

Structure Factor Check

3H1J

Title: STIGMATELLIN-BOUND CYTOCHROME BC1 COMPLEX FROM CHICKEN
Date: 12-APR-09
PDB code: 3H1J

Crystal

Cell parameters:

a: 173.46 Å b: 182.45 Å c: 241.33 Å
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Model

32679 atoms (14 water molecules)

Number of chains: 51

Volume not occupied by model: 63.4 %

 (for atomic model): 77.3 Å²

σ (B): 17.81 Å²

Matthews coefficient: 4.17

Corresponding solvent % : 70.30

Refinement

Program: CNS 1.1

Nominal resolution range: 42.7 – 3.00 Å

Reported R-factor: 0.243

Number of reflections used: 141718

Reported Rfree: 0.28

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 42.7 – 3.00 Å

Reflections in file: 141717

Unique reflections above 0: 141717

above 1 σ : 138899

above 3 σ : 81483

SF CHECK

Nominal resolution range: 42.7 – 3.00 Å

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

Used reflections: 141716

Reflections out of resolution: 1

Completeness: 92.6 %

R_{stand}(F) = $\langle \sigma(F) \rangle / \langle F \rangle$: 0.106

Anisotropic distribution of Structure Factors

ratio of eigen values: 1.0000 0.5954 0.6935

B_{overall} (by Patterson): 53.Å²

Optical resolution: 2.23 Å

Expected opt. resol. for complete data set: 2.23 Å

Estimated minimal error: 0.106 Å

Model vs. Structure Factors

R-factor for all reflections: 0.291

Correlation factor: 0.849

R-factor: 0.296

for $F > 2.0 \sigma$

nom. resolution range: 42.68 – 3.00 Å

reflections used: 138910

Rfree: 0.321

Nfree: 2736

R-factor without free-refl.: 0.295

Non free-reflections: 136174

<u> (error in coords by Luzzati plot): 0.476 Å

Estimated maximal error: 0.290 Å

DPI: 0.409 Å

Scaling

Scale: 0.602

Bdiff: -9.31

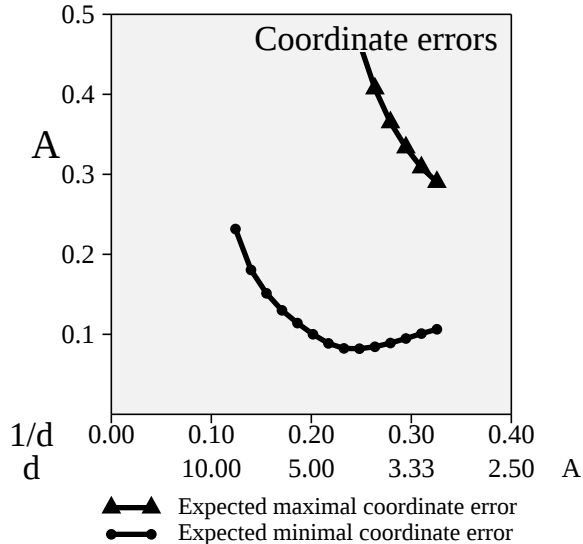
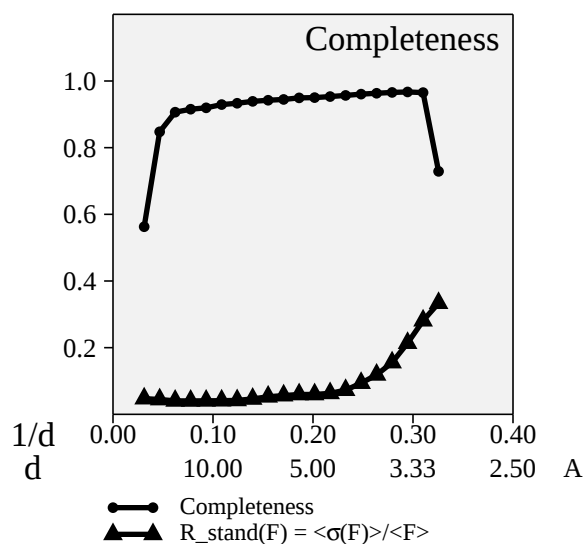
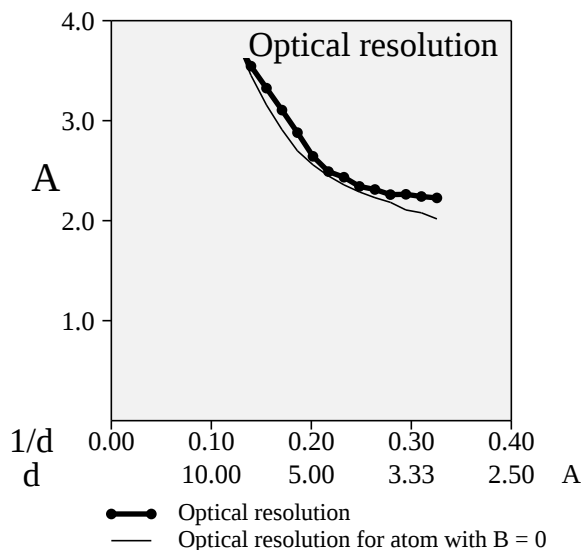
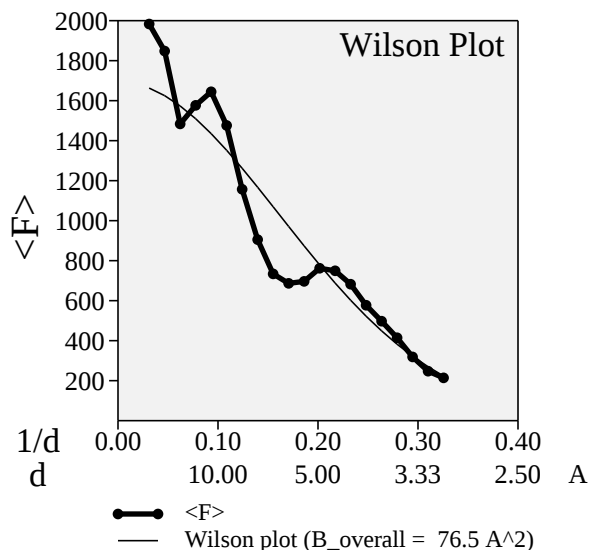
Anisothermal Scaling (Beta):

7.7360 -2.3366 1.2297 0.0000 0.0000 0.0000

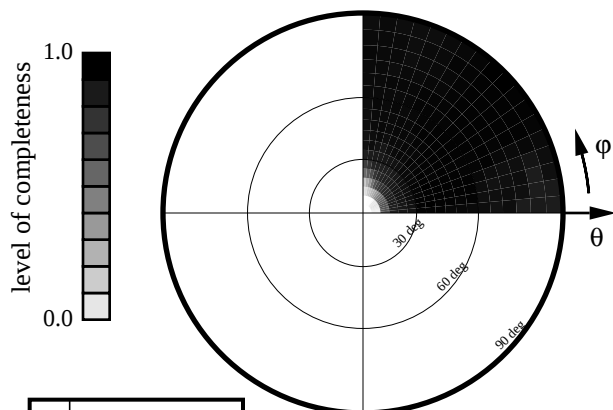
Solvent correction – Ks,Bs: 0.642 250.136

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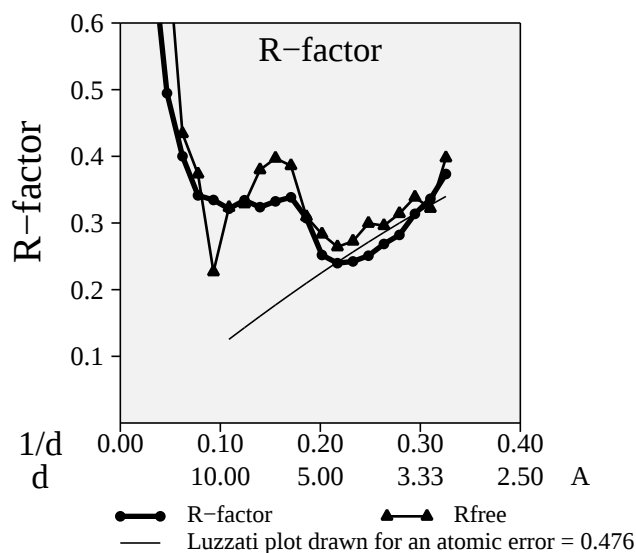


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

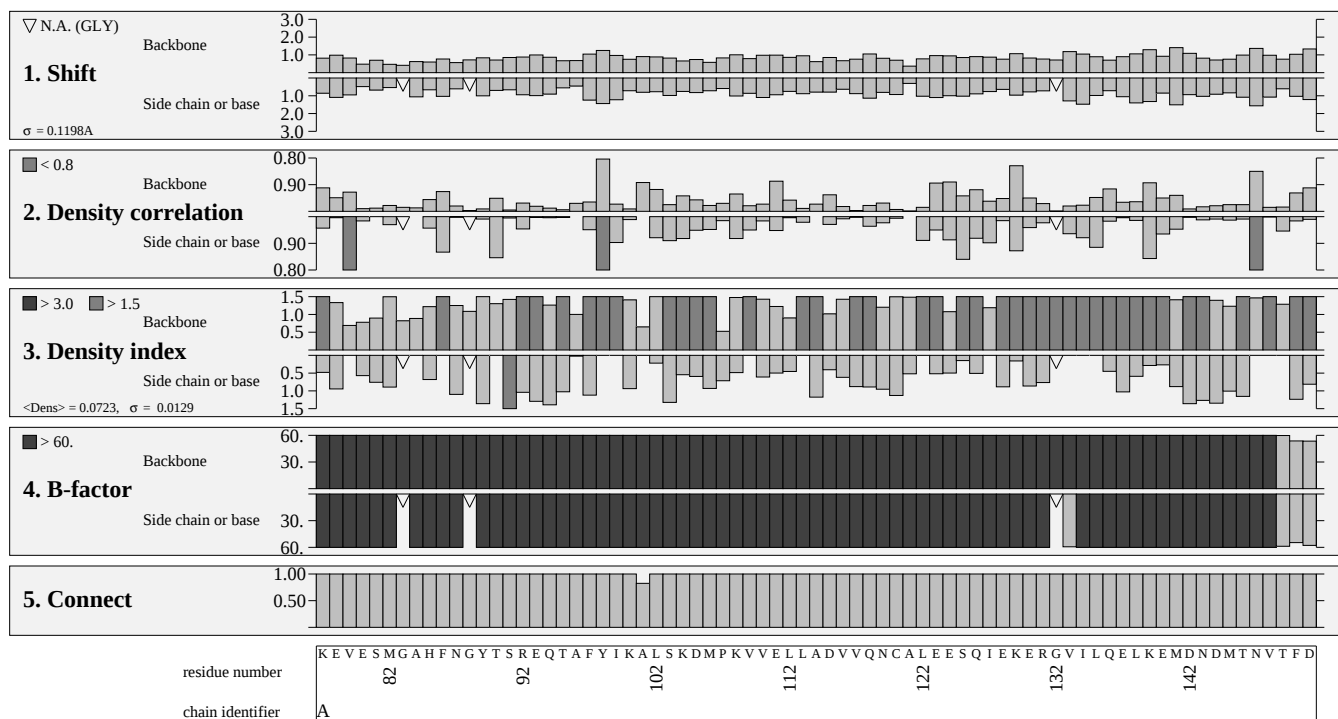
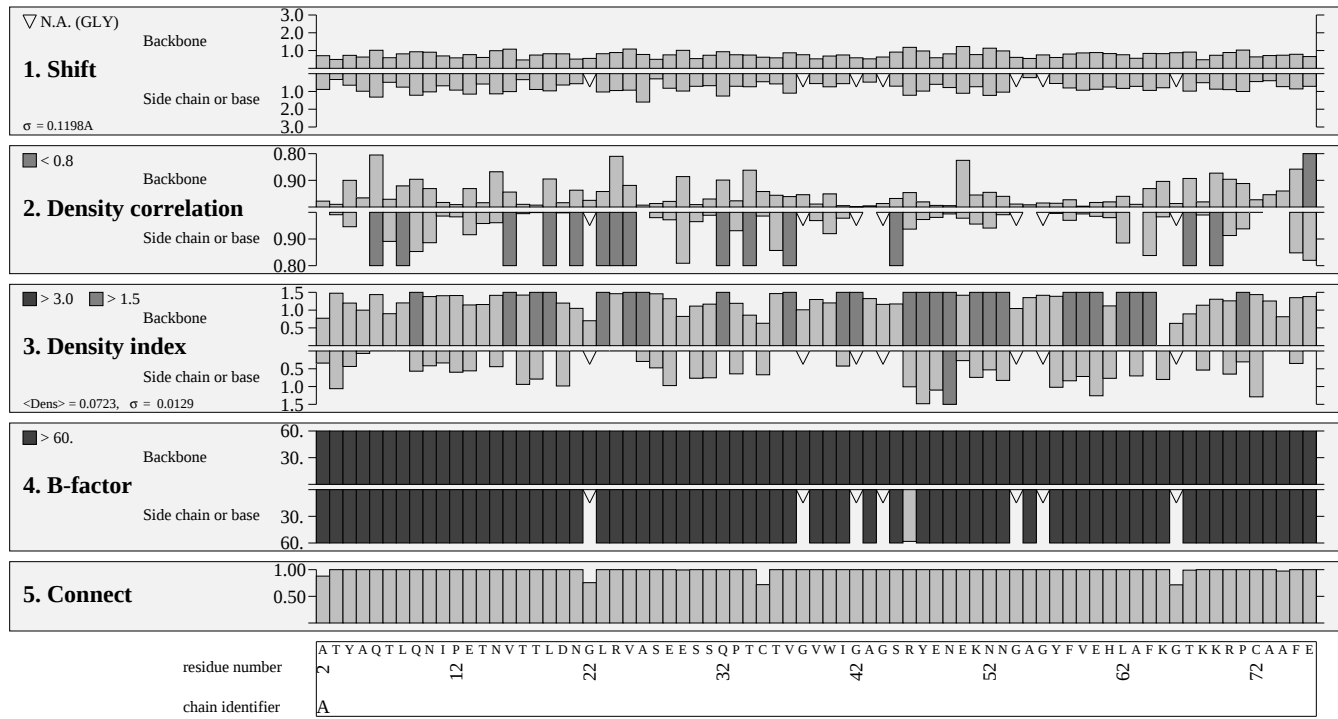
polar coordinates of the crystallographical axes



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3H1J

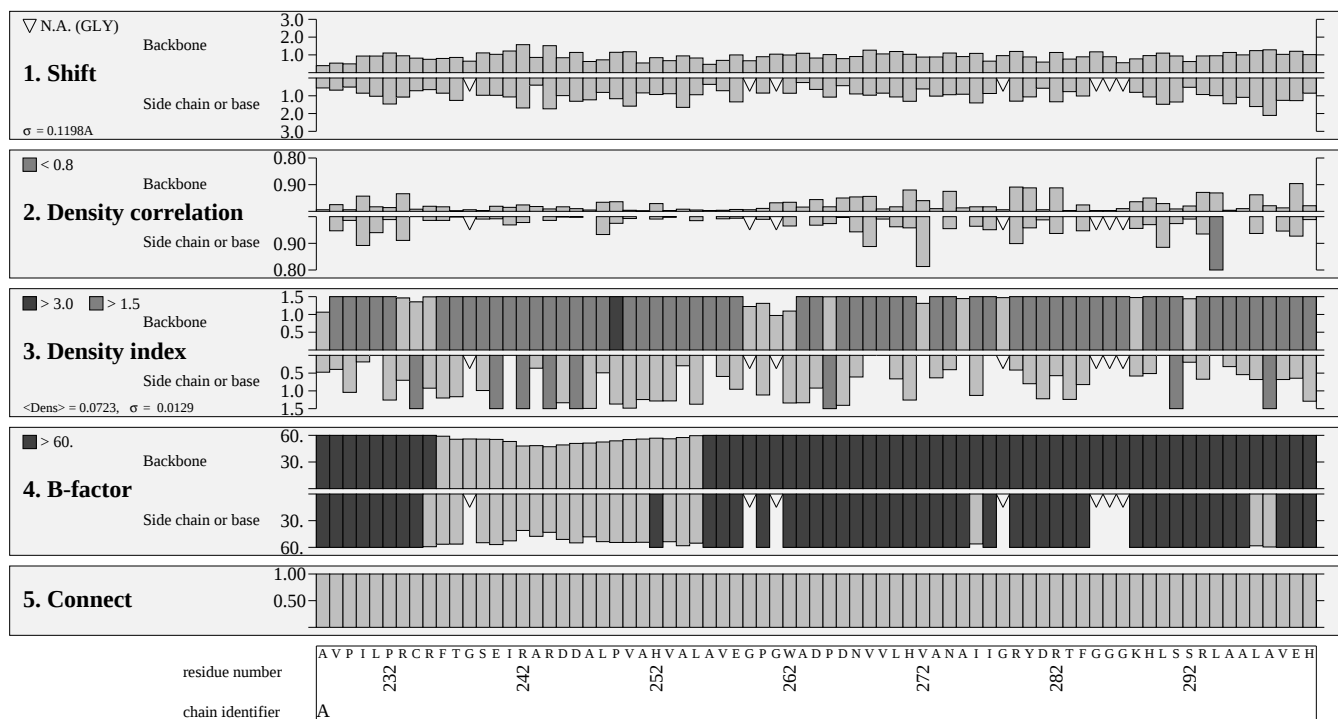
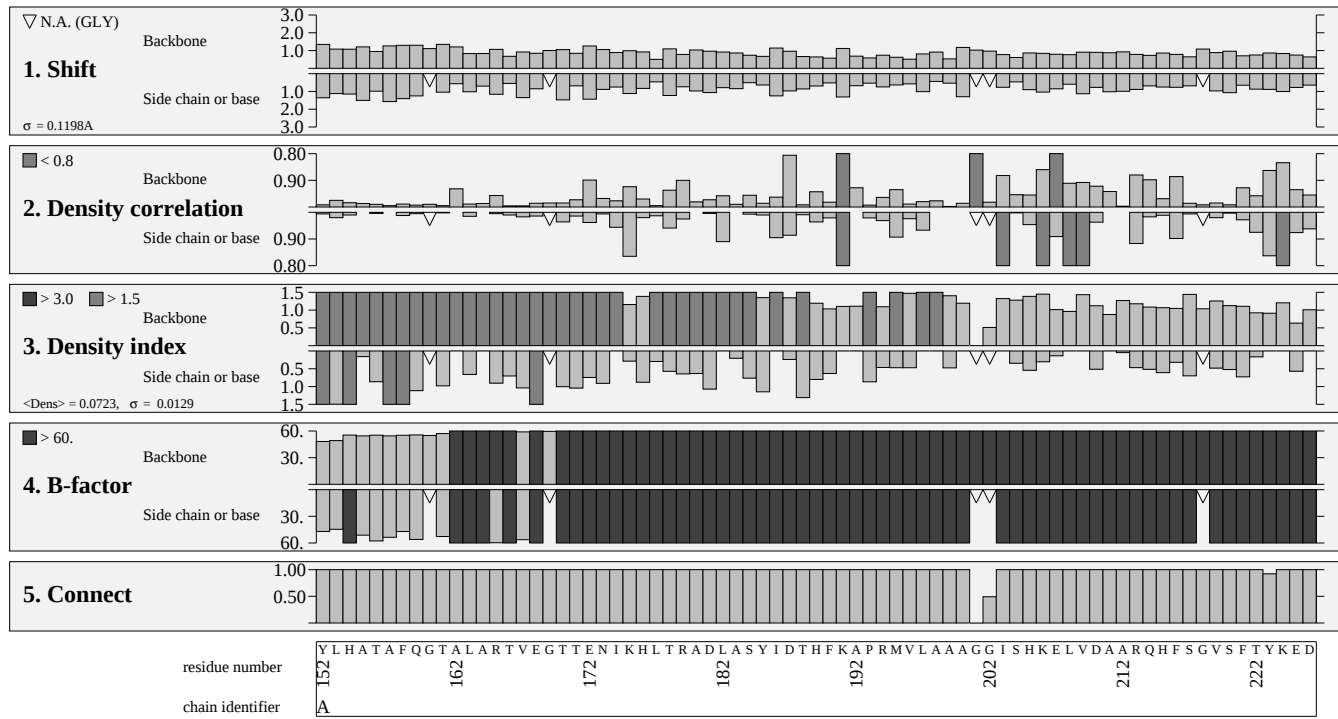
Local estimation



