

Structure Factor Check

3TGU

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH PFVS-DESIGNED MOA I
BOUND
Date: 17-AUG-11
PDB code: 3TGU

Crystal

Cell parameters:

a: 172.68 Å b: 183.30 Å c: 241.94 Å
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Model

32733 atoms (21 water molecules)

Number of chains: 51

Volume not occupied by model: 62.9 %

 (for atomic model): 73.9 Å²

σ (B): 19.86 Å²

Matthews coefficient: 4.18

Corresponding solvent % : 70.33

Refinement

Program: CNS 1.1

Nominal resolution range: 25.0 – 2.70 Å

Reported R-factor: 0.258

Number of reflections used: 191170

Reported Rfree: 0.29

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 25.0 – 2.70 Å

Reflections in file: 191170

Unique reflections above 0: 191170

above 1 σ : 184592

above 3 σ : 104833

SFCHECK

Nominal resolution range: 25.0 – 2.70 Å

\05max. from input data, min. from author\05

Used reflections: 191170

Completeness: 91.2 %

R_stand(F) = $\langle \sigma(F) \rangle / \langle F \rangle$: 0.091

Anisotropic distribution of Structure Factors

ratio of eigen values: 1.0000 0.4697 0.4702

B_overall (by Patterson): 48.Å²

Optical resolution: 2.07 Å

Expected opt. resol. for complete data set: 2.07 Å

Estimated minimal error: 0.095 Å

Model vs. Structure Factors

R-factor for all reflections: 0.307

Correlation factor: 0.867

R-factor: 0.305

for $F > 2.0\sigma$

nom. resolution range: 24.98 – 2.70Å

reflections used: 184724

Rfree: 0.332

Nfree: 3620

R-factor without free-refl.: 0.304

Non free-reflections: 181104

<u> (error in coords by Luzzati plot): 0.489 Å

Estimated maximal error: 0.349 Å

DPI: 0.333 Å

Scaling

Scale: 0.647

Bdiff: -10.25

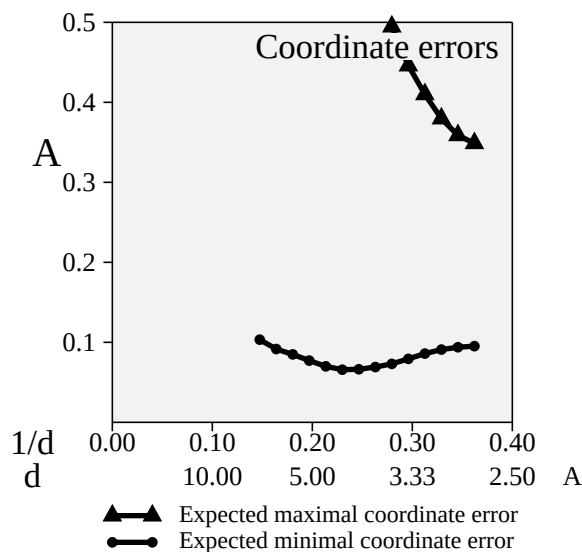
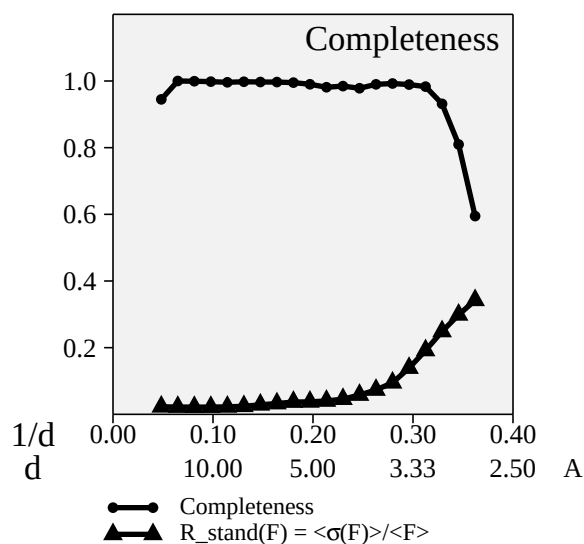
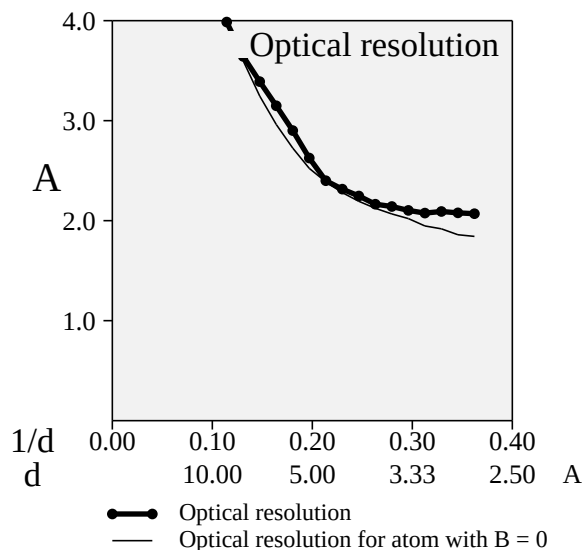
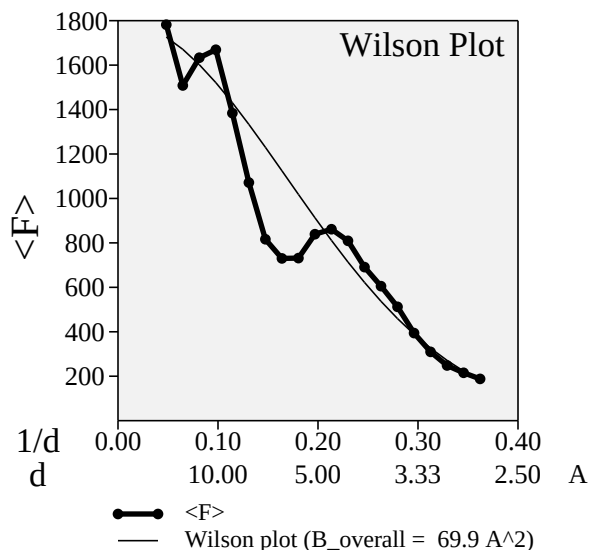
Anisothermal Scaling (Beta):

11.3750 -3.4908 -3.1882 0.0000 0.0000 0.0000

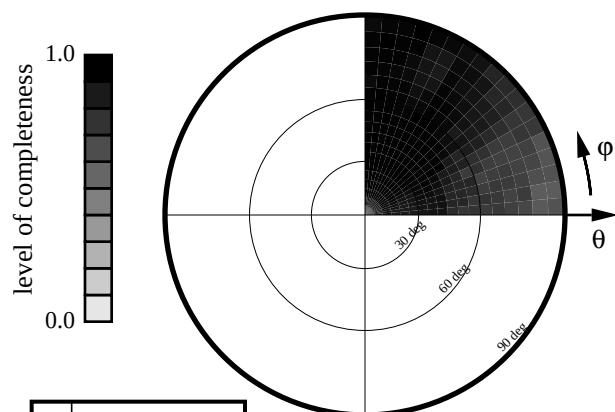
Solvent correction – Ks,Bs: 0.594 250.062

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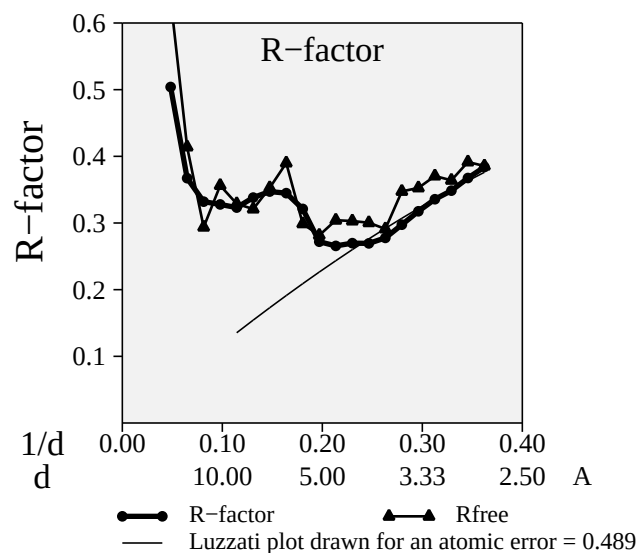


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

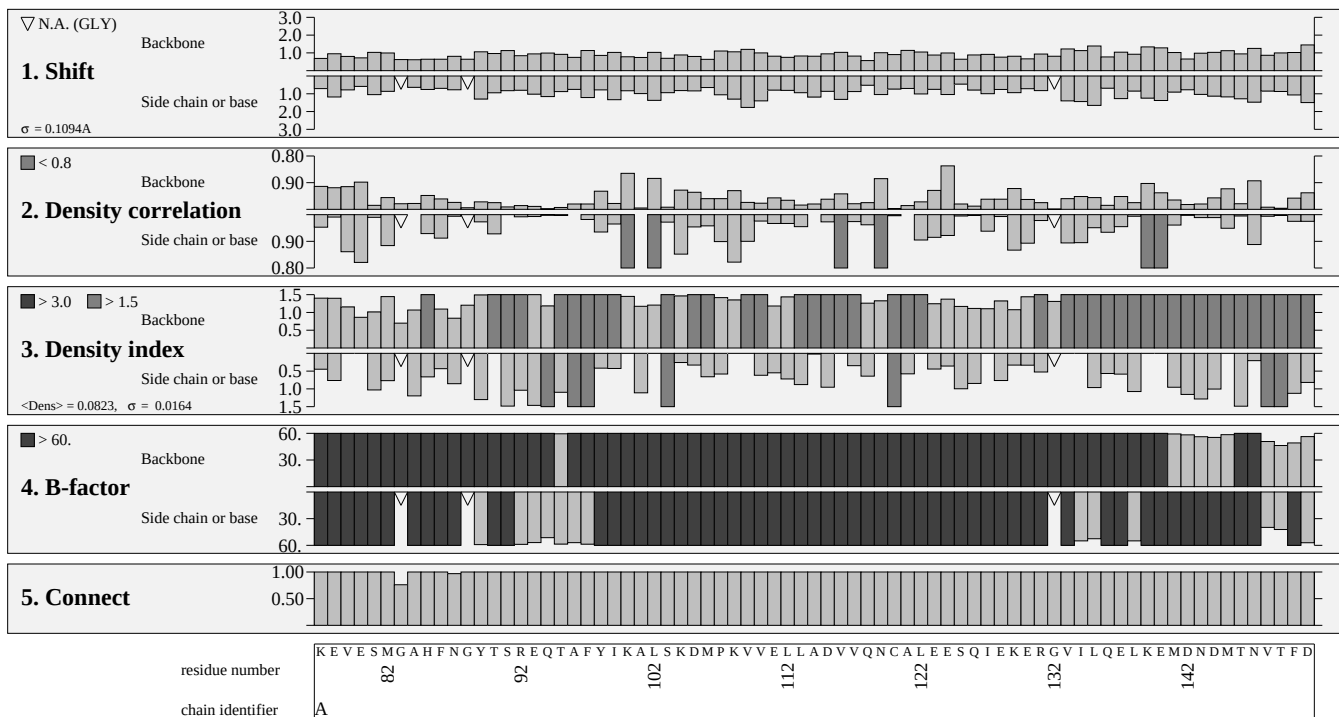
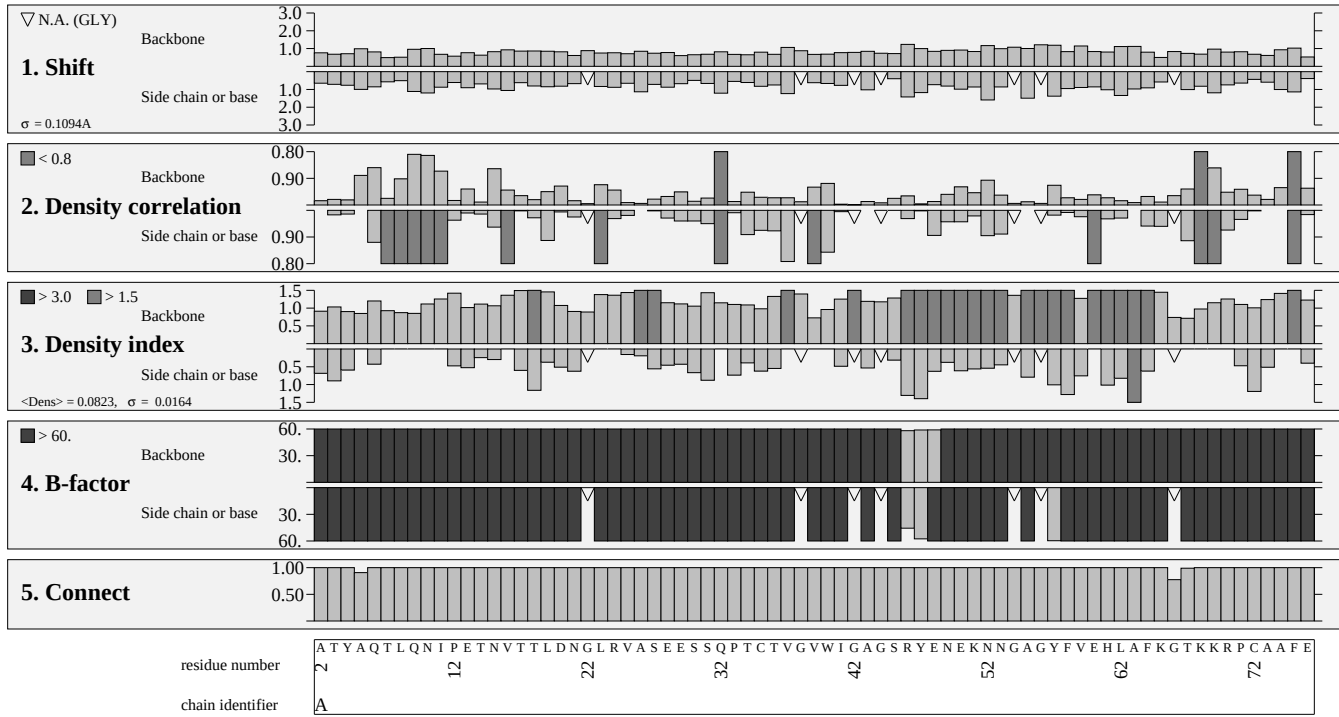
polar coordinates of the crystallographical axes



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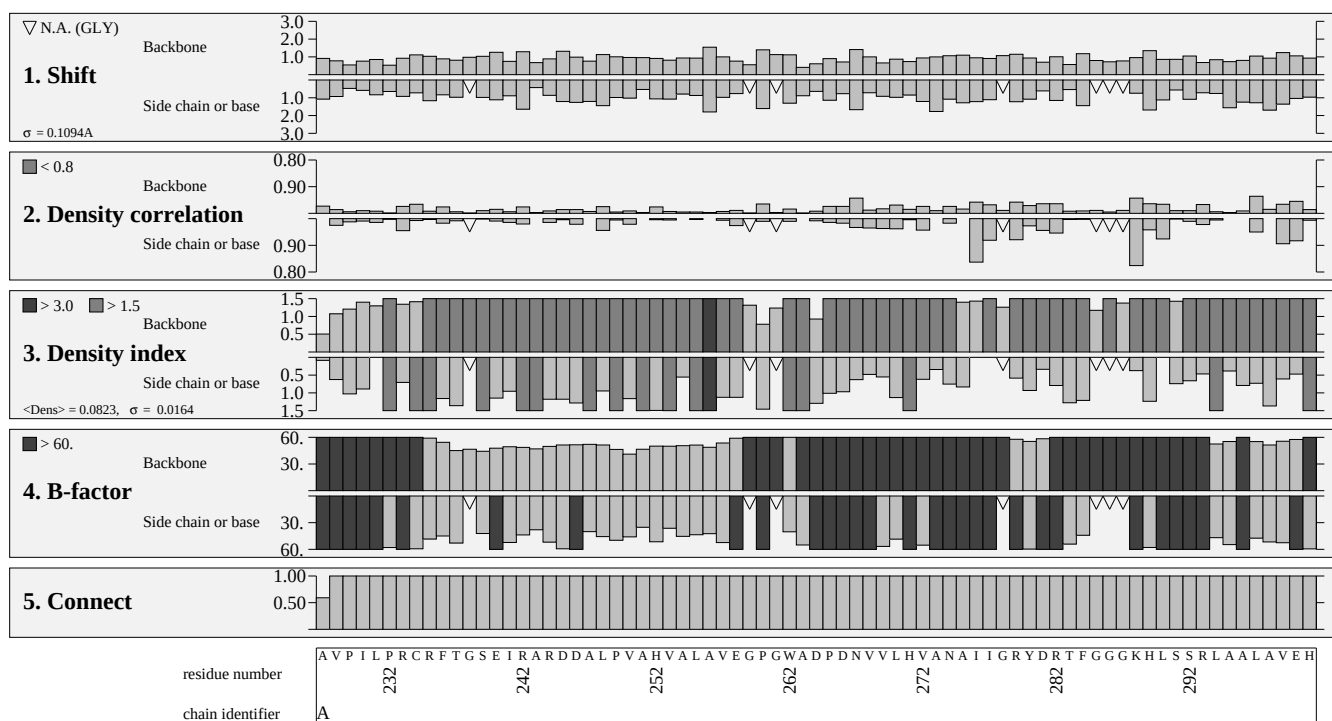
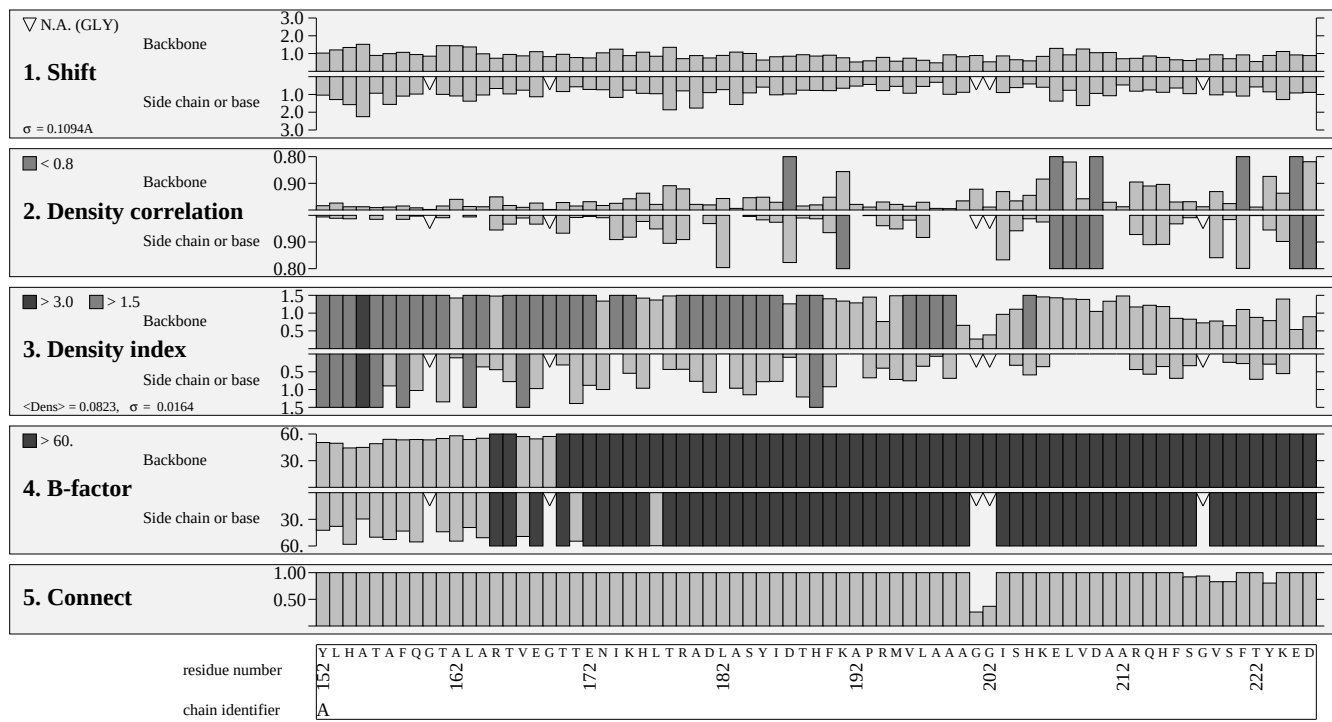
Local estimation



