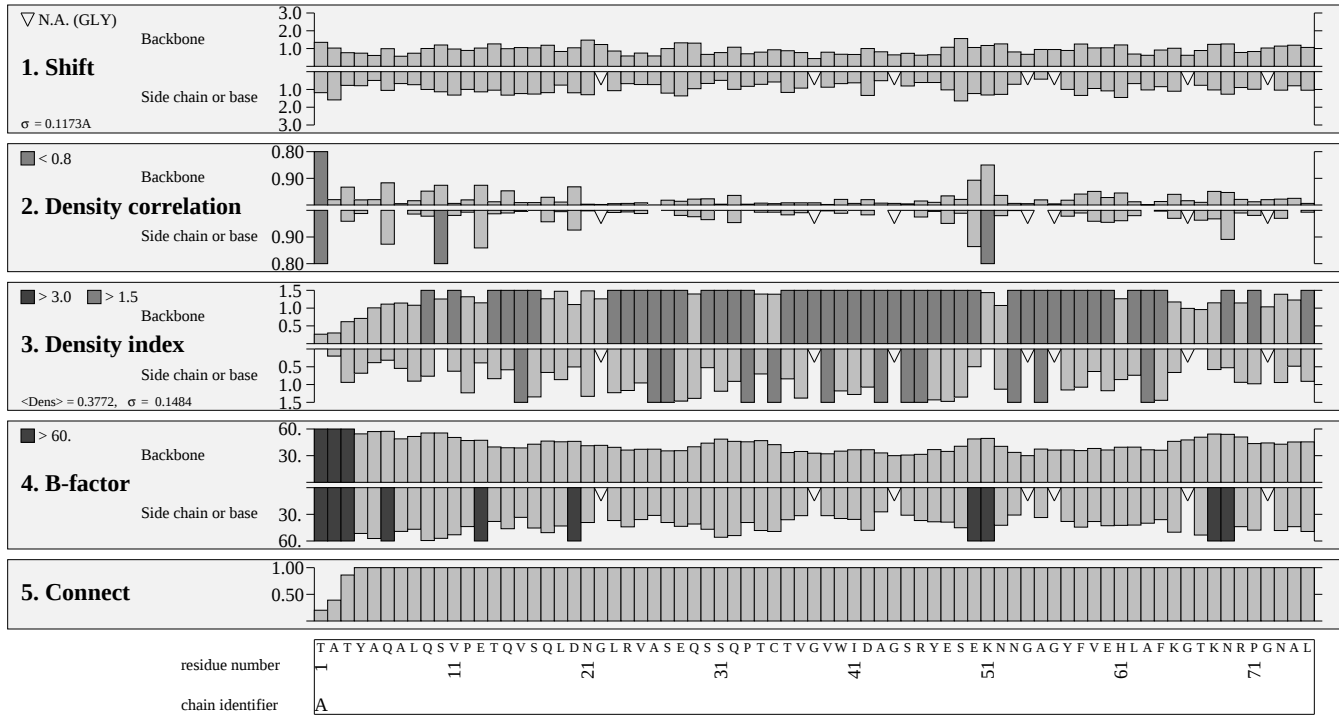
polar coordinates of the crystallographical axes



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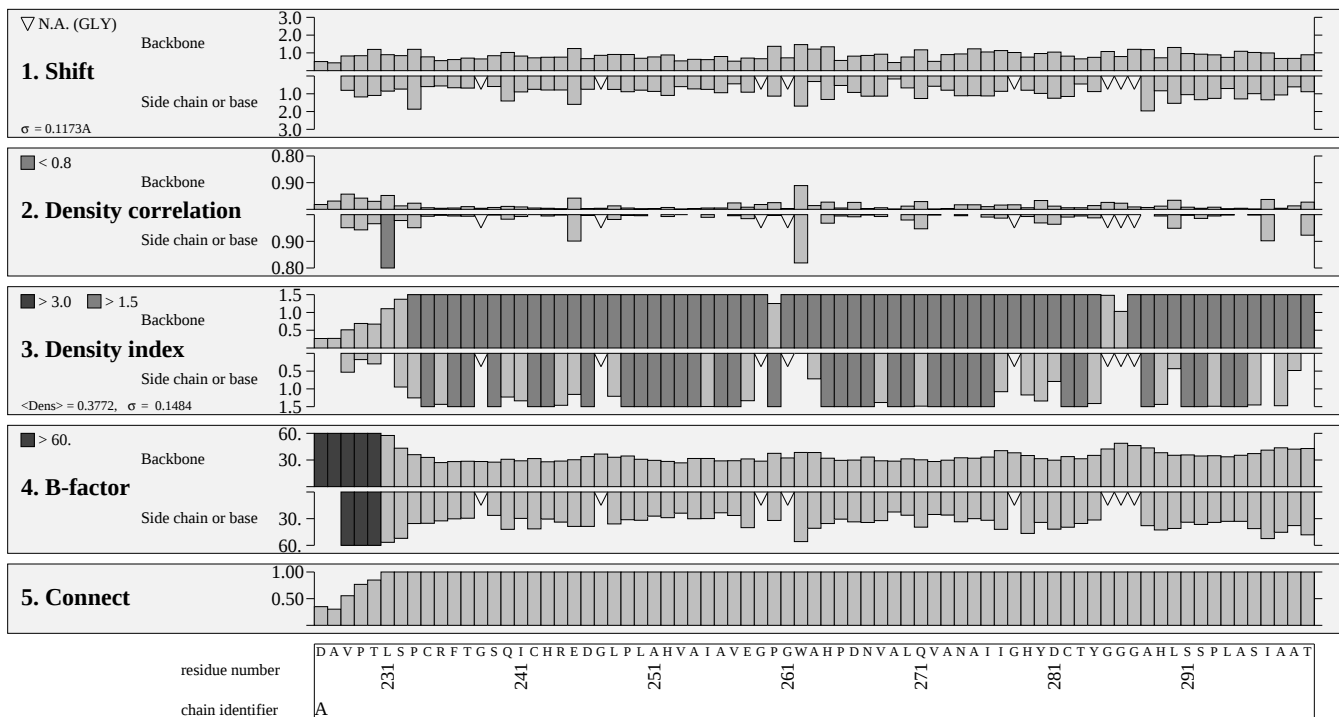
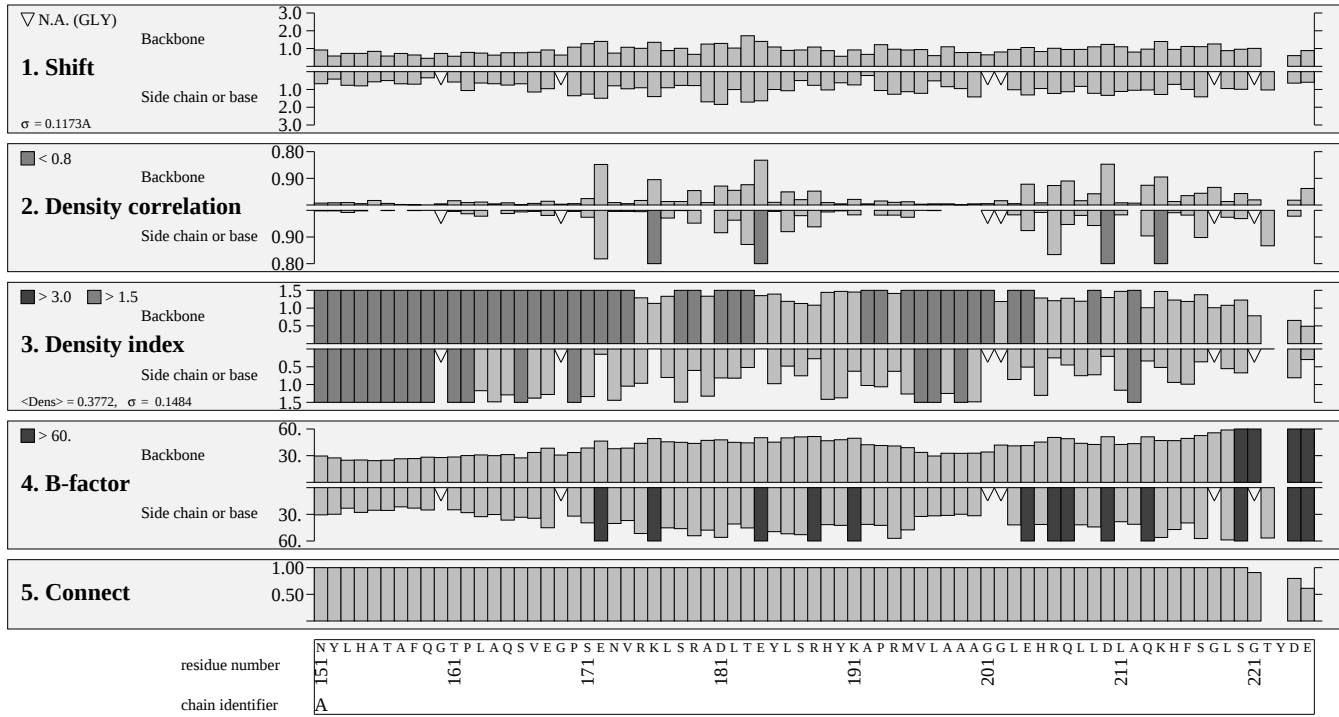
Local estimation



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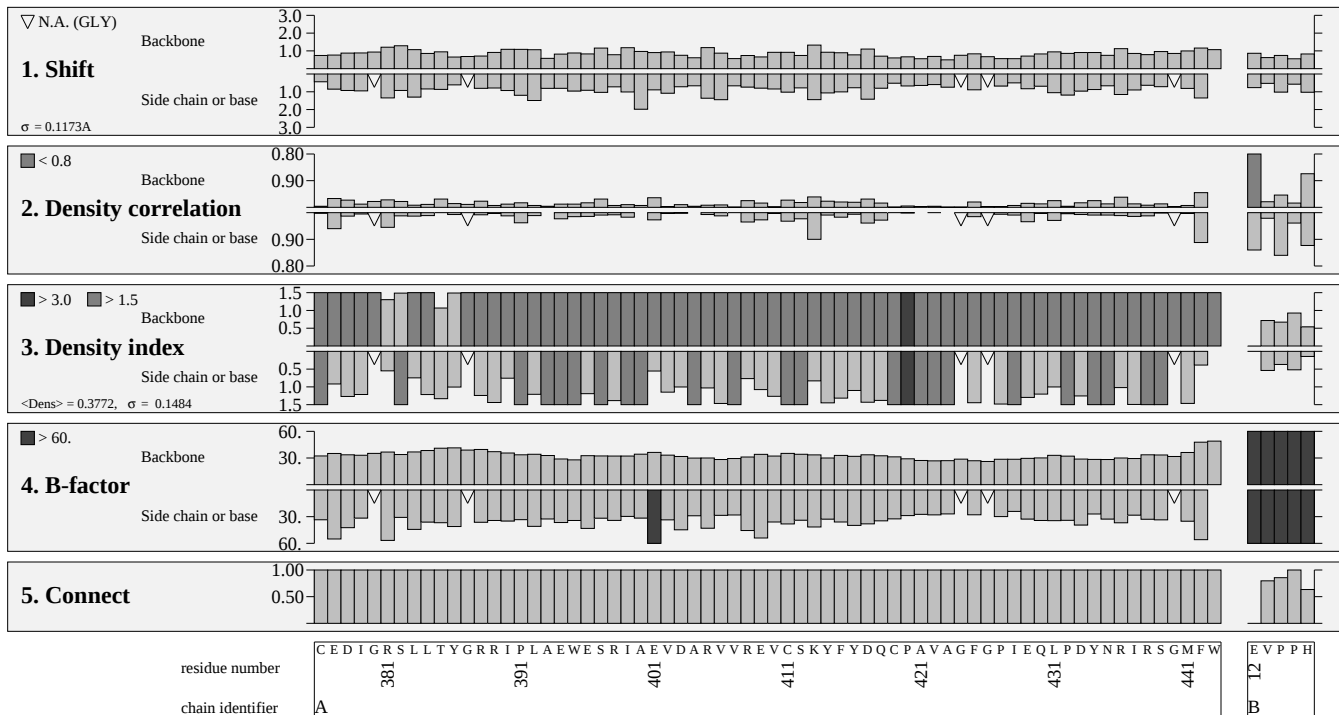
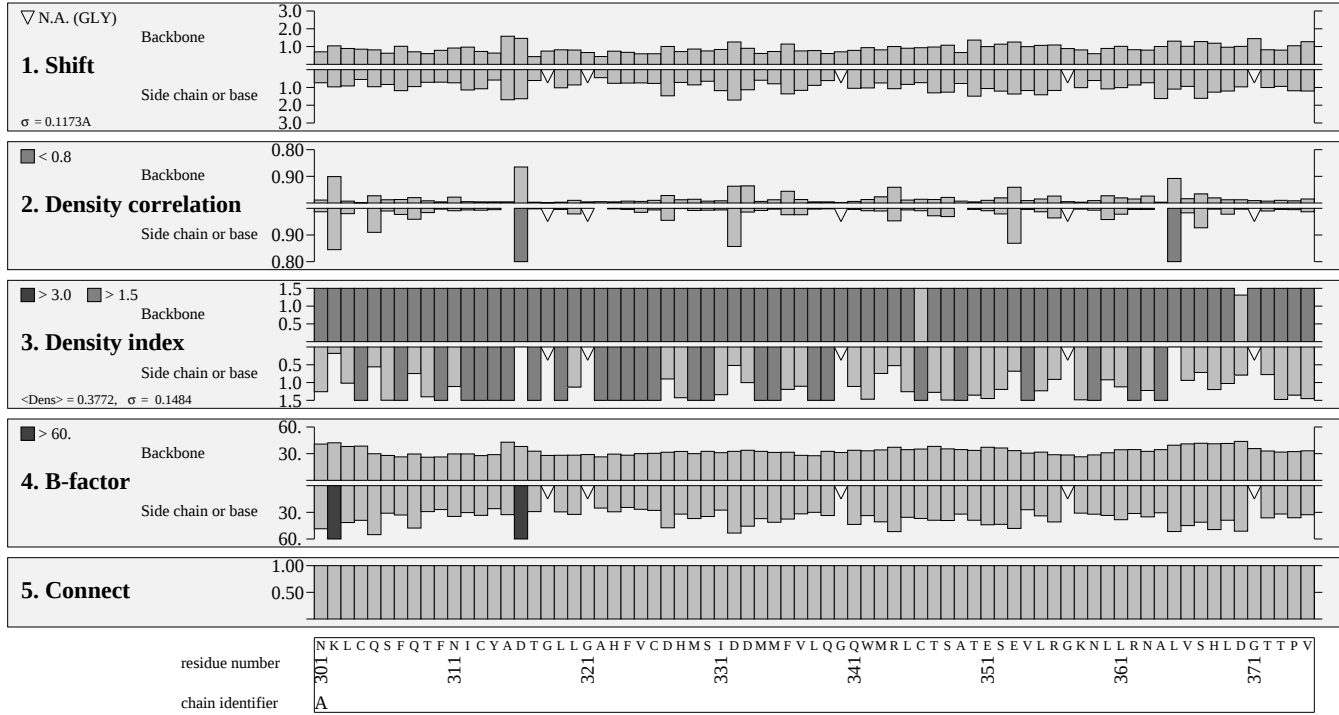
Local estimation (2)



Structure Factor Check

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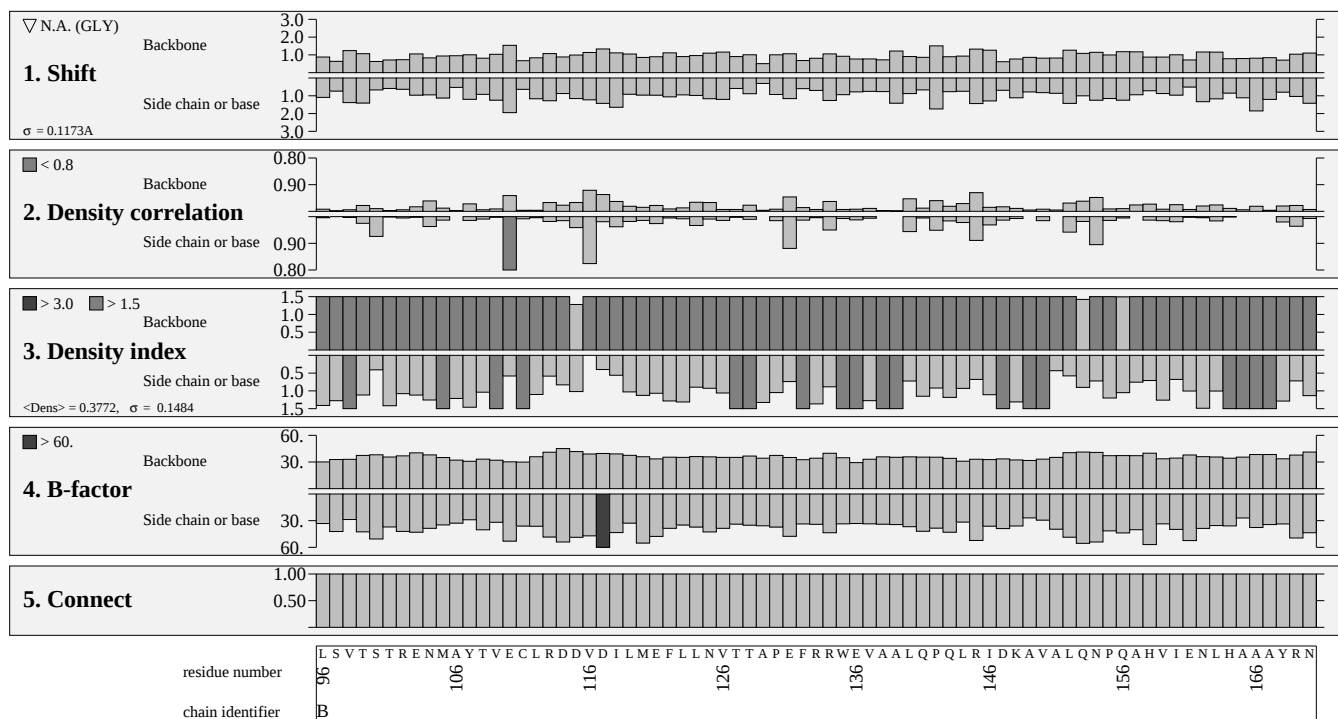
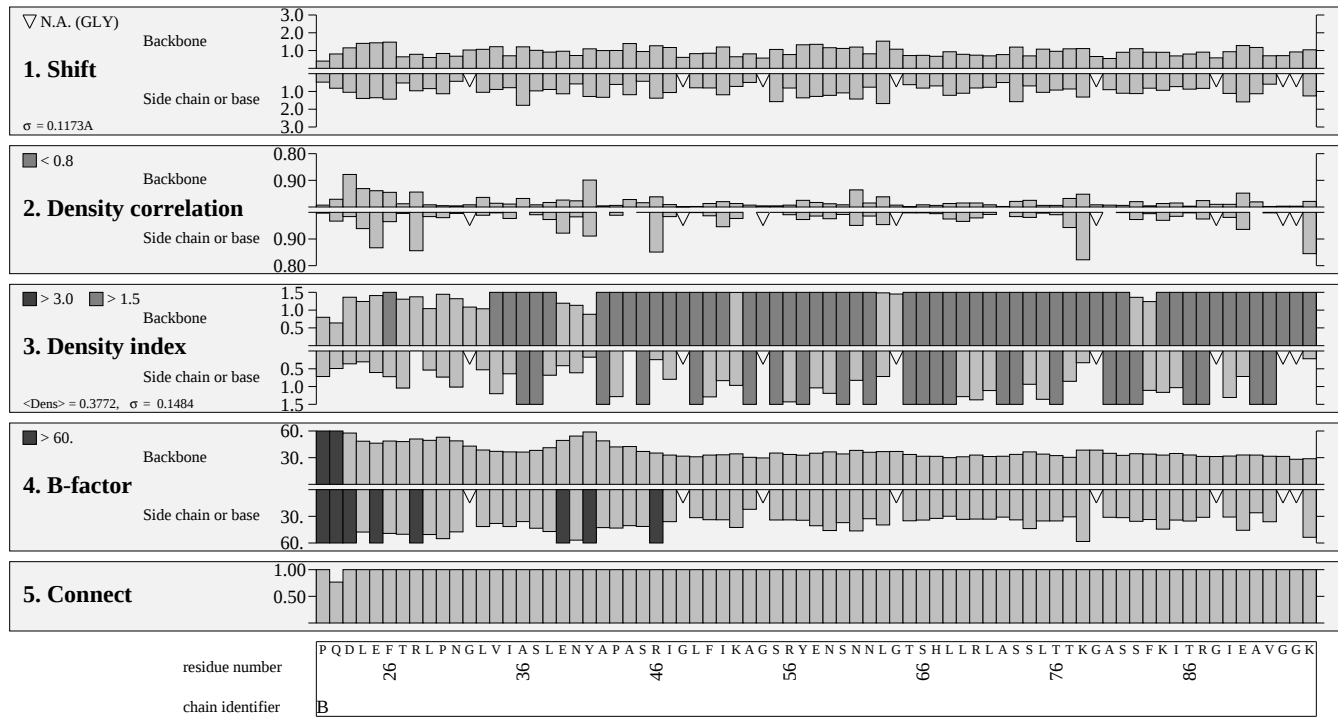
Local estimation (3)



Structure Factor Check

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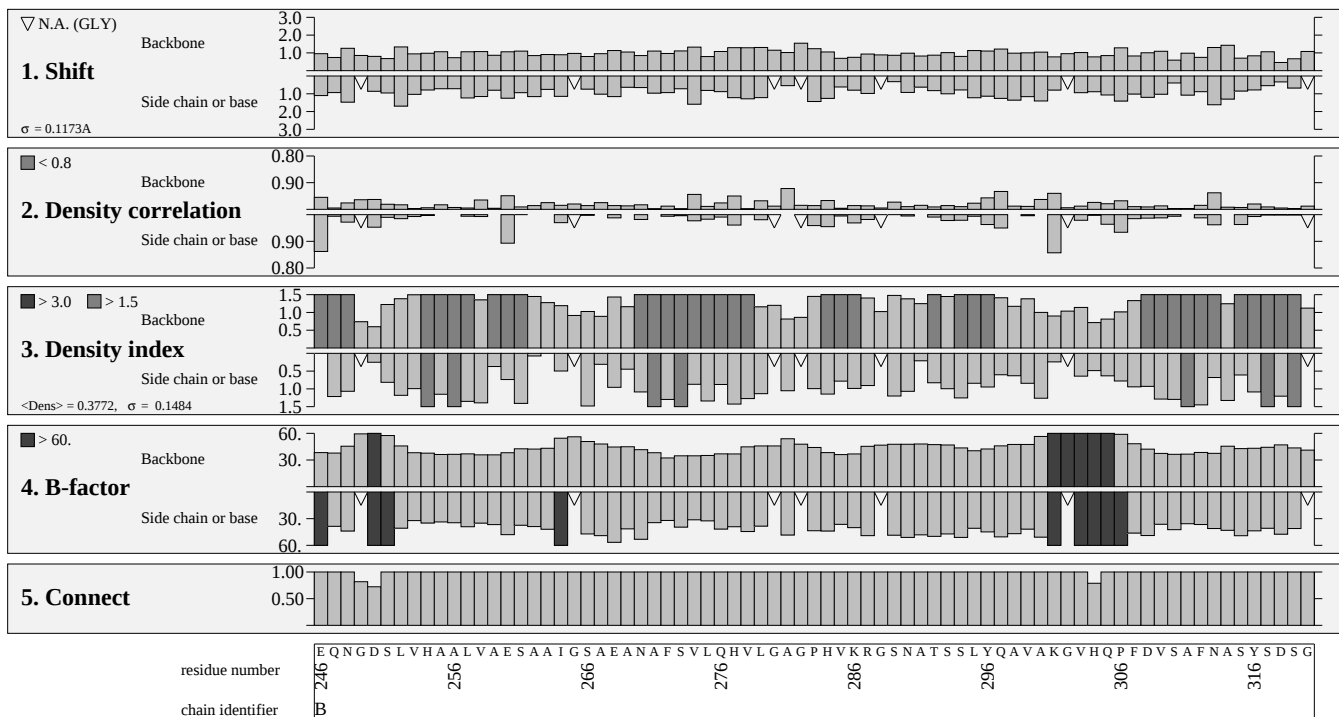
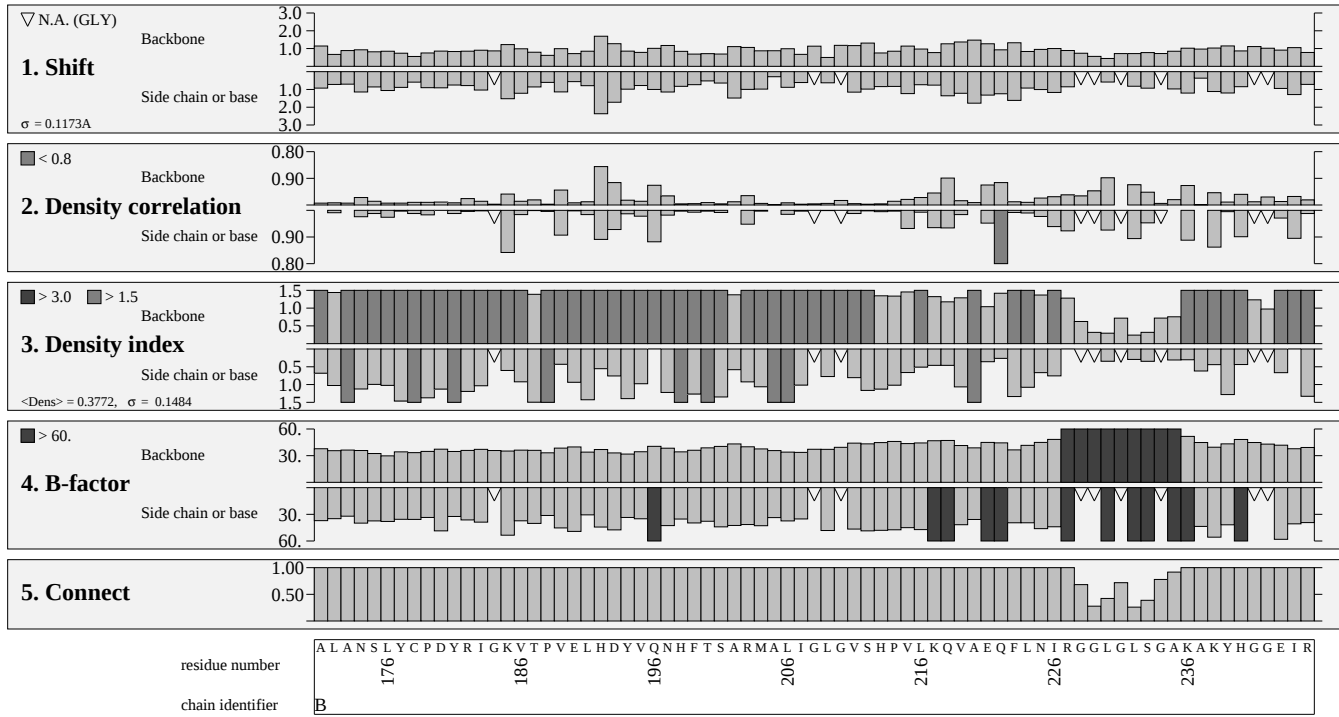
Local estimation (4)