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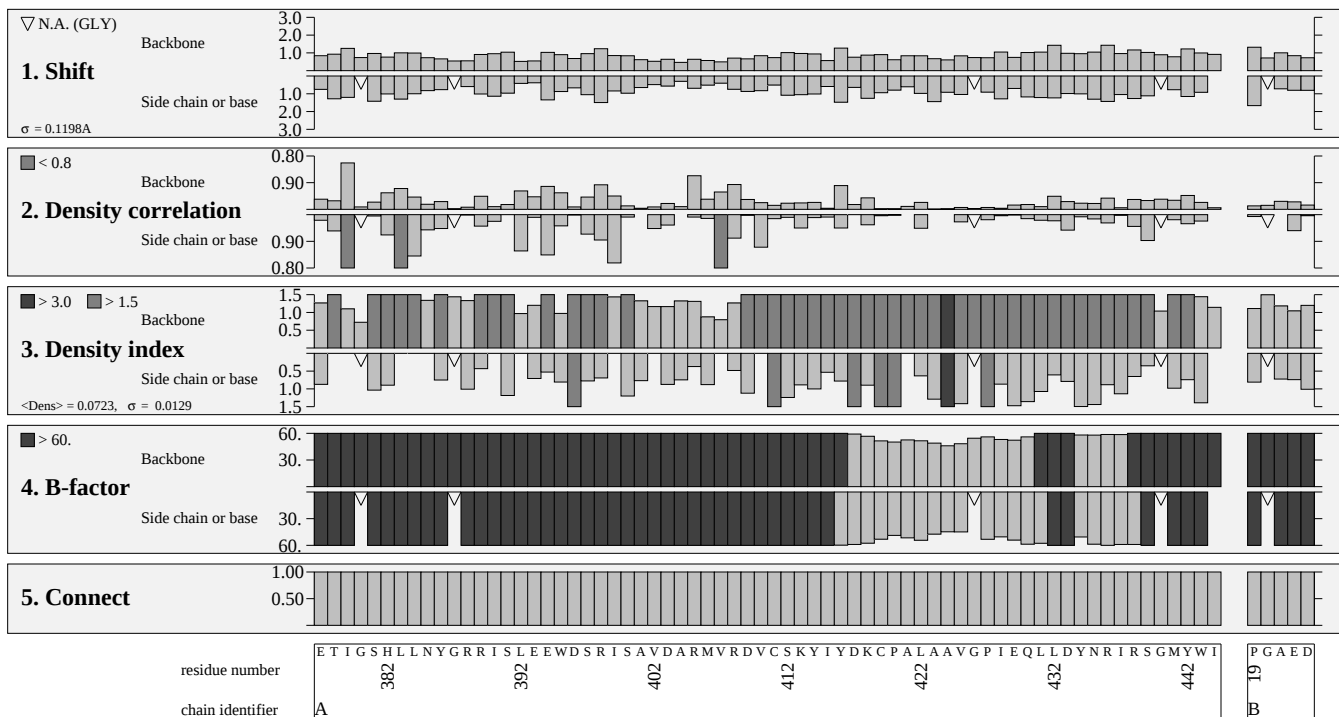
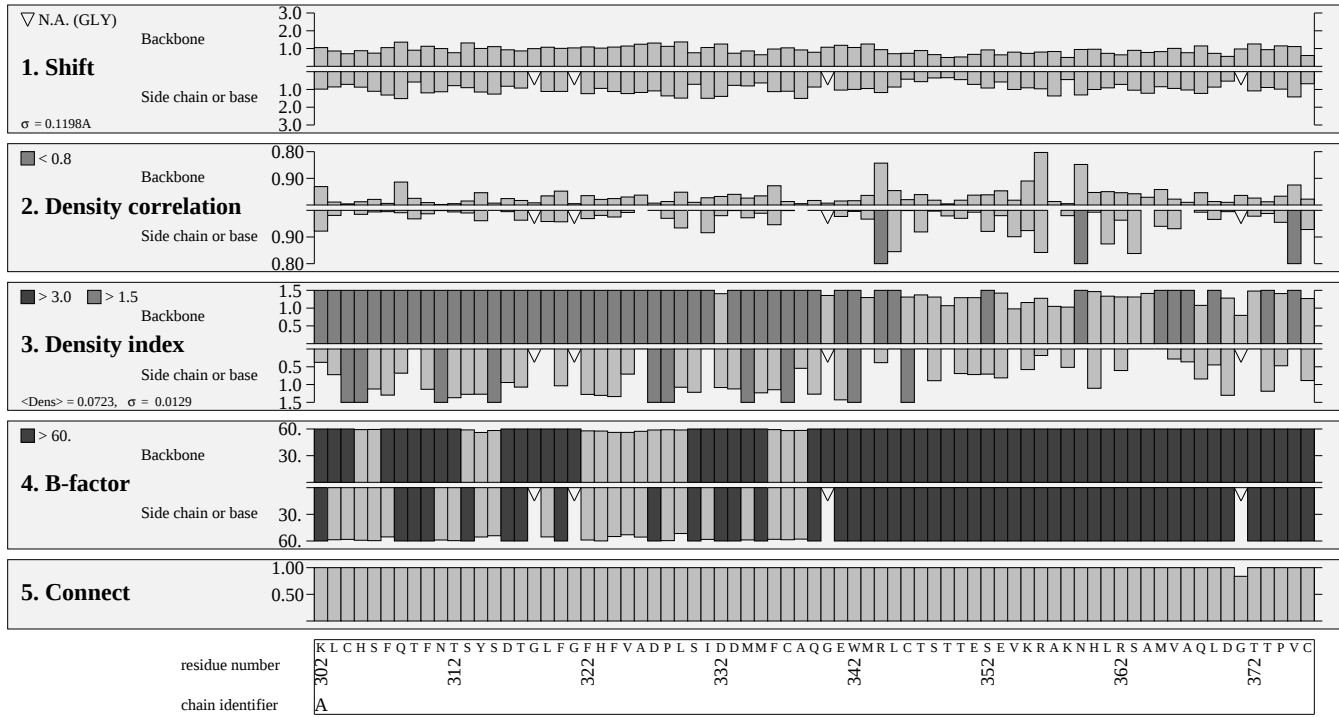
Local estimation (2)



Structure Factor Check

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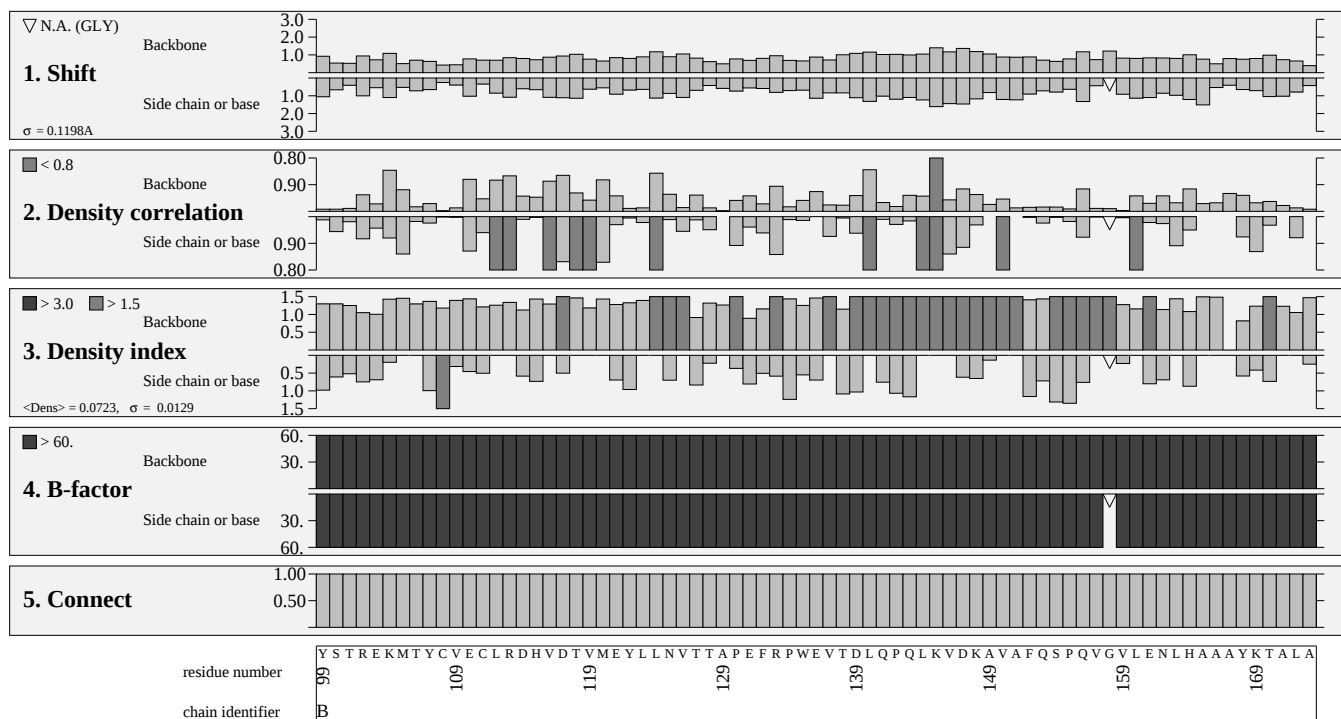
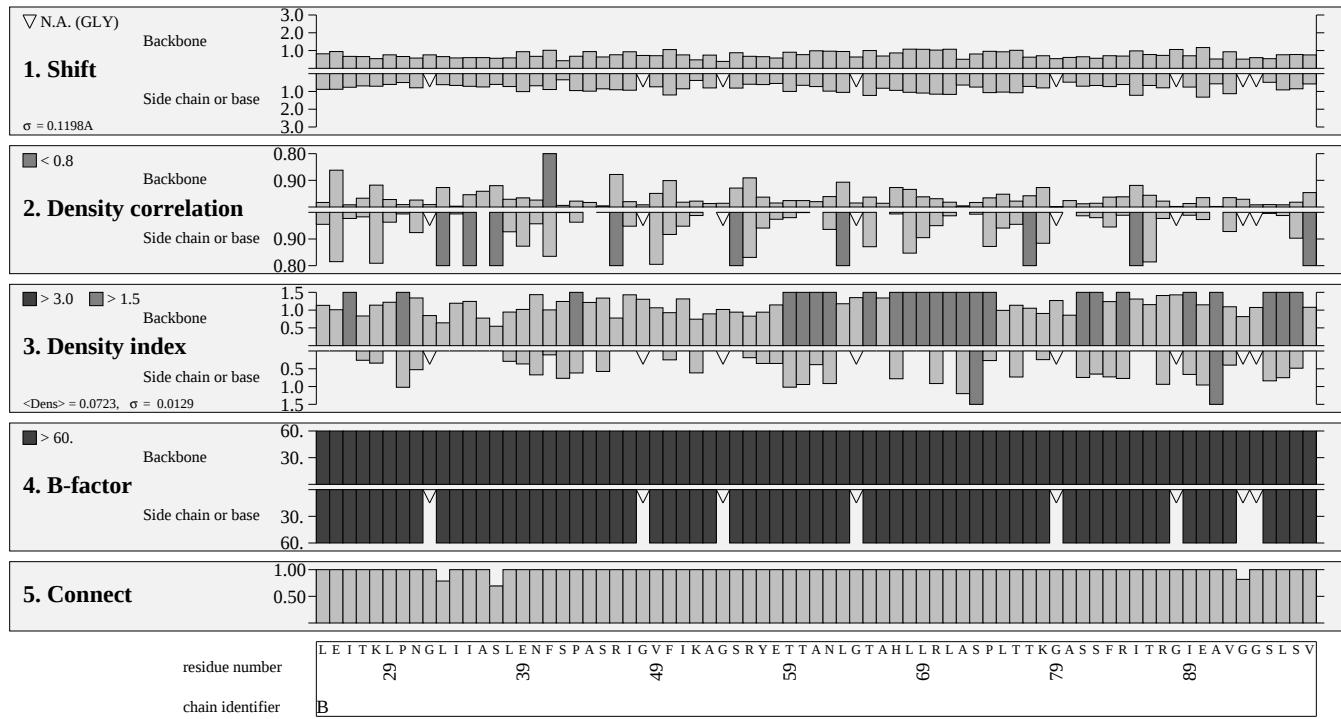
Local estimation (3)



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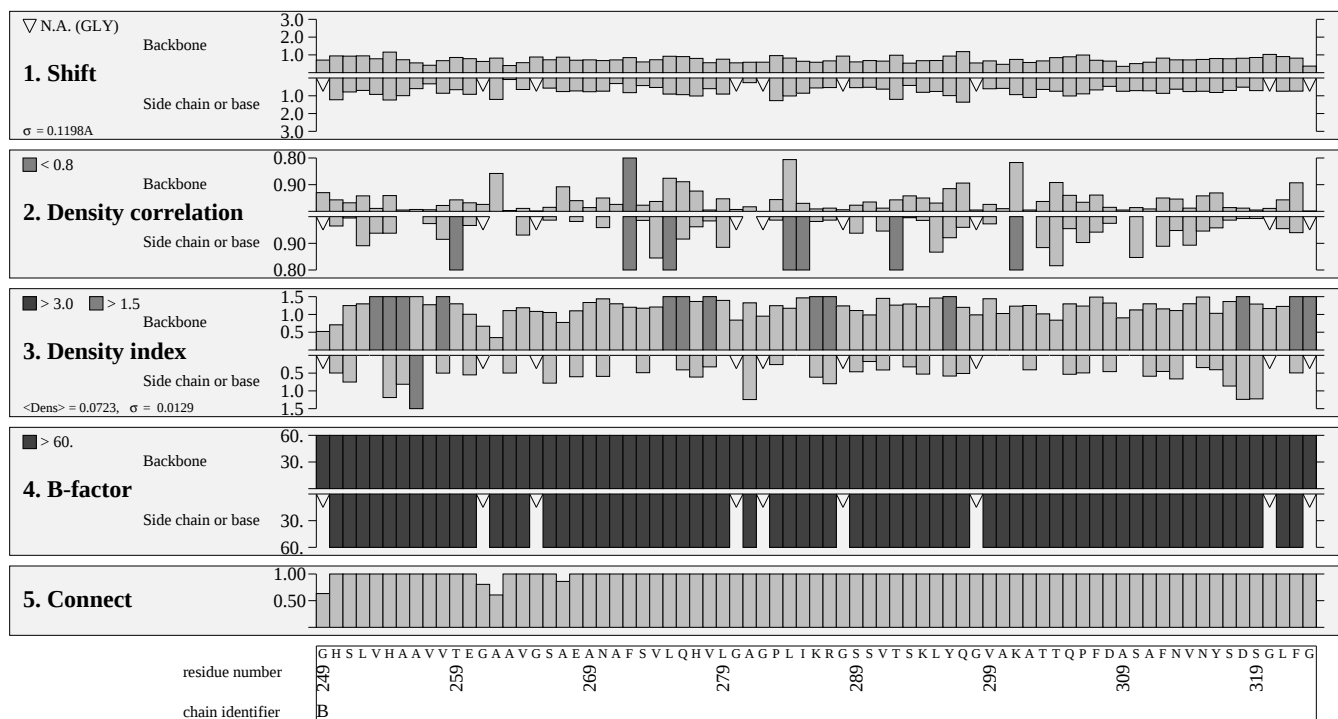
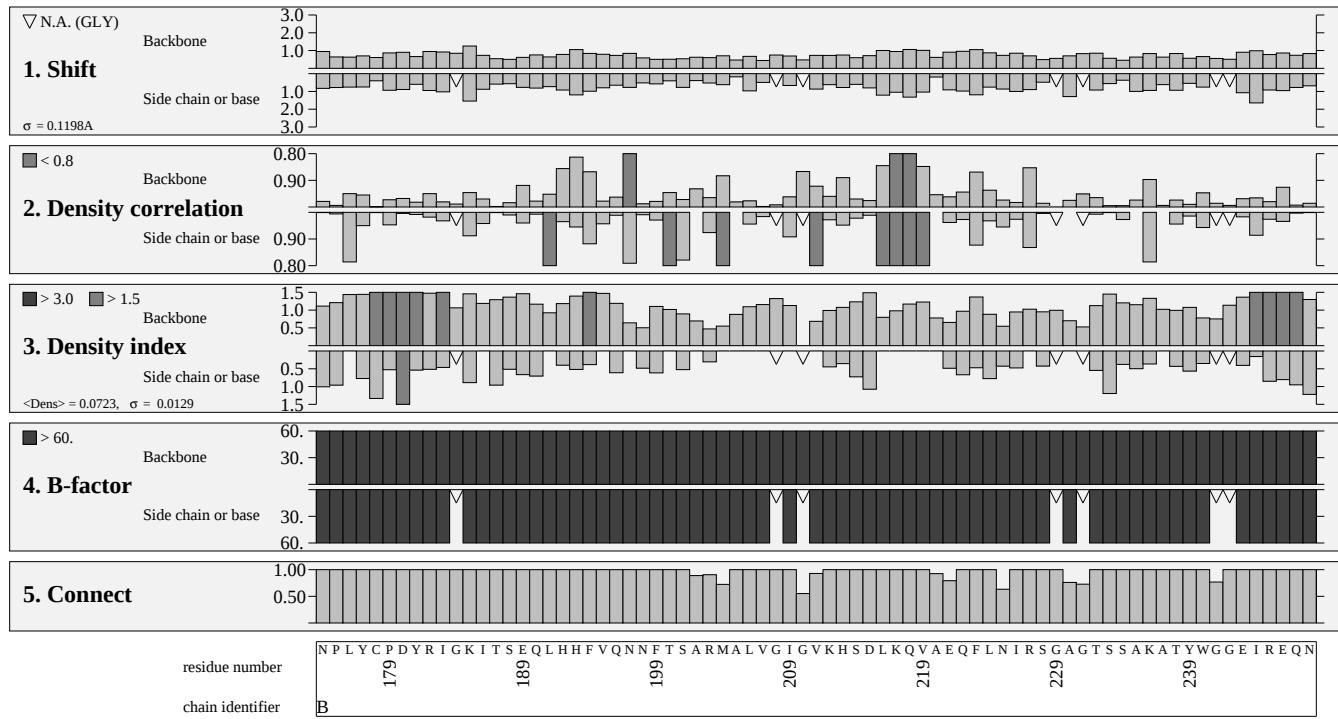
Local estimation (4)



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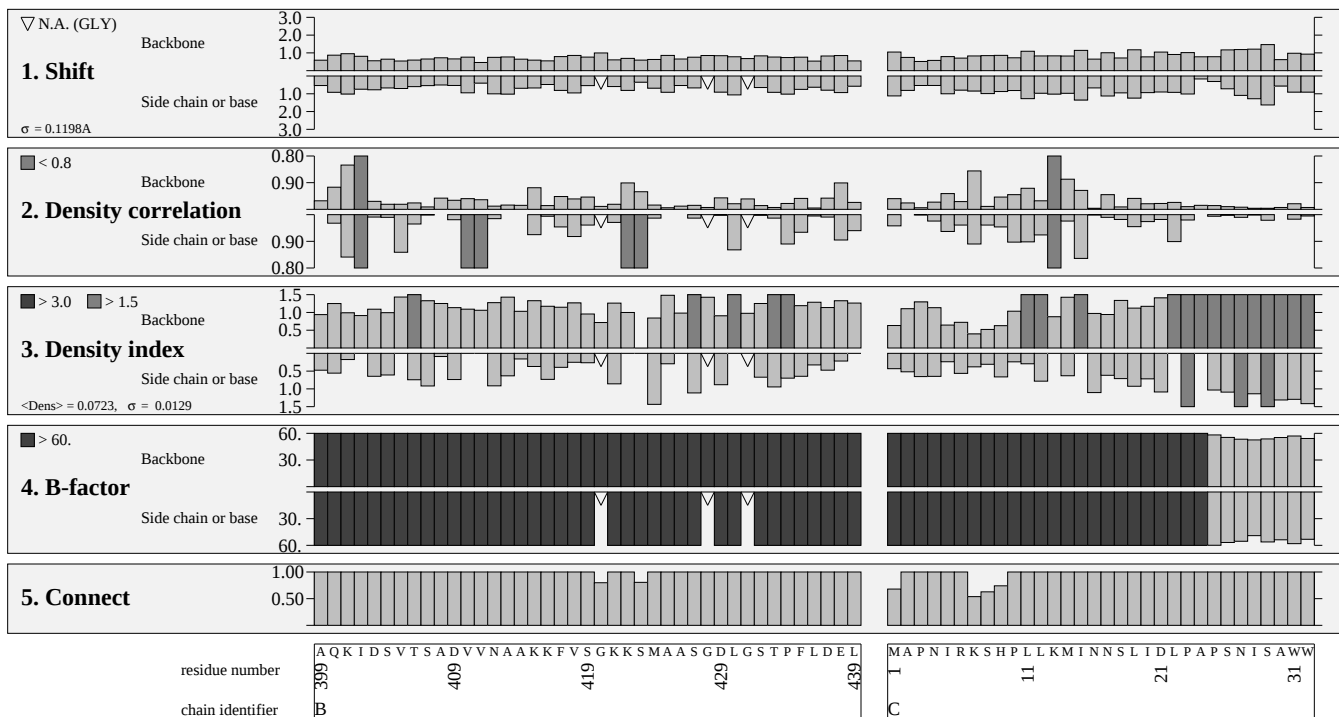
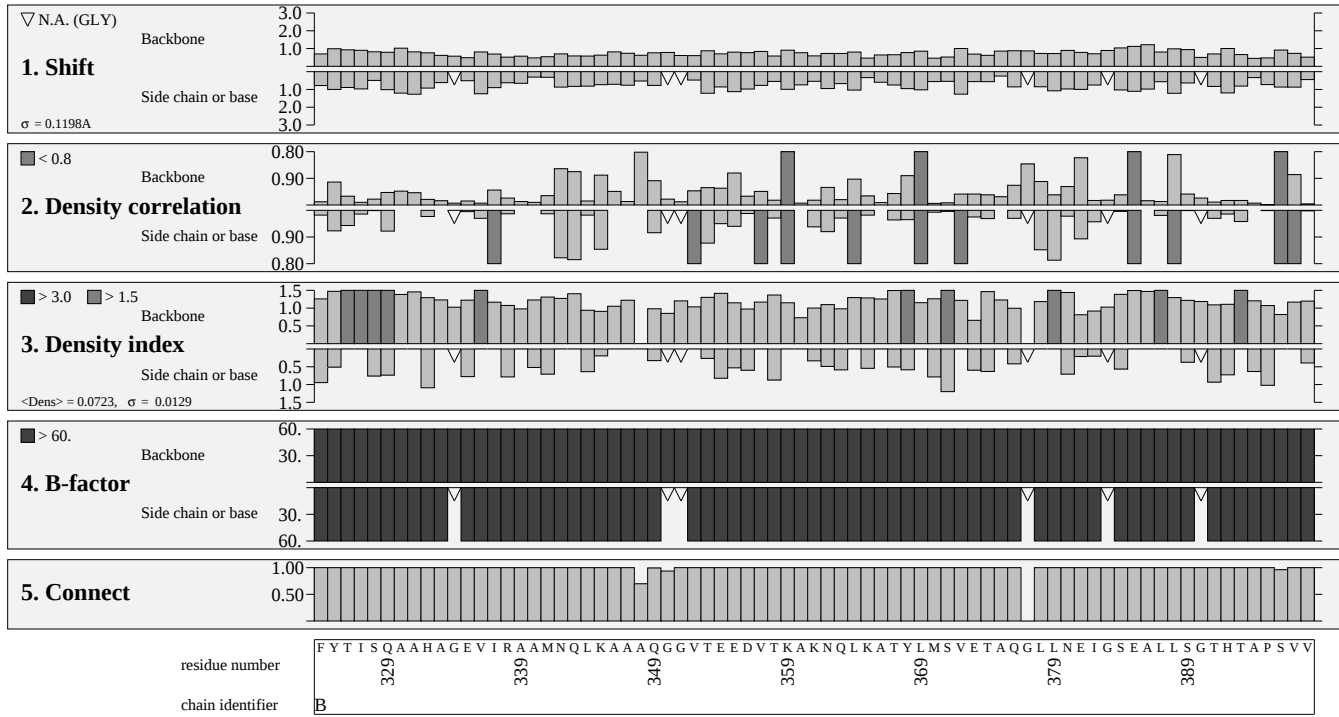
Local estimation (5)



