

Structure Factor Check

3H1I

Title: STIGMATELLIN AND ANTIMYCIN BOUND CYTOCHROME BC1 COMPLEX FROM
 Date: 12-APR-09
 PDB code: 3H1I

Crystal

Cell parameters:

a: 174.69 Å b: 181.67 Å c: 240.73 Å
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Model

32701 atoms

Number of chains: 51

Volume not occupied by model: 62.7 %

 (for atomic model): 78.7 Å²

σ (B): 21.96 Å²

Matthews coefficient: 4.17

Corresponding solvent % : 70.29

Refinement

Program: CNS 1.1

Nominal resolution range: 20.0 – 3.53 Å

Reported R-factor: 0.263

Number of reflections used: 85111

Reported Rfree: 0.31

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 49.5 – 3.53 Å

Reflections in file: 85472

Unique reflections above 0: 85472

above 1 σ : 82734

above 3 σ : 38800

SF CHECK

Nominal resolution range: 49.5 – 3.53 Å

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

Used reflections: 85472

Completeness: 90.5 %

R_{stand}(F) = $\langle \sigma(F) \rangle / \langle F \rangle$: 0.149

Anisotropic distribution of Structure Factors

ratio of eigen values: 1.0000 0.5035 0.5470

B_{overall} (by Patterson): 60.Å²

Optical resolution: 2.50 Å

Expected opt. resol. for complete data set: 2.50 Å

Estimated minimal error: 0.224 Å

Model vs. Structure Factors

R-factor for all reflections: 0.321

Correlation factor: 0.777

R-factor: 0.319

for $F > 2.0 \sigma$

nom. resolution range: 19.99 – 3.53 Å

reflections used: 82388

Rfree: 0.351

Nfree: 2477

R-factor without free-refl.: 0.318

Non free-reflections: 79911

<u> (error in coords by Luzzati plot): 0.715 Å

Estimated maximal error: 0.470 Å

DPI: 0.691 Å

Scaling

Scale: 0.883

Bdiff: -7.32

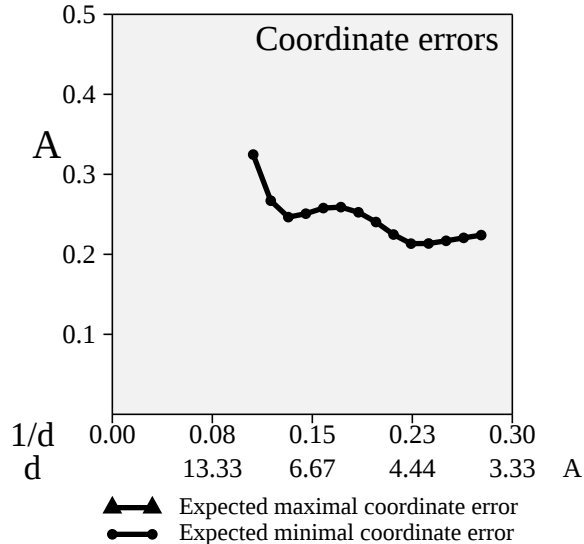
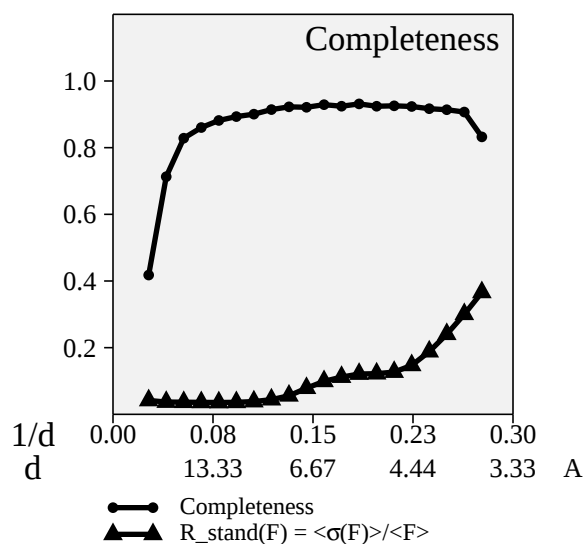
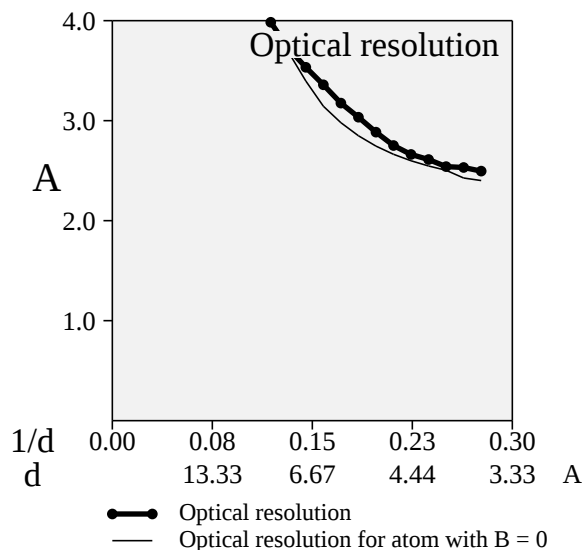
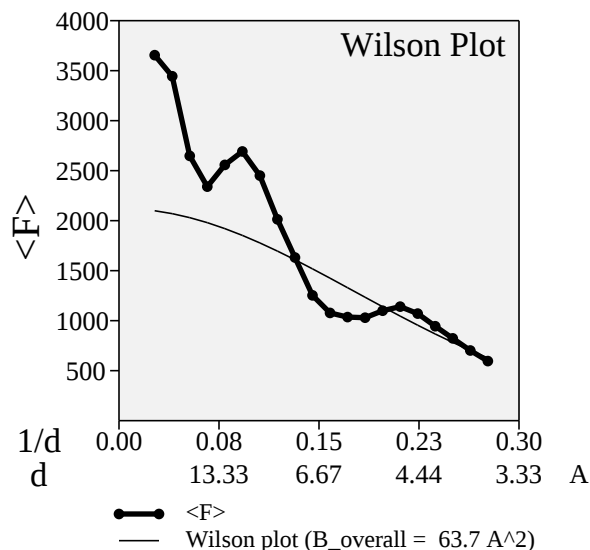
Anisothermal Scaling (Beta):

13.0670 0.6489 2.3767 0.0000 0.0000 0.0000

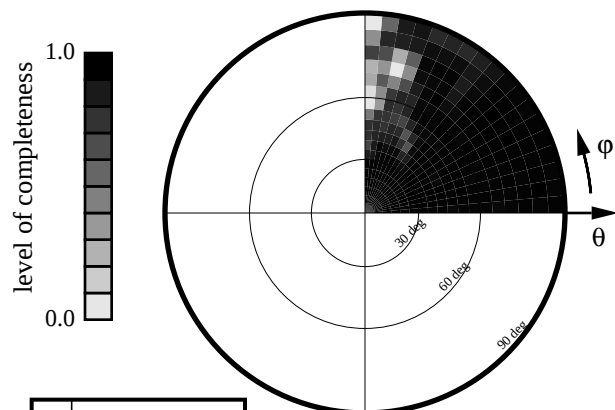
Solvent correction – Ks,Bs: 0.655 250.453

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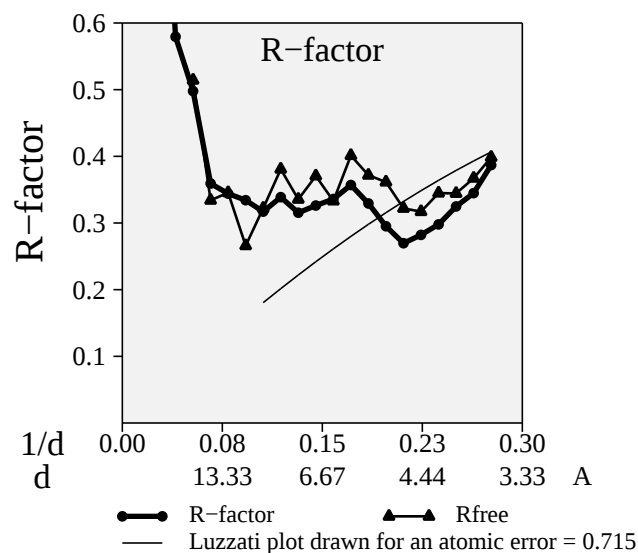


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

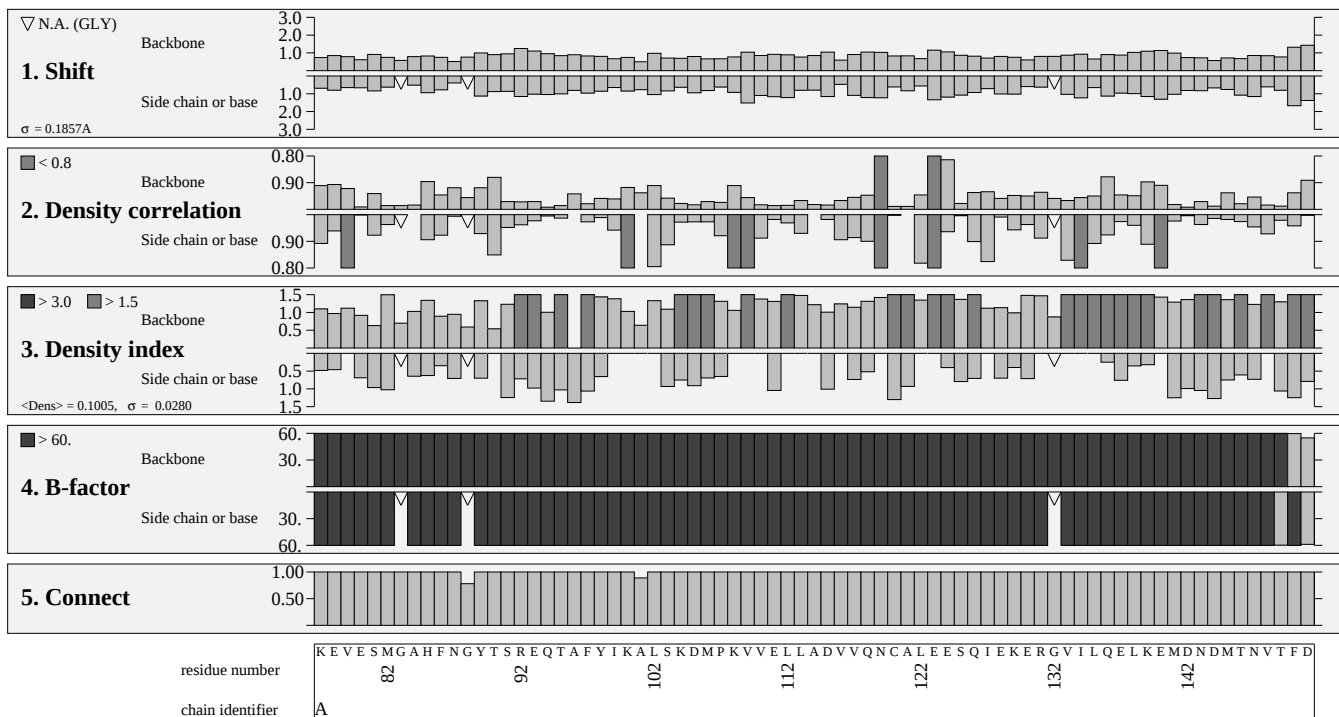
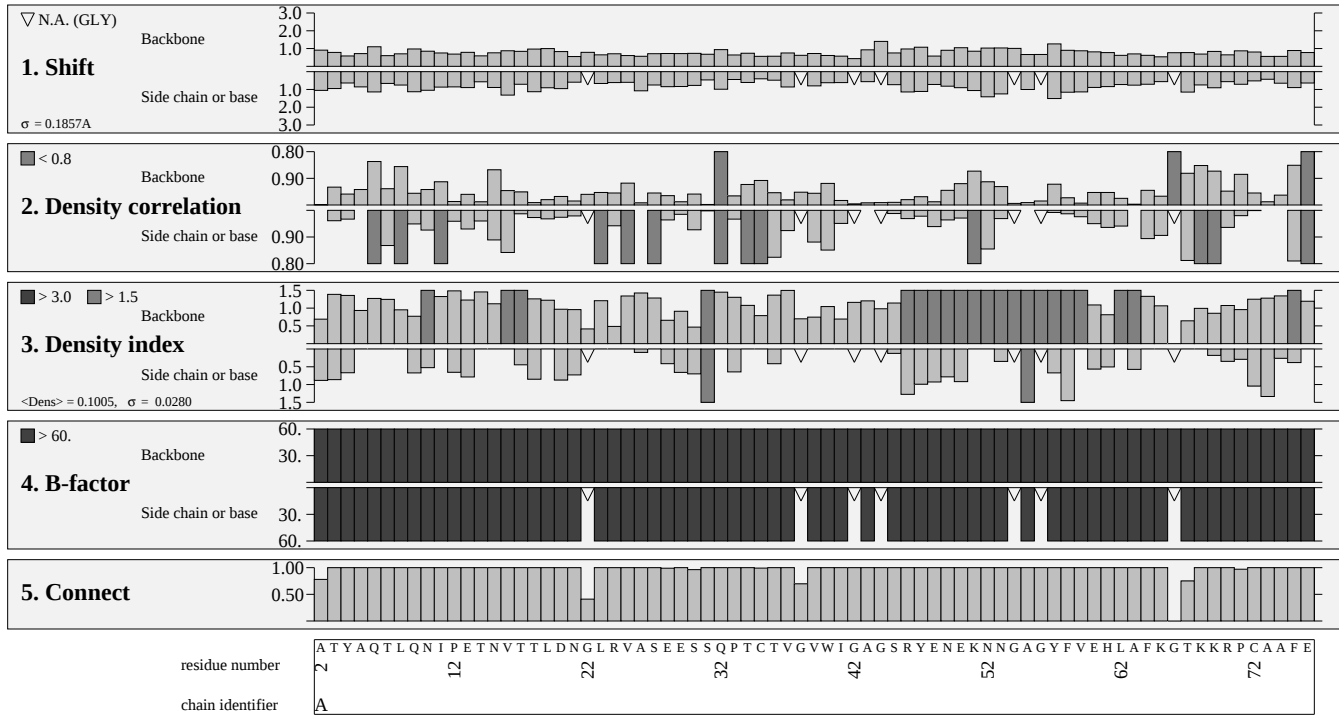
polar coordinates of the crystallographical axes



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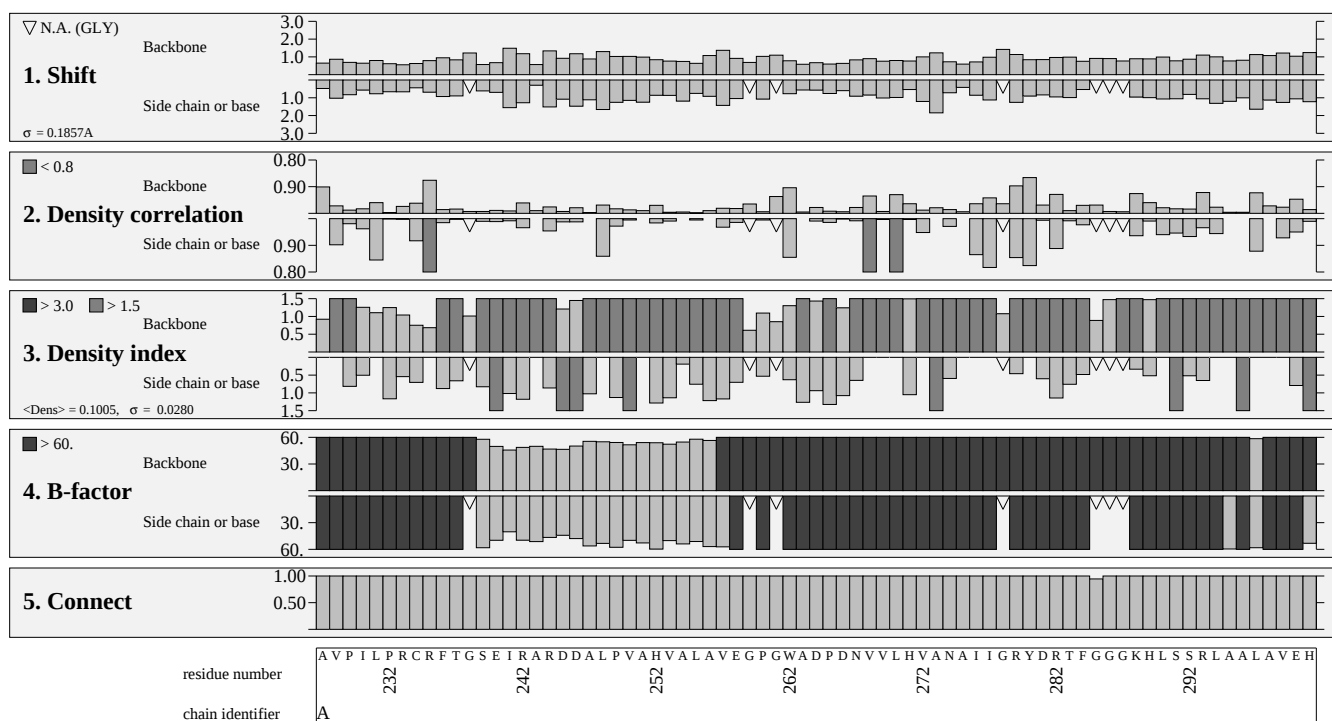
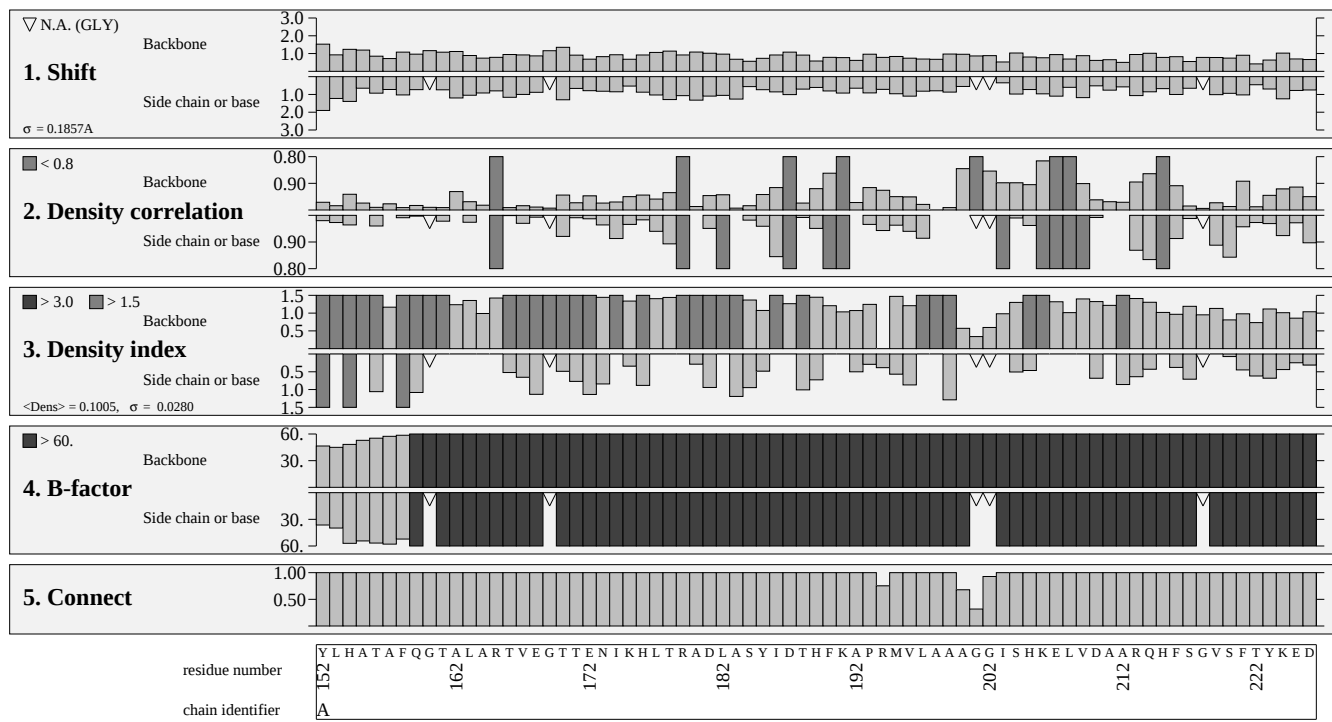
Local estimation