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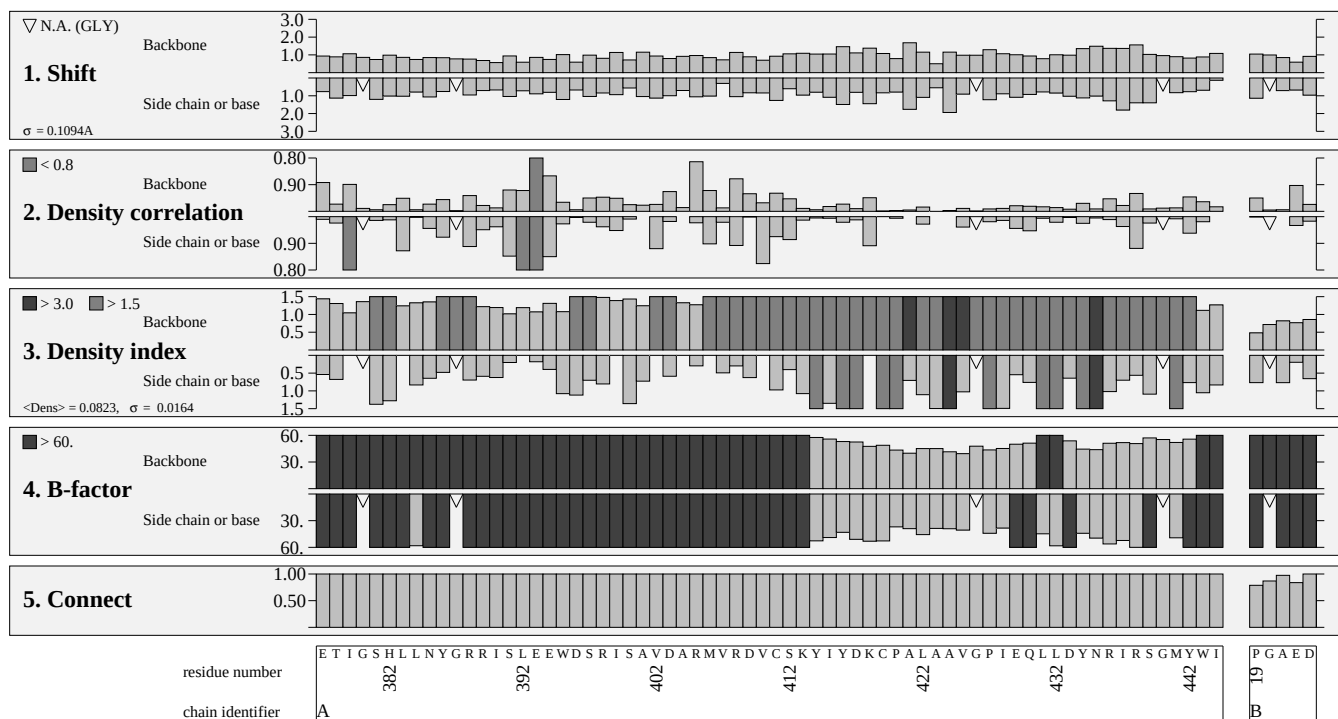
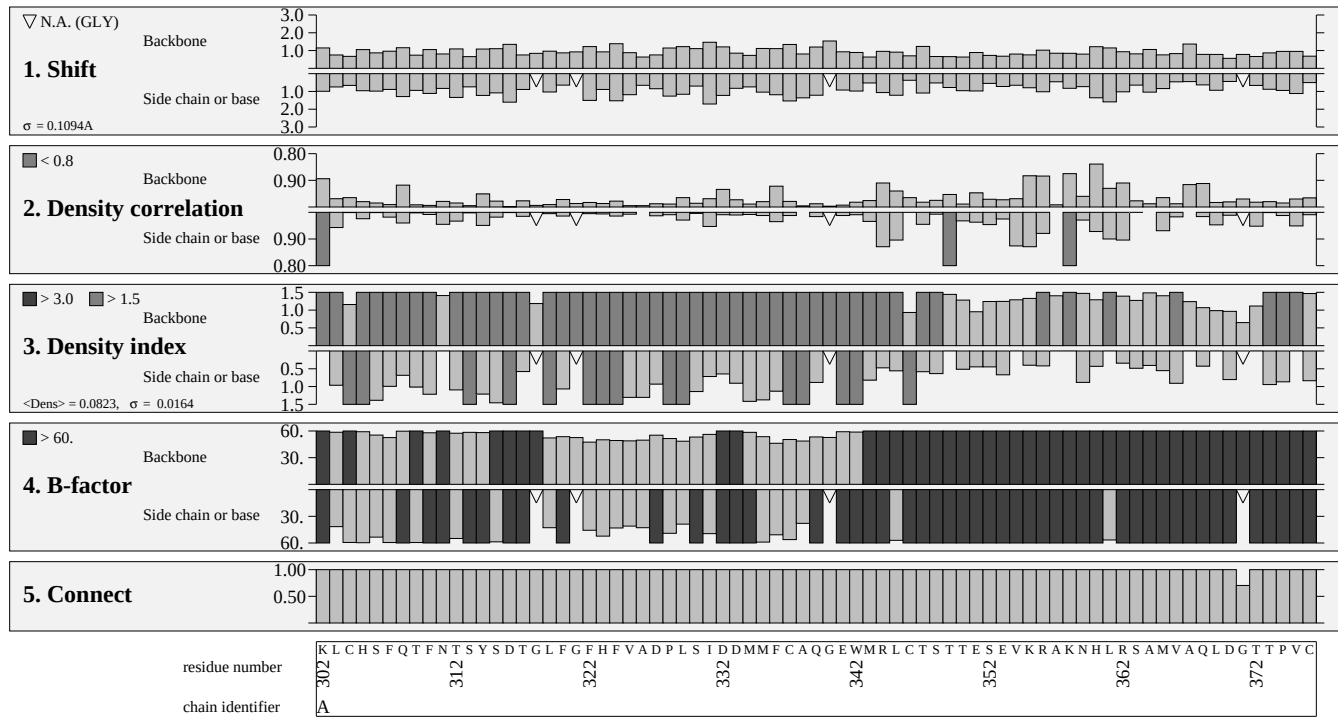
Local estimation (2)



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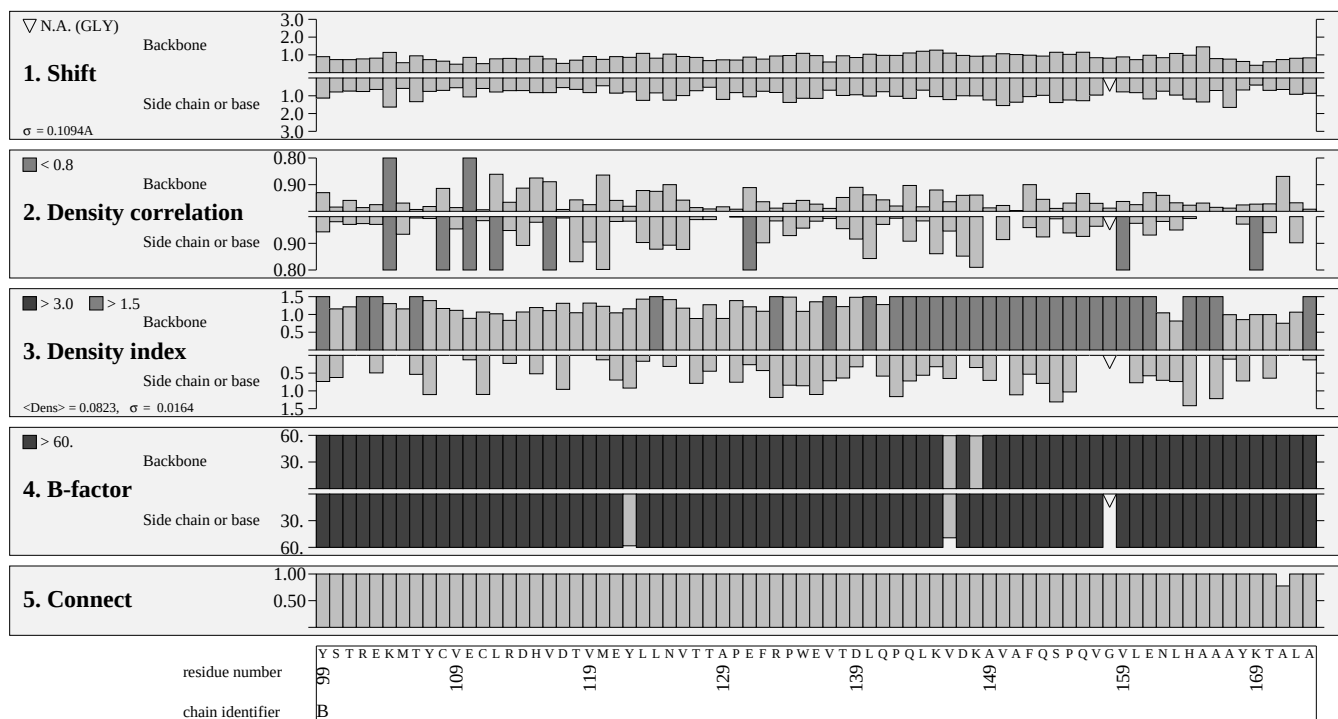
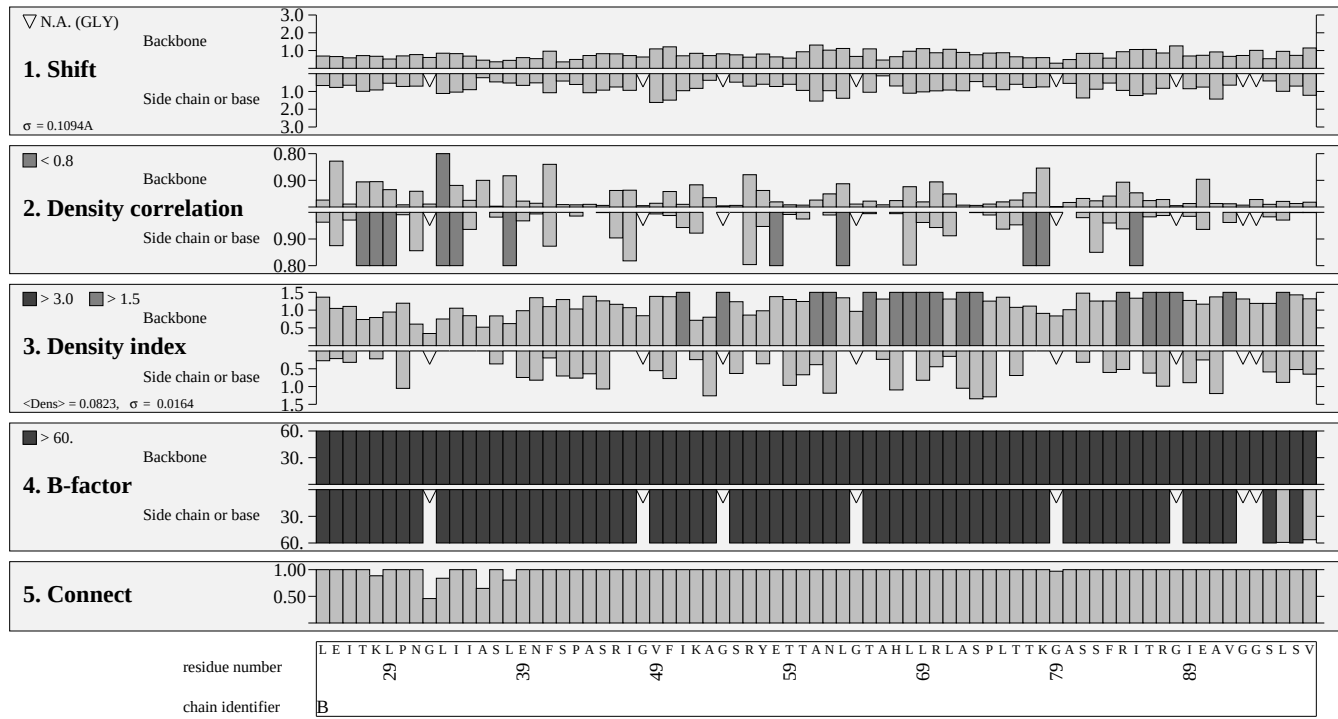
Local estimation (3)



Structure Factor Check

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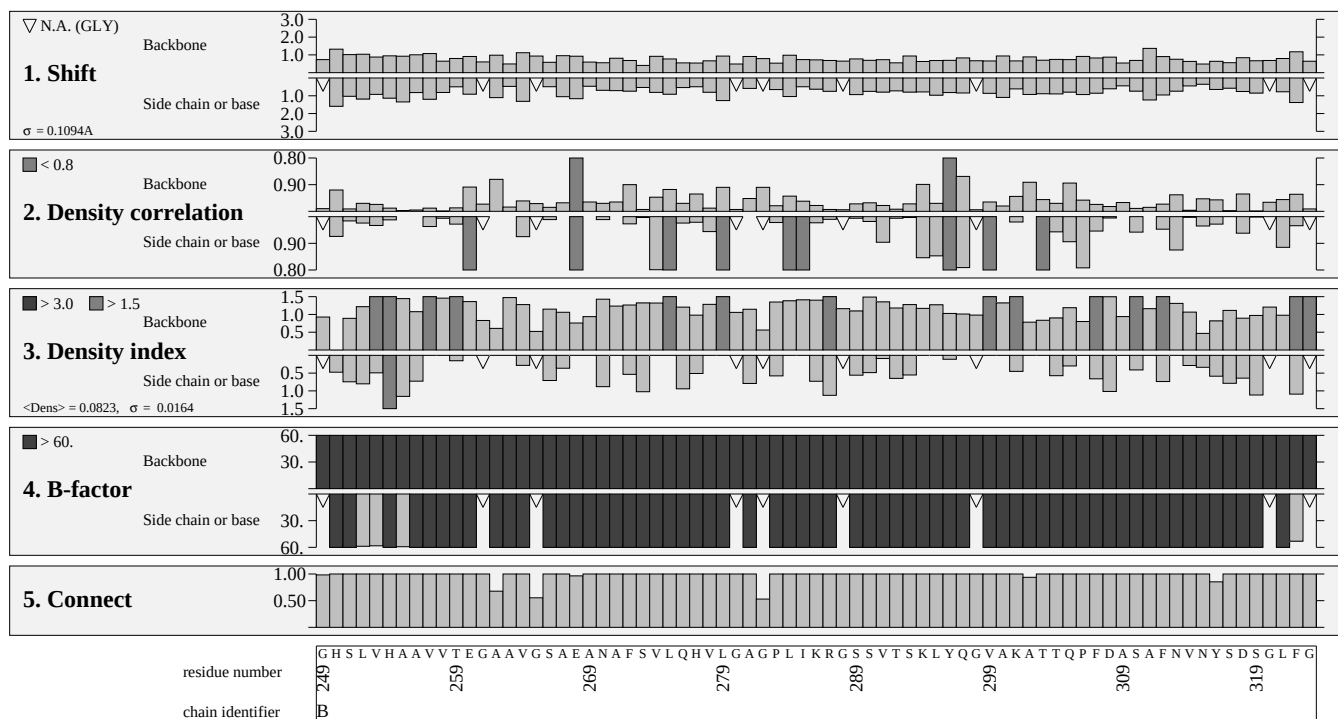
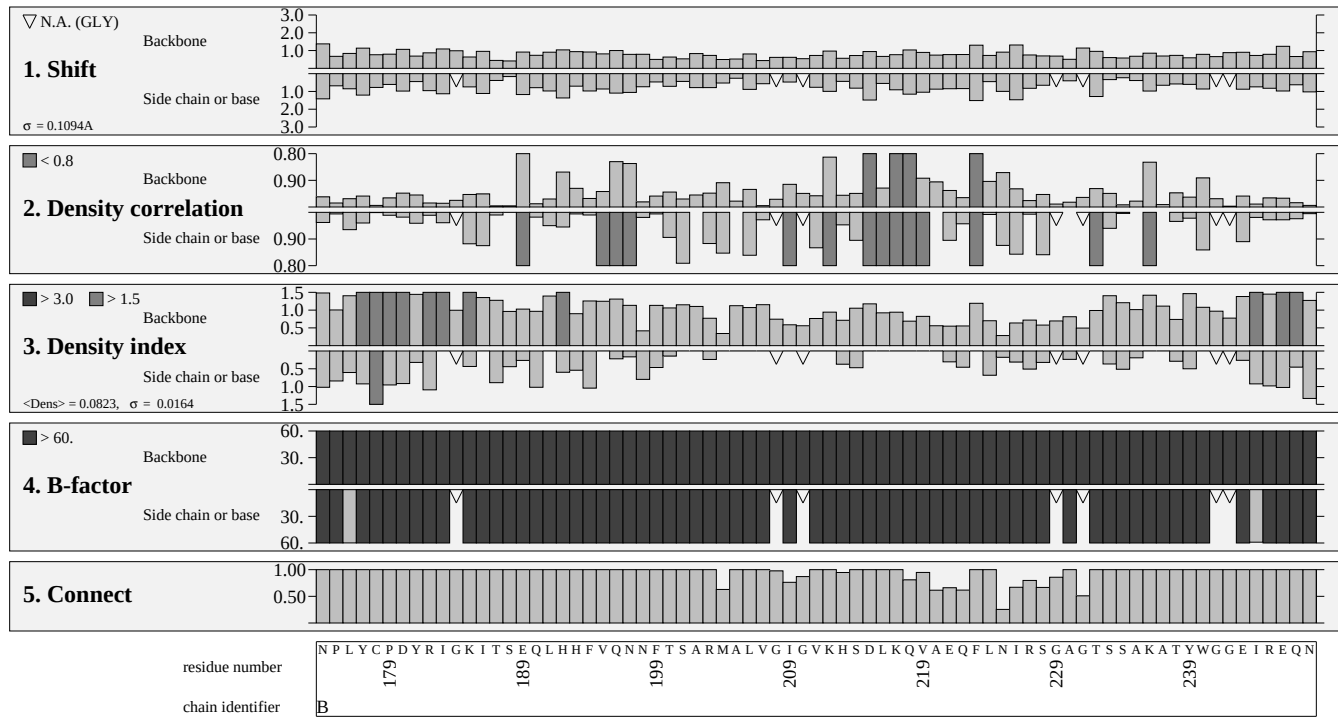
Local estimation (4)



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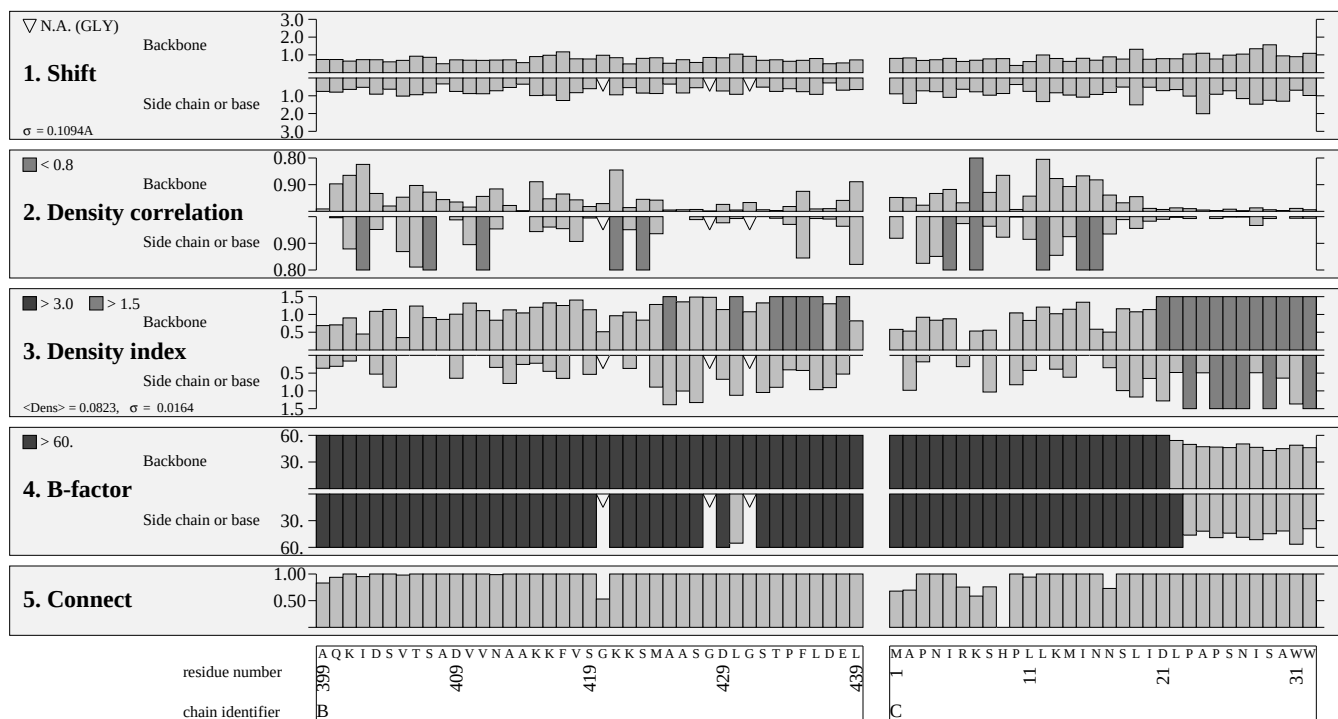
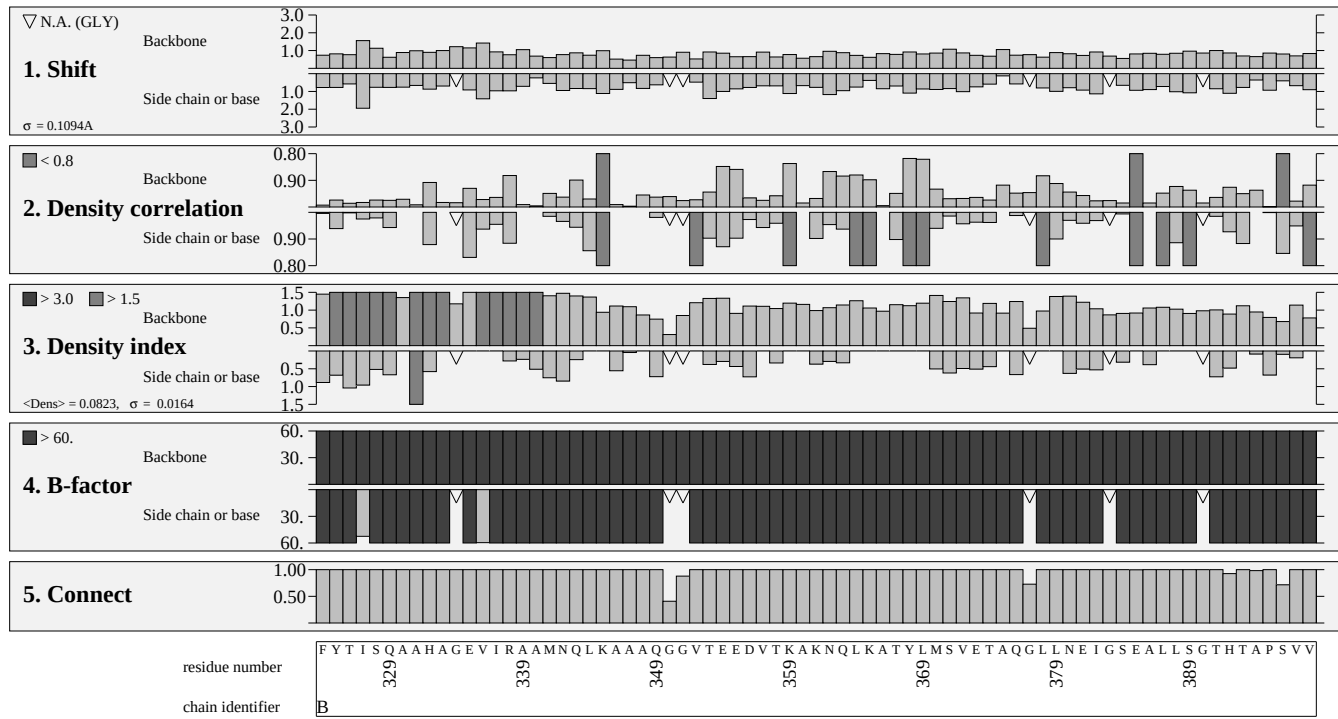
Local estimation (5)