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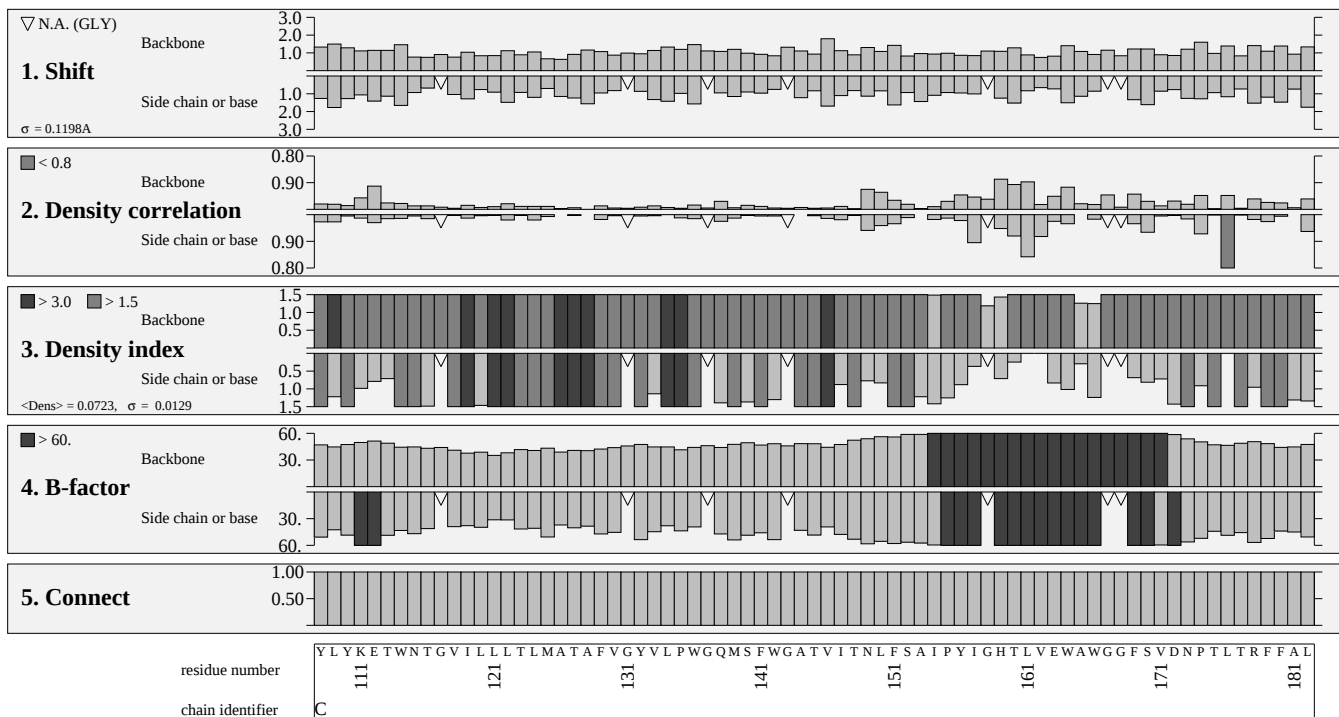
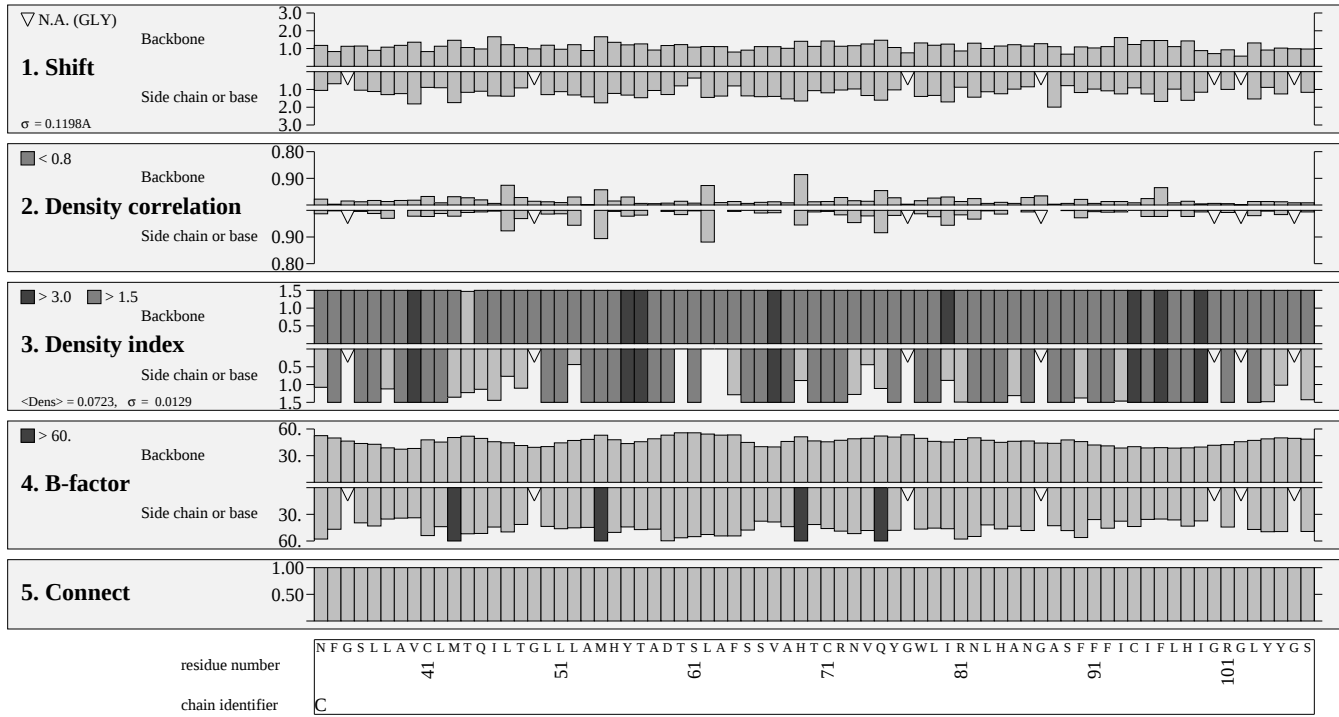
Local estimation (6)



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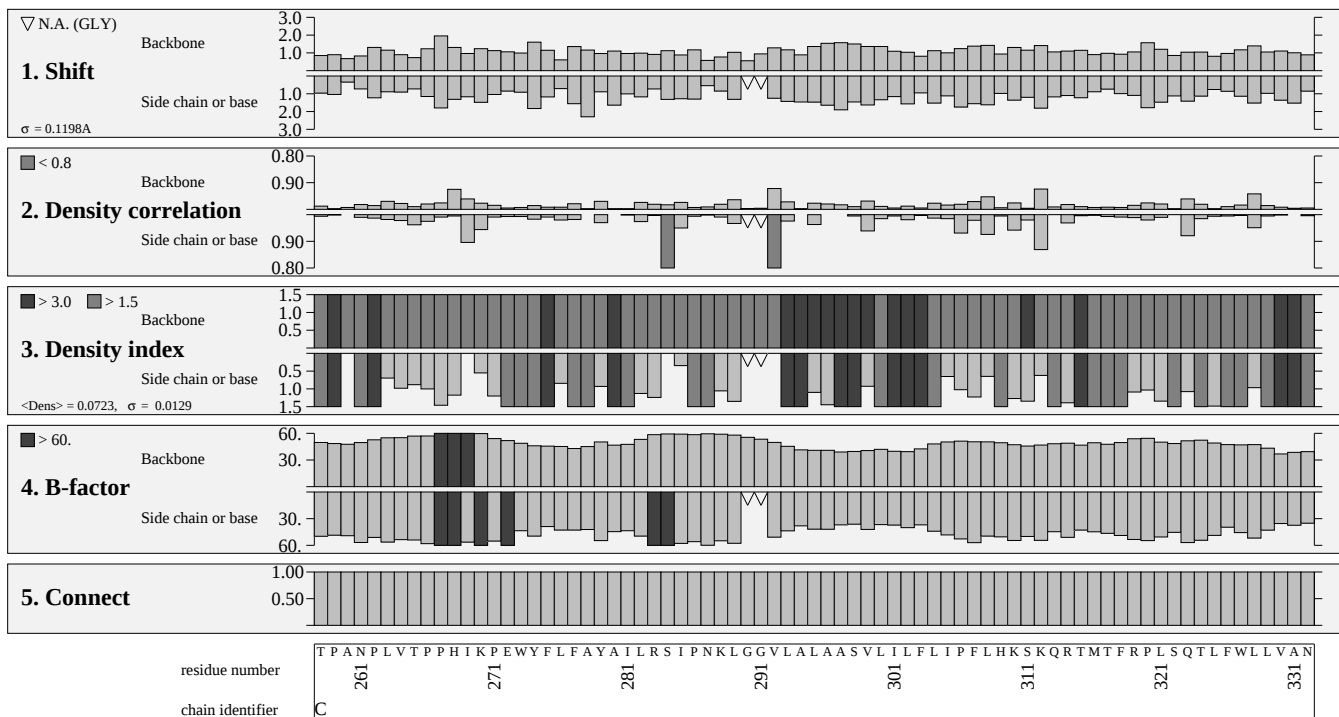
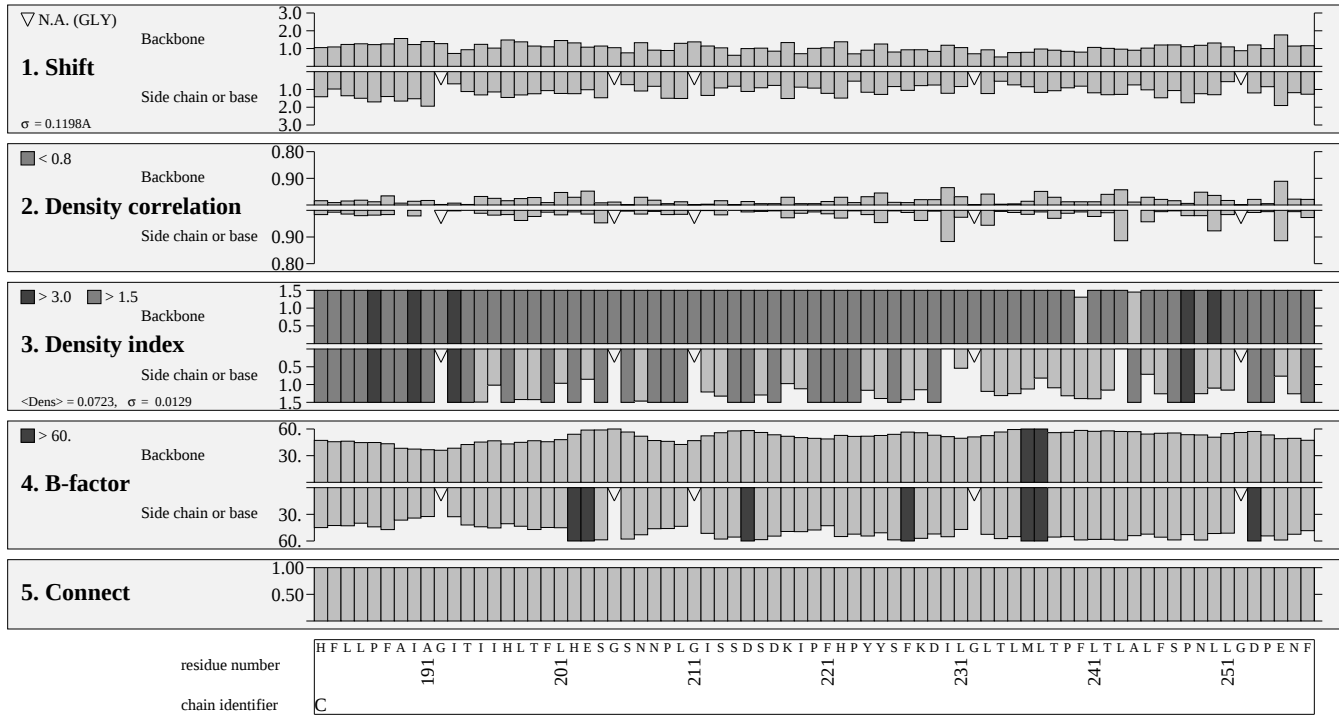
Local estimation (7)



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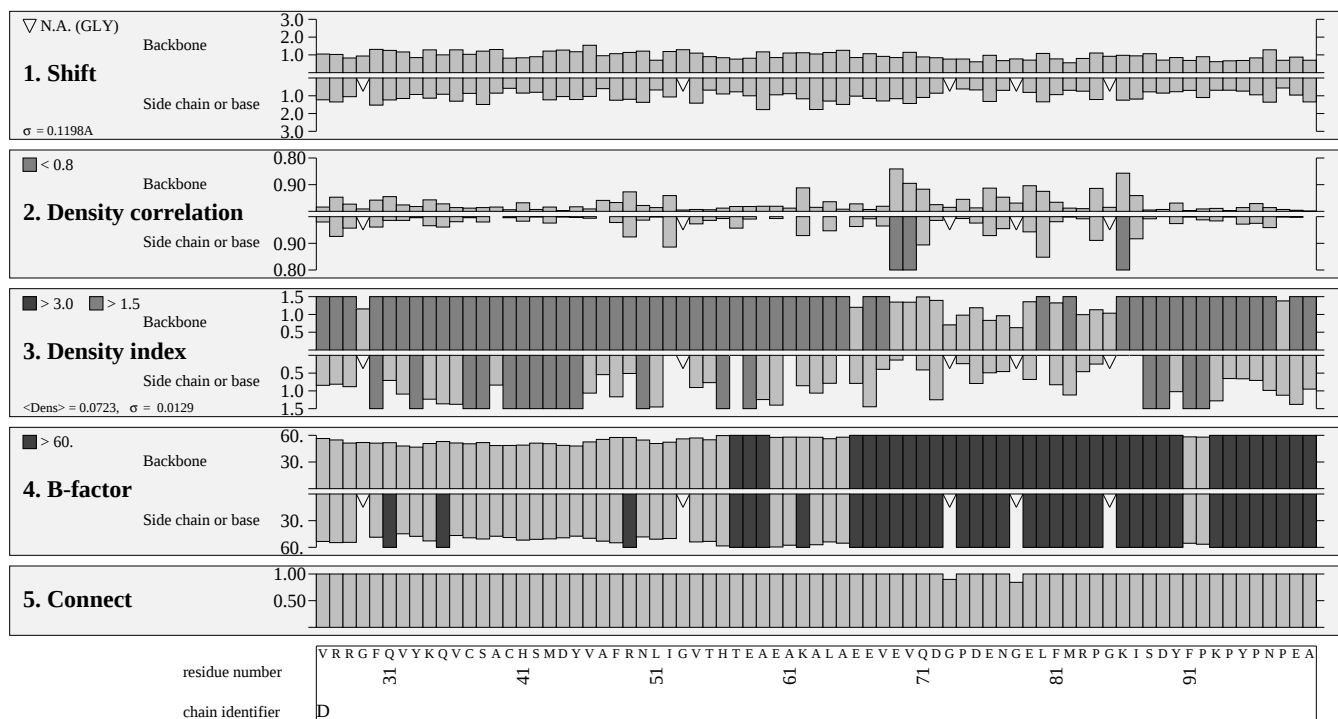
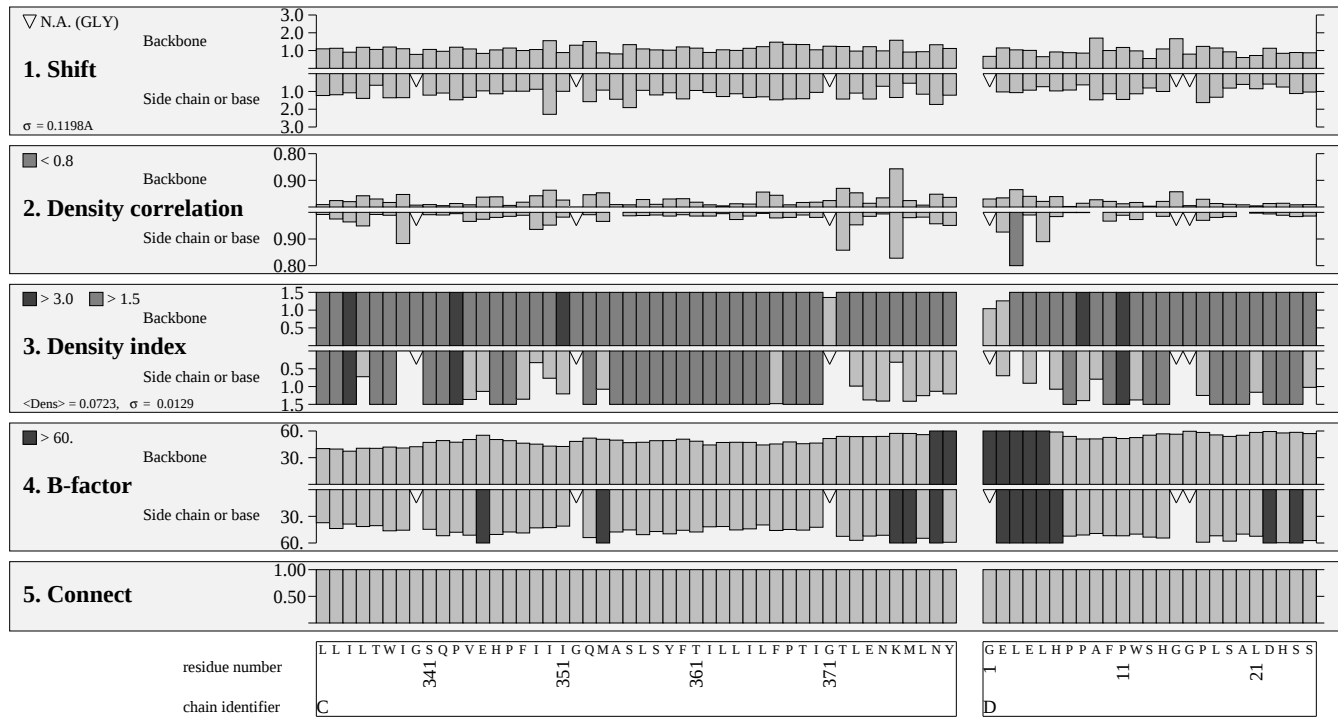
Local estimation (8)



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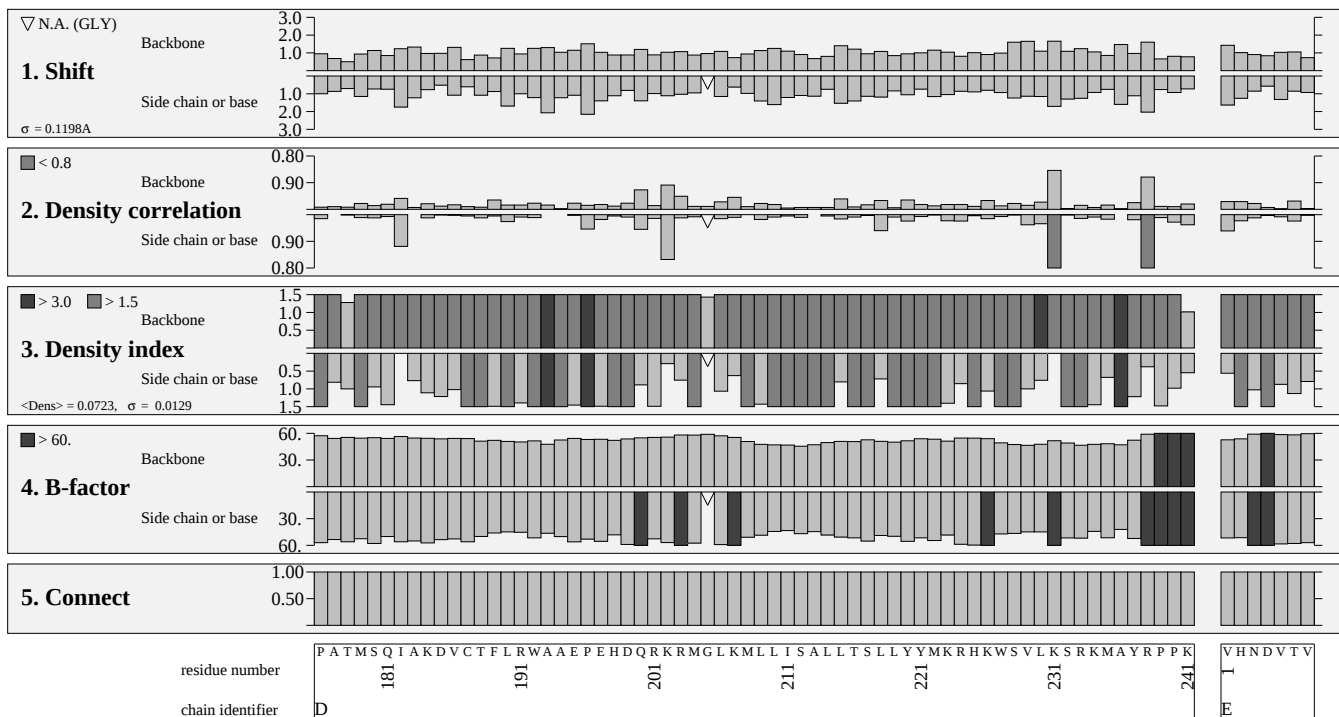
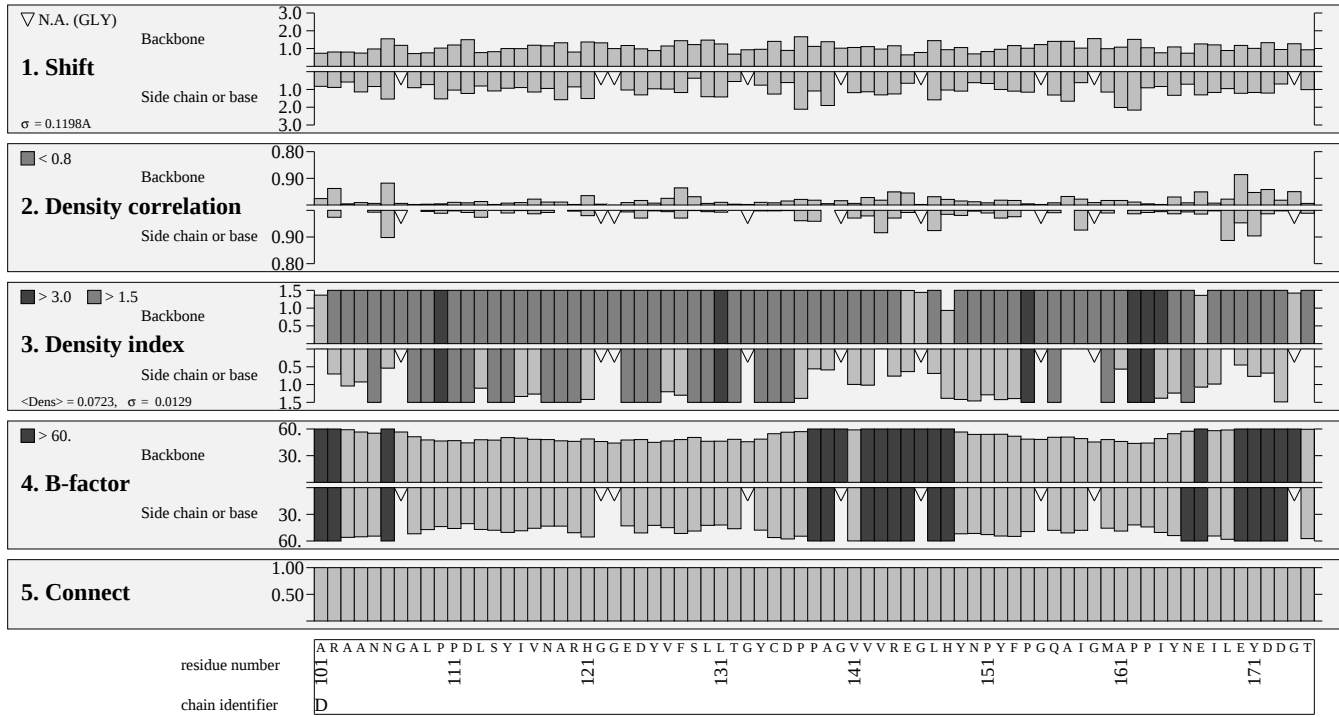
Local estimation (9)



