

Structure Factor Check

3H1K

Title: CHICKEN CYTOCHROME BC1 COMPLEX WITH ZN++ AND AN IODINATED DE
OF KRESOXIM-METHYL BOUND
Date: 12-APR-09
PDB code: 3H1K

Crystal

Cell parameters:

a: 171.72 Å b: 181.30 Å c: 241.29 Å
α: 90.00 β: 90.00 γ: 90.00

Space group: P 21 21 21

Model

32673 atoms (17 water molecules)

Number of chains: 51

Volume not occupied by model: 62.0 %

 (for atomic model): 89.7 Å²

σ(B): 14.10 Å²

Matthews coefficient: 4.11

Corresponding solvent % : 69.80

Refinement

Program: CNS 1.1

Nominal resolution range: 18.0 – 3.48 Å

Reported R-factor: 0.239

Number of reflections used: 86369

Reported Rfree: 0.28

Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 42.6 – 3.48 Å

Reflections in file: 86926

Unique reflections above 0: 86926

above 1σ: 84850

above 3σ: 43497

SF CHECK

Nominal resolution range: 42.6 – 3.48 Å

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

Used reflections: 86926

Completeness: 89.6 %

R_{stand}(F) = <σ(F)>/<F> : 0.099

Anisotropic distribution of Structure Factors

ratio of eigen values: 1.0000 0.5227 0.6748

B_{overall} (by Patterson): 63.Å²

Optical resolution: 2.51 Å

Expected opt. resol. for complete data set: 2.51 Å

Estimated minimal error: 0.205 Å

Model vs. Structure Factors

R-factor for all reflections: 0.315

Correlation factor: 0.799

R-factor: 0.313

for F > 2.0σ

nom. resolution range: 18.00 – 3.48Å

reflections used: 84309

Rfree: 0.340

Nfree: 2500

R-factor without free-refl.: 0.312

Non free-reflections: 81809

<u> (error in coords by Luzzati plot): 0.684 Å

Estimated maximal error: 0.539 Å

DPI: 0.628 Å

Scaling

Scale: 0.655

Bdiff: -8.11

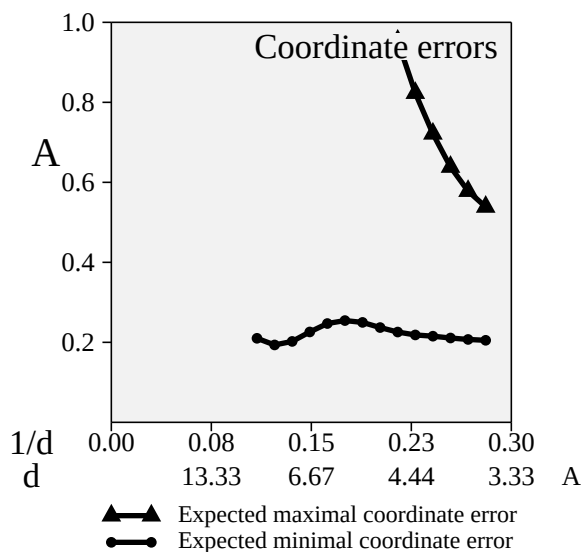
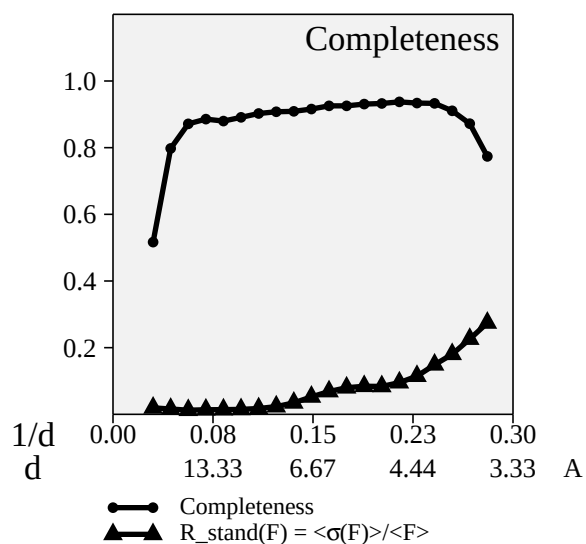
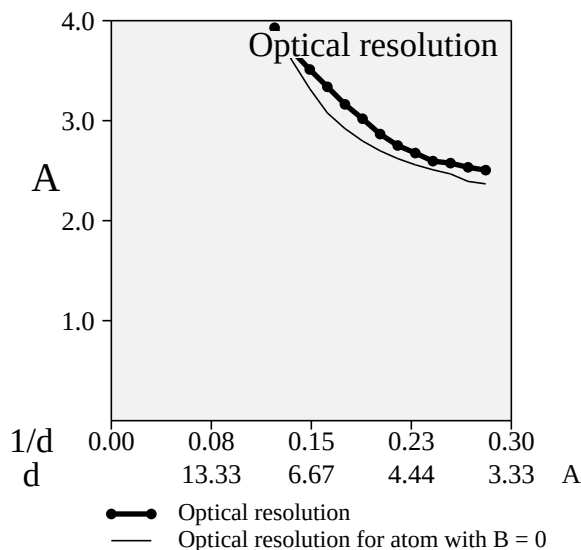
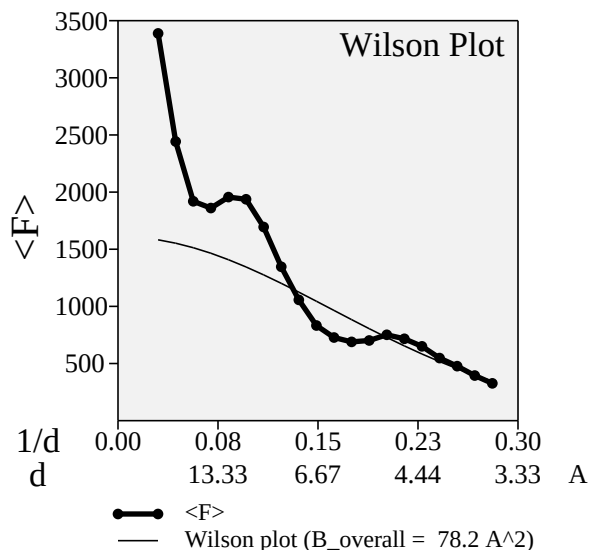
Anisothermal Scaling (Beta):

16.0876 -1.3143 4.7515 0.0000 0.0000 0.0000

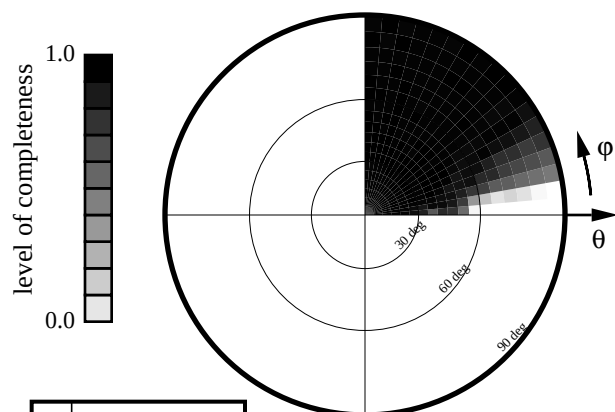
Solvent correction – Ks,Bs: 0.576 250.570

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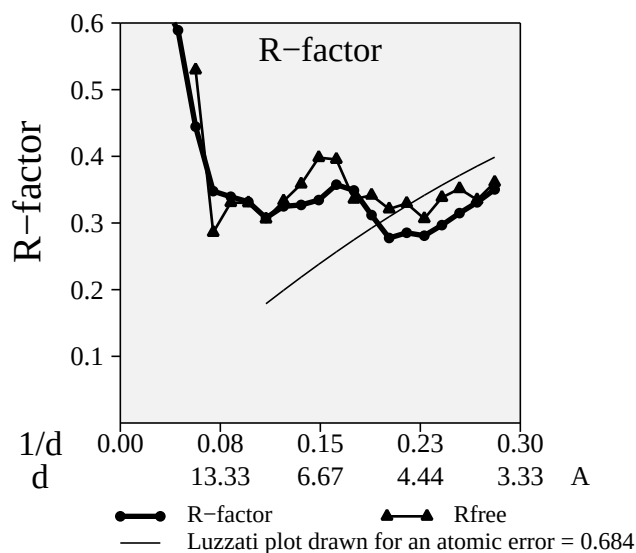


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

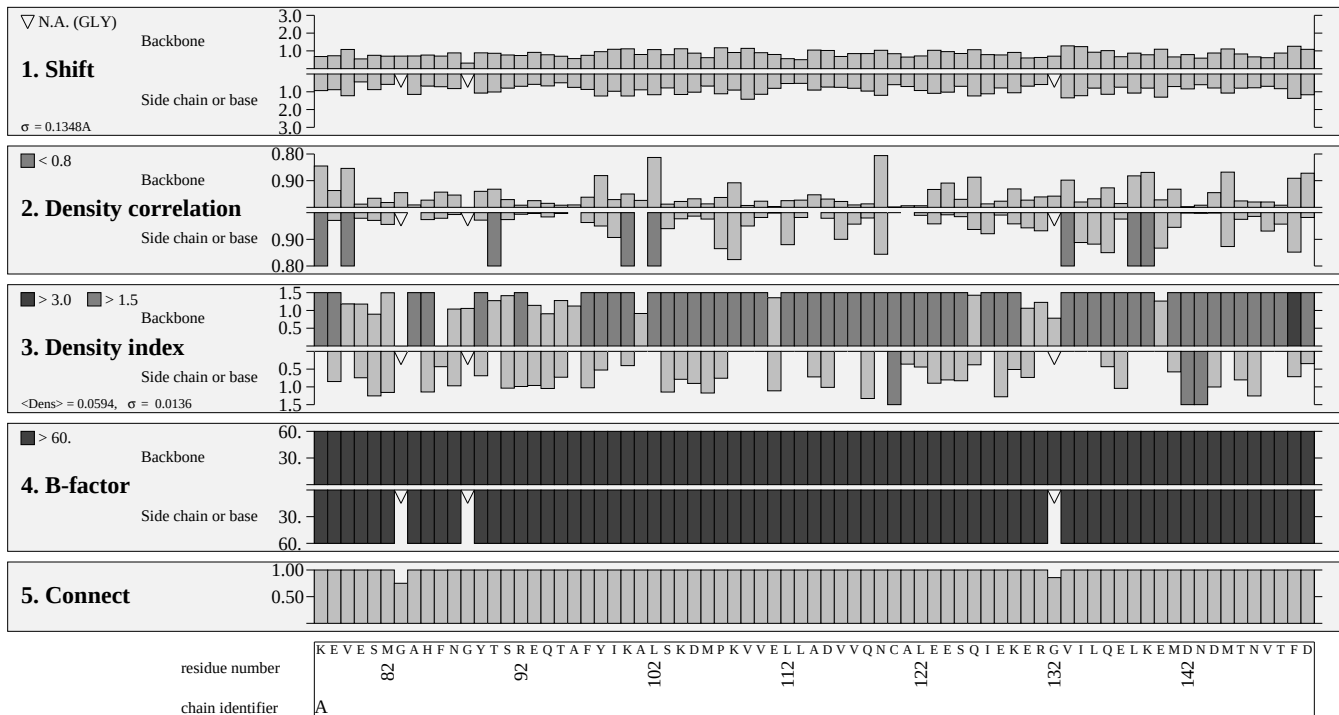
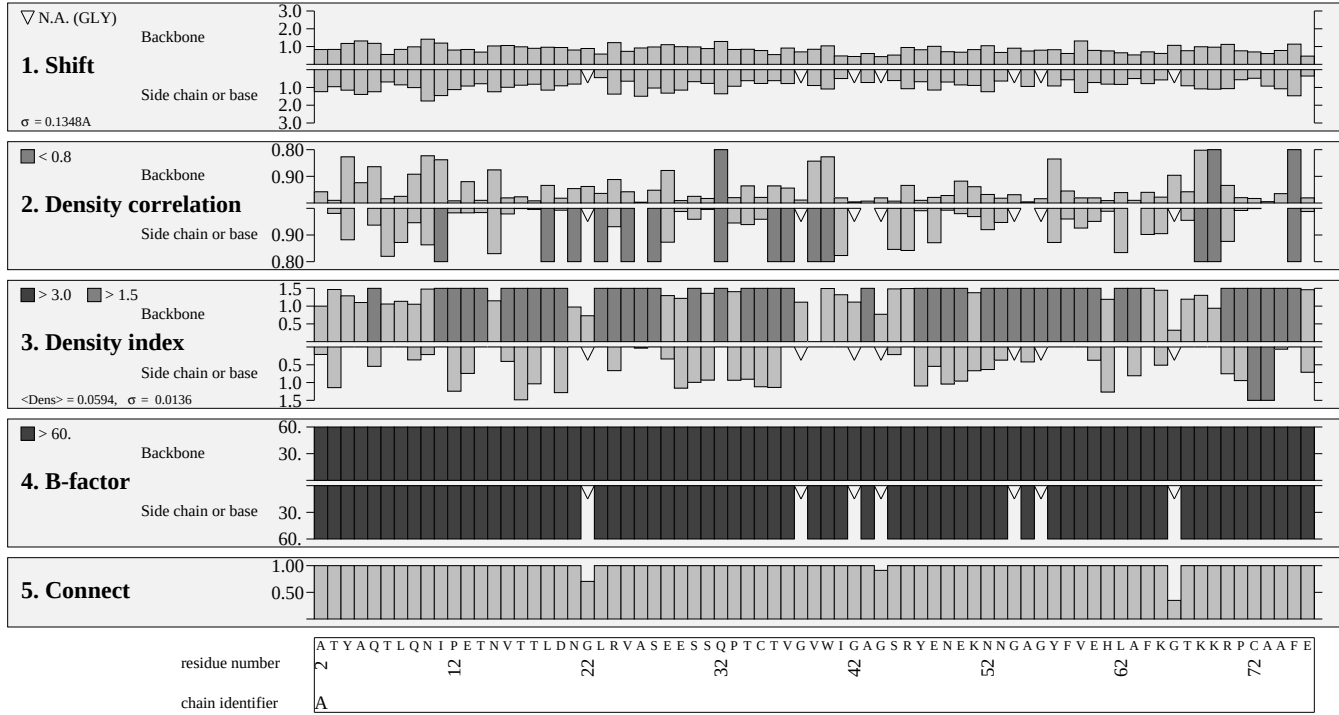
polar coordinates of the crystallographical axes