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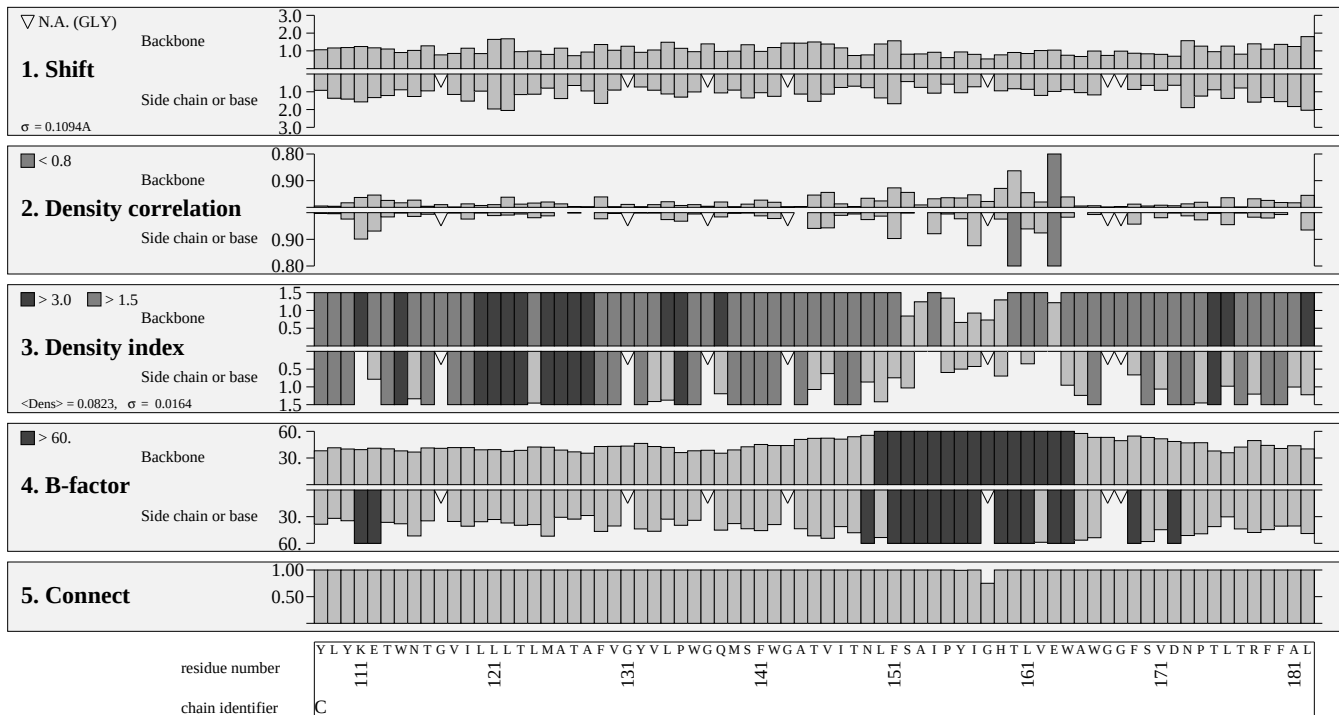
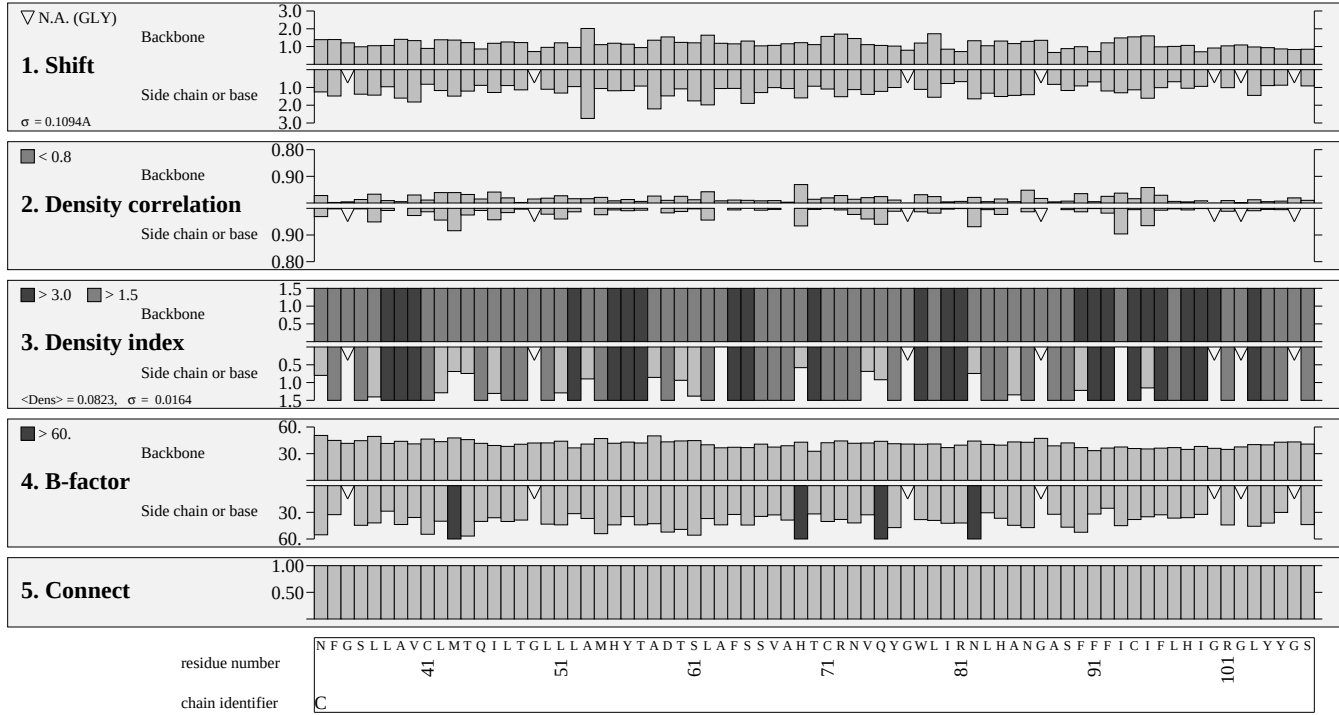
Local estimation (6)



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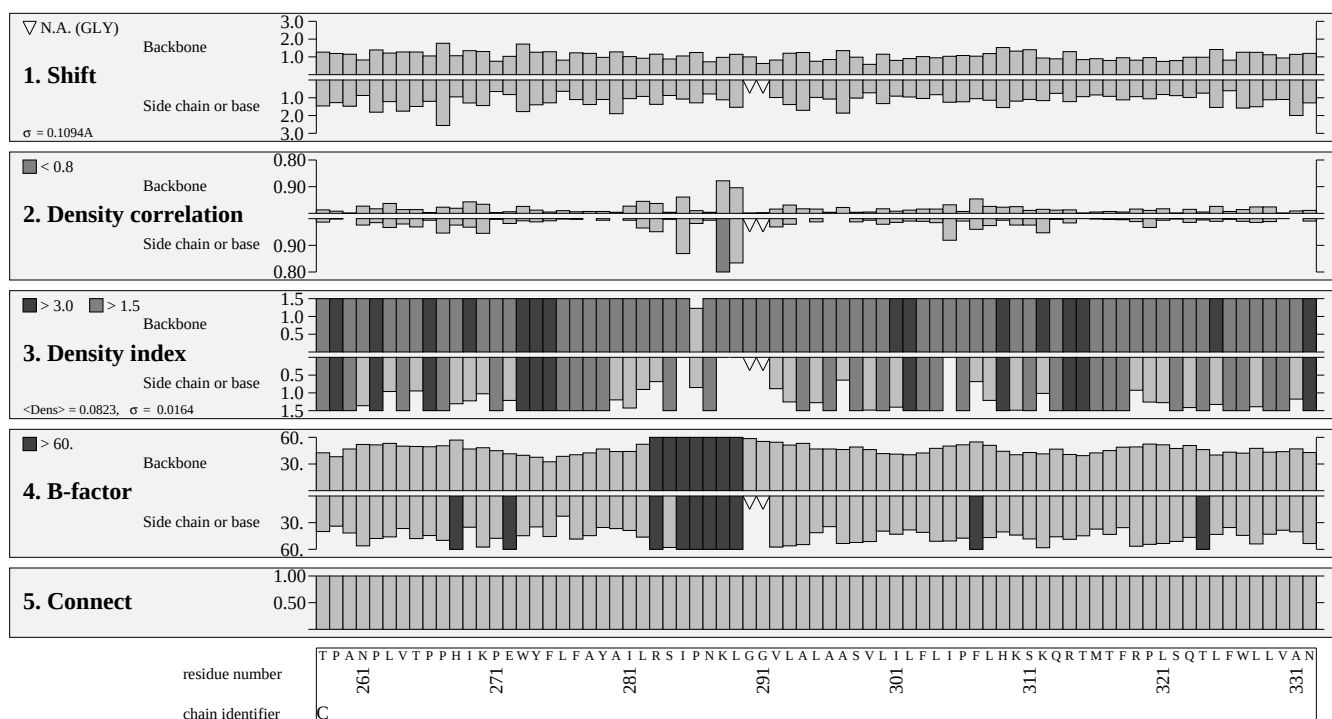
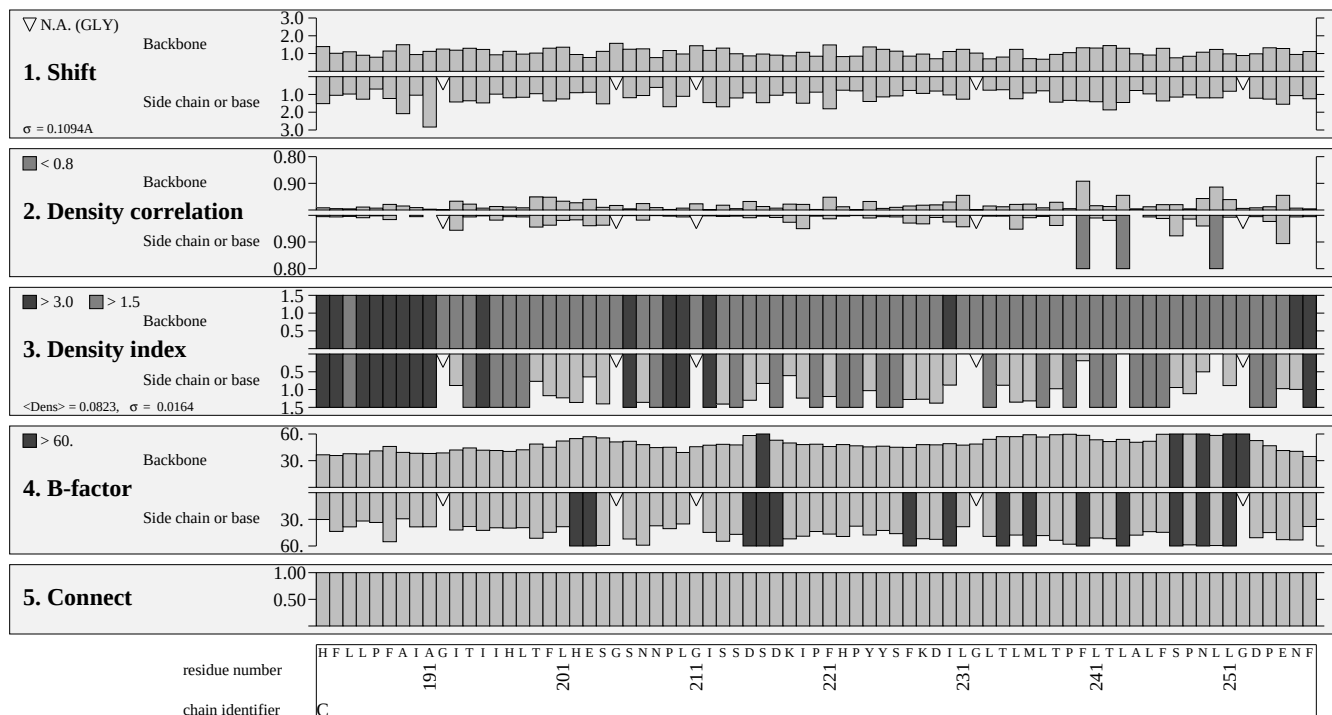
Local estimation (7)



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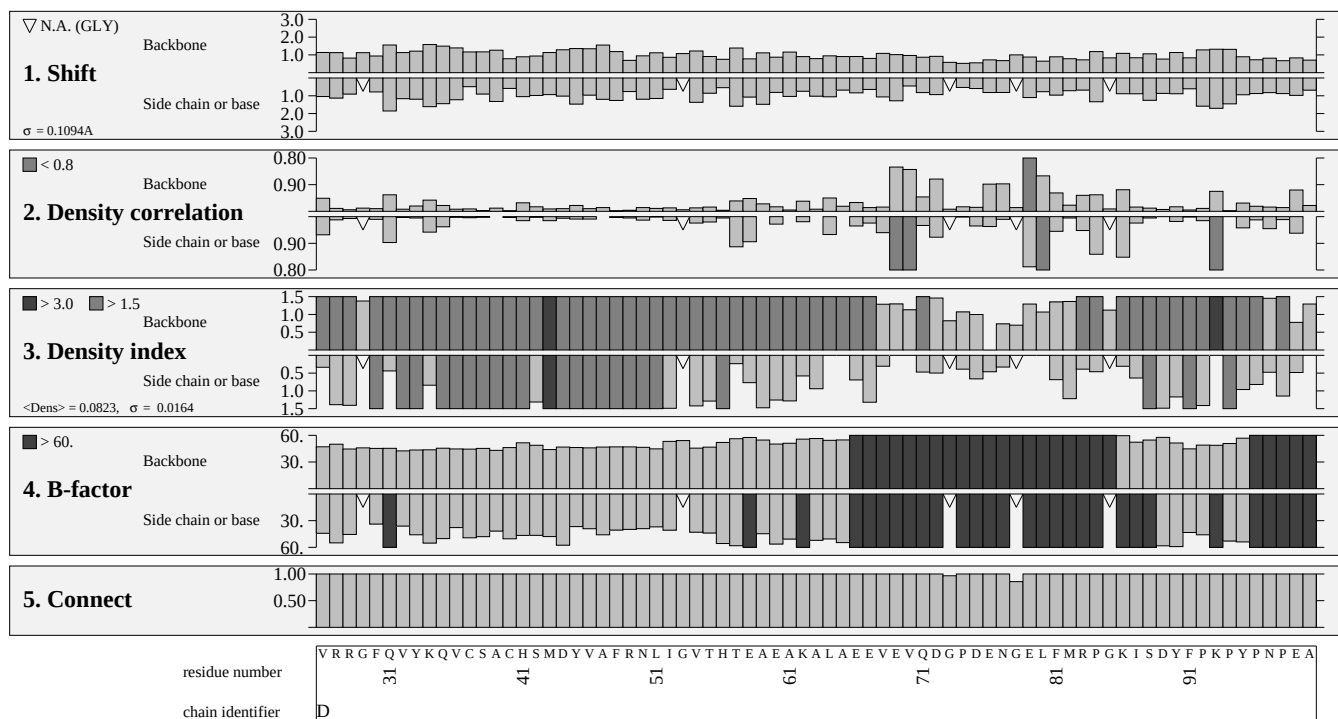
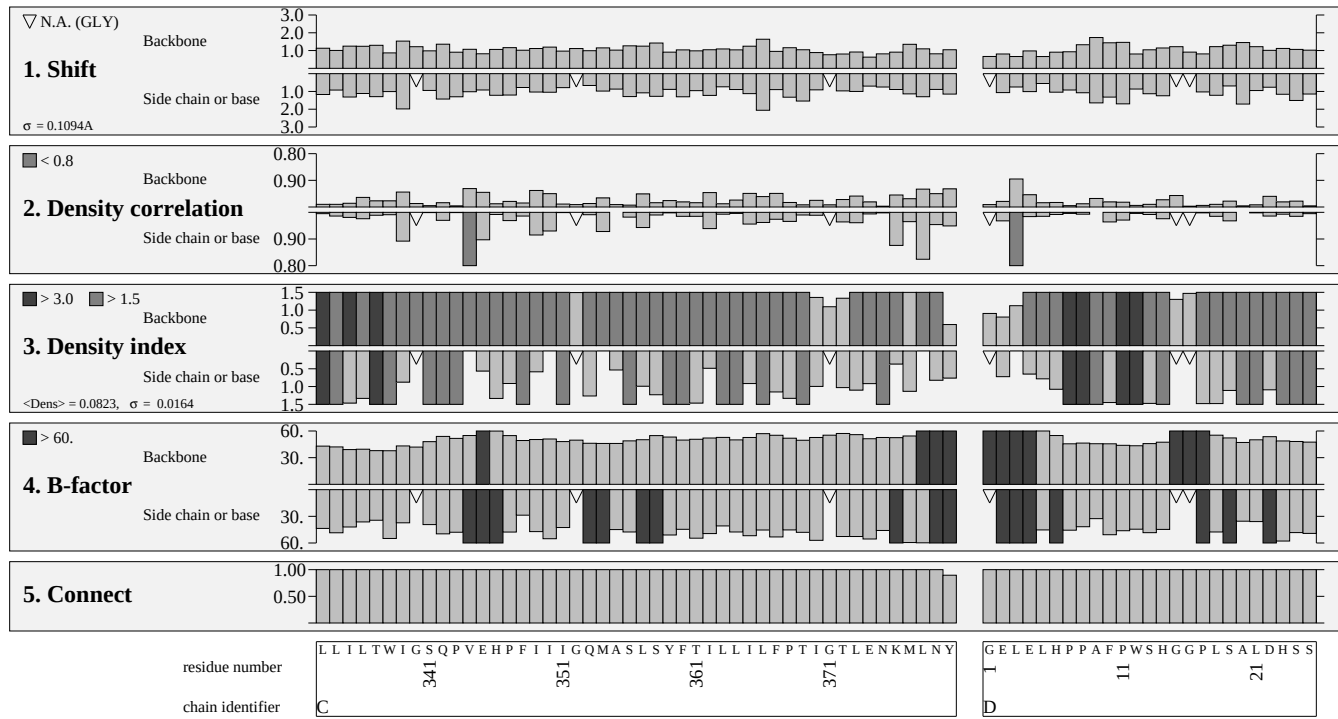
Local estimation (8)