Structure Factor Check

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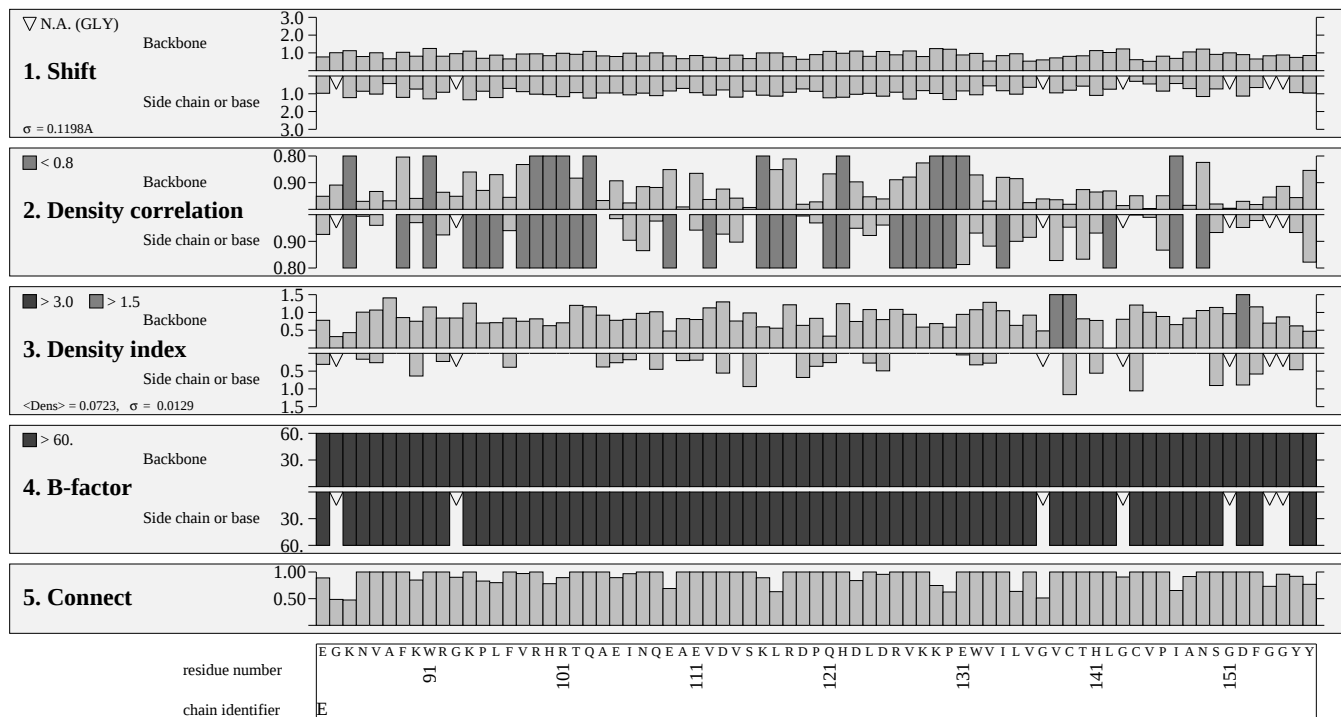
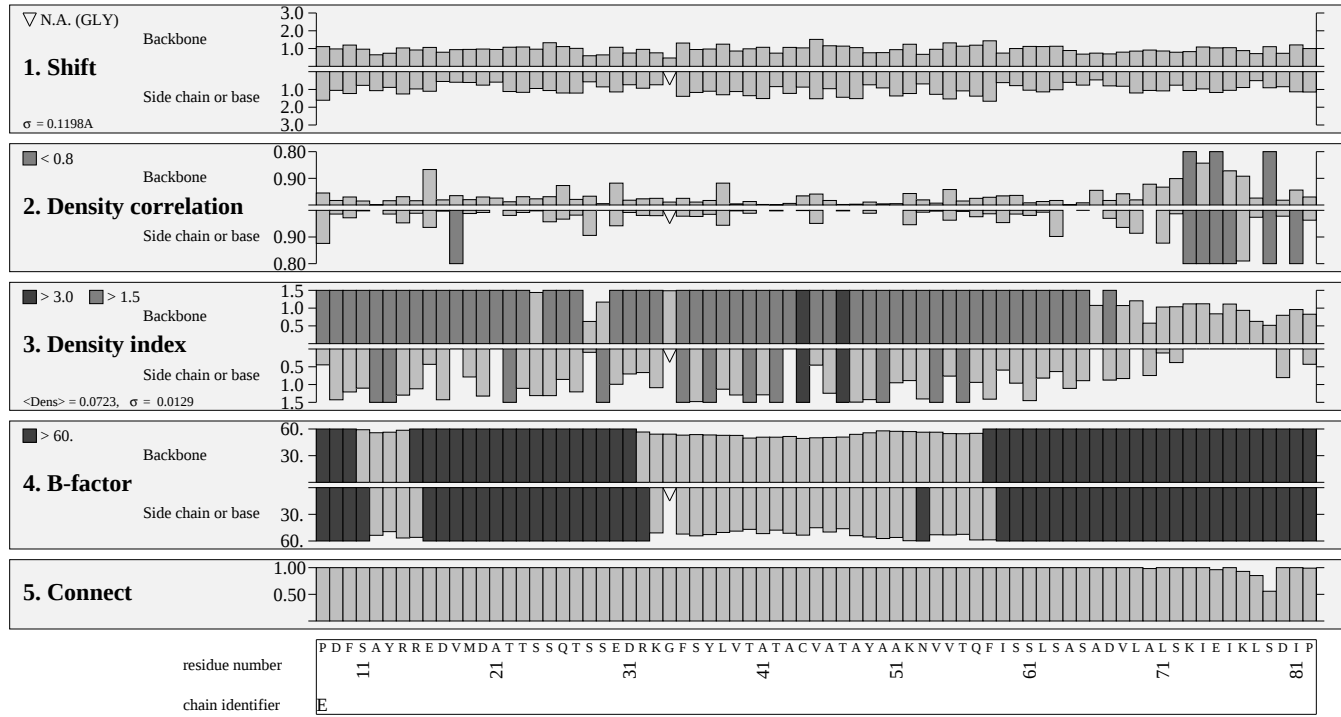
Local estimation (10)



Structure Factor Check

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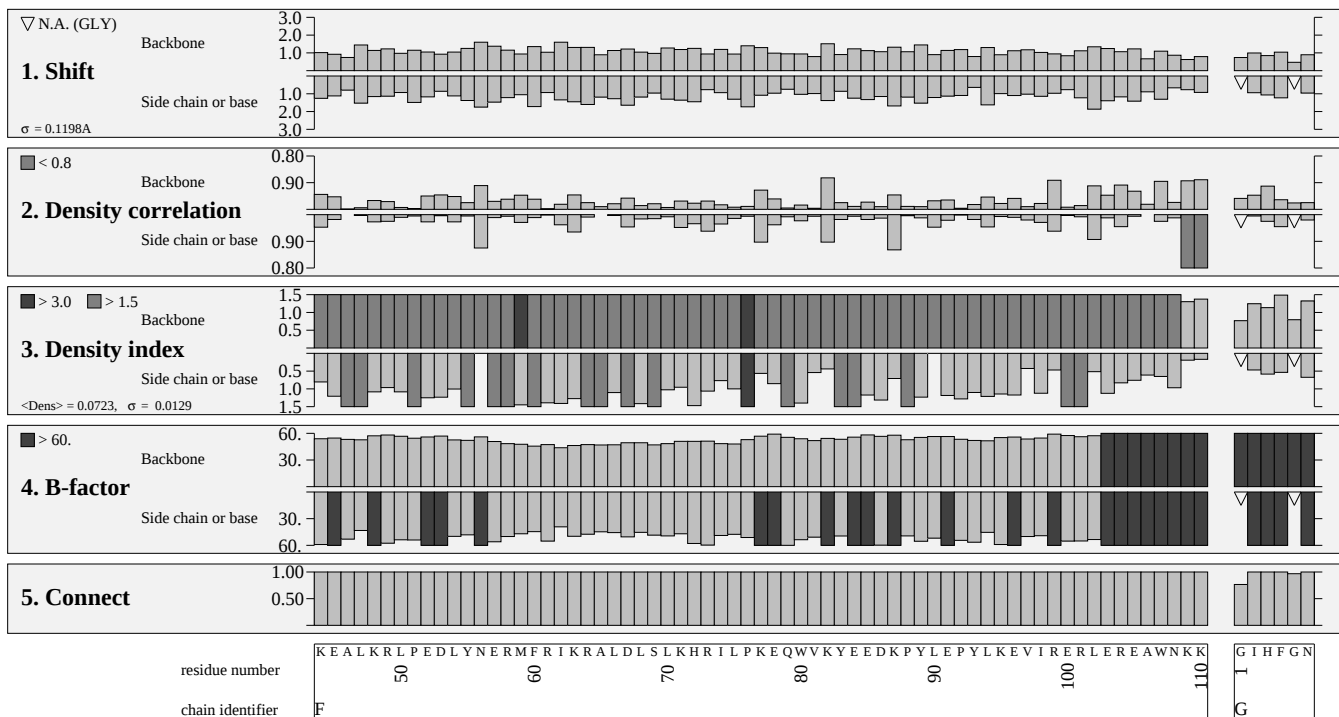
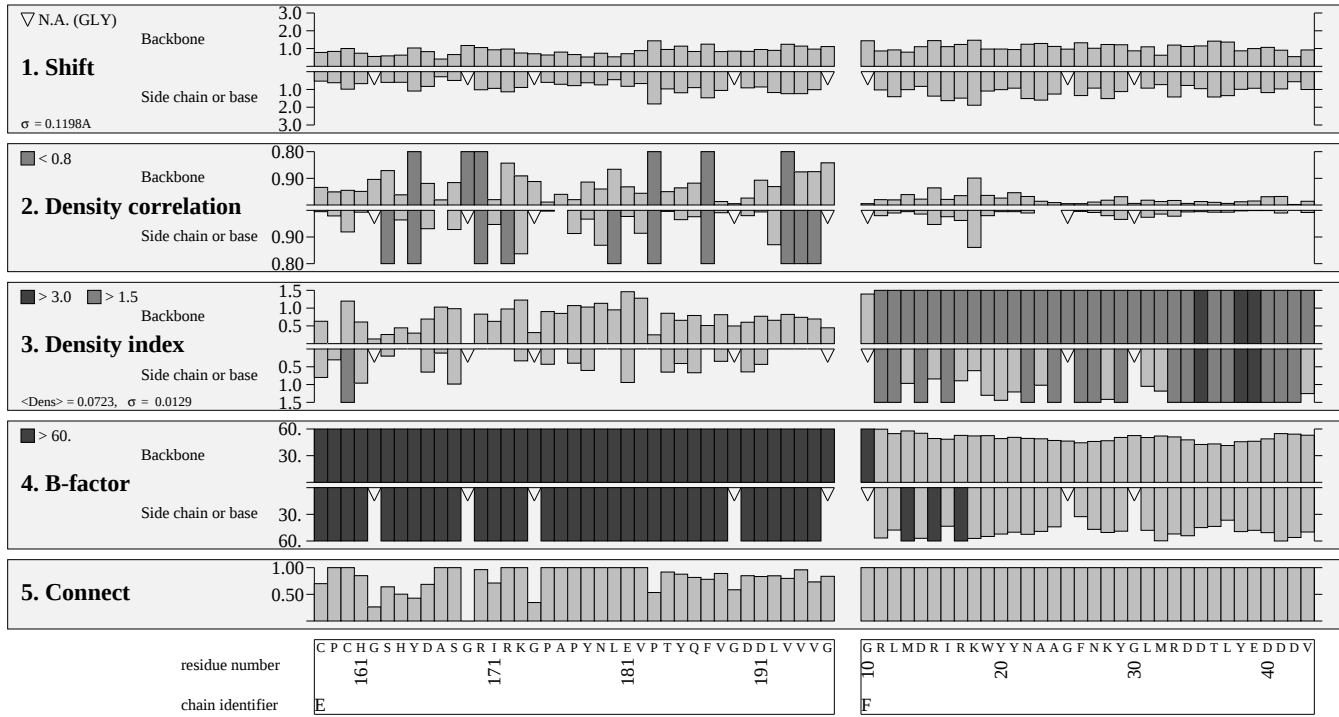
Local estimation (11)



Structure Factor Check

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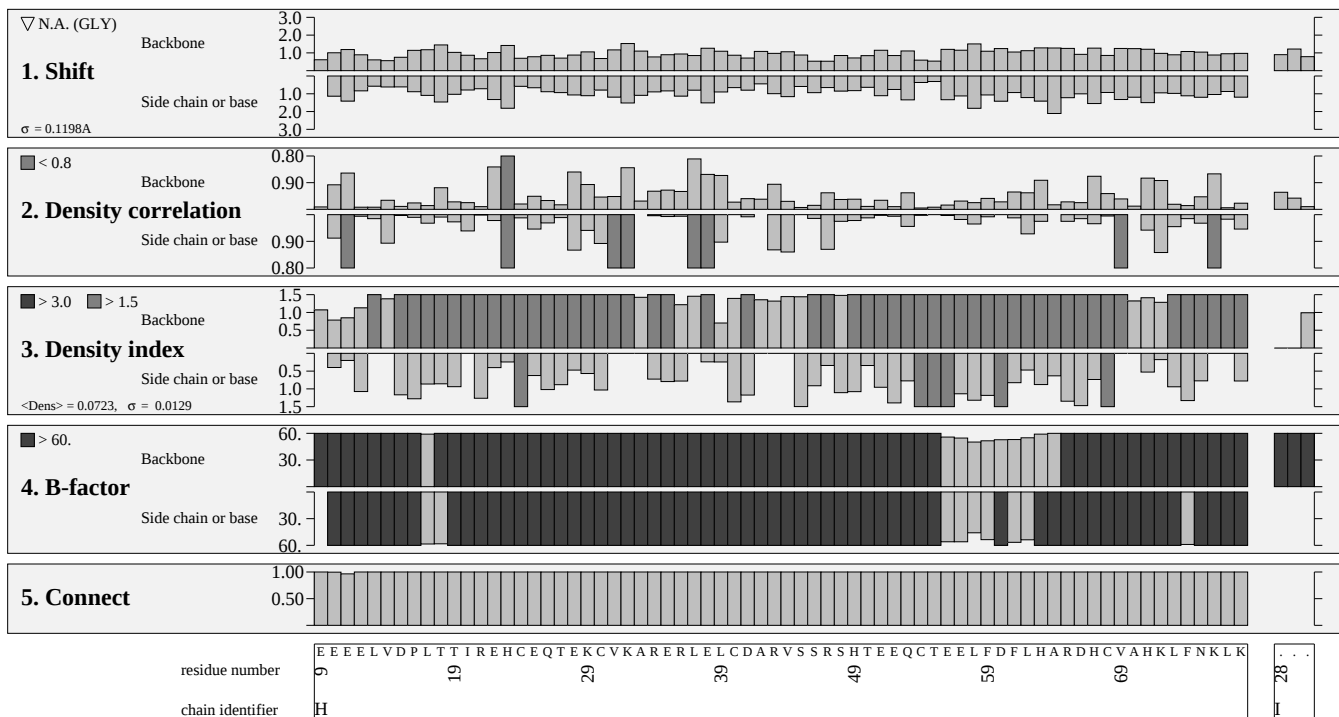
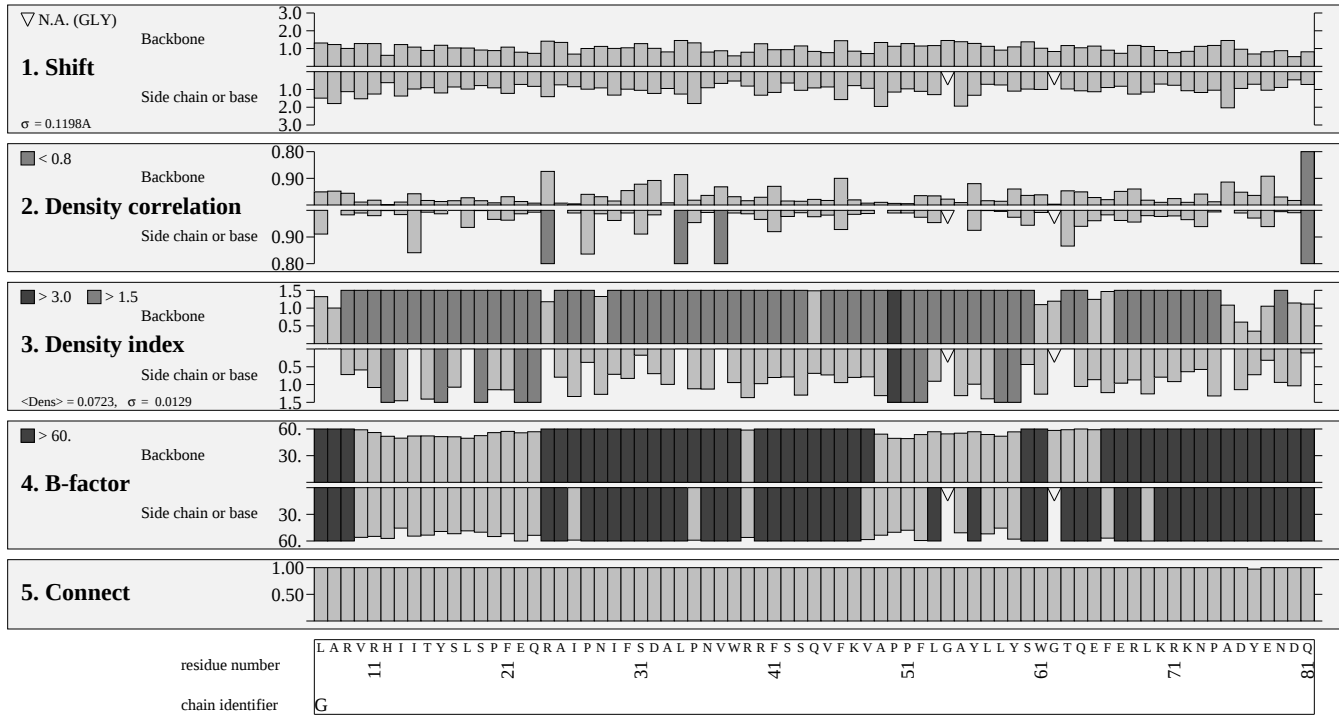
Local estimation (12)



Structure Factor Check

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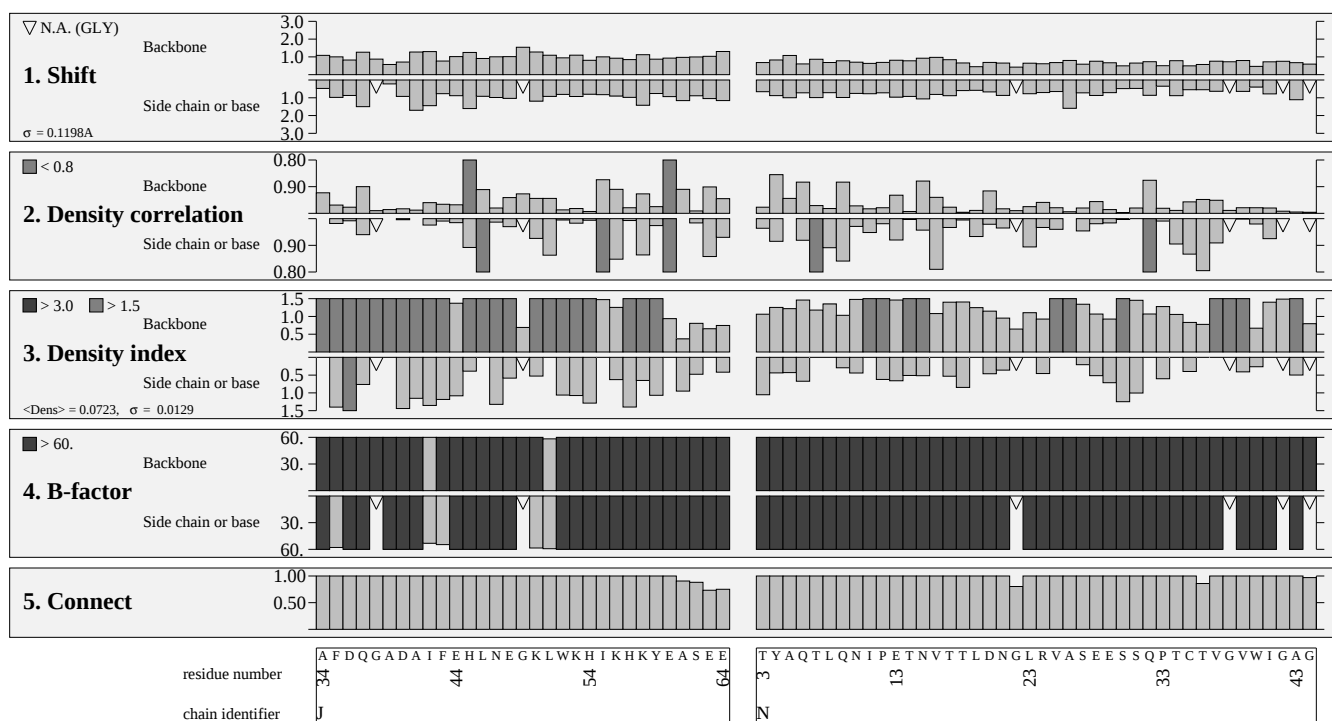
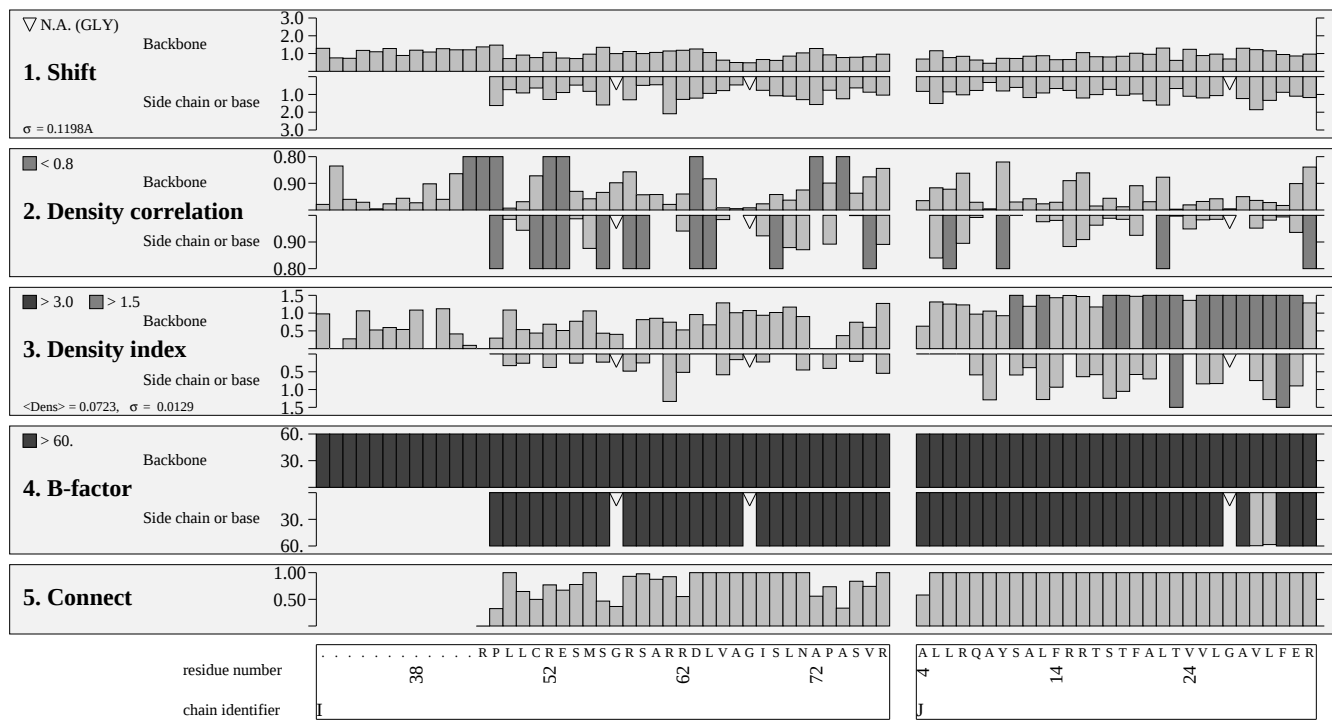
Local estimation (13)