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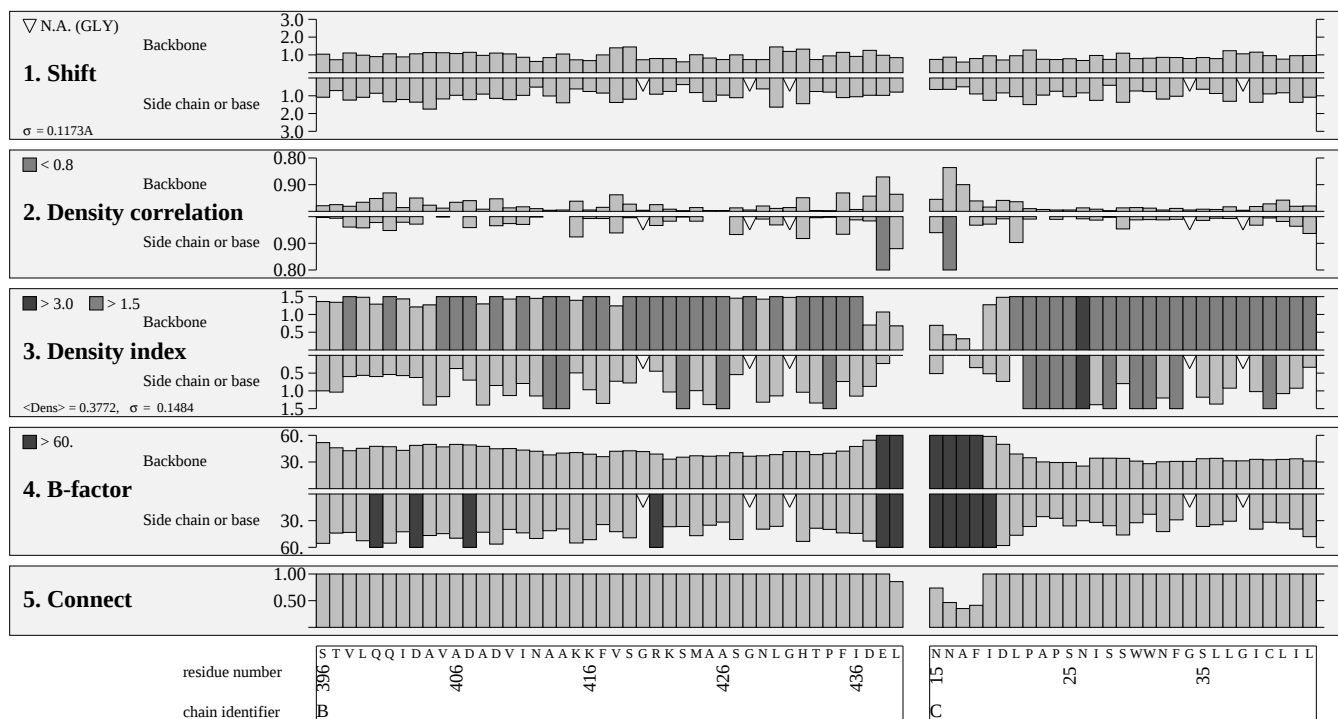
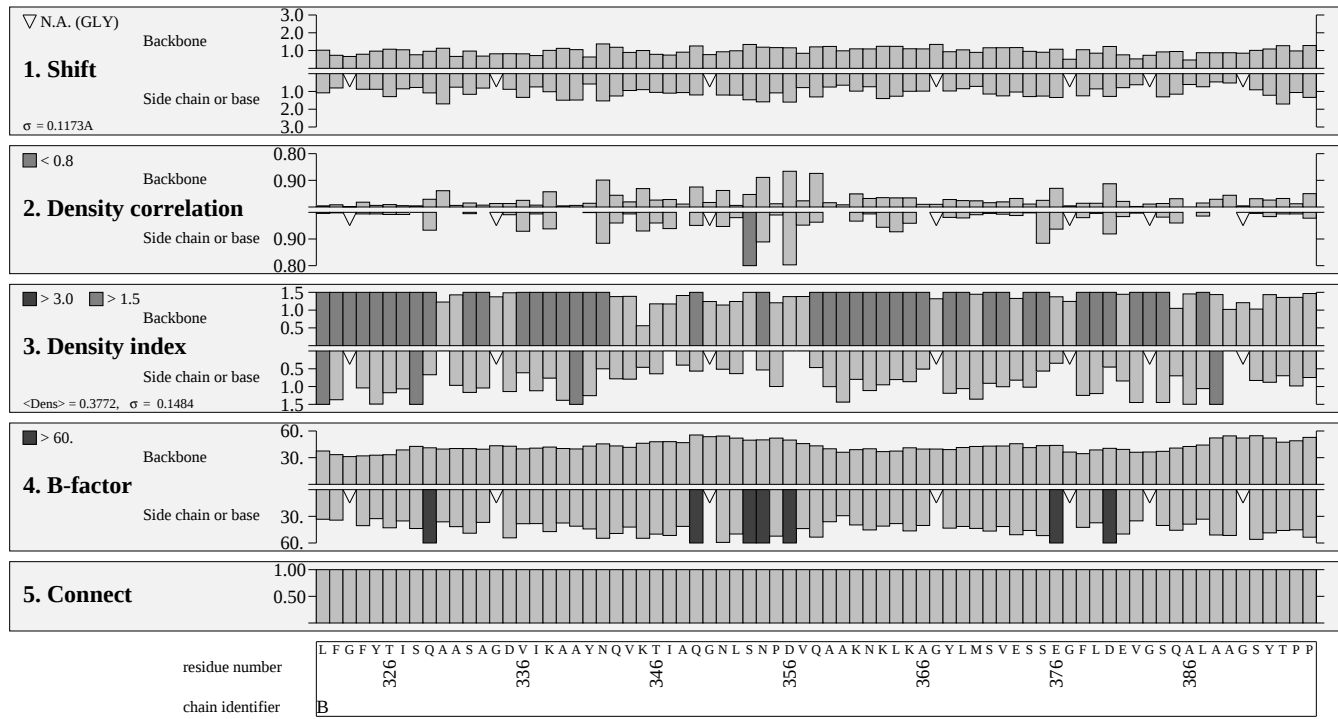
Local estimation (5)



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2A06

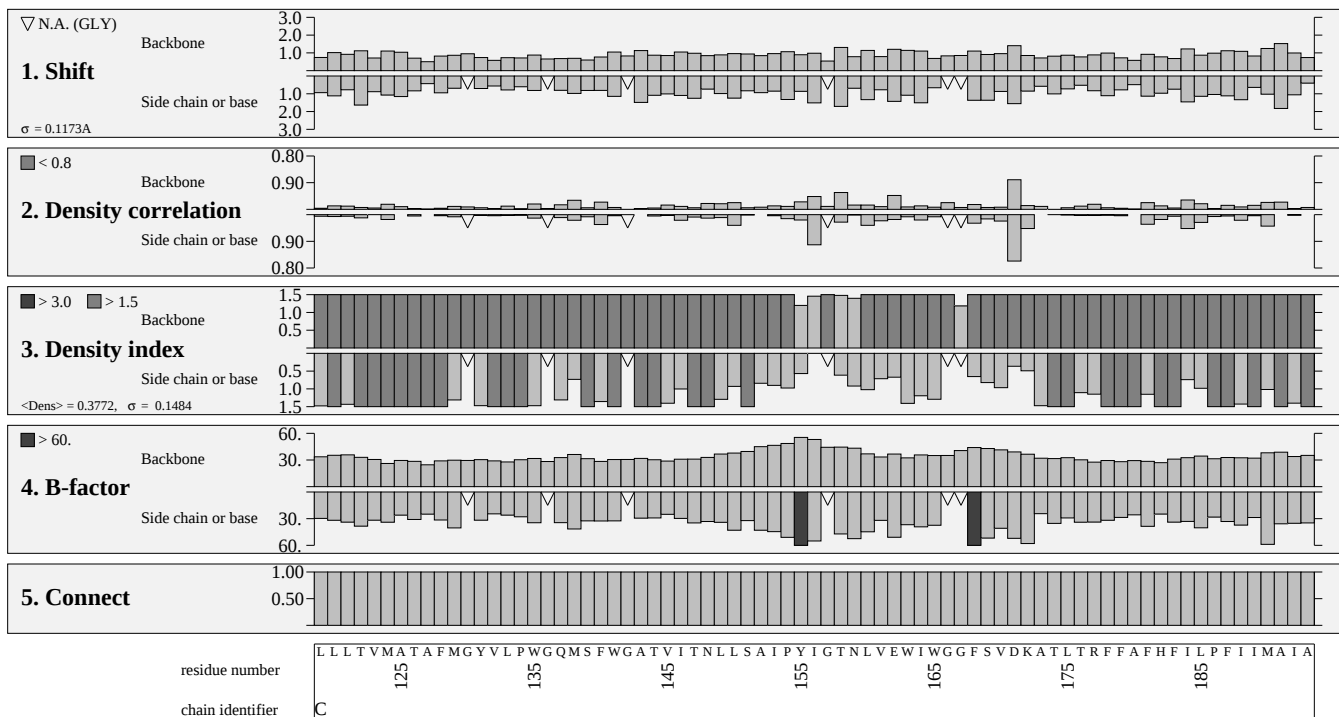
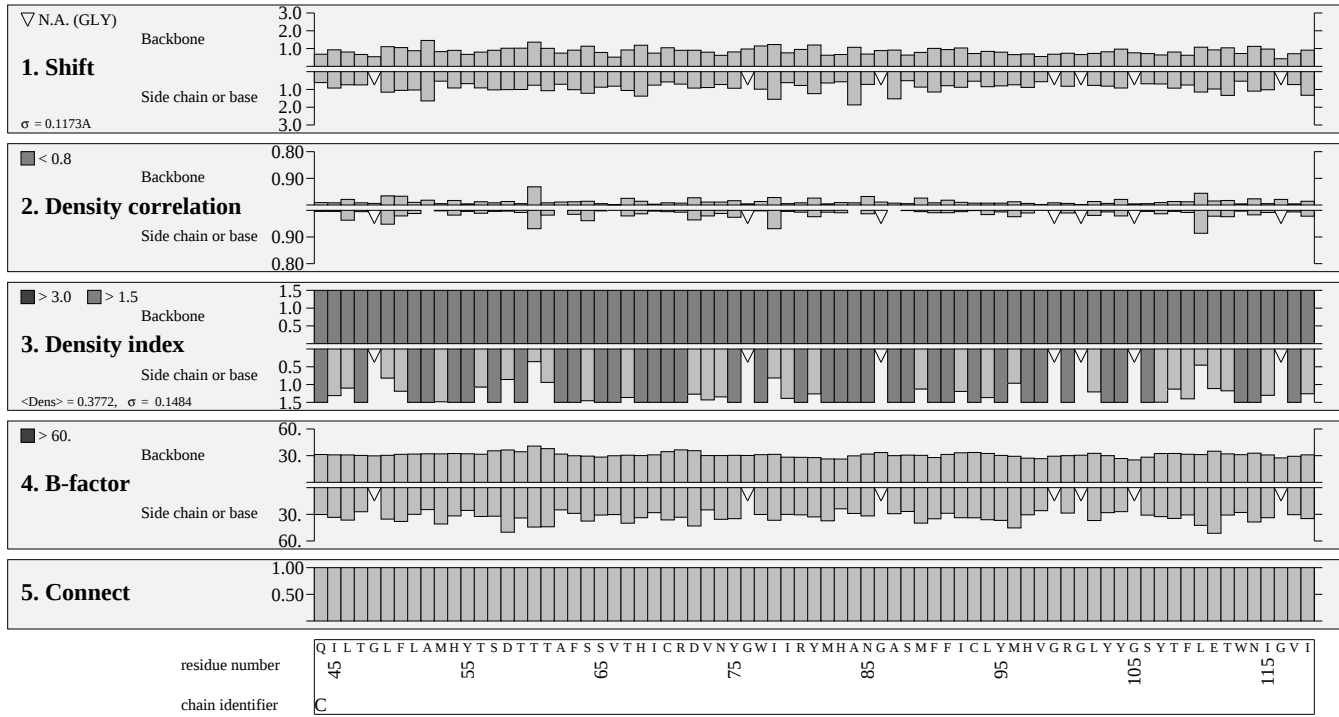
Local estimation (6)



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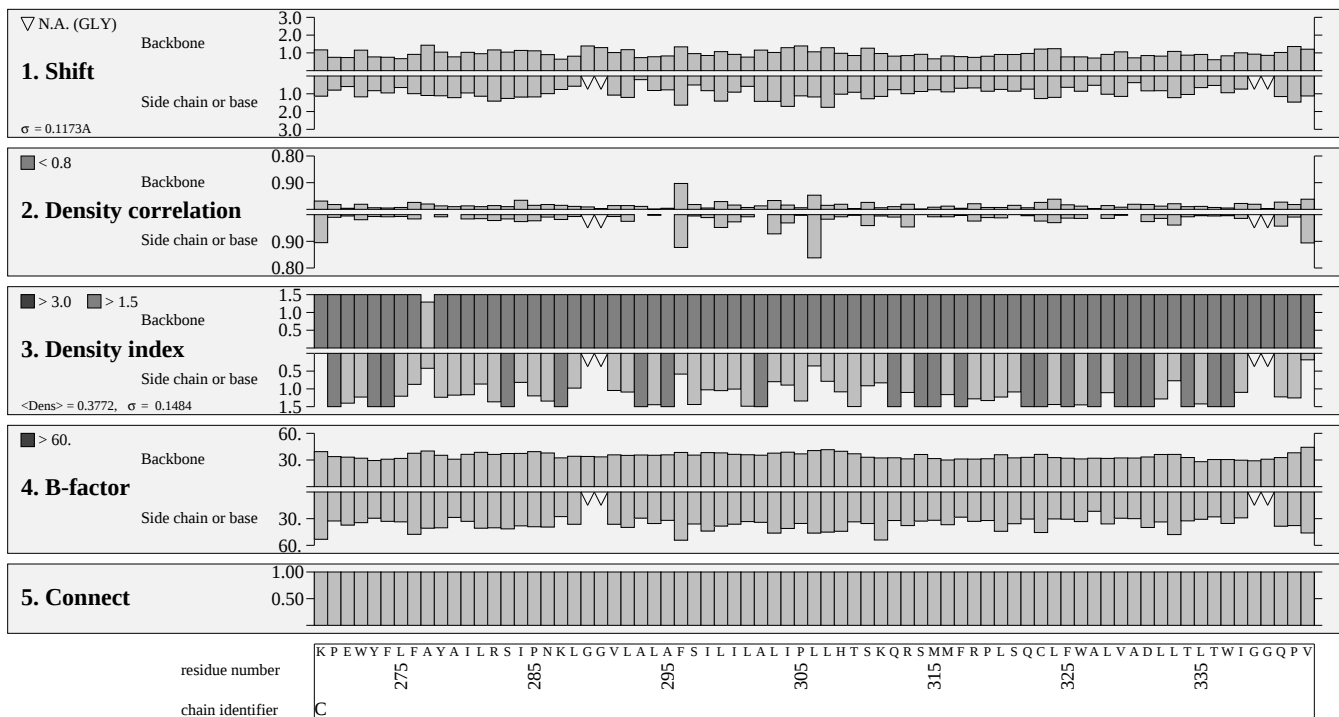
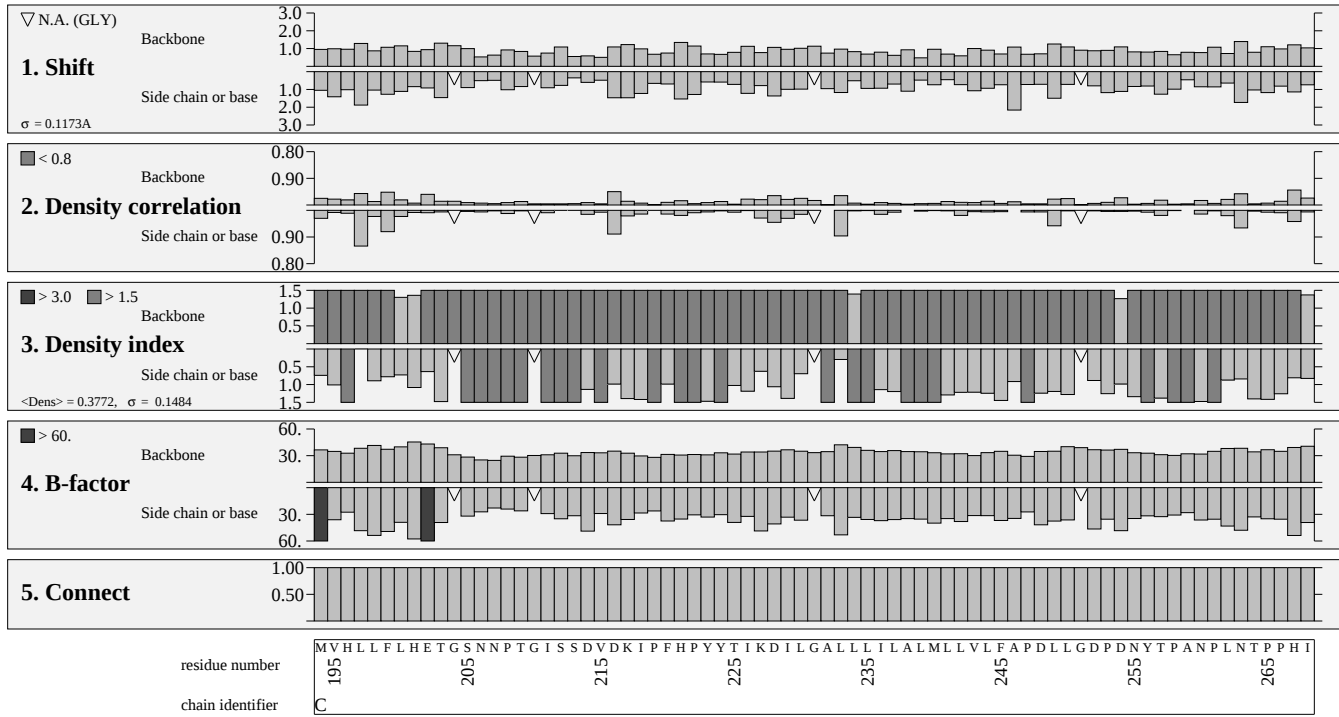
Local estimation (7)



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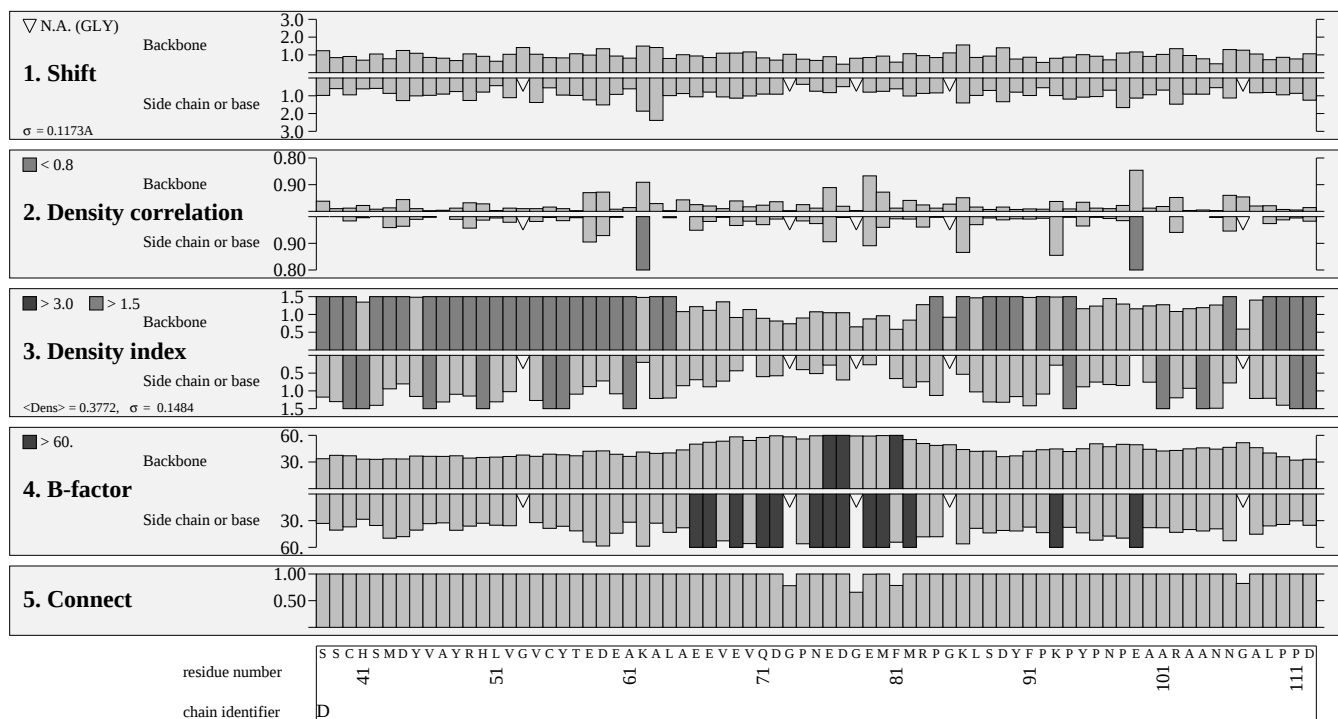
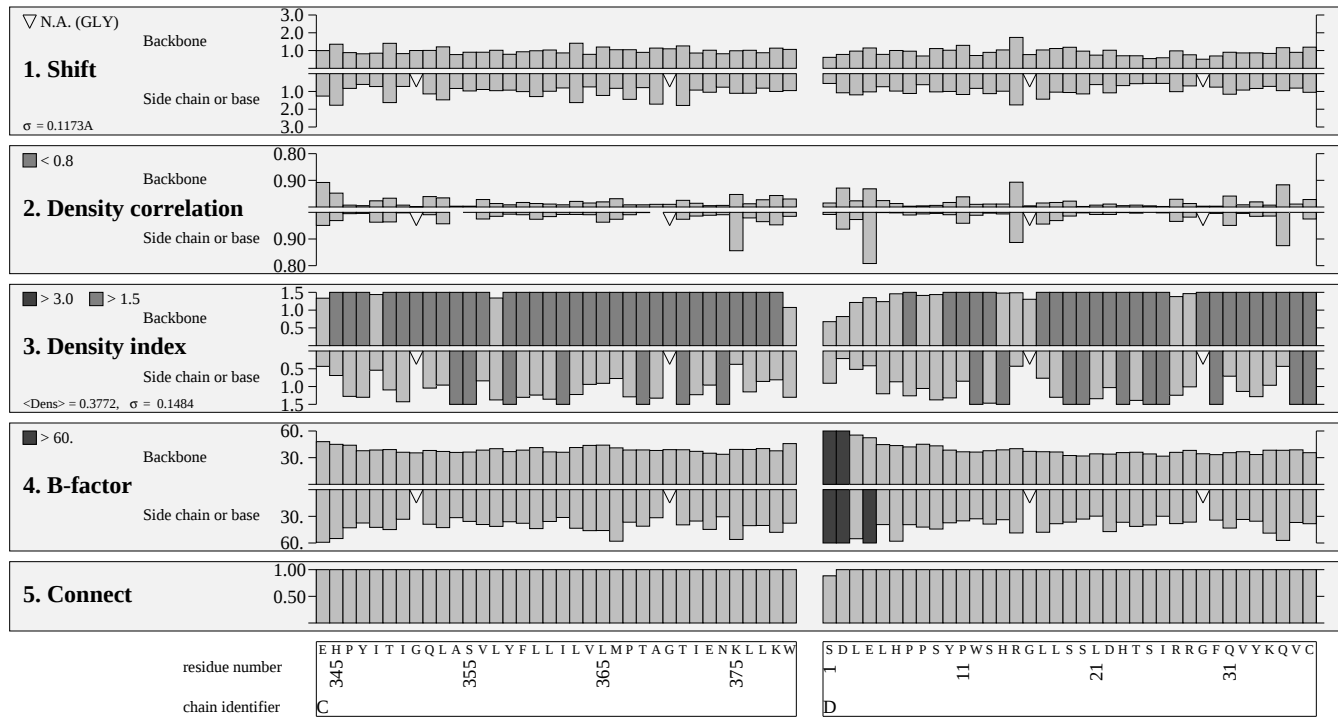
Local estimation (8)



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2A06

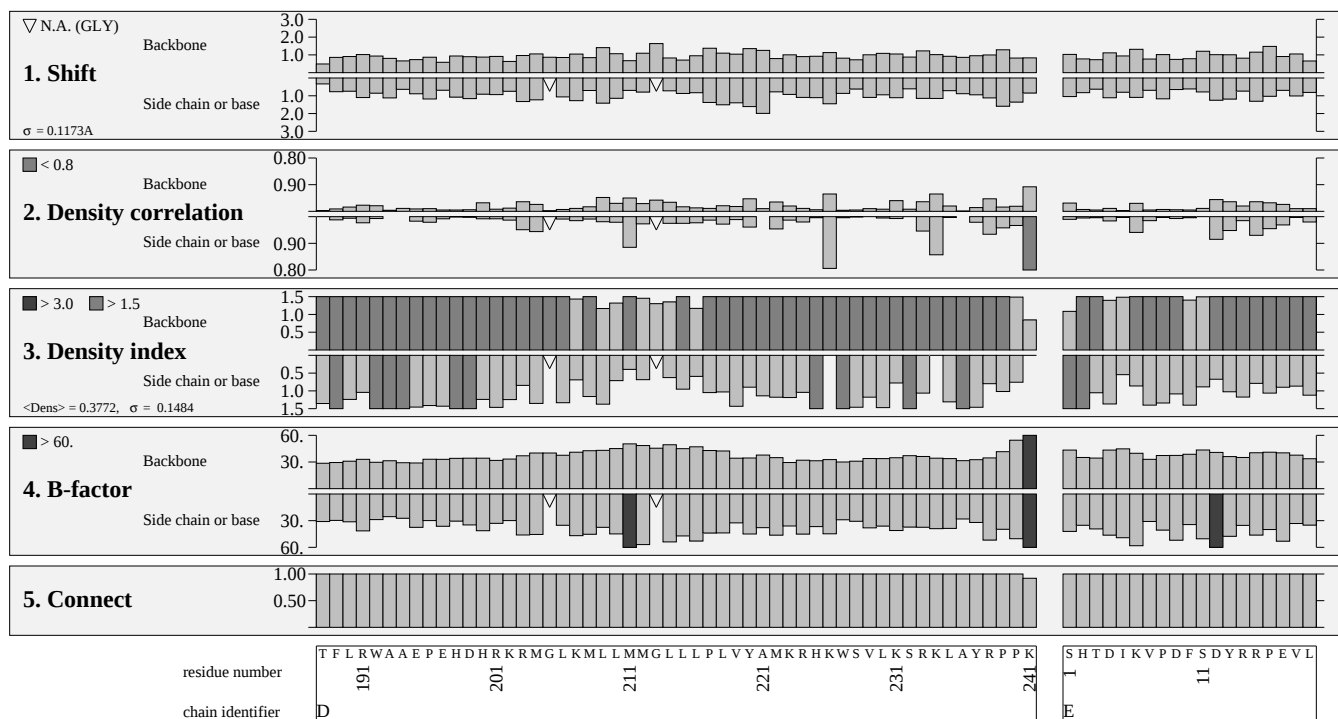
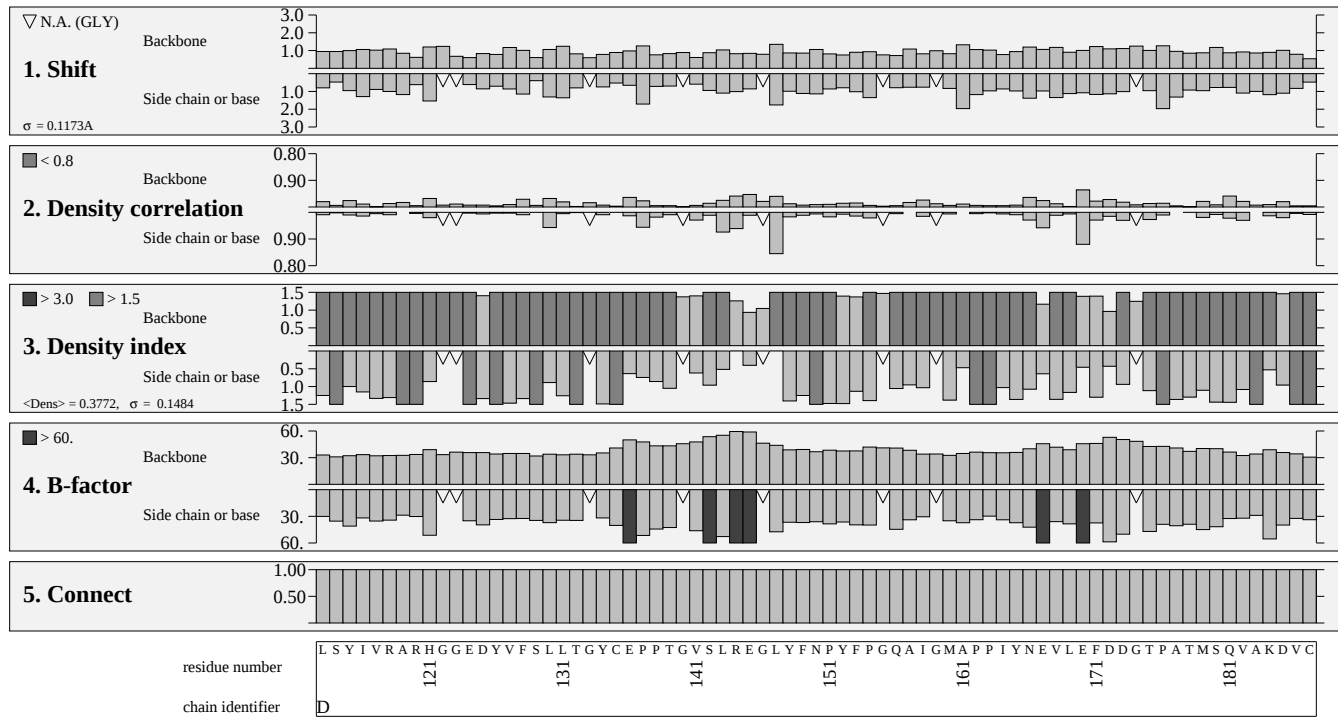
Local estimation (9)