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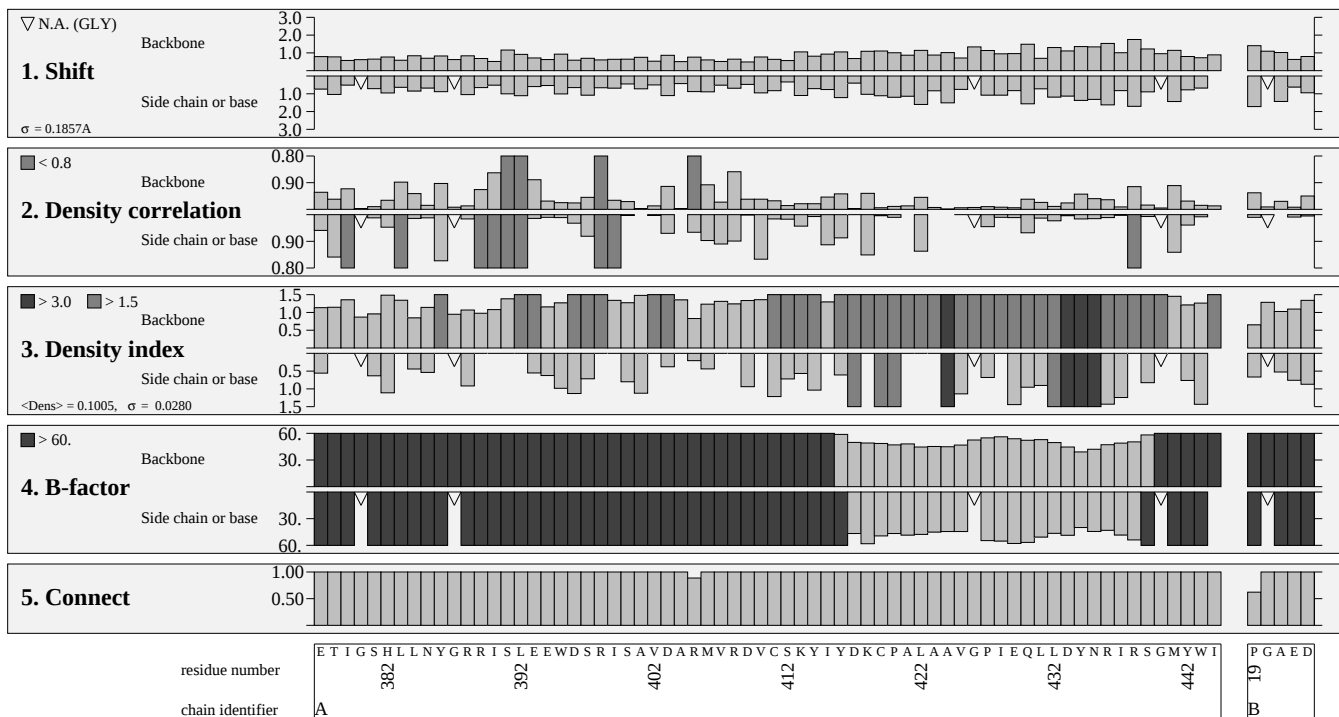
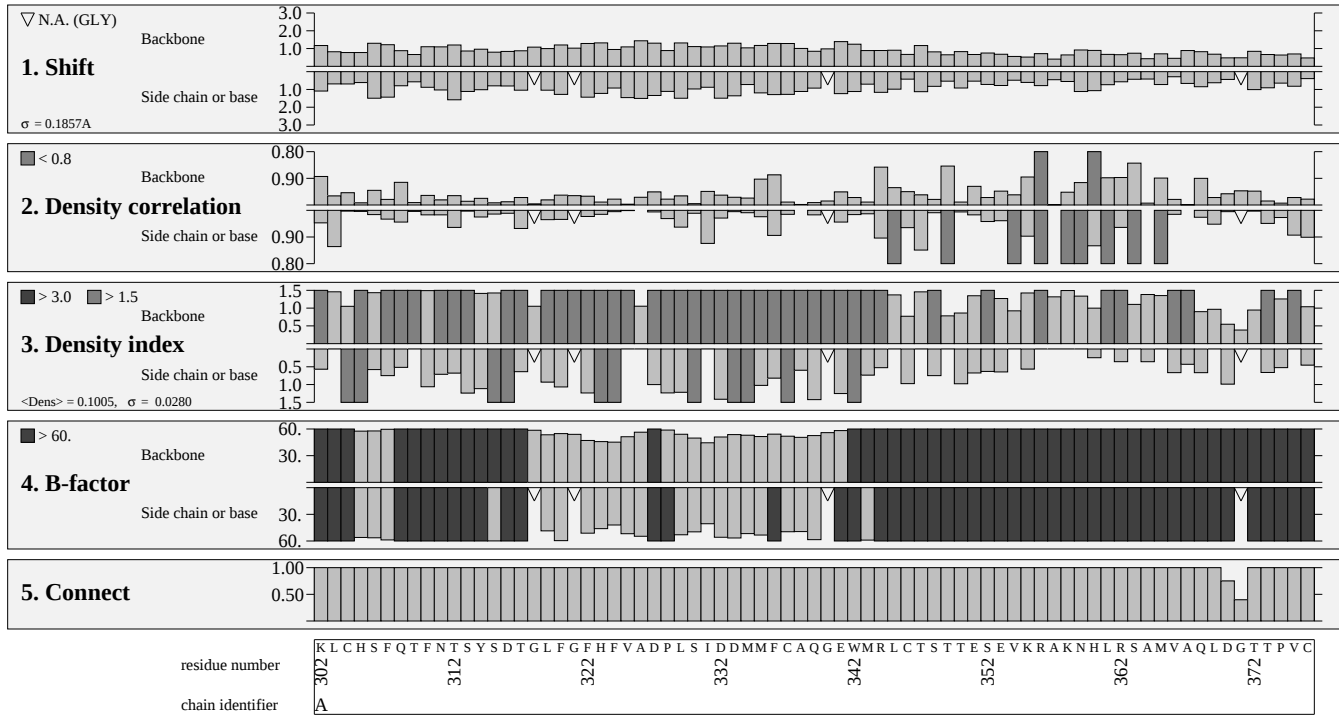
Local estimation (2)



Structure Factor Check

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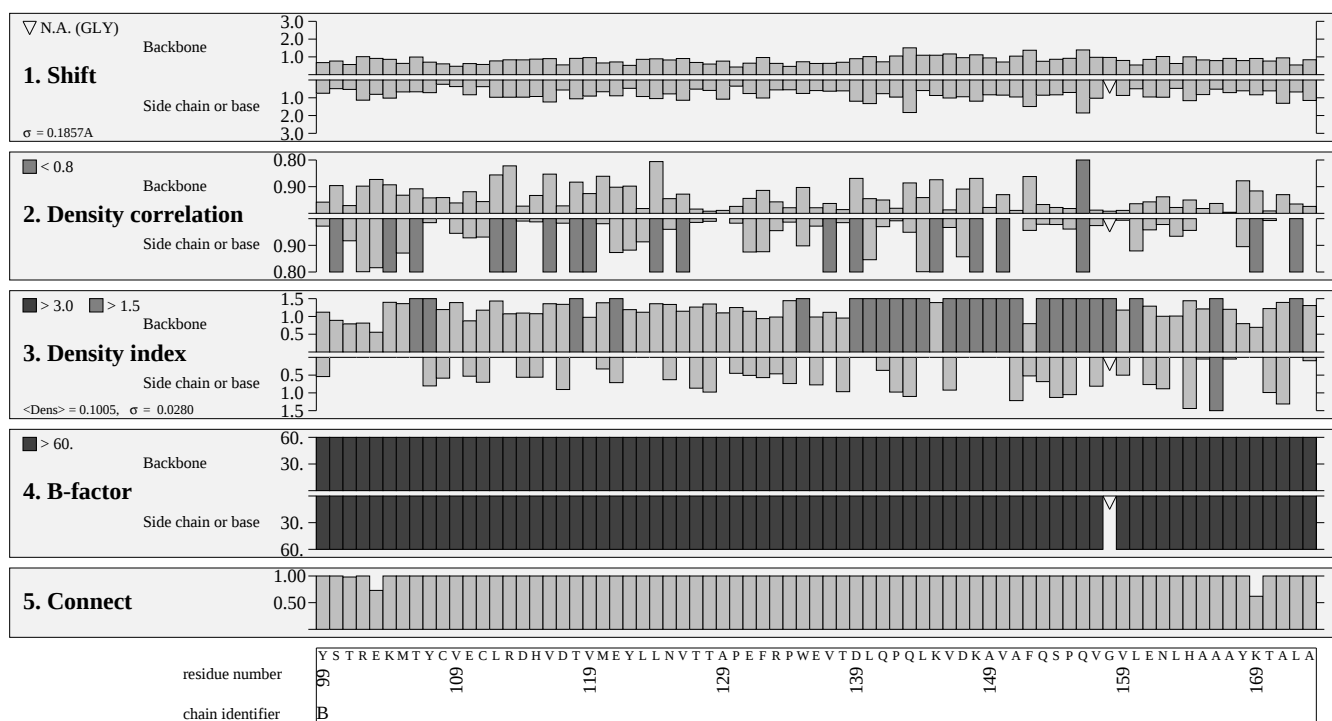
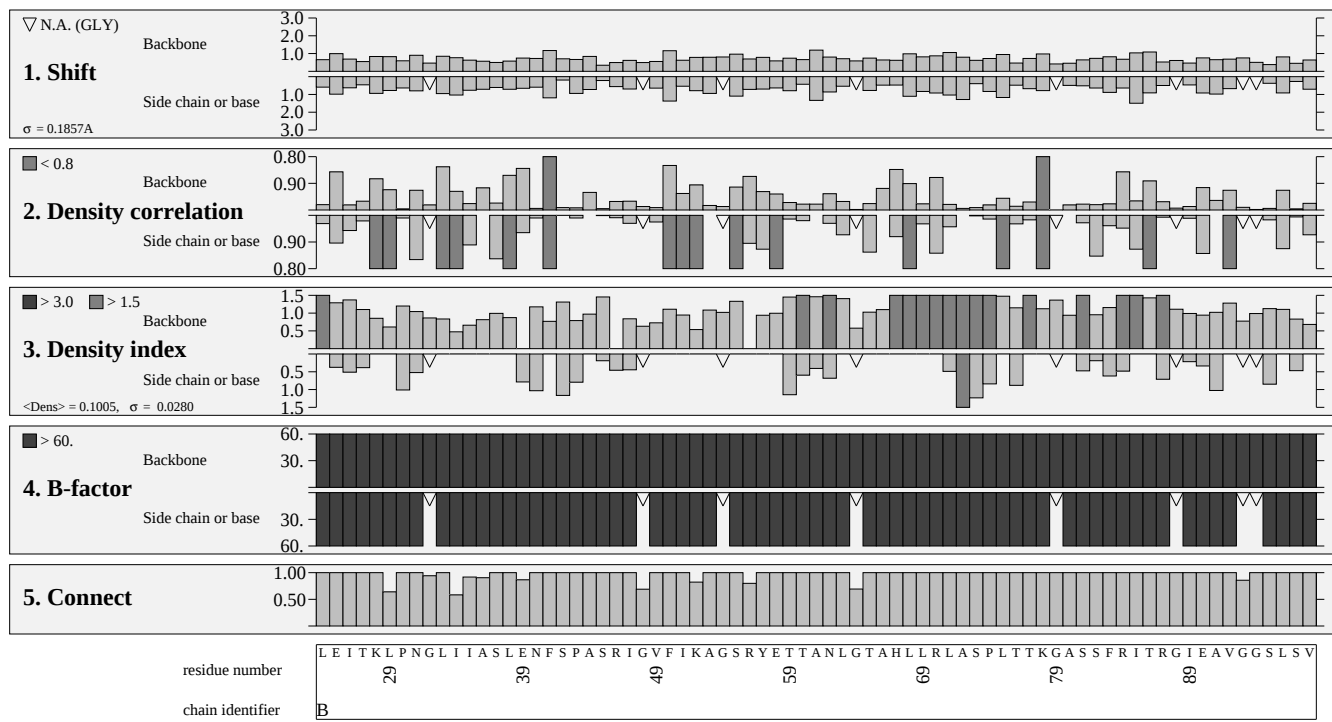
Local estimation (3)



Structure Factor Check

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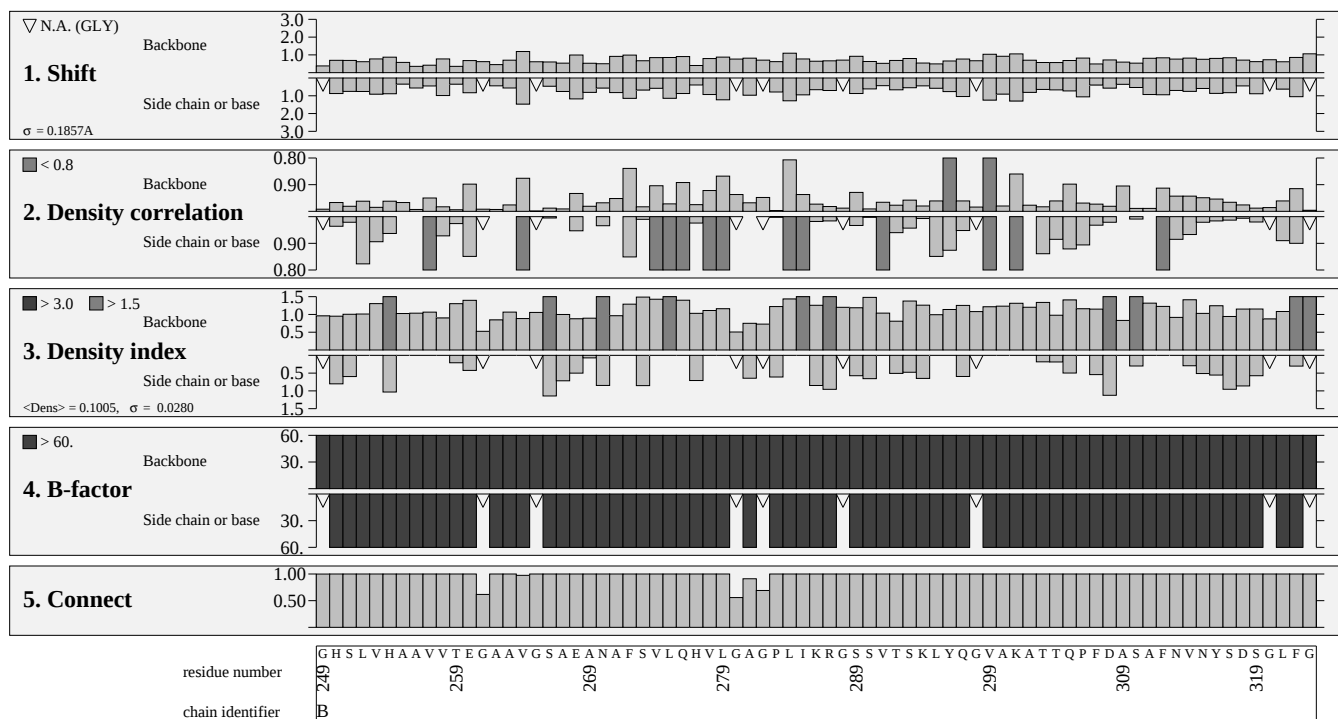
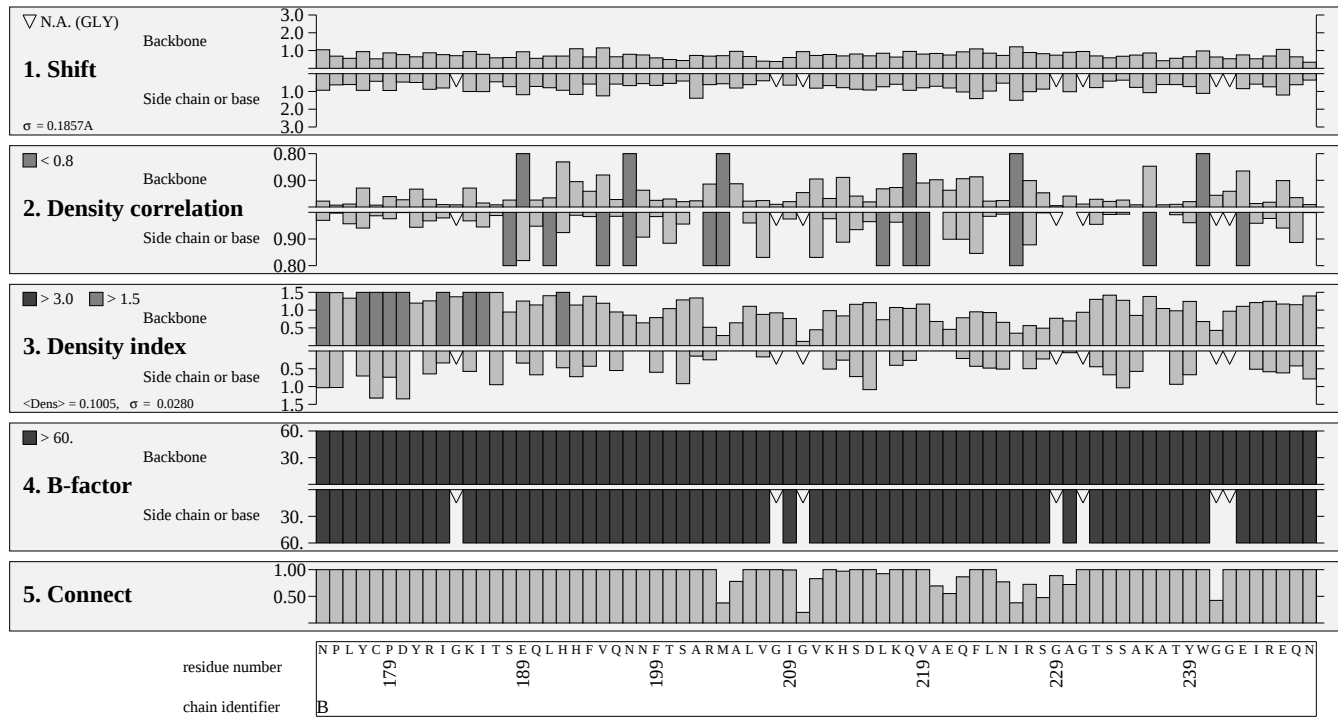
Local estimation (4)



Structure Factor Check

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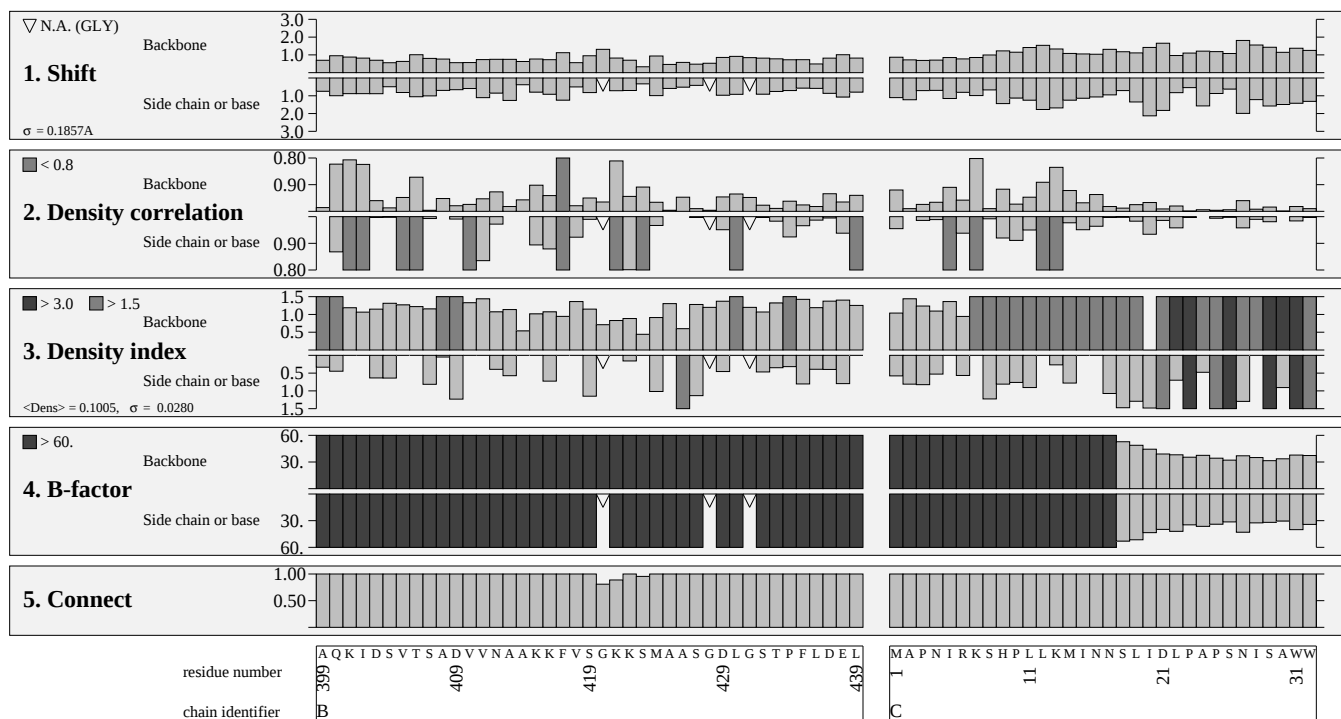
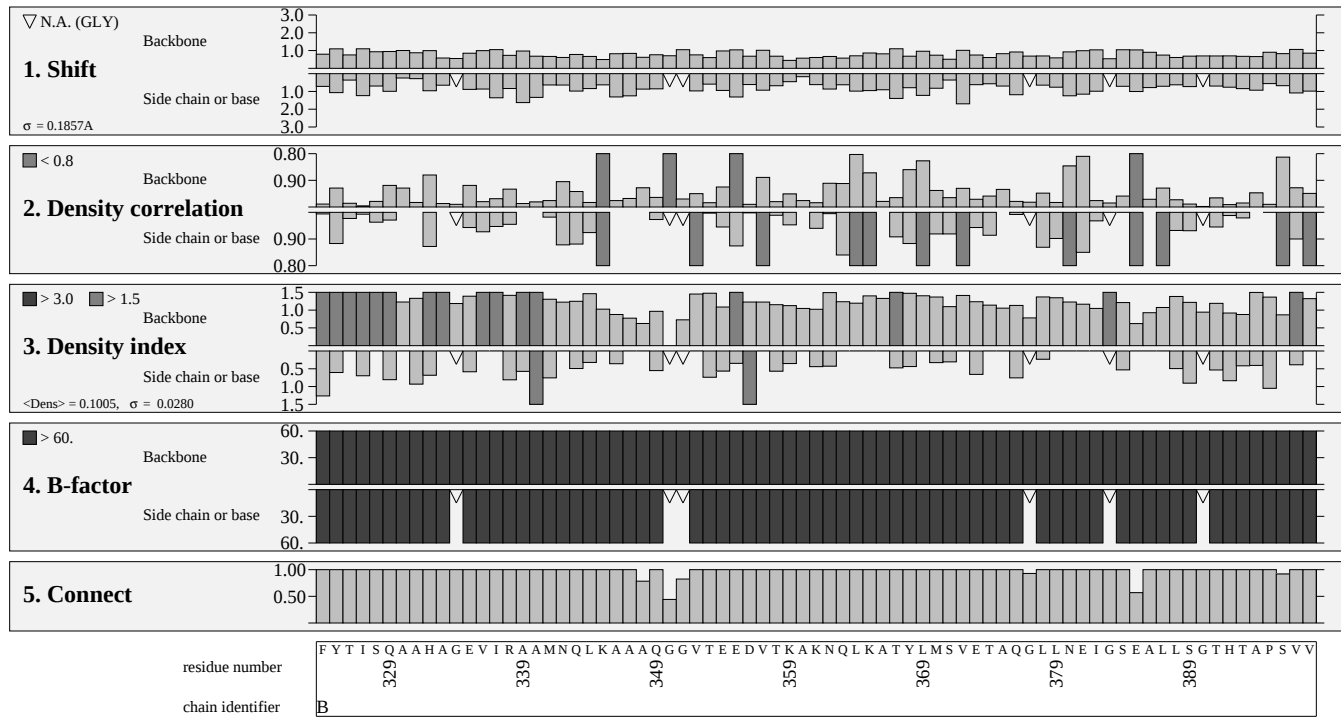
Local estimation (5)