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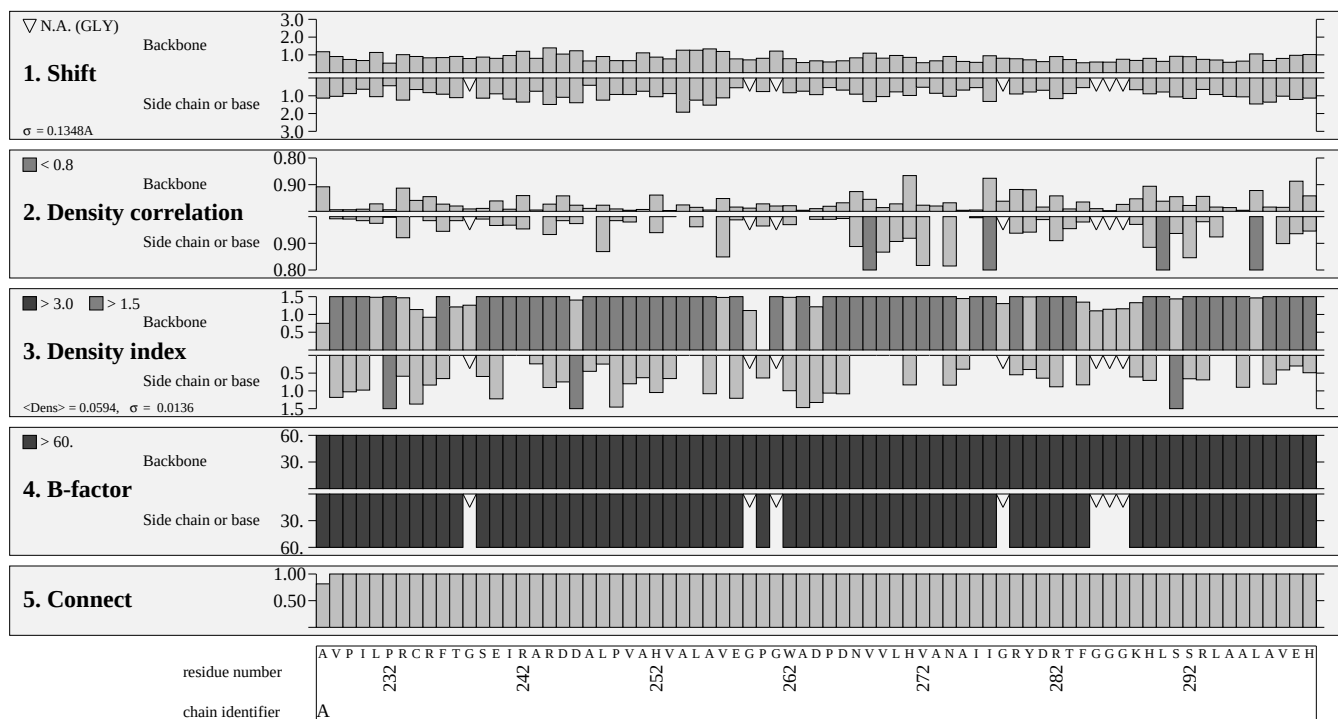
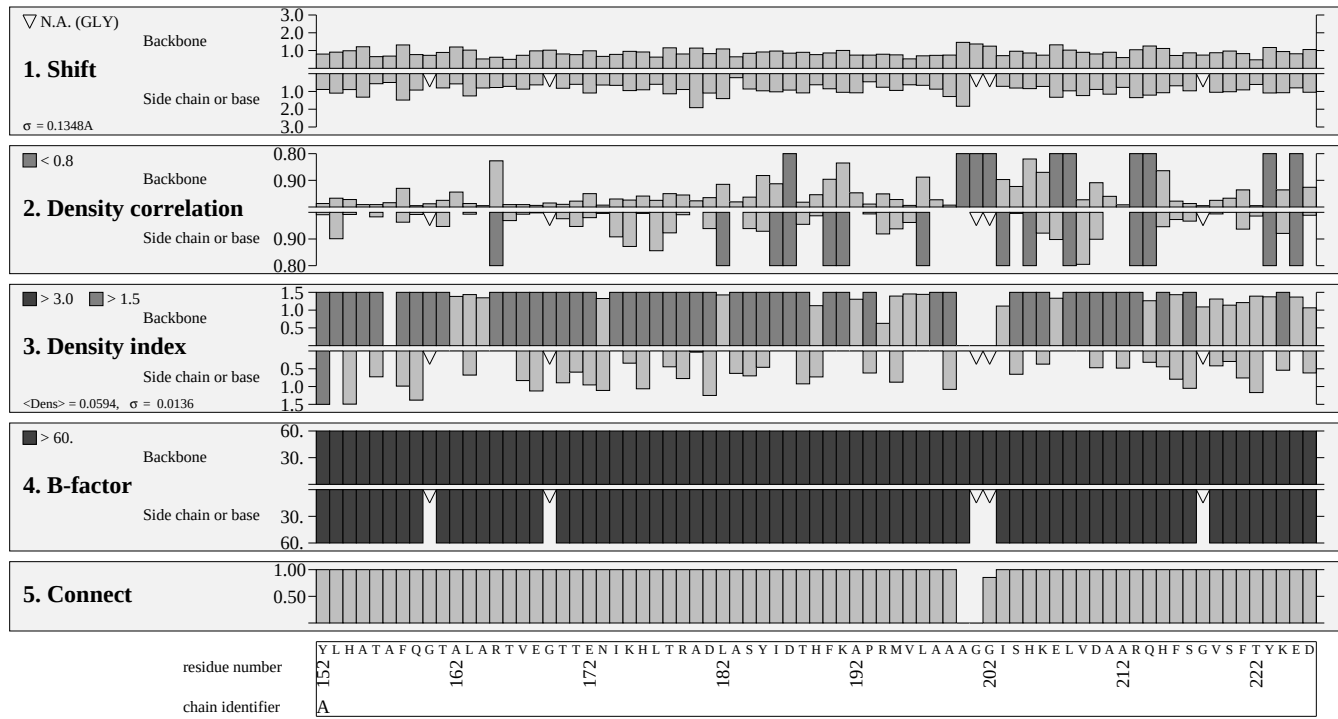
Local estimation



Structure Factor Check

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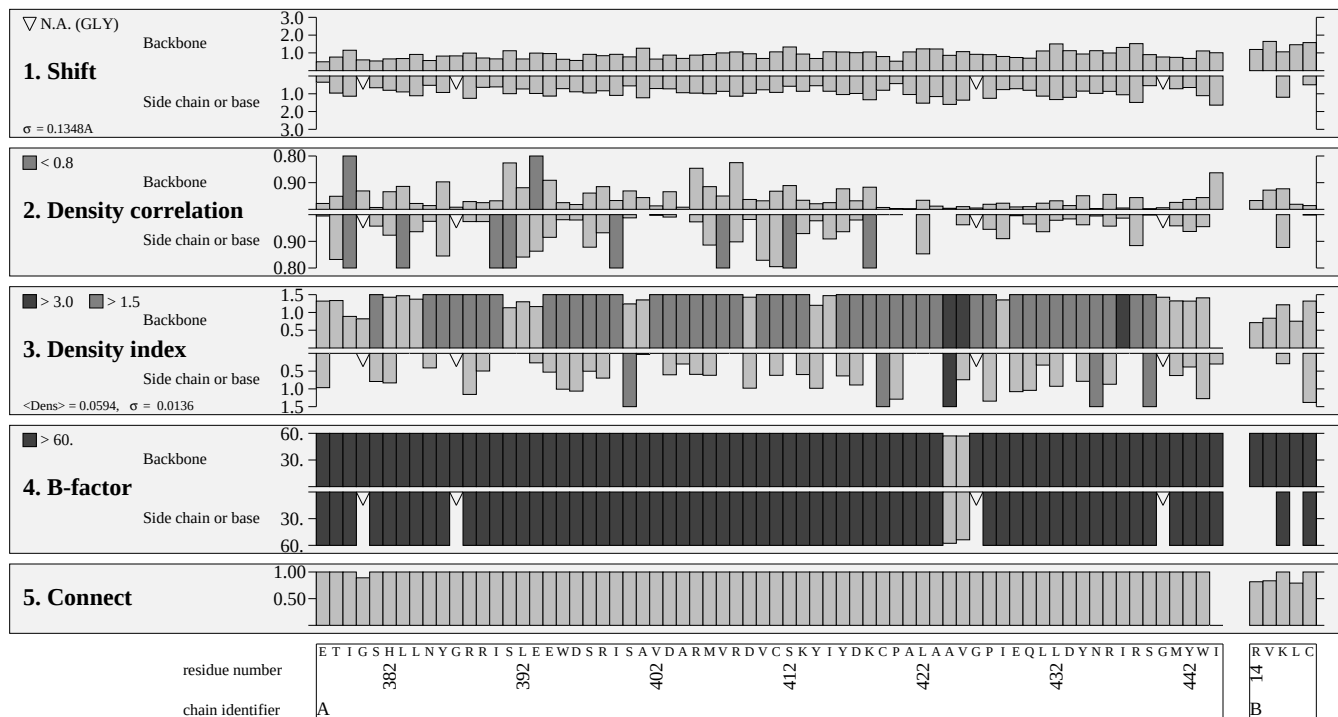
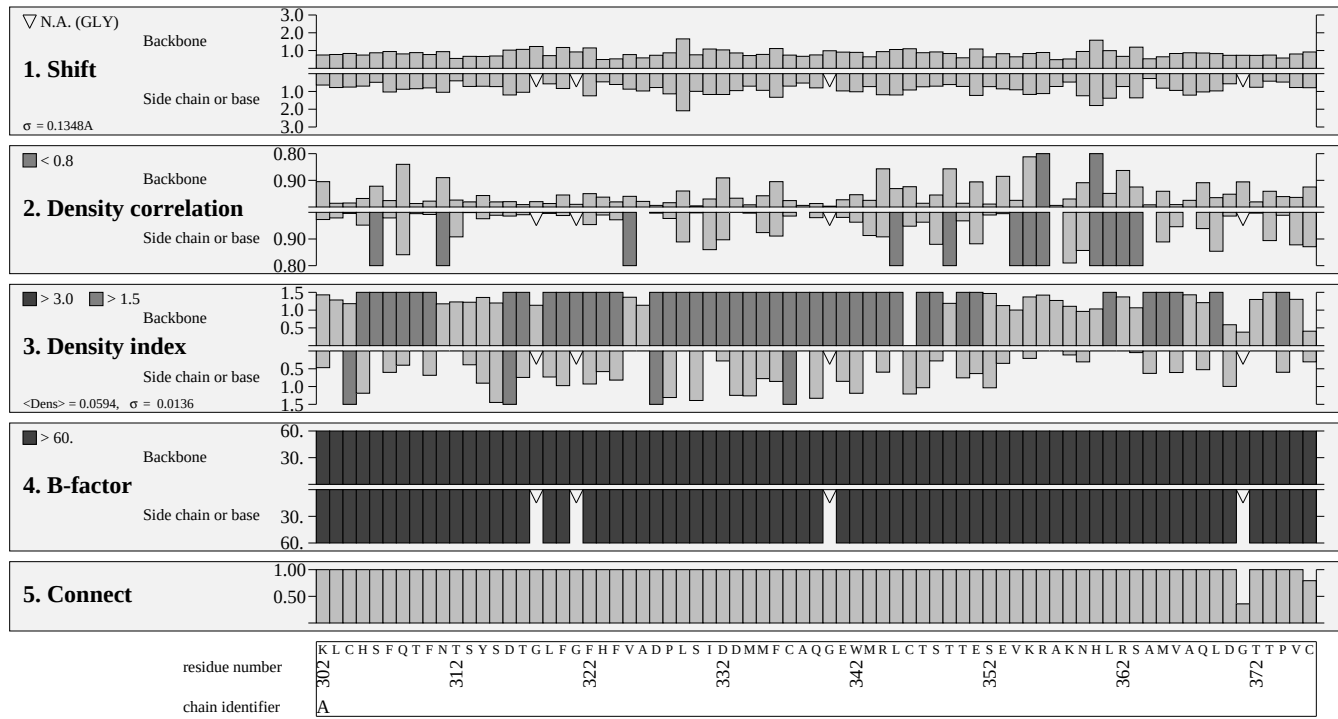
Local estimation (2)