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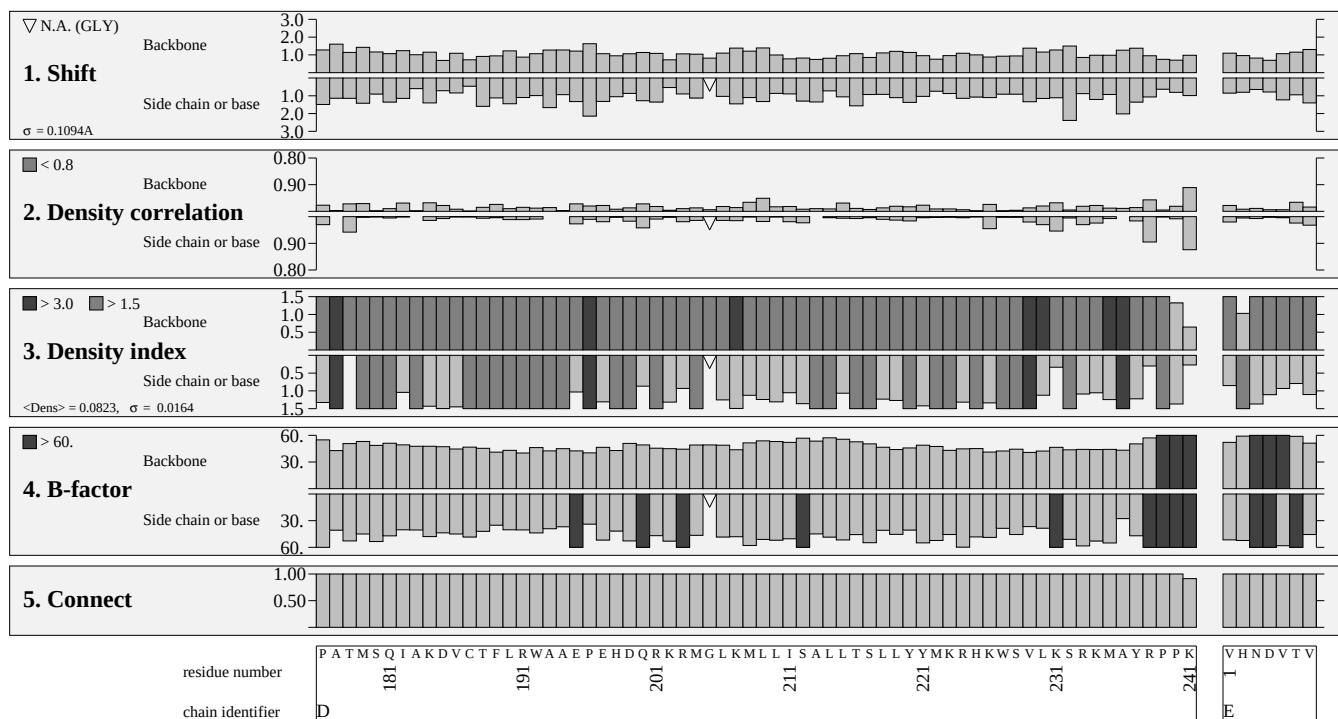
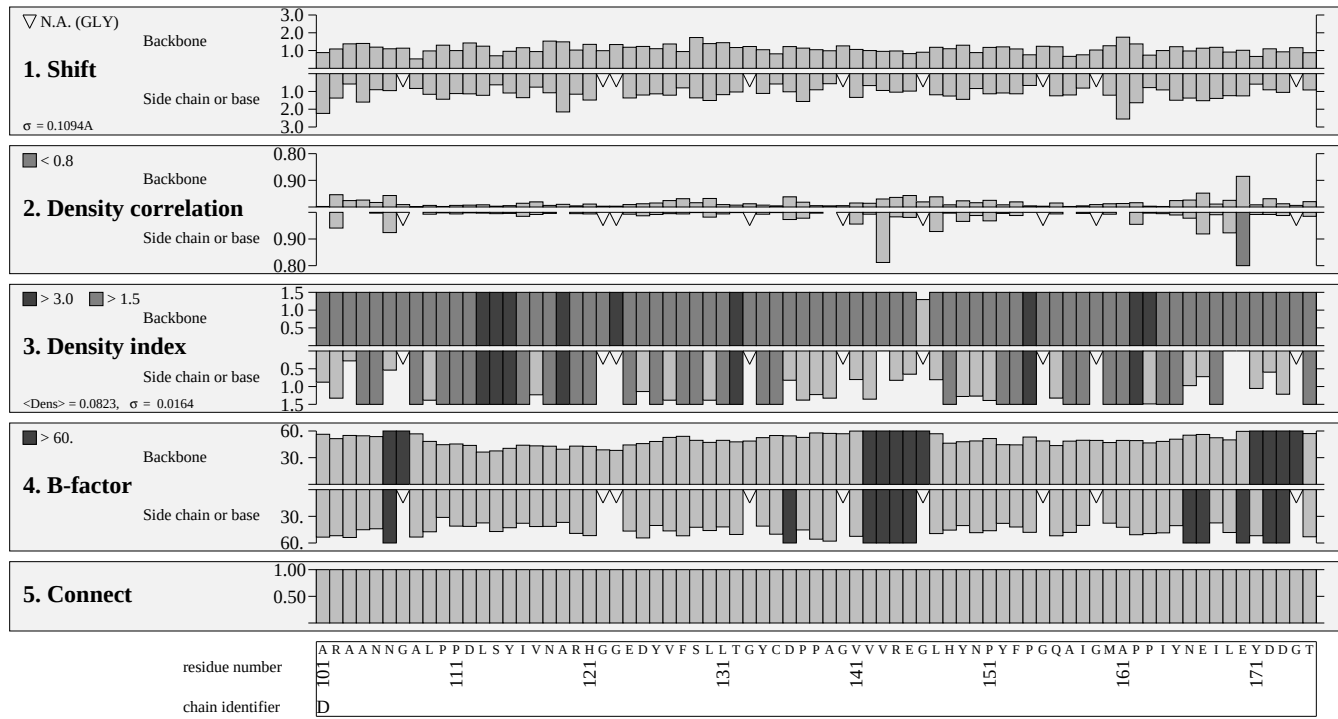
Local estimation (9)



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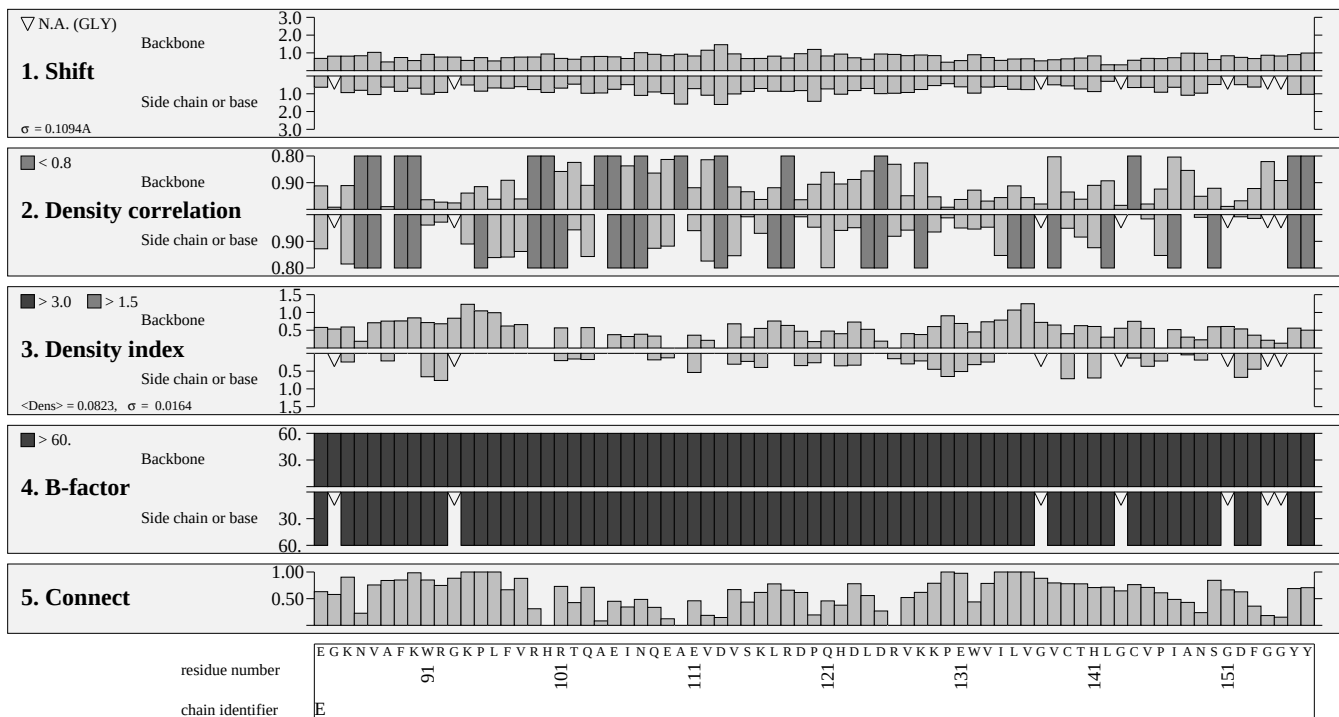
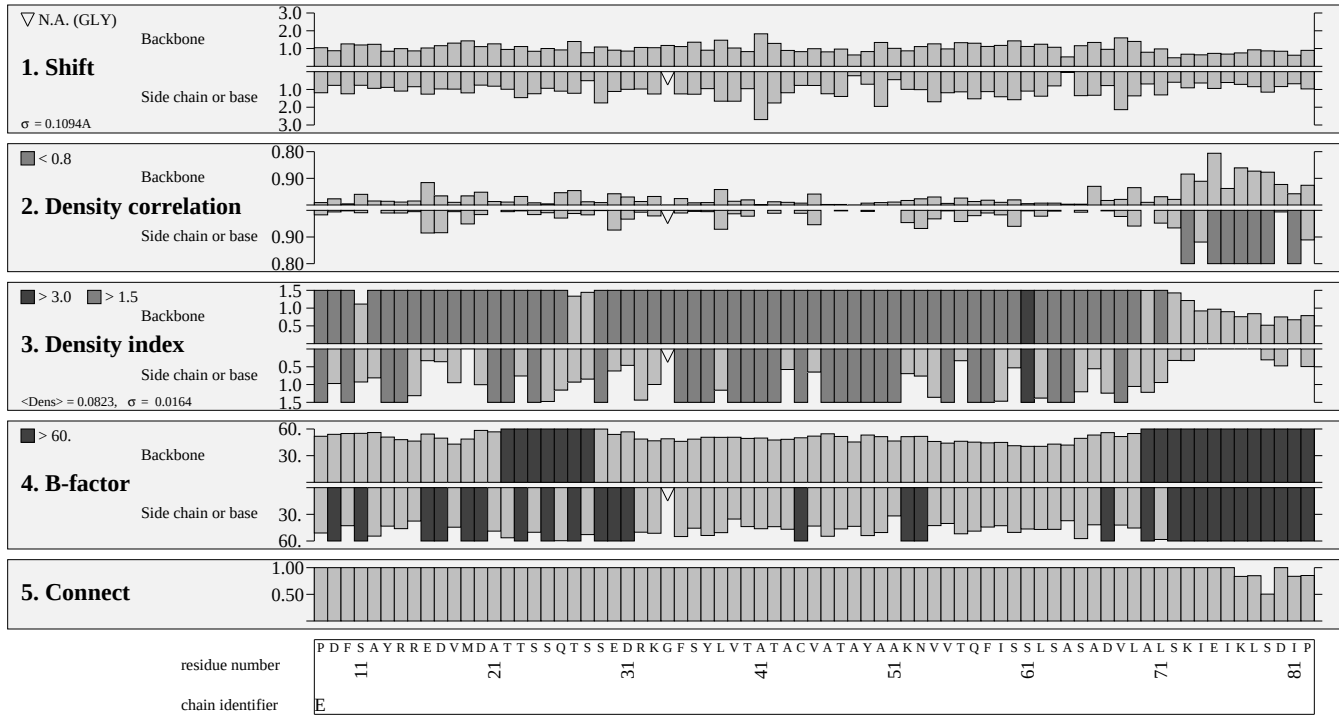
Local estimation (10)



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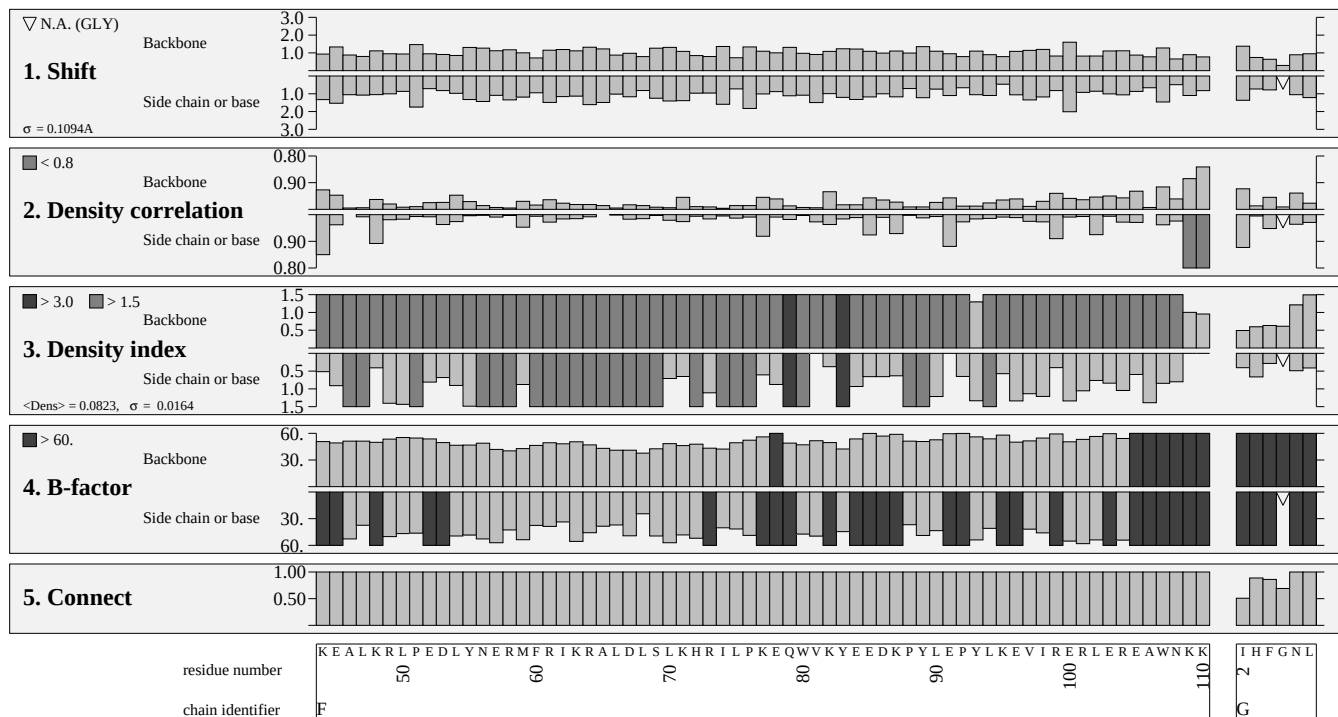
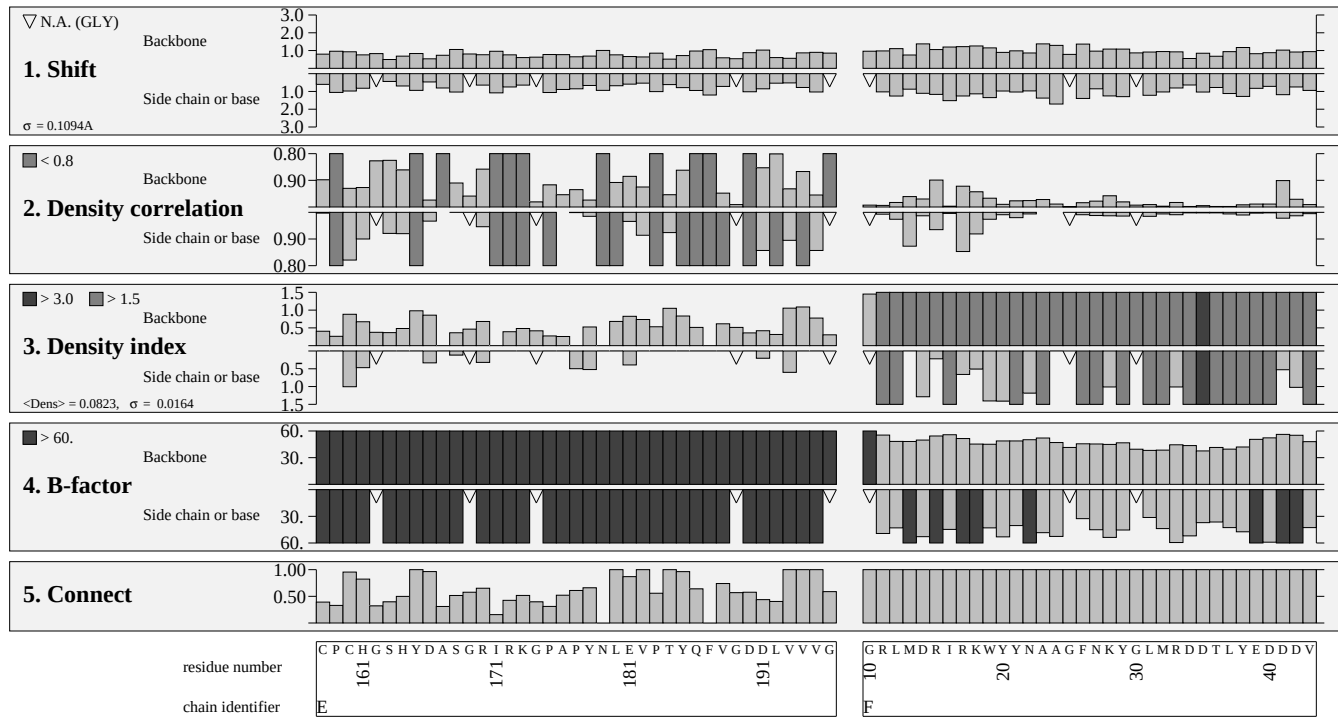
Local estimation (11)



Structure Factor Check

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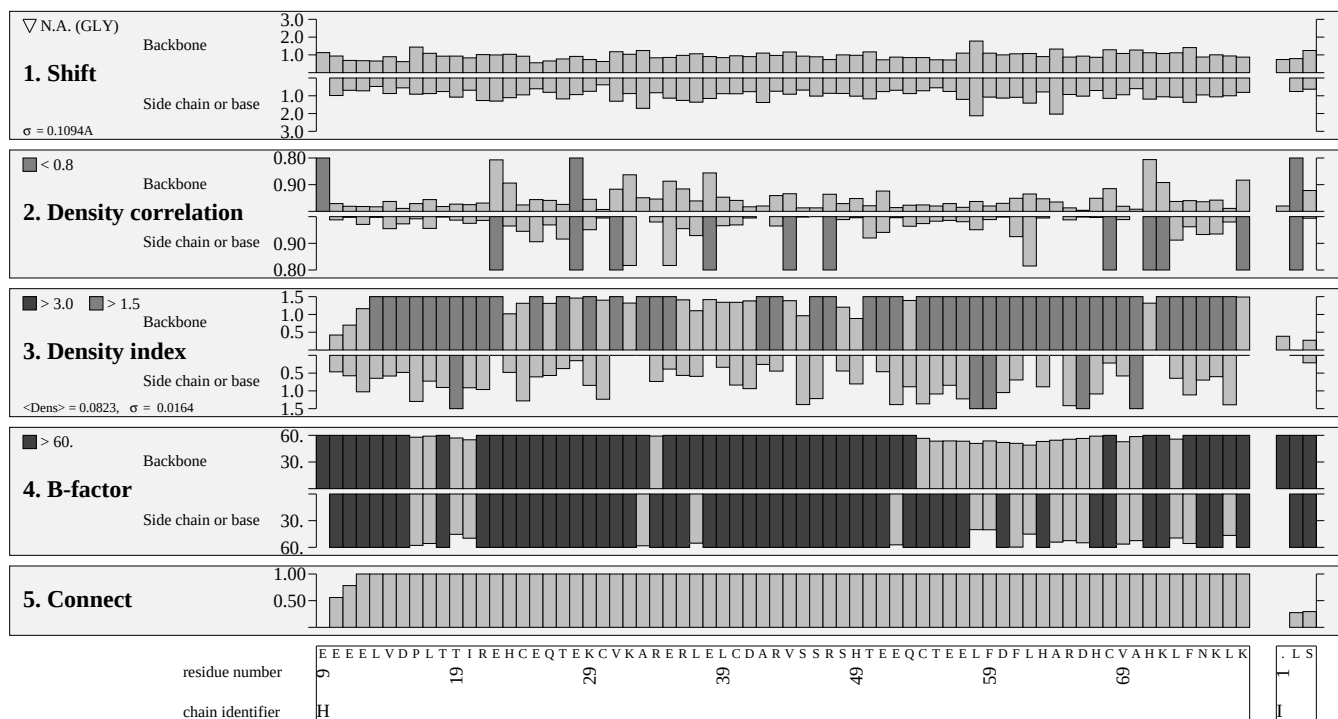
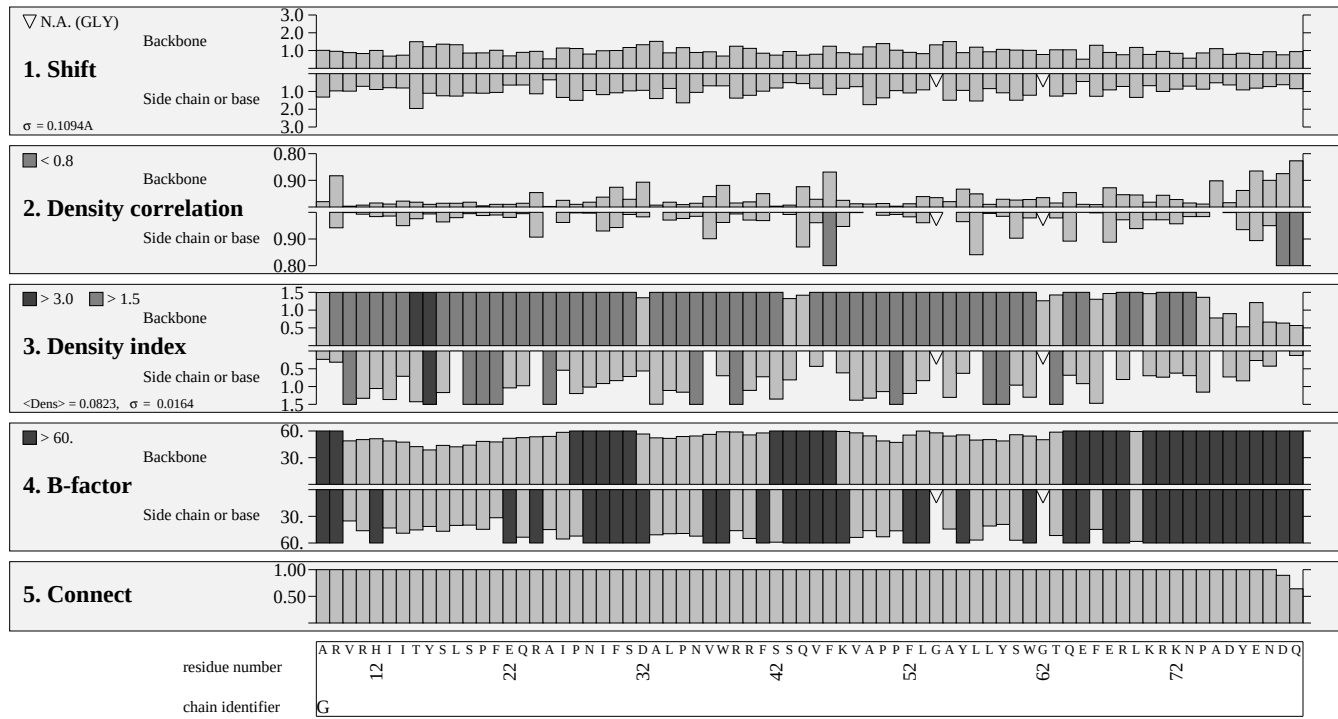
Local estimation (12)