Structure Factor Check

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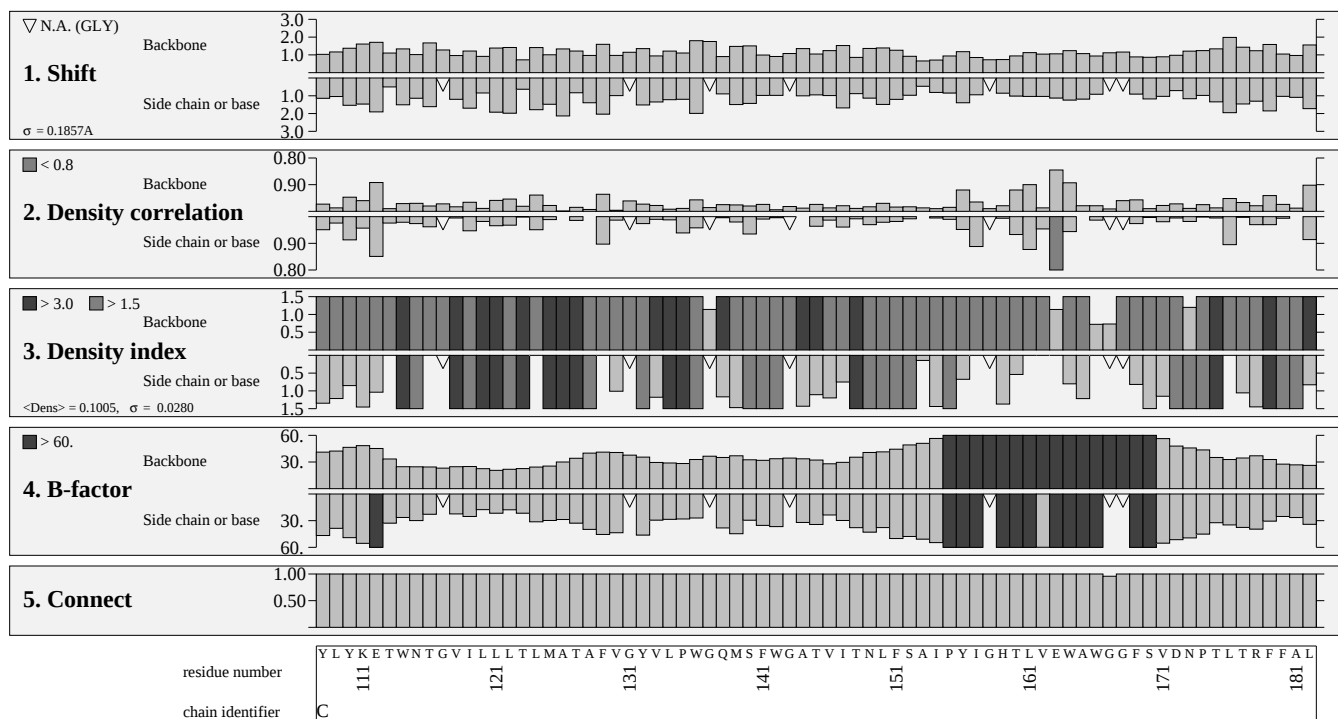
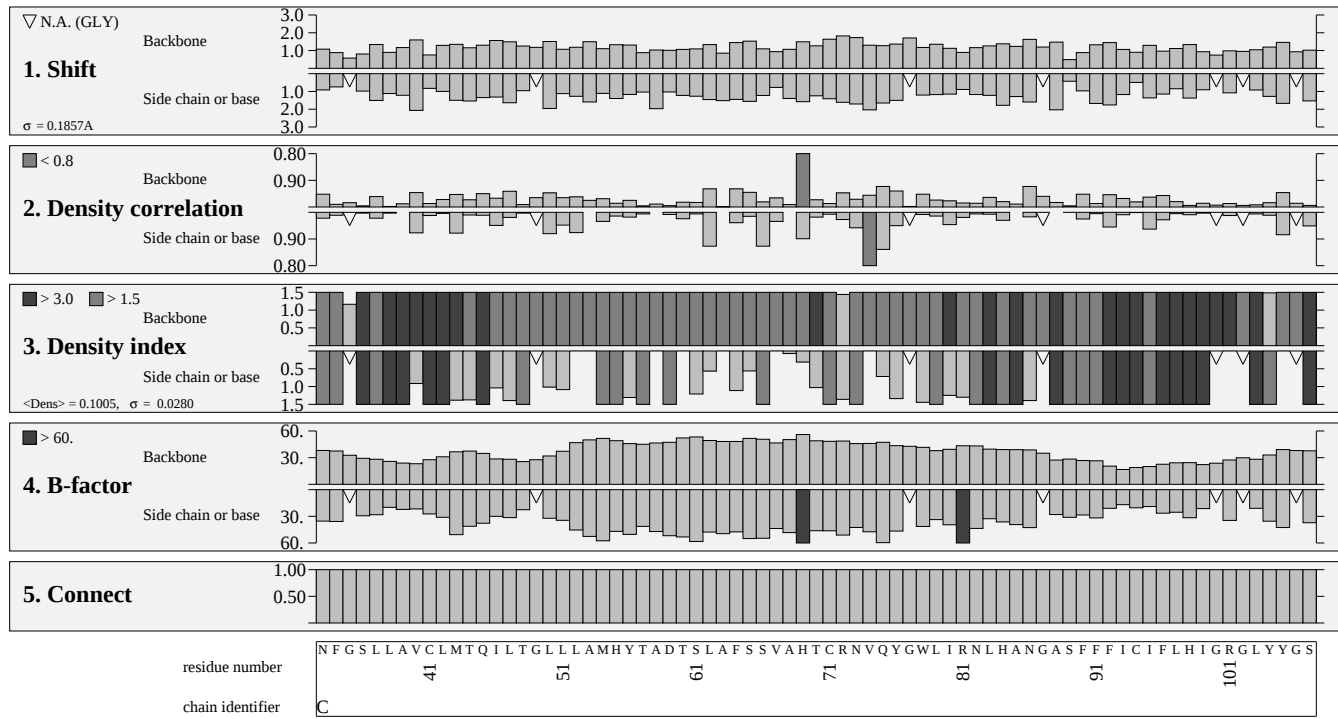
Local estimation (6)



Structure Factor Check

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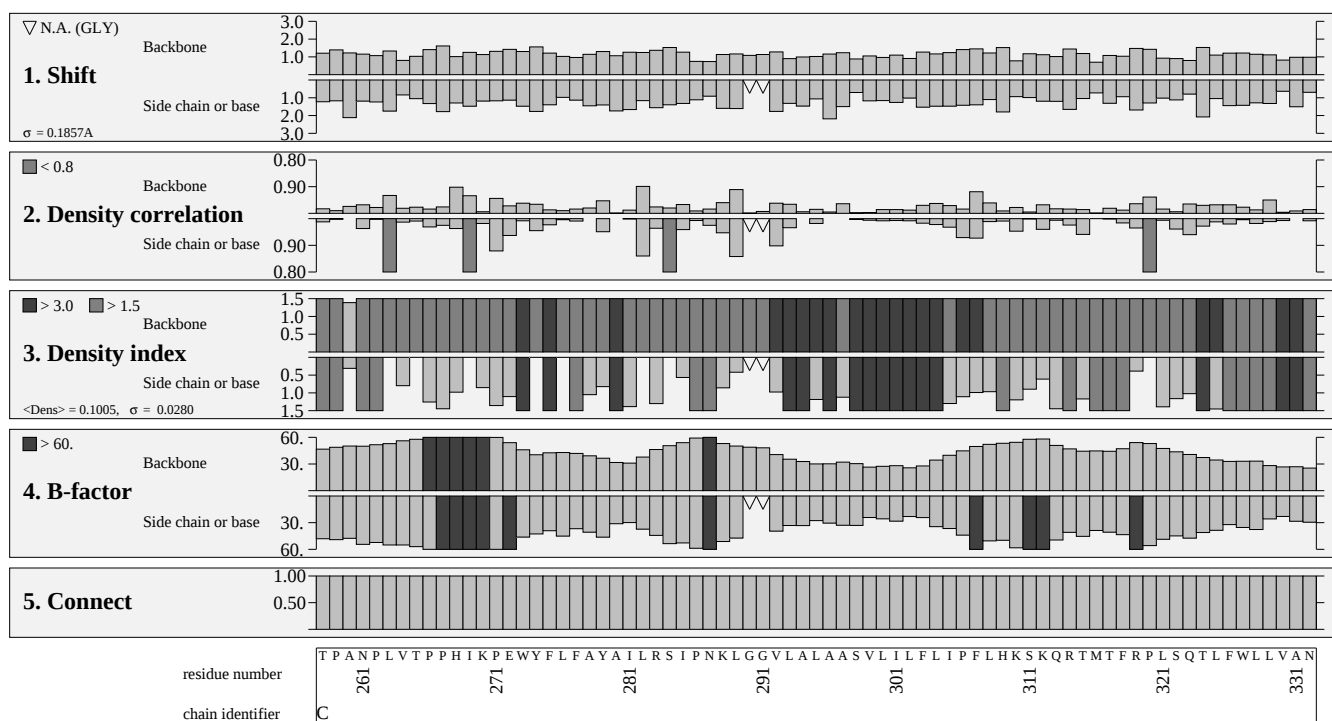
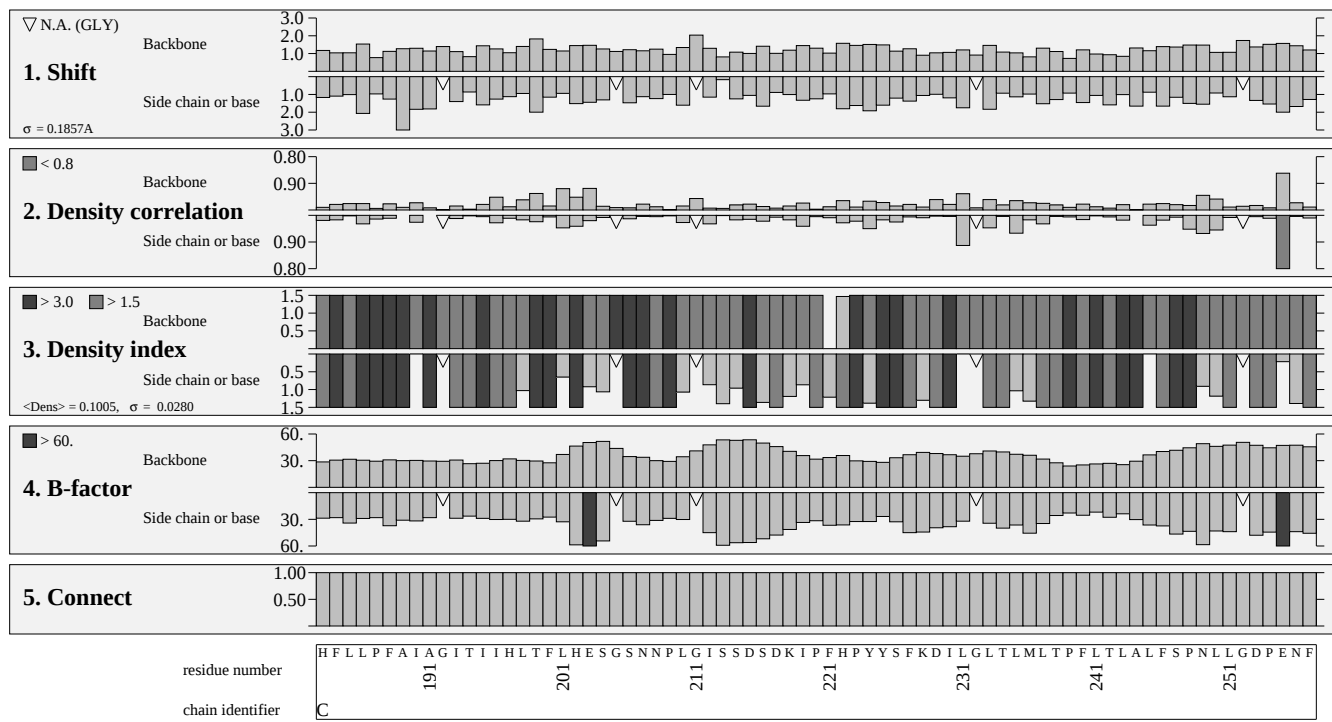
Local estimation (7)



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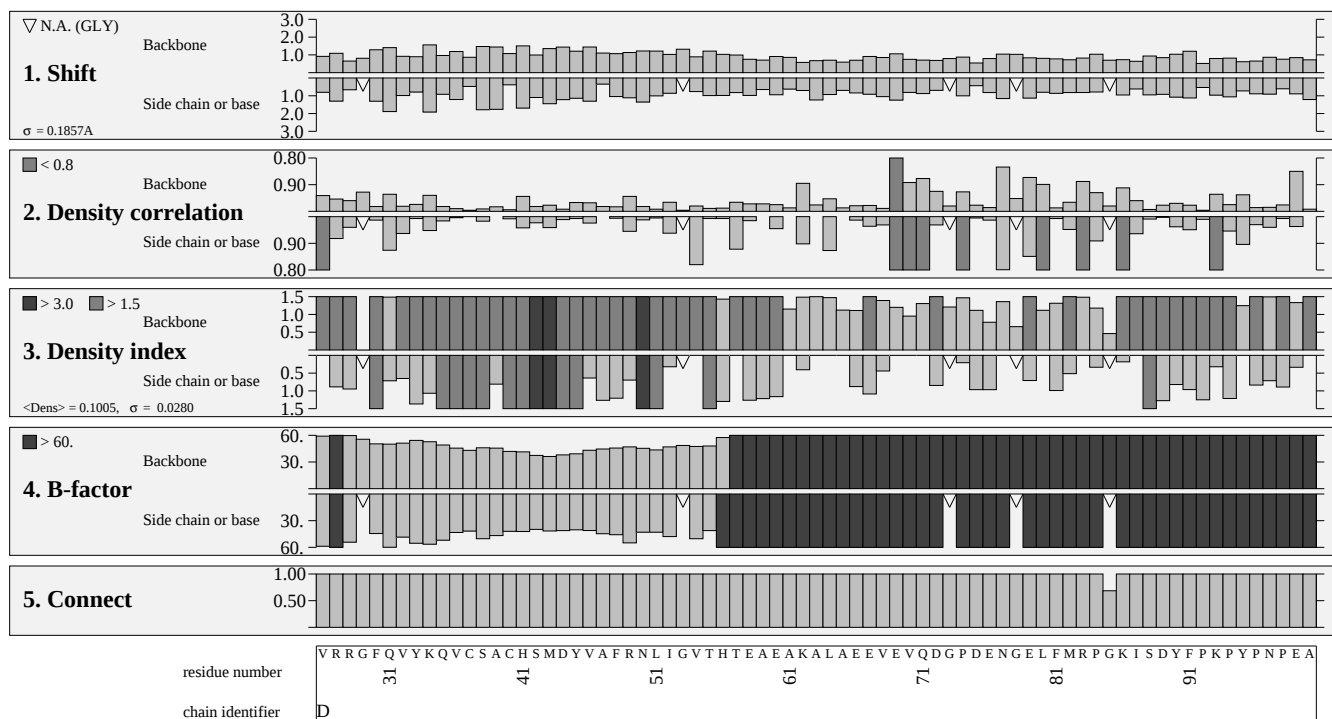
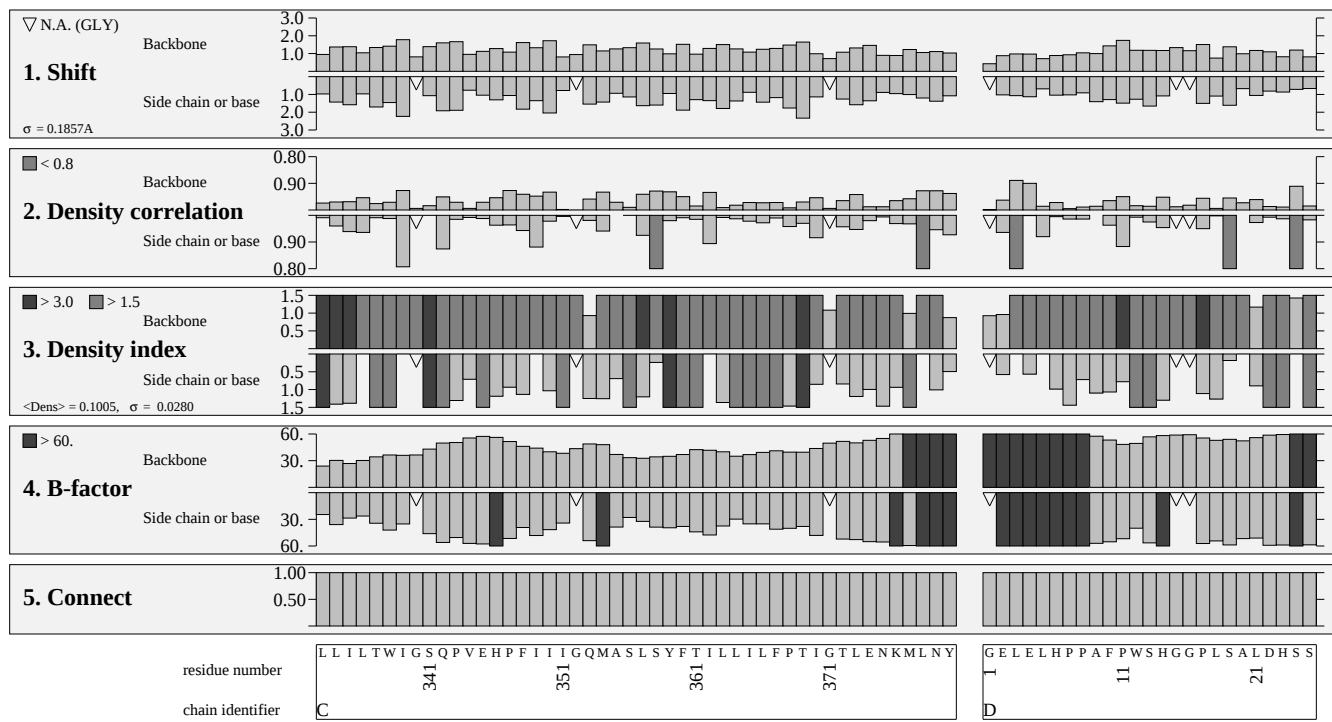
Local estimation (8)



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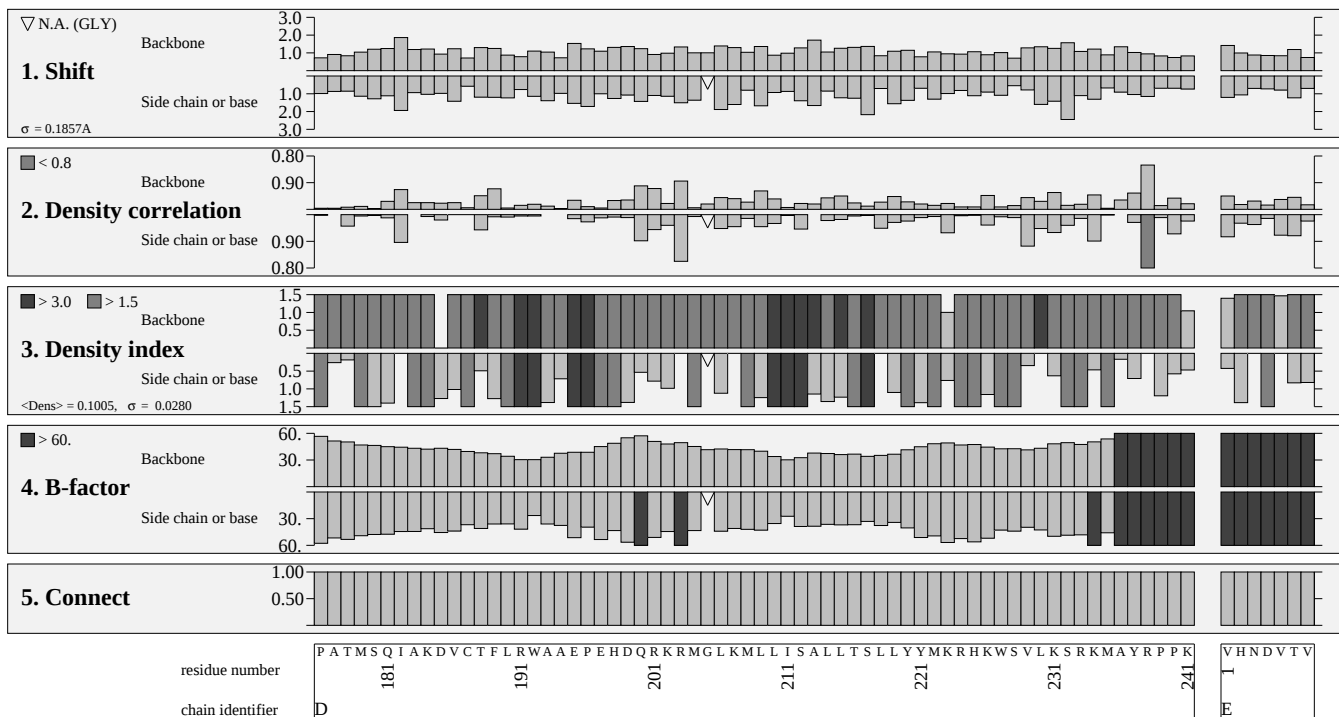
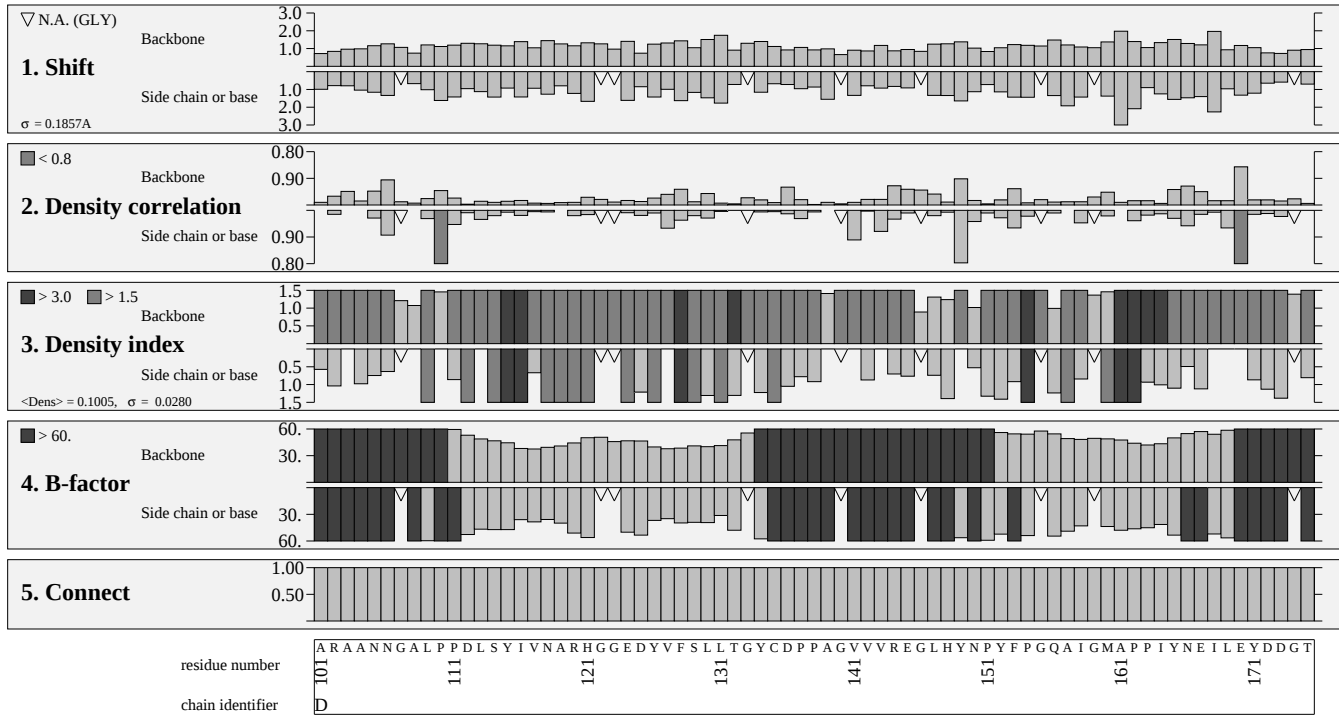
Local estimation (9)