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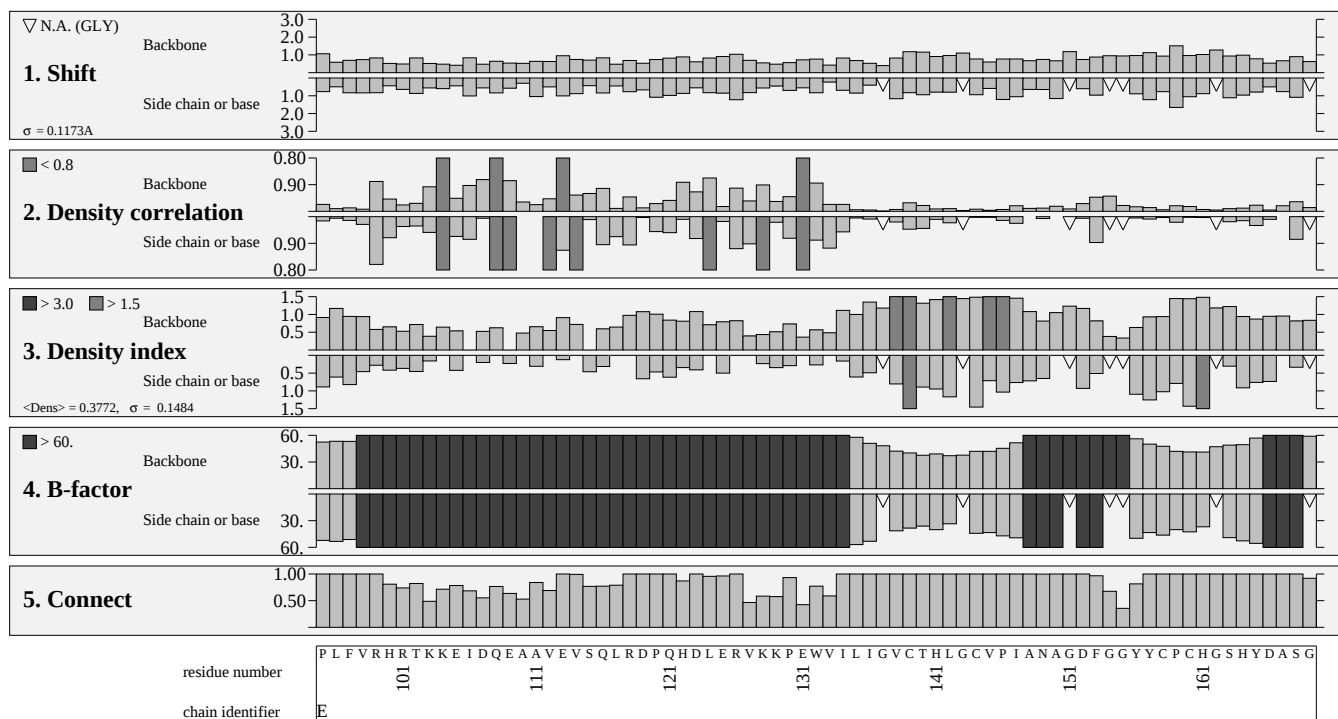
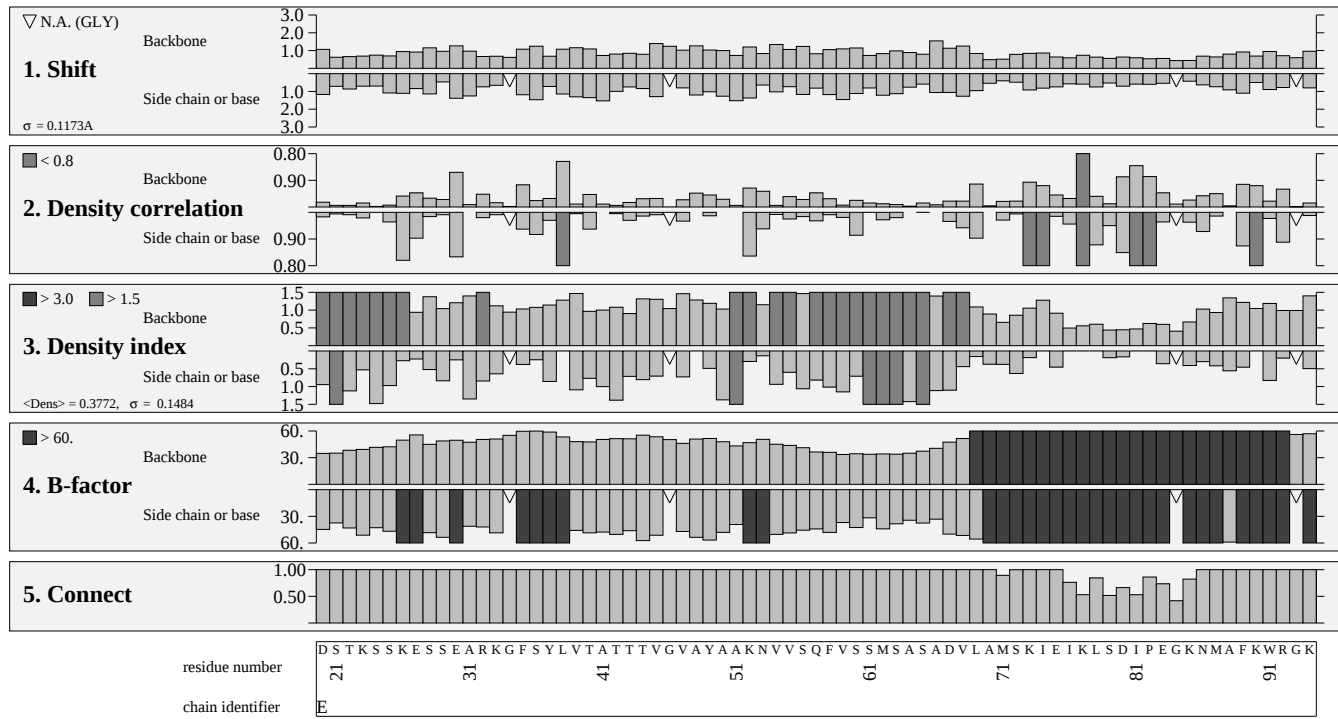
Local estimation (10)



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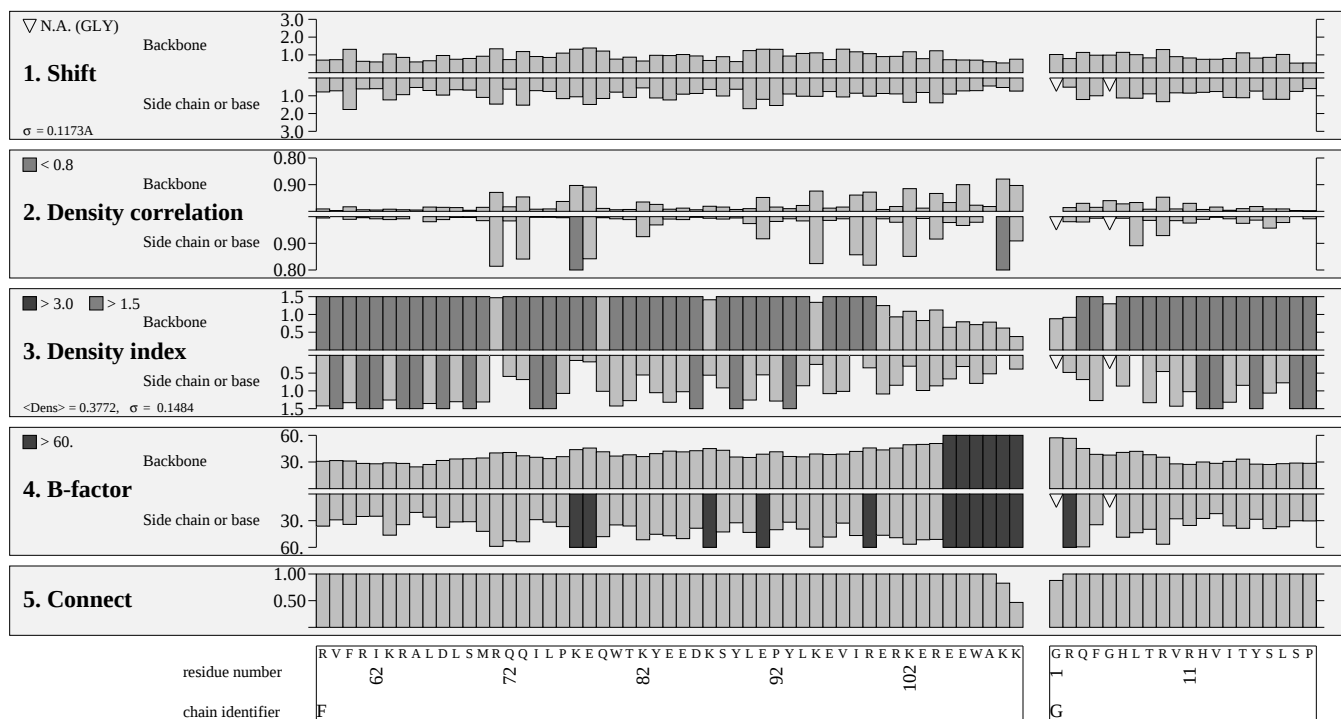
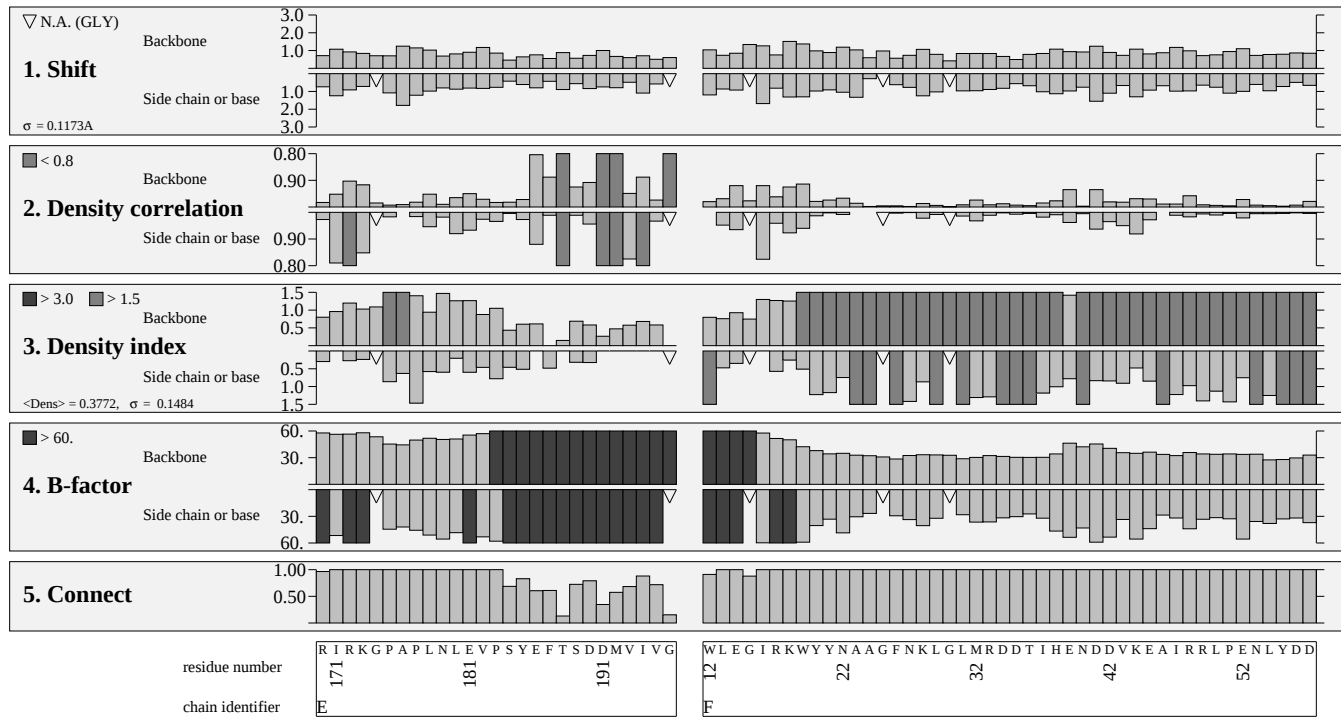
Local estimation (11)



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2A06

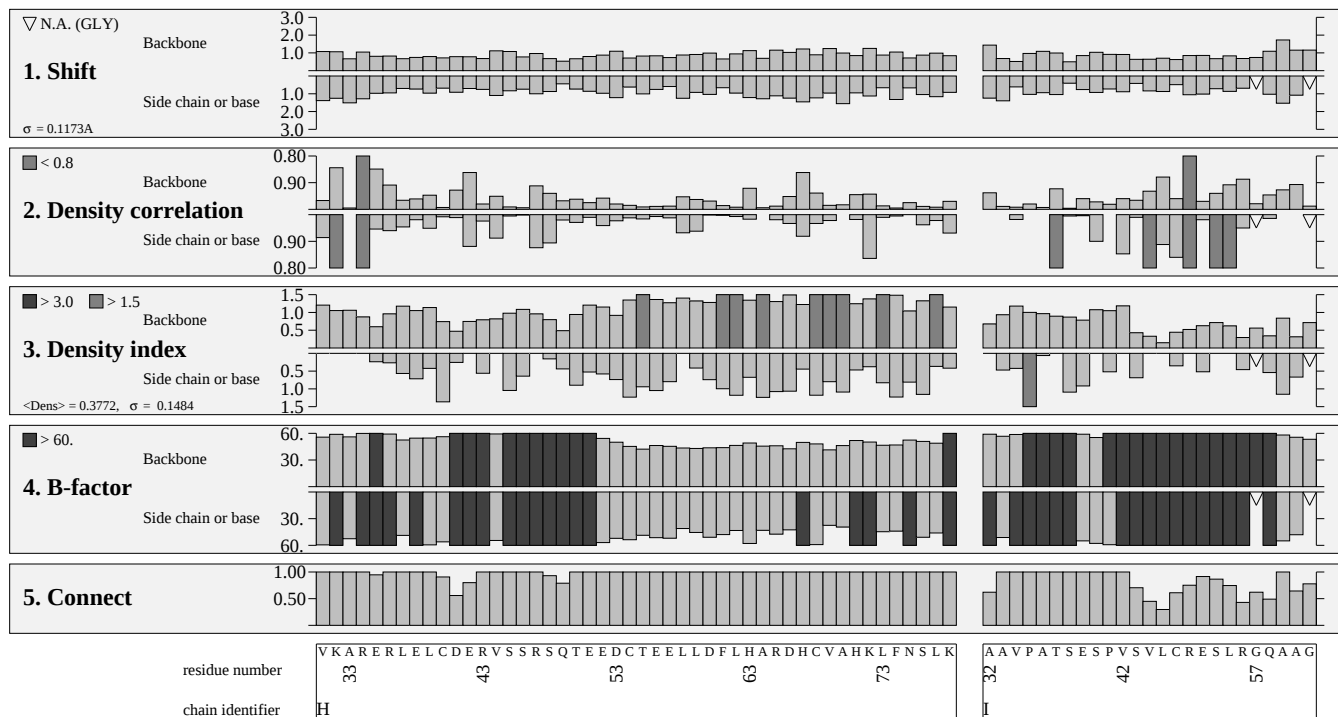
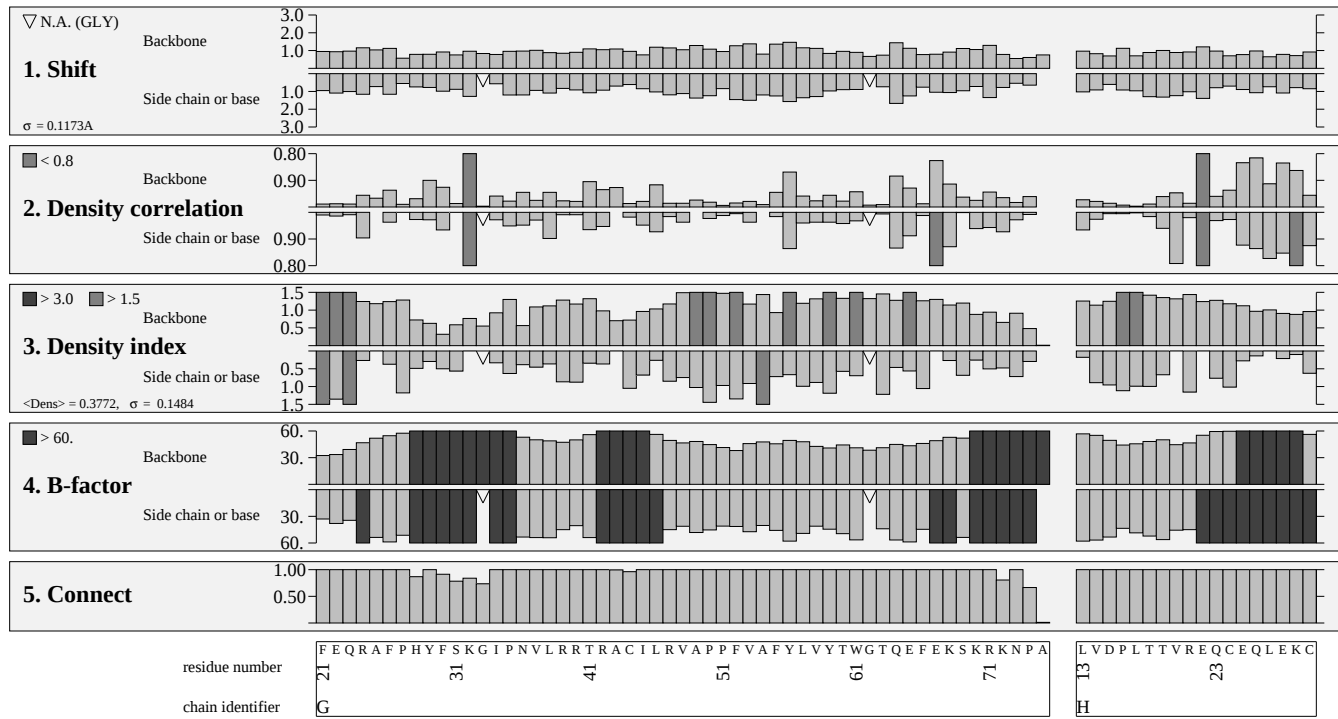
Local estimation (12)



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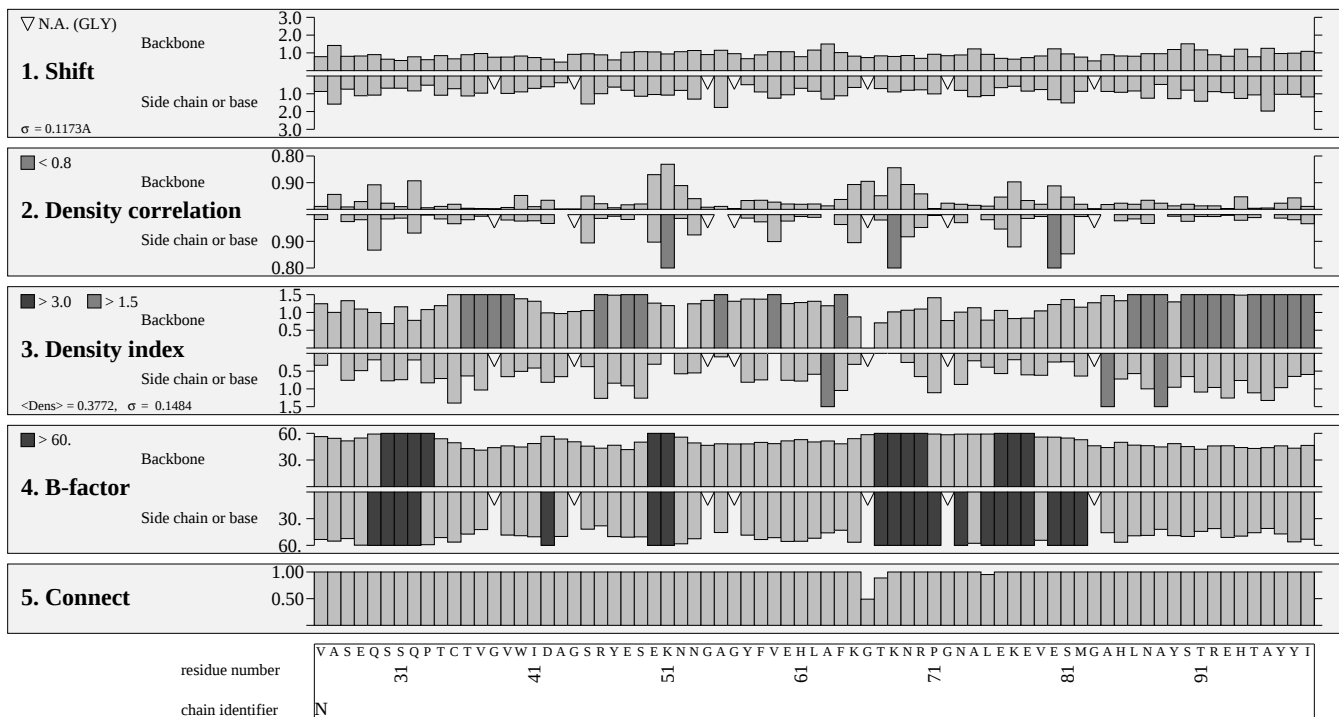
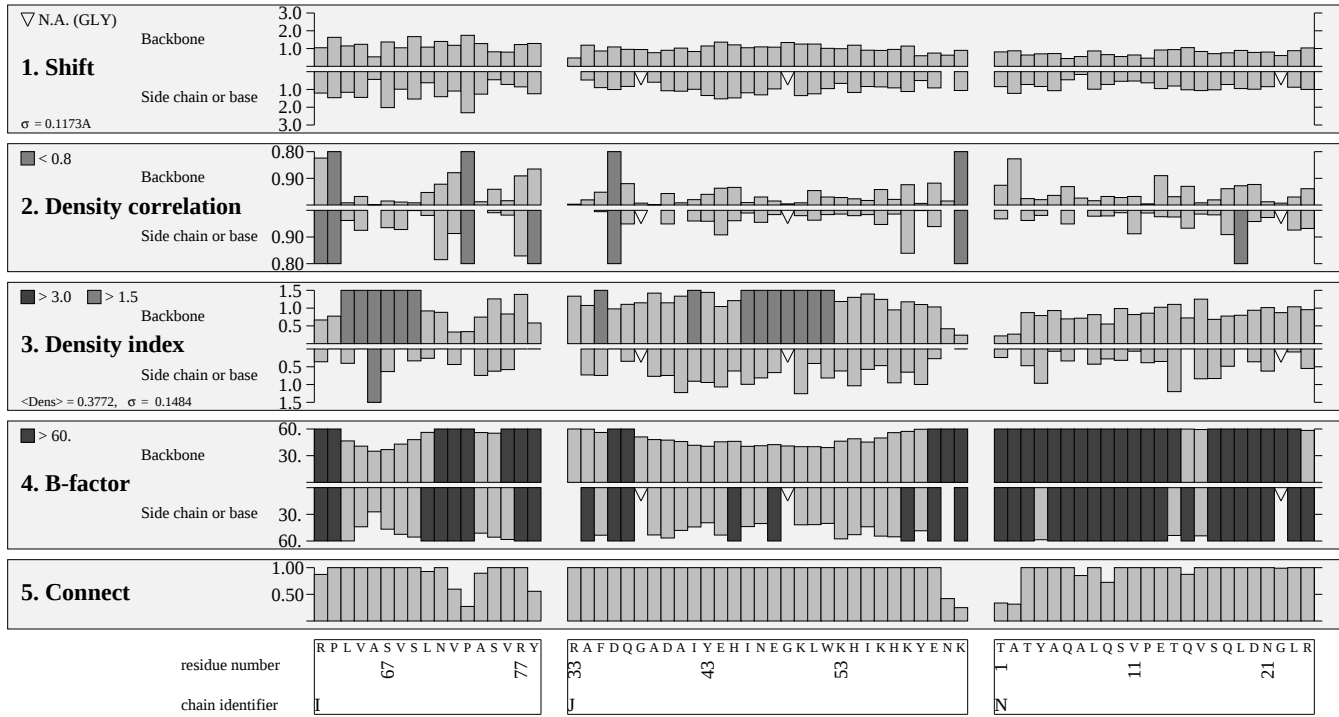
Local estimation (13)



Structure Factor Check

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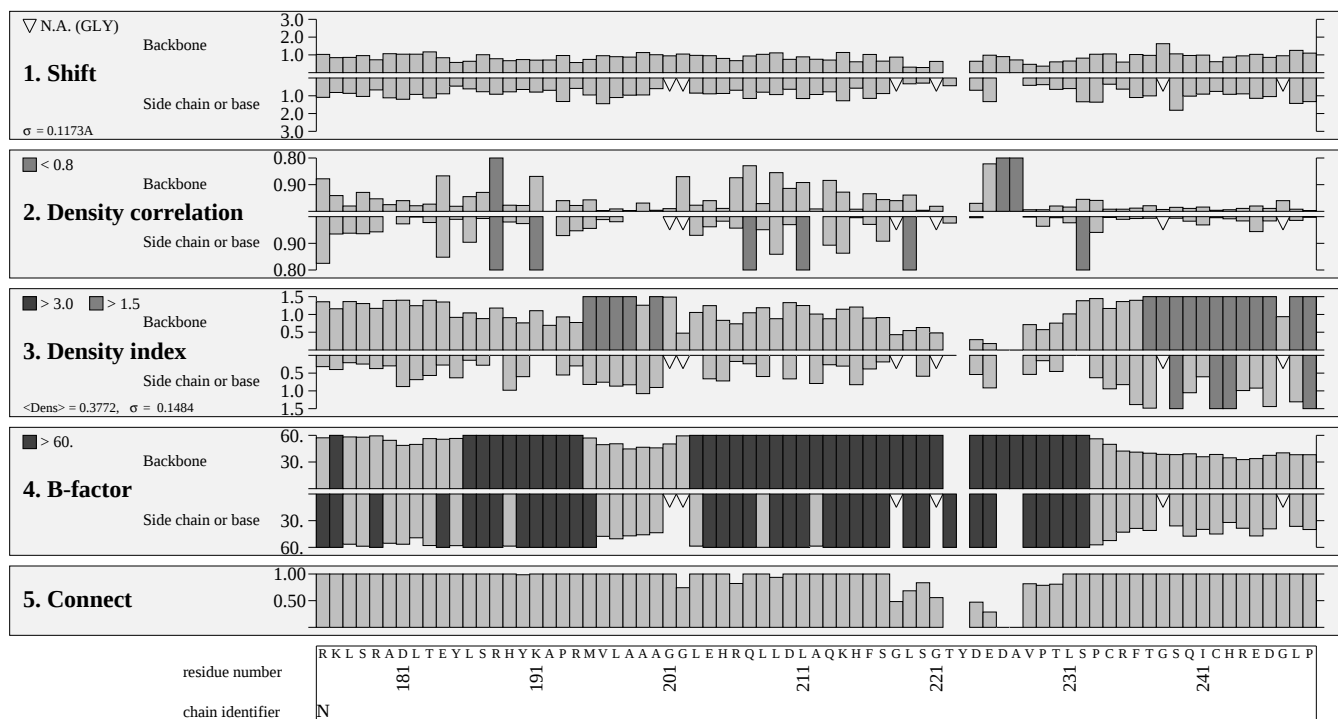
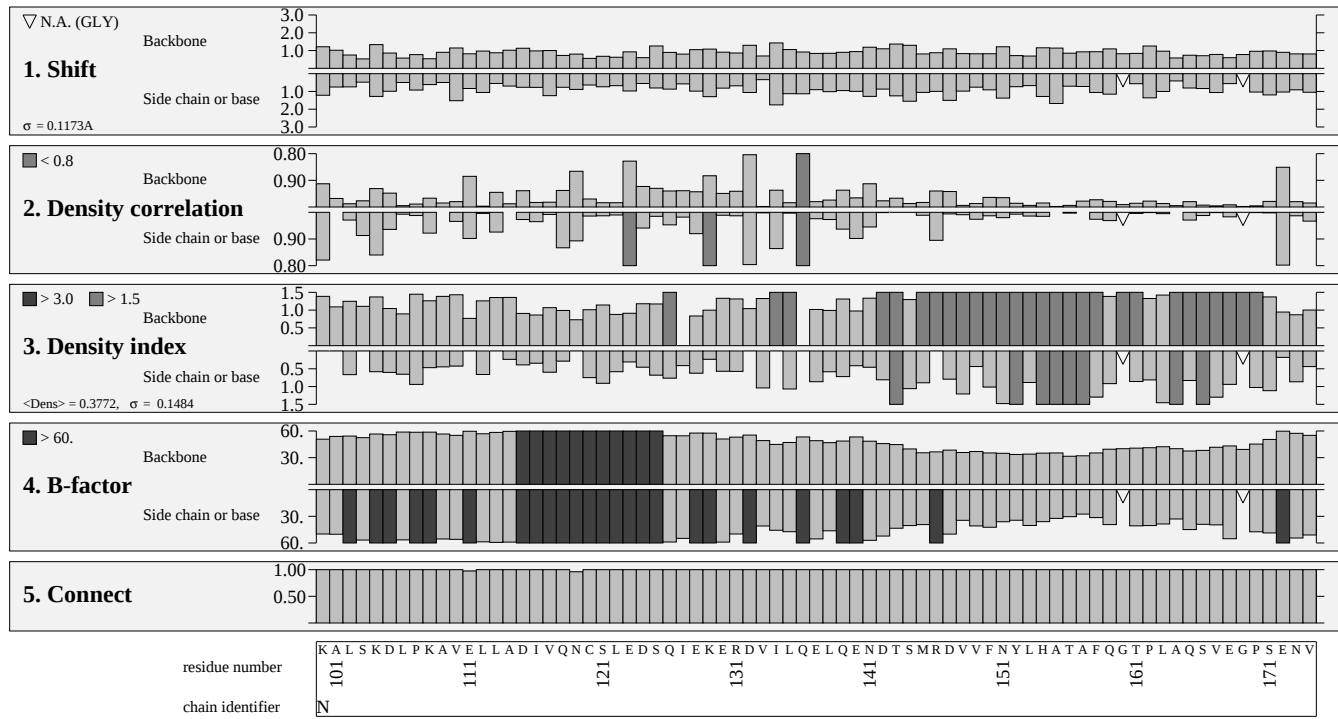
Local estimation (14)