Structure Factor Check

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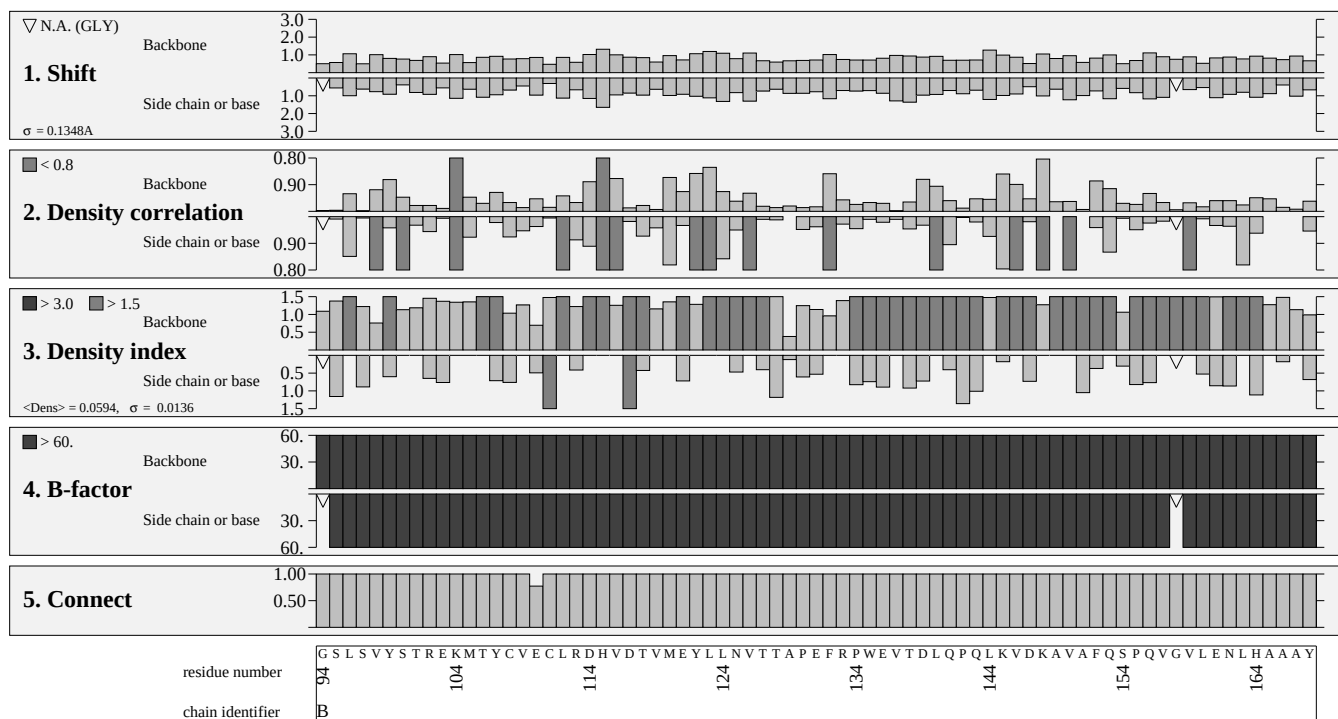
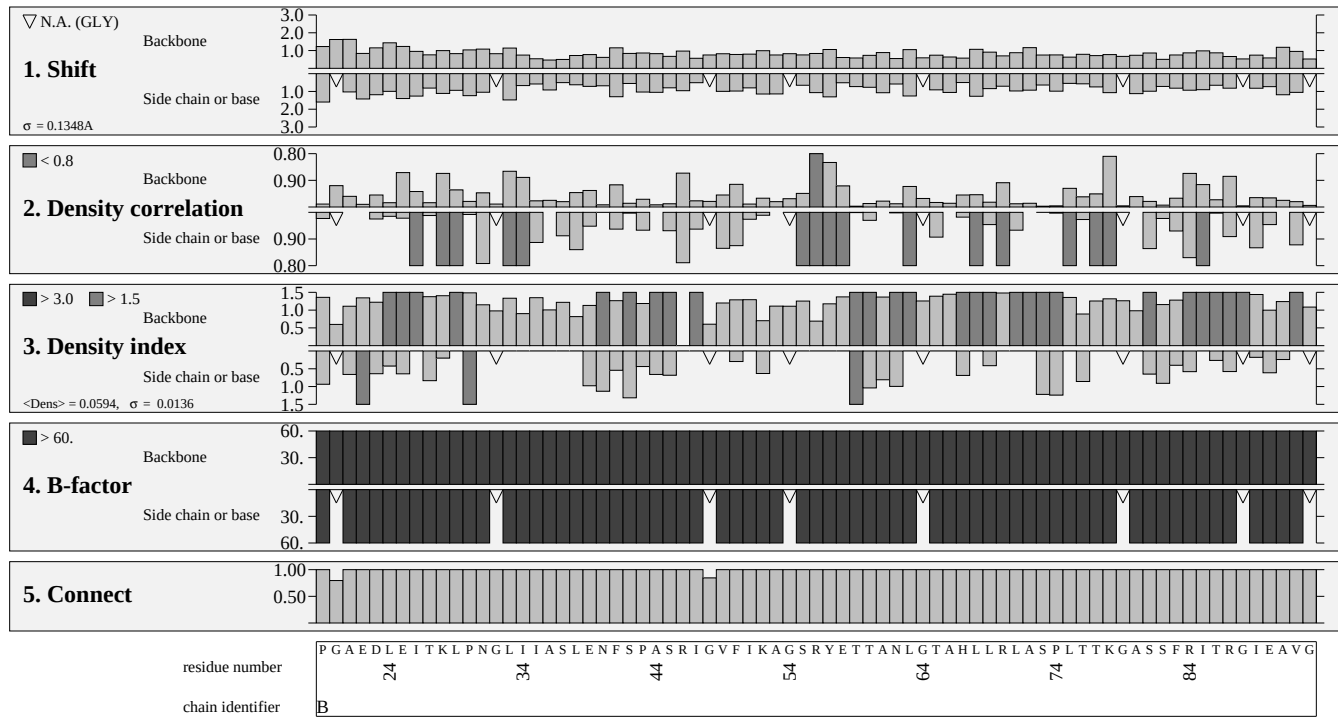
Local estimation (3)



Structure Factor Check

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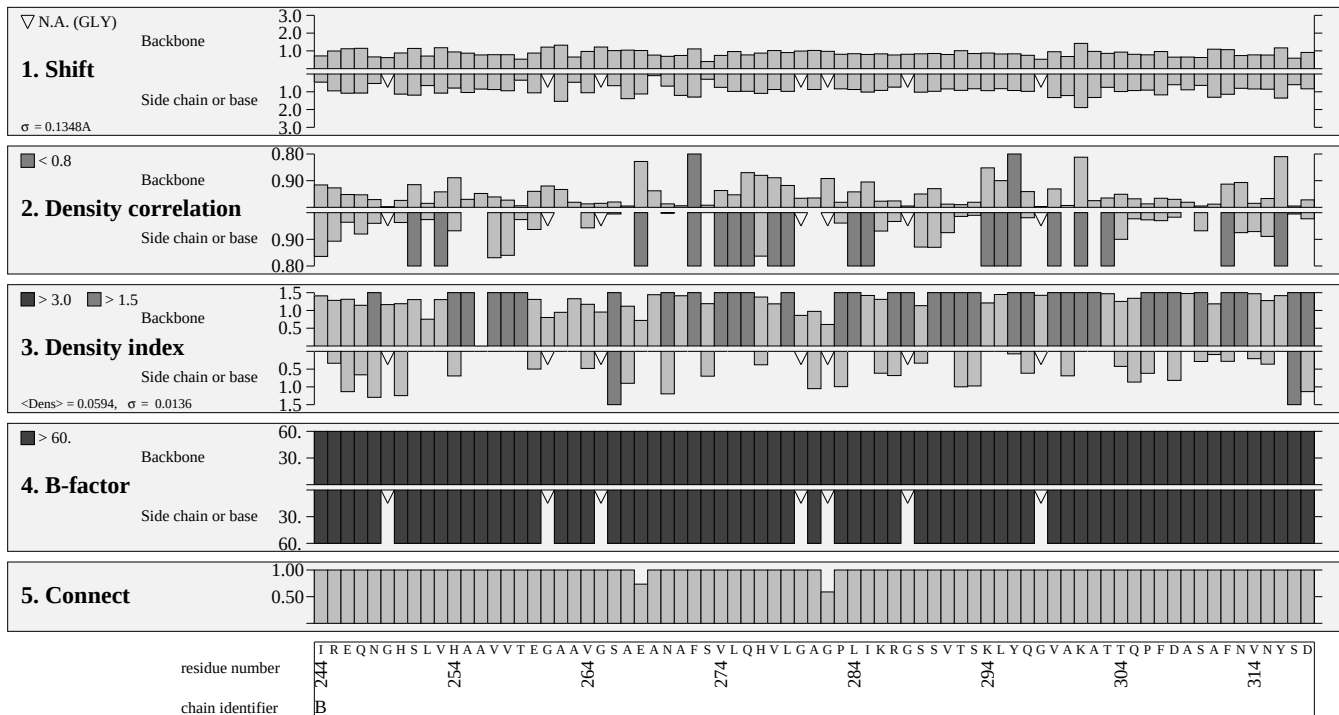
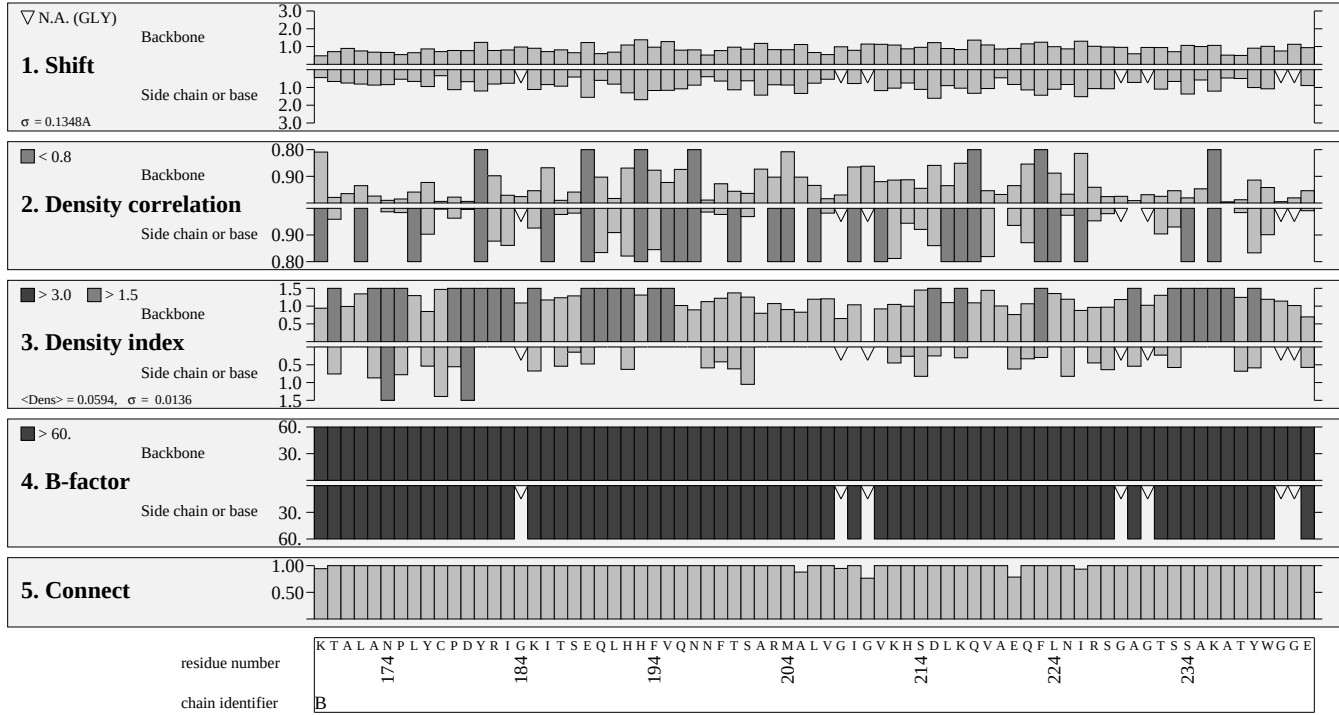
Local estimation (4)



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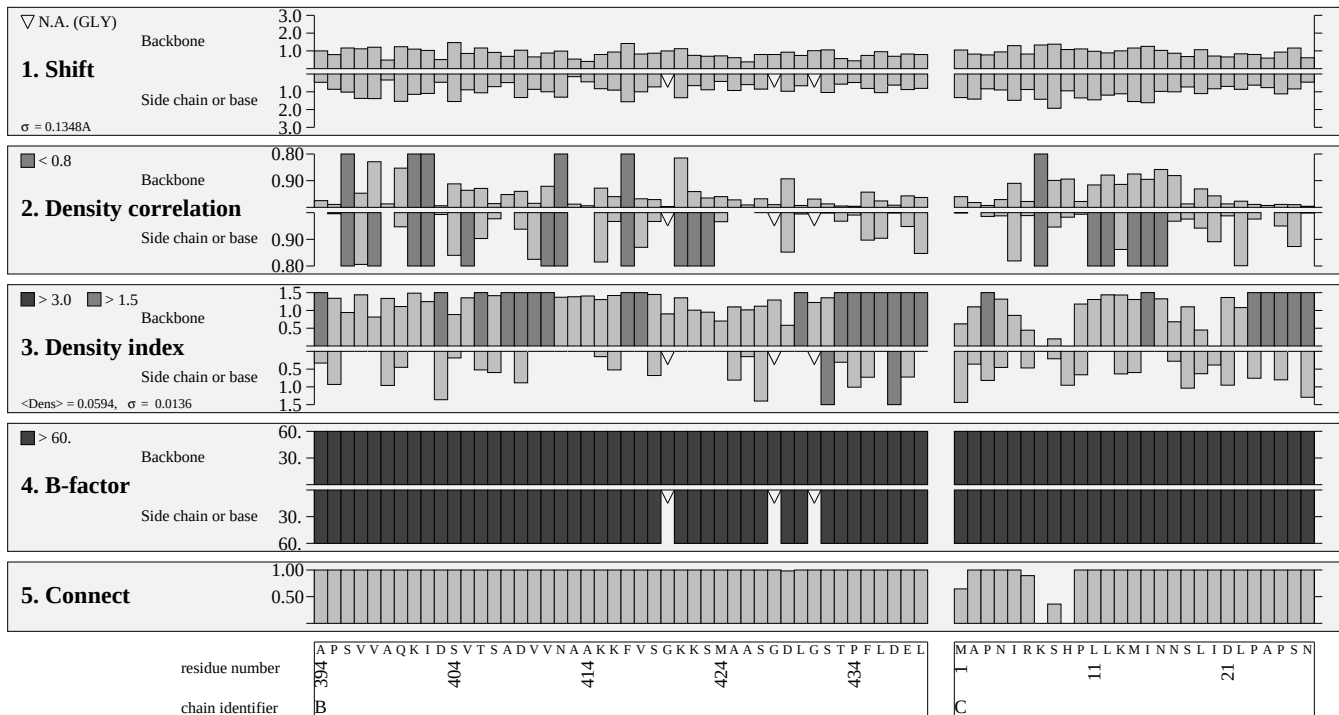
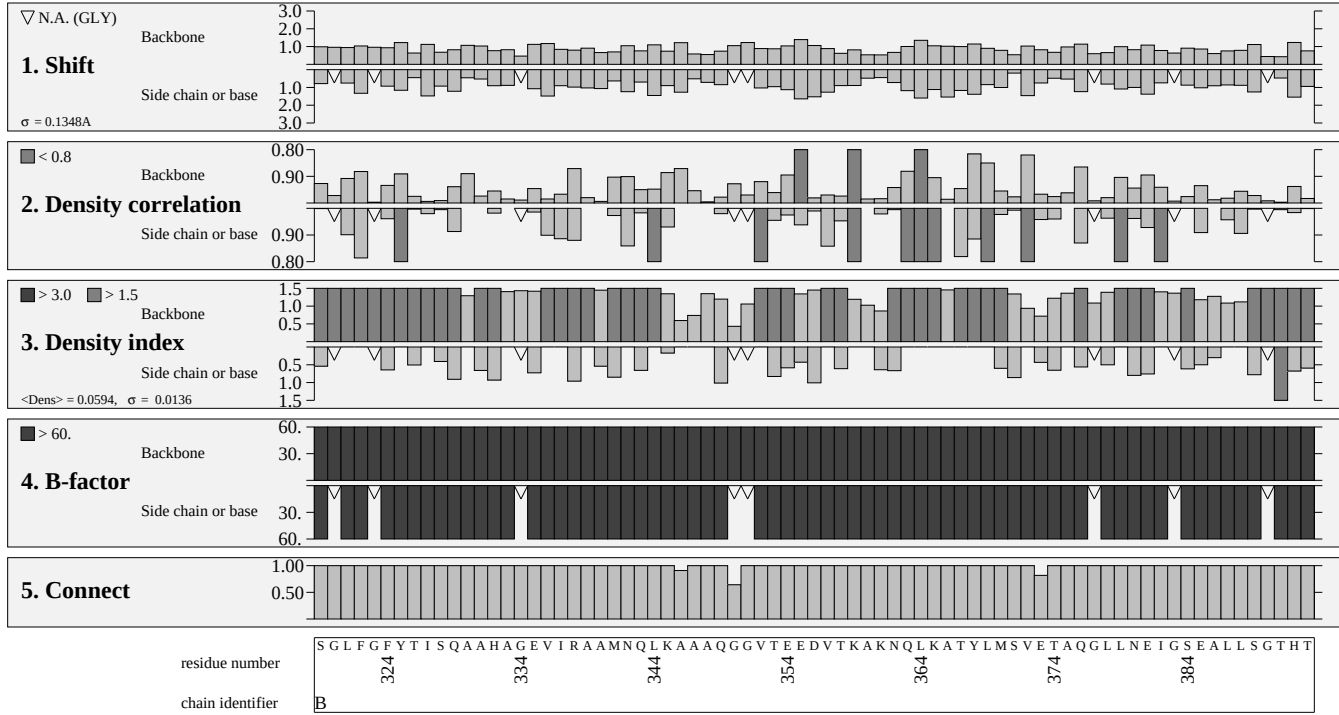
Local estimation (5)