Structure Factor Check

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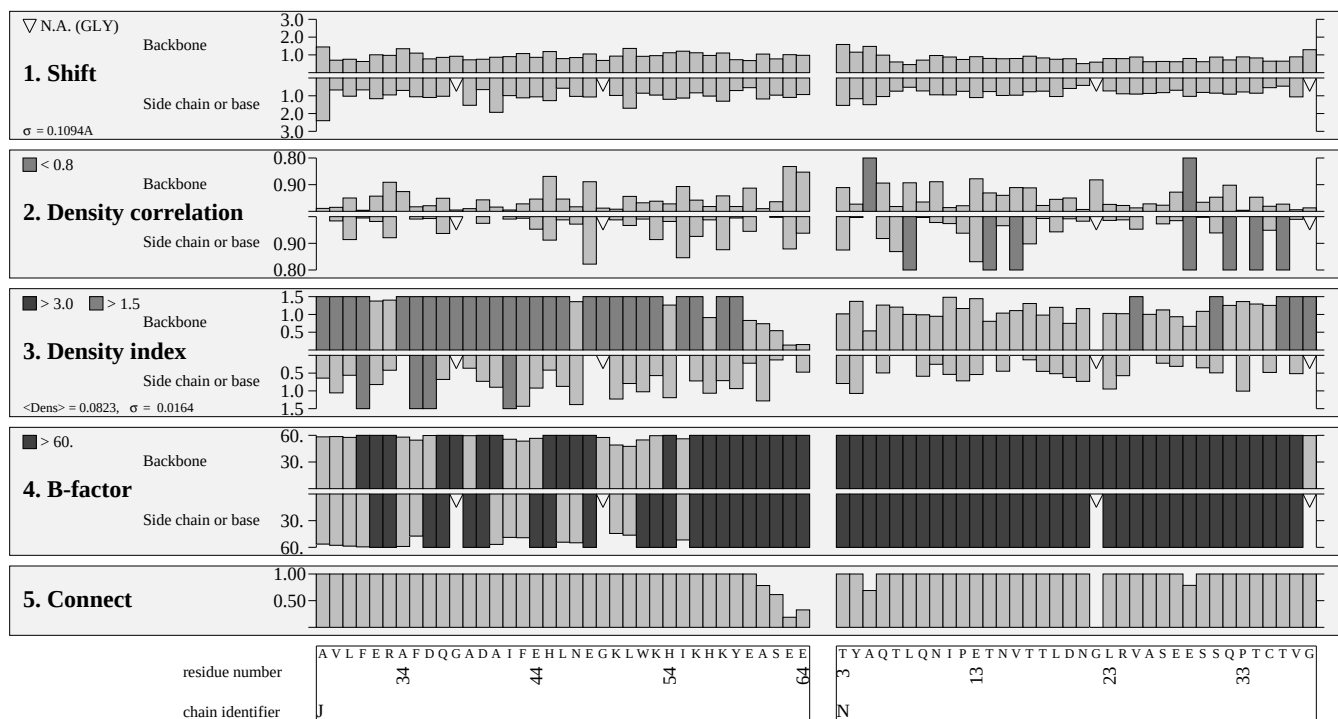
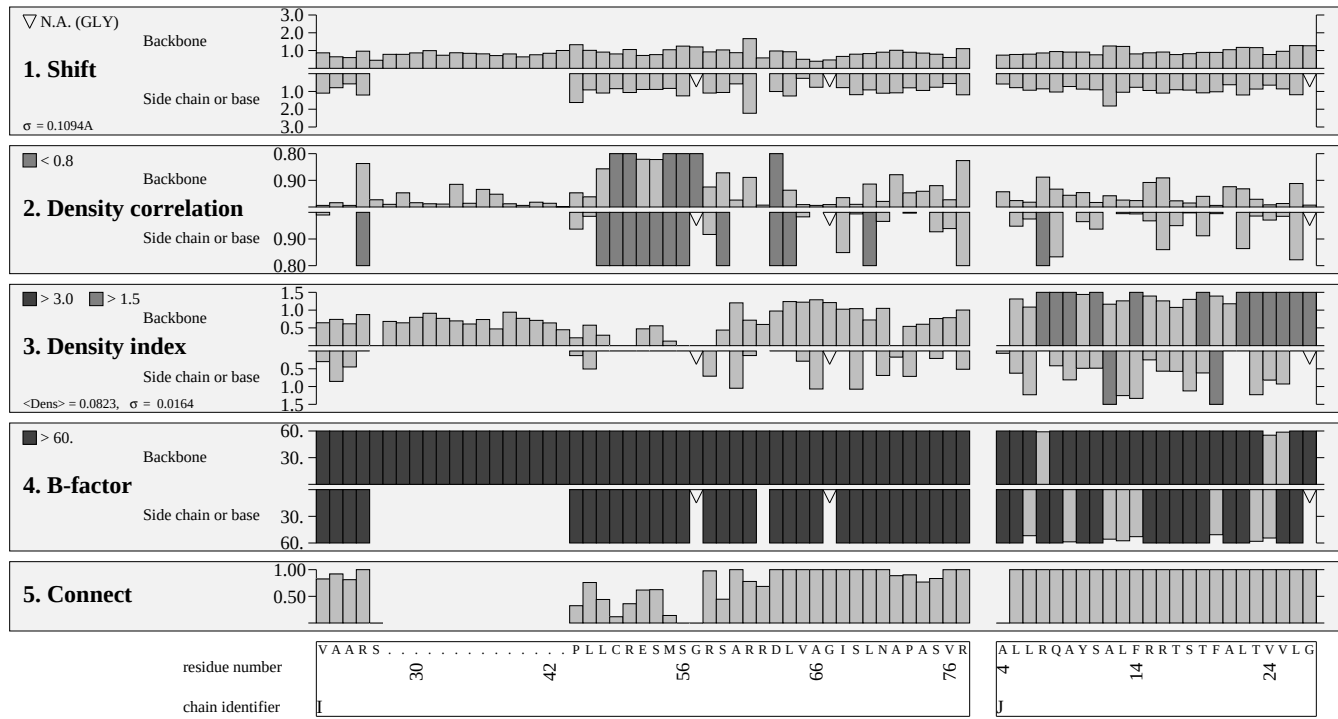
Local estimation (13)



Structure Factor Check

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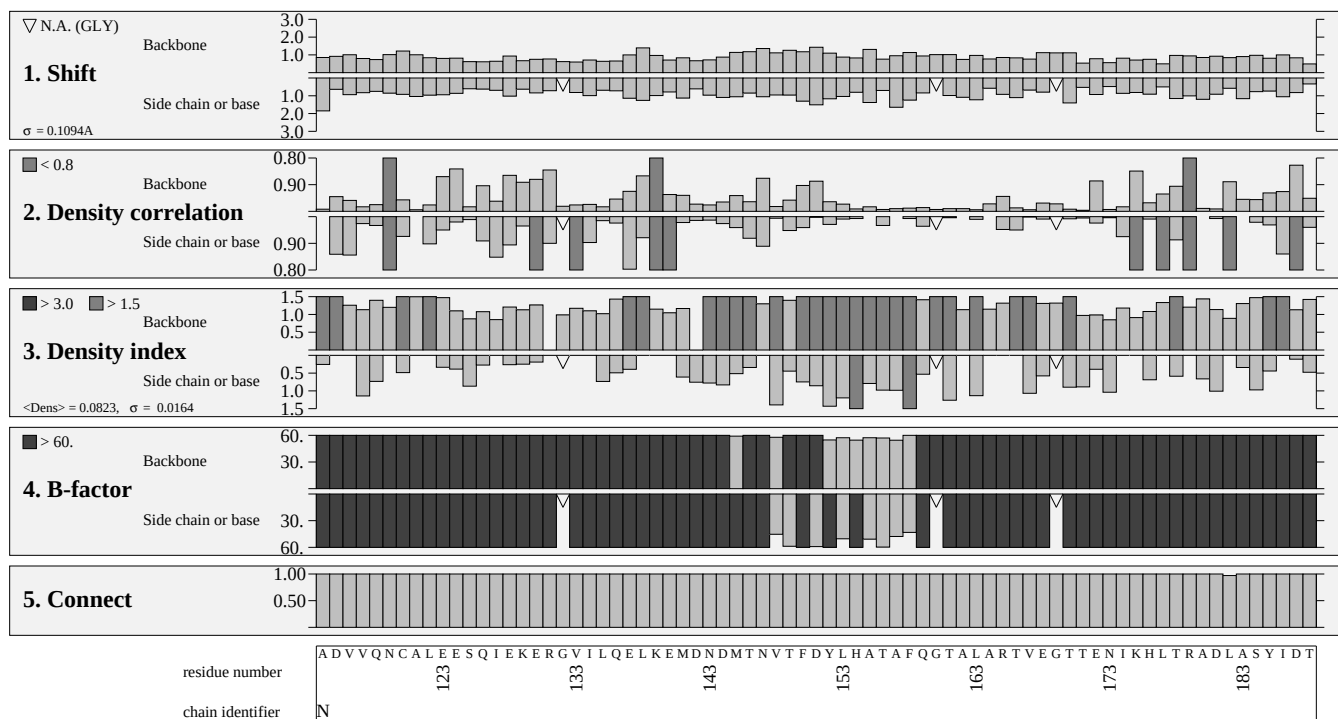
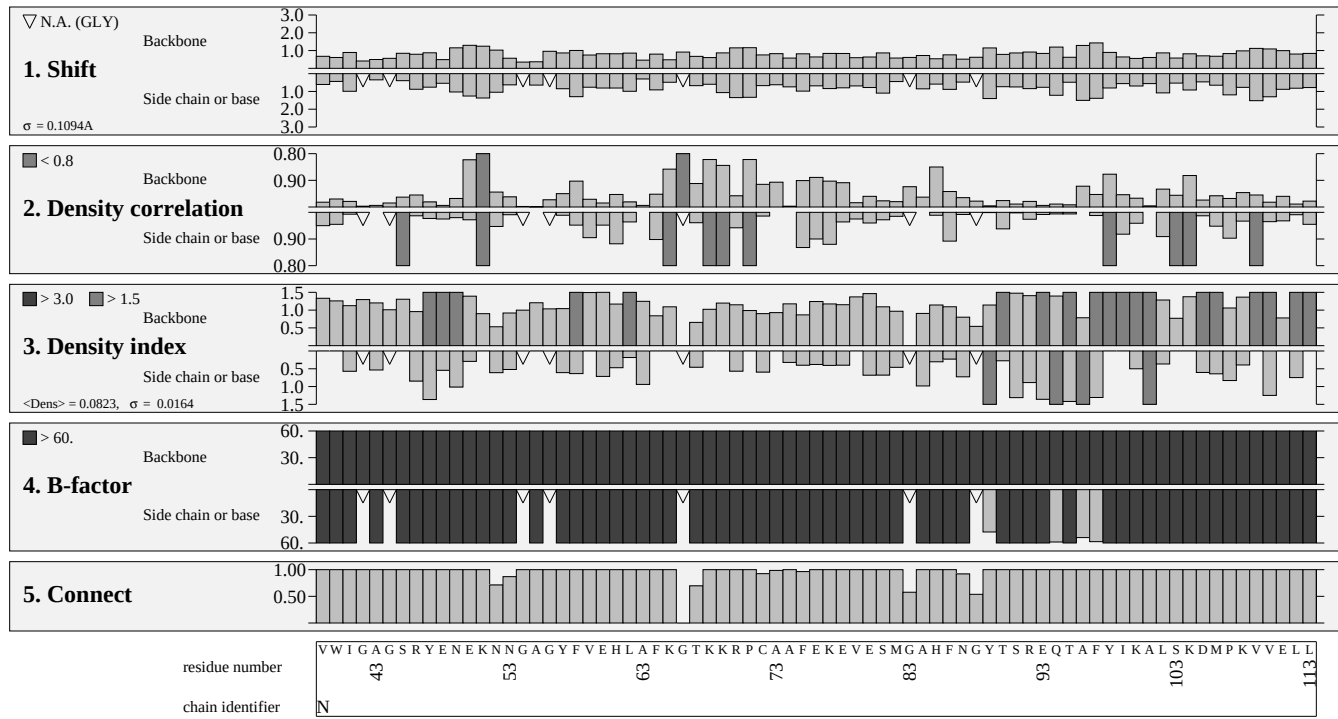
Local estimation (14)



Structure Factor Check

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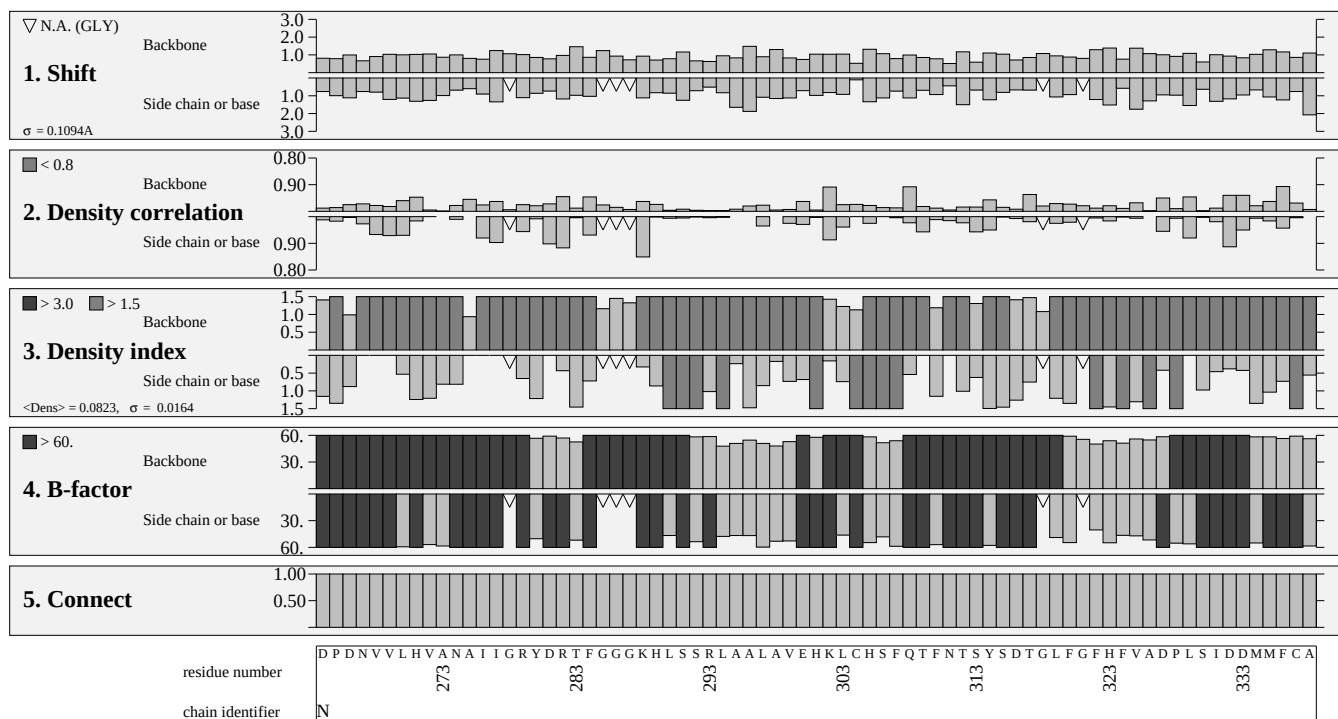
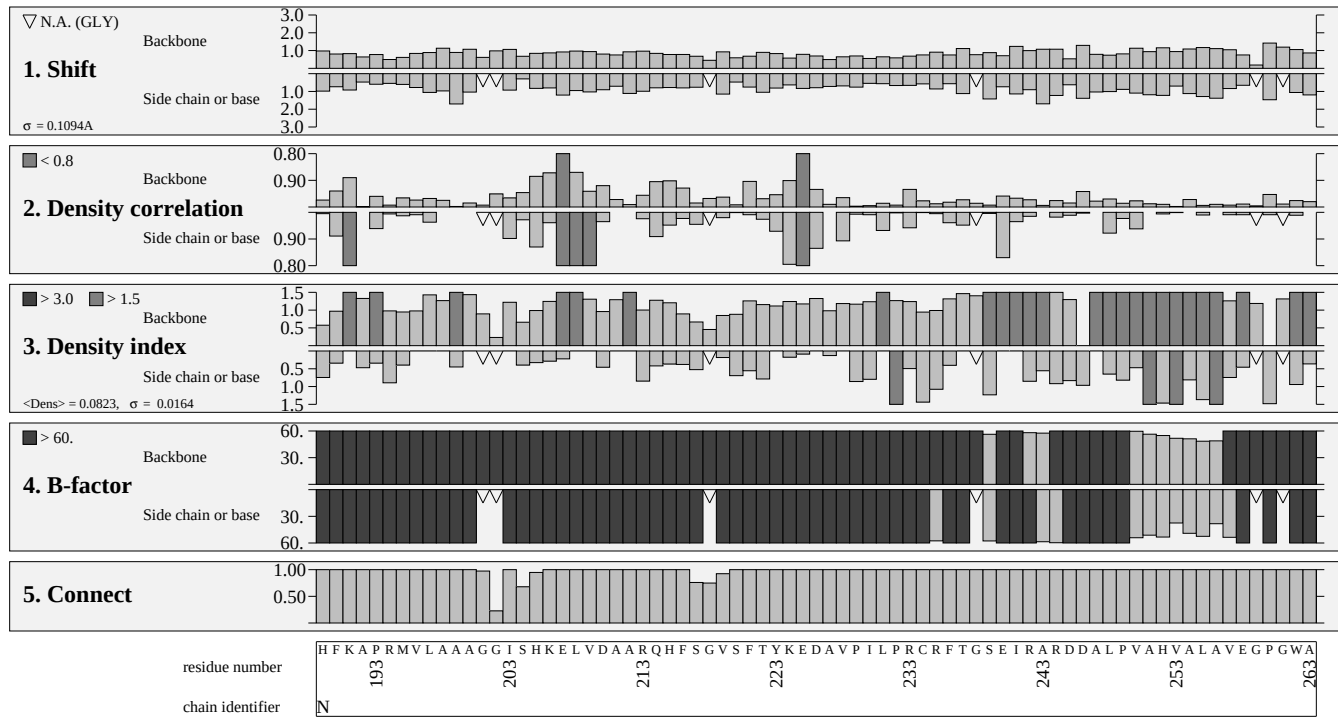
Local estimation (15)