Structure Factor Check

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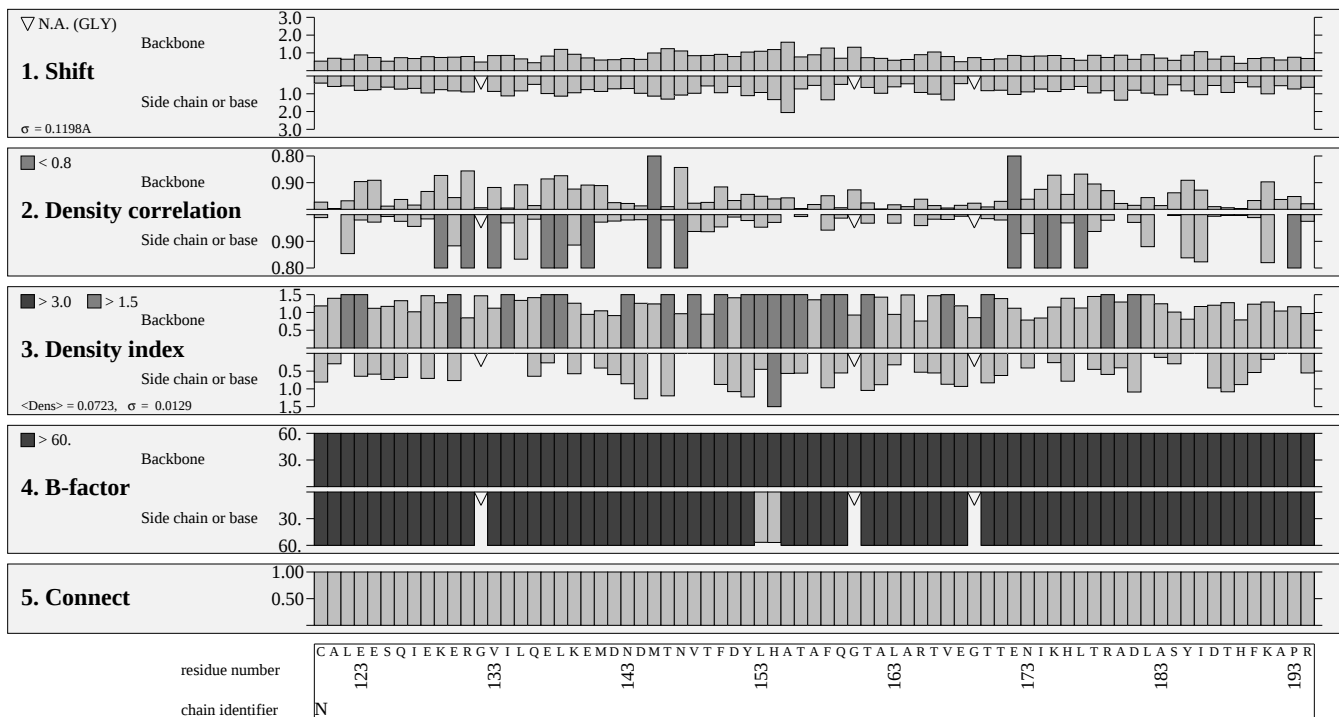
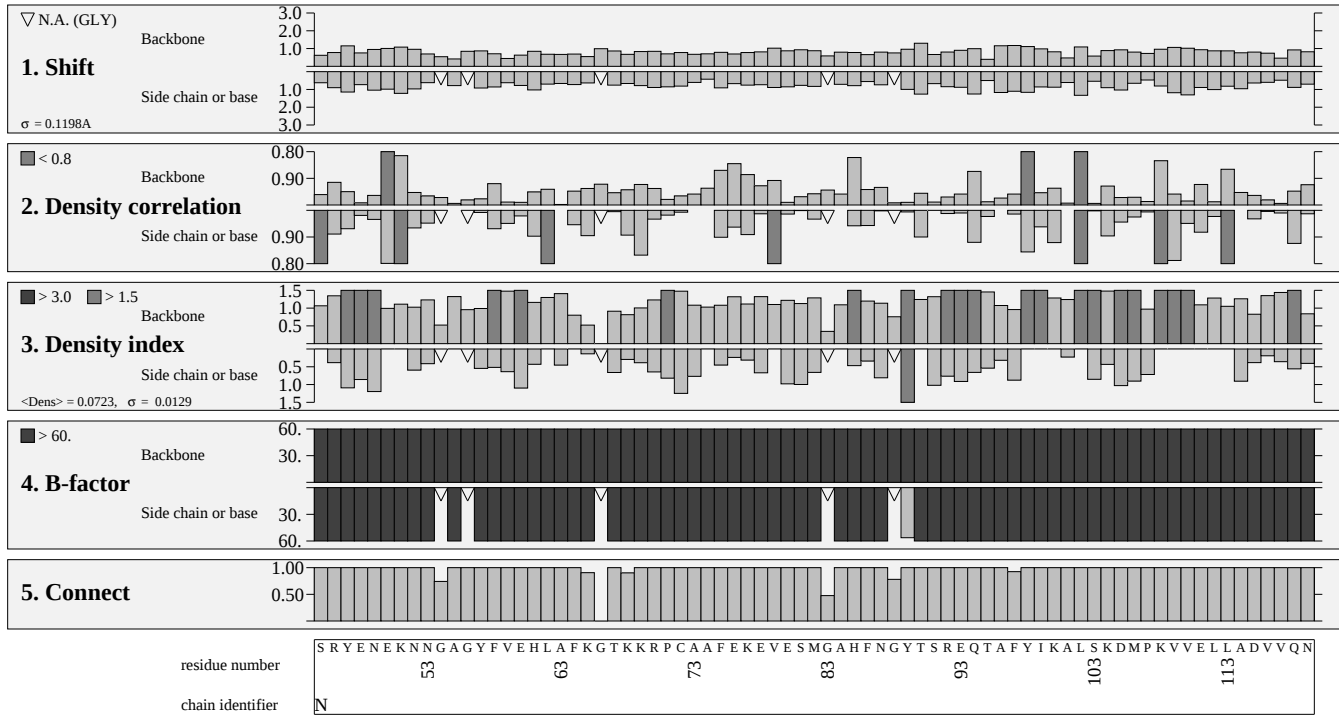
Local estimation (14)



Structure Factor Check

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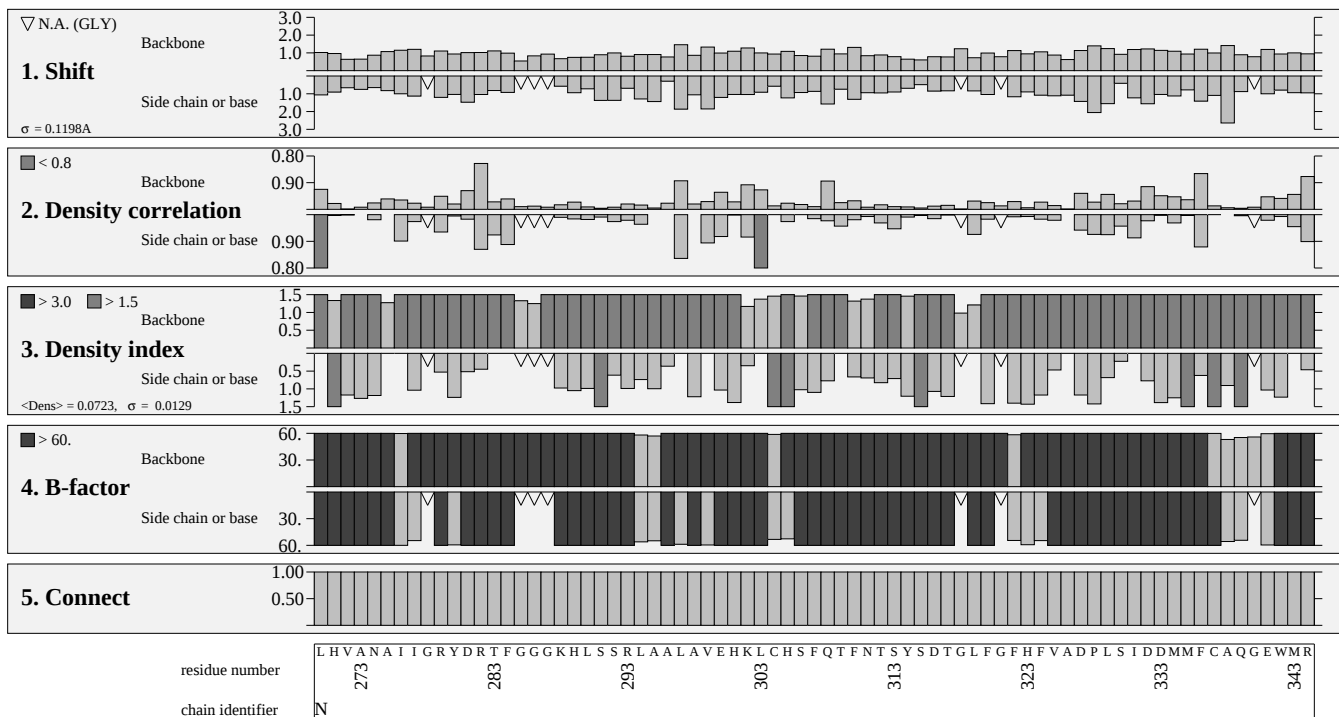
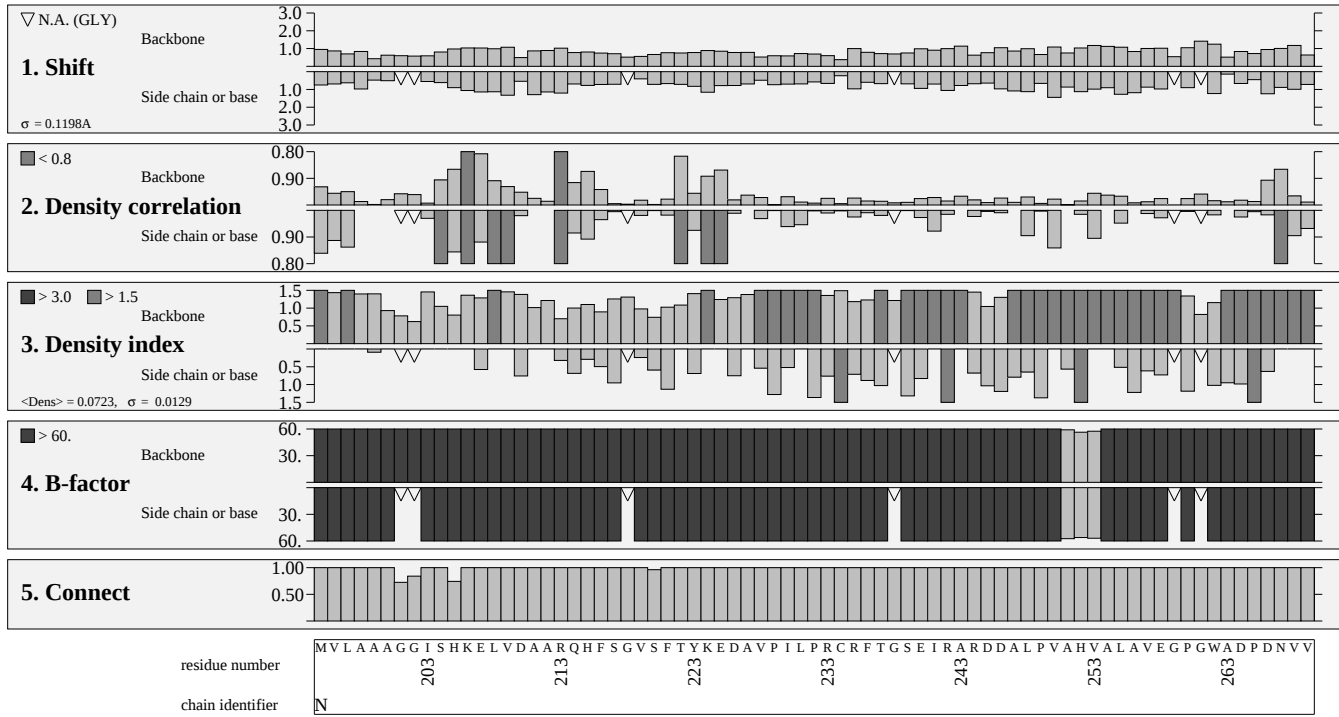
Local estimation (15)



Structure Factor Check

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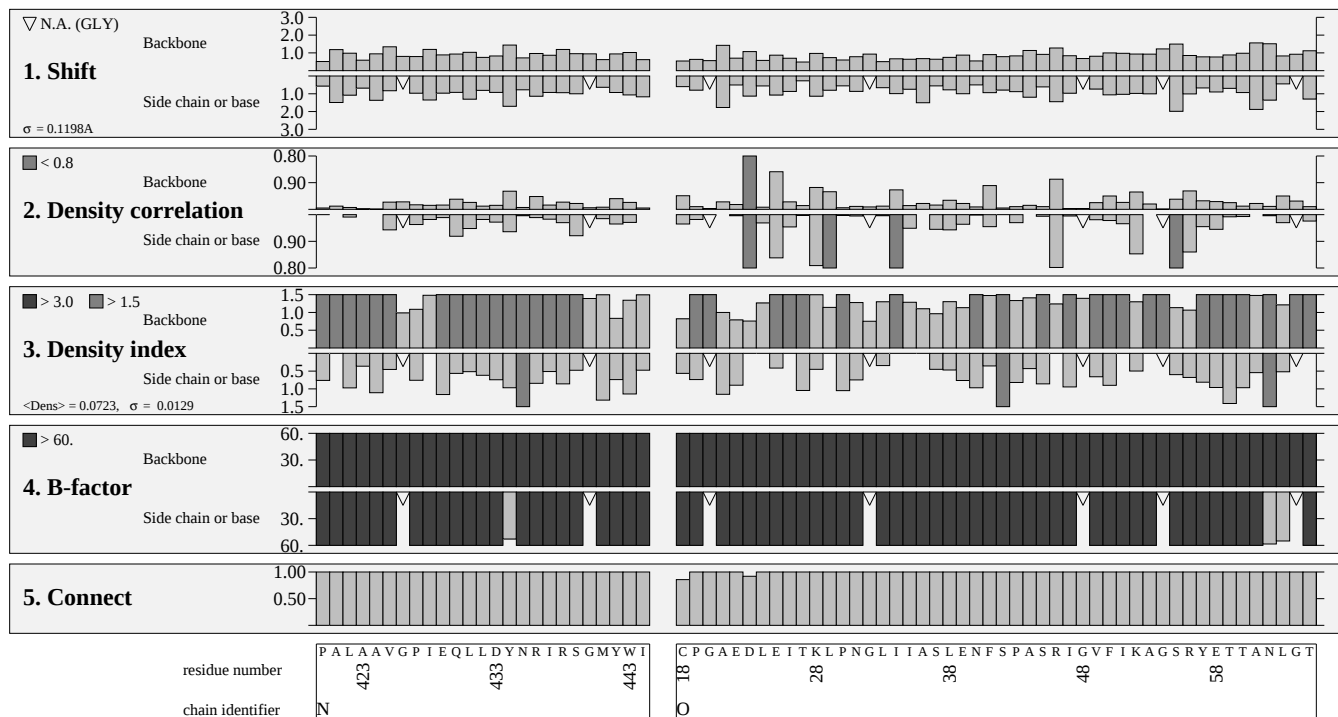
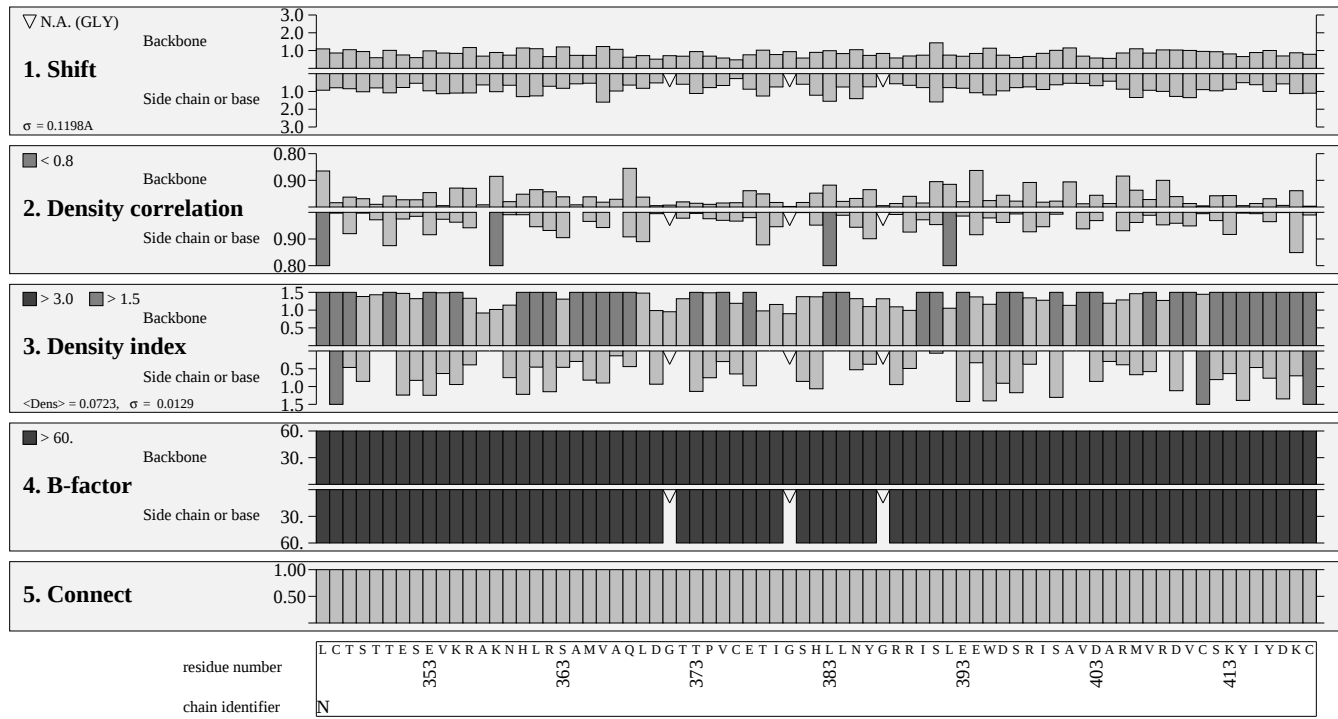
Local estimation (16)