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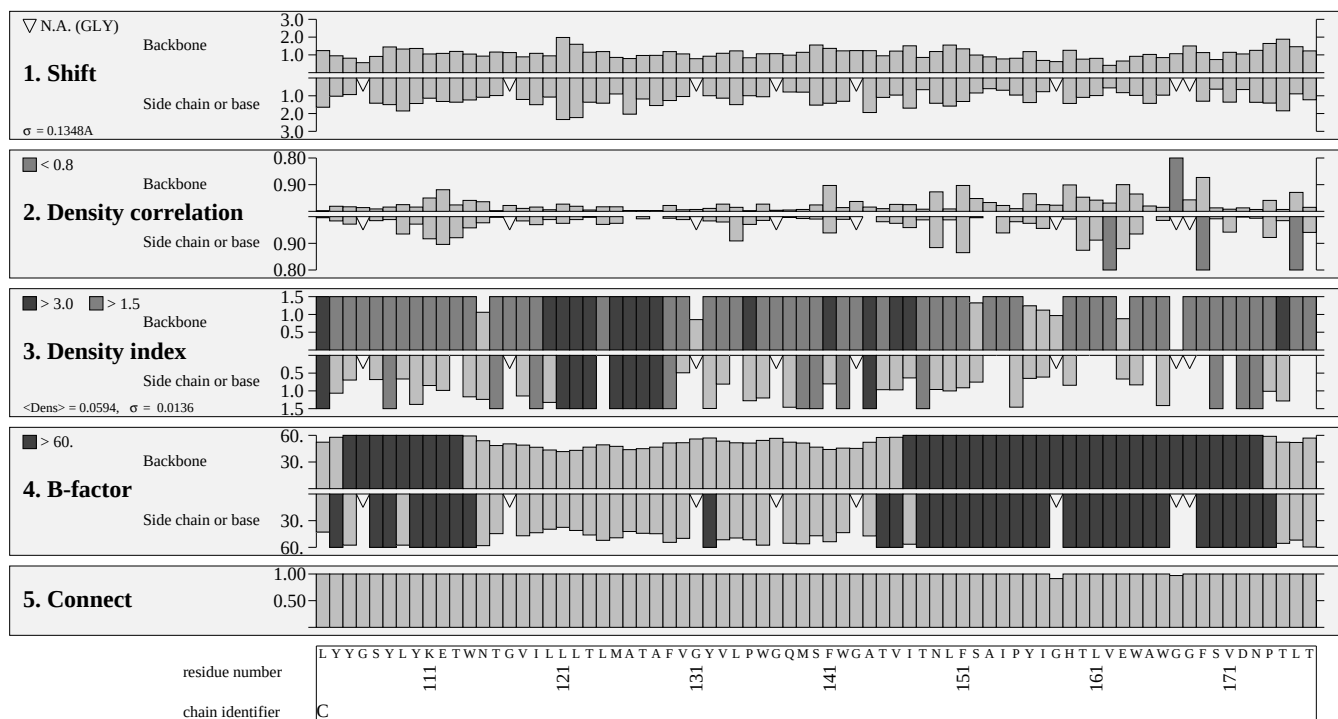
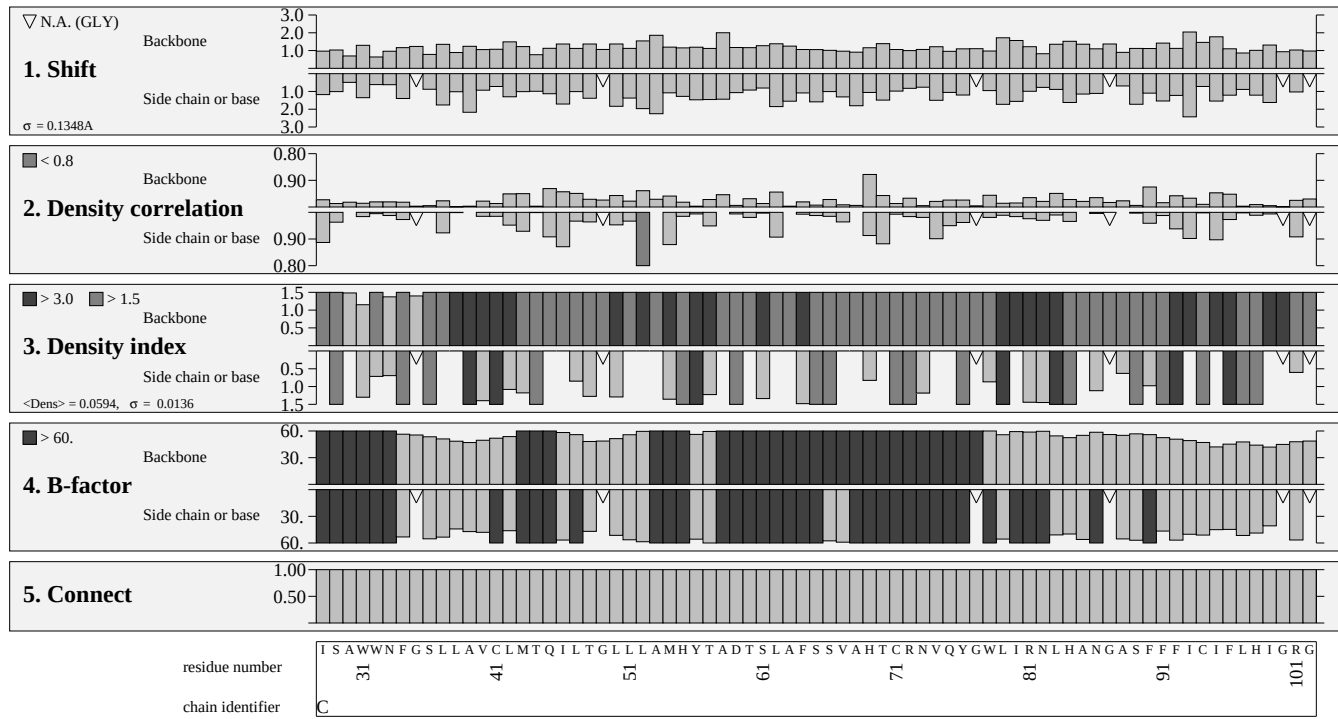
Local estimation (6)



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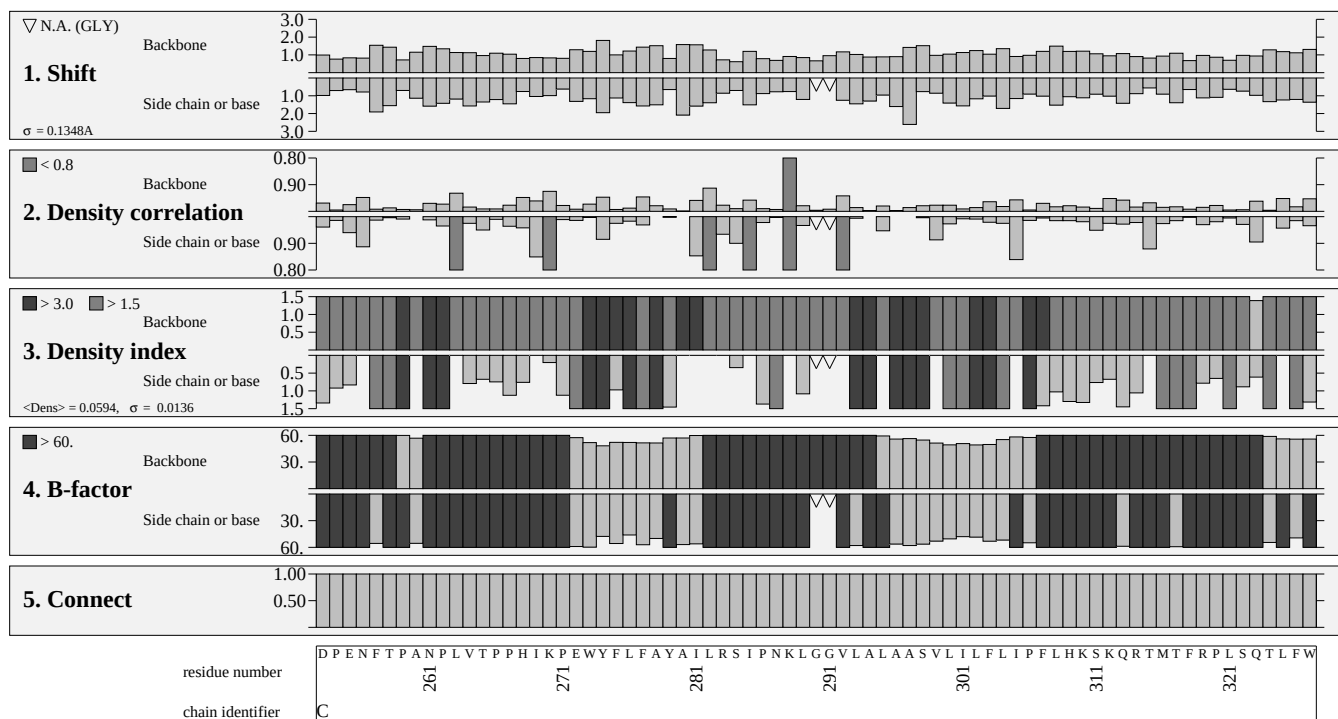
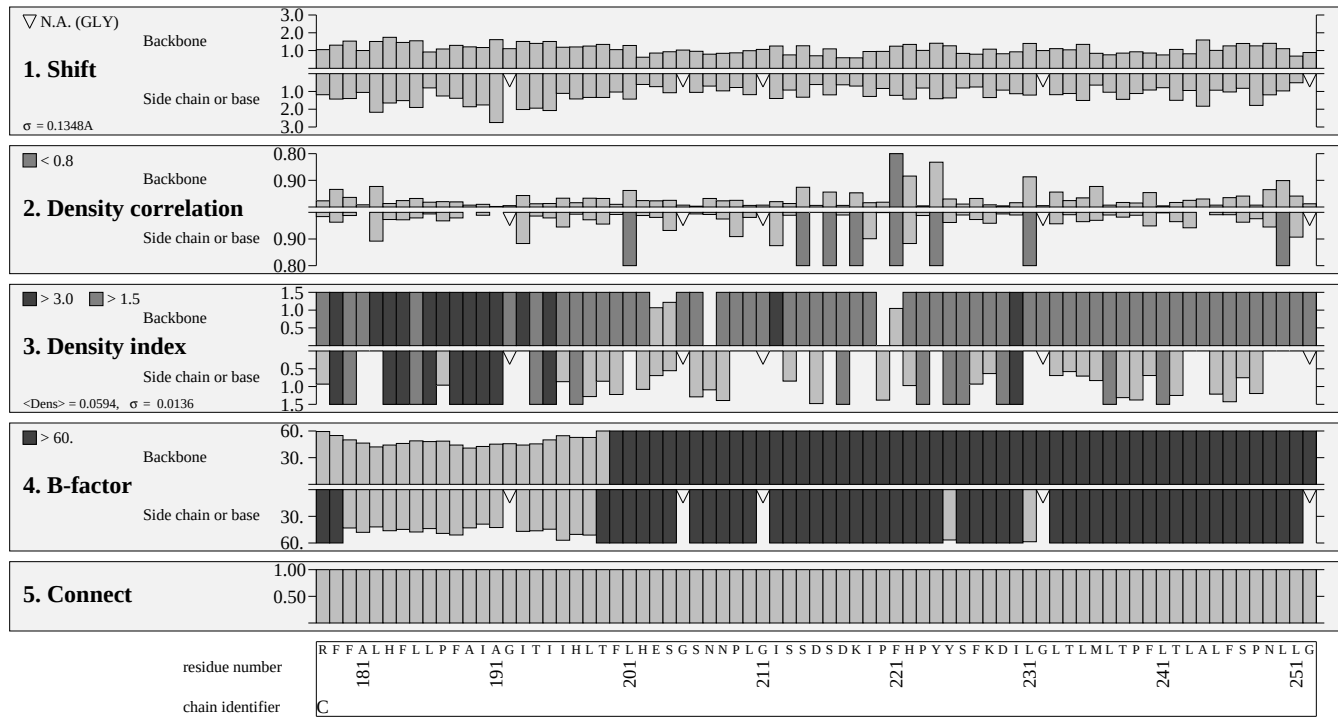
Local estimation (7)