Structure Factor Check

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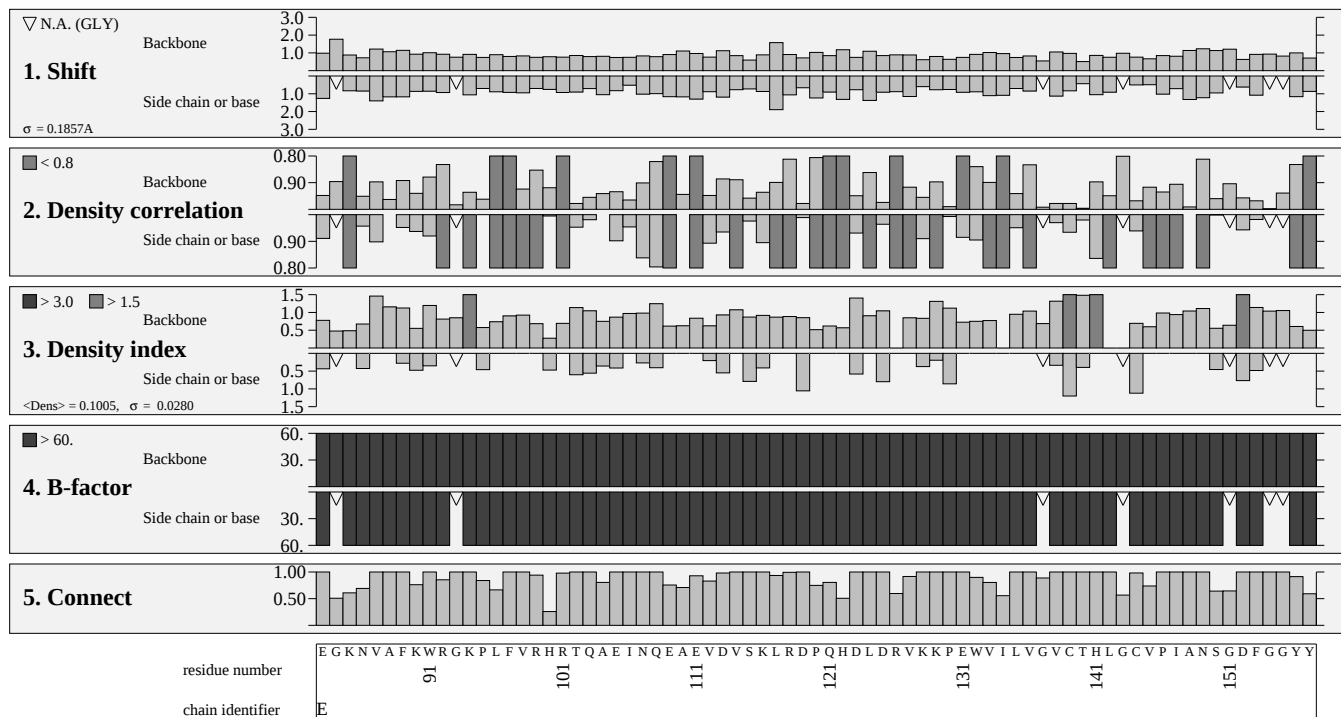
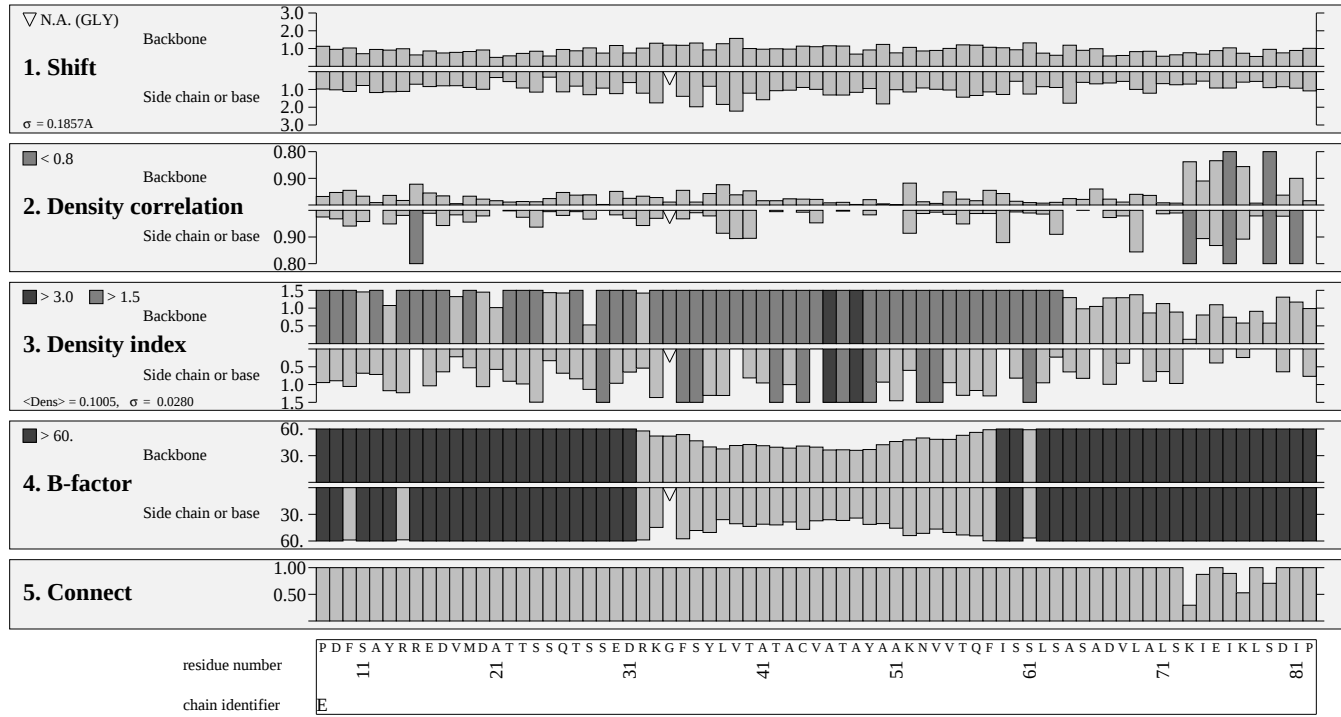
Local estimation (10)



Structure Factor Check

3H1I

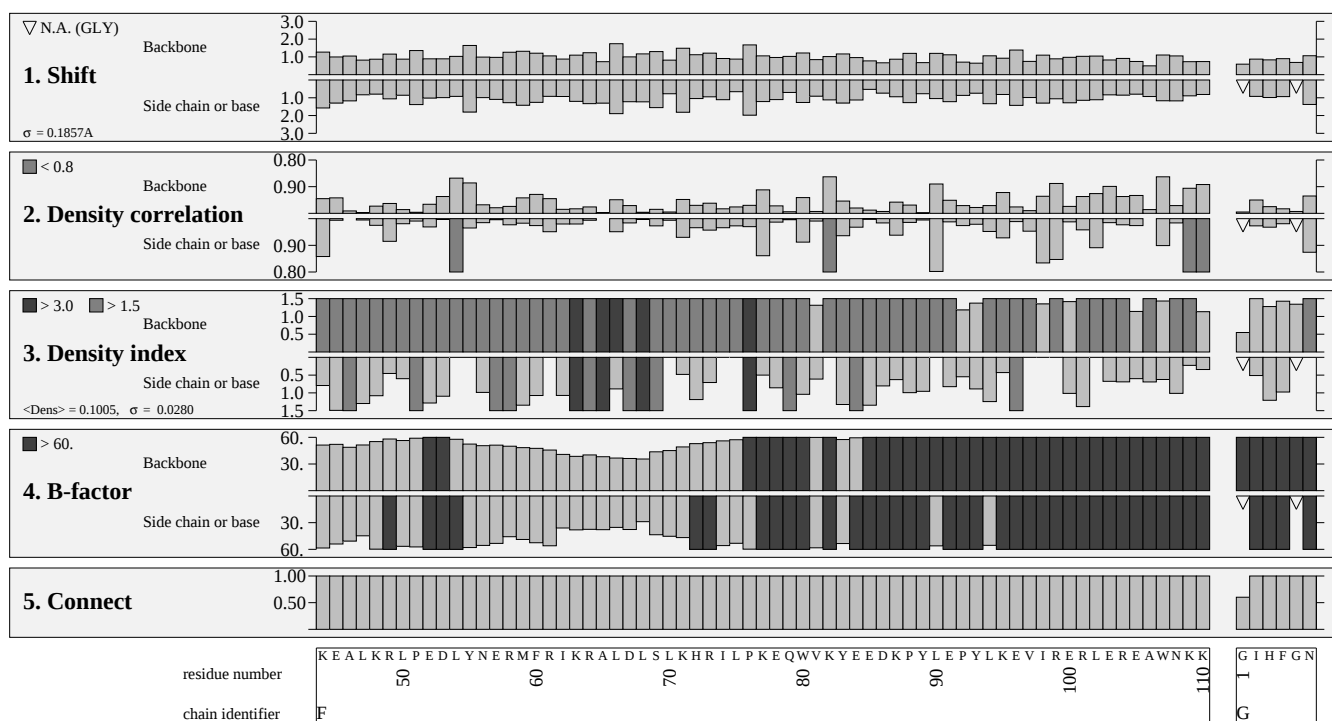
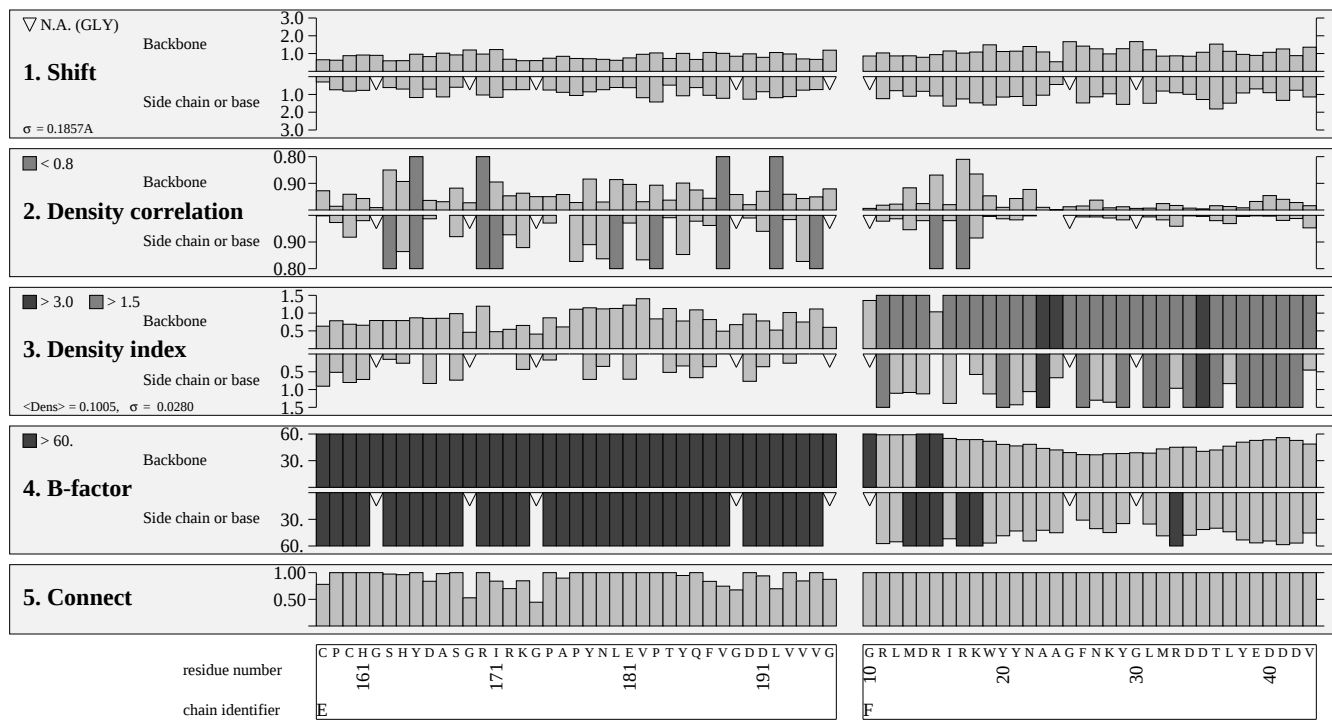
Local estimation (11)



Structure Factor Check

3H1I

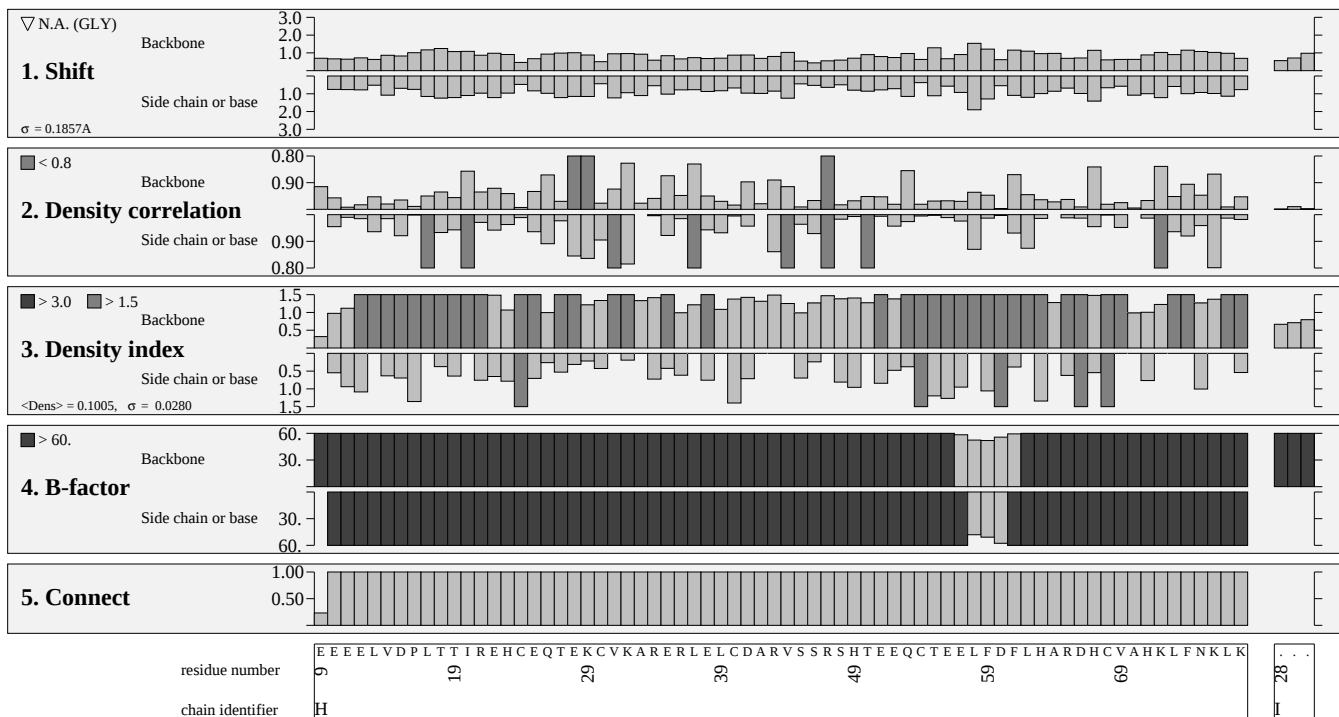
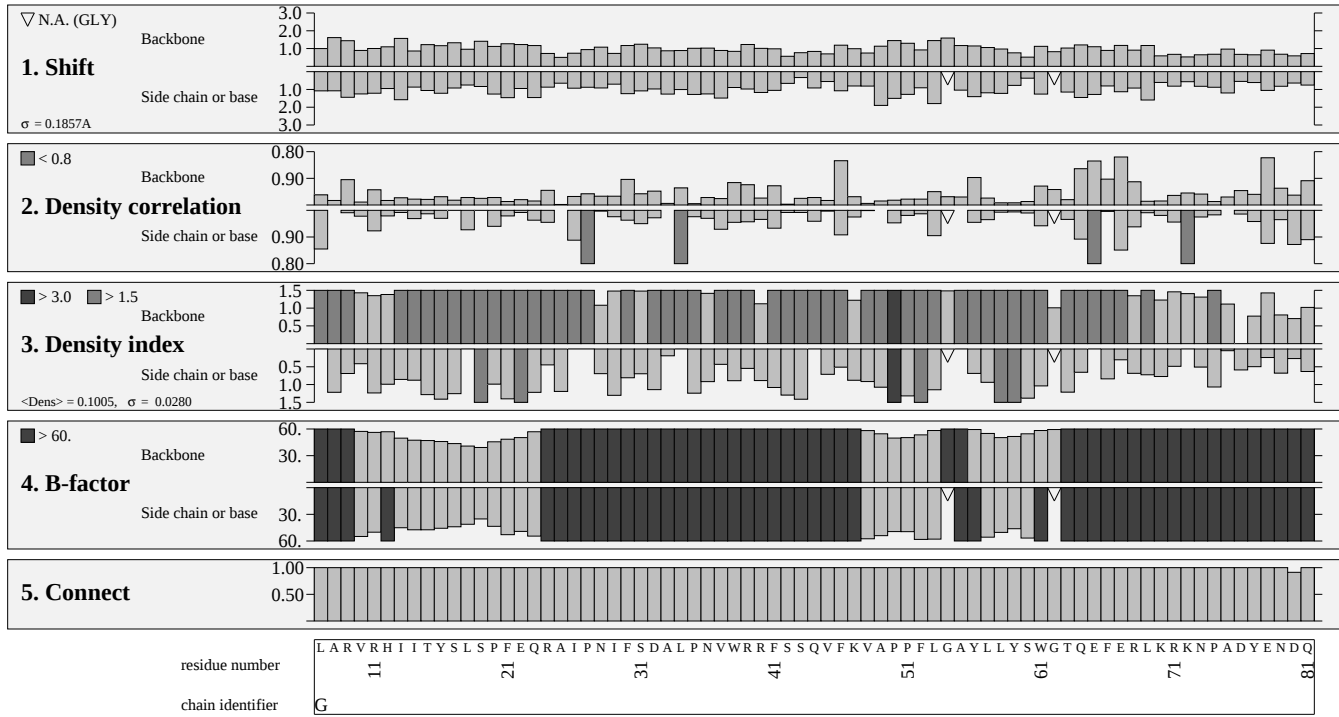
Local estimation (12)