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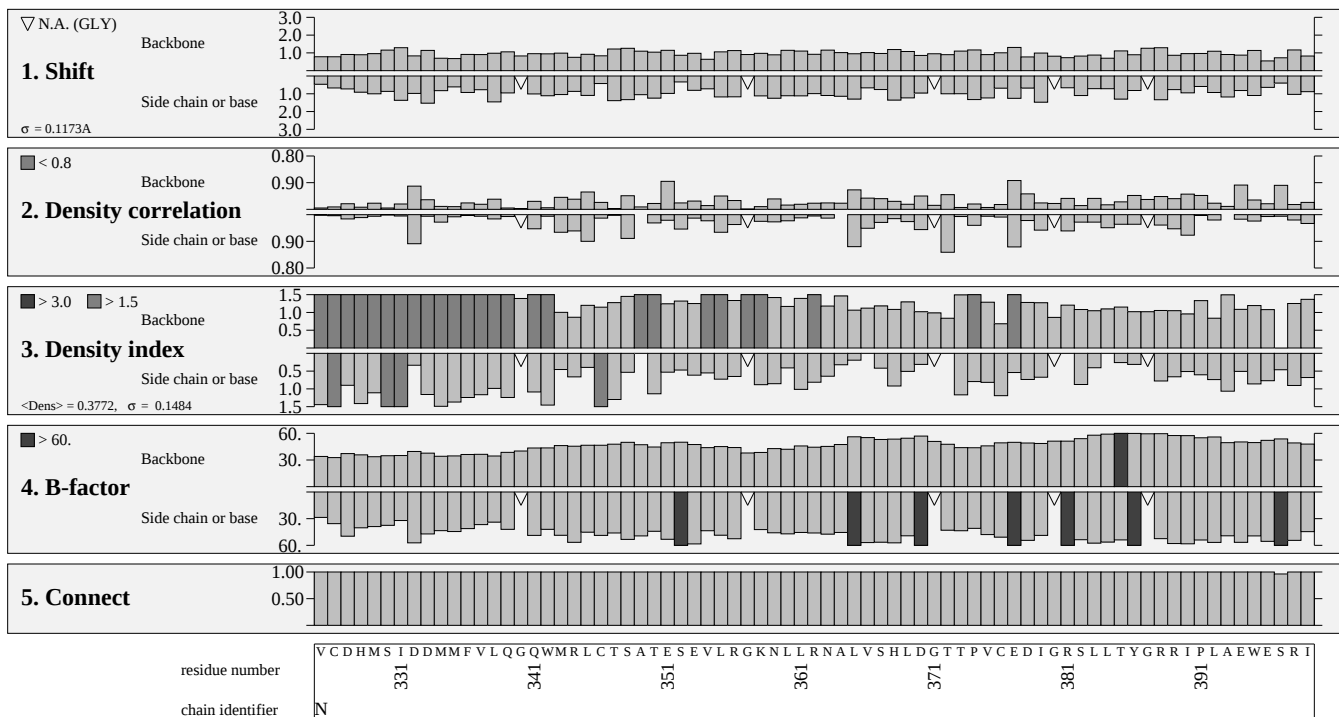
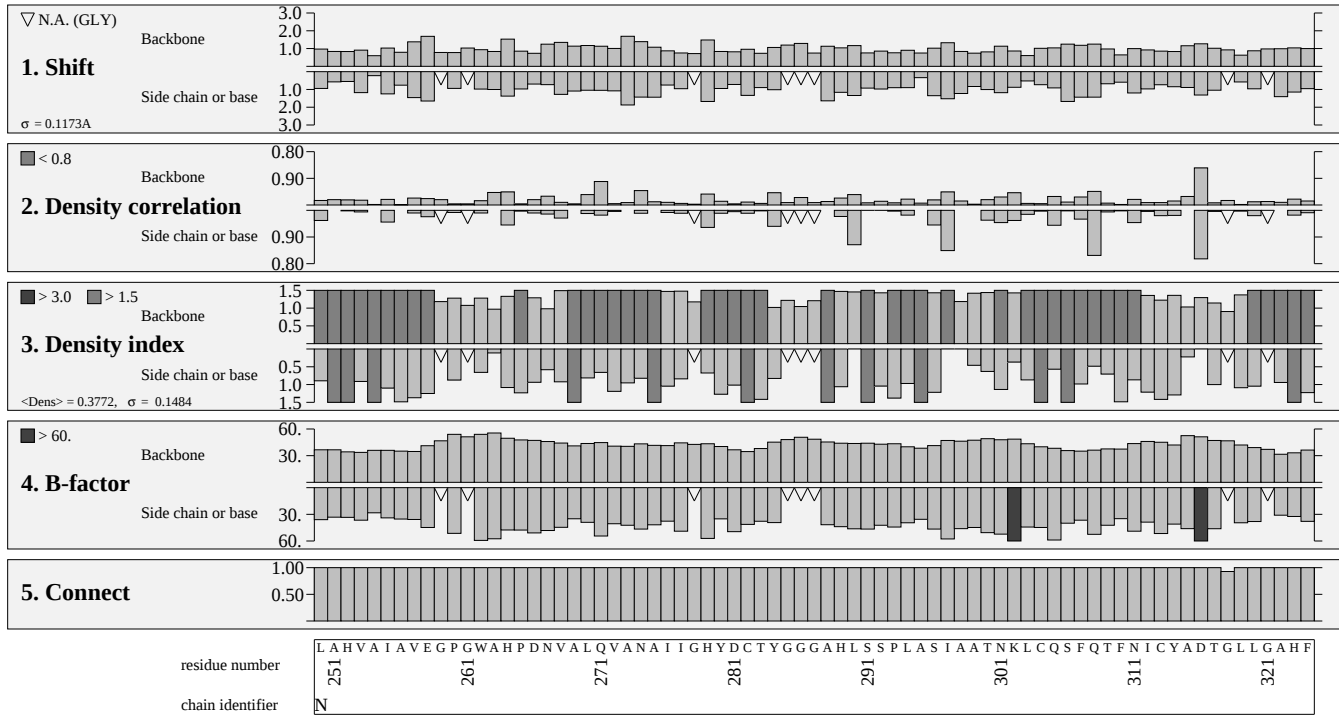
Local estimation (15)



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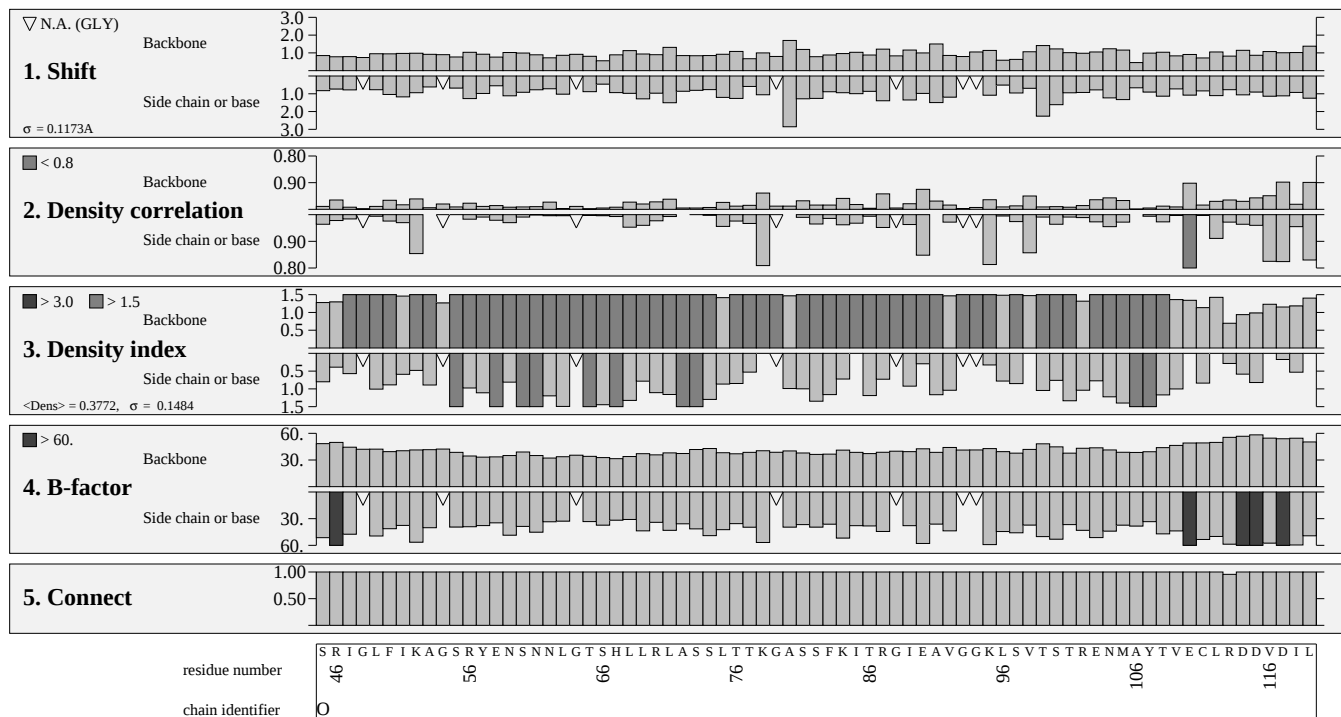
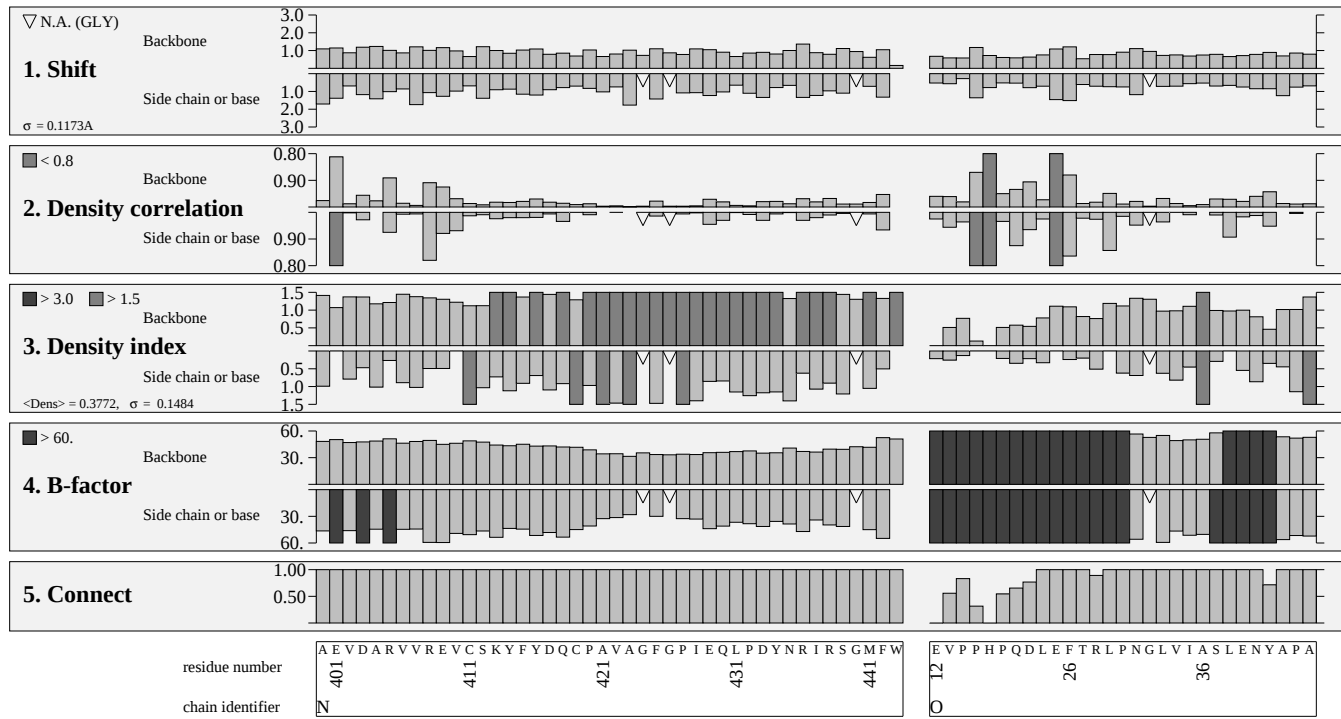
Local estimation (16)



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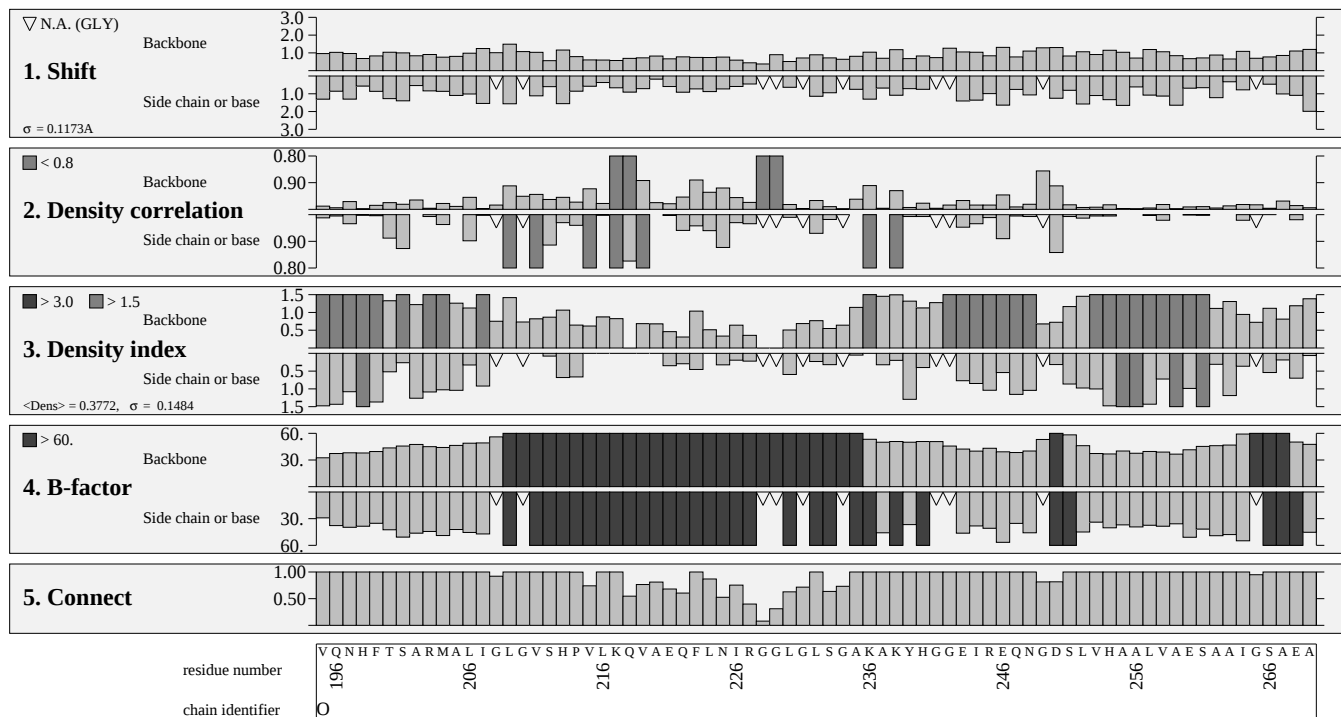
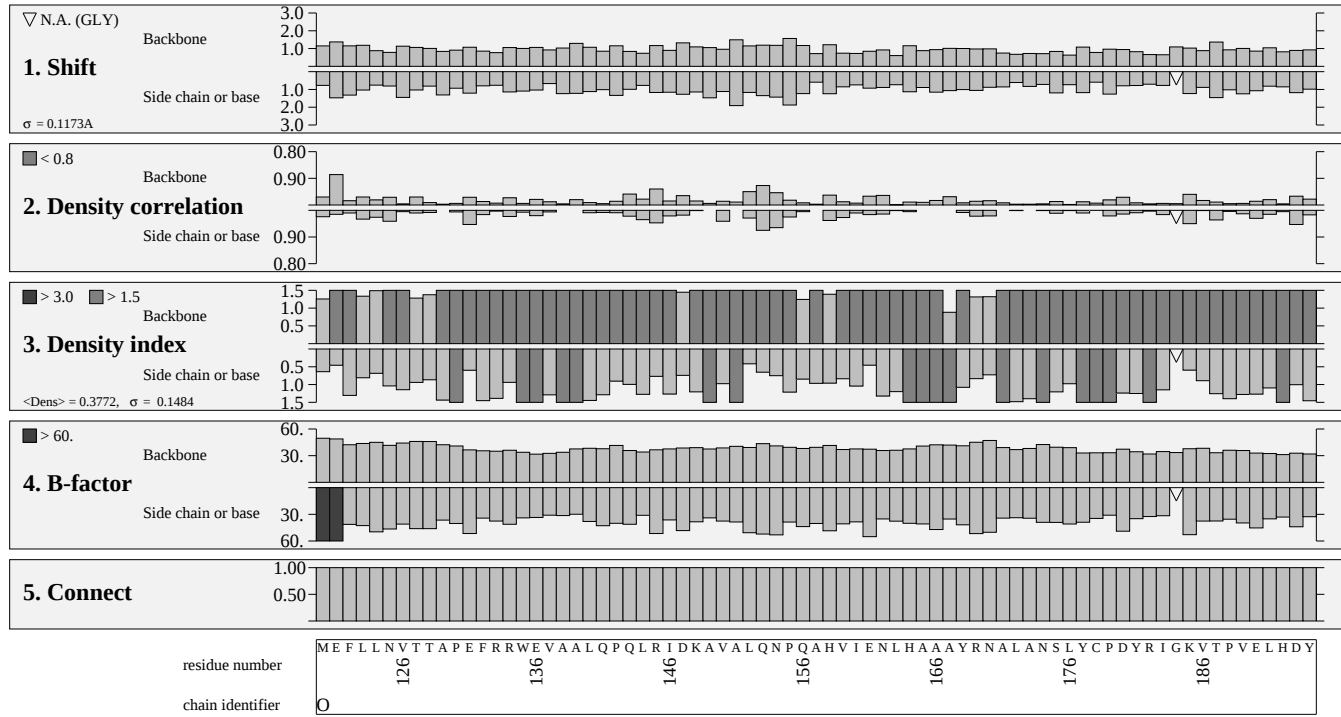
Local estimation (17)



Structure Factor Check

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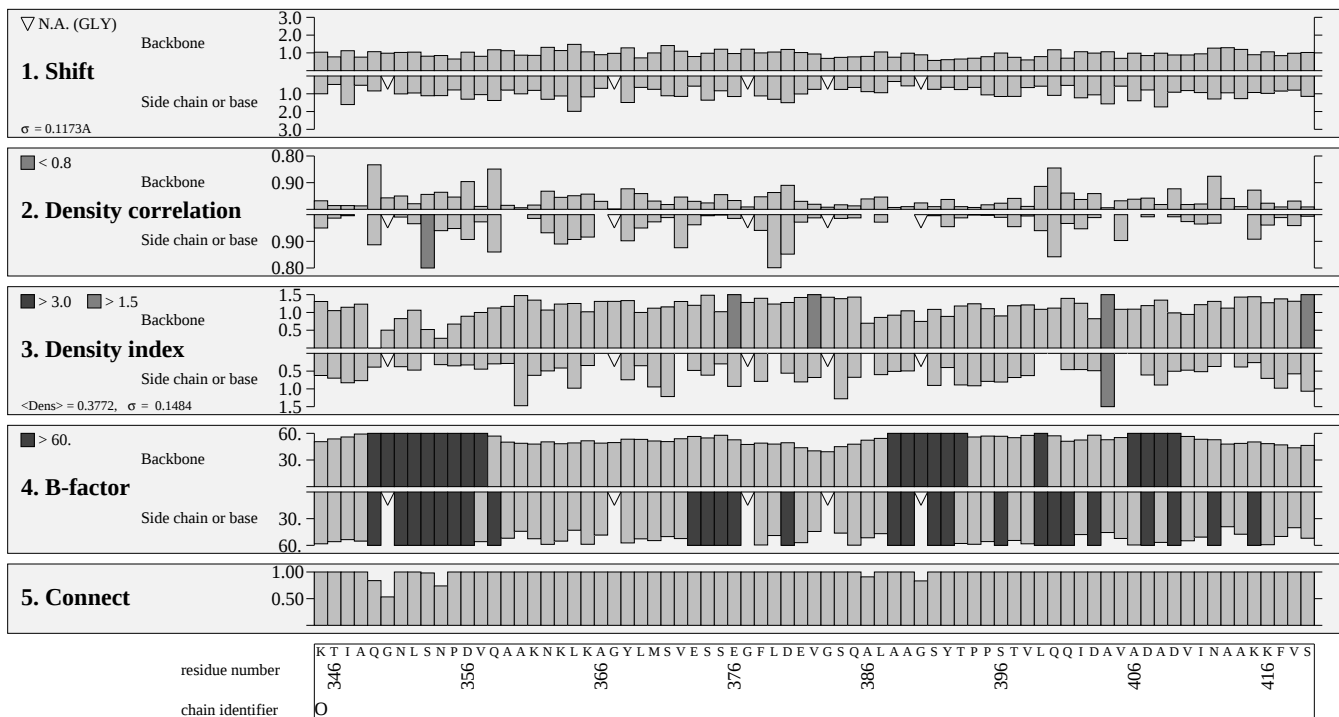
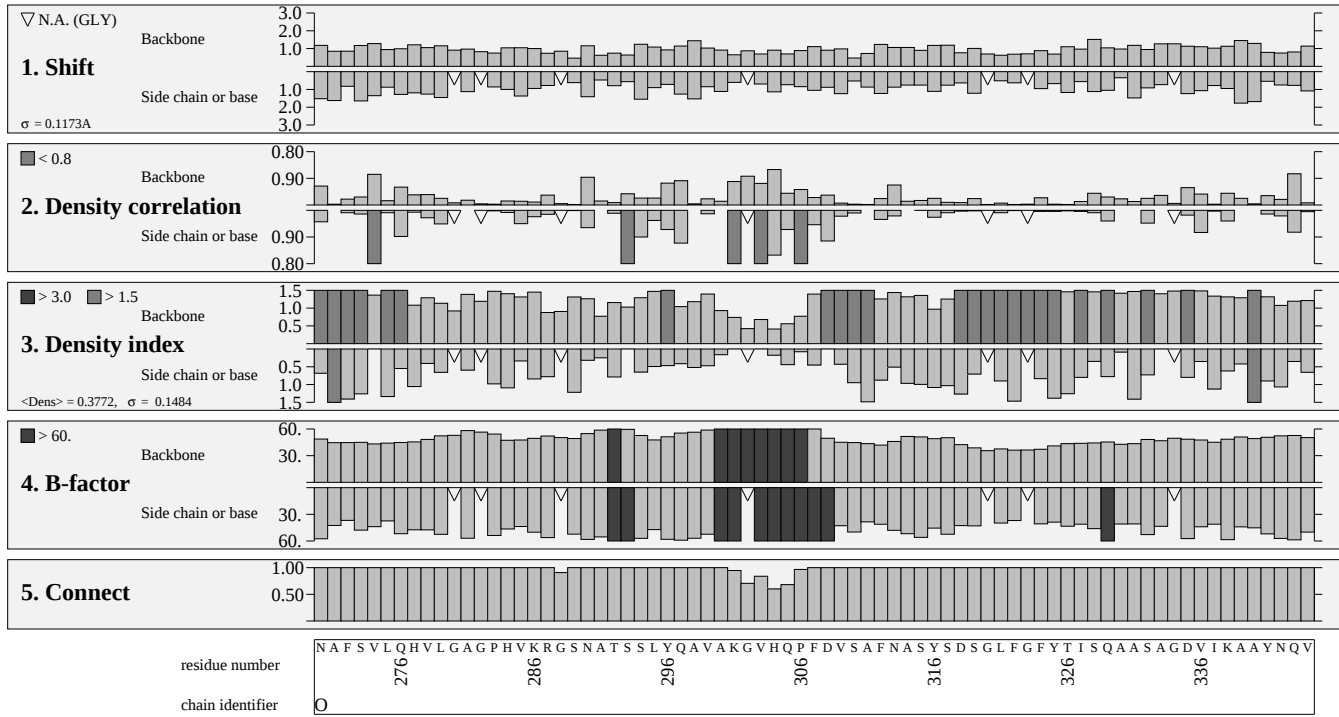
Local estimation (18)