Structure Factor Check

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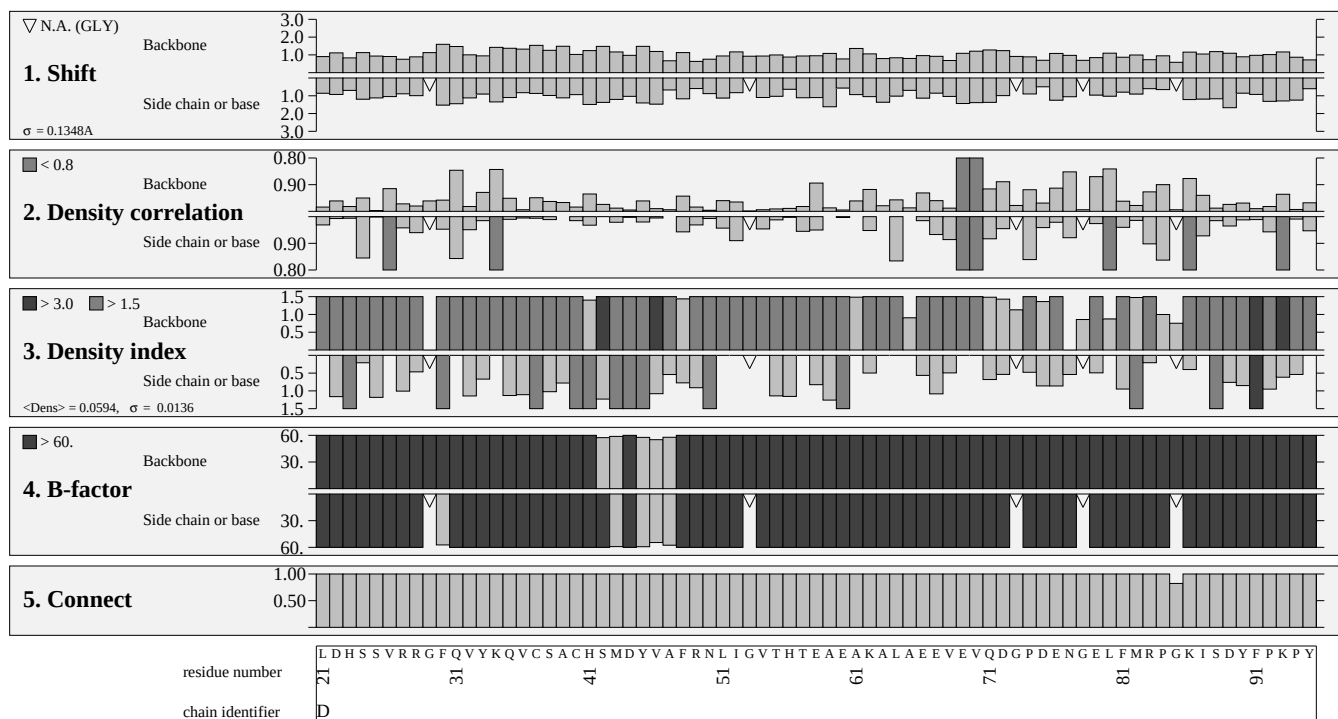
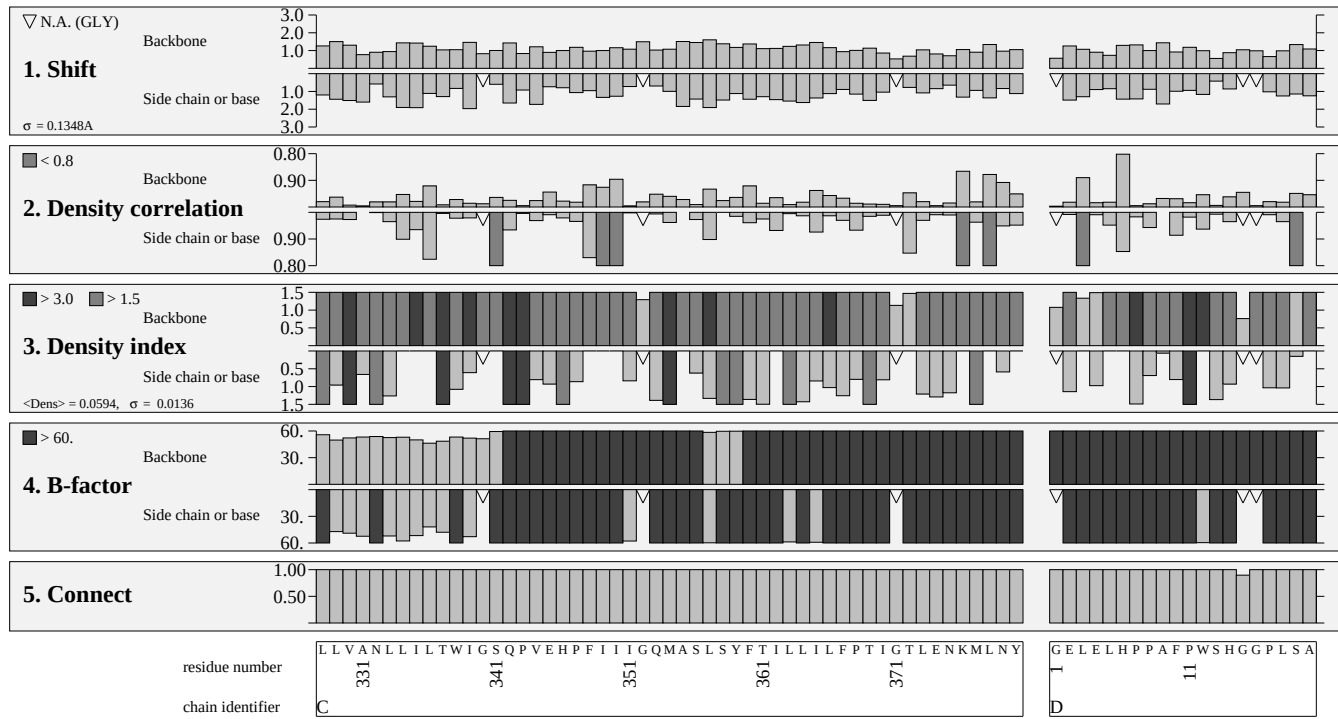
Local estimation (8)



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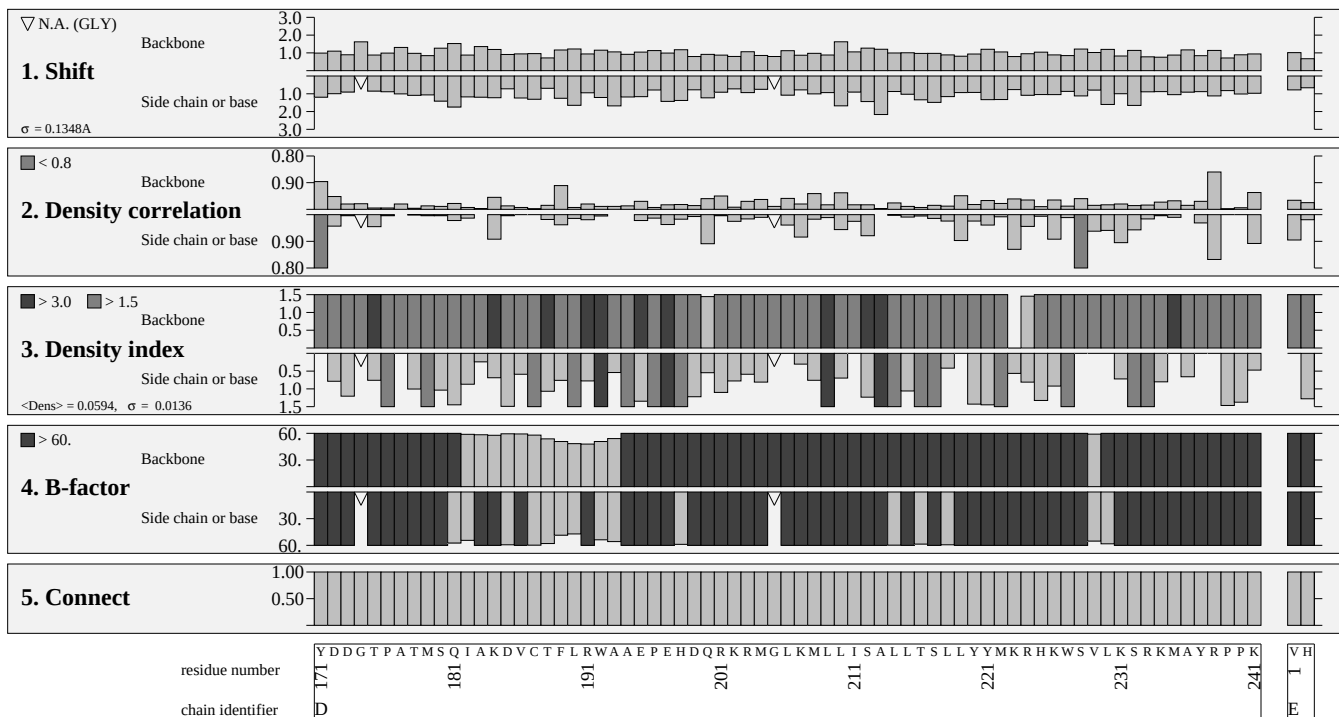
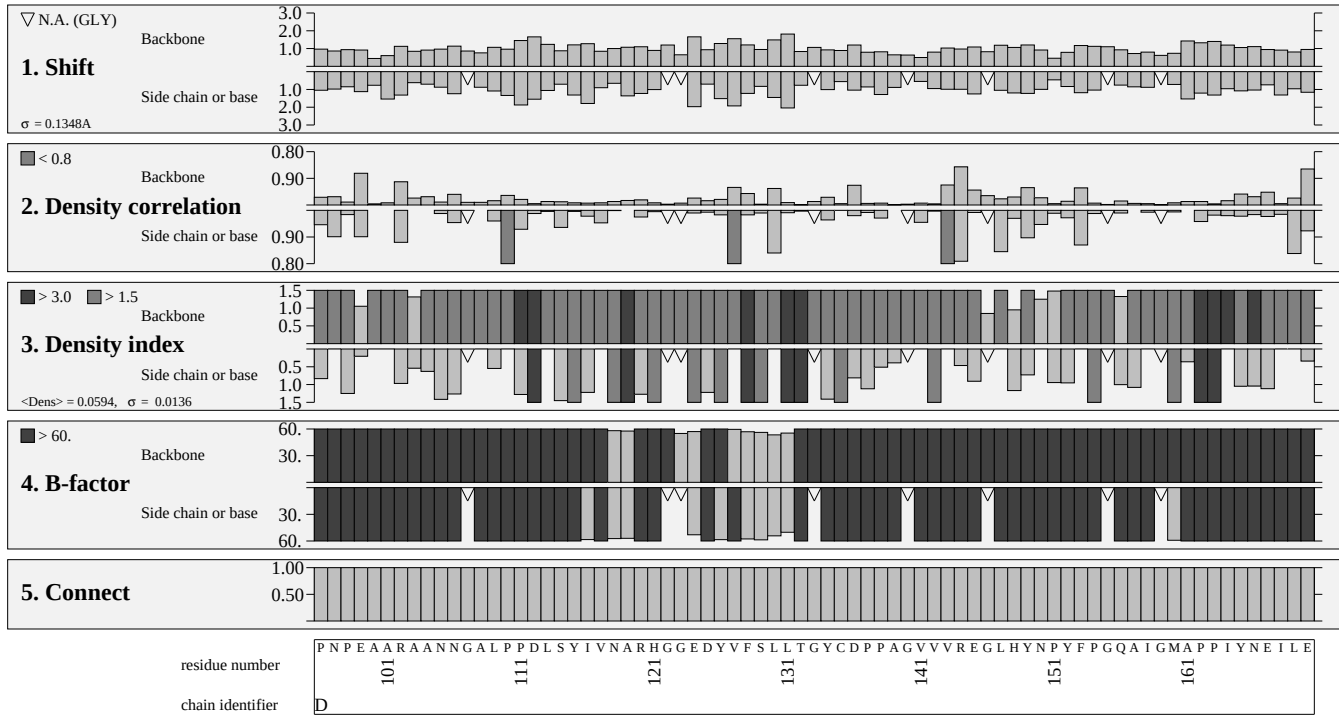
Local estimation (9)



Structure Factor Check

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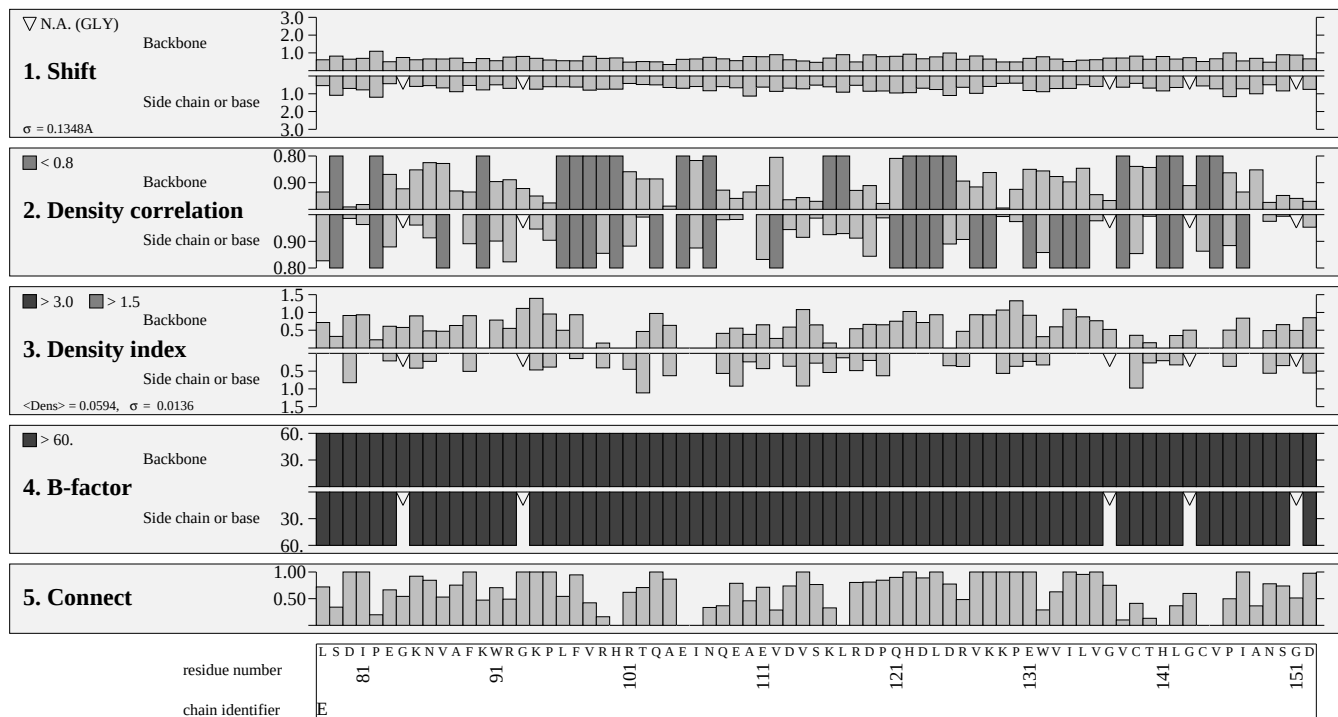
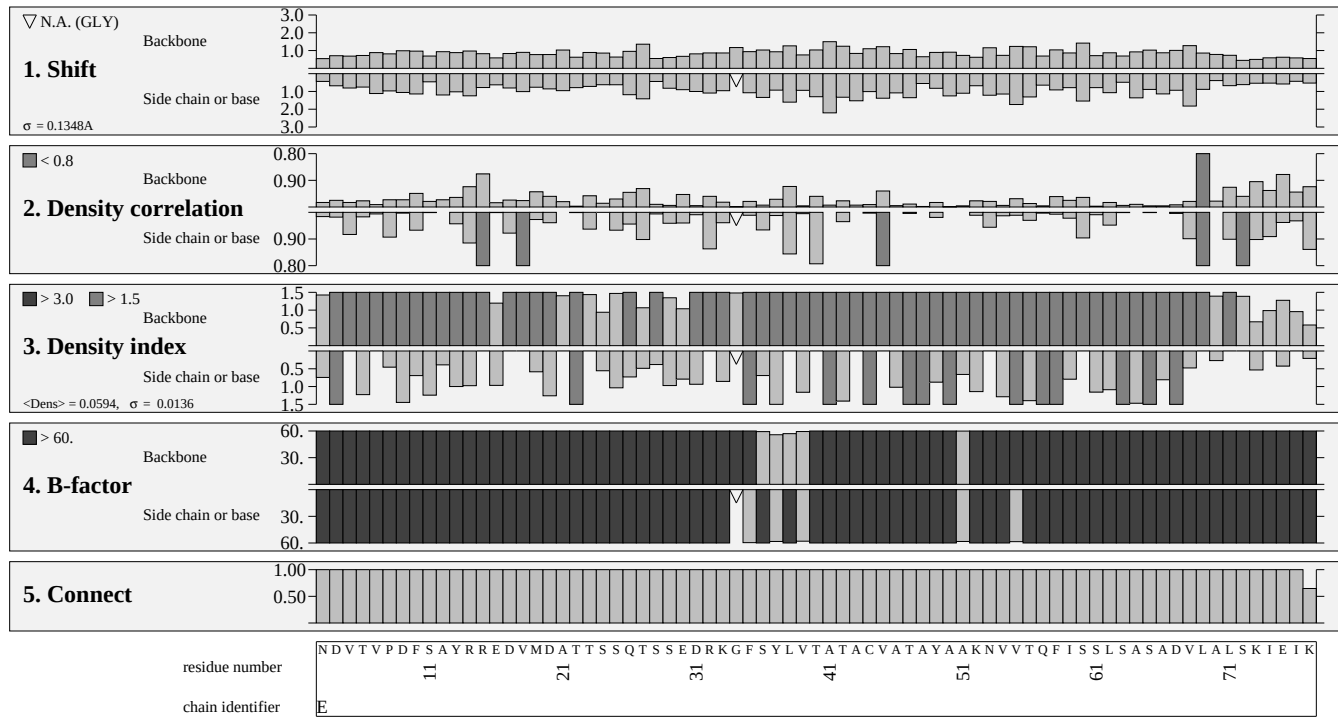
Local estimation (10)