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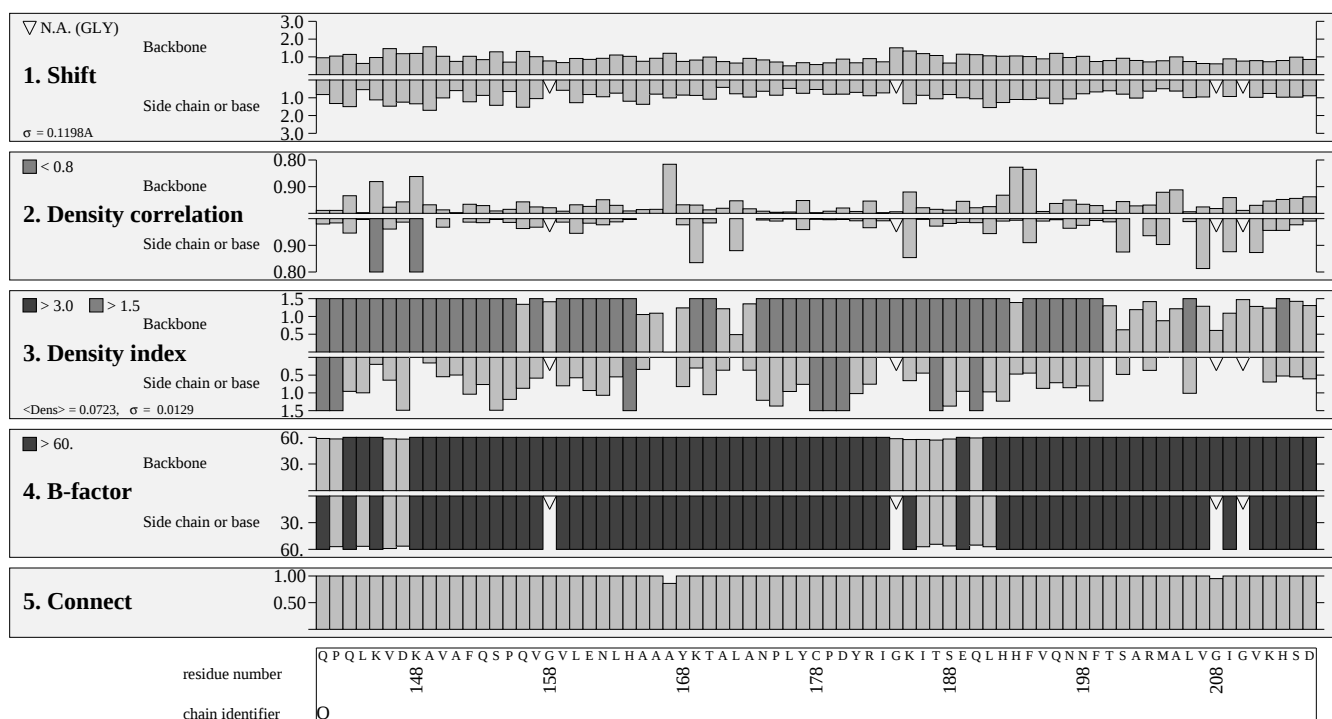
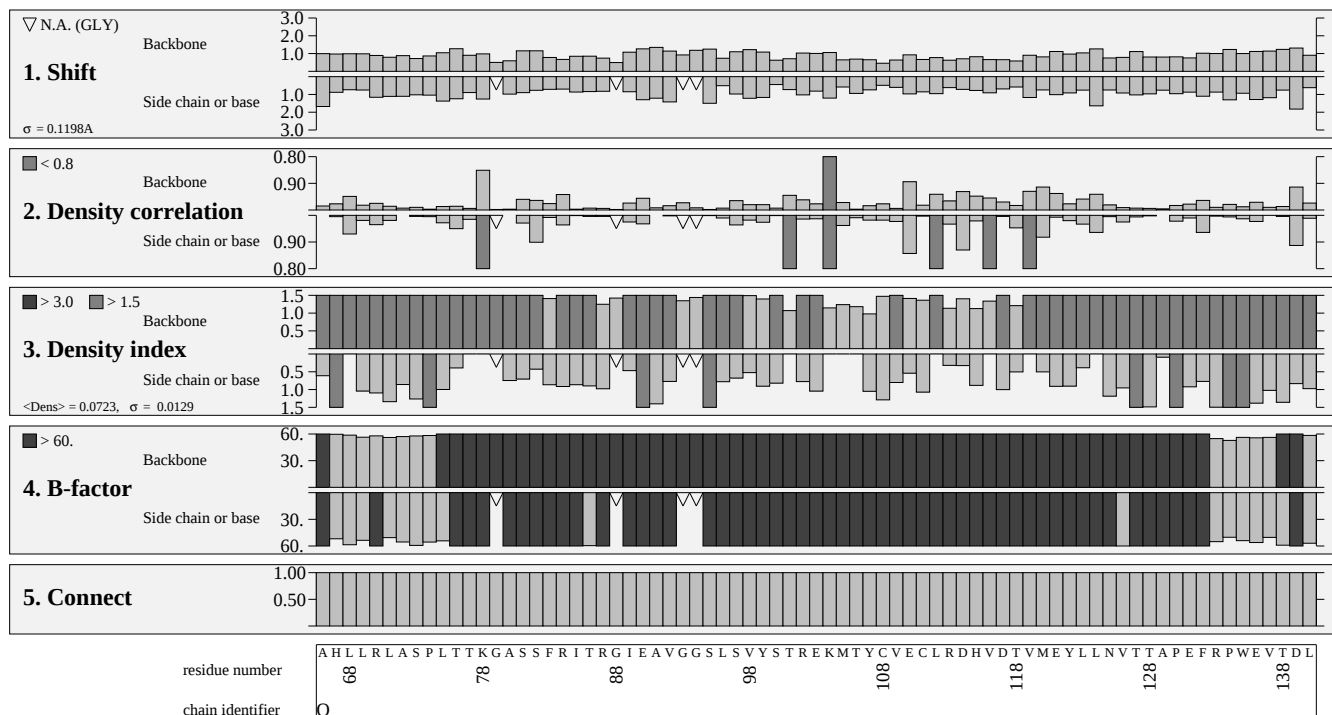
Local estimation (17)



Structure Factor Check

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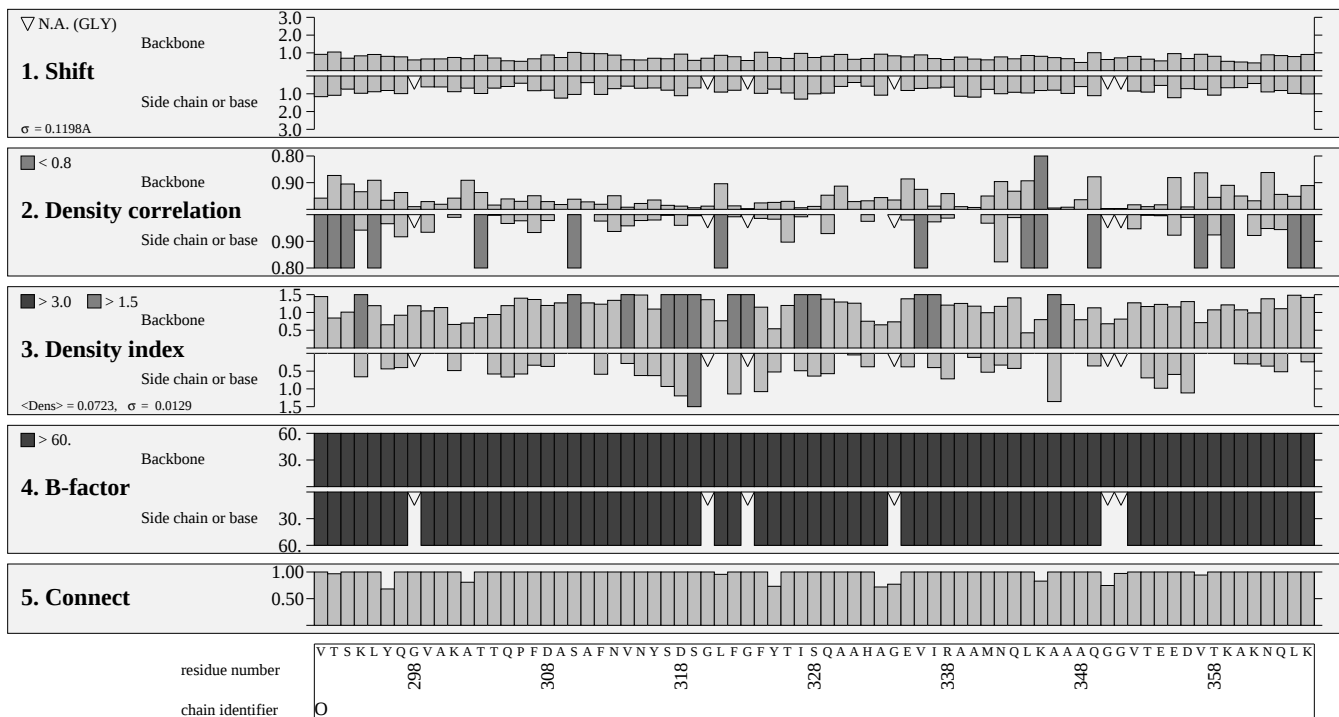
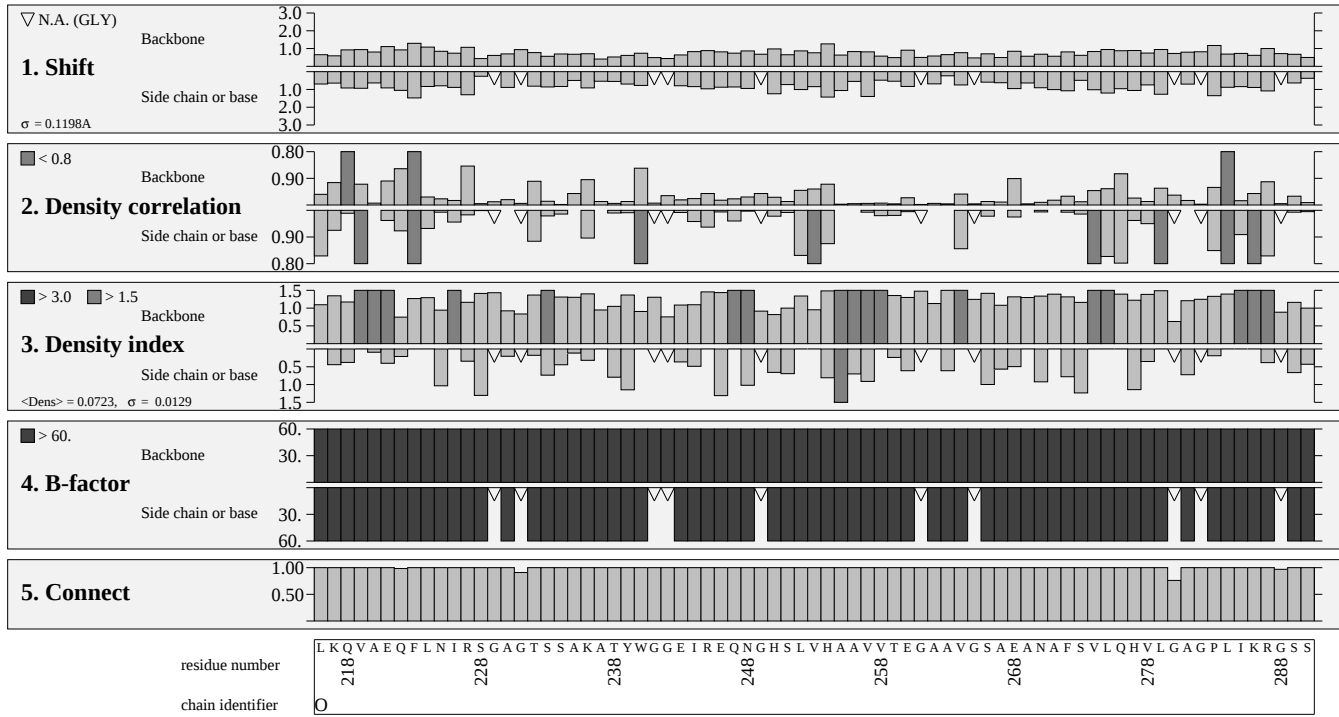
Local estimation (18)



Structure Factor Check

3H1J

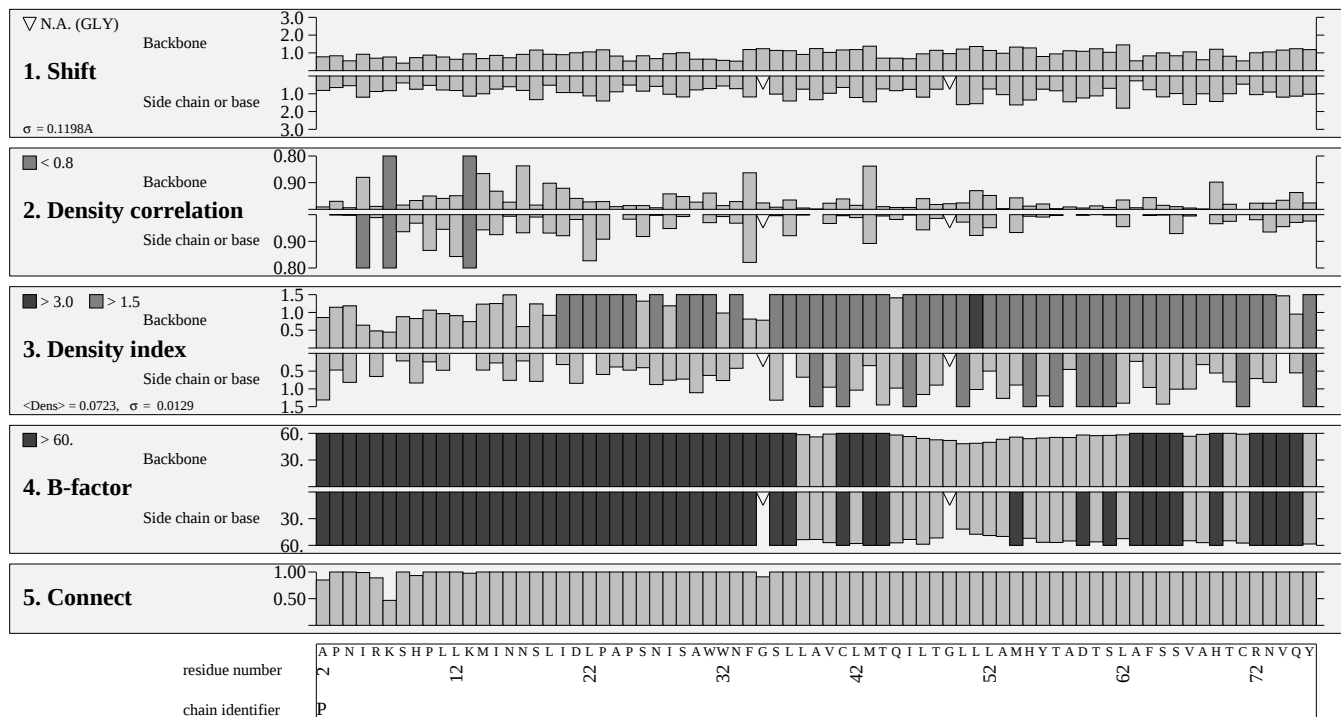
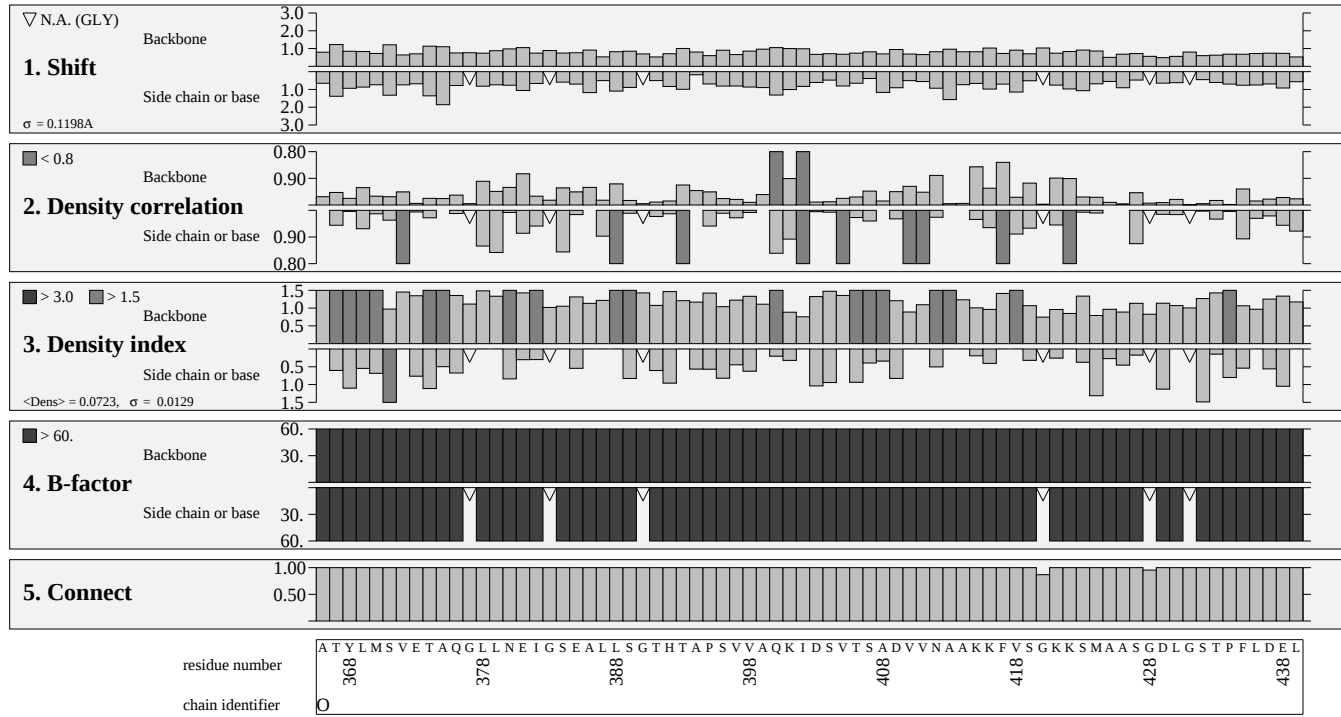
Local estimation (19)



Structure Factor Check

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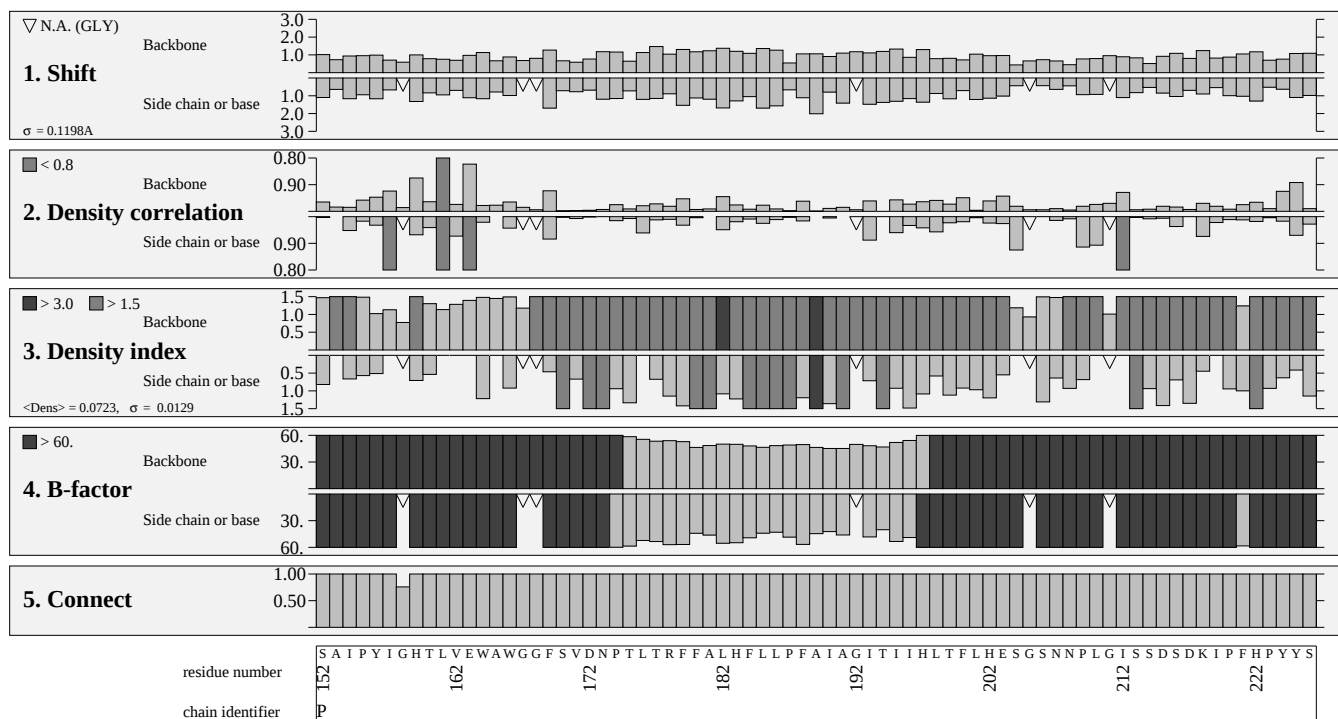
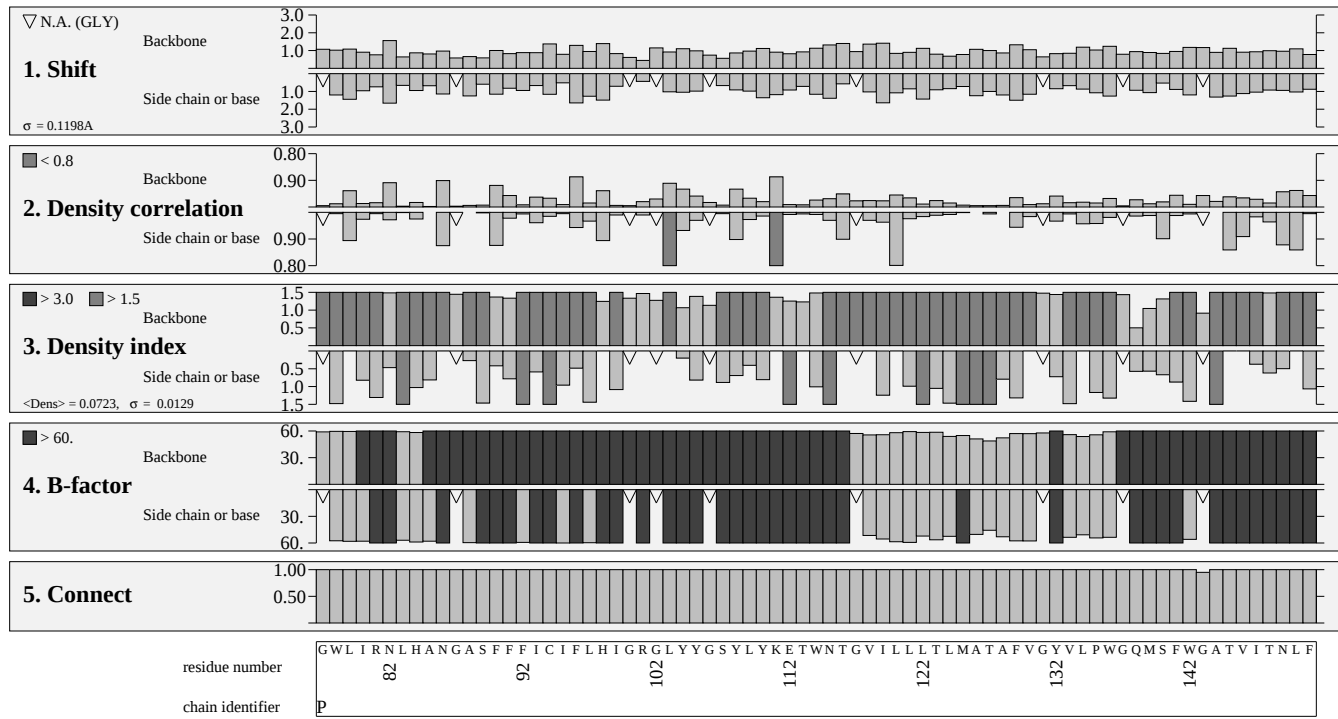
Local estimation (20)