Structure Factor Check

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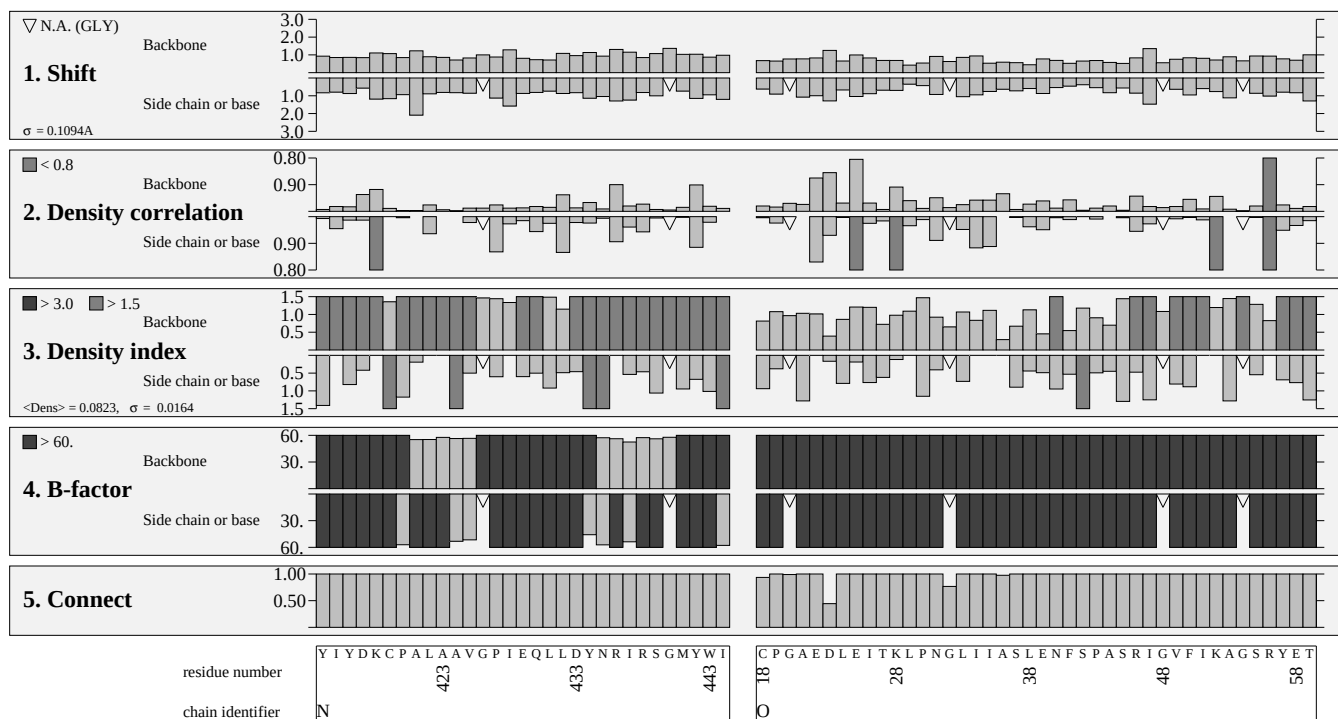
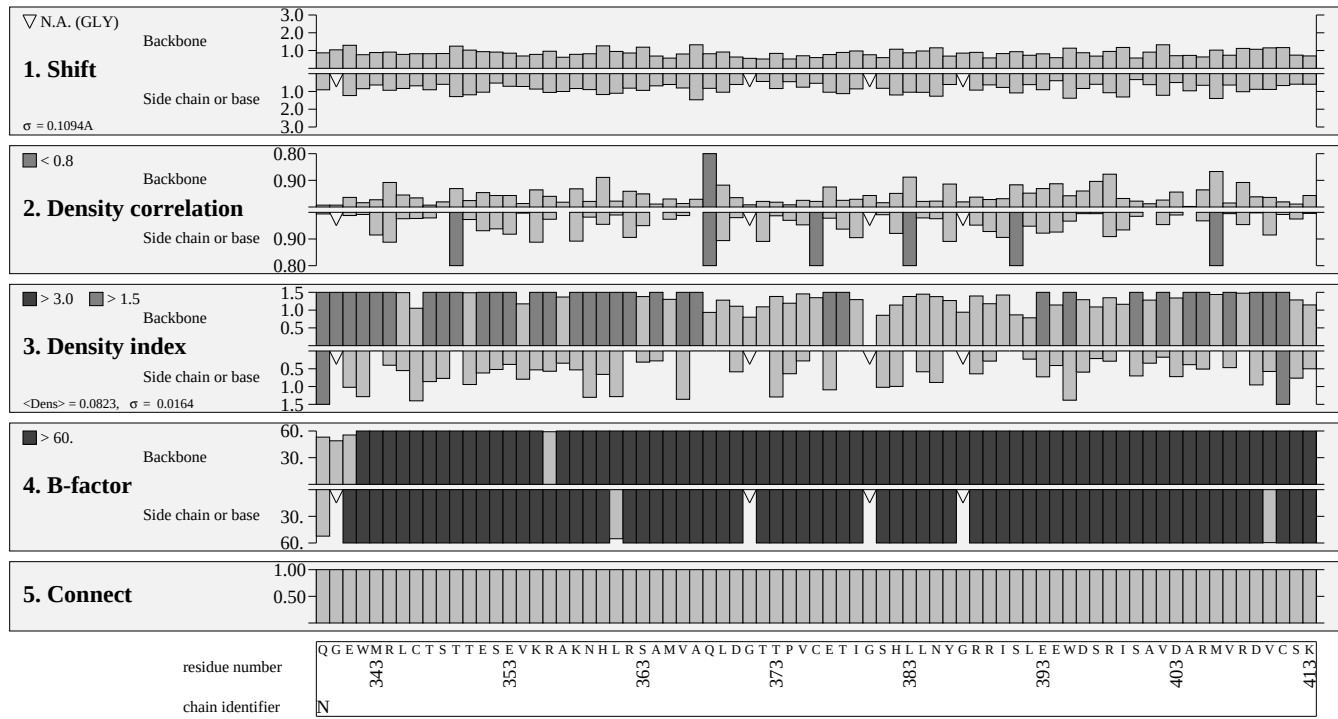
Local estimation (16)



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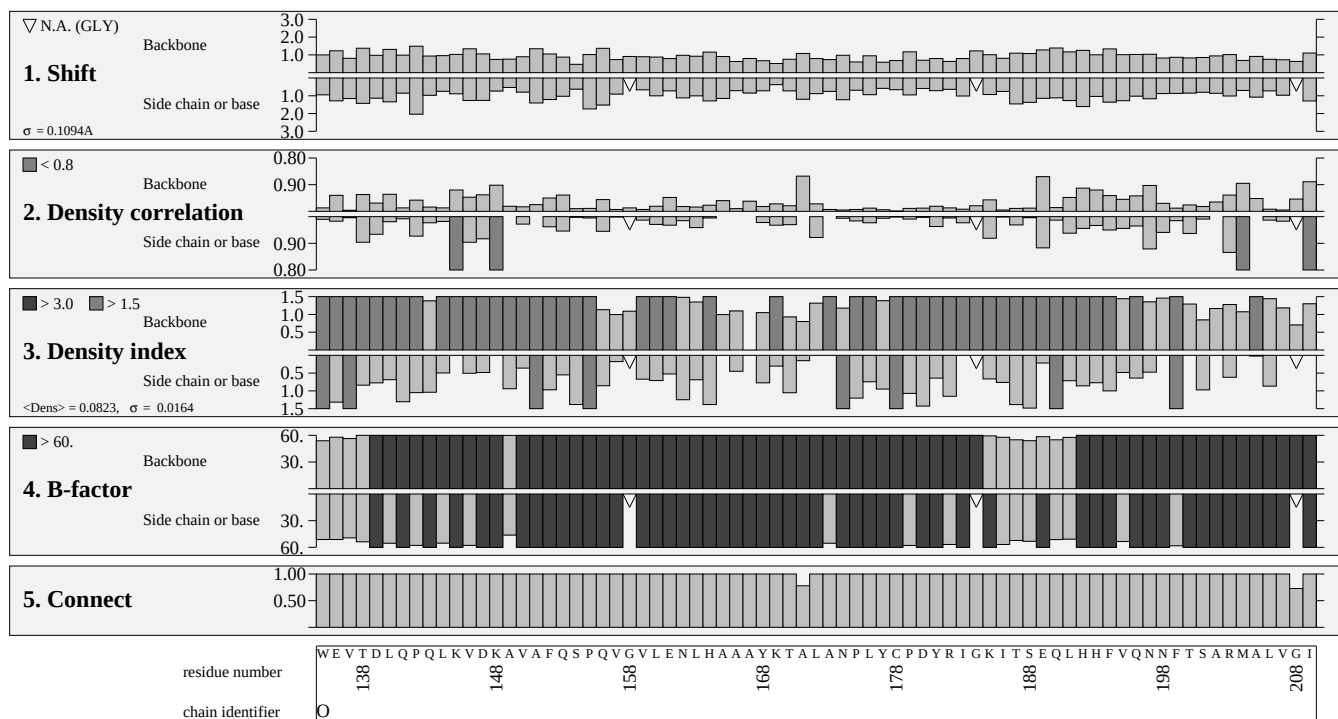
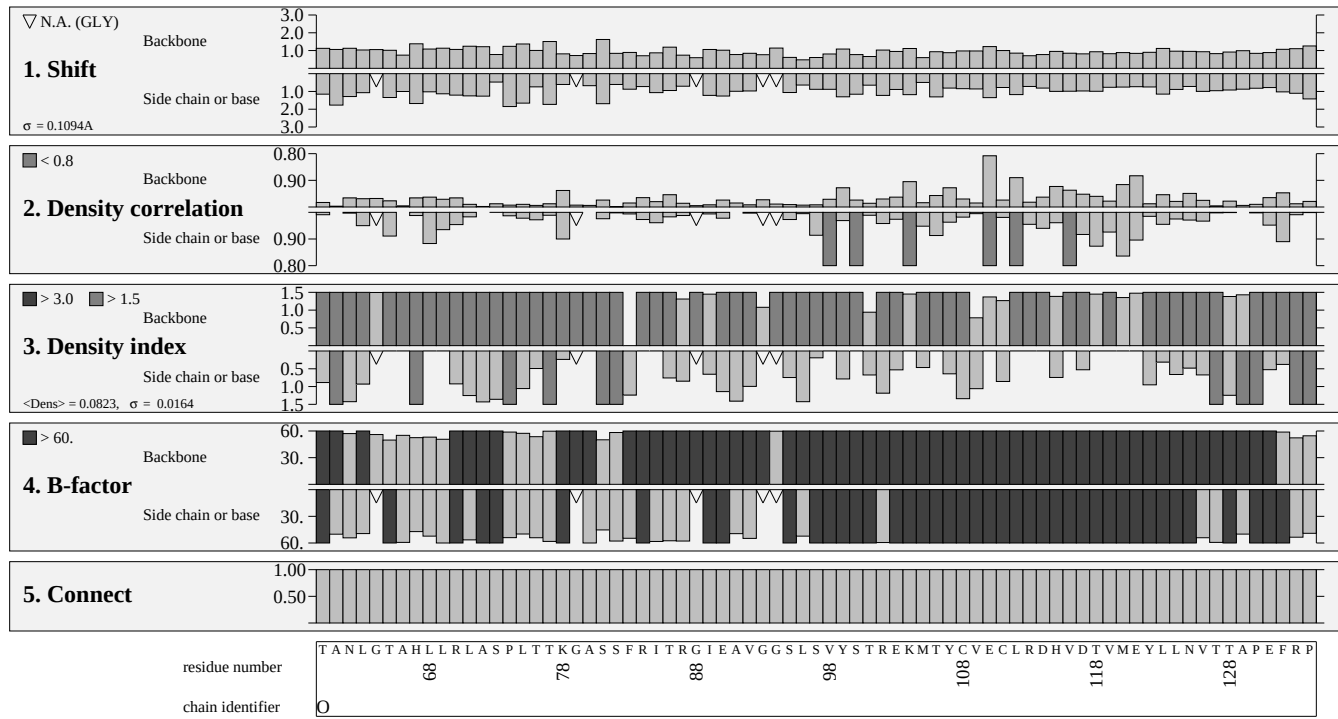
Local estimation (17)



Structure Factor Check

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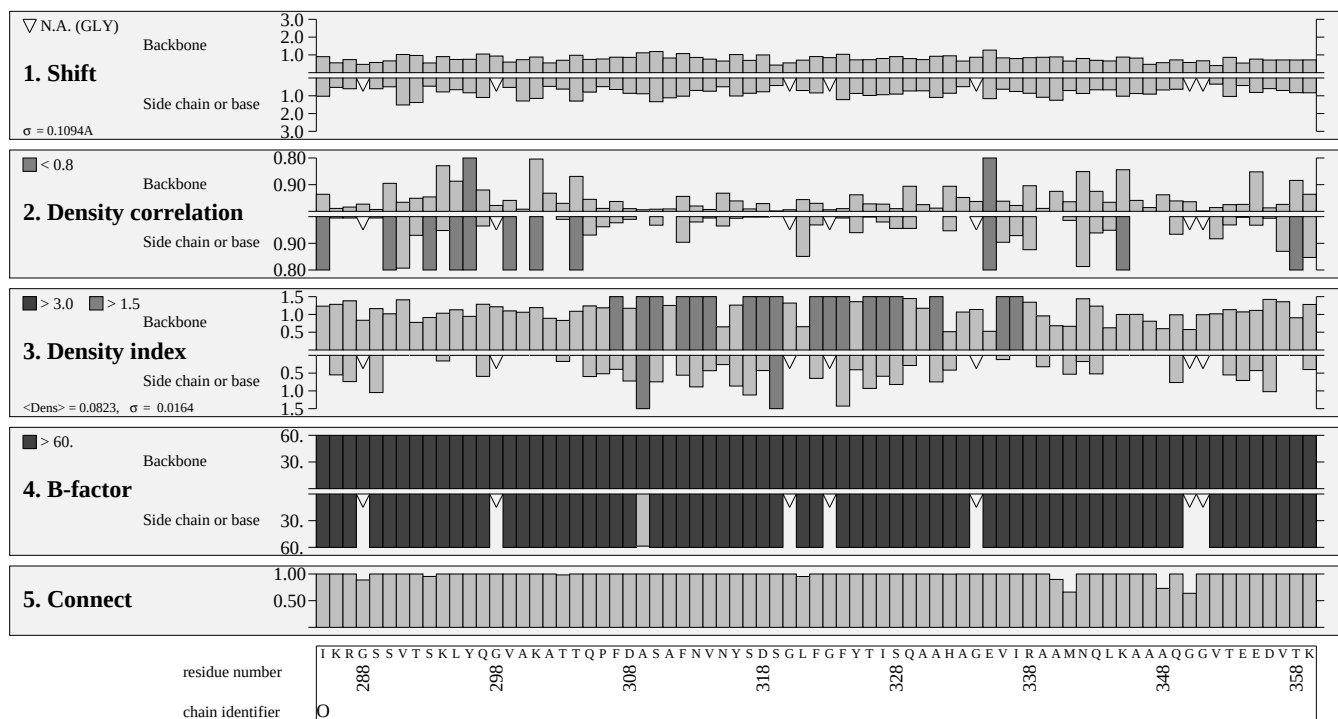
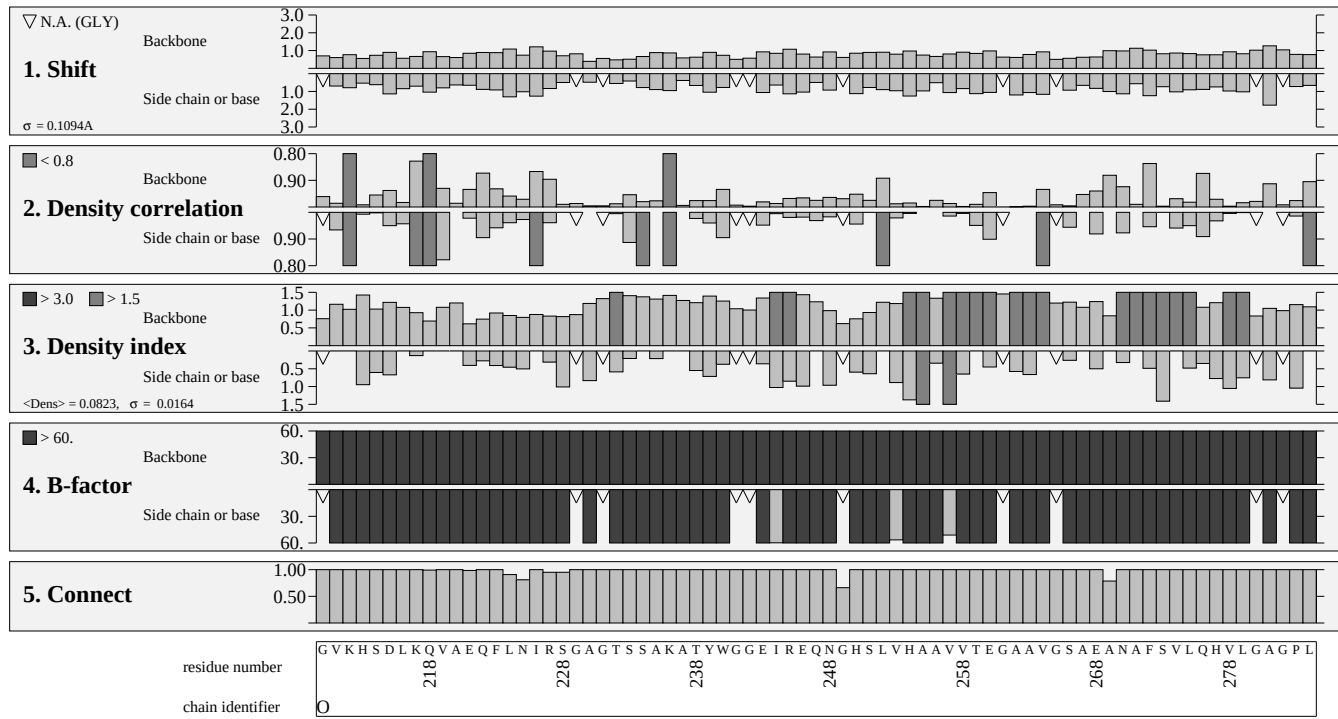
Local estimation (18)



Structure Factor Check

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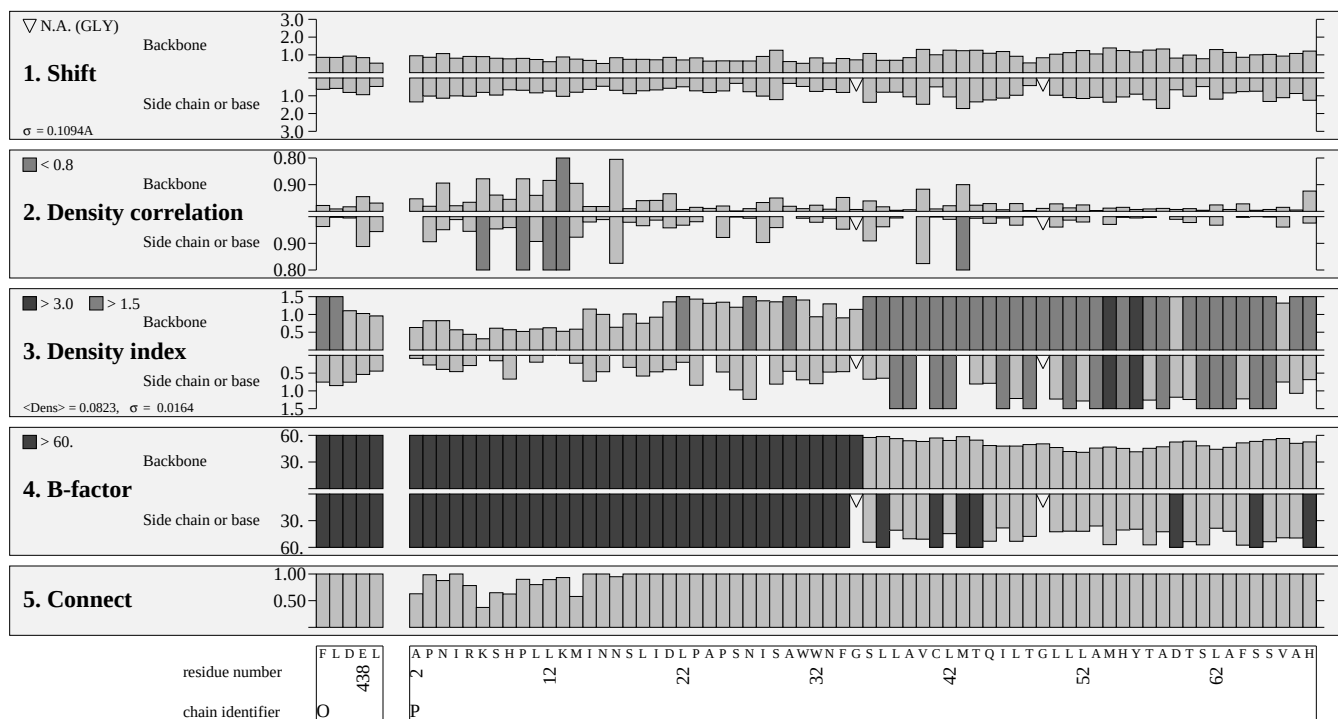
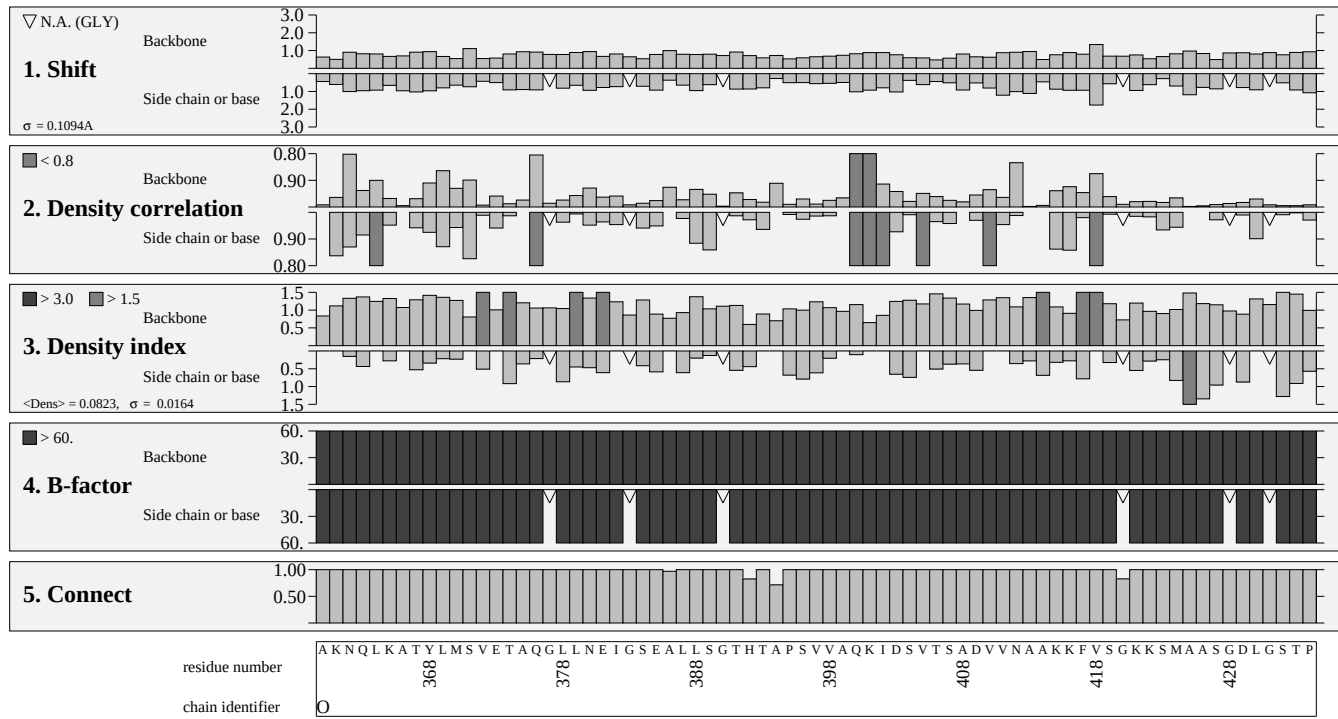
Local estimation (19)