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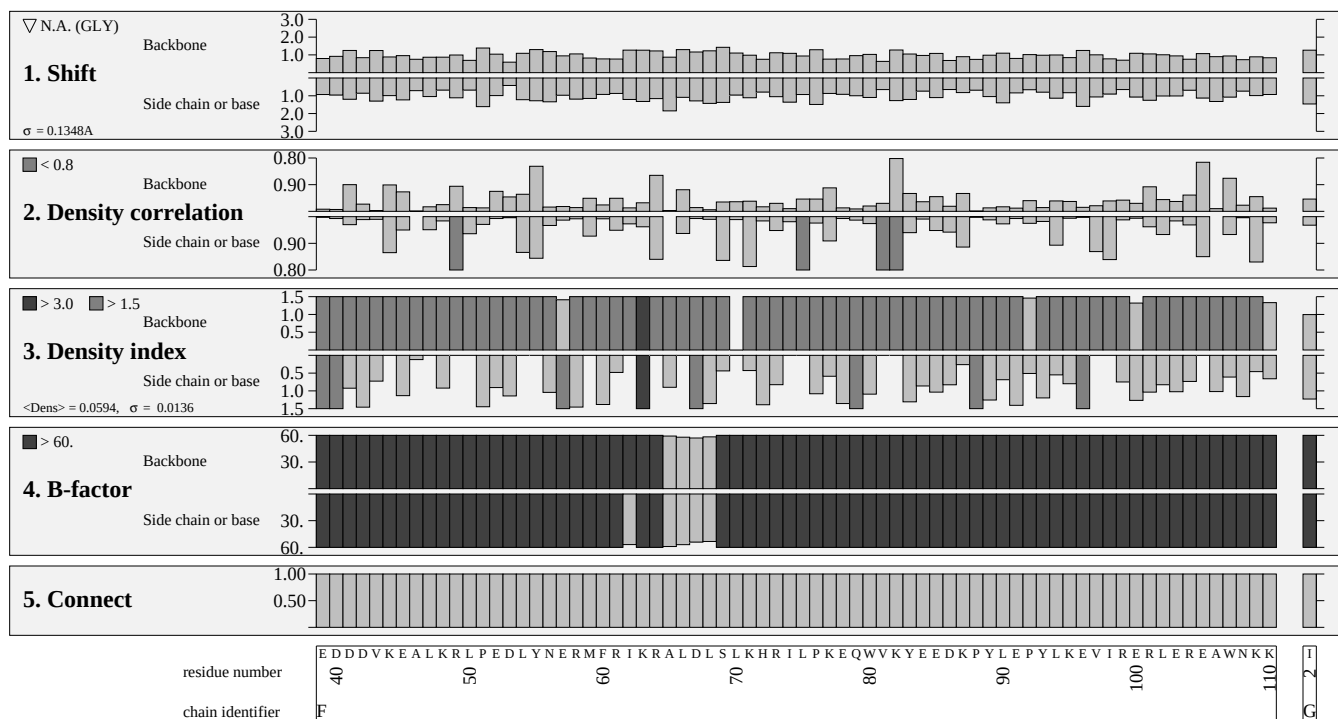
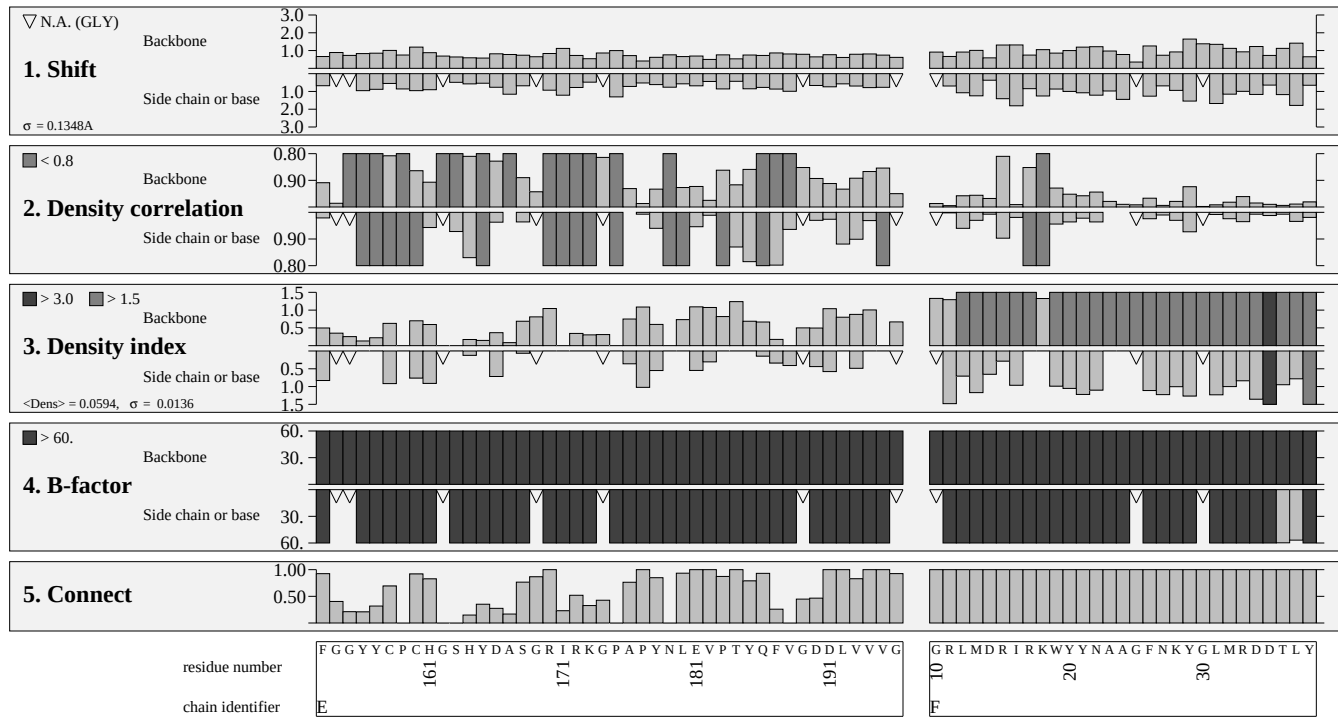
Local estimation (11)



Structure Factor Check

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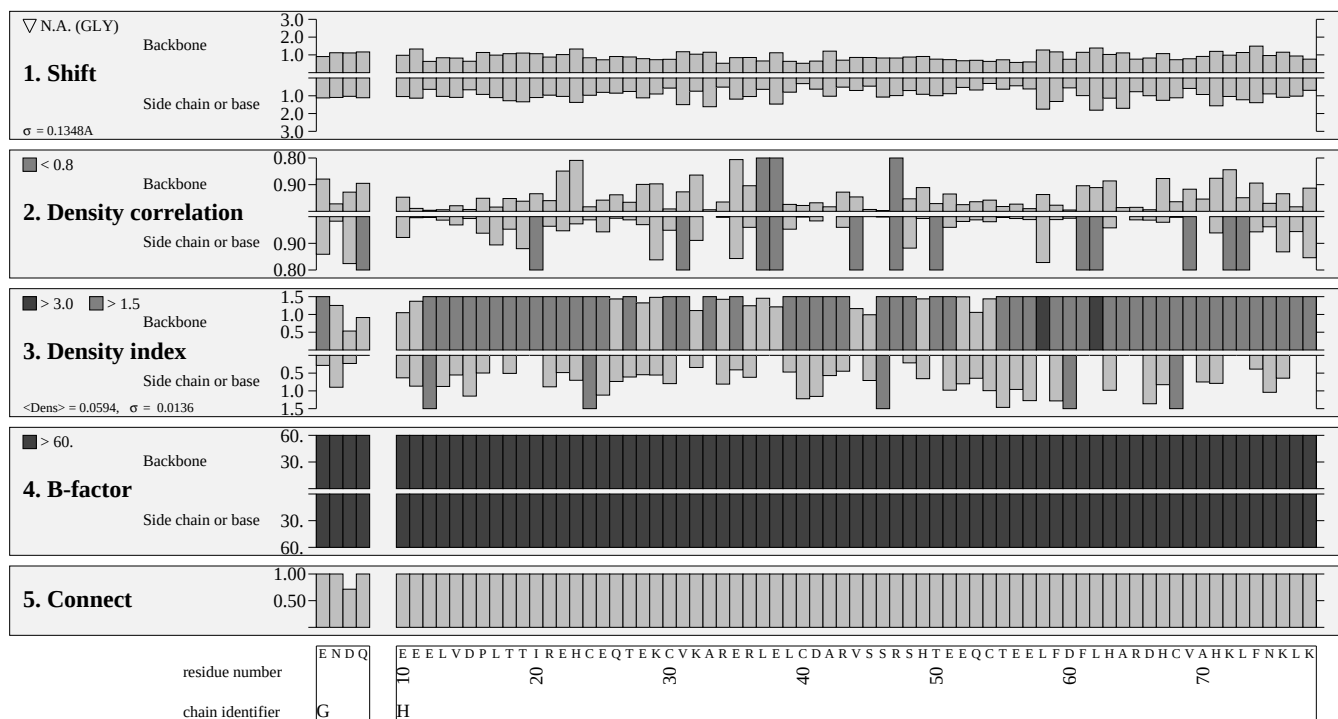
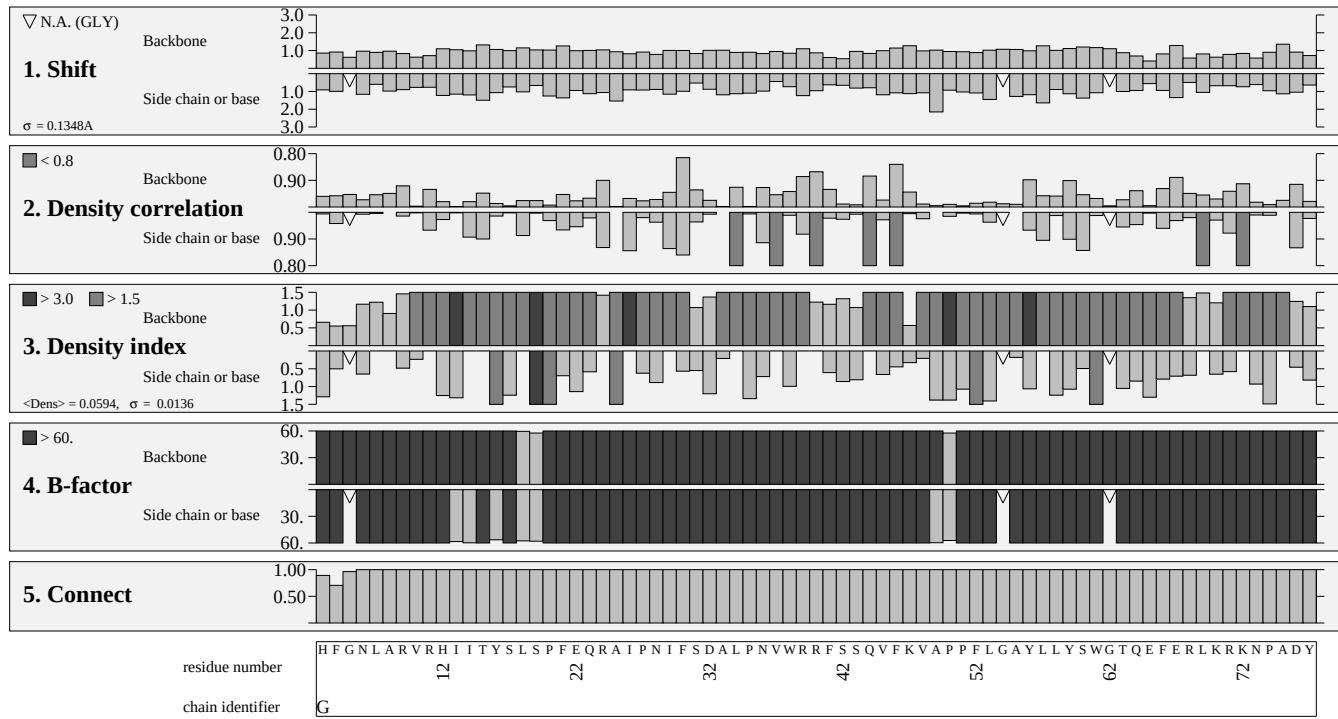
Local estimation (12)