Structure Factor Check

3H1I

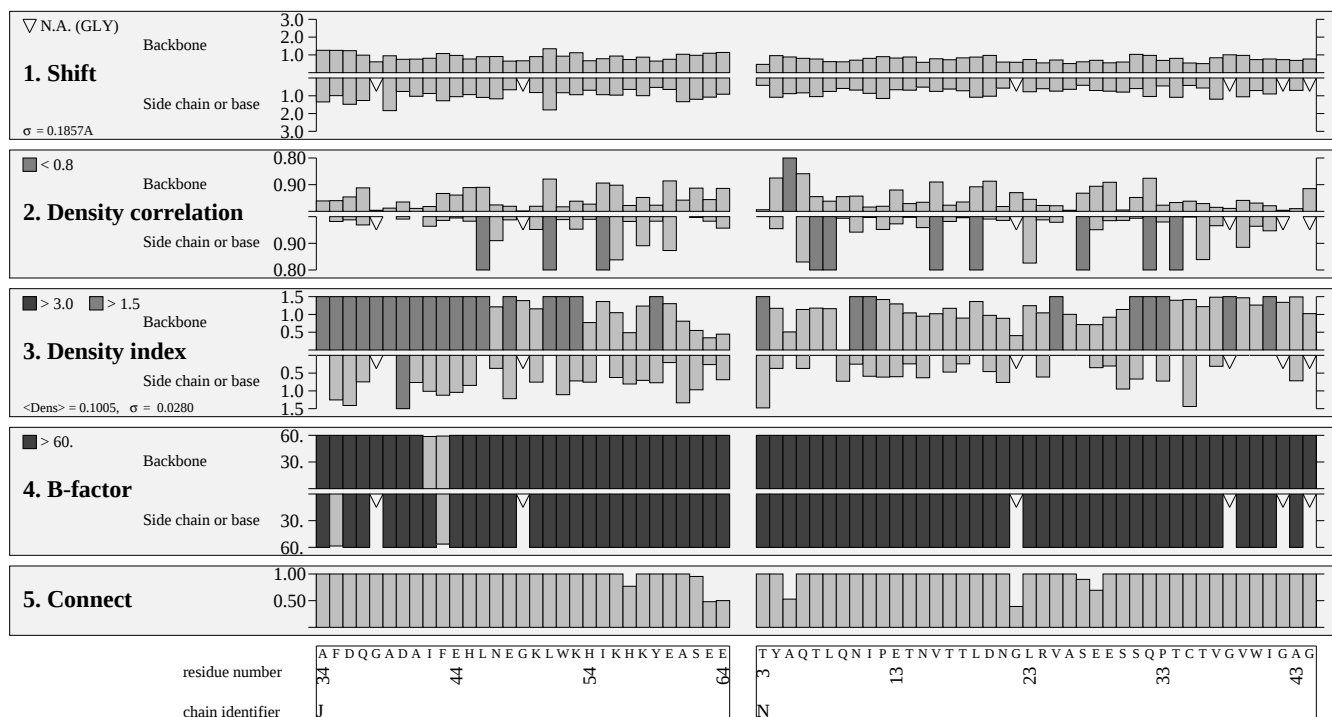
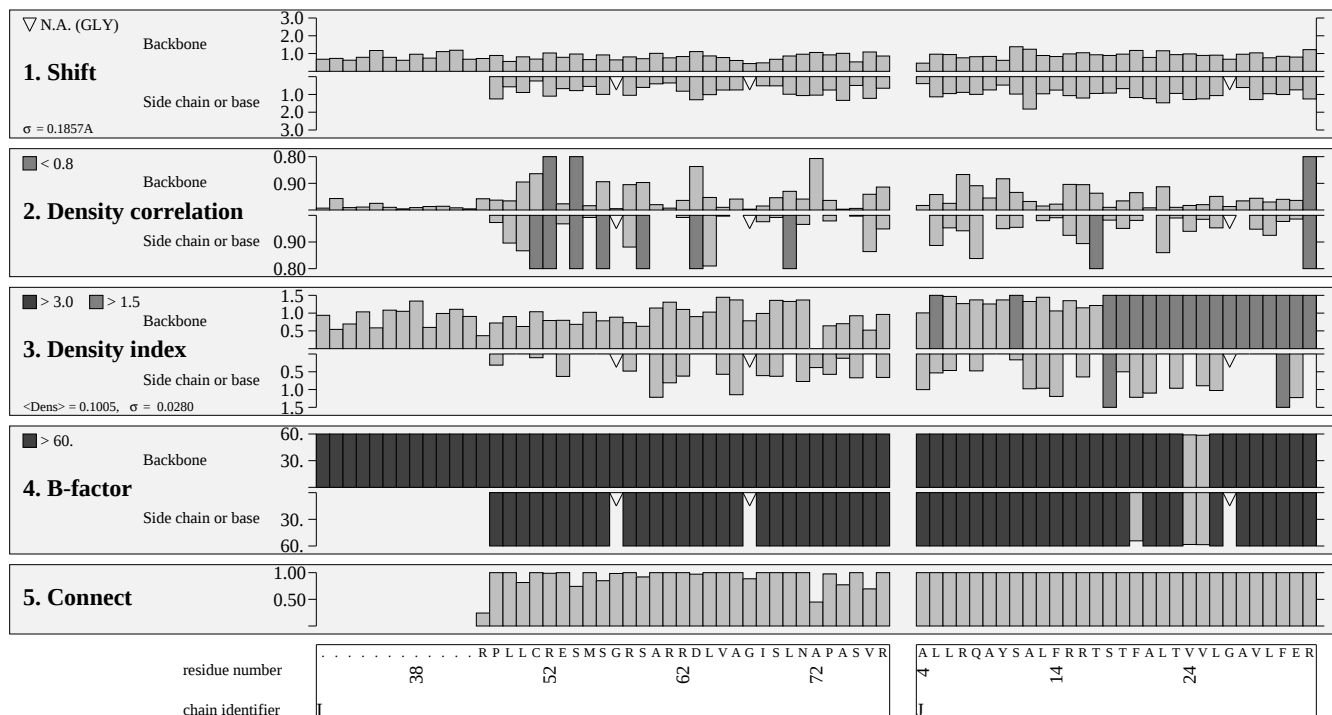
Local estimation (13)



Structure Factor Check

3H1I

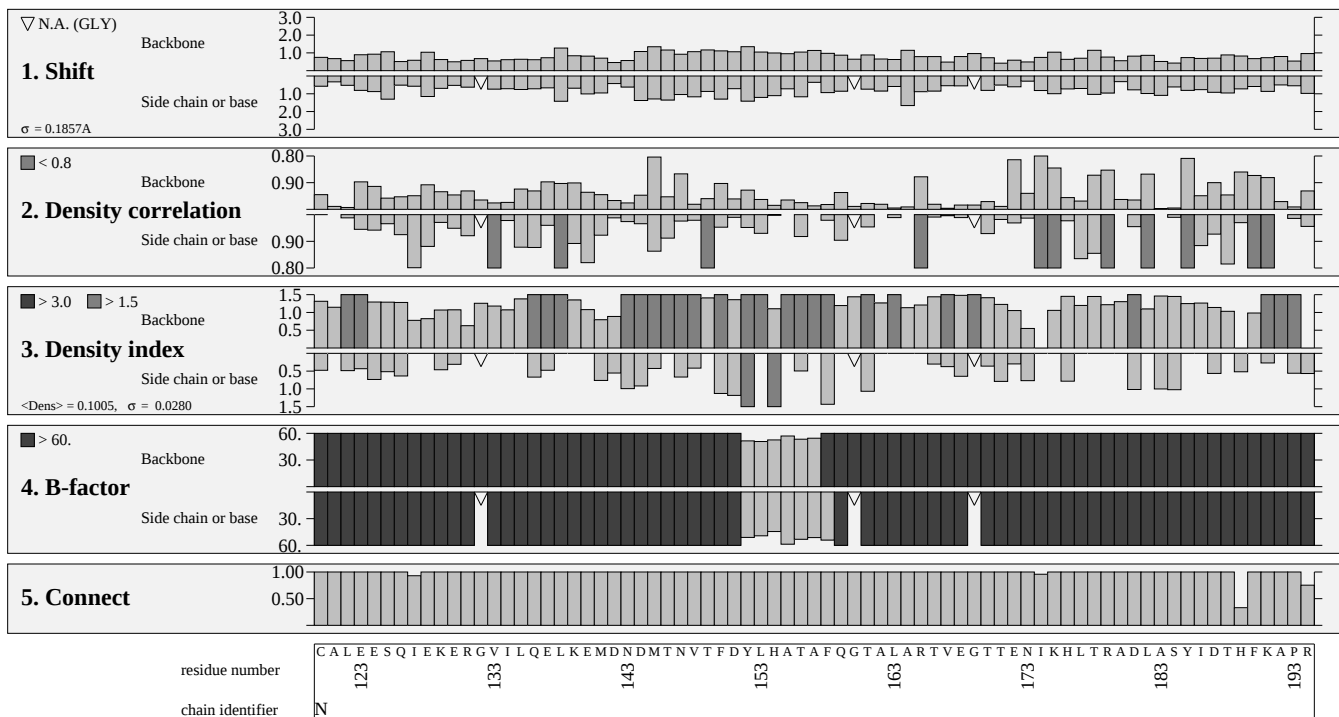
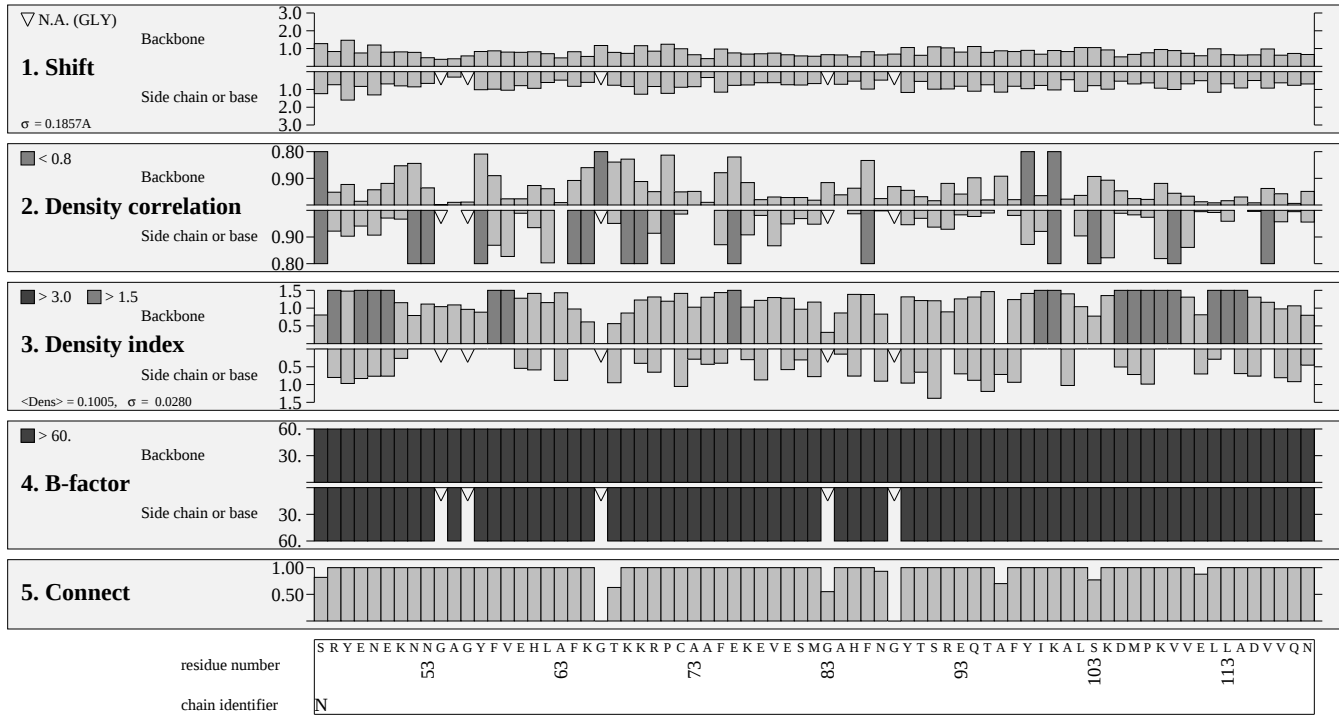
Local estimation (14)



Structure Factor Check

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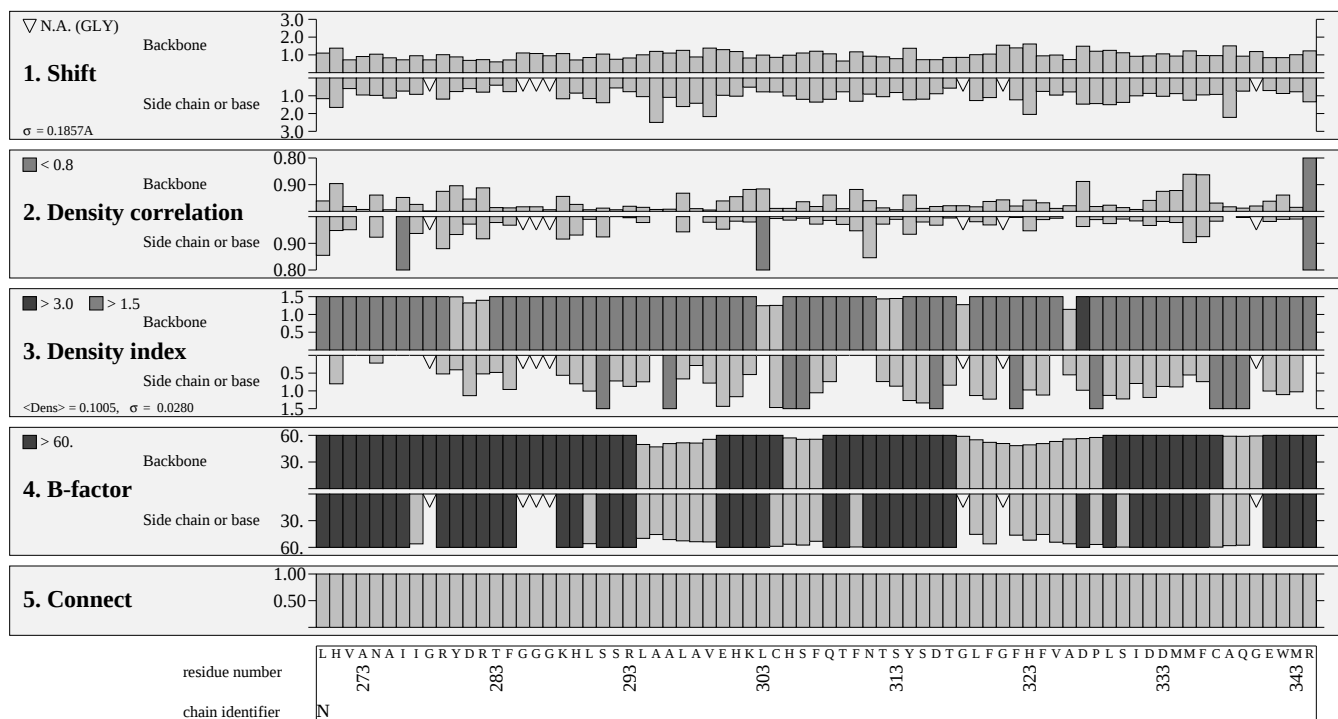
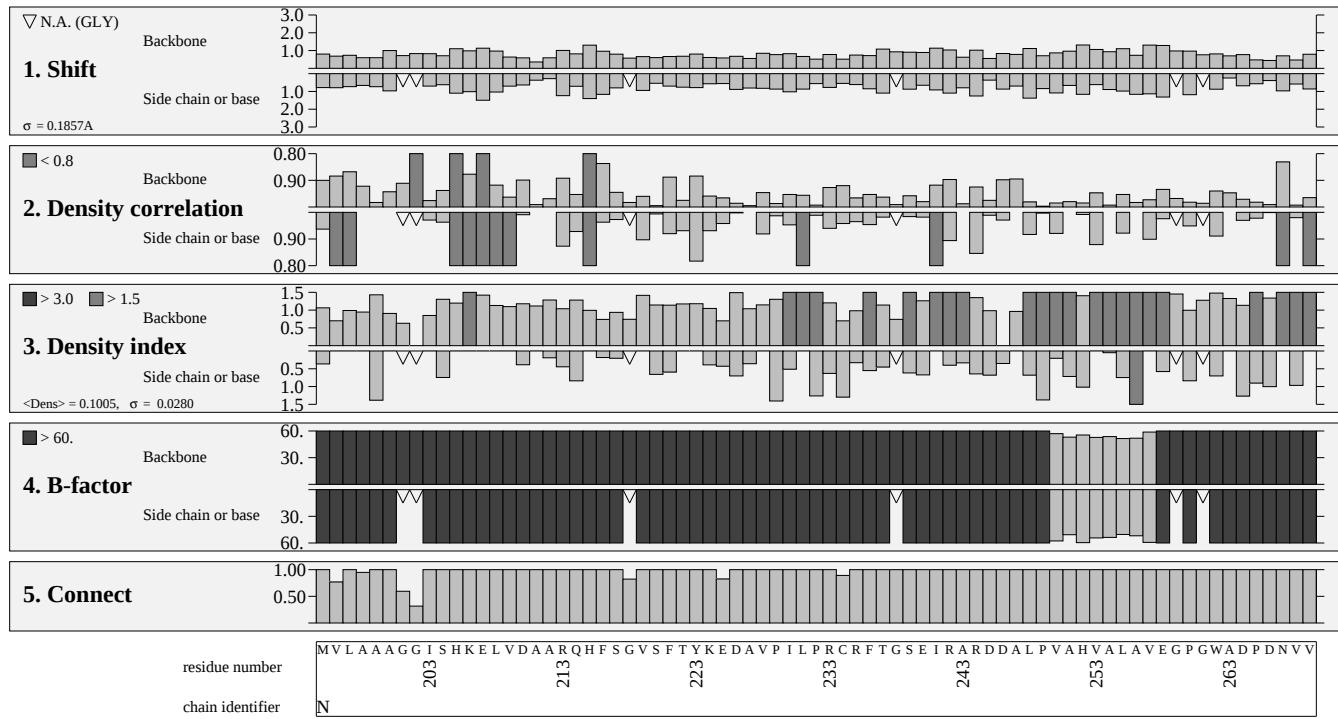
Local estimation (15)



Structure Factor Check

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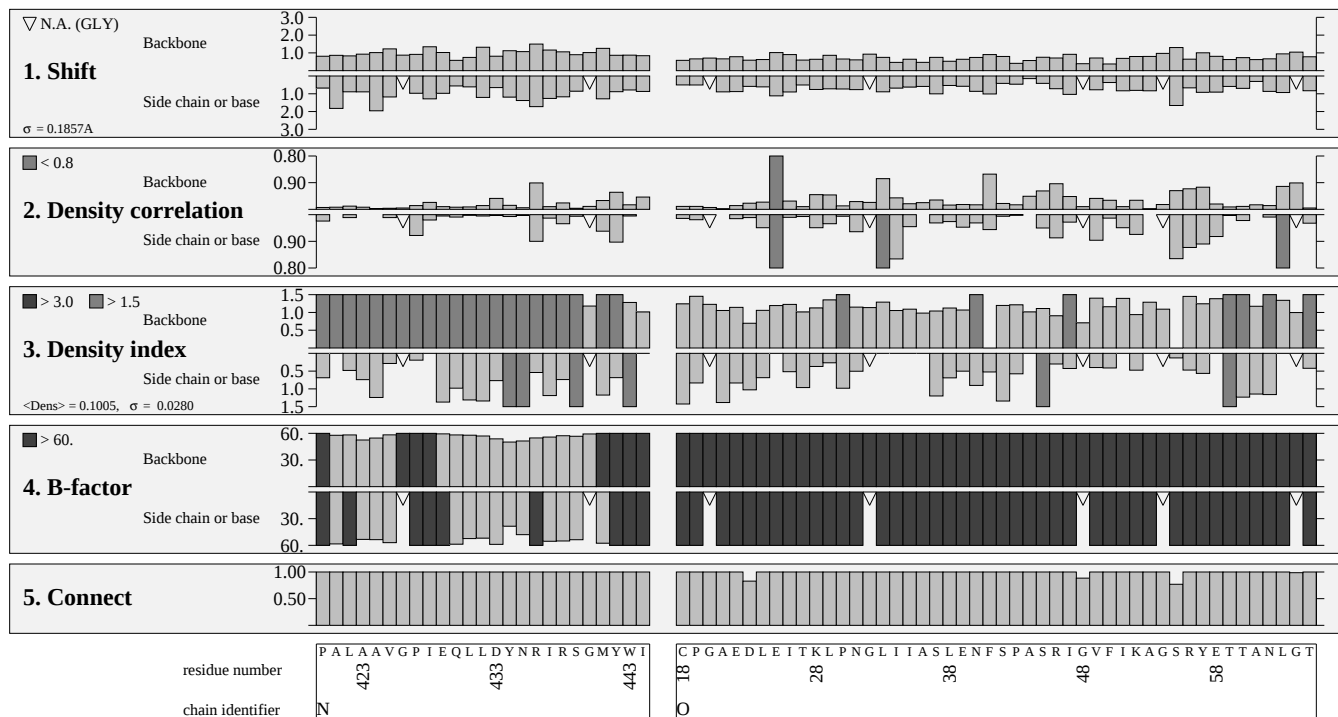
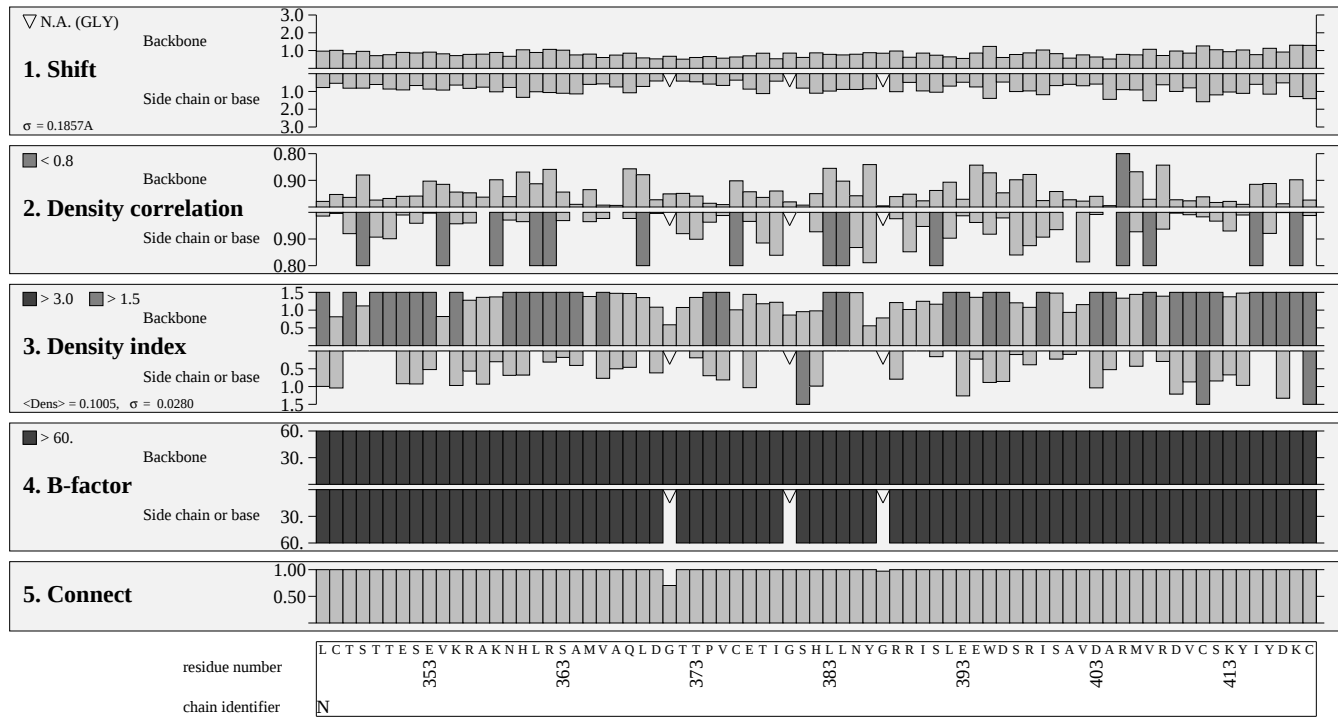
Local estimation (16)