Structure Factor Check

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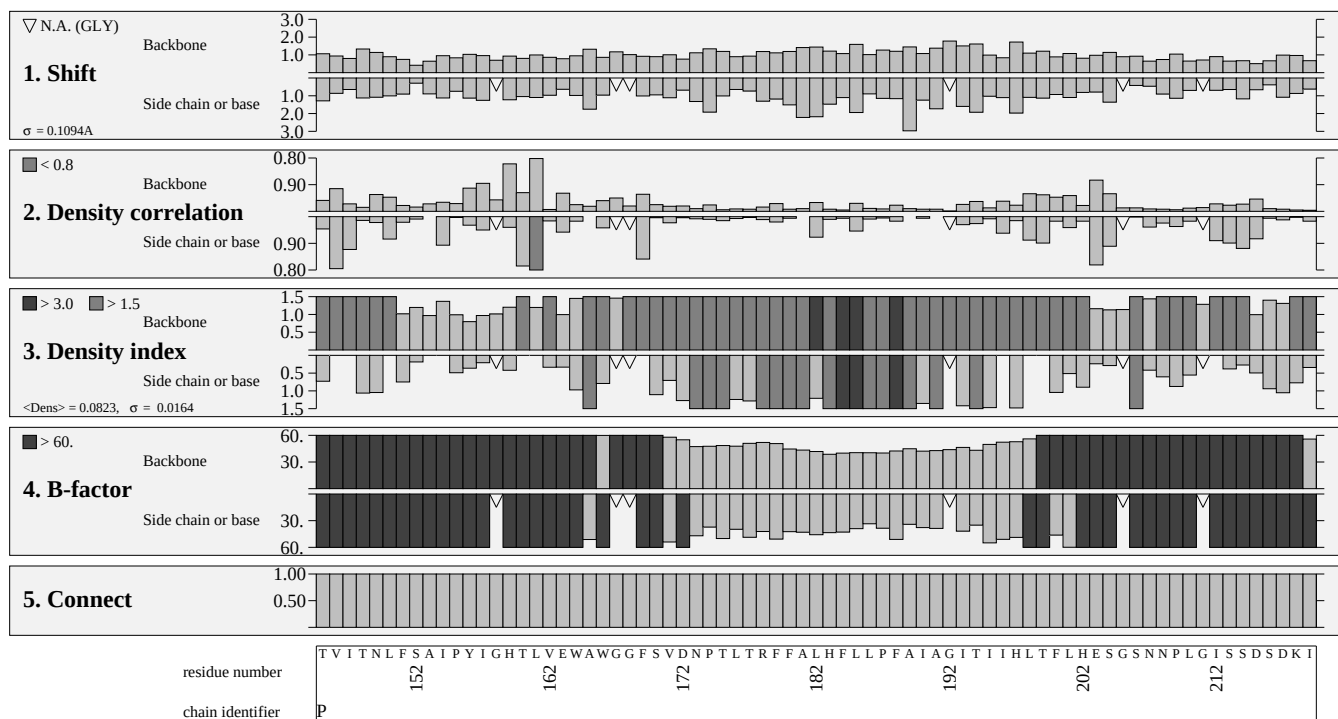
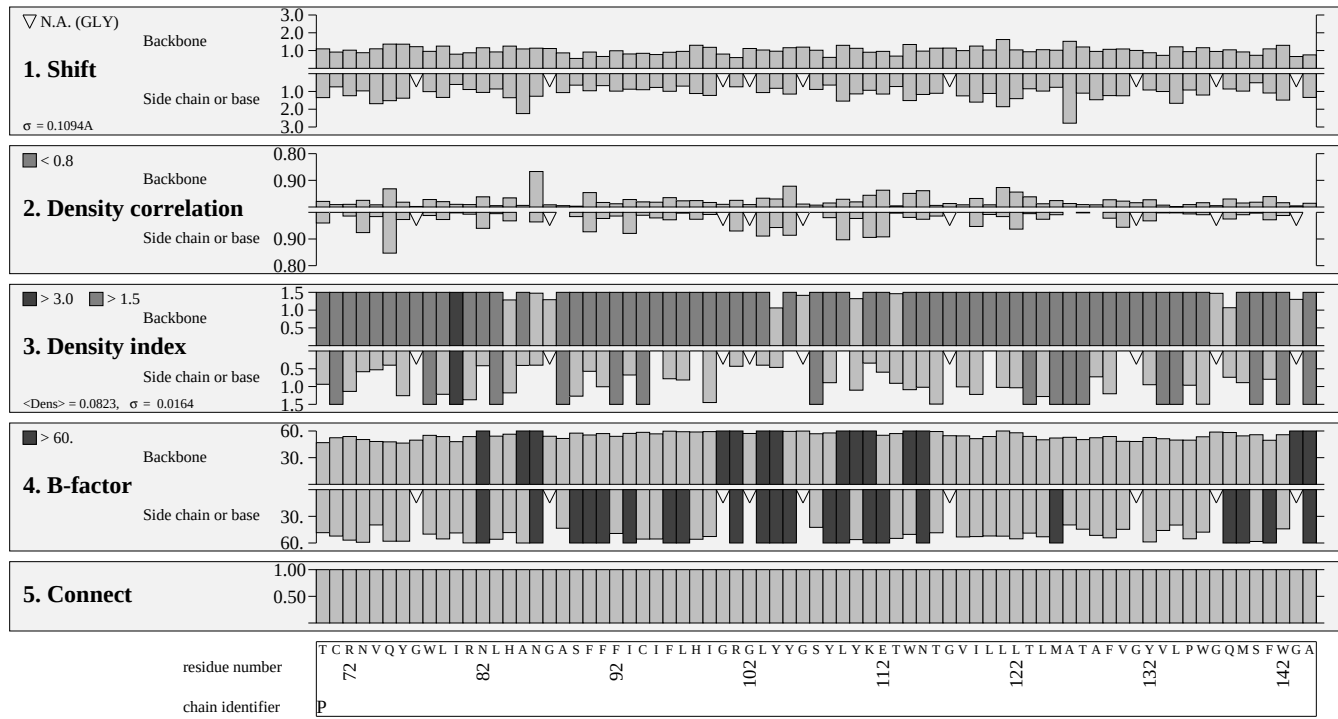
Local estimation (20)



Structure Factor Check

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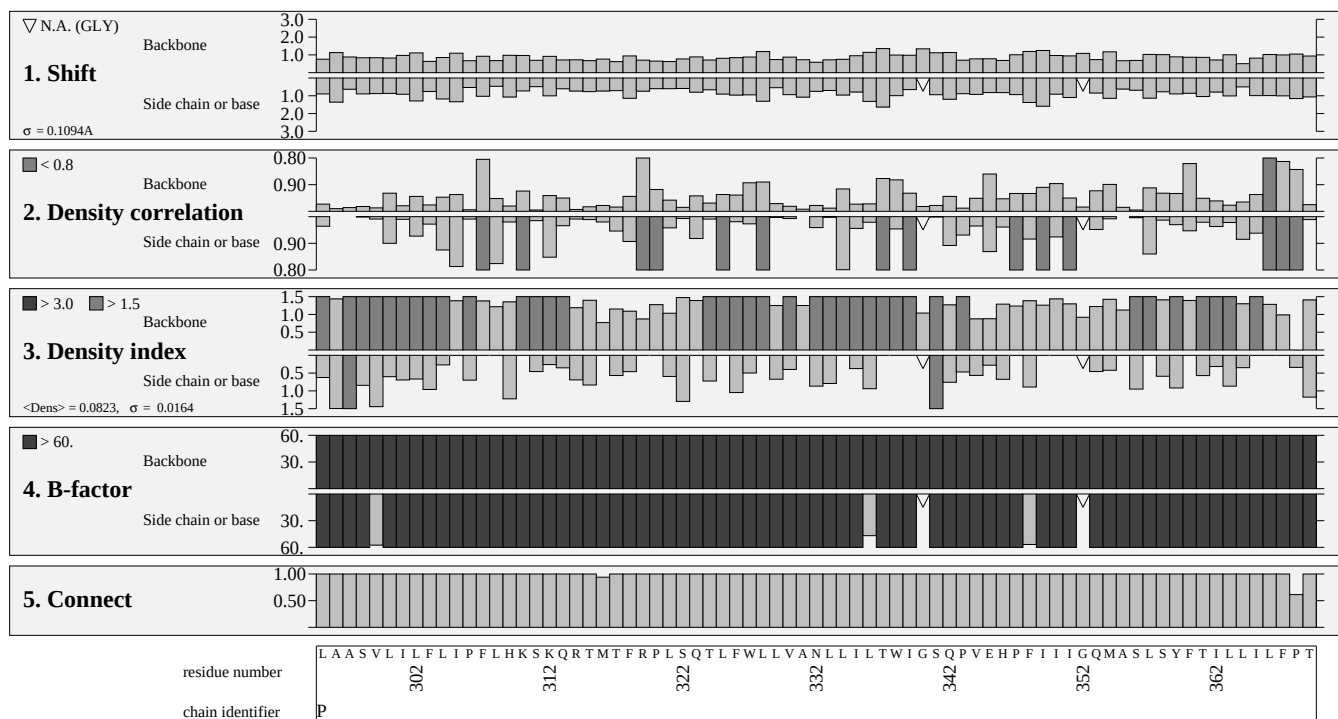
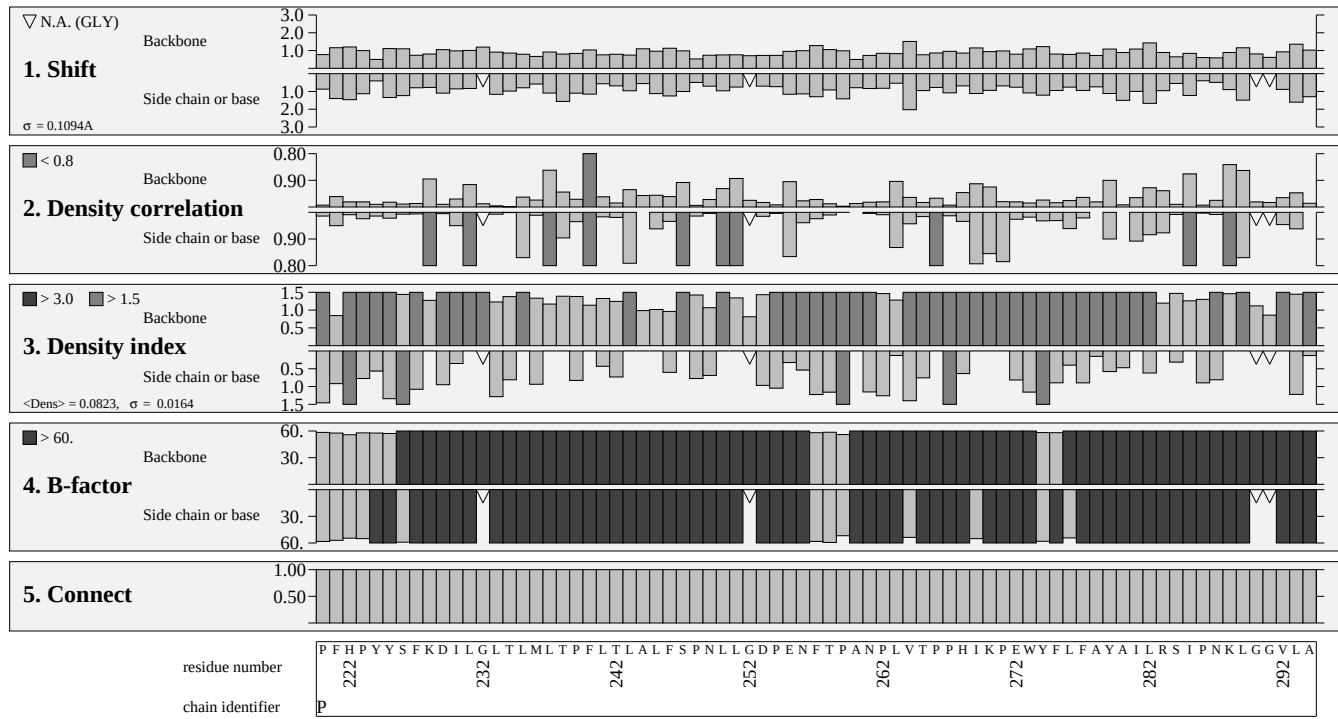
Local estimation (21)



Structure Factor Check

3TGU

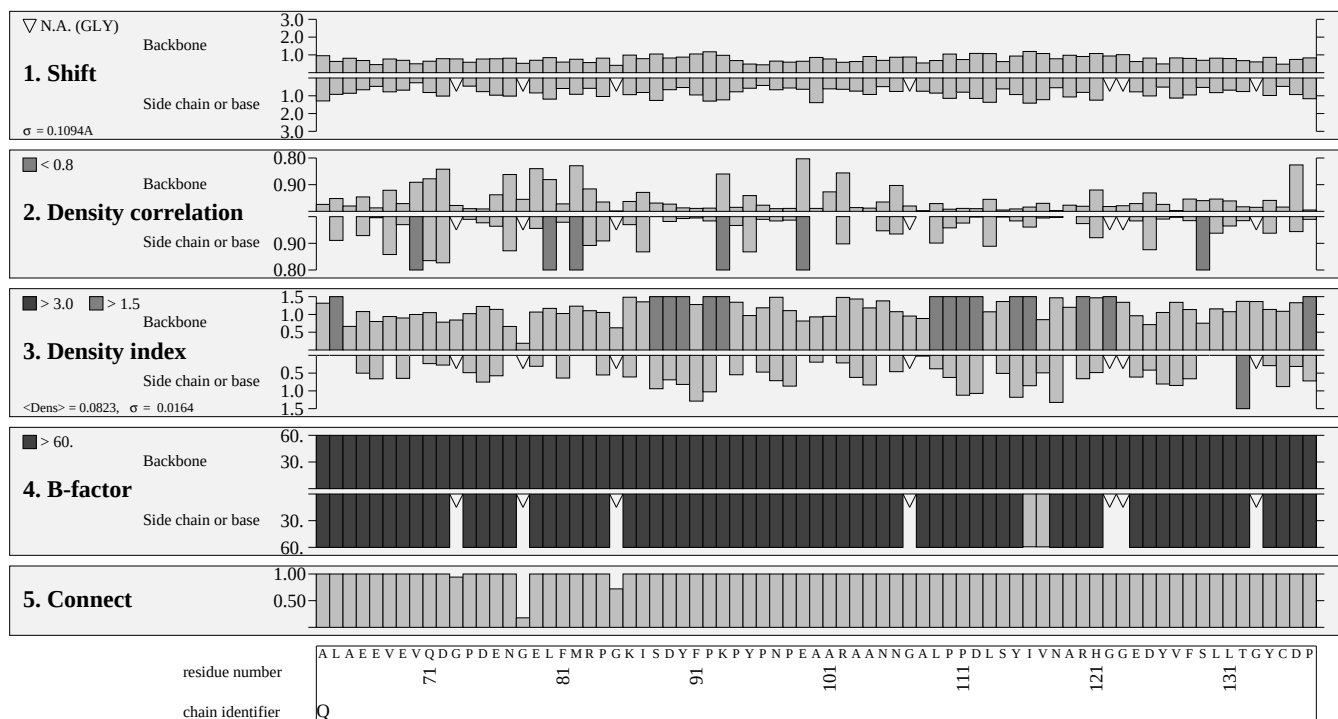
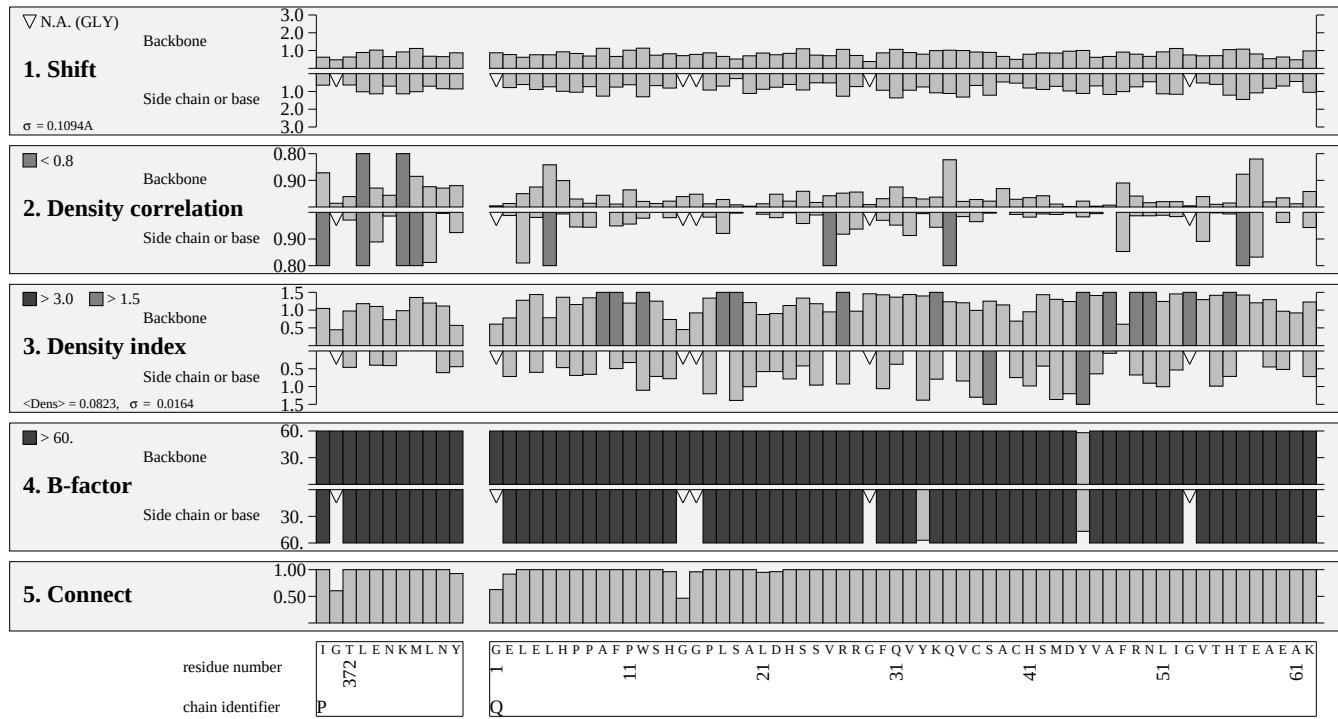
Local estimation (22)