Structure Factor Check

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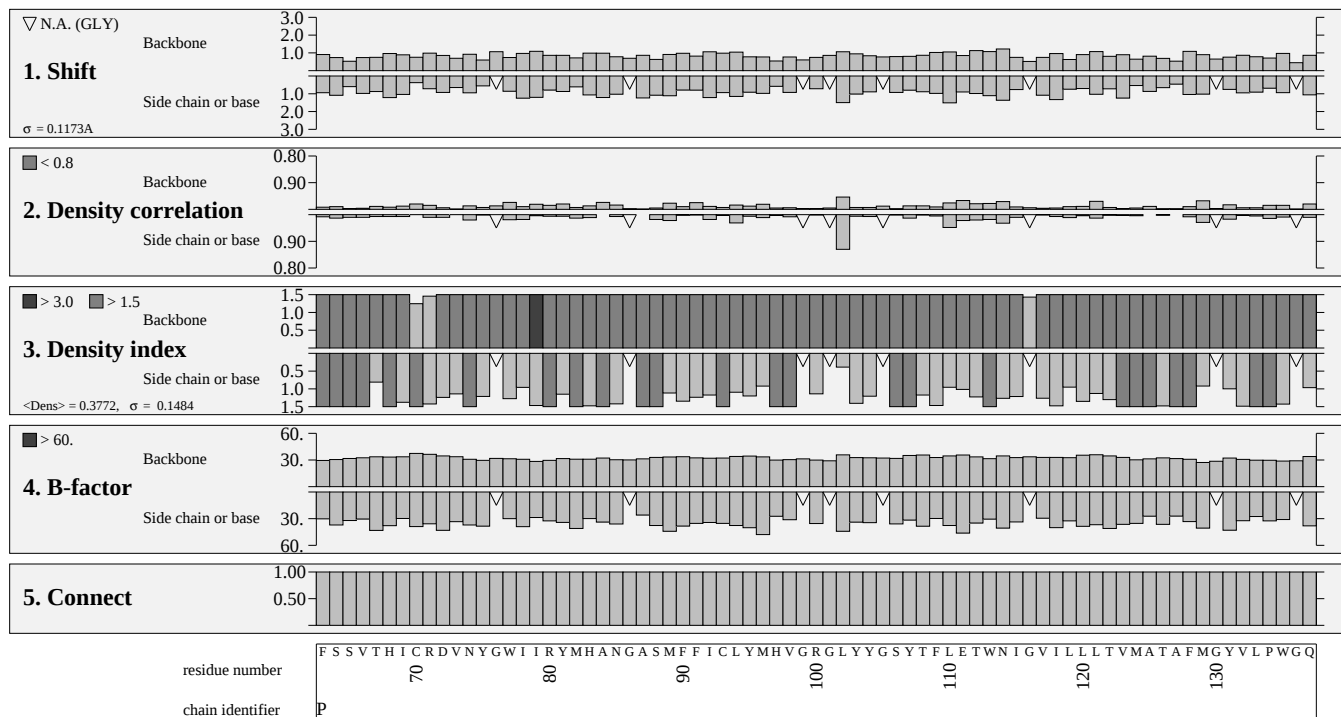
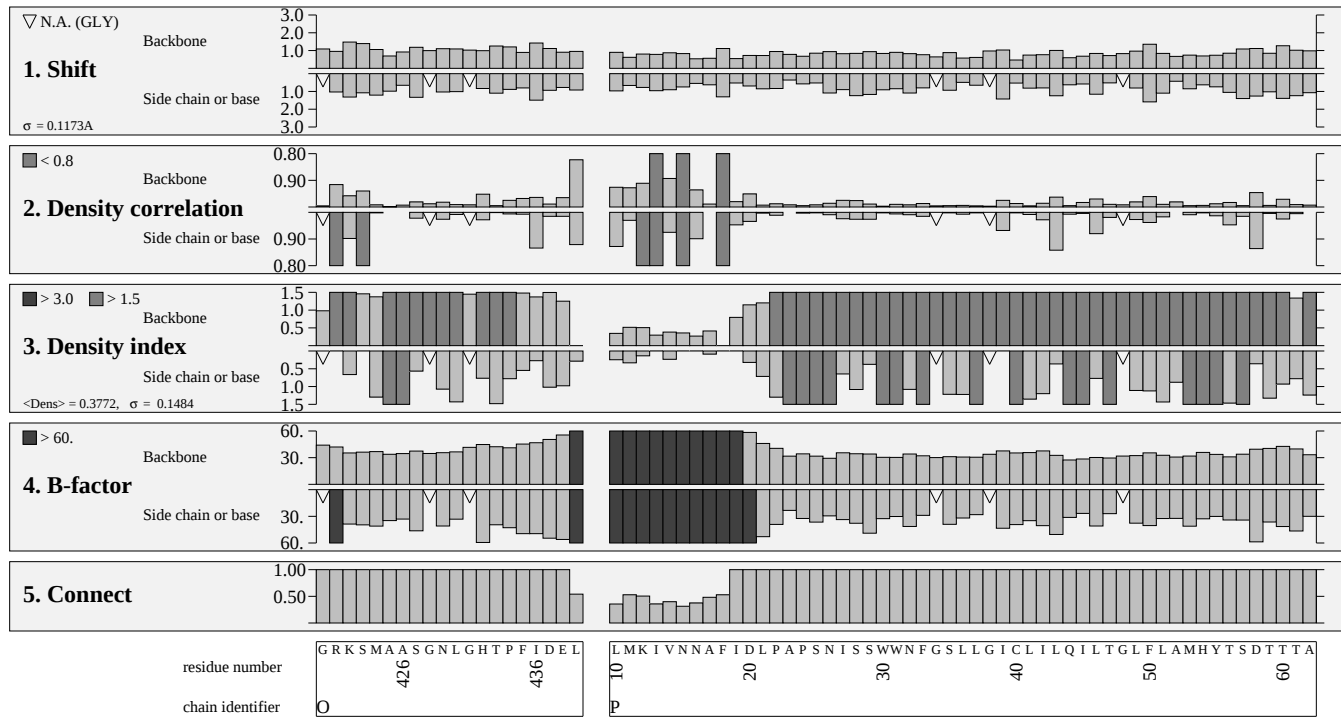
Local estimation (19)



Structure Factor Check

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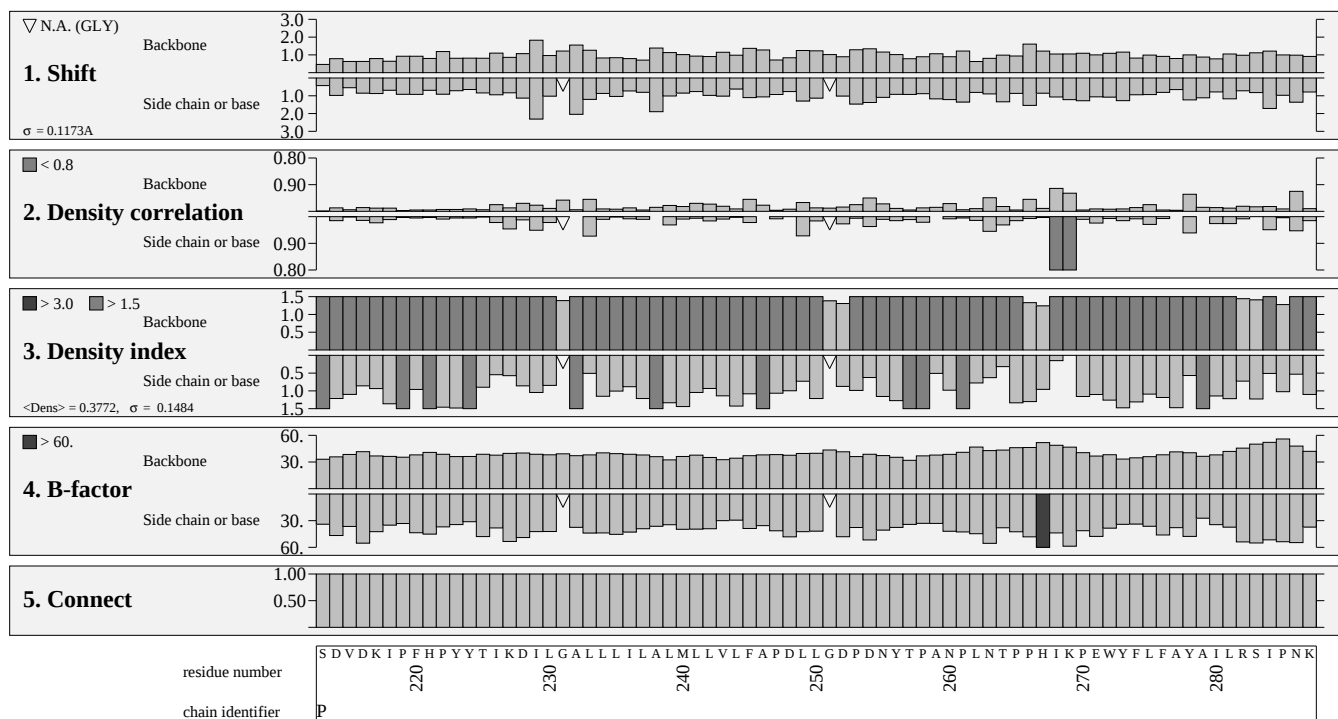
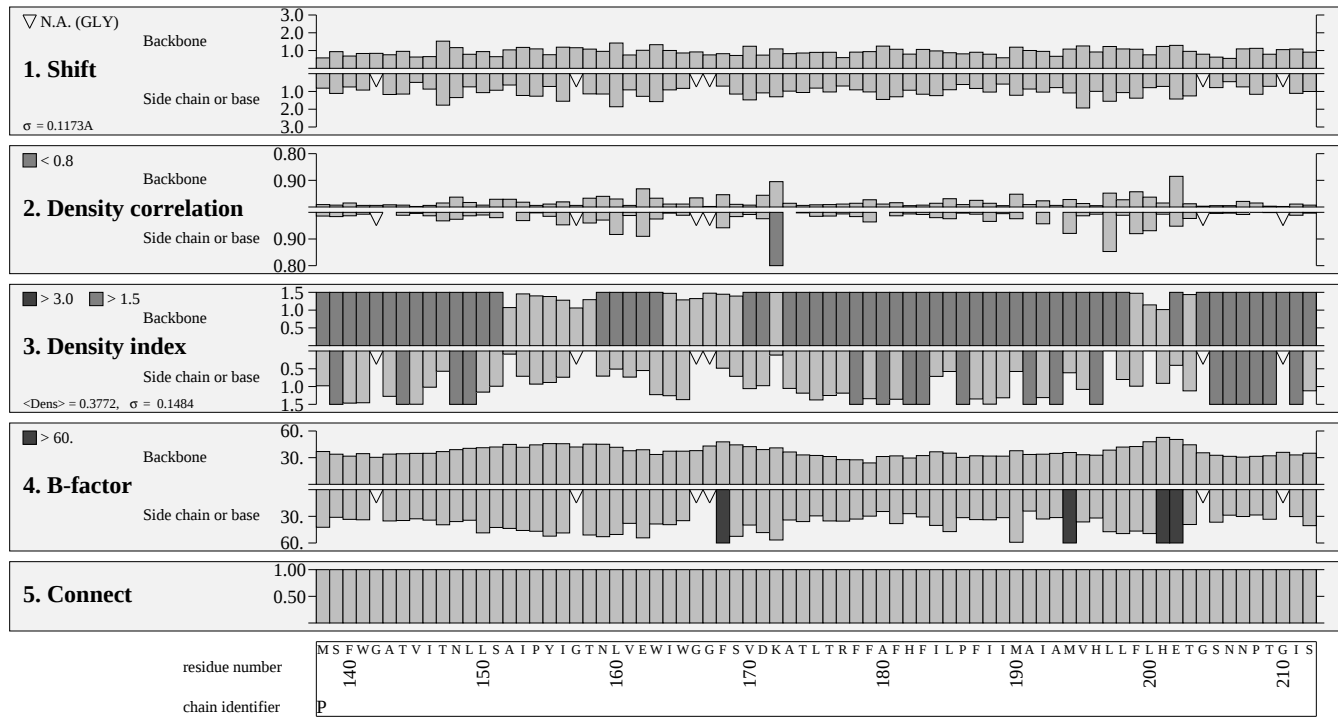
Local estimation (20)



Structure Factor Check

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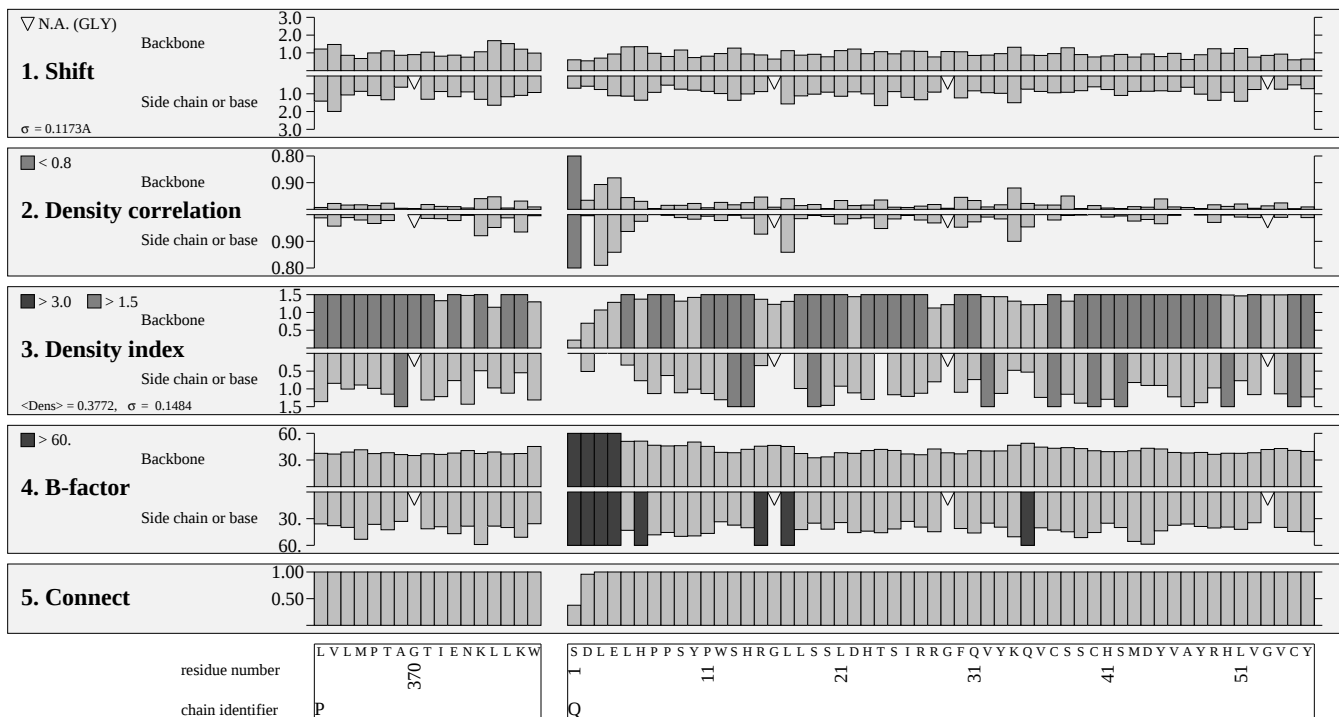
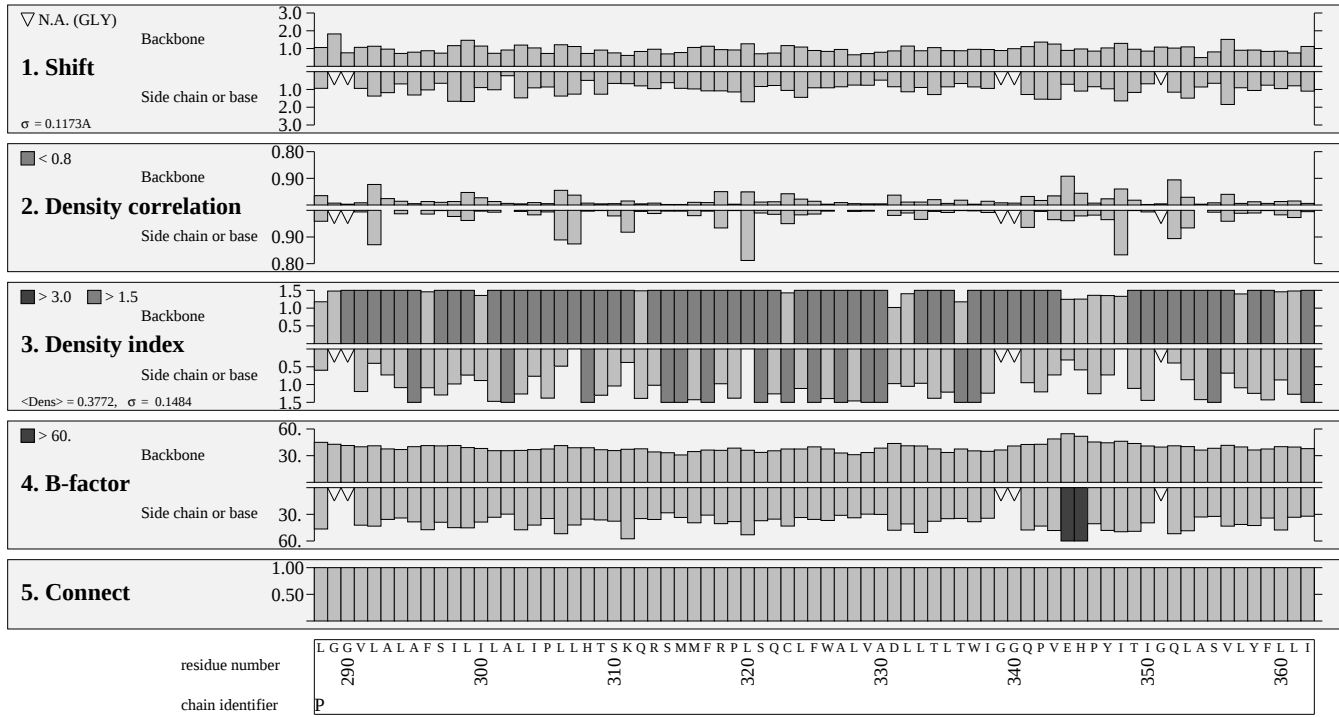
Local estimation (21)



Structure Factor Check

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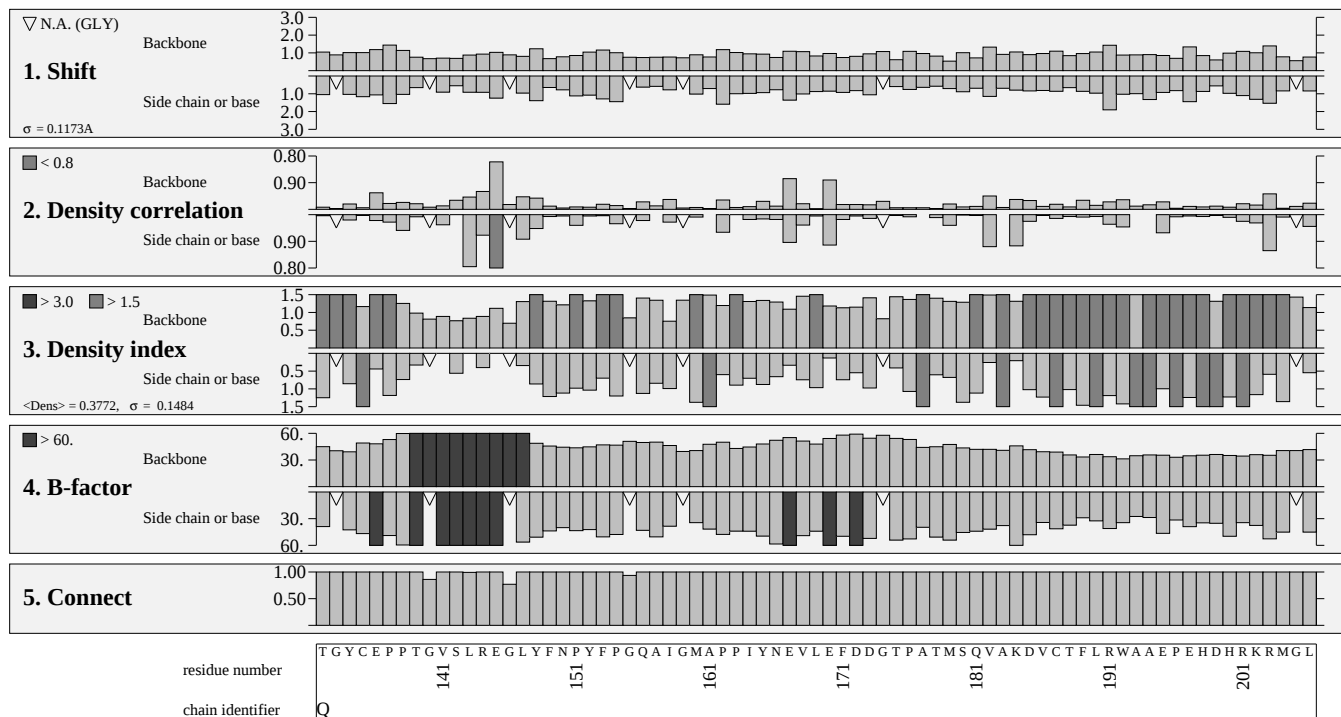
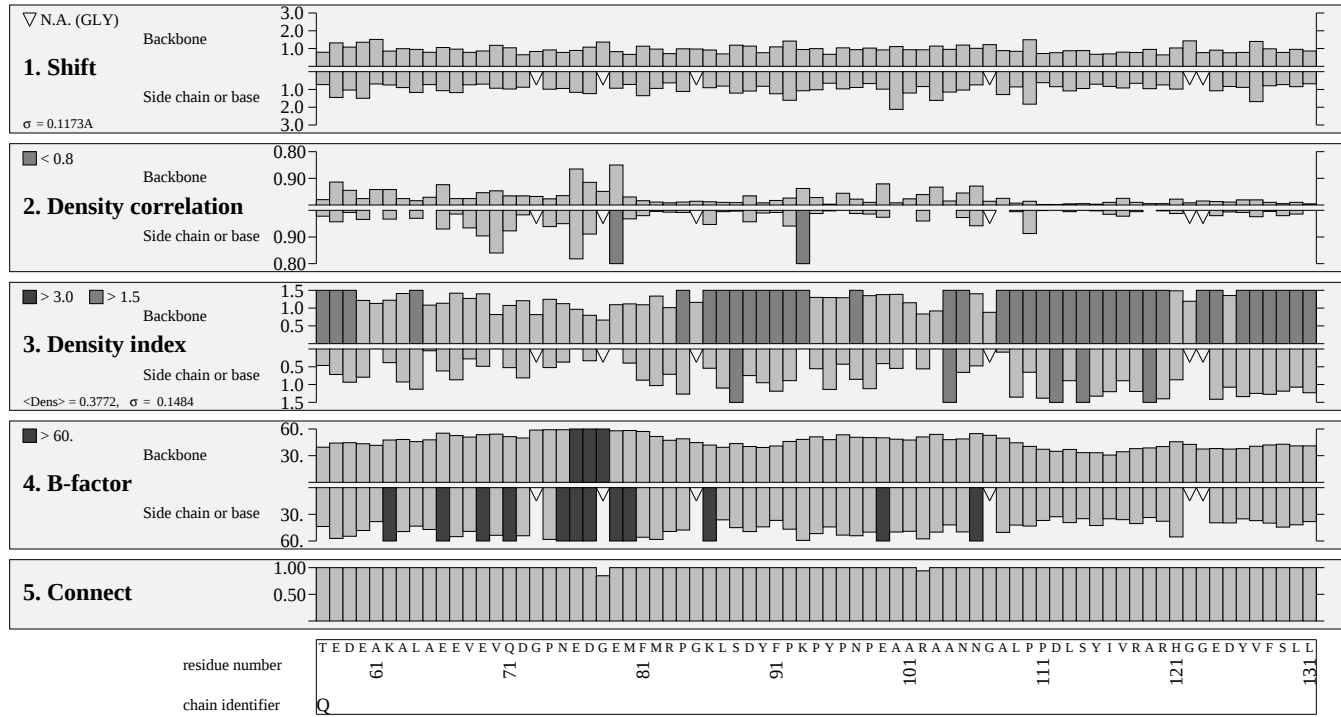
Local estimation (22)



Structure Factor Check

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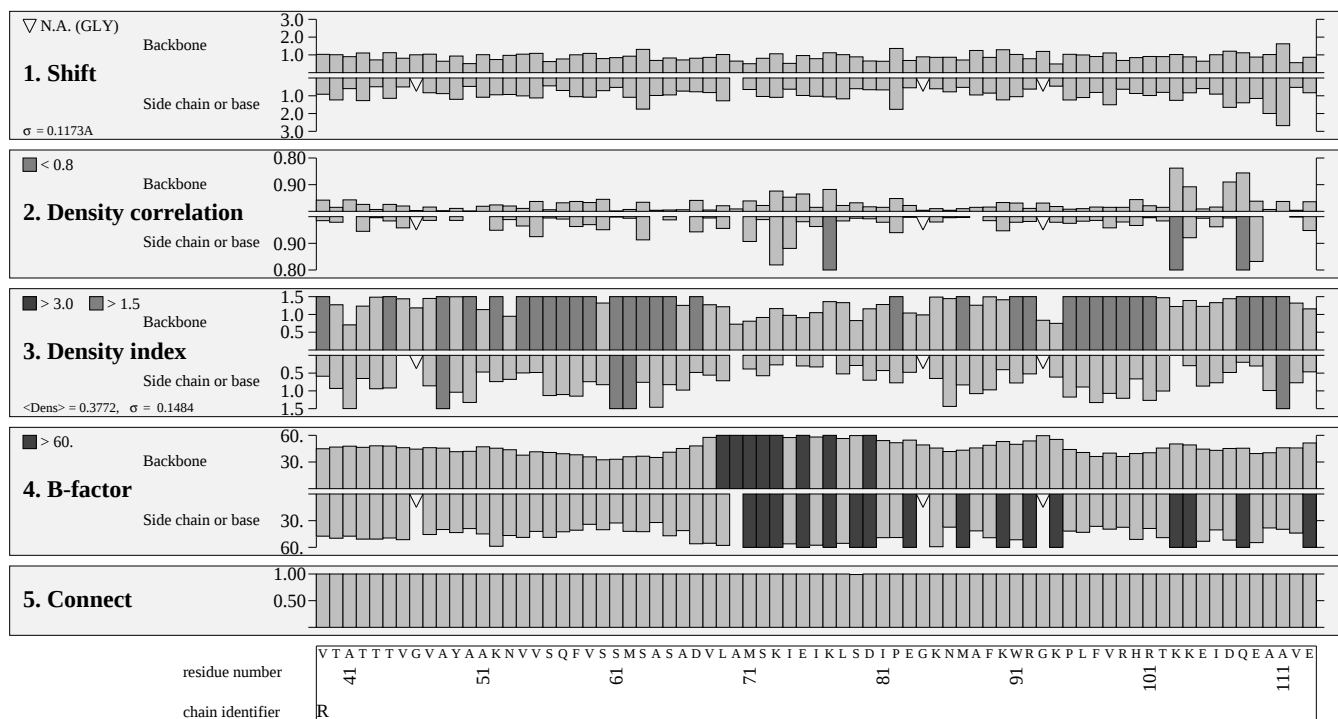
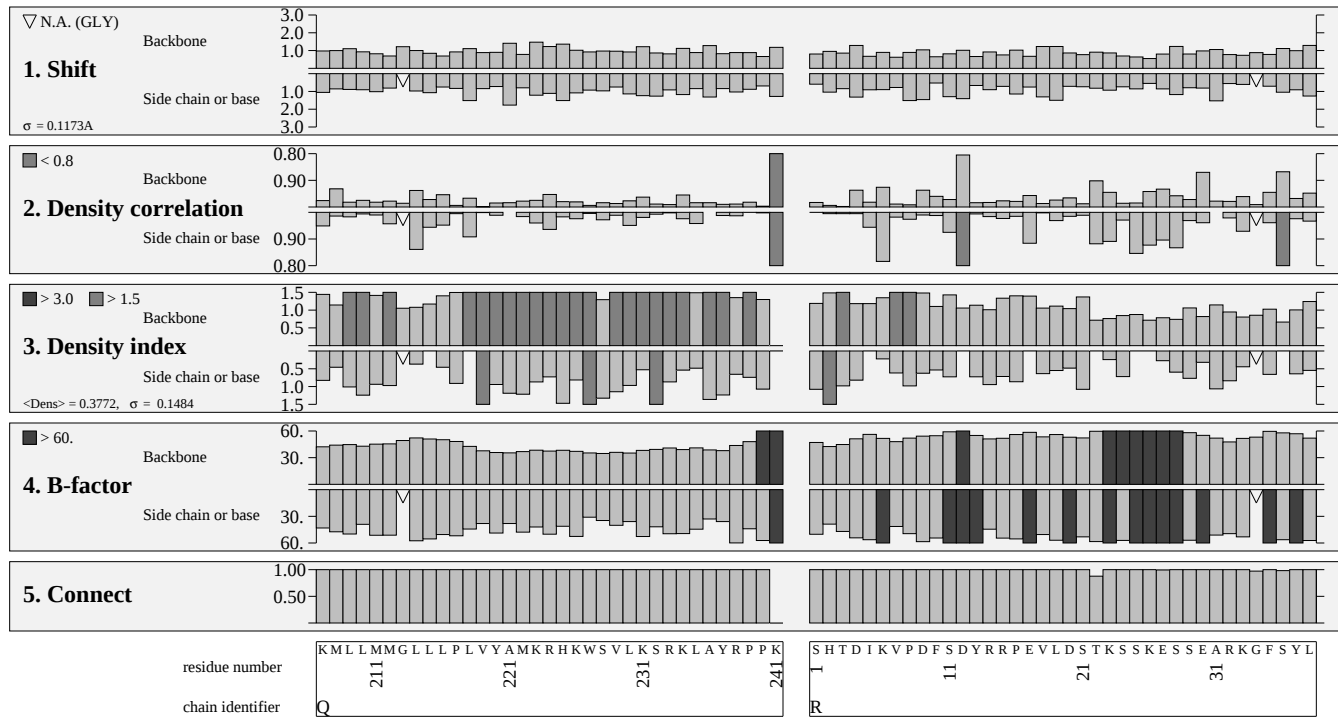
Local estimation (23)