Structure Factor Check

3H1J

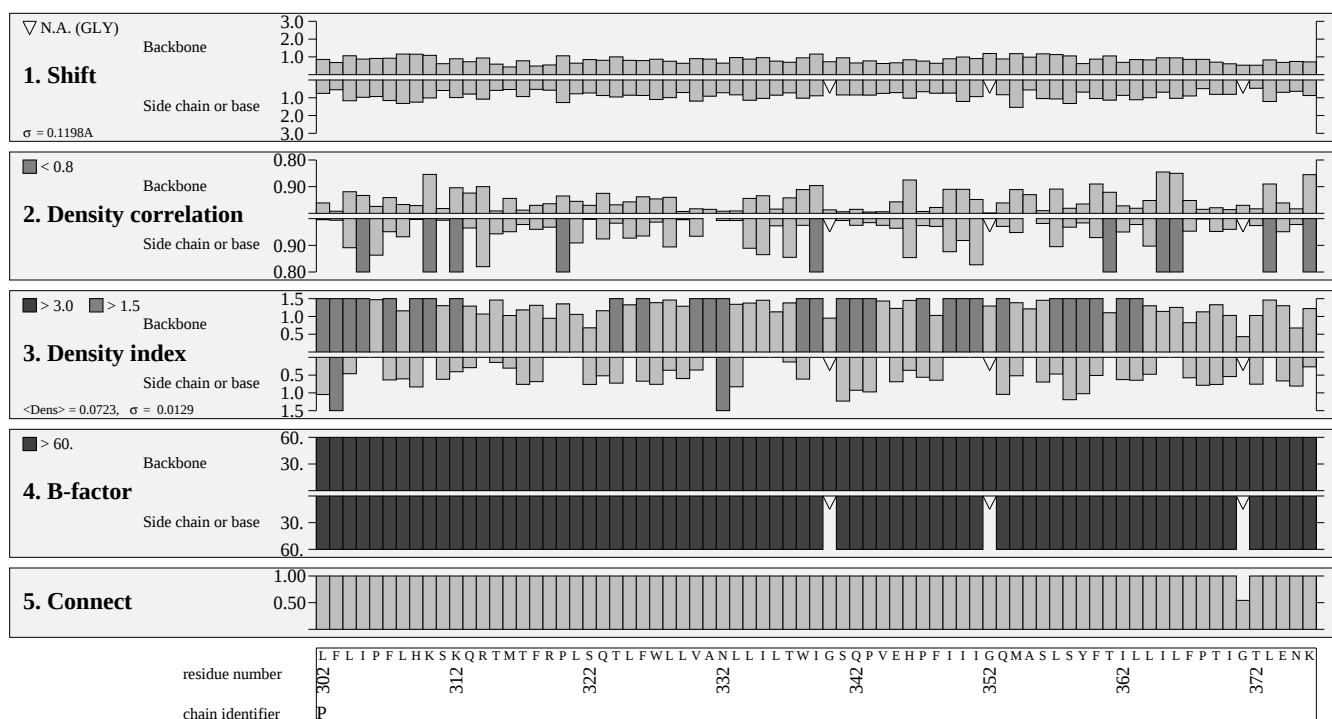
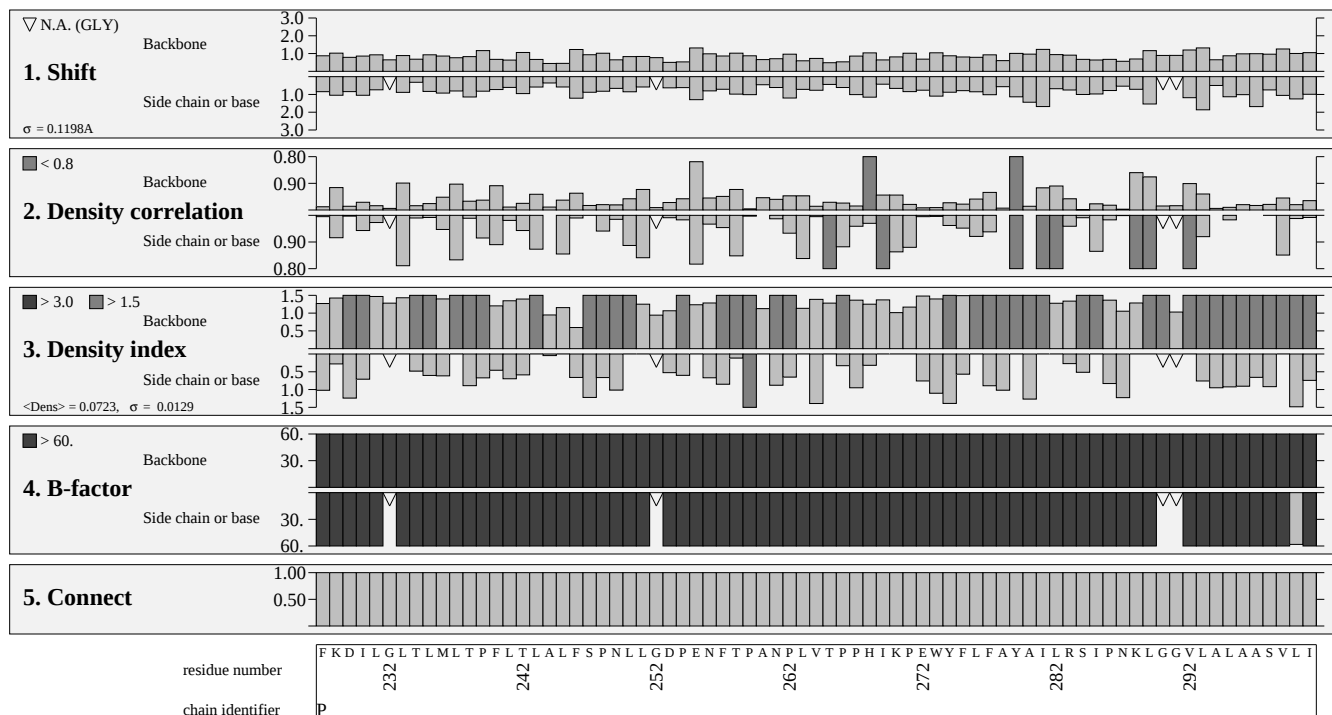
Local estimation (21)



Structure Factor Check

3H1J

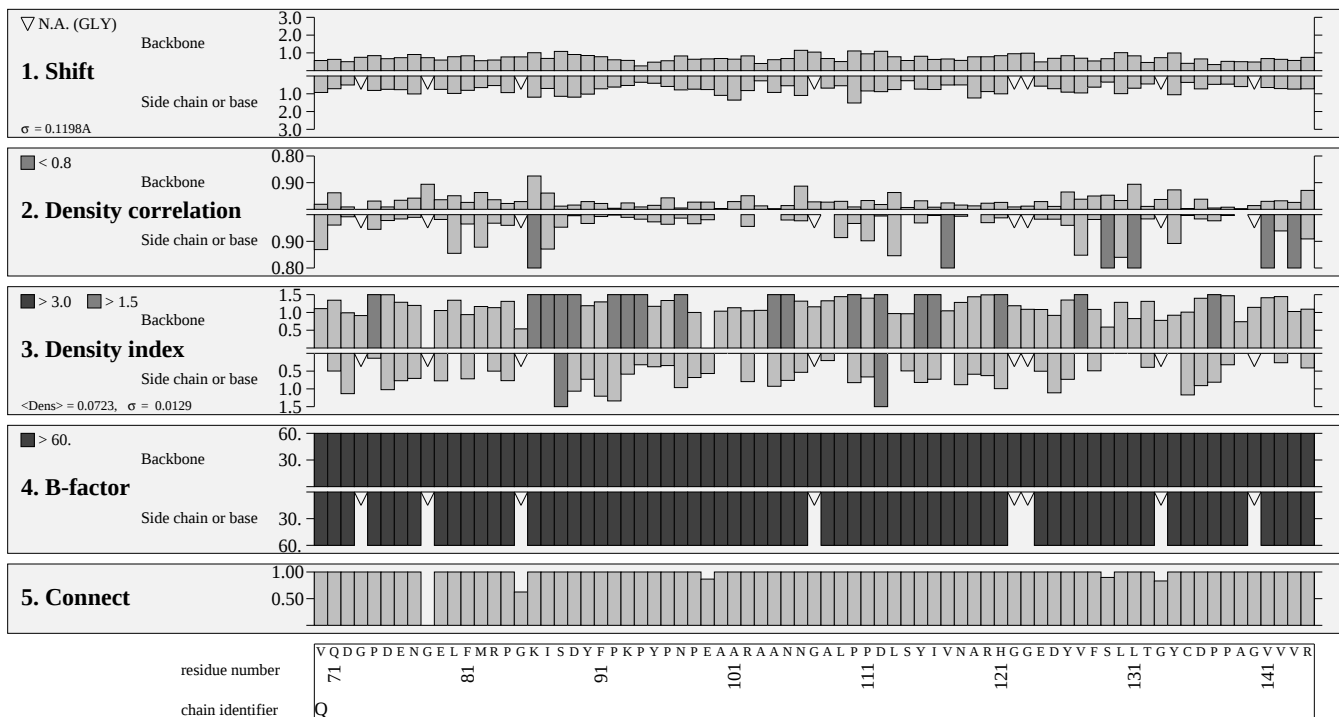
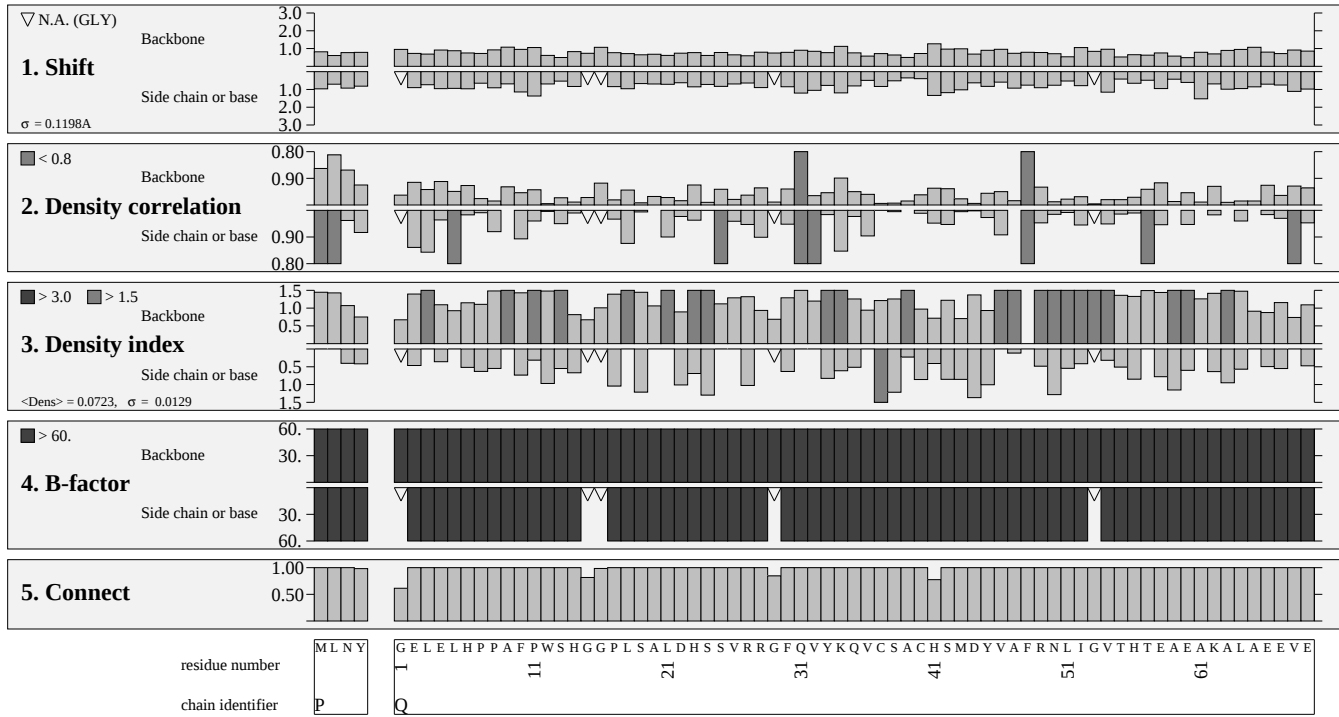
Local estimation (22)



Structure Factor Check

3H1J

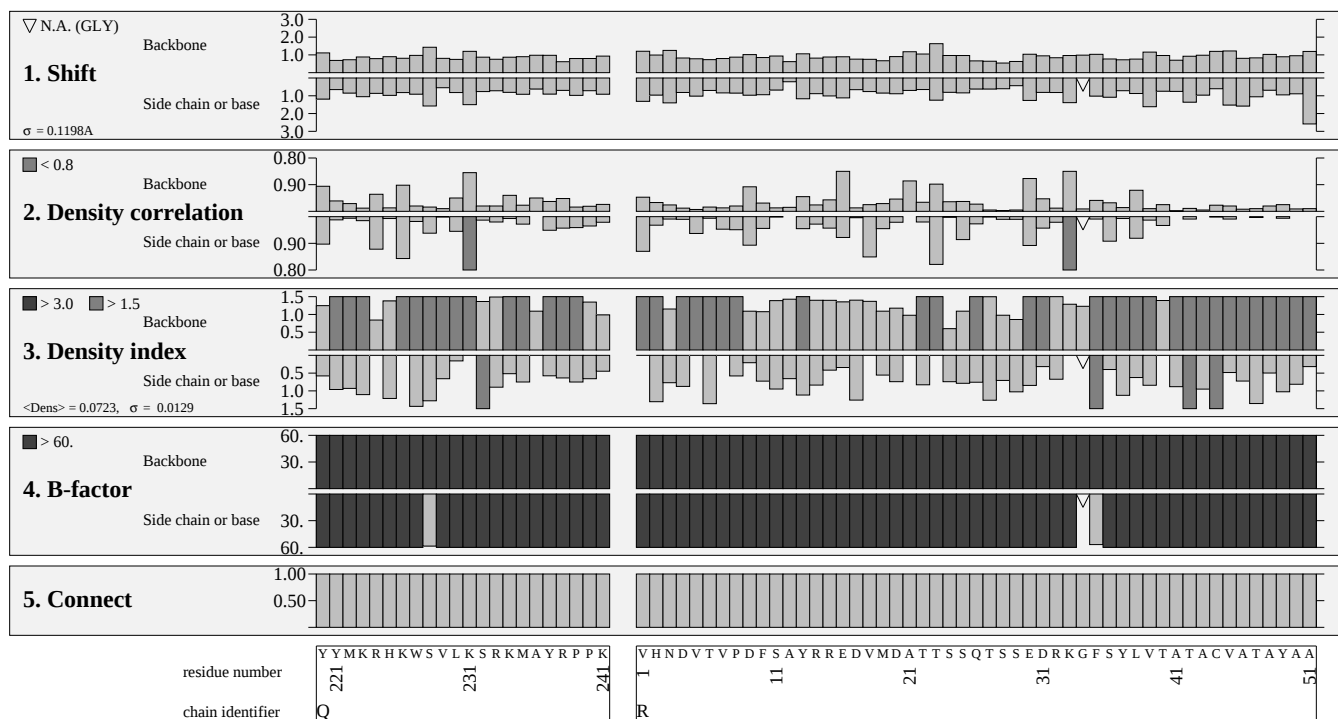
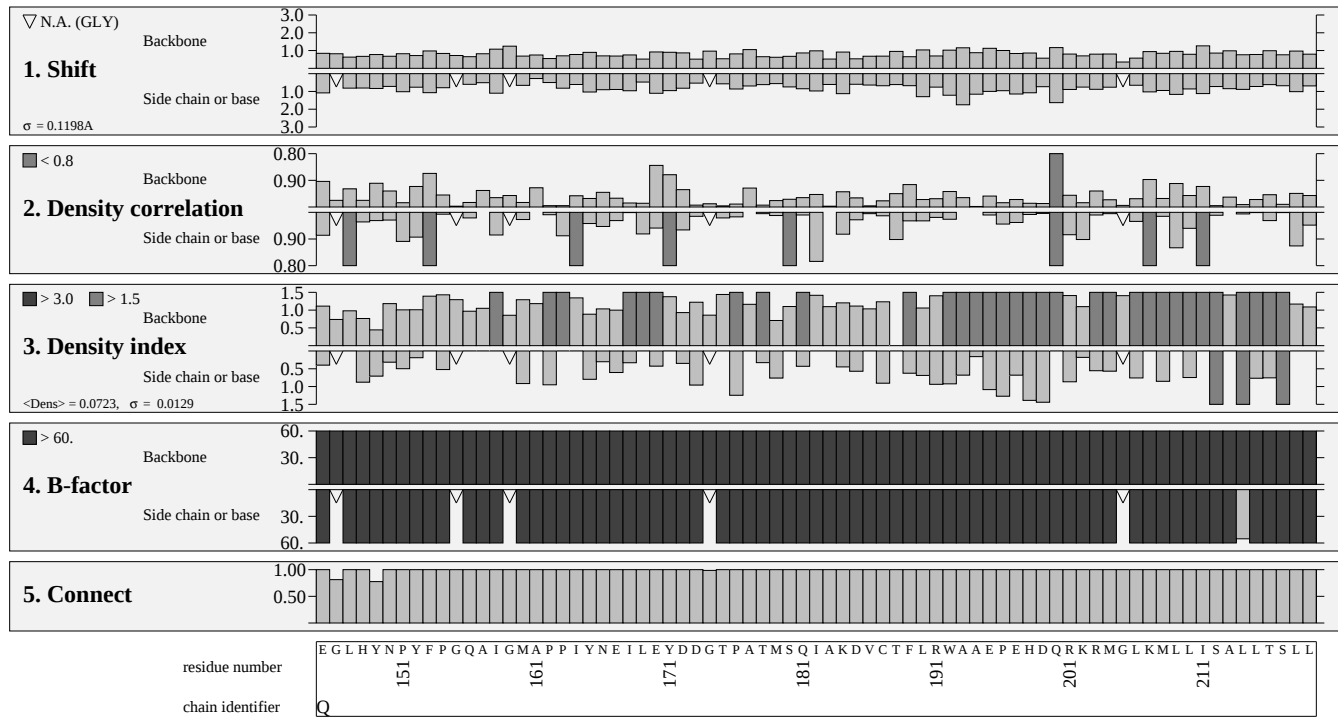
Local estimation (23)



Structure Factor Check

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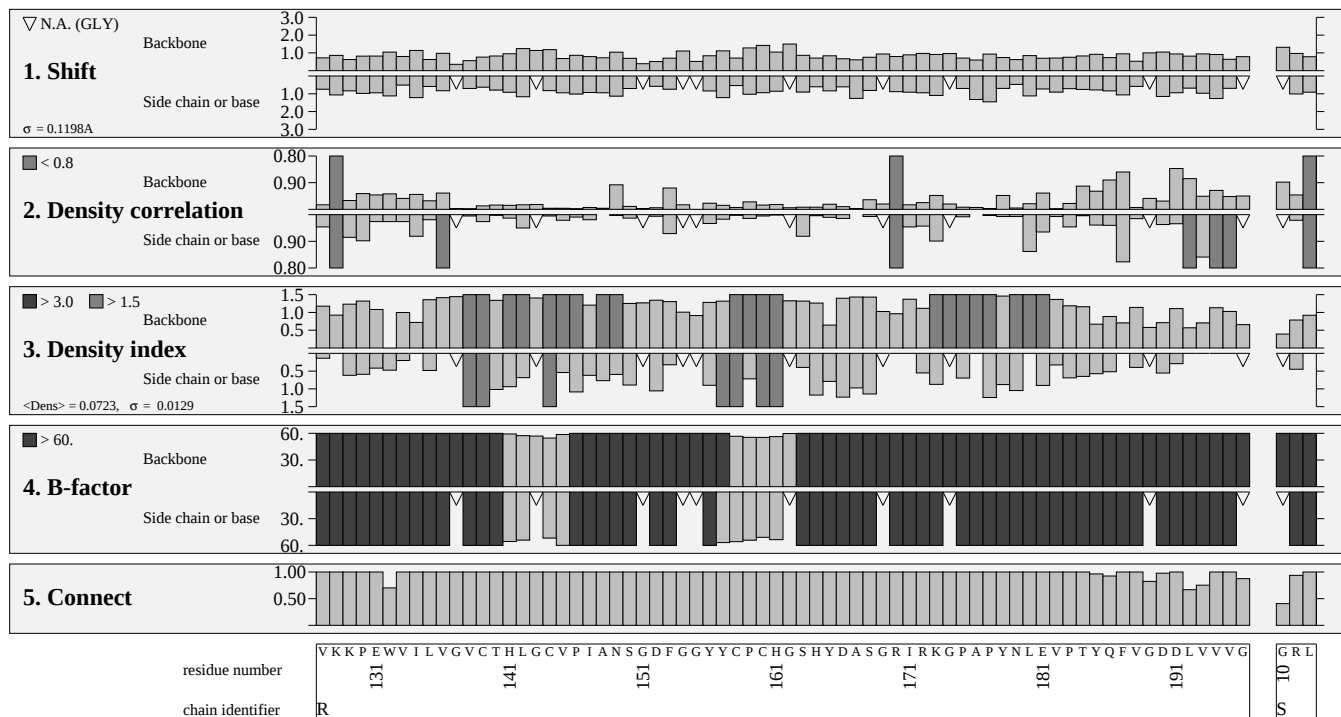
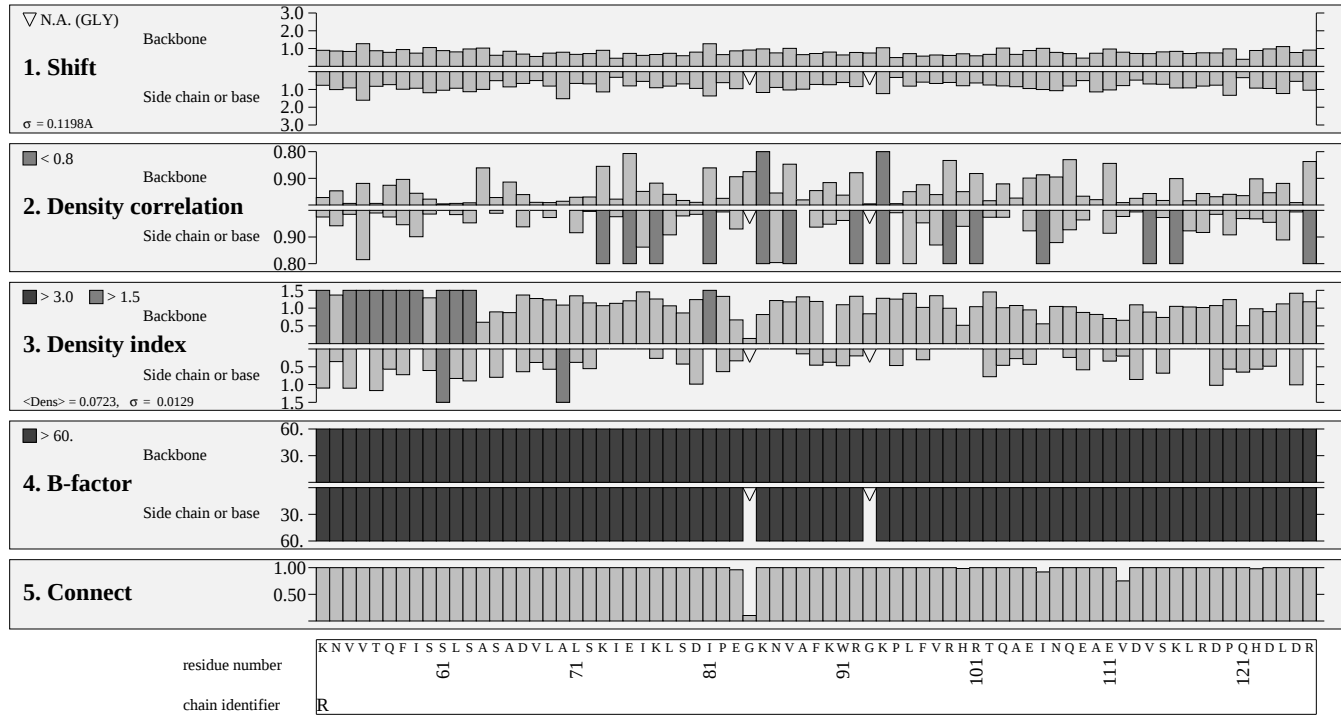
Local estimation (24)