Structure Factor Check

3TGU

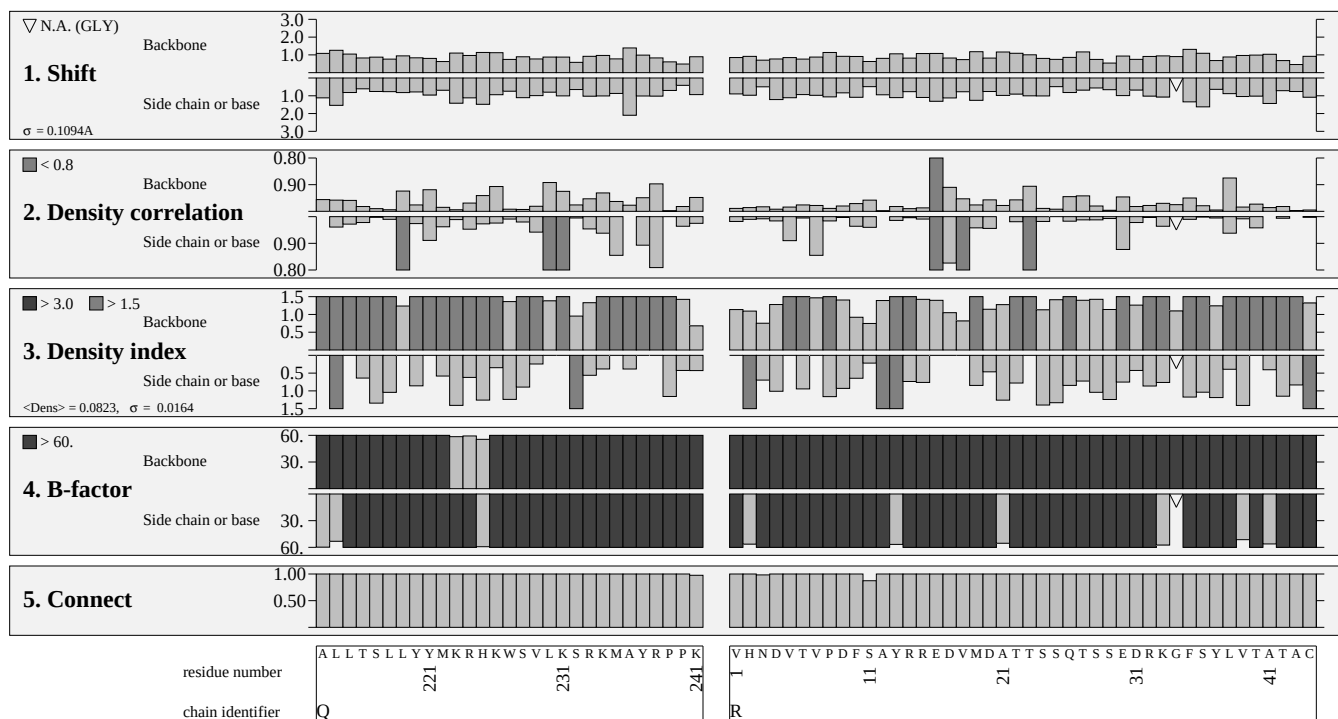
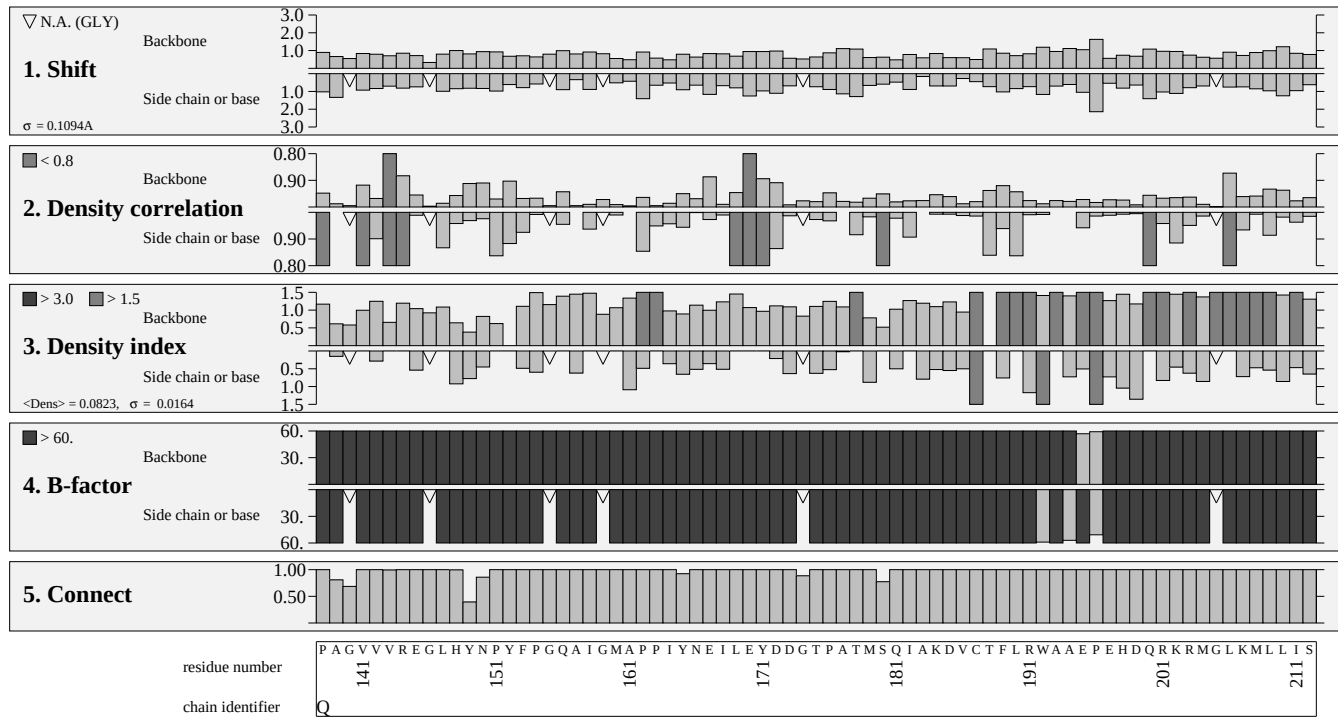
Local estimation (23)



Structure Factor Check

3TGU

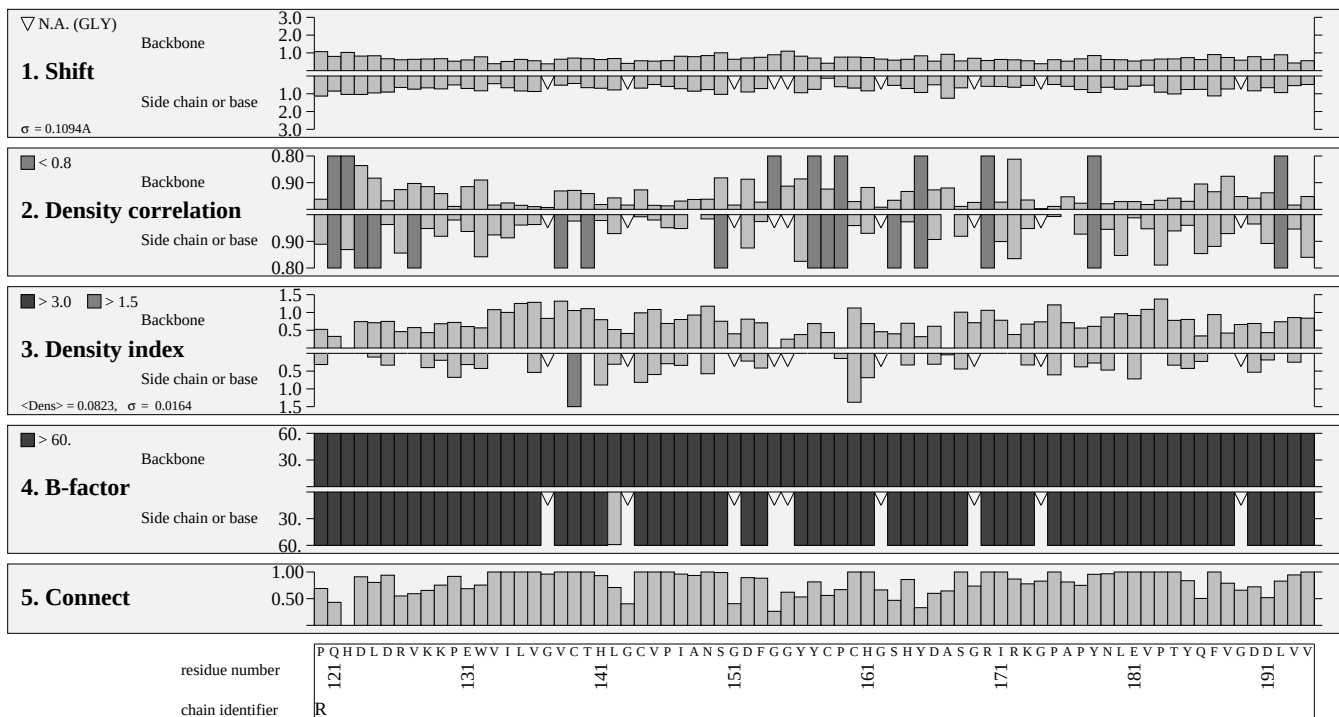
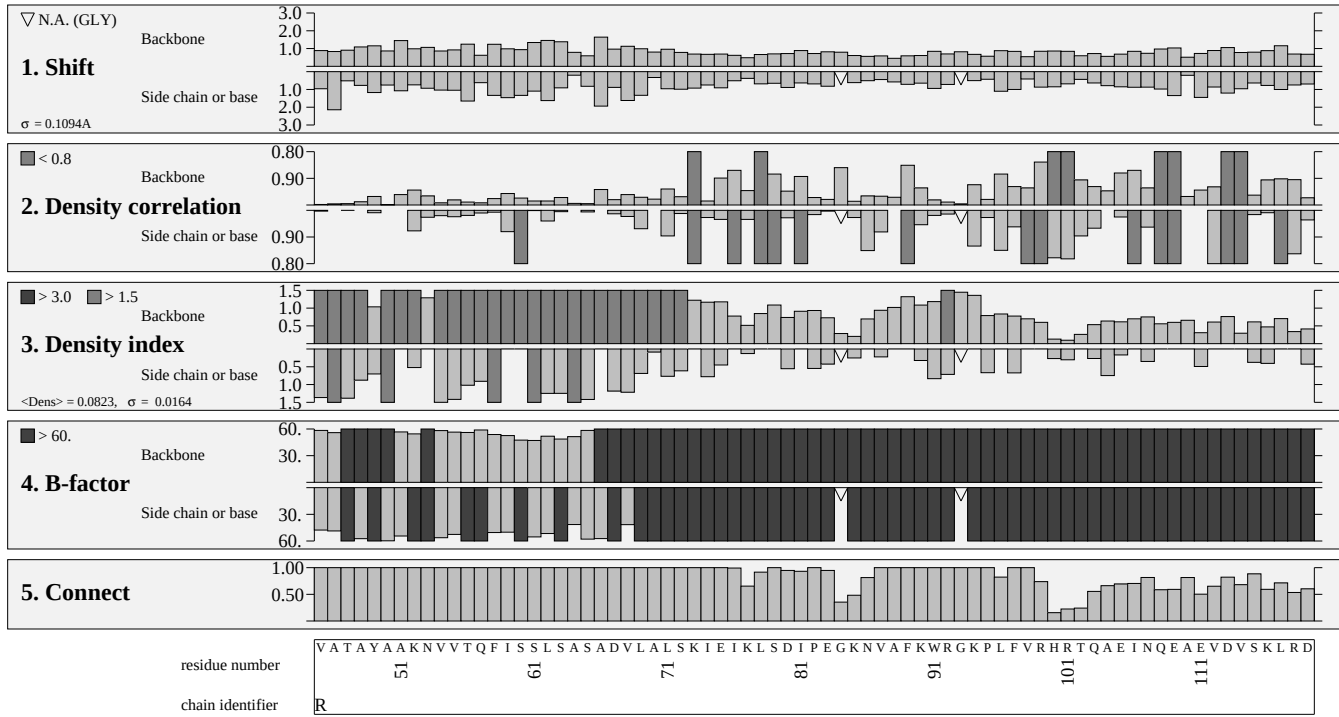
Local estimation (24)



Structure Factor Check

3TGU

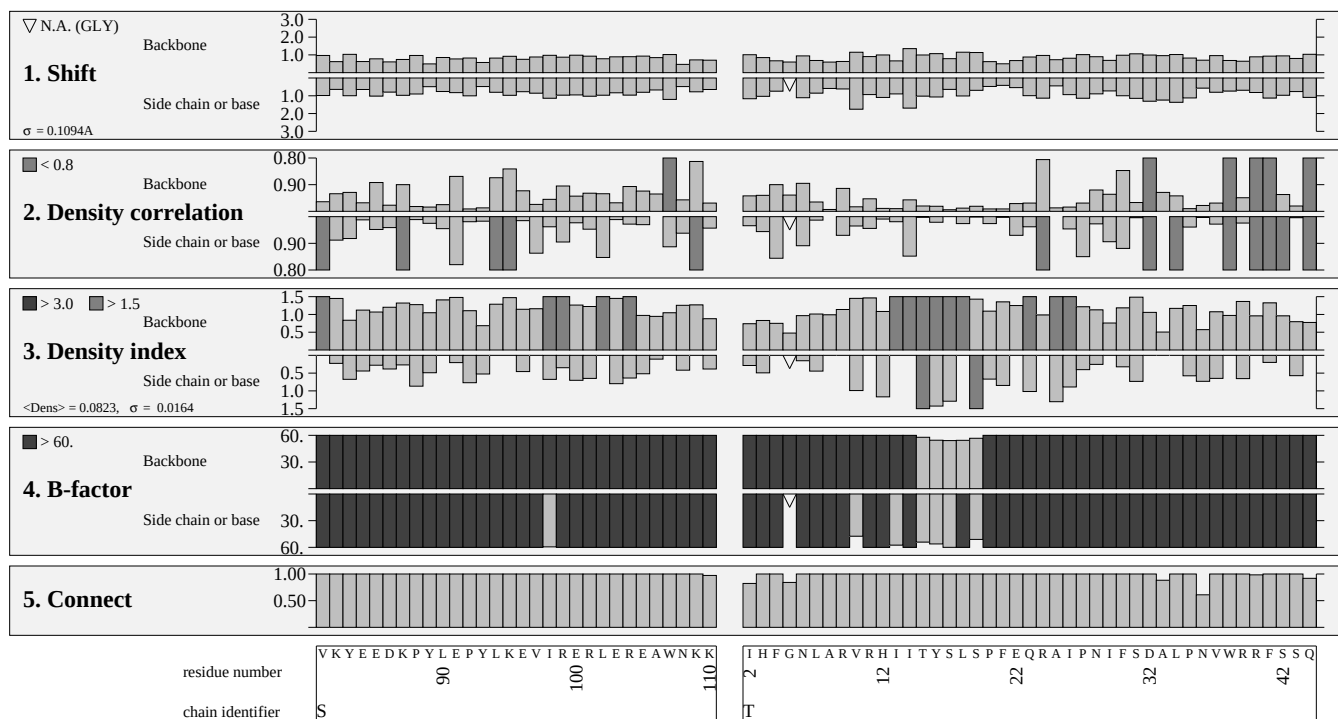
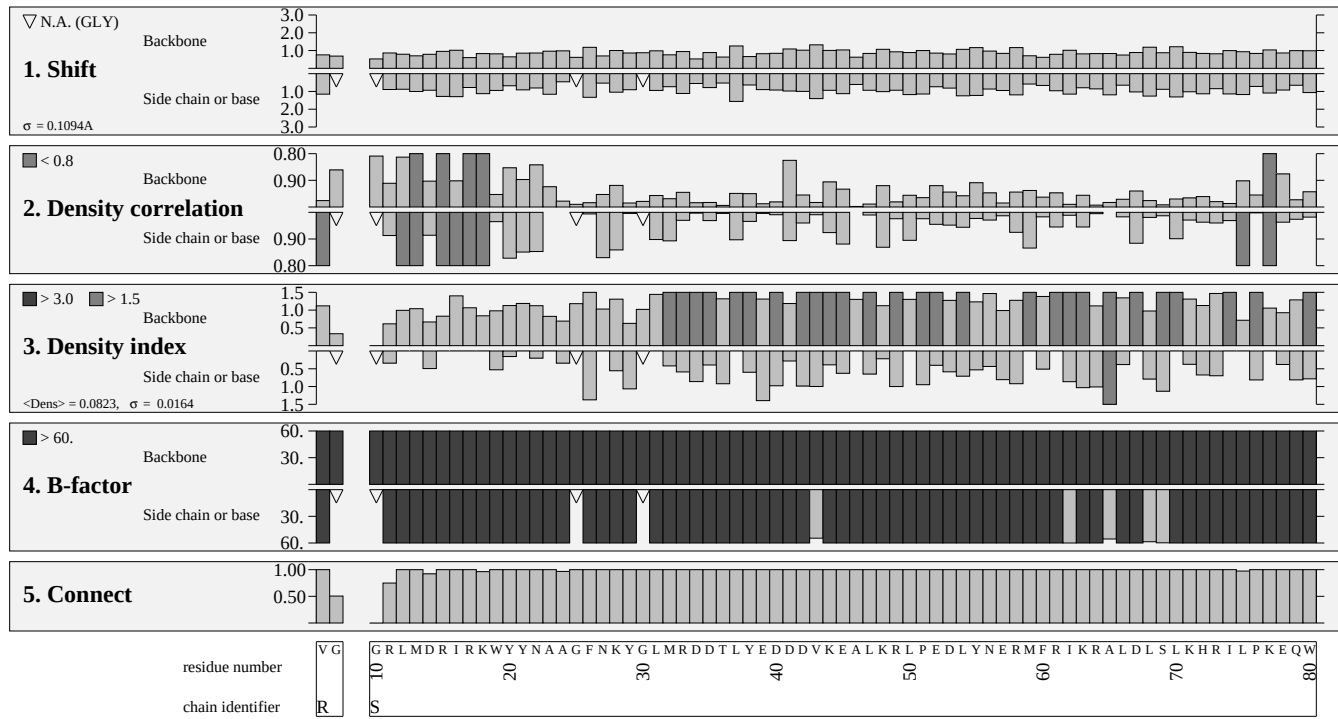
Local estimation (25)



Structure Factor Check

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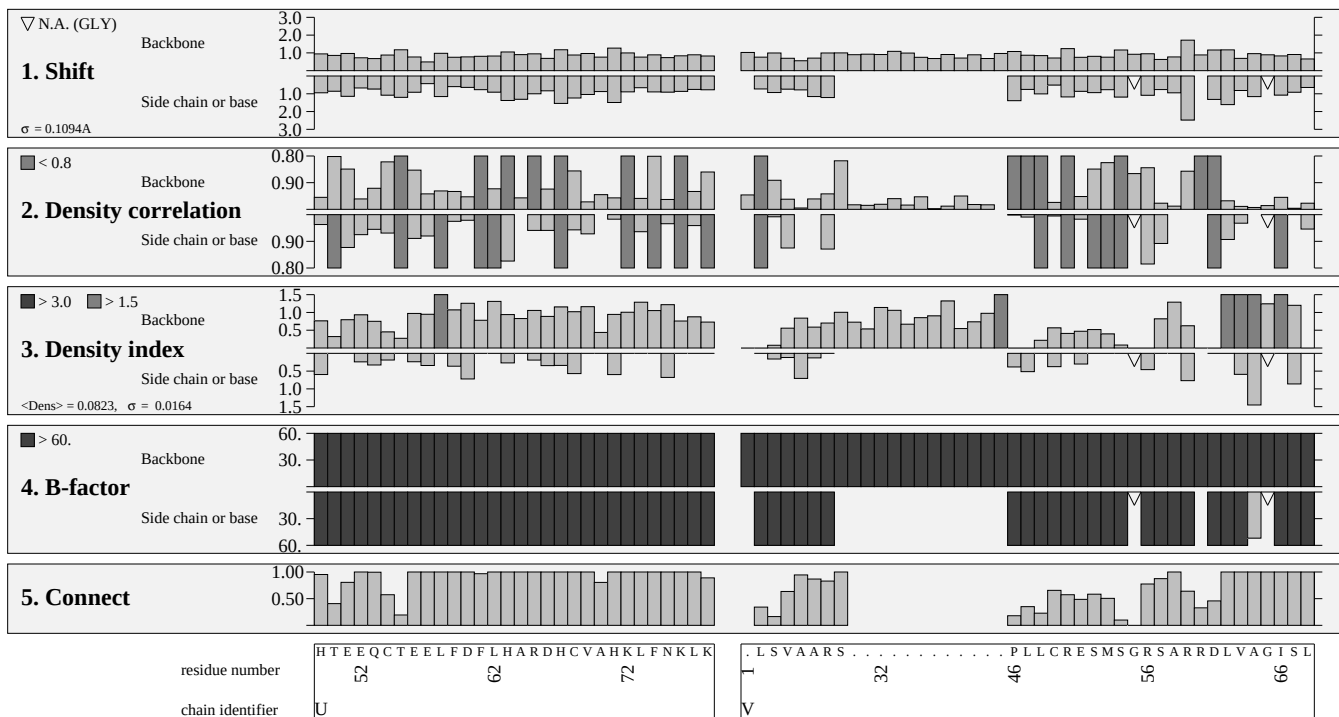
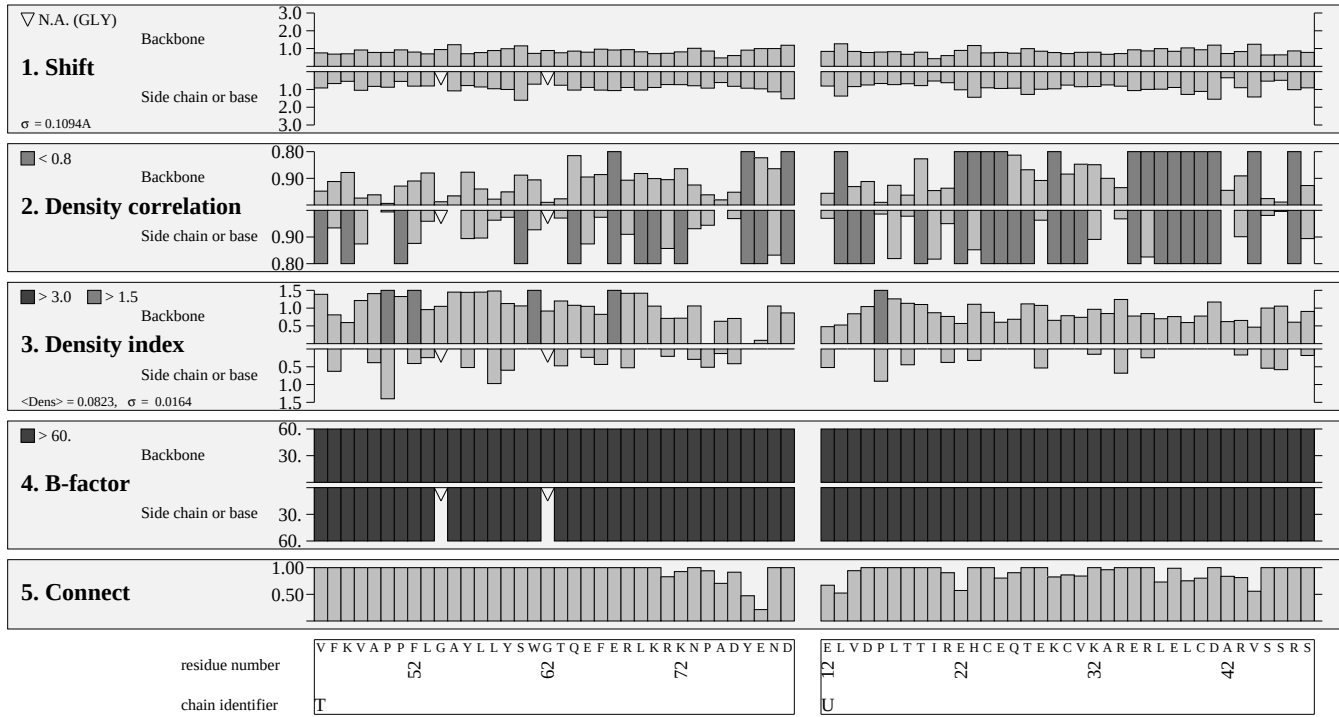
Local estimation (26)



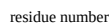
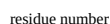
Structure Factor Check

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Local estimation (27)



Local estimation (28)



Local estimation (29)