Structure Factor Check

3H1K

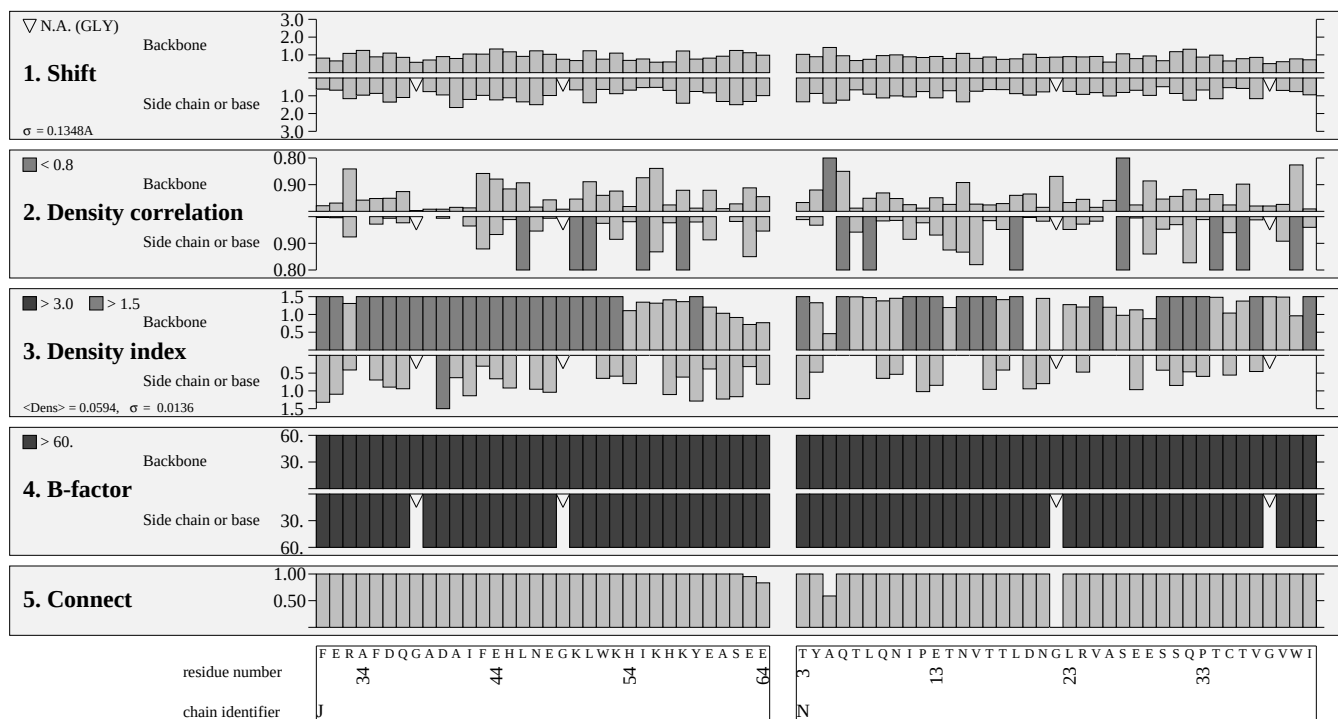
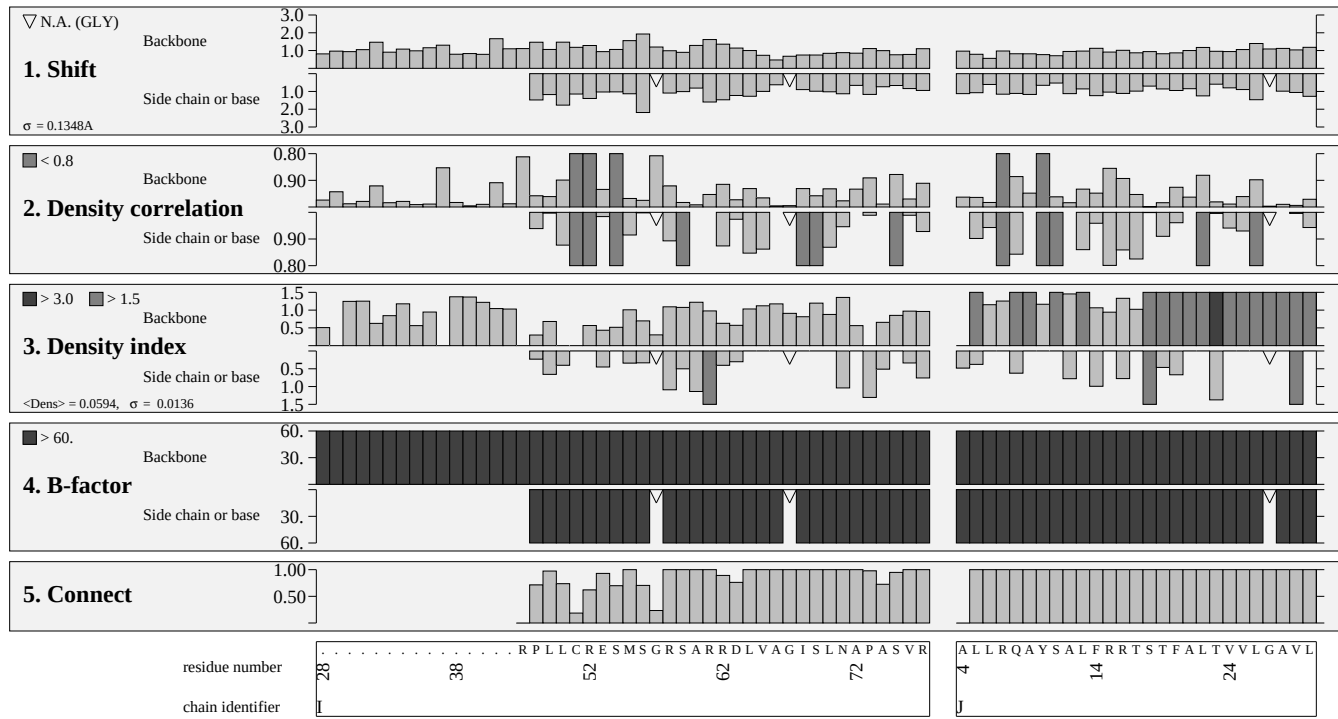
Local estimation (13)



Structure Factor Check

3H1K

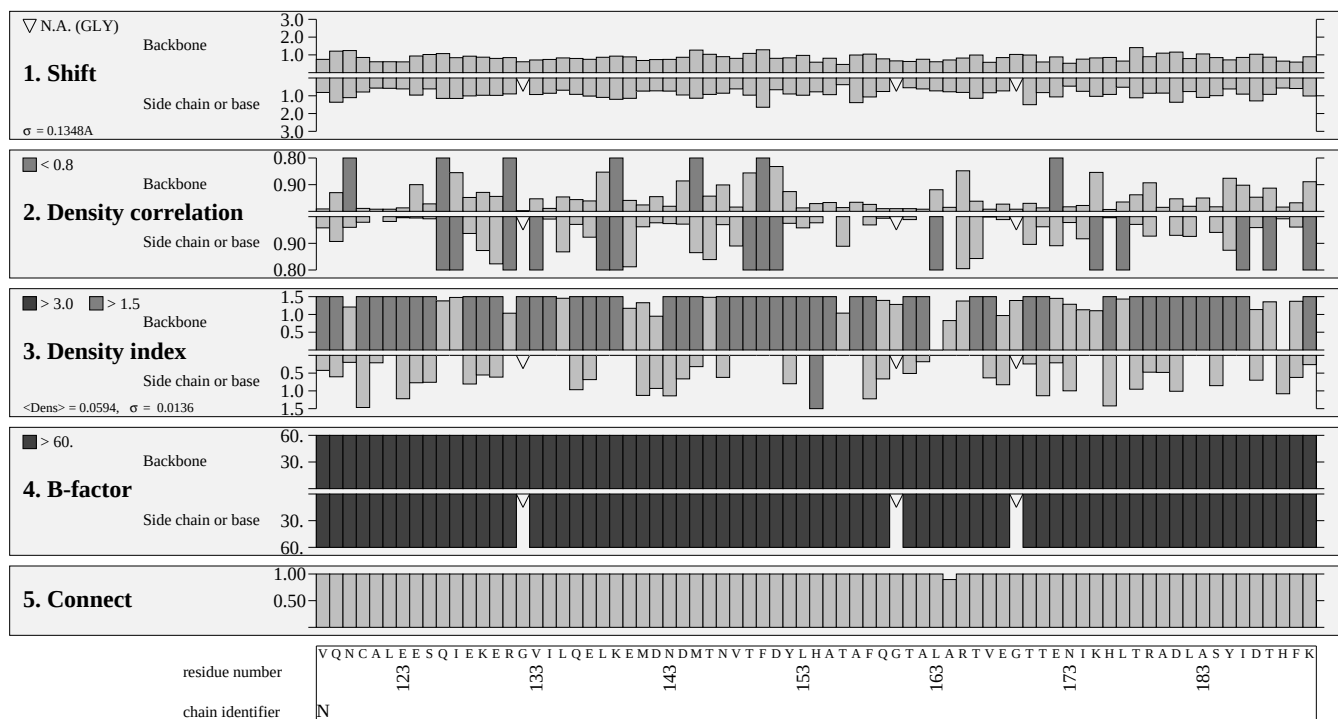
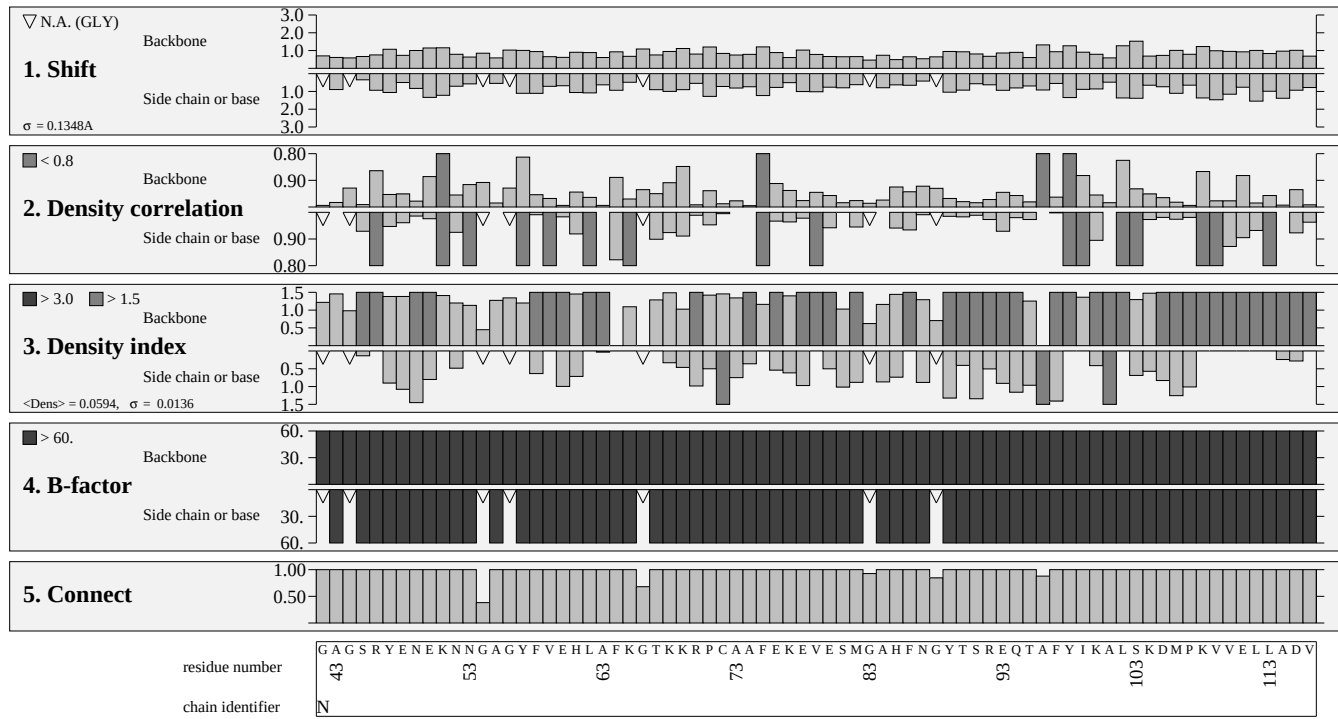
Local estimation (14)



Structure Factor Check

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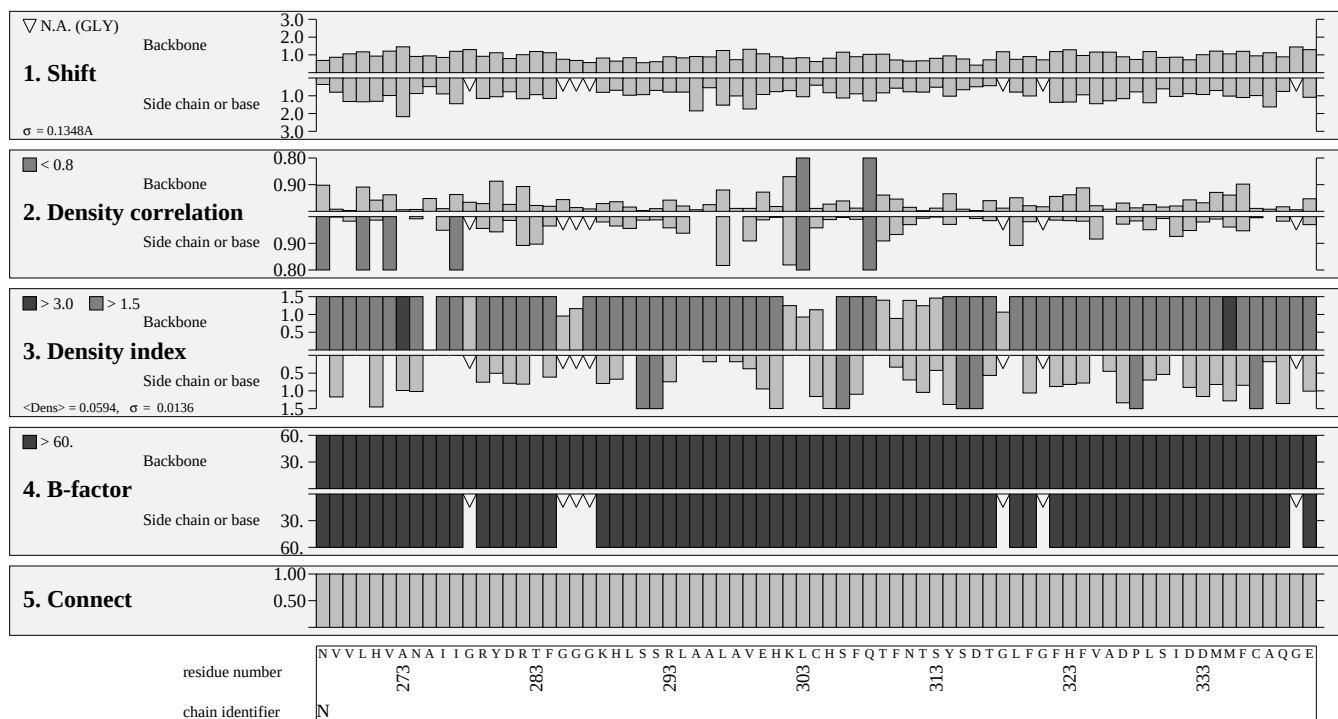
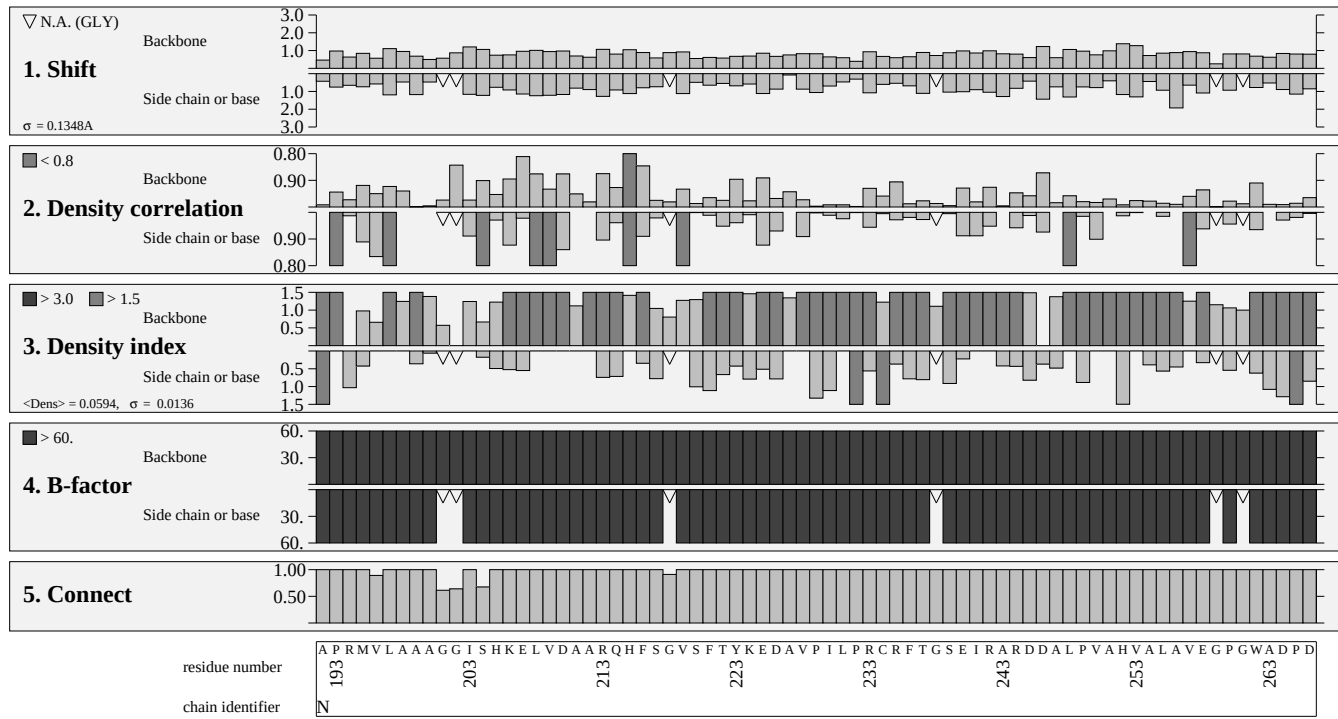
Local estimation (15)