Structure Factor Check

3H1J

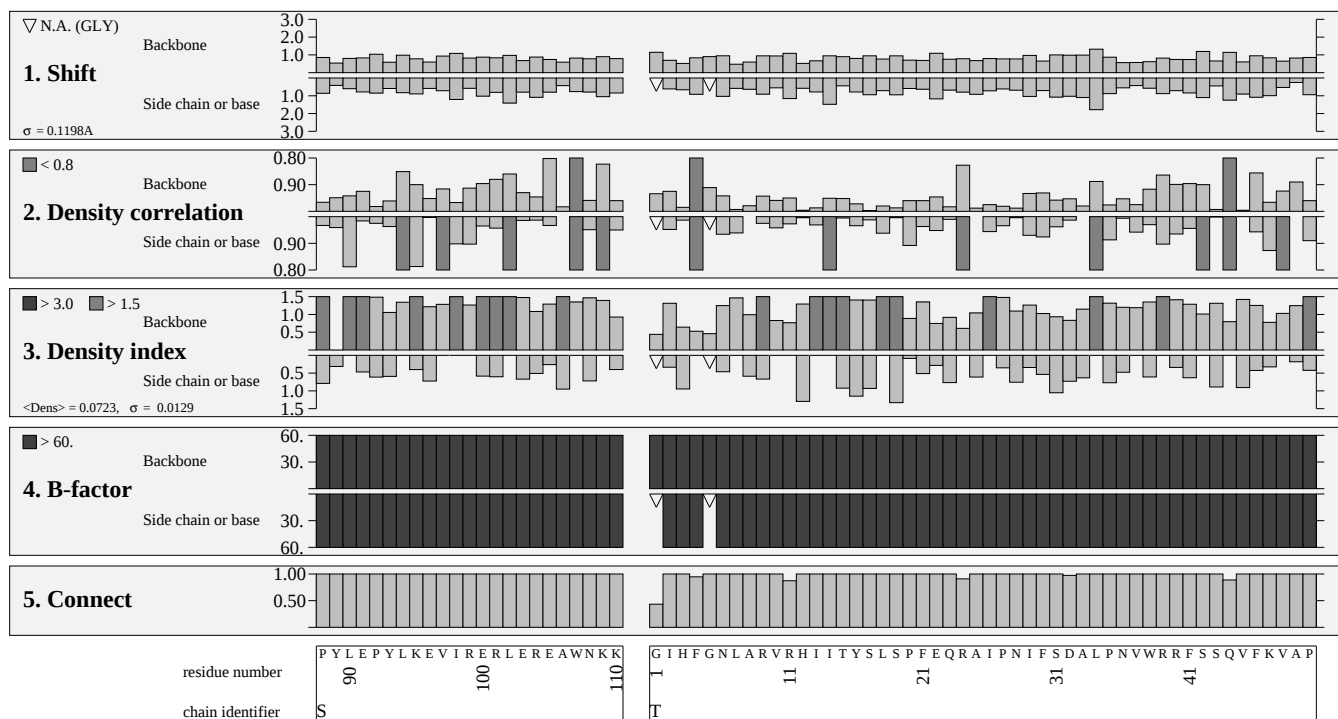
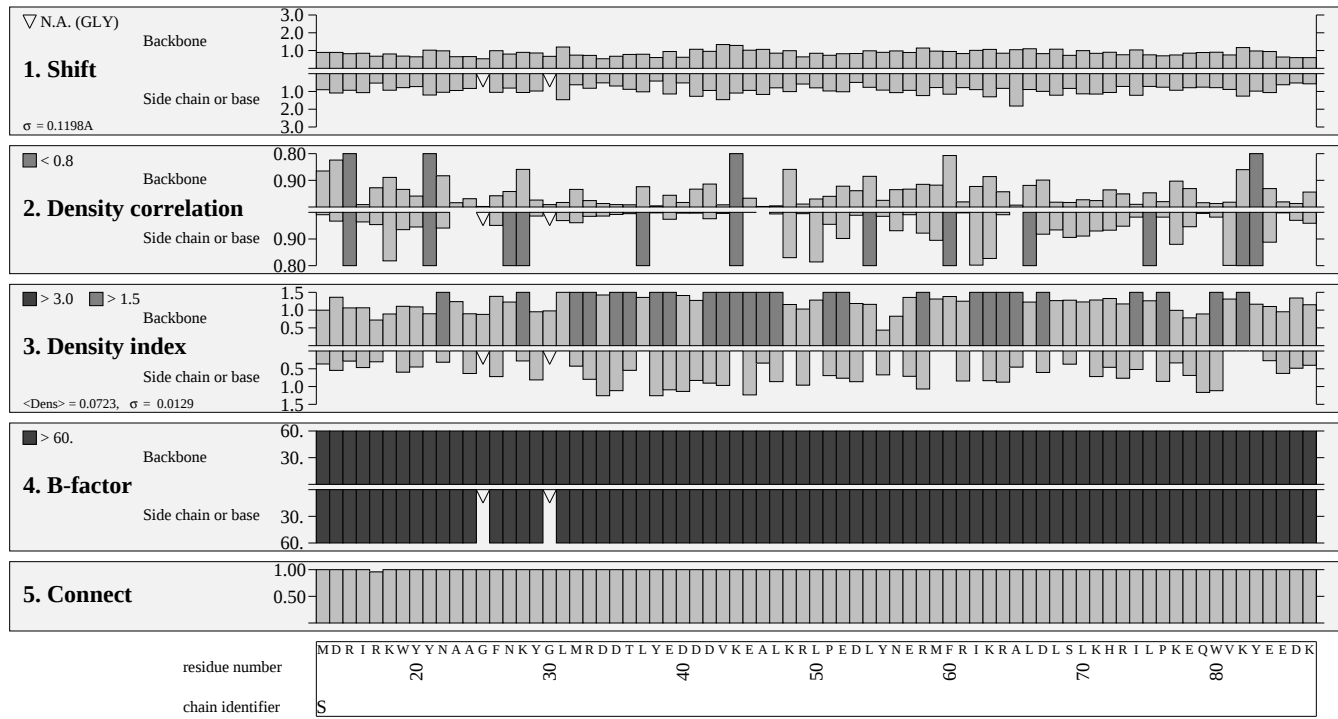
Local estimation (25)



Structure Factor Check

3H1J

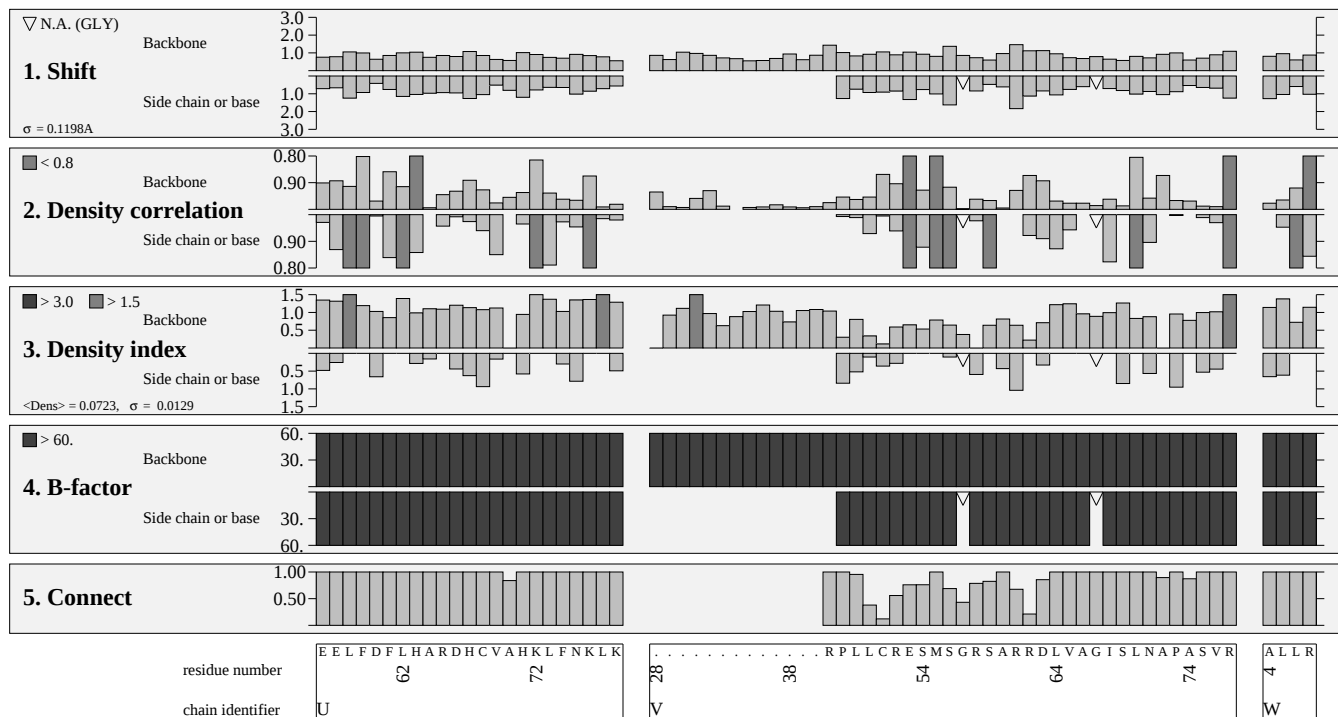
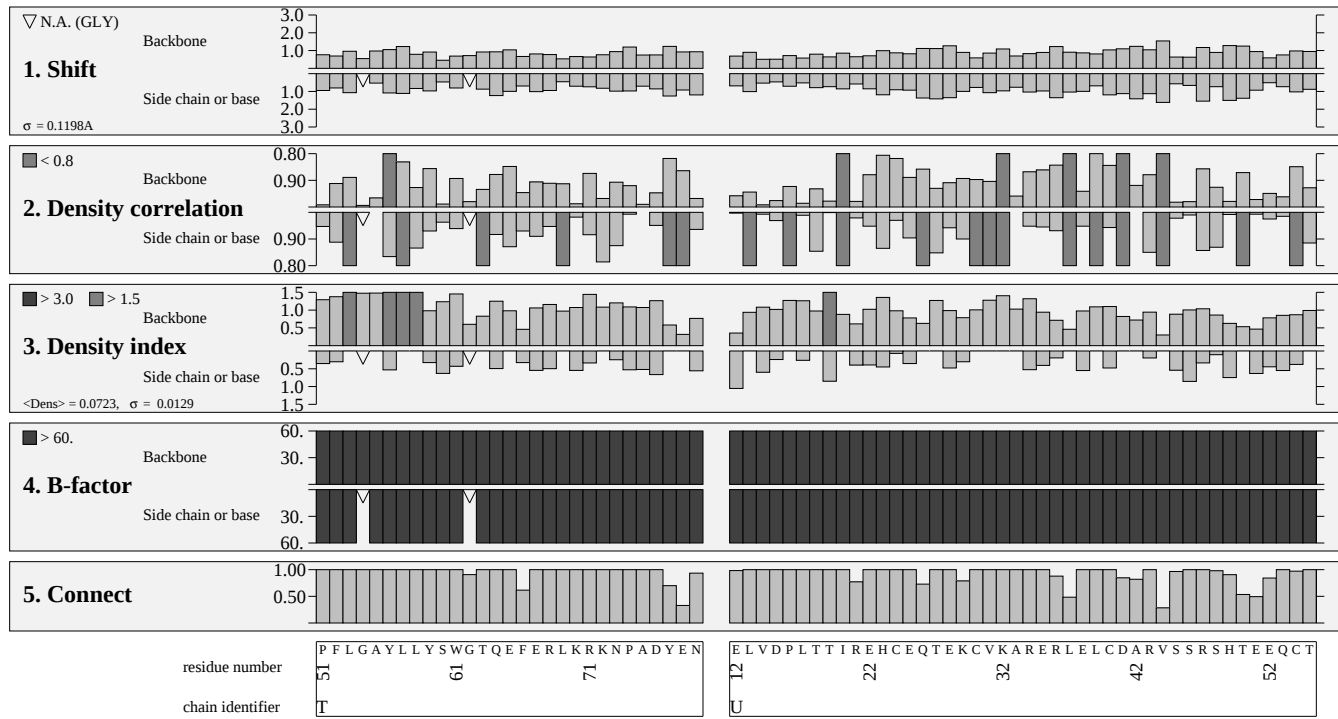
Local estimation (26)



Structure Factor Check

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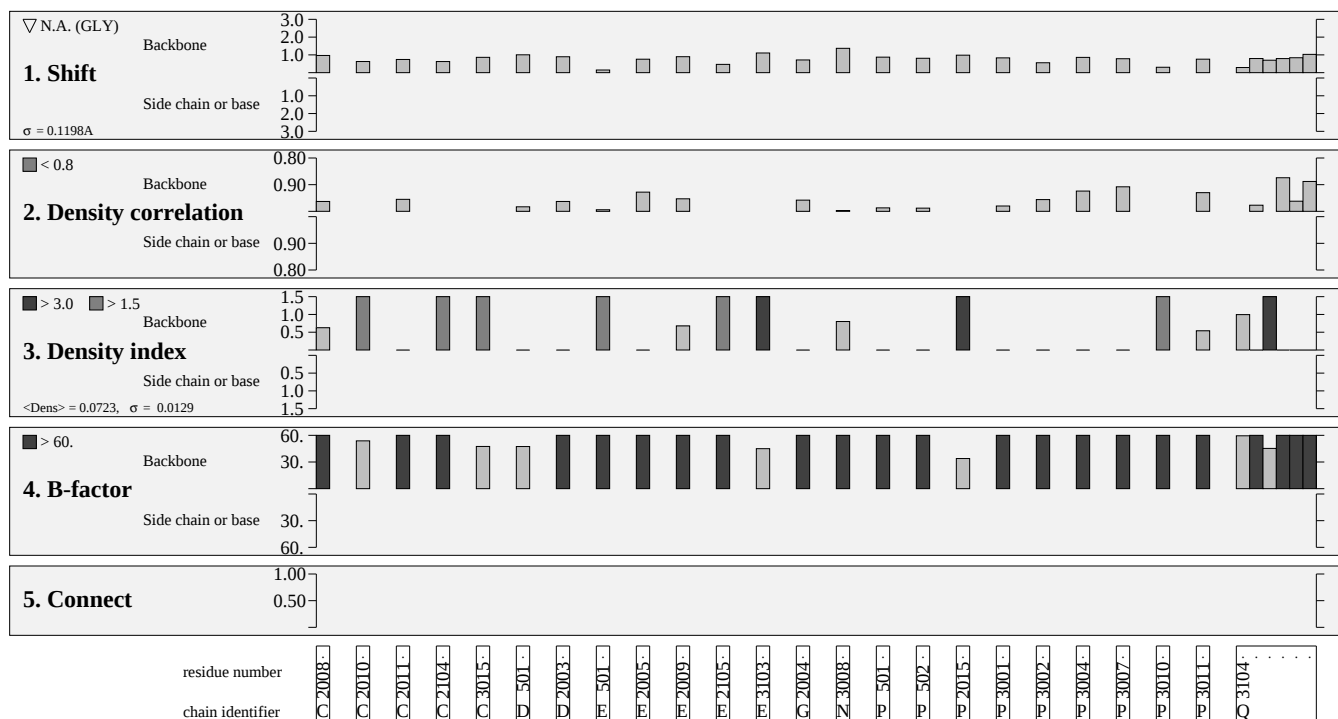
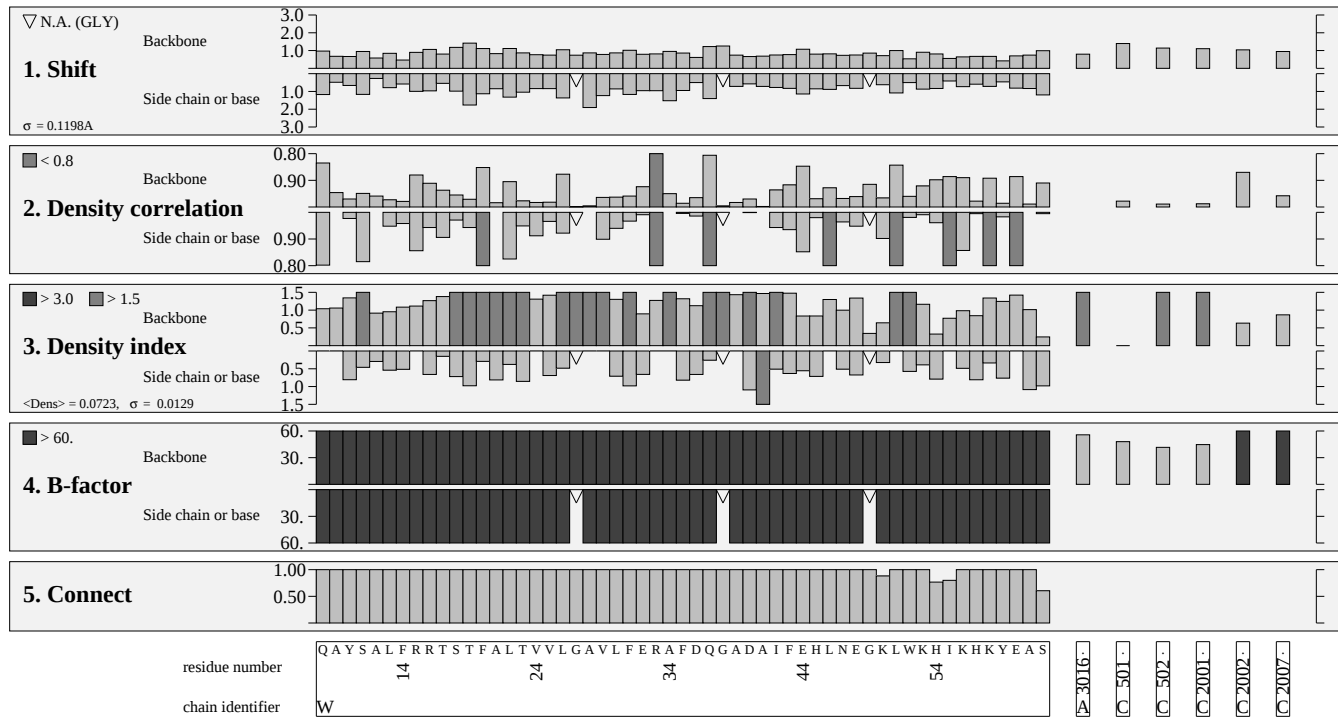
Local estimation (27)



Structure Factor Check

3H1J

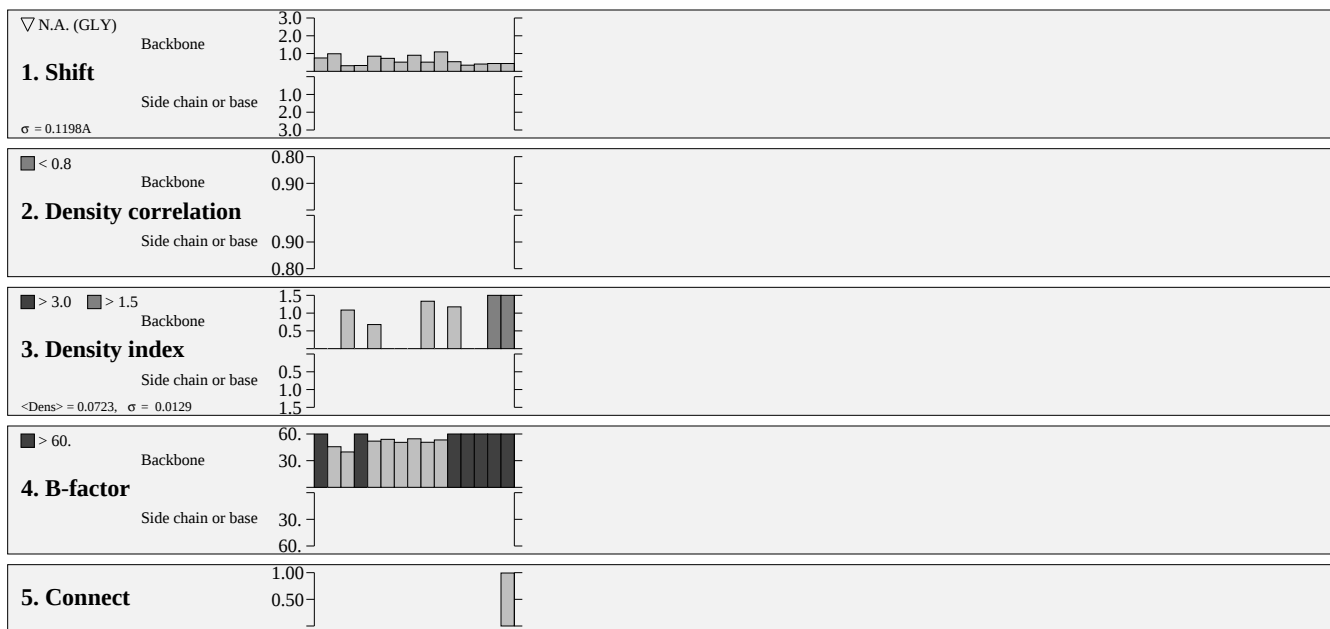
Local estimation (28)



Structure Factor Check

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Local estimation (29)



residue number

chain identifier