Structure Factor Check

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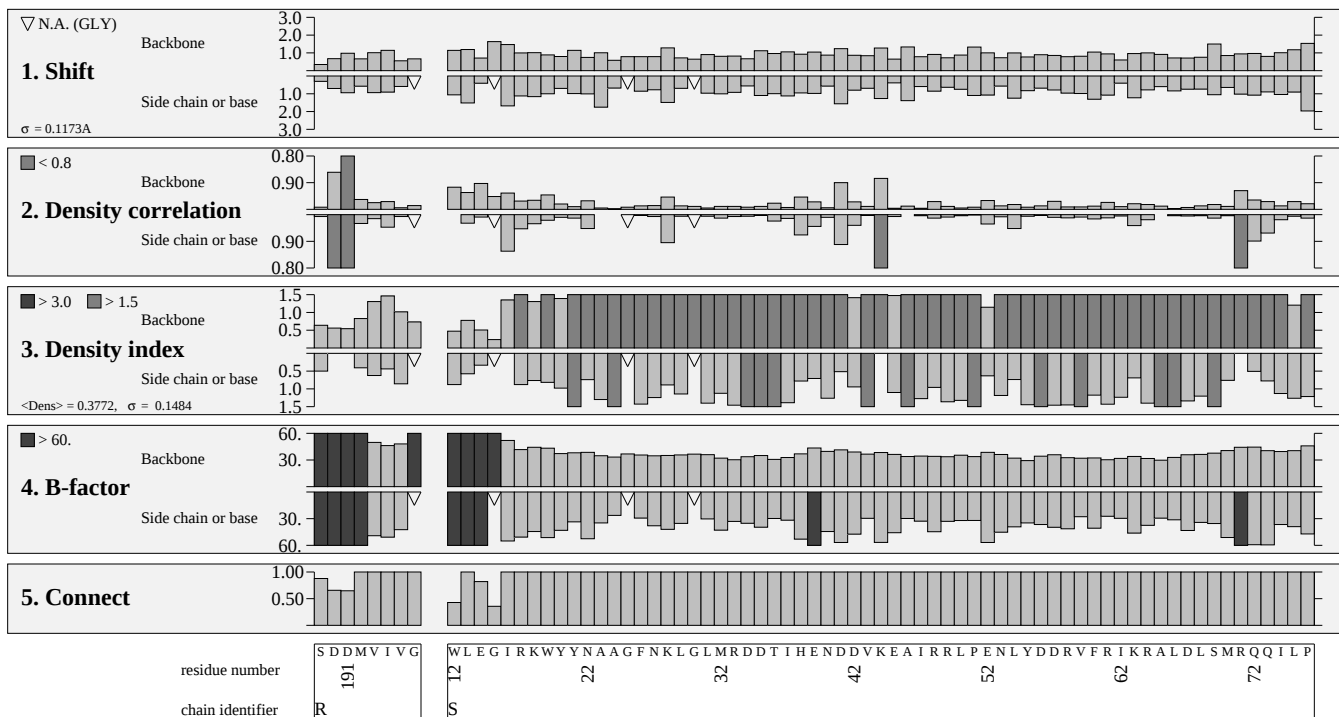
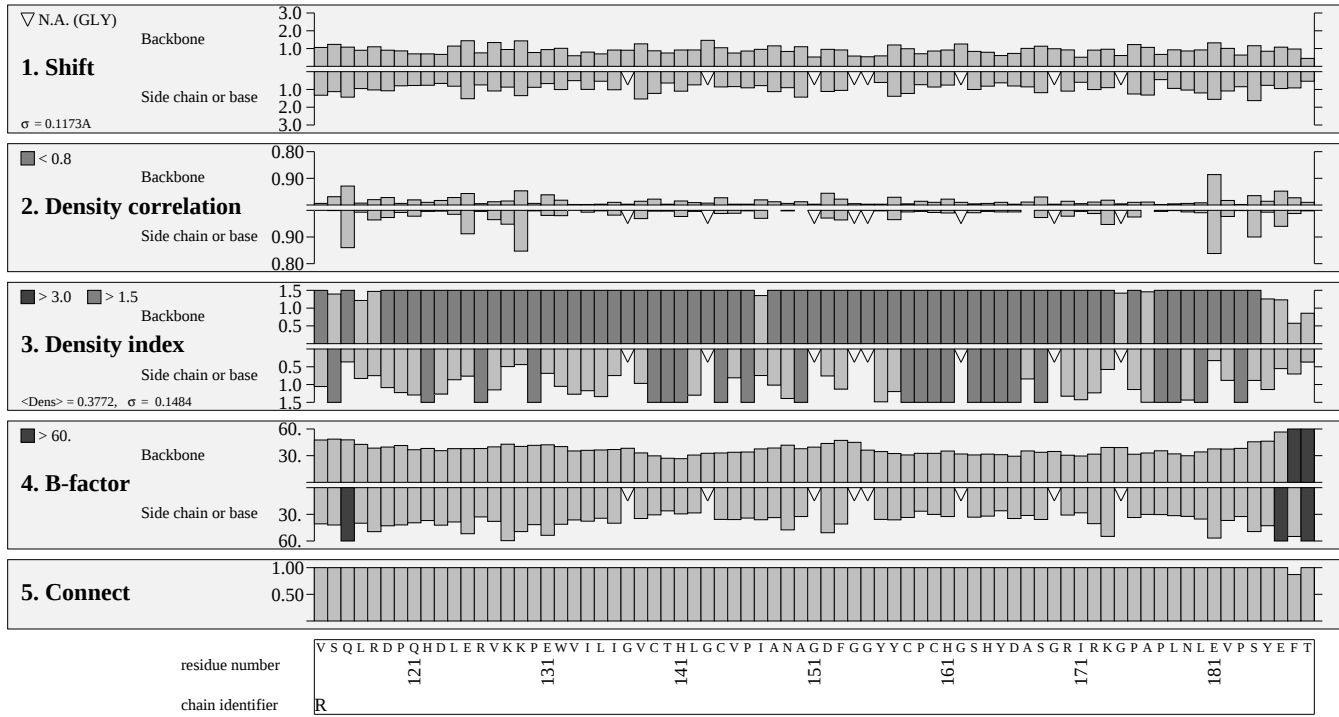
Local estimation (24)



Structure Factor Check

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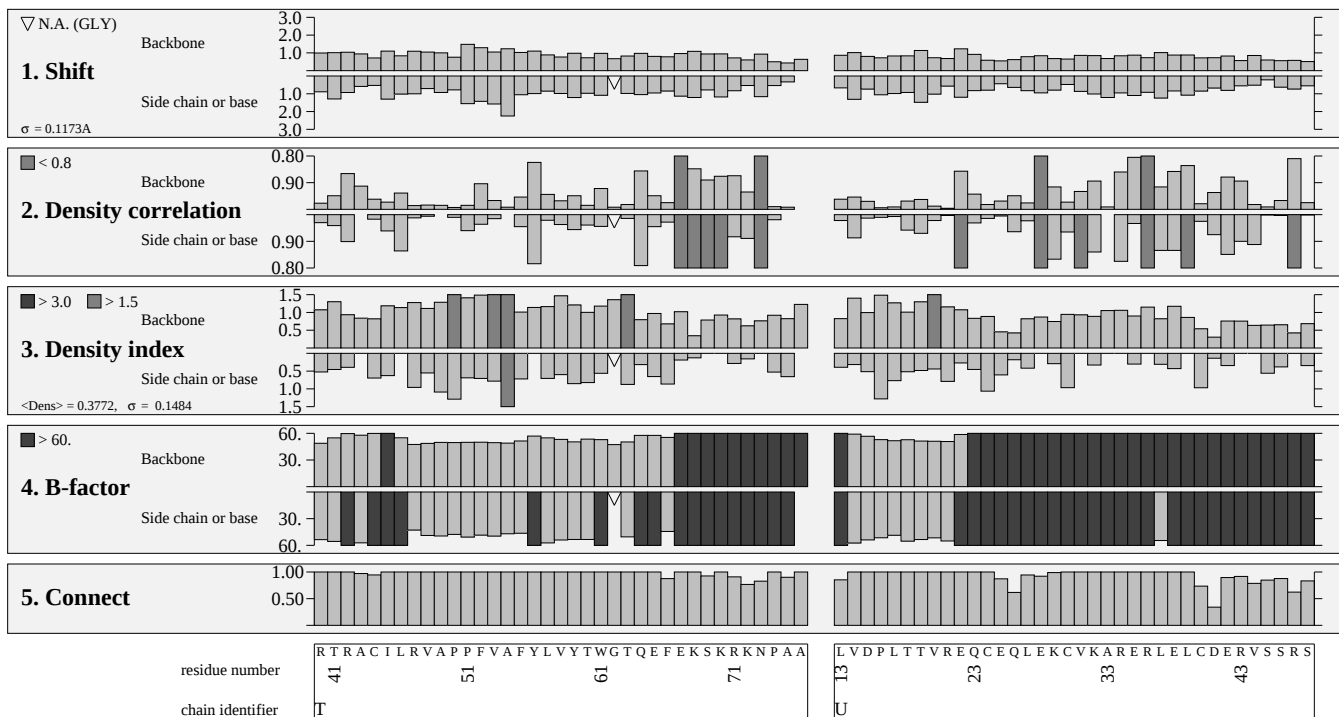
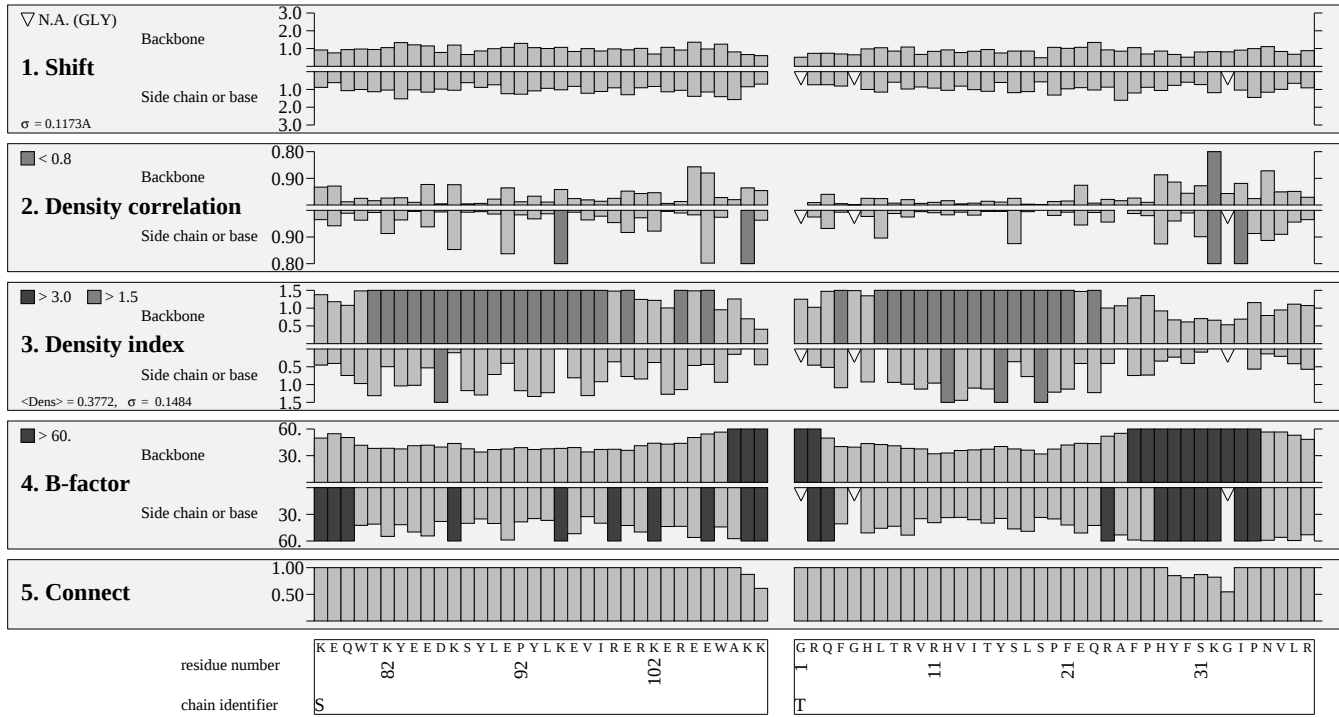
Local estimation (25)



Structure Factor Check

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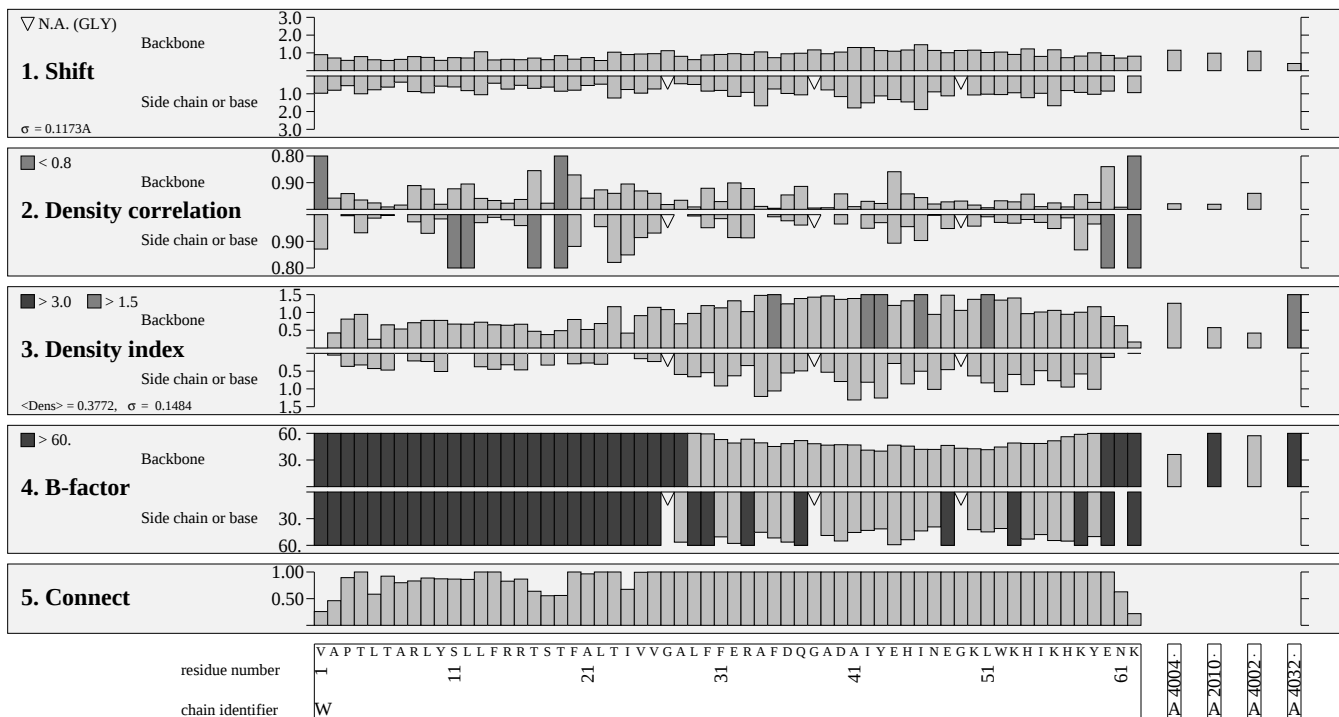
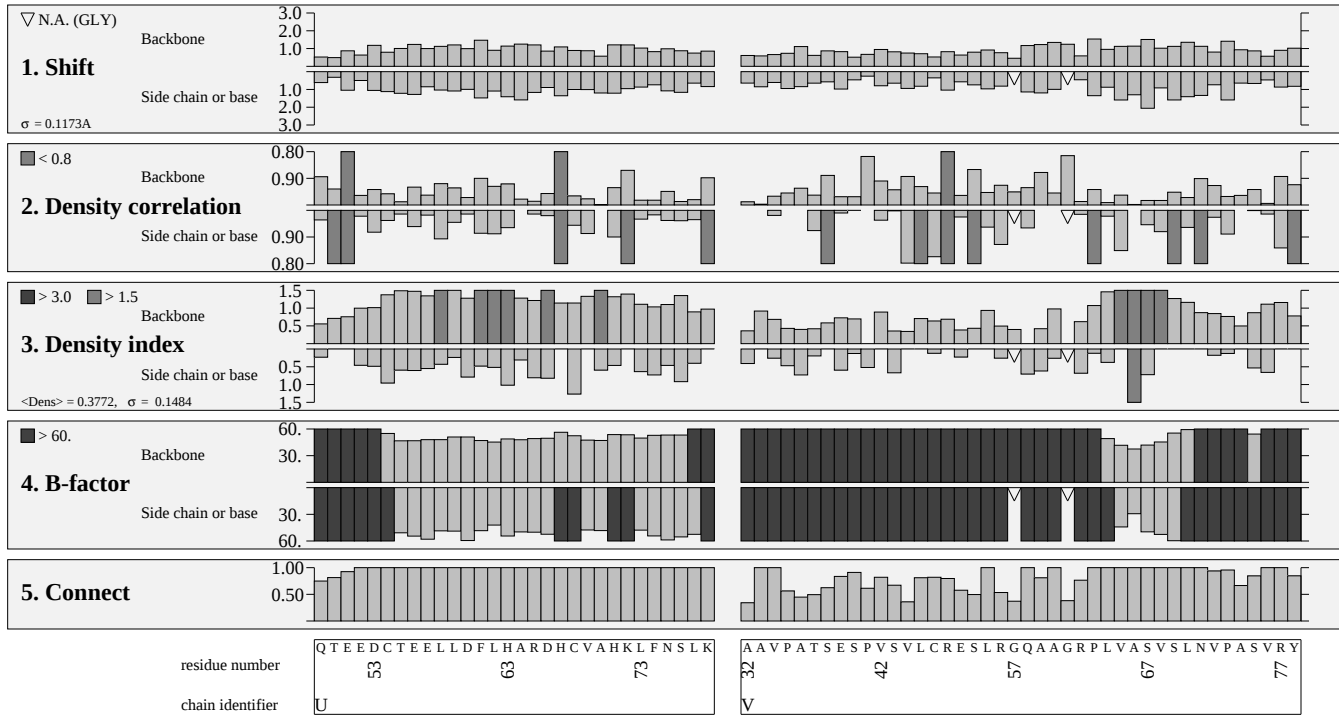
Local estimation (26)



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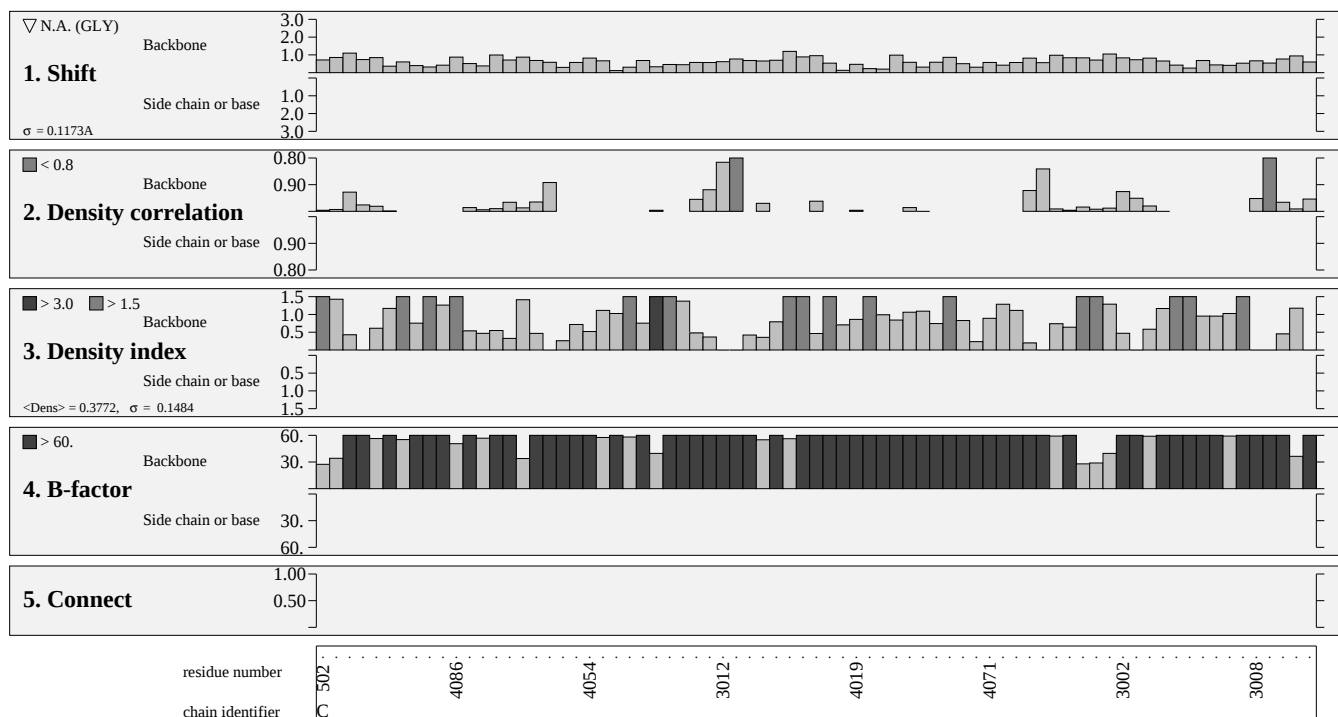
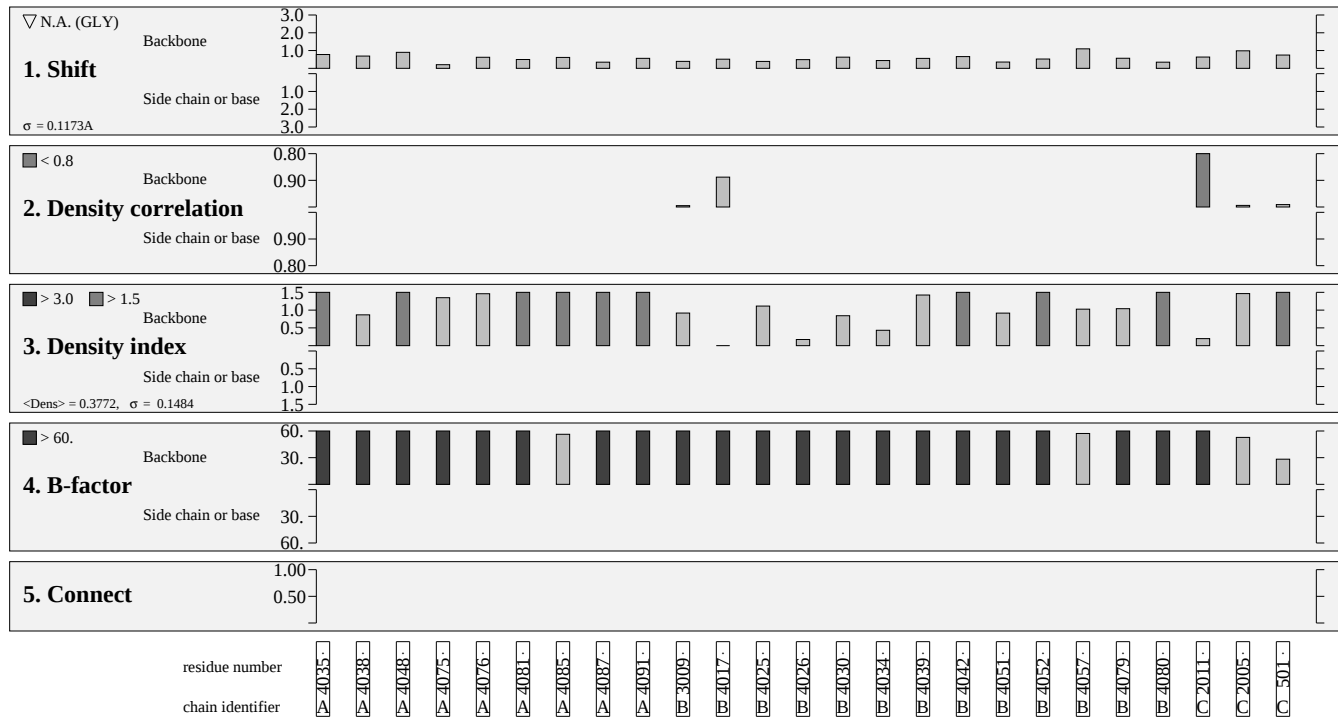
Local estimation (27)



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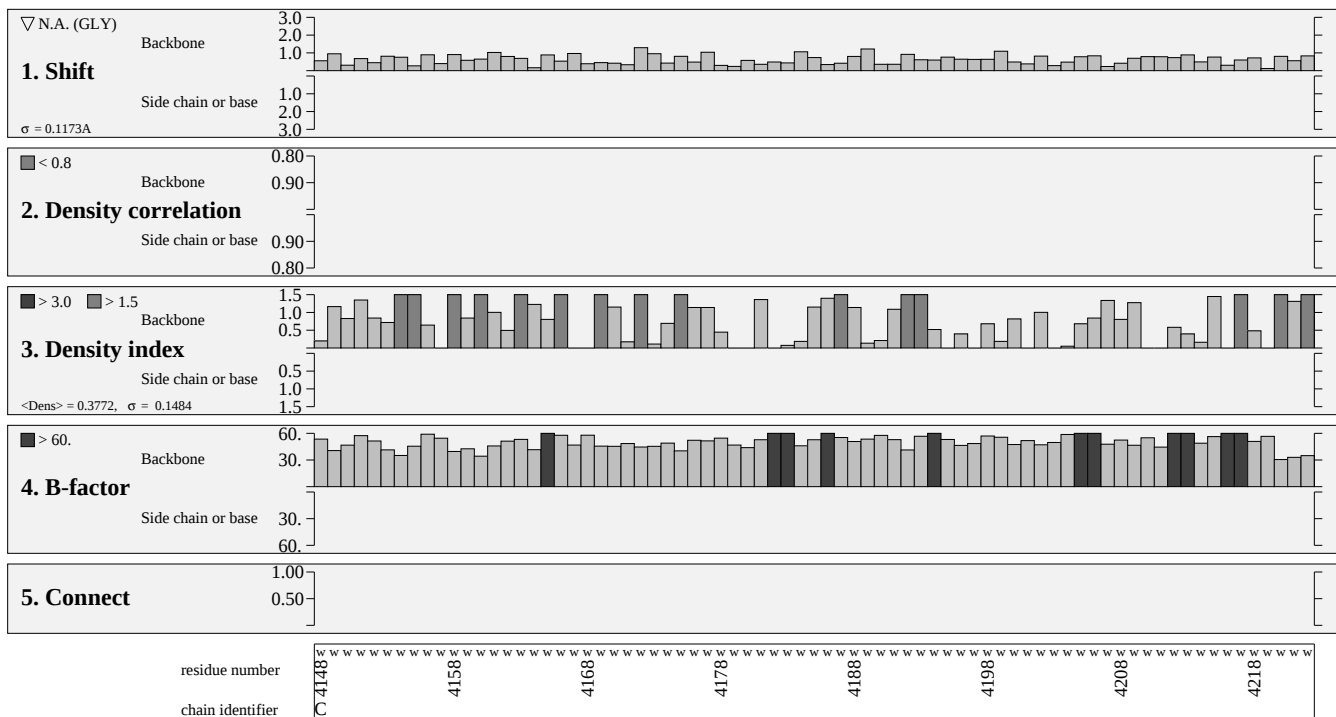
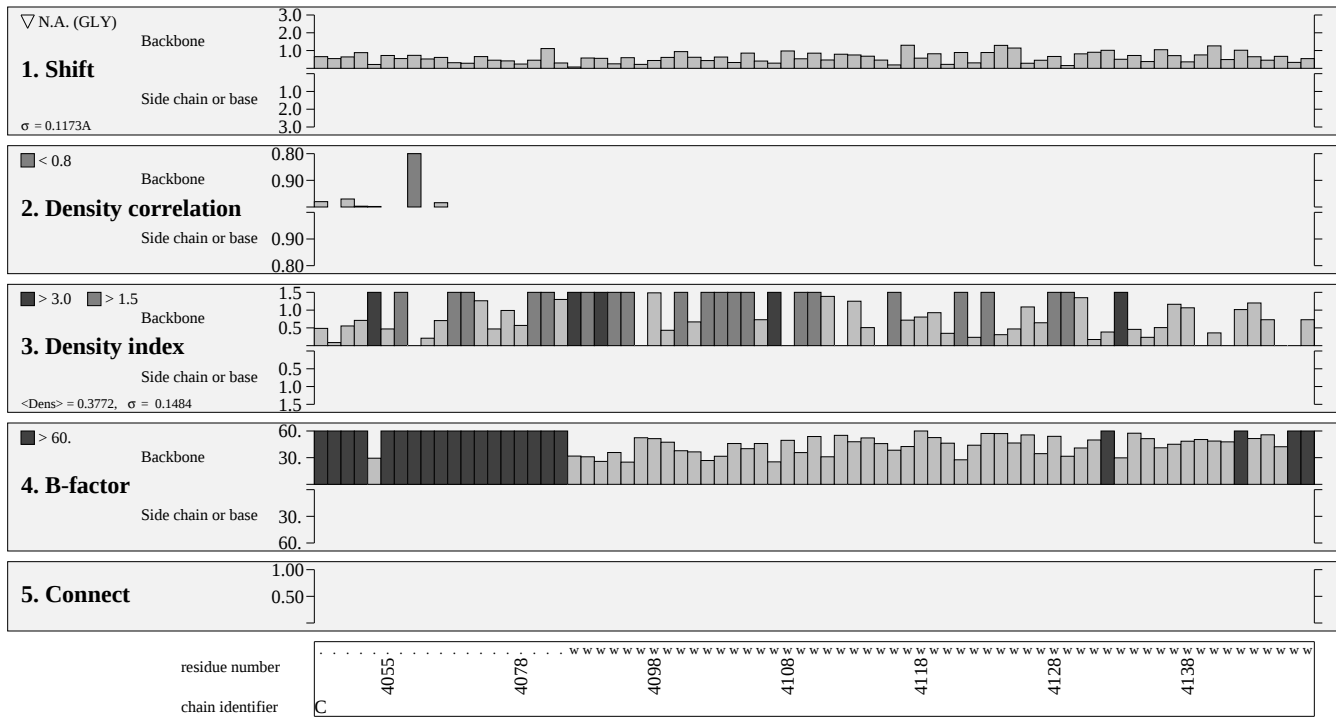
Local estimation (28)