Structure Factor Check

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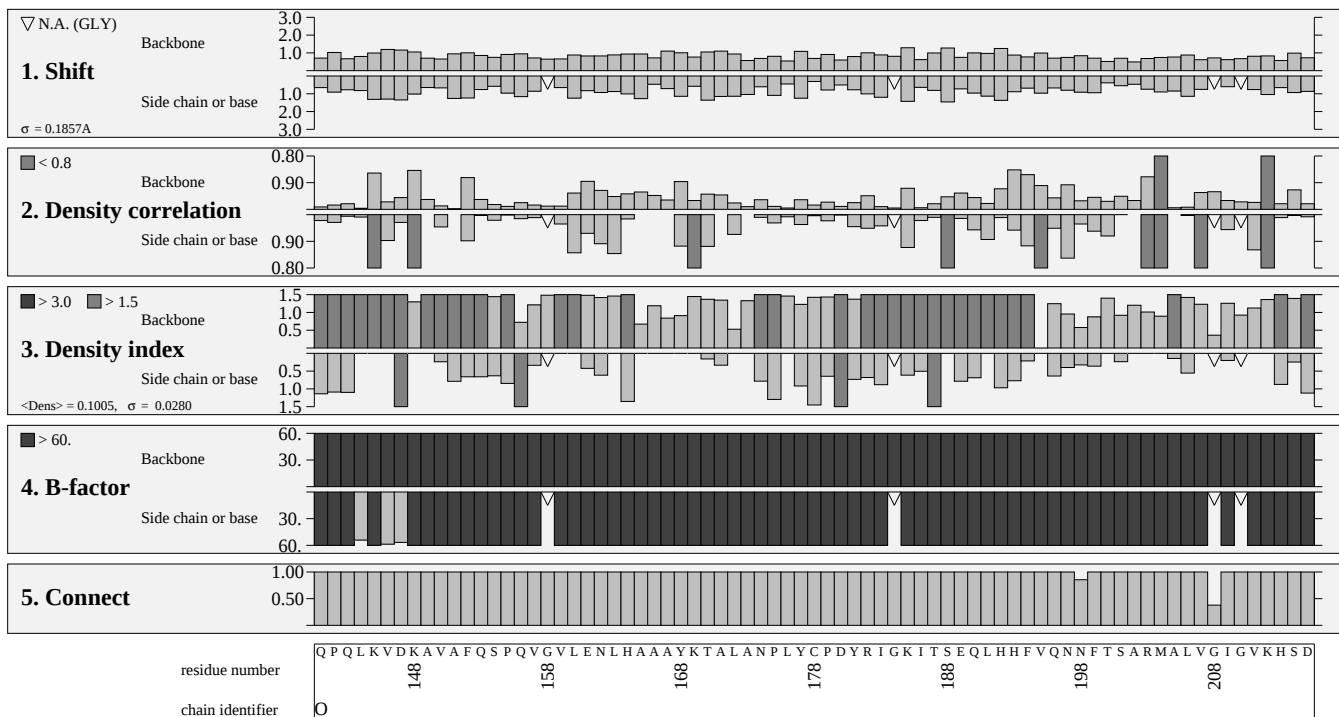
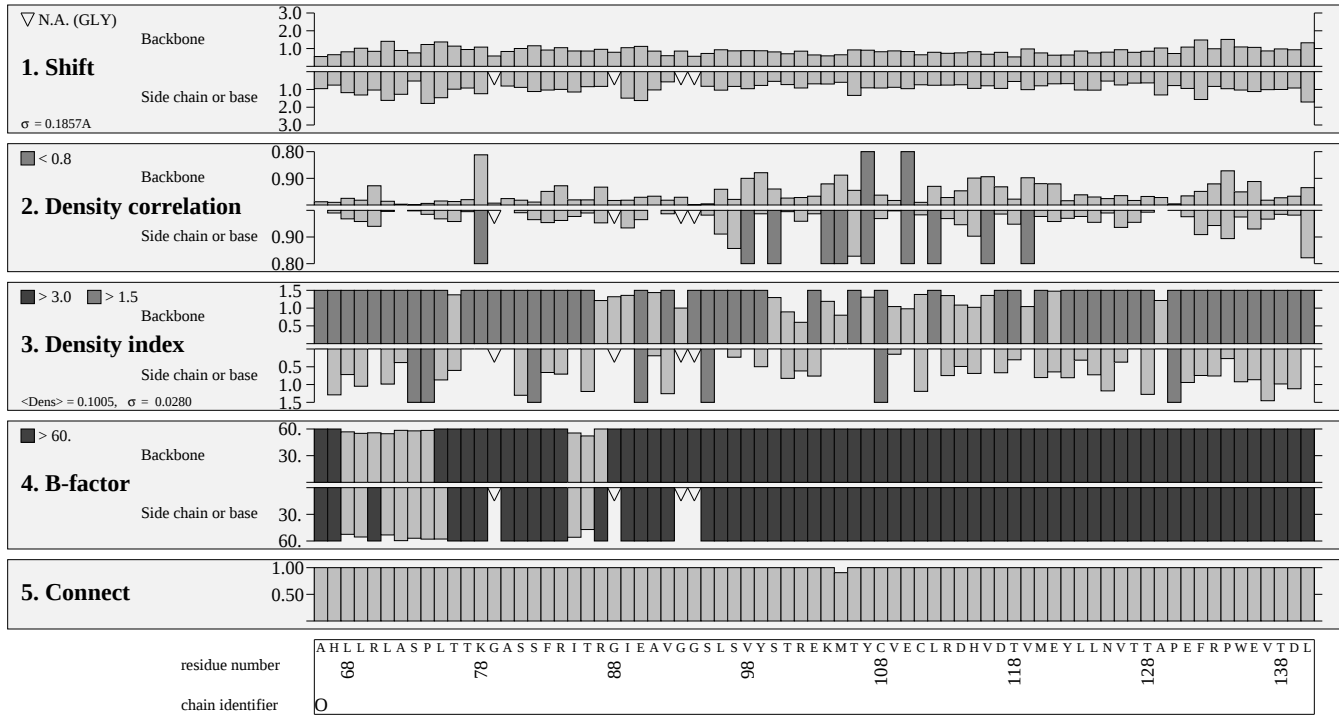
Local estimation (17)



Structure Factor Check

3H1I

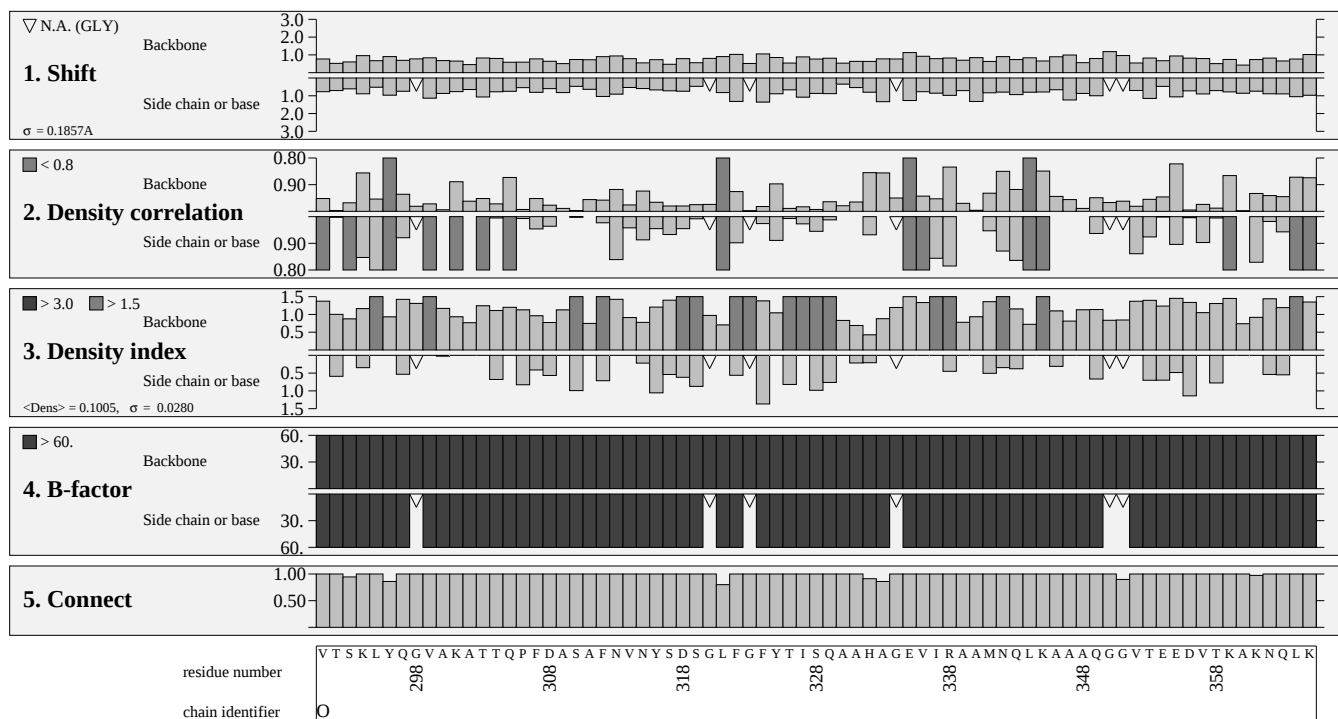
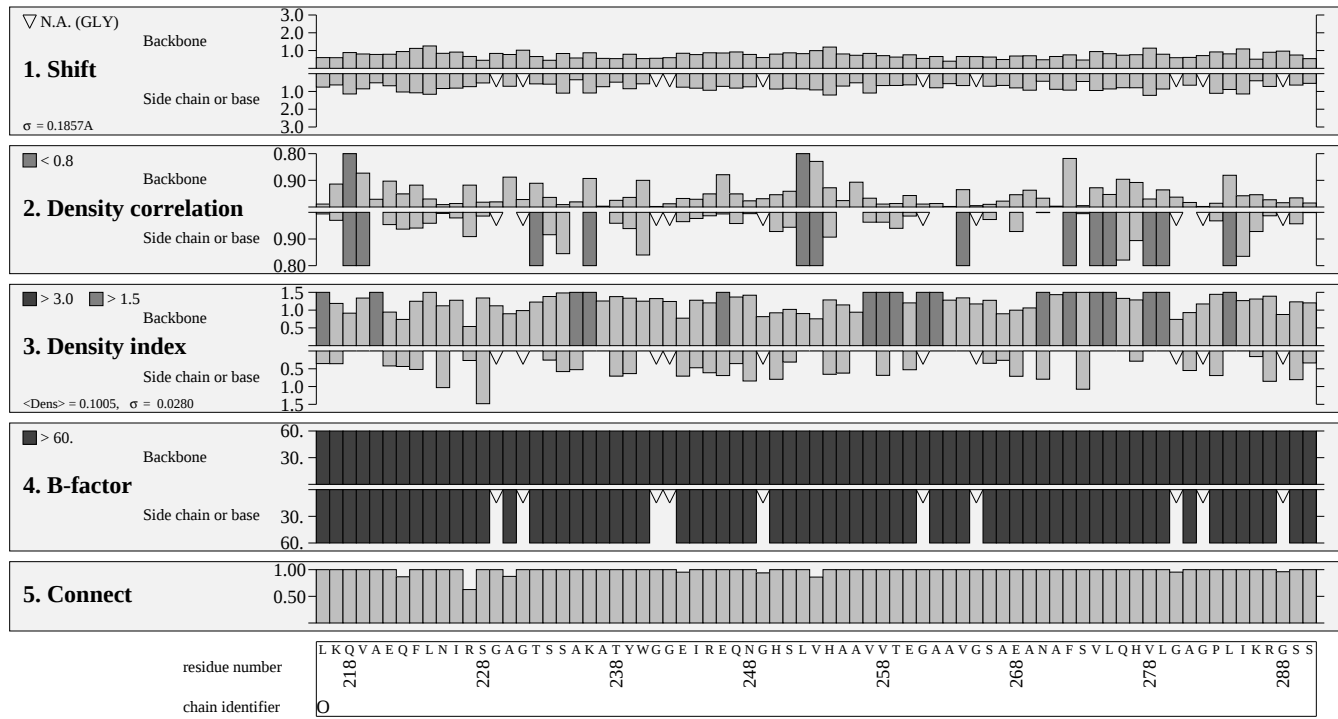
Local estimation (18)



Structure Factor Check

3H1I

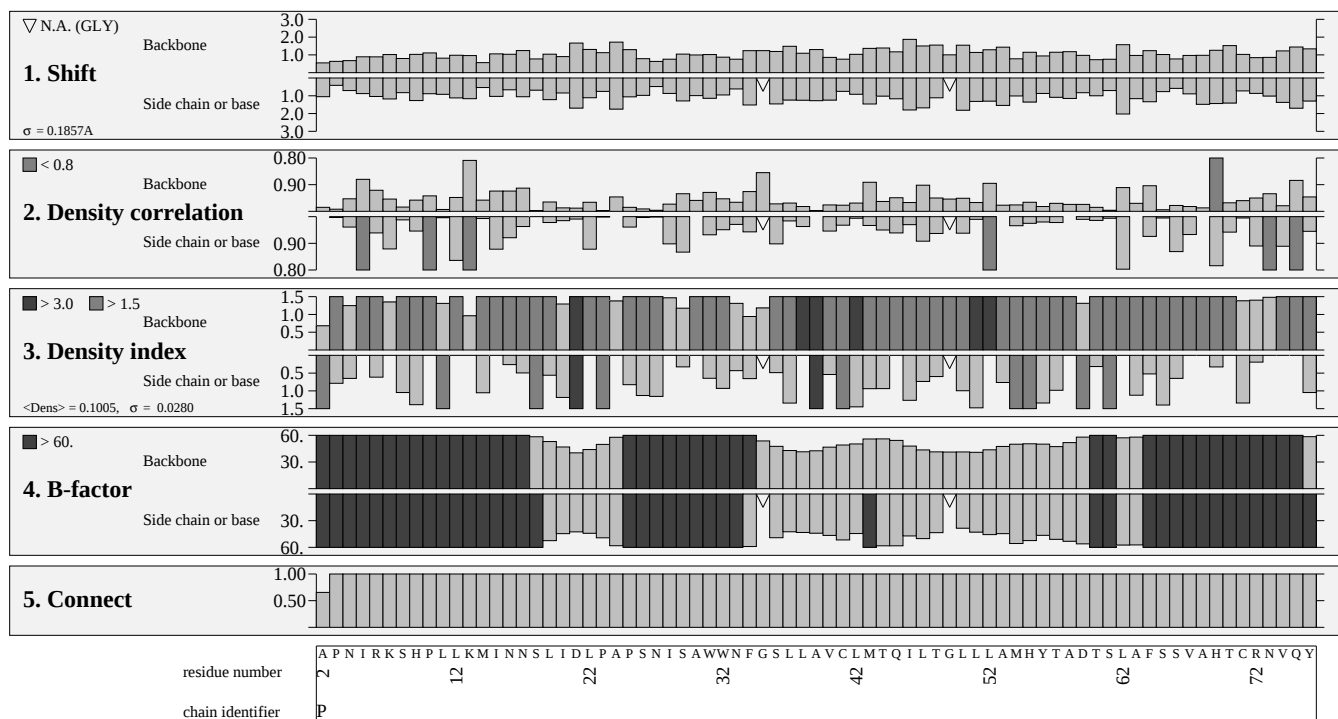
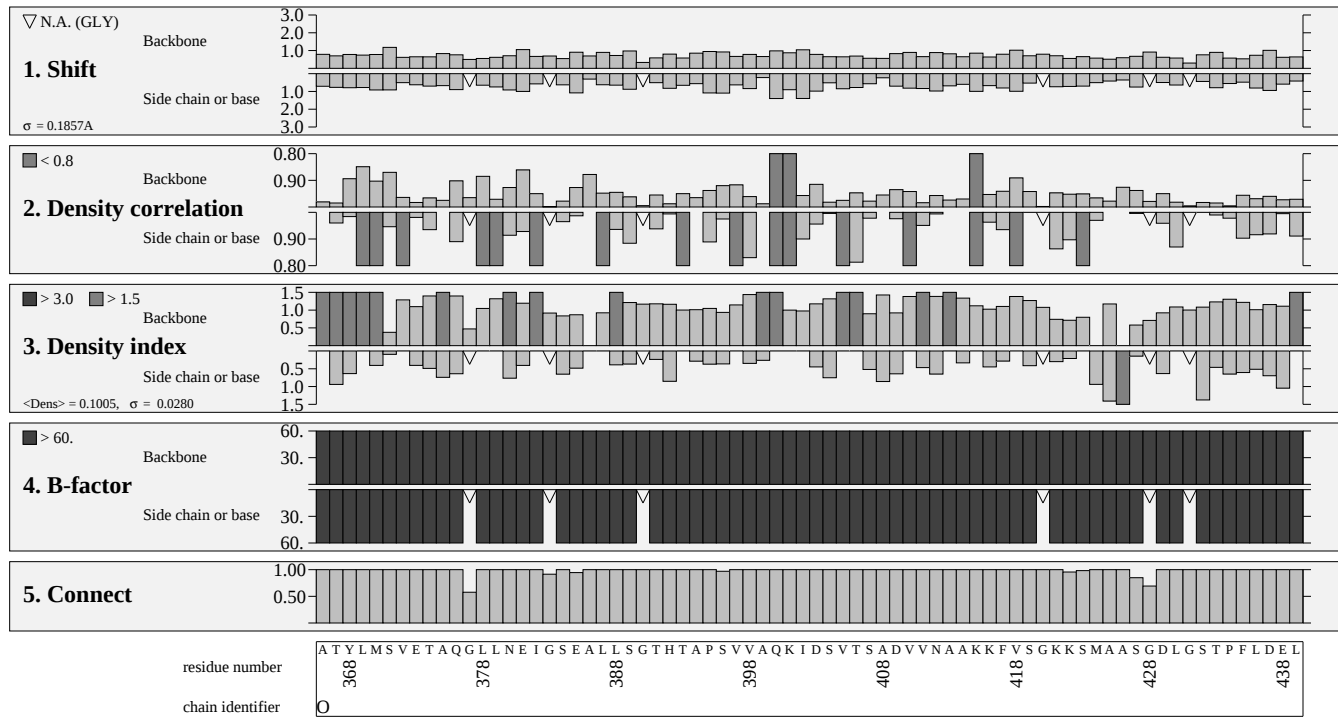
Local estimation (19)



Structure Factor Check

3H1I

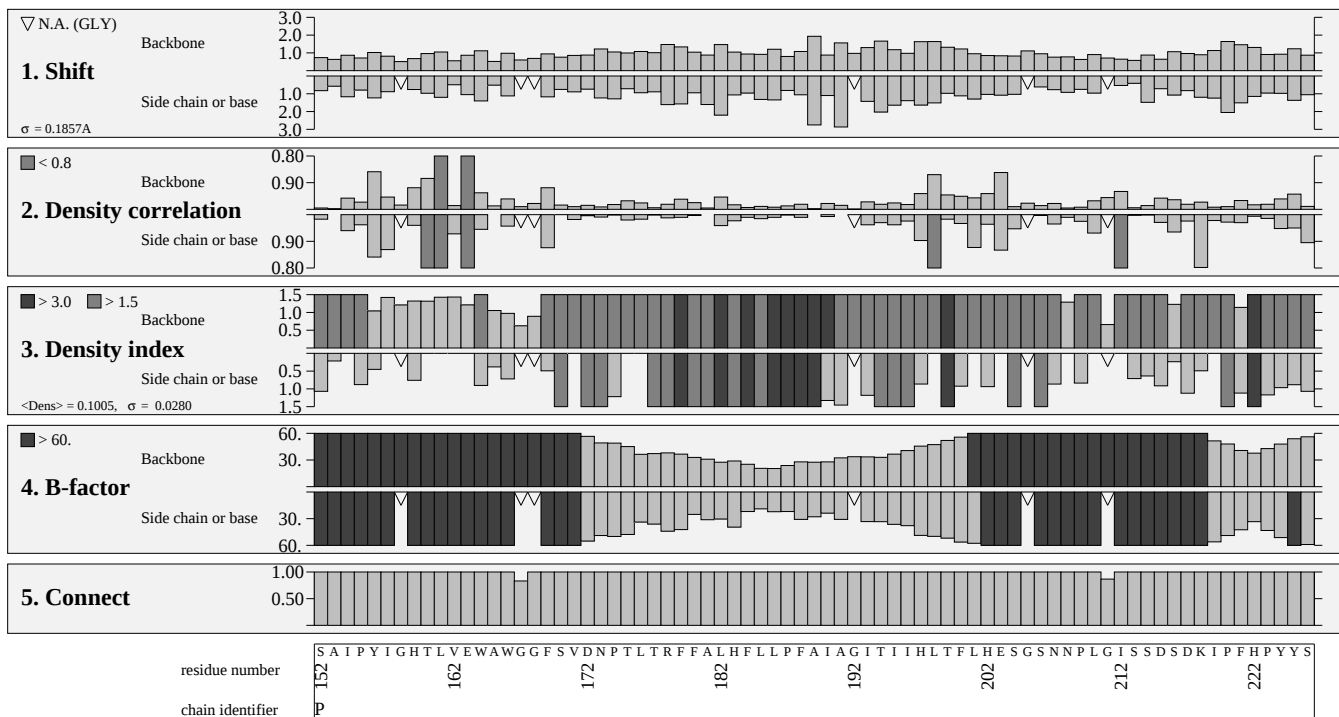
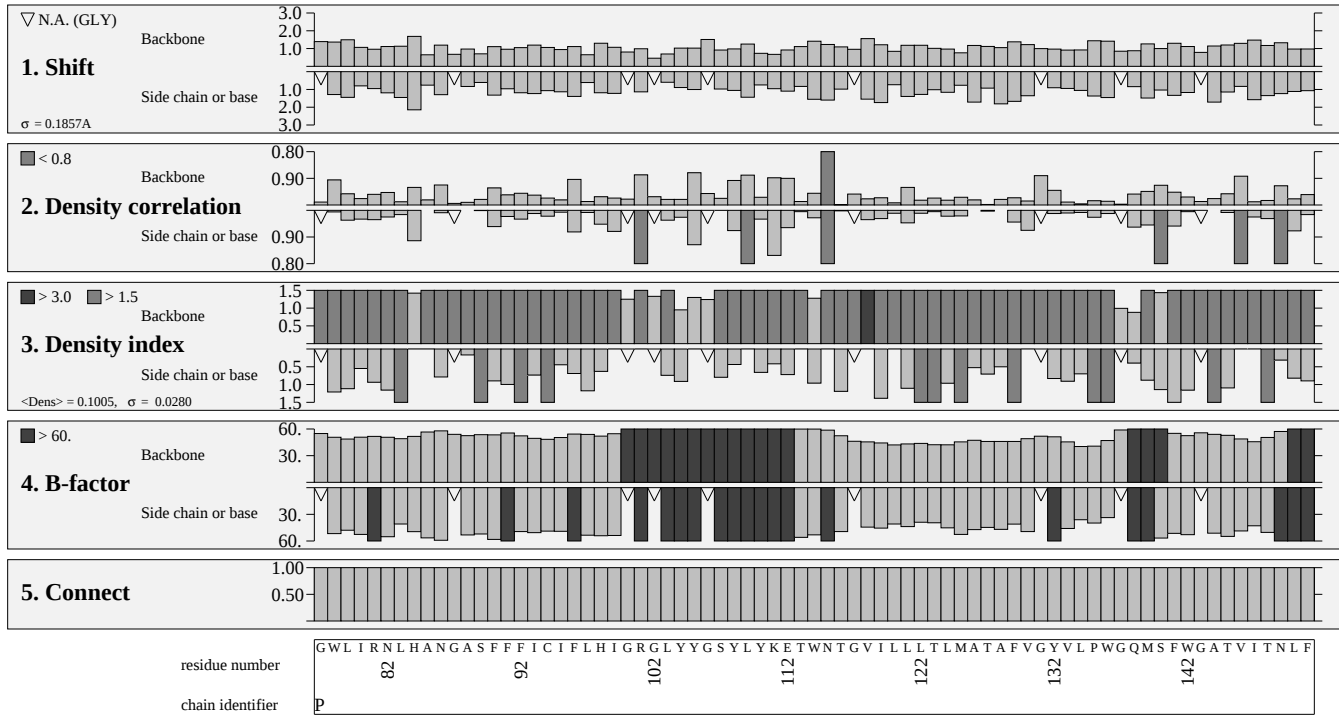
Local estimation (20)