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2A06

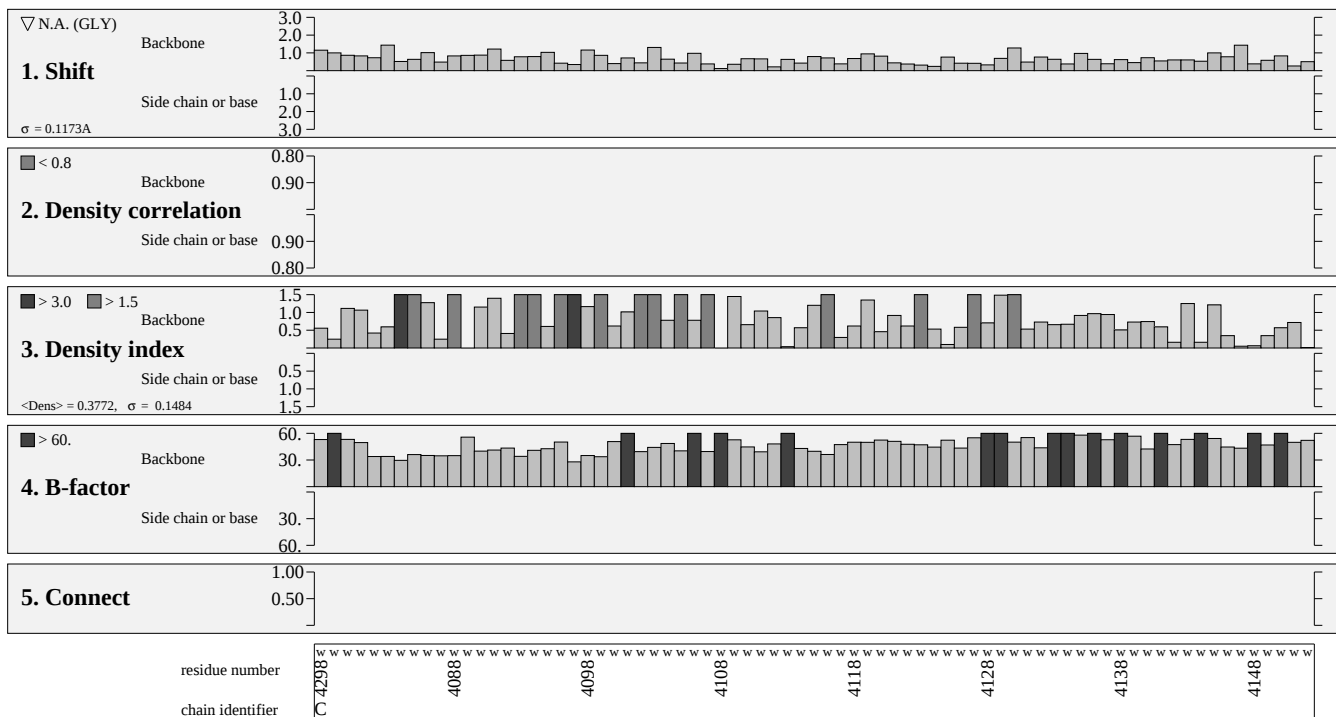
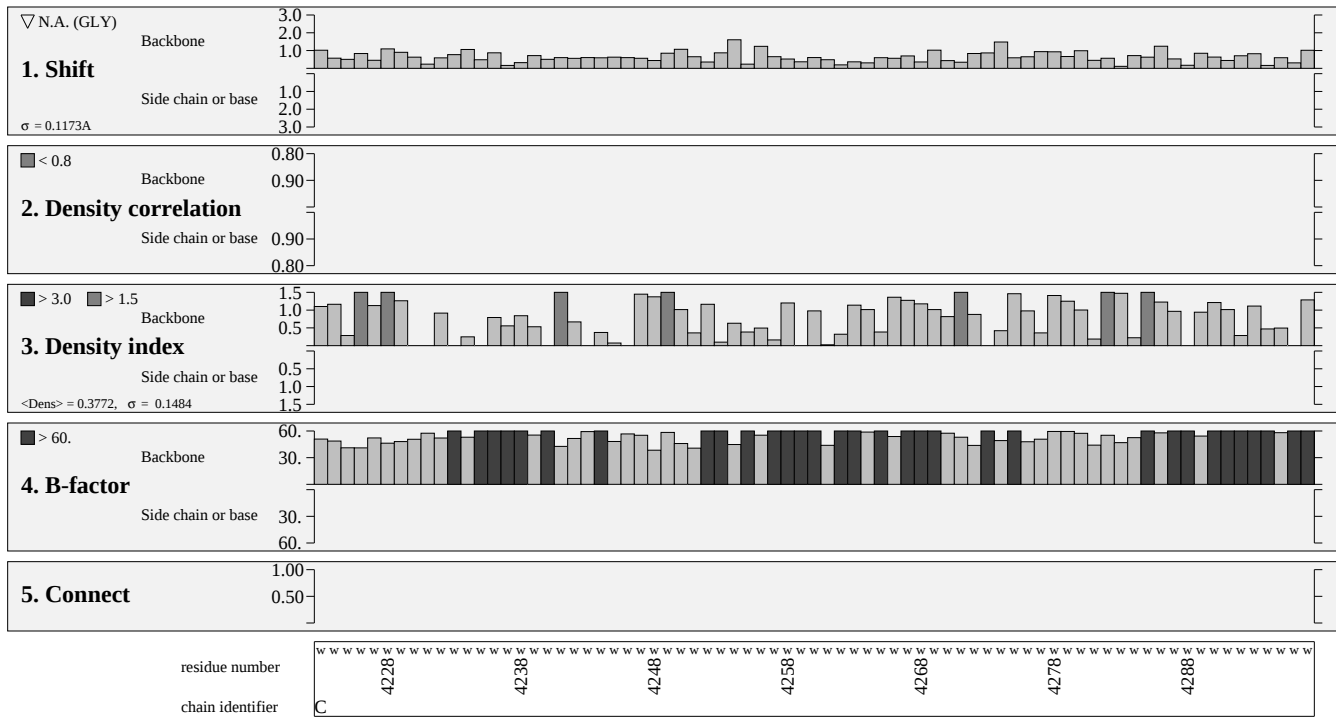
Local estimation (29)



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2A06

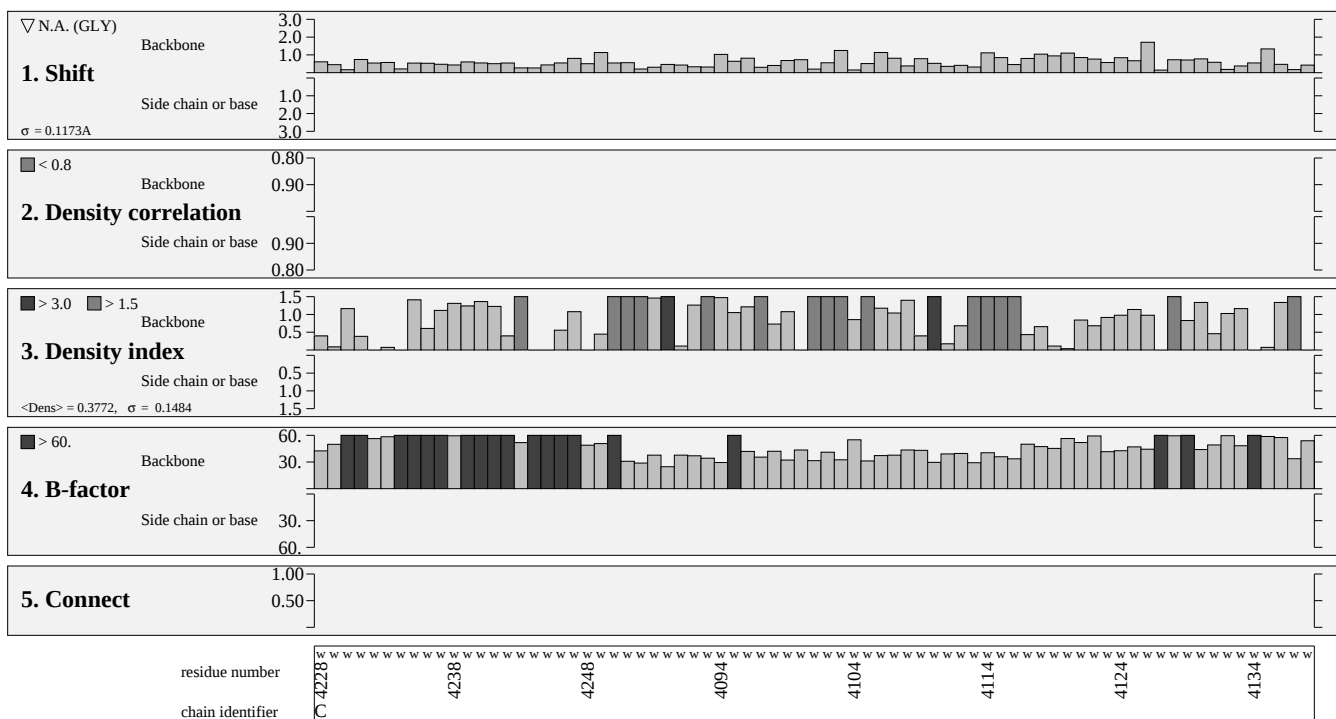
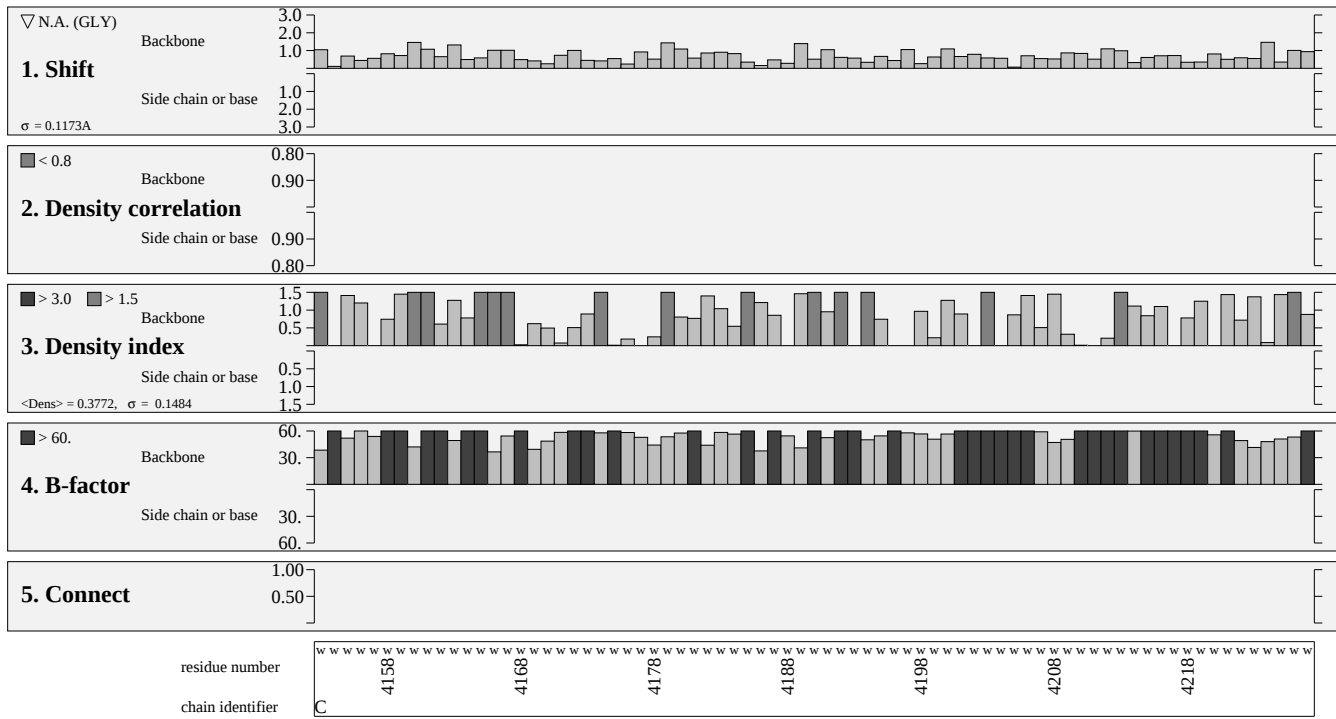
Local estimation (30)



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2A06

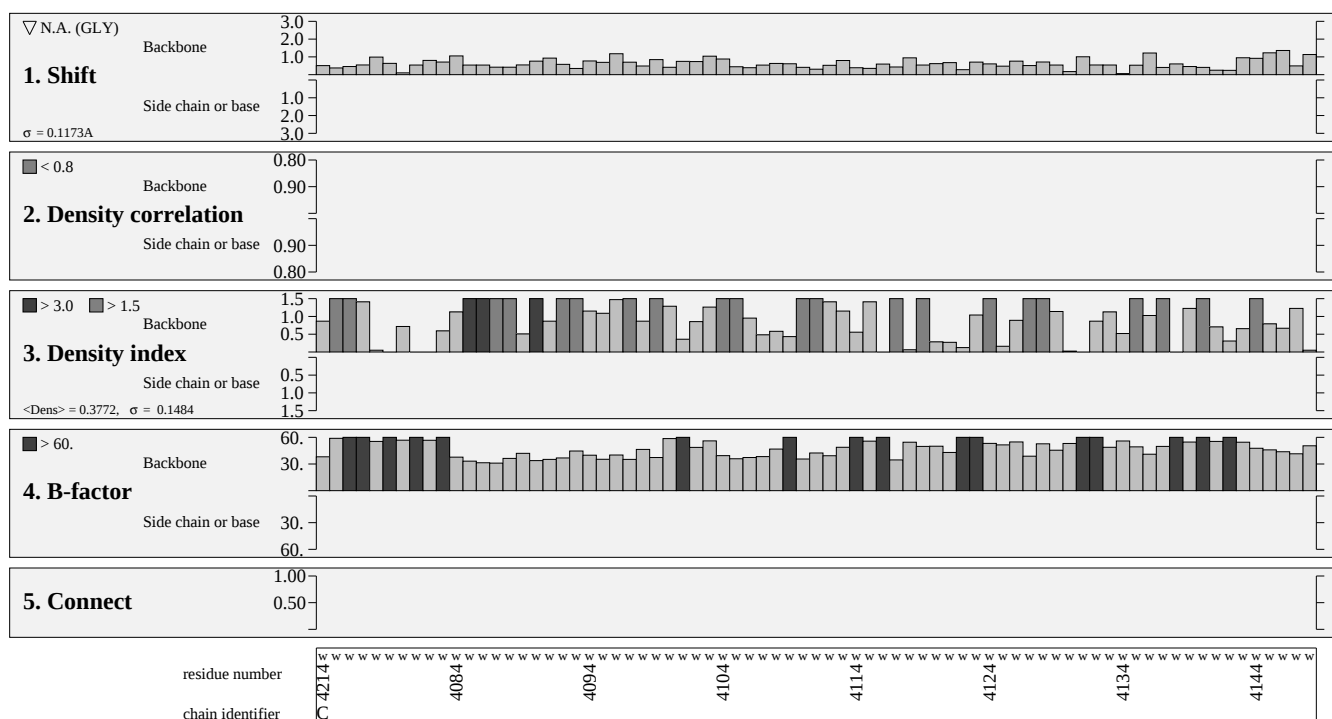
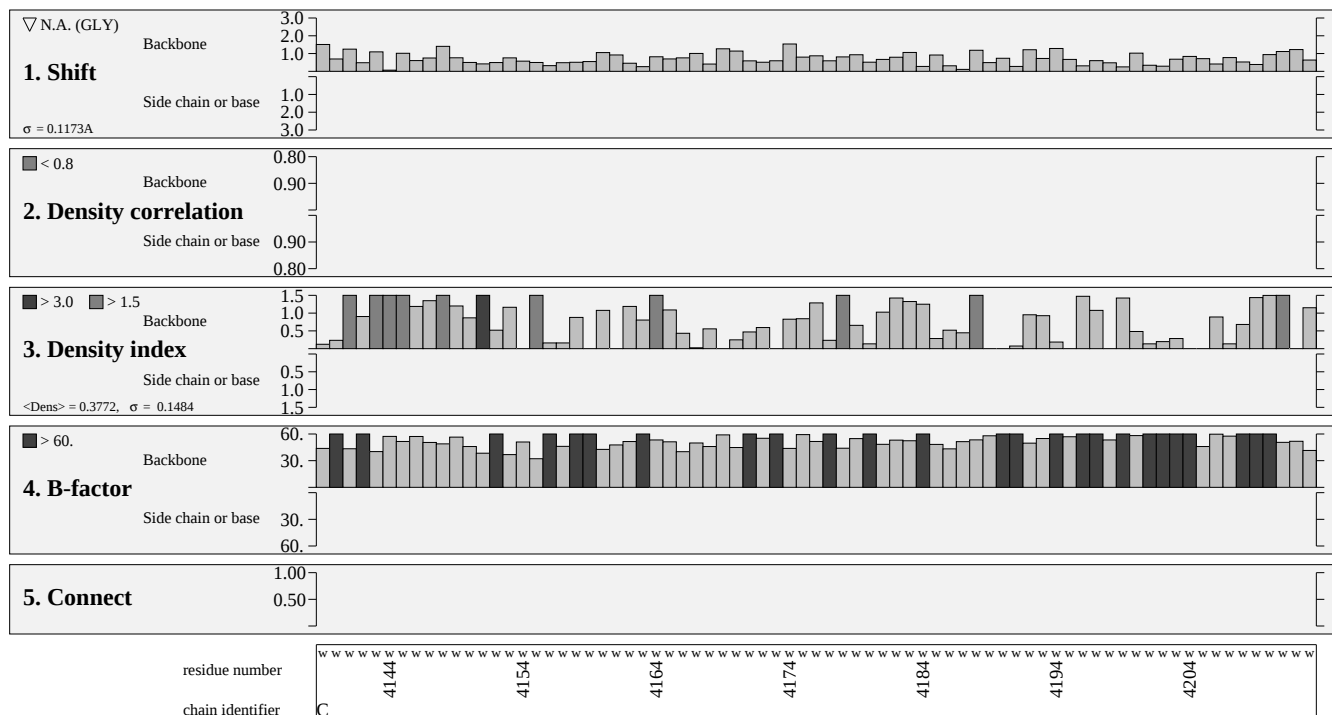
Local estimation (31)



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2A06

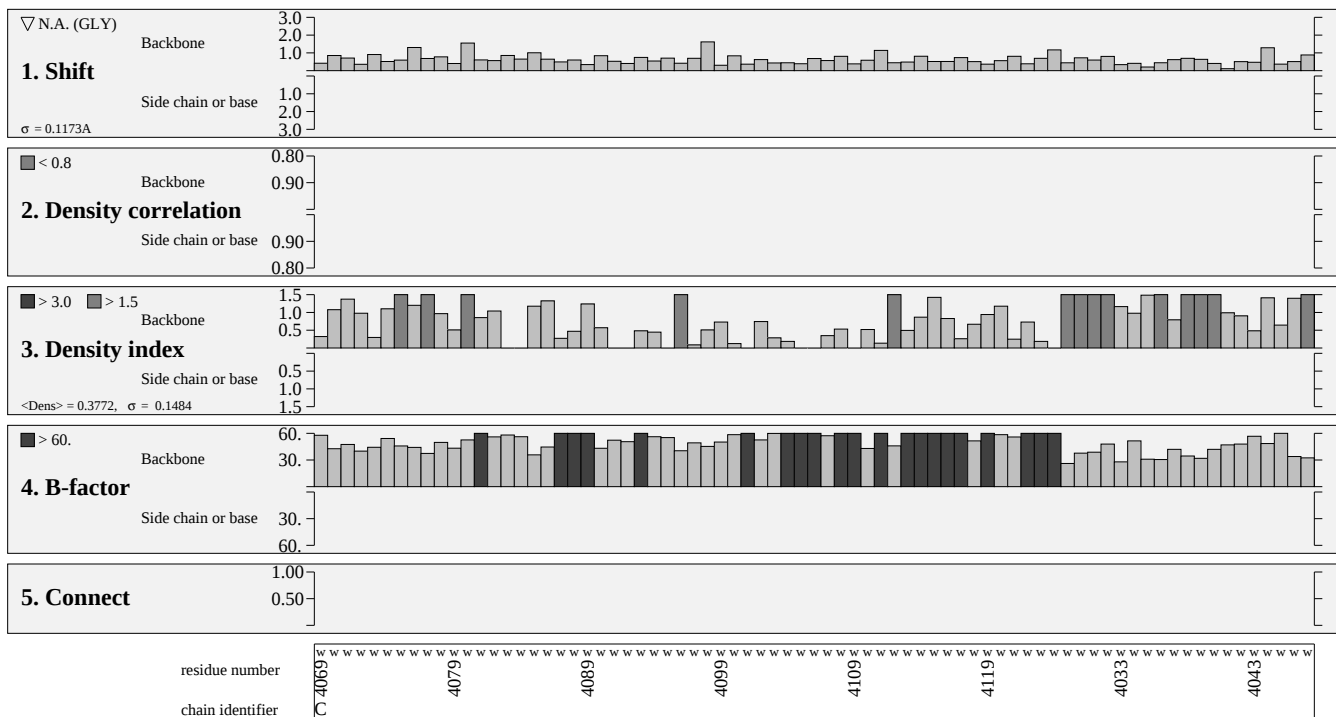
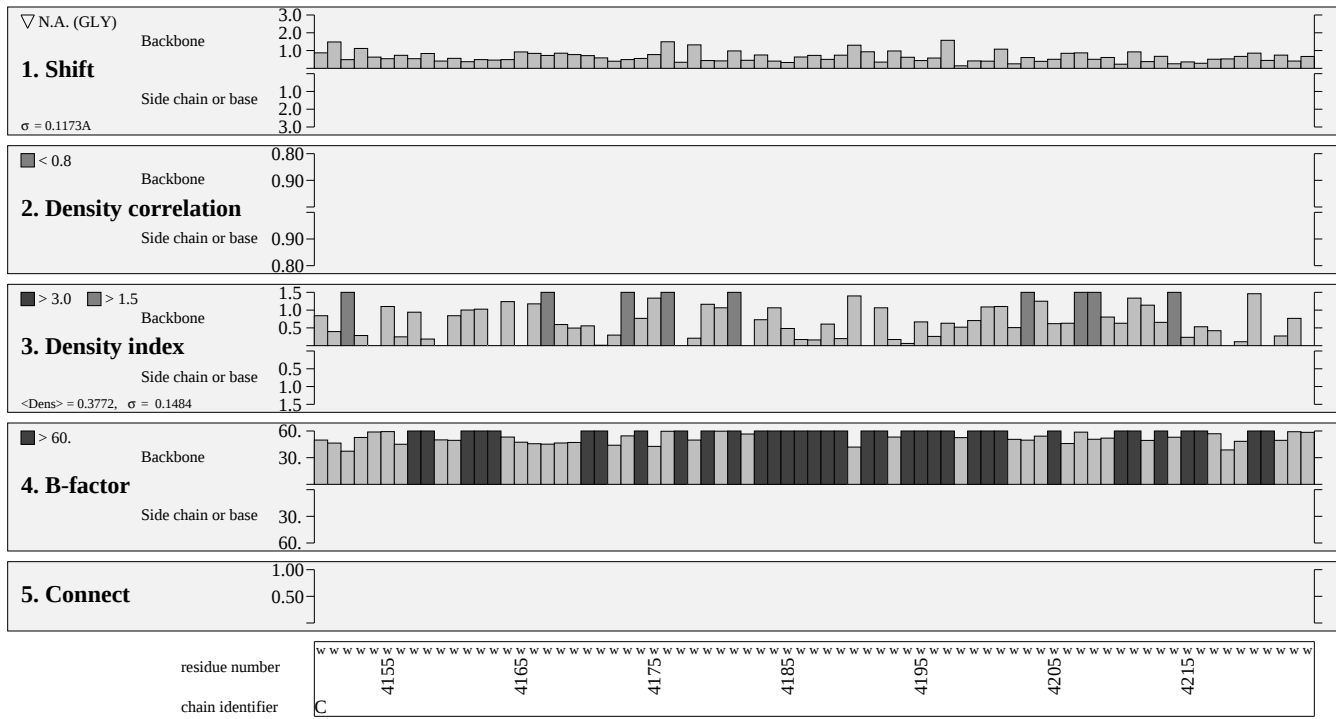
Local estimation (32)