Structure Factor Check

3H1I

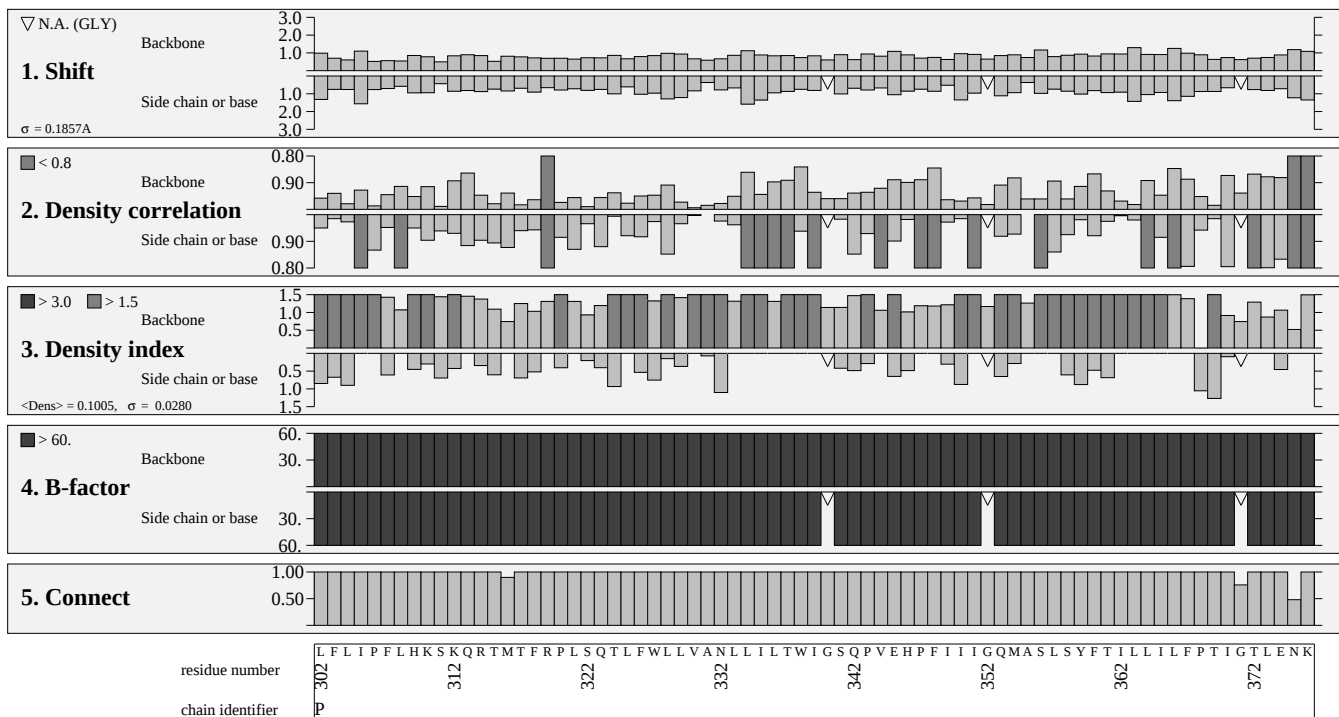
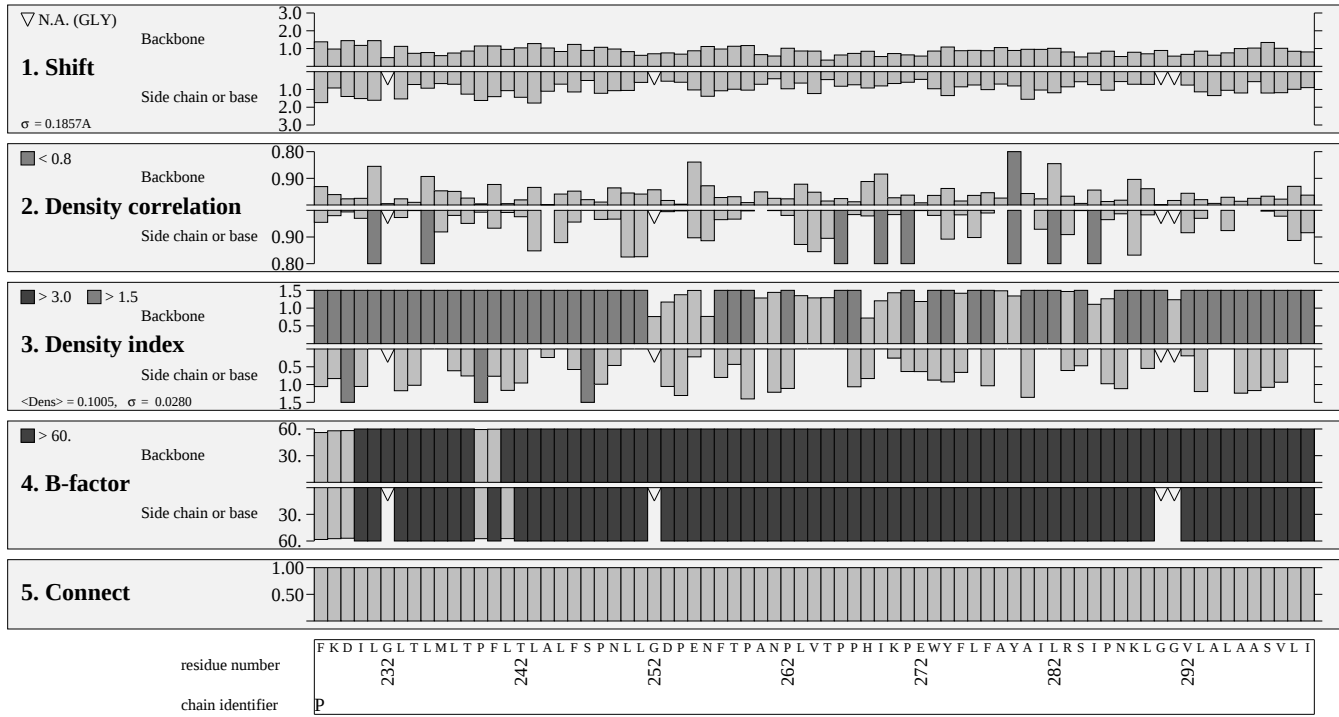
Local estimation (21)



Structure Factor Check

3H1I

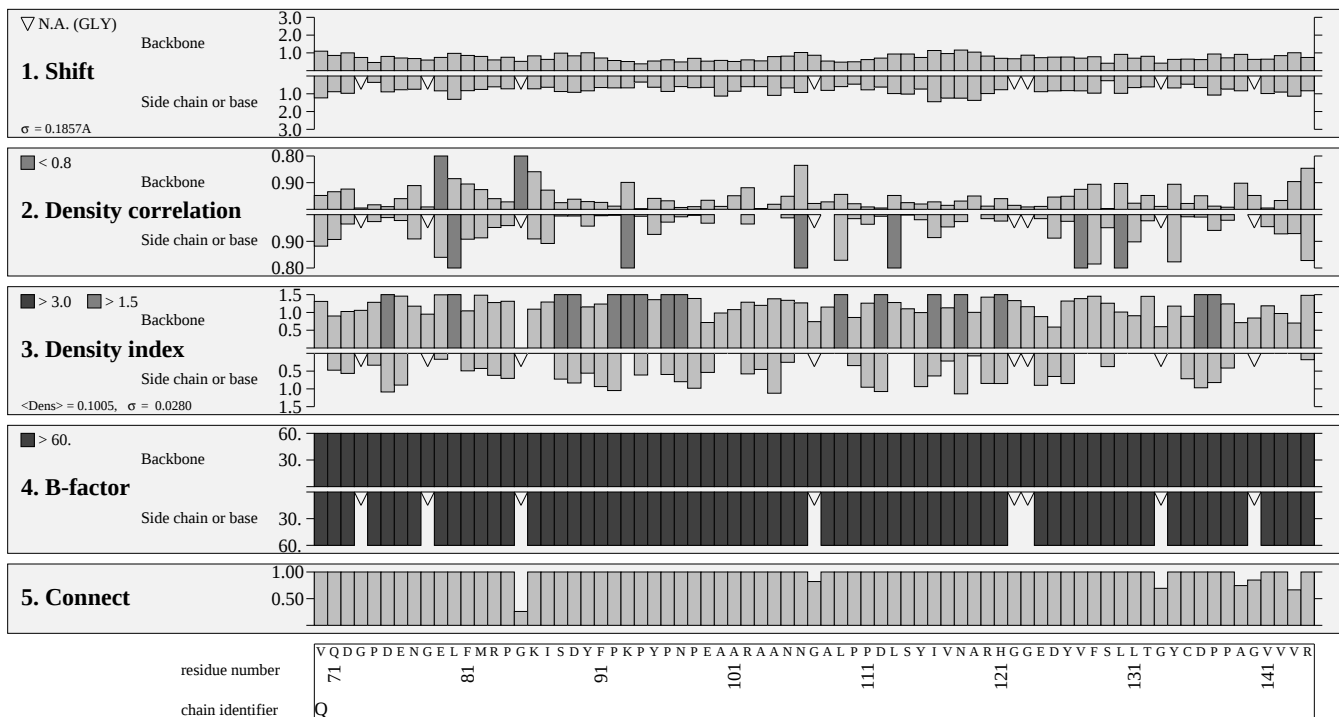
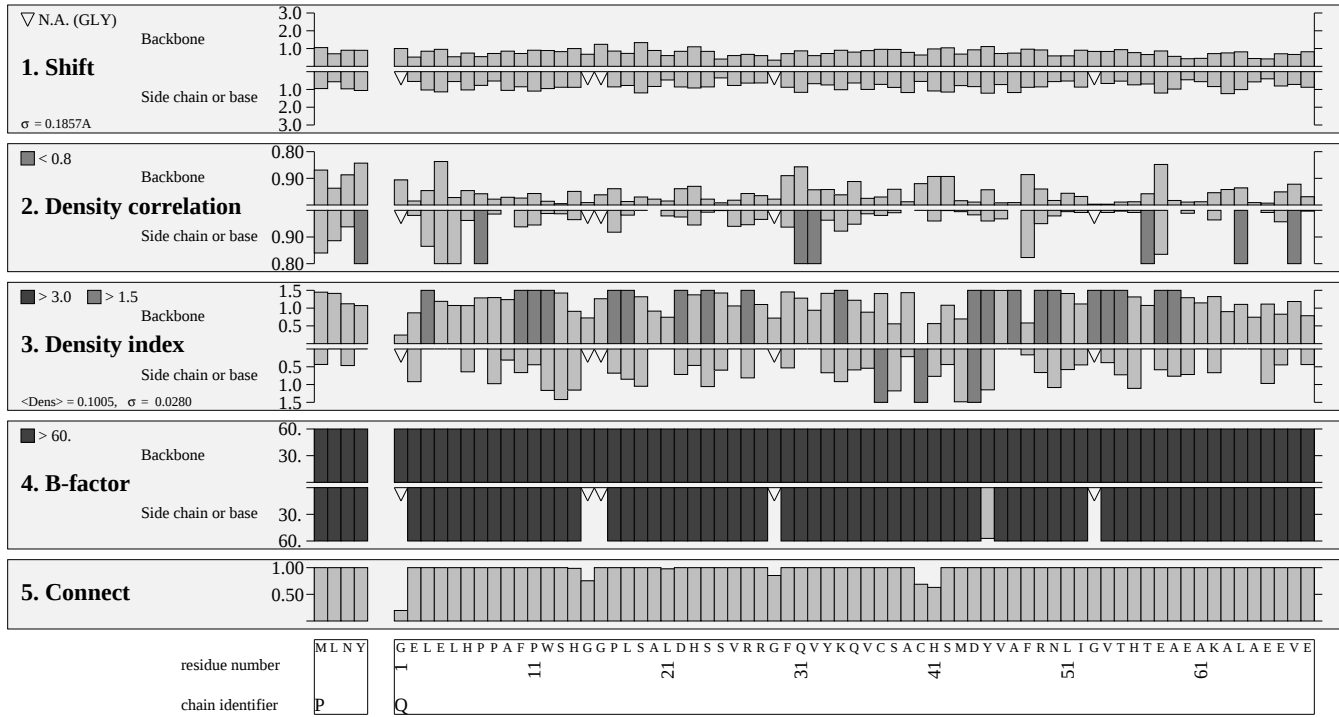
Local estimation (22)



Structure Factor Check

3H1I

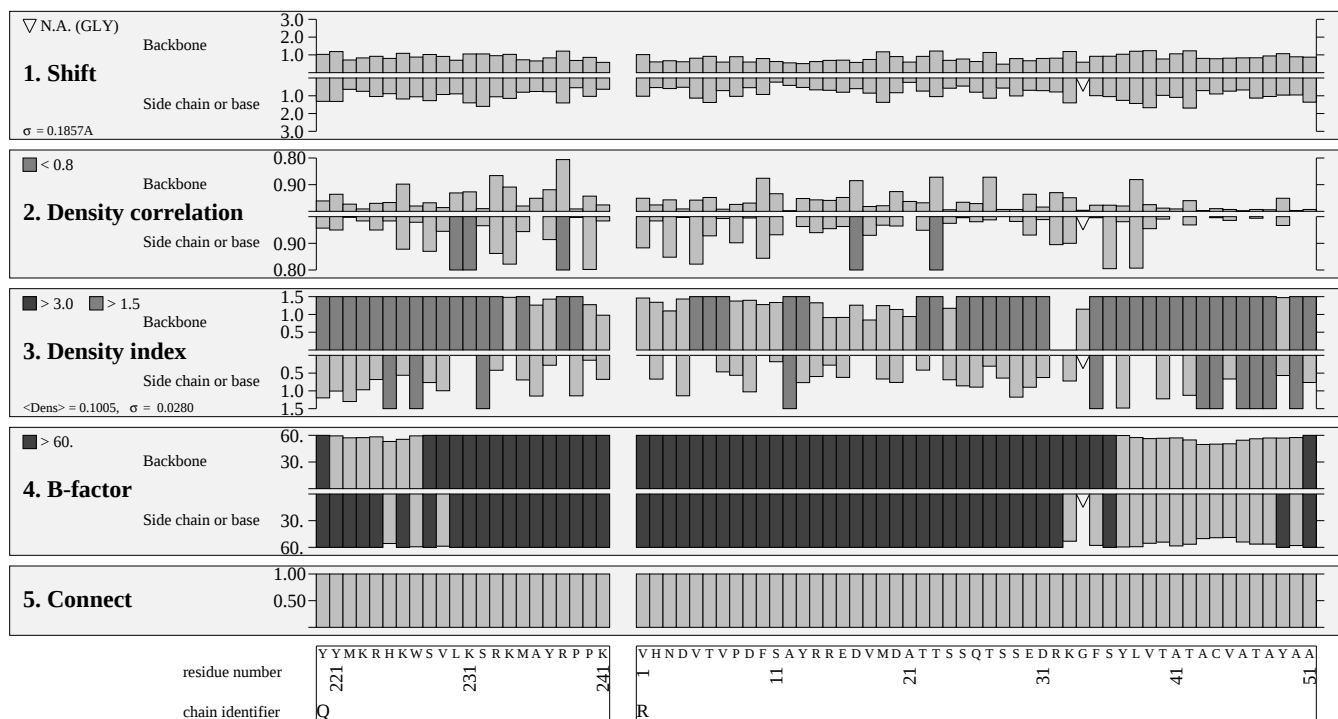
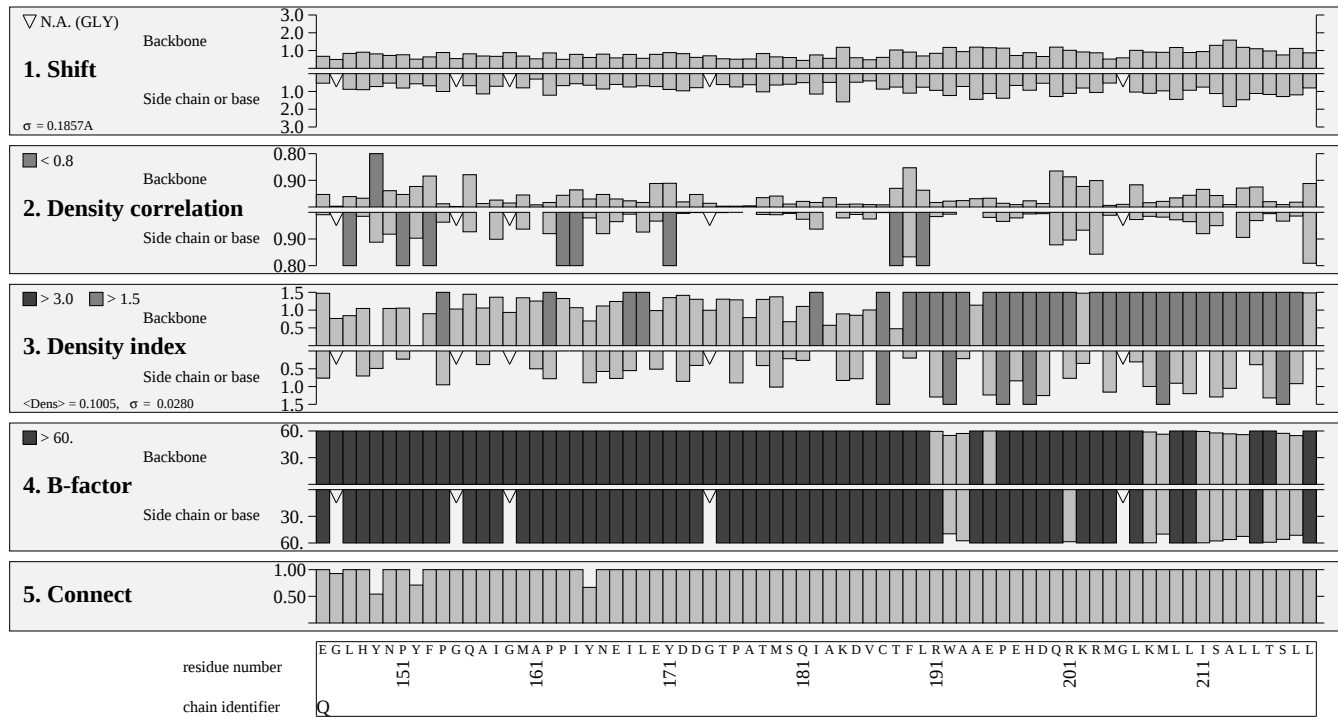
Local estimation (23)



Structure Factor Check

3H1I

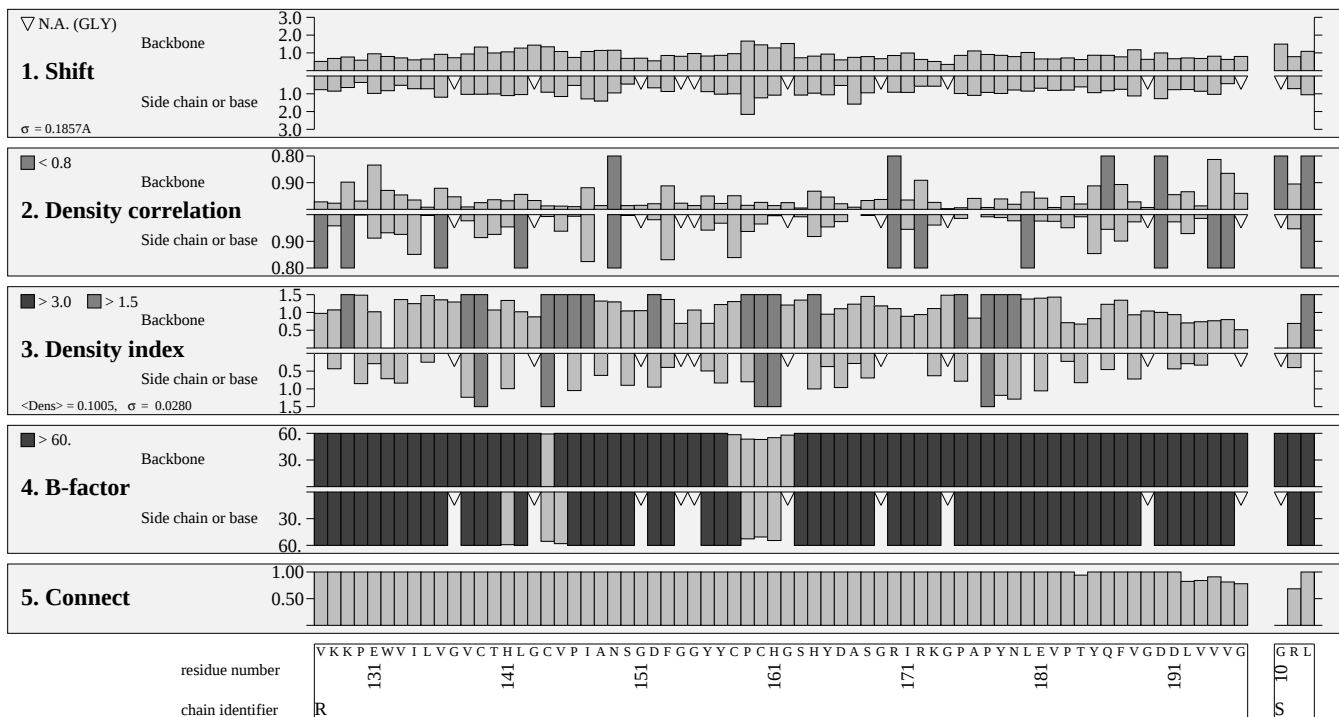
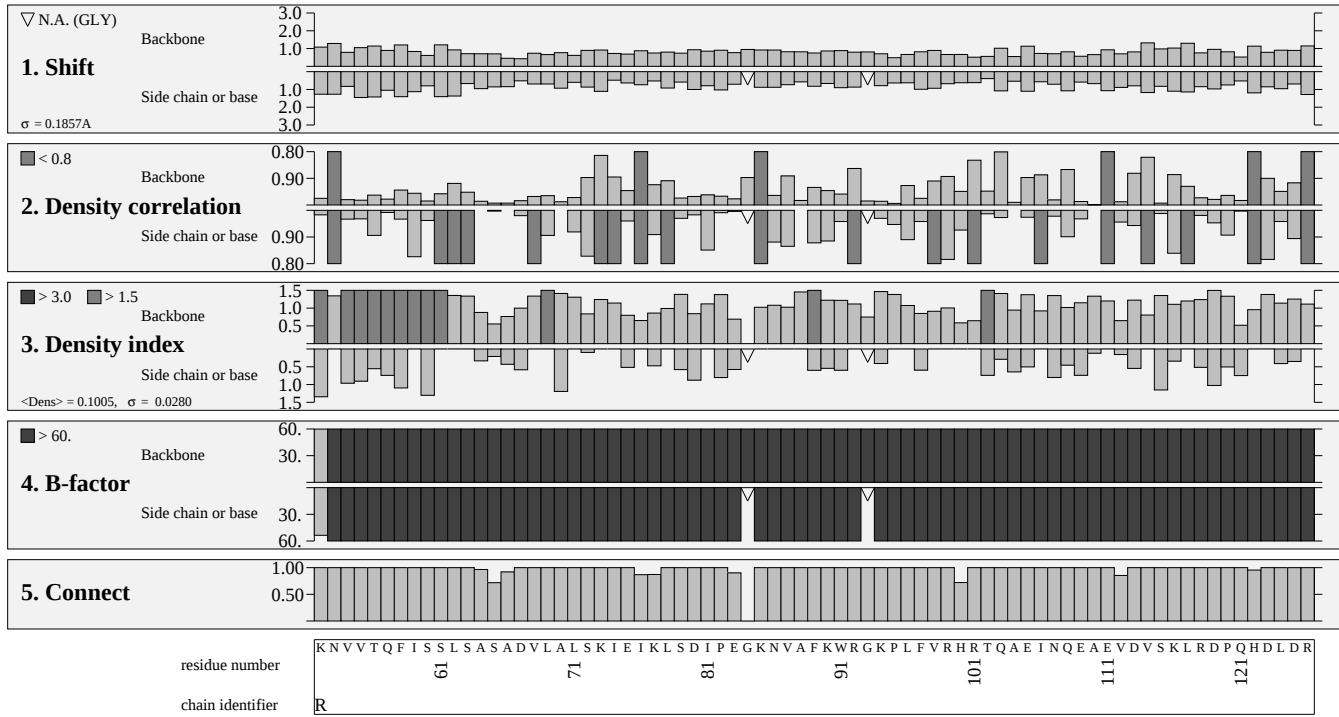
Local estimation (24)



Structure Factor Check

3H1I

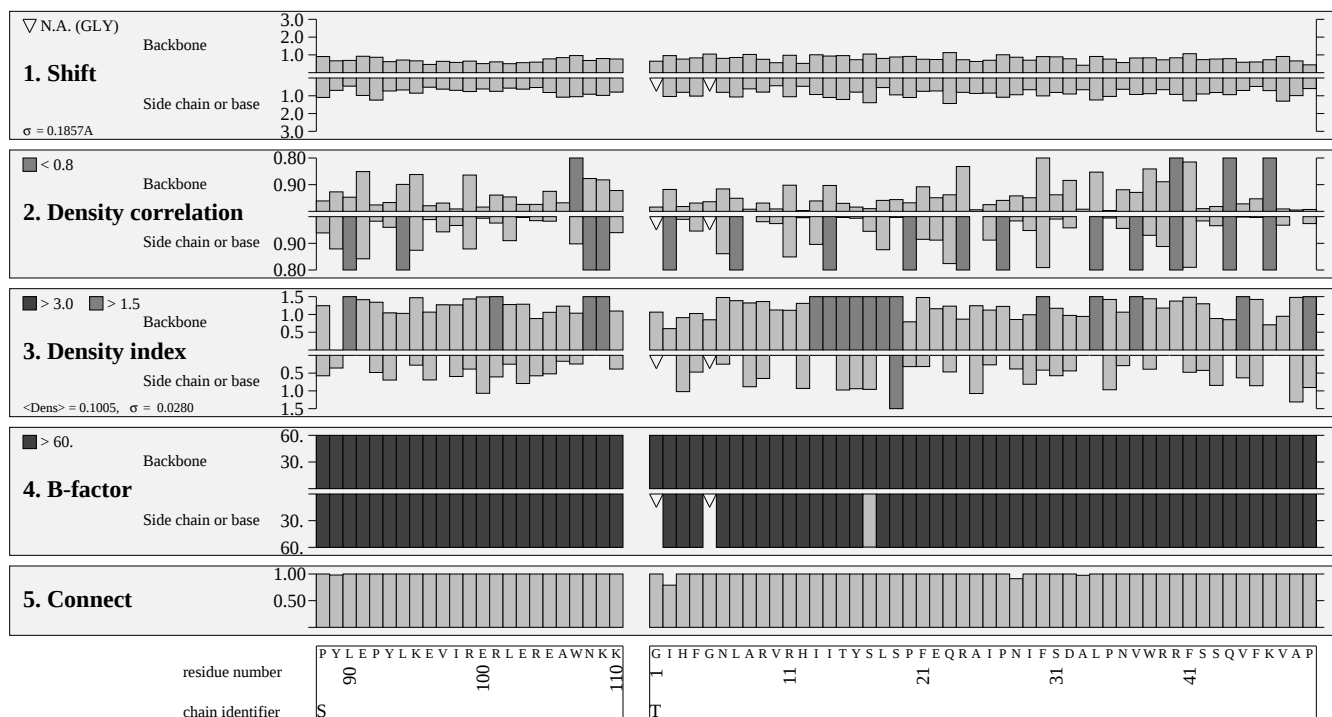
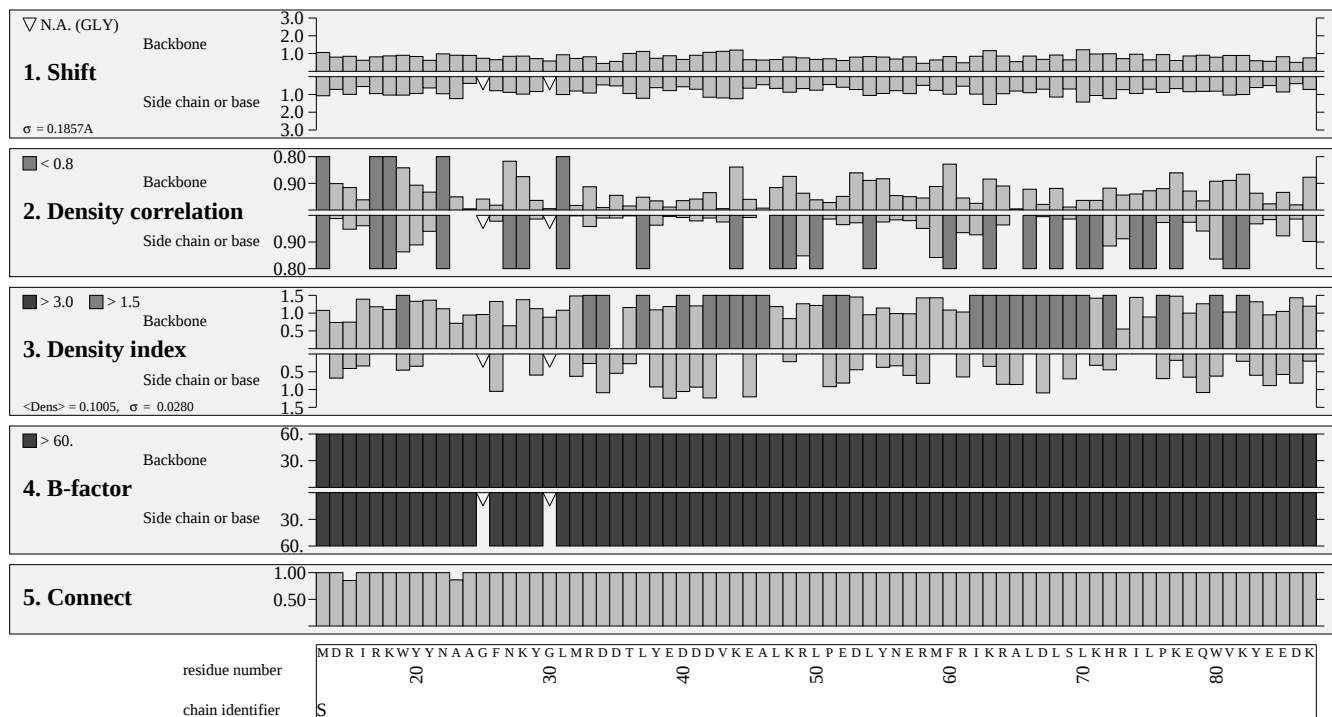
Local estimation (25)



Structure Factor Check

3H1I

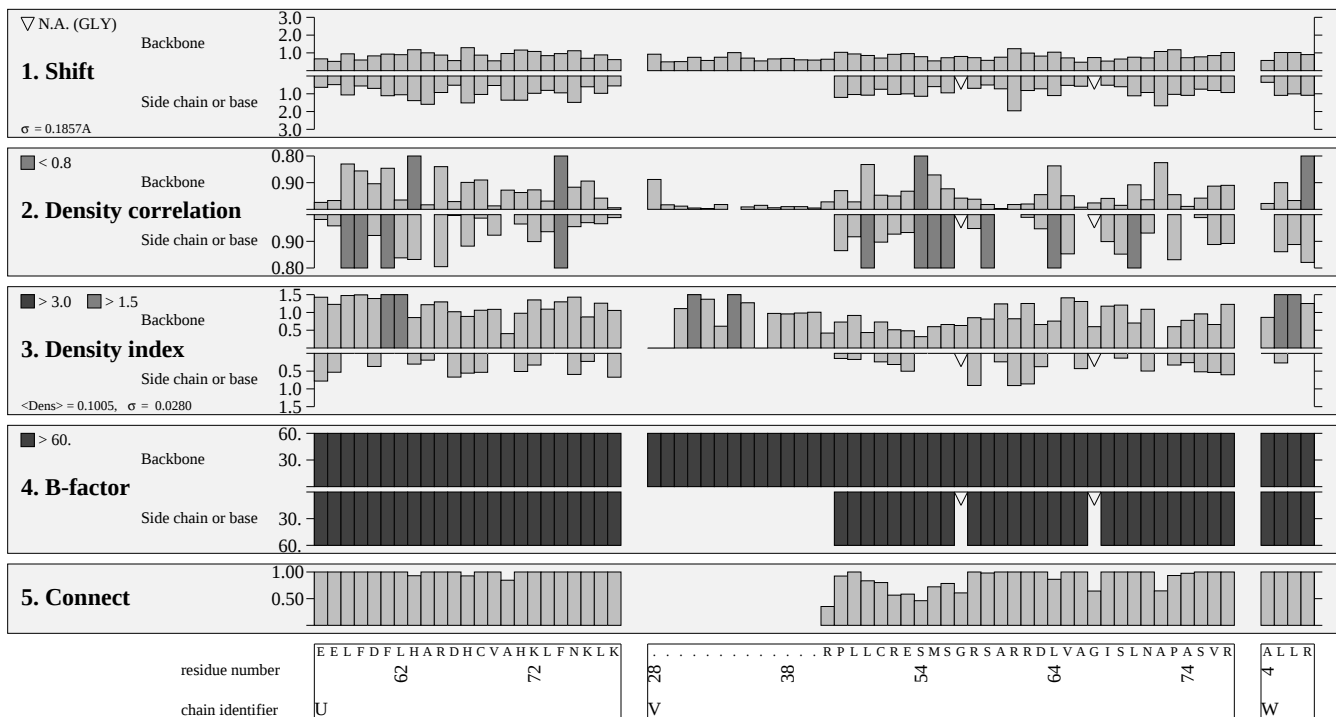
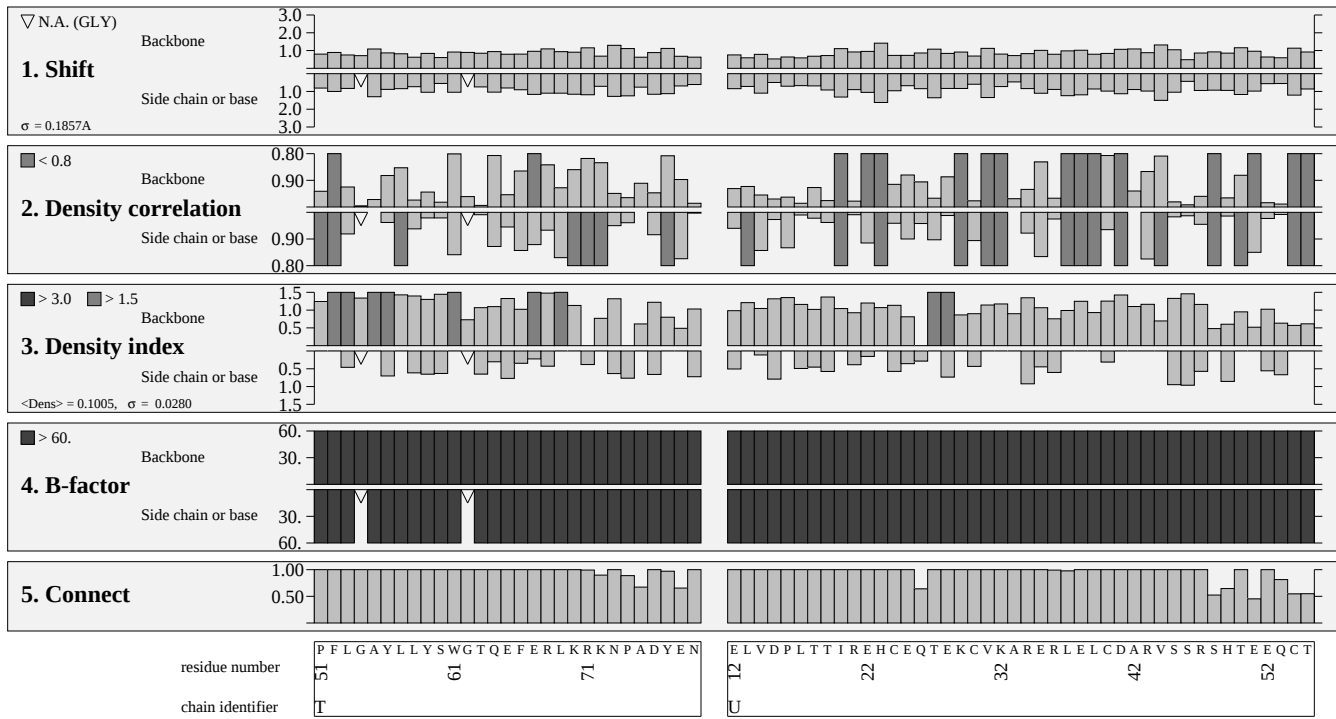
Local estimation (26)



Structure Factor Check

3H1I

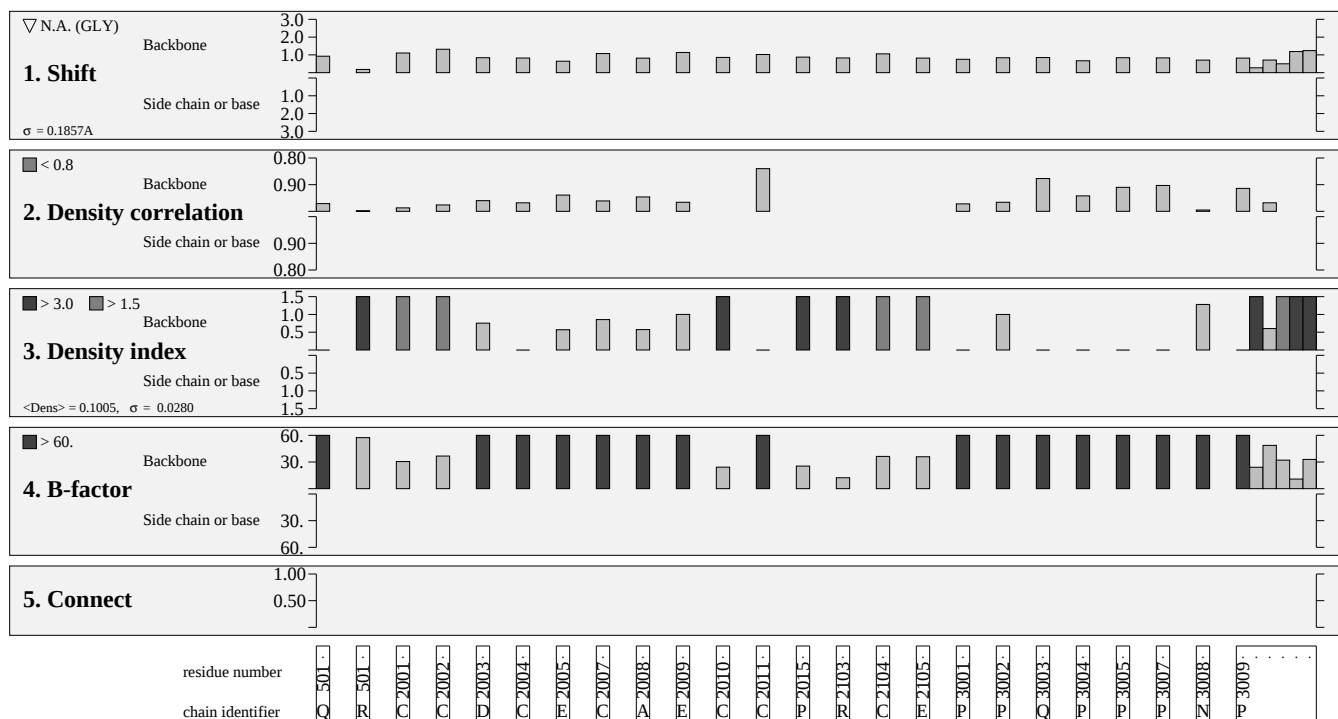
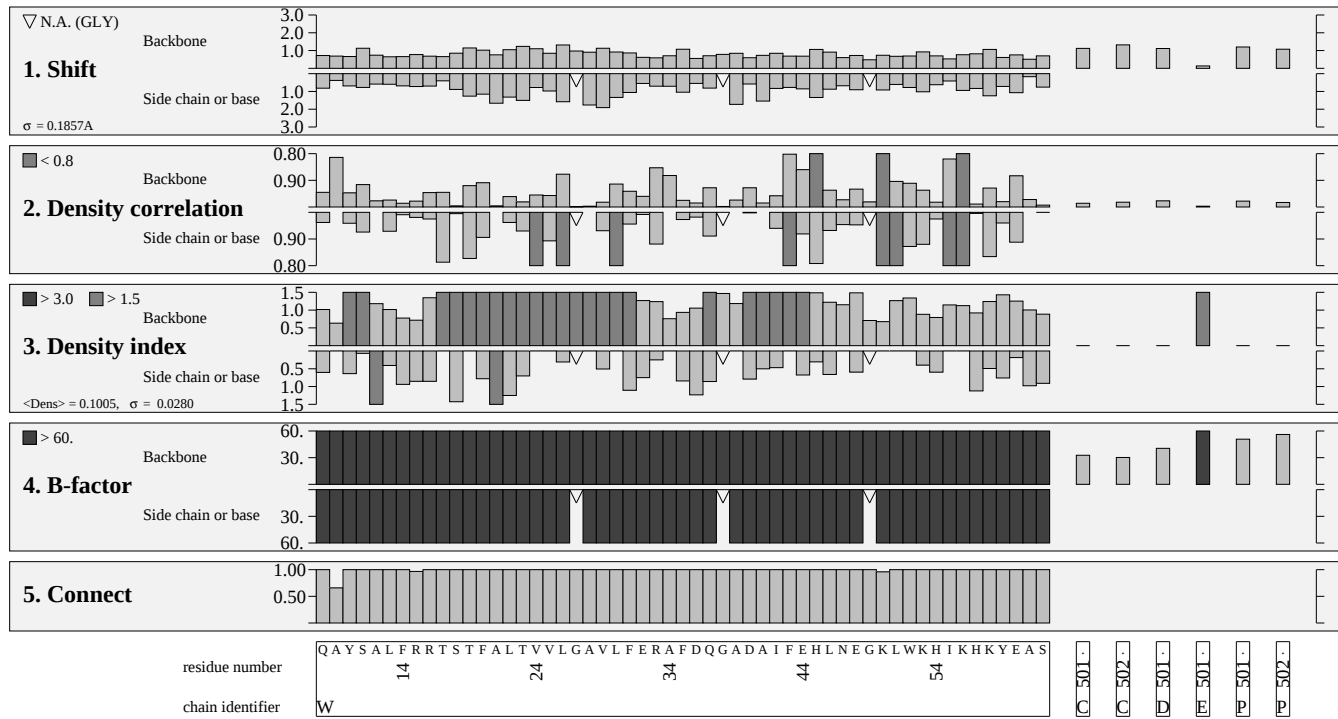
Local estimation (27)



Structure Factor Check

3H1I

Local estimation (28)



Structure Factor Check

3H1I

Local estimation (29)



residue number

chain identifier