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2A06

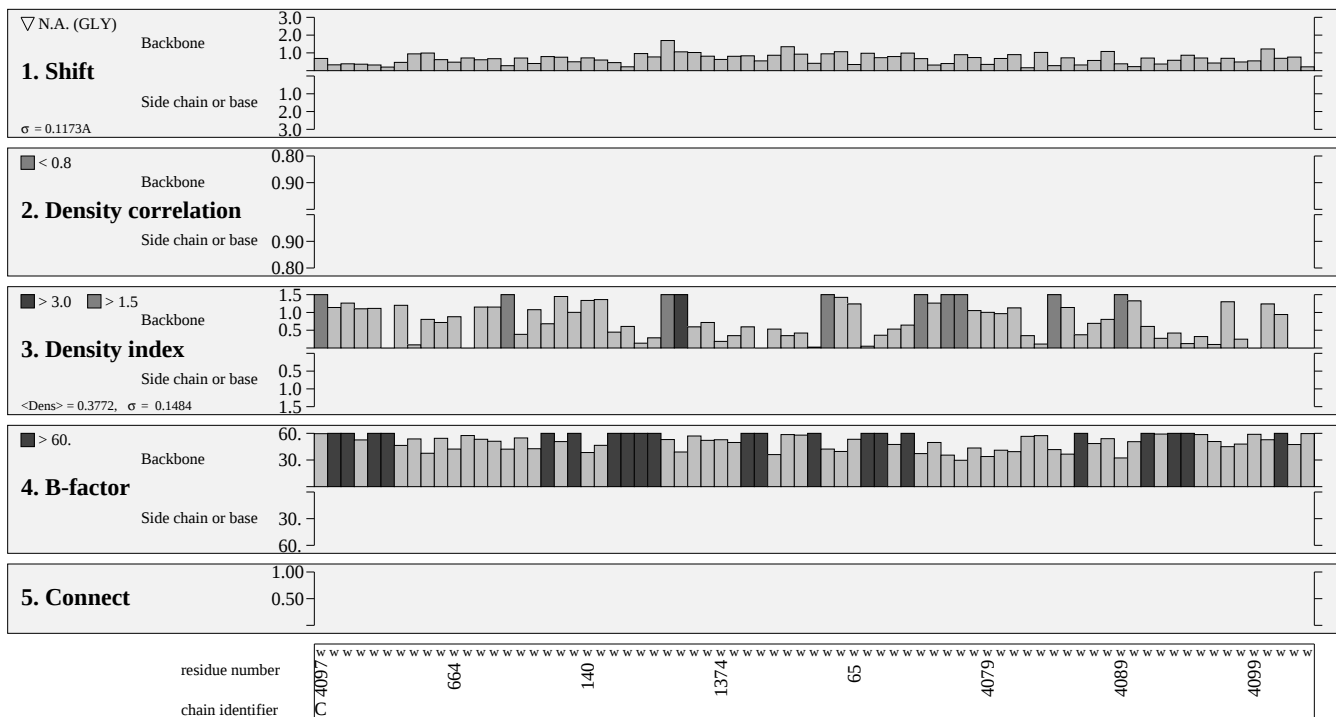
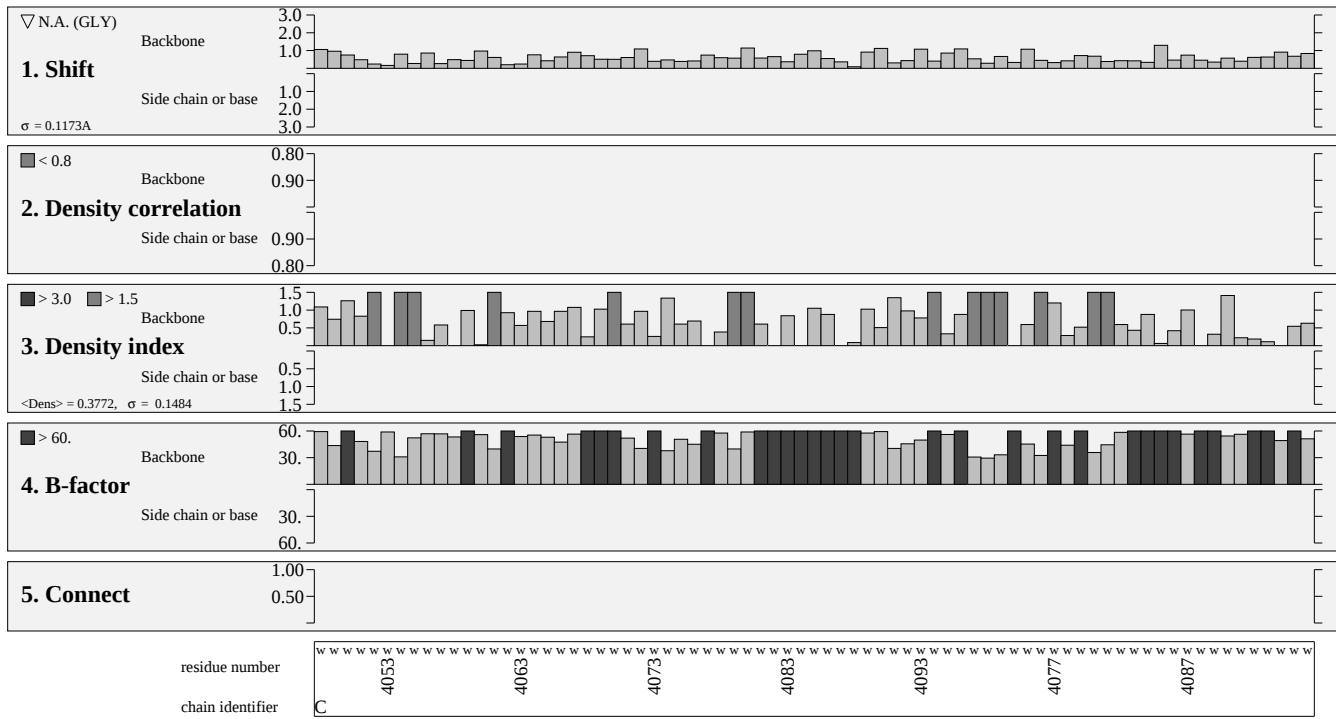
Local estimation (33)



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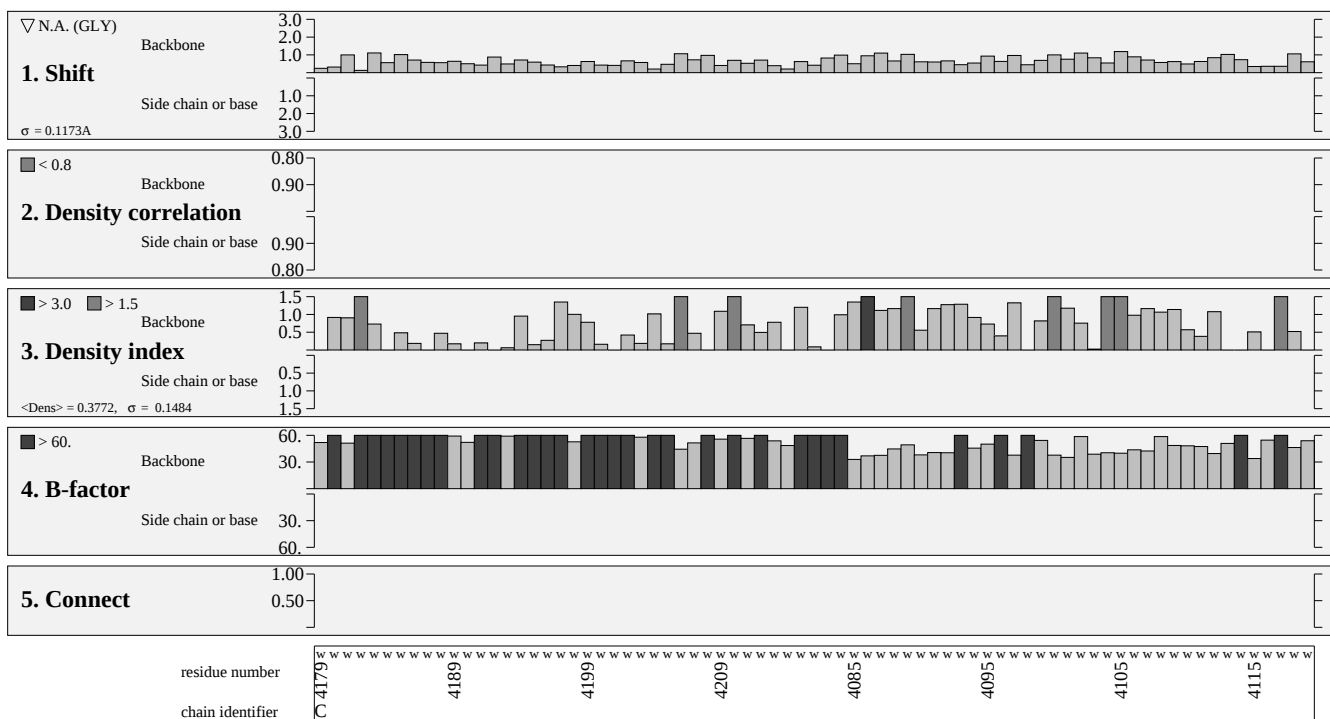
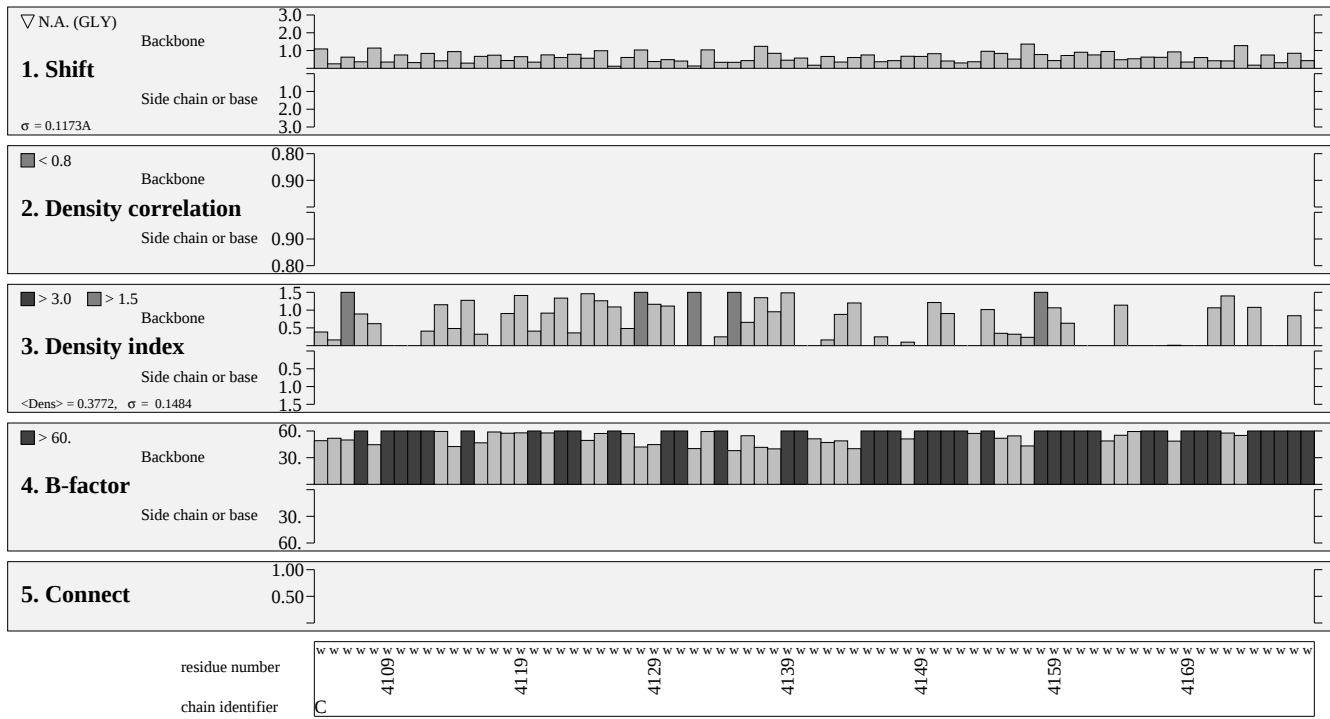
Local estimation (34)



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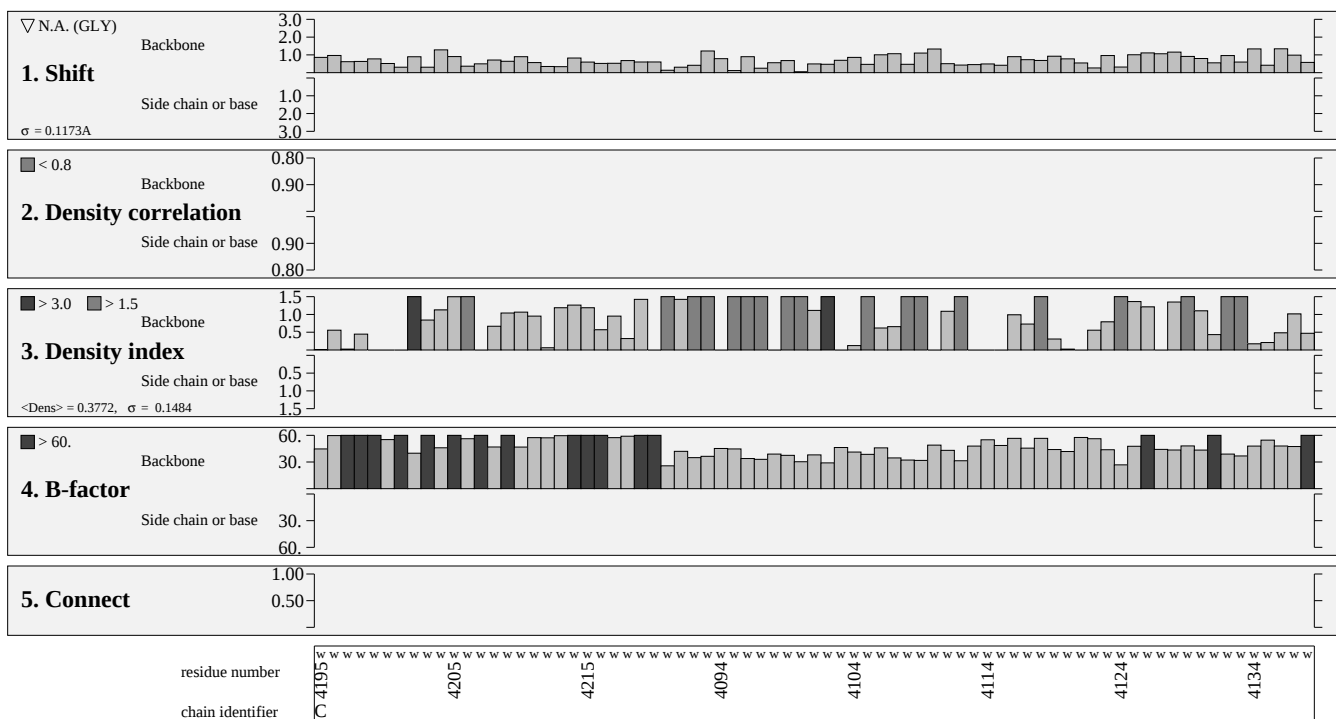
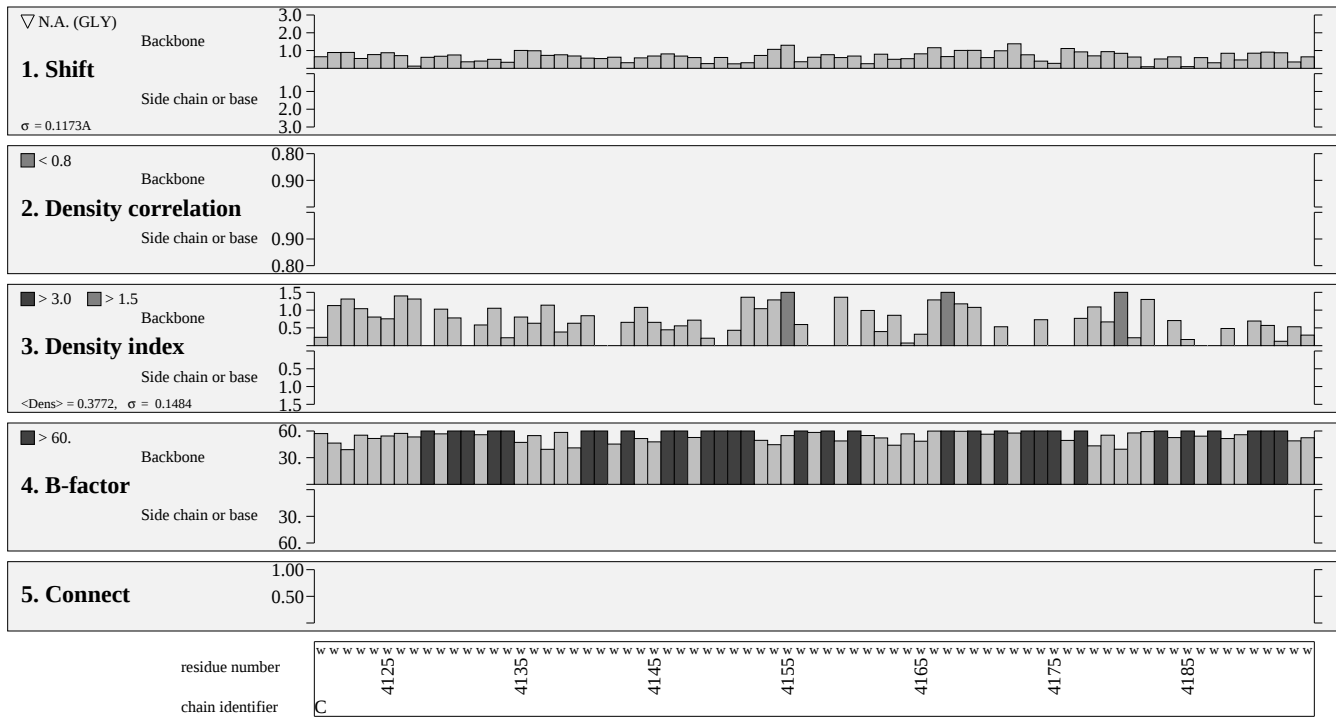
Local estimation (35)



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2A06

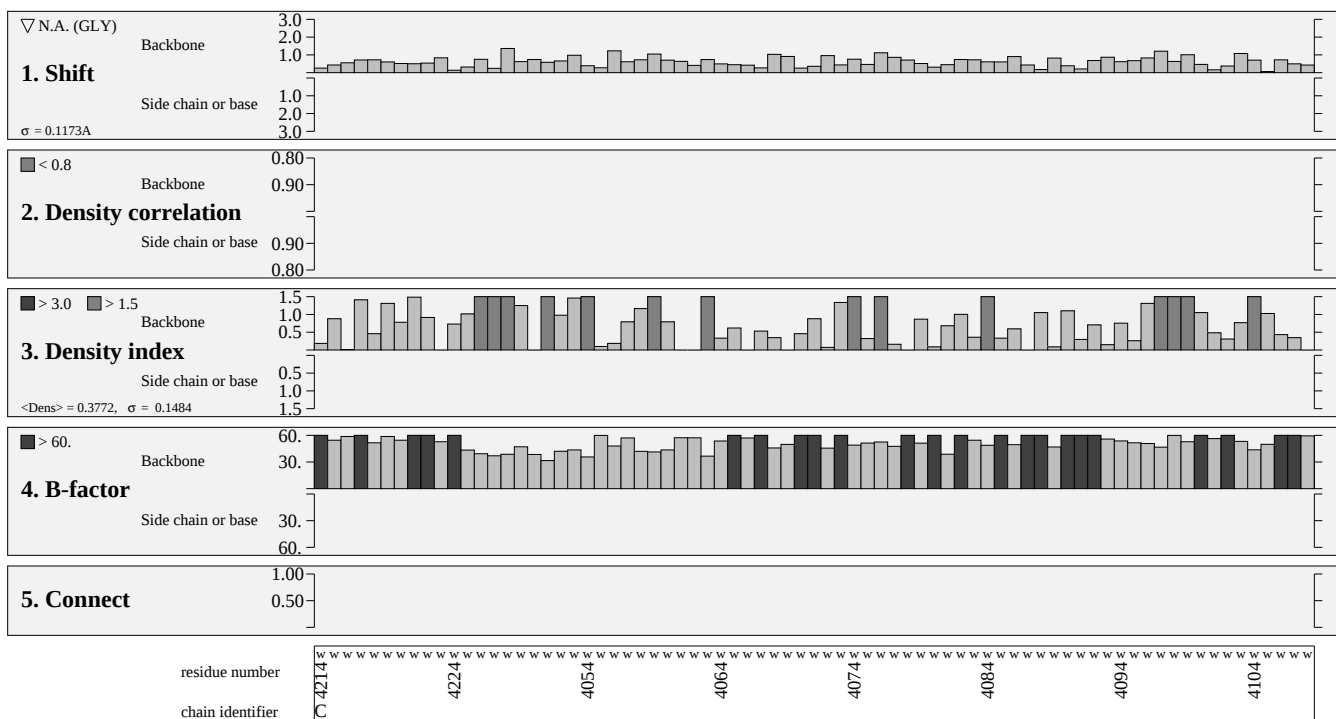
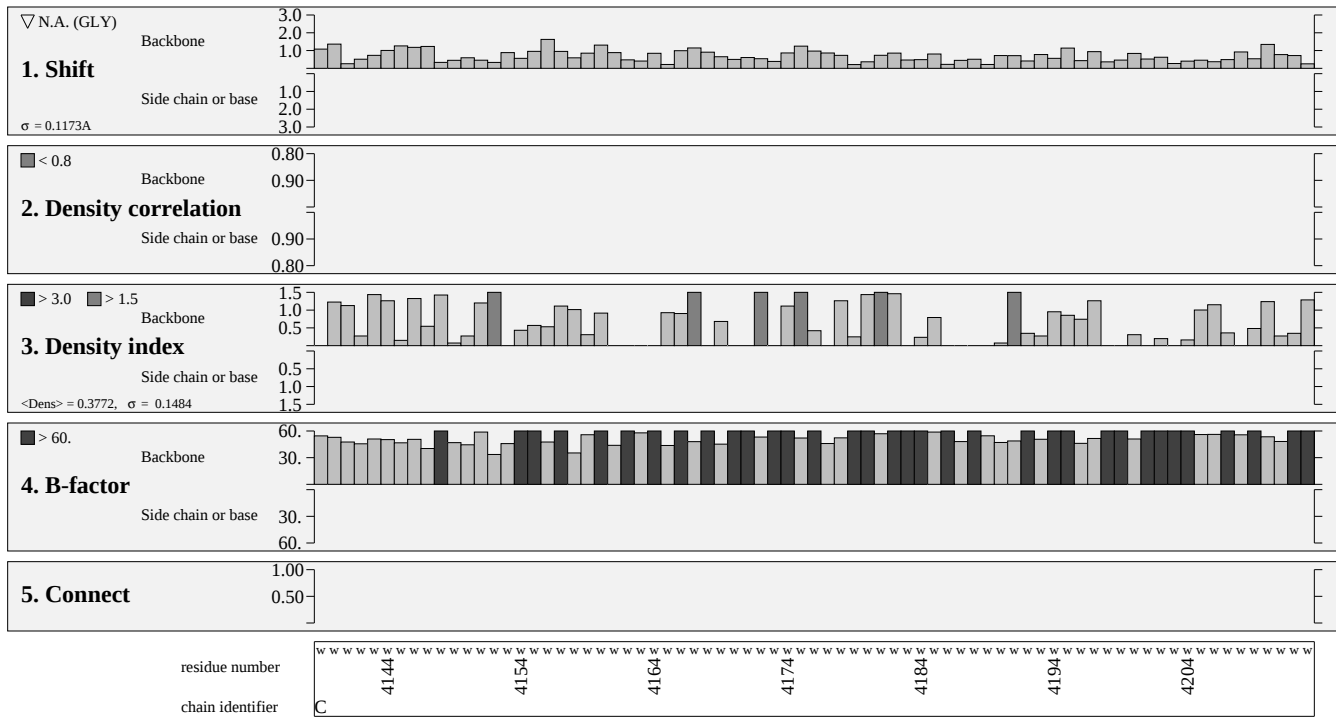
Local estimation (36)



Structure Factor Check

2A06

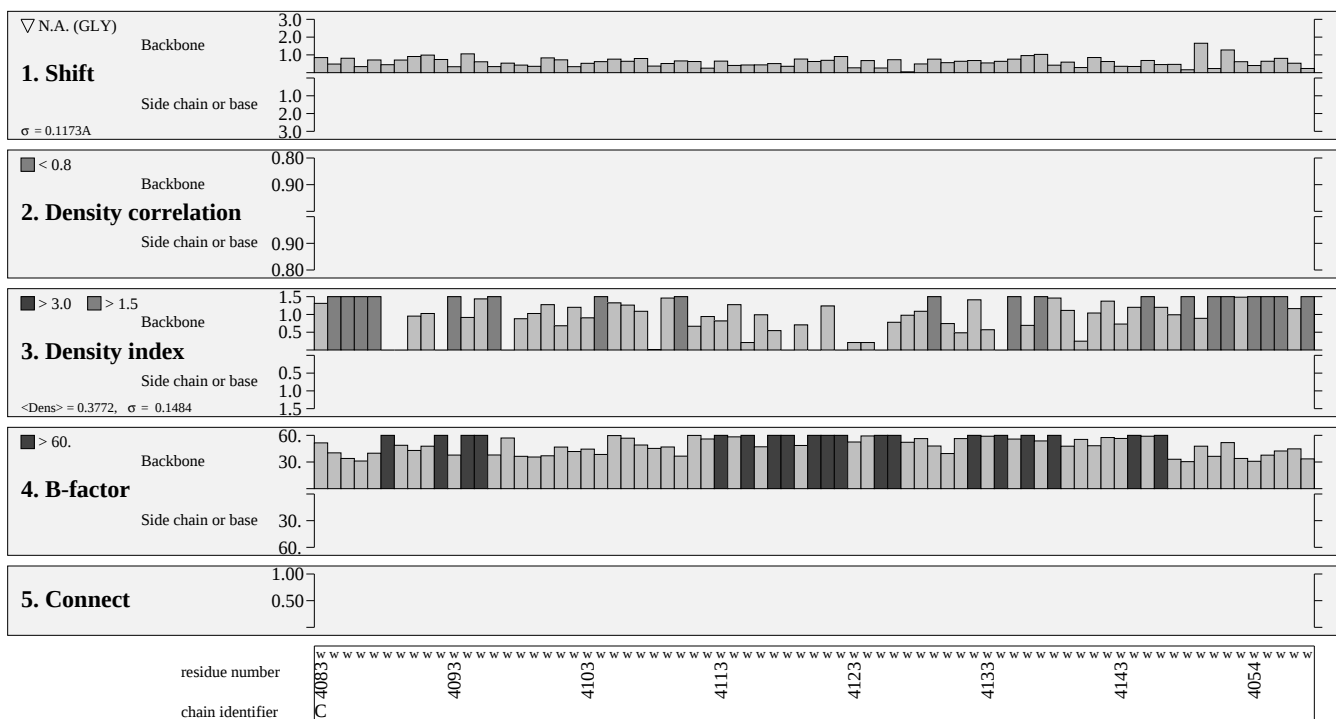
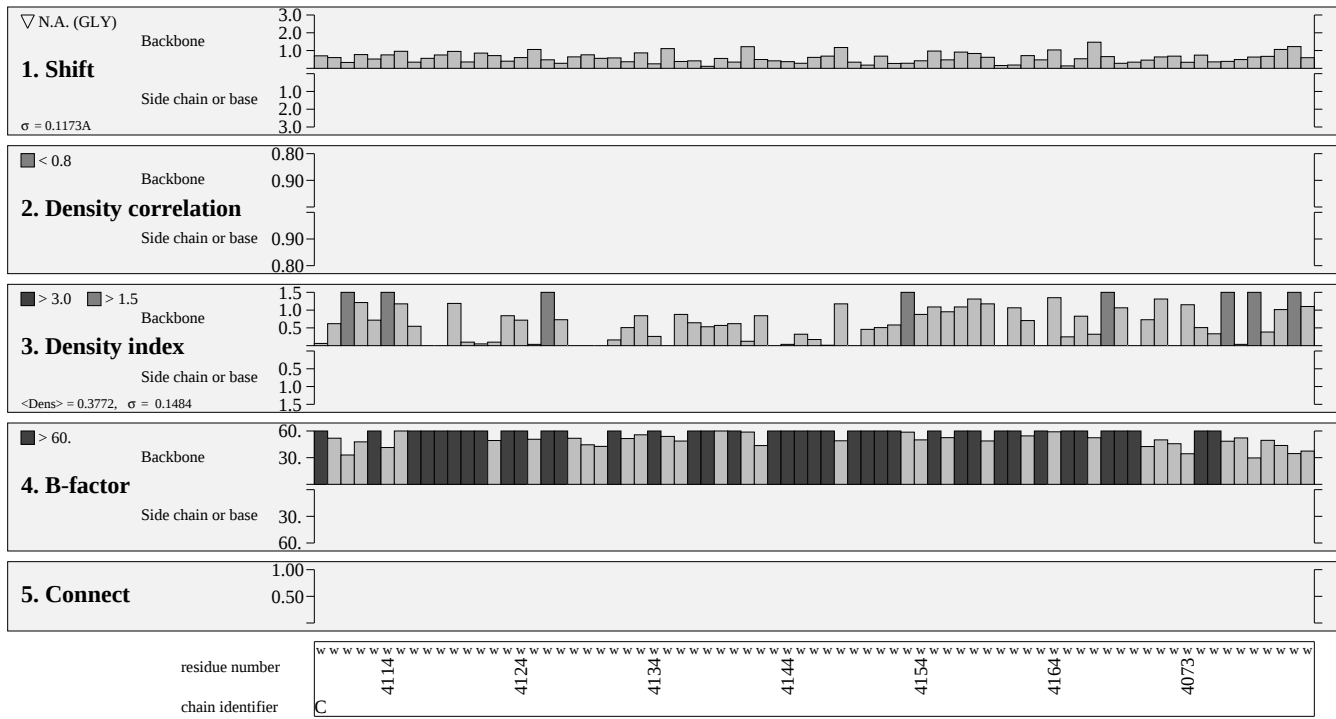
Local estimation (37)



Structure Factor Check

2A06

Local estimation (38)



Structure Factor Check

2A06

Local estimation (39)