Structure Factor Check

3H1K

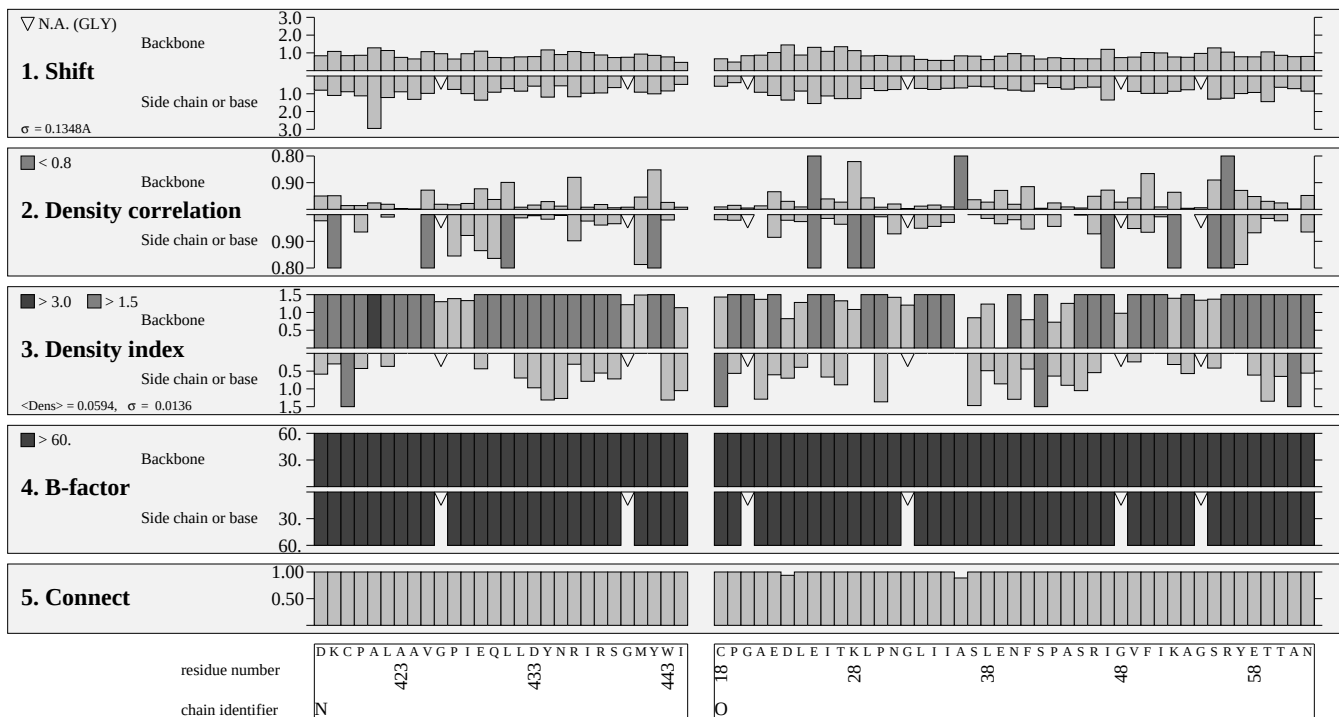
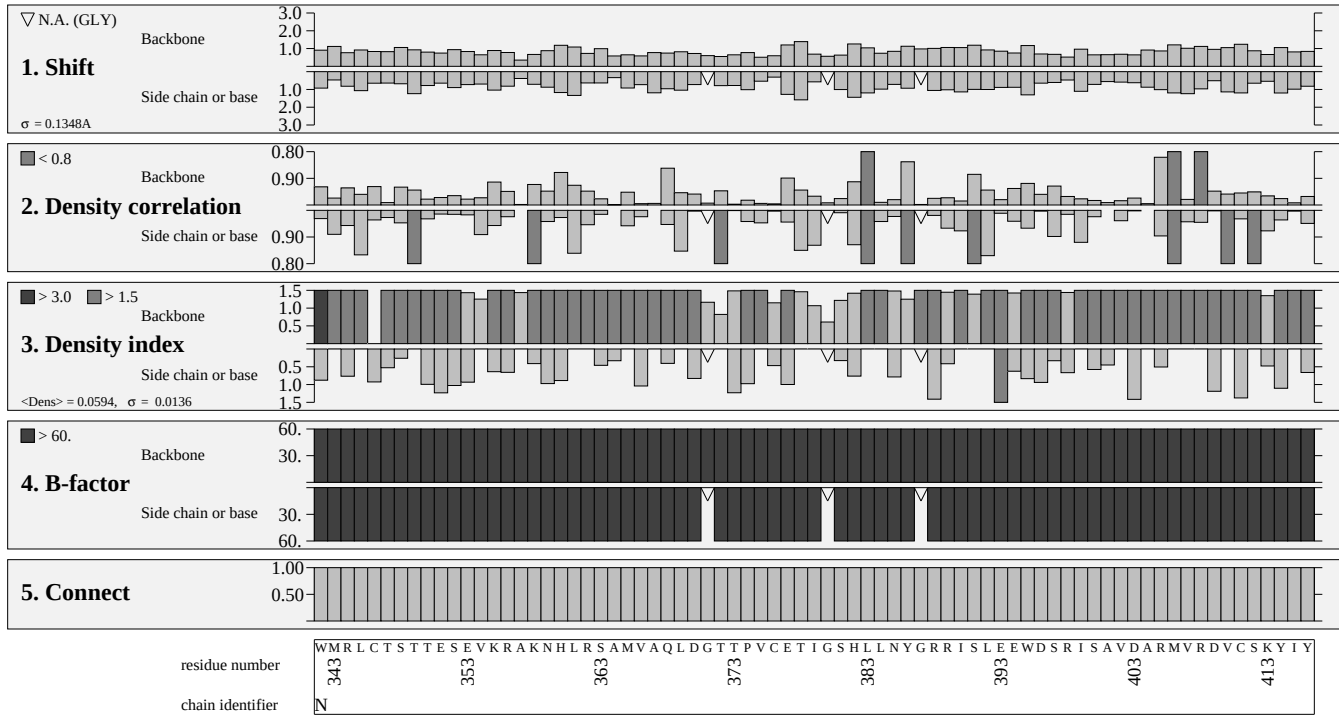
Local estimation (16)



Structure Factor Check

3H1K

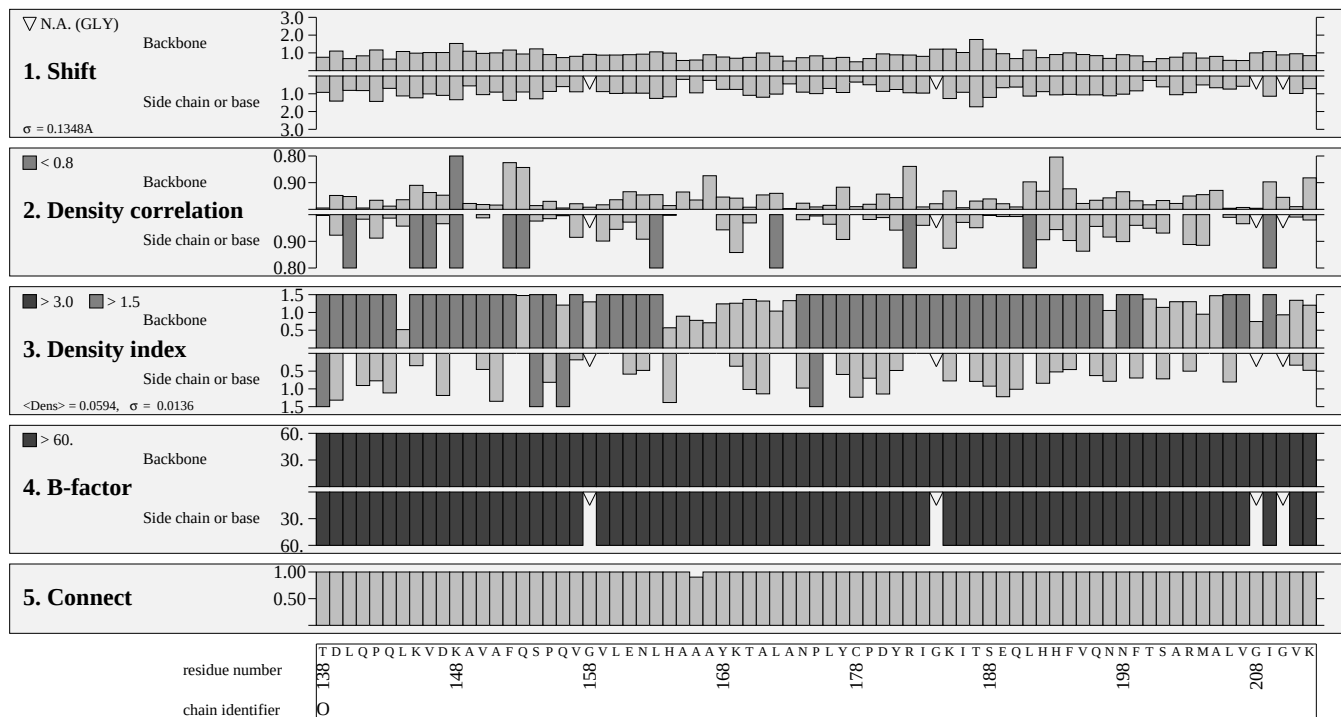
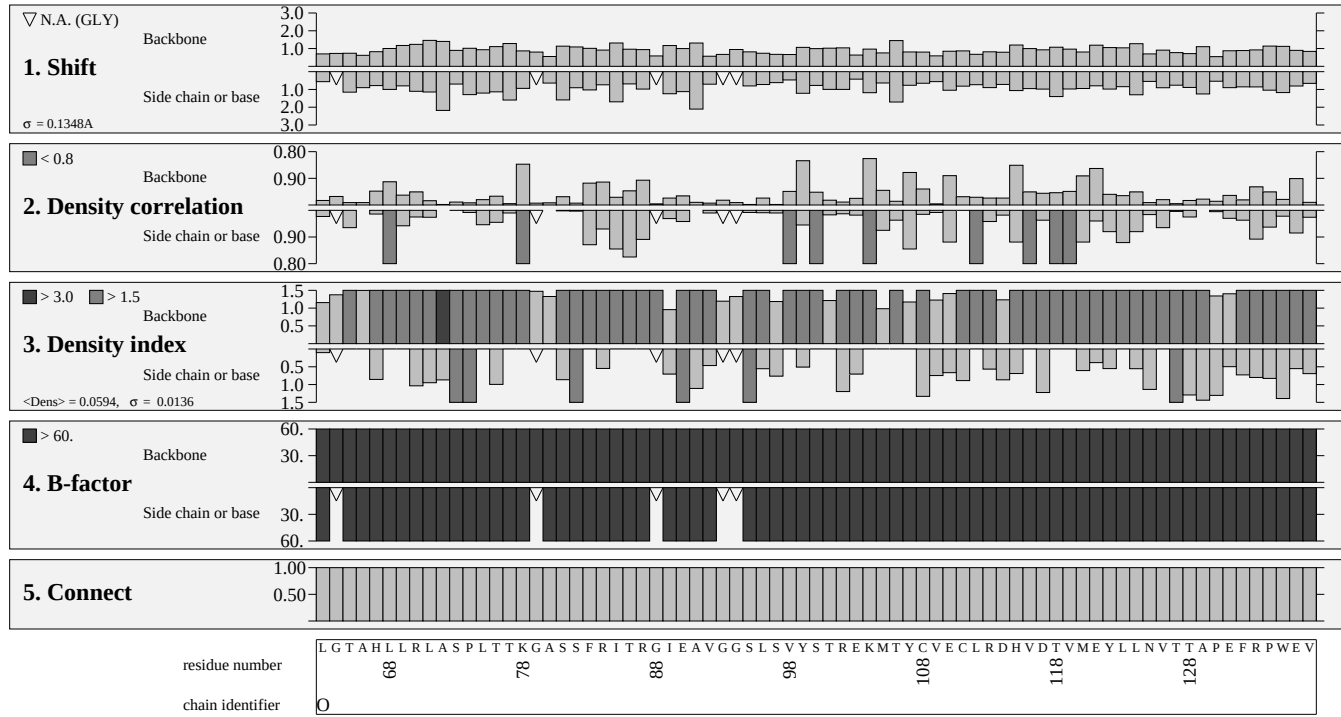
Local estimation (17)



Structure Factor Check

3H1K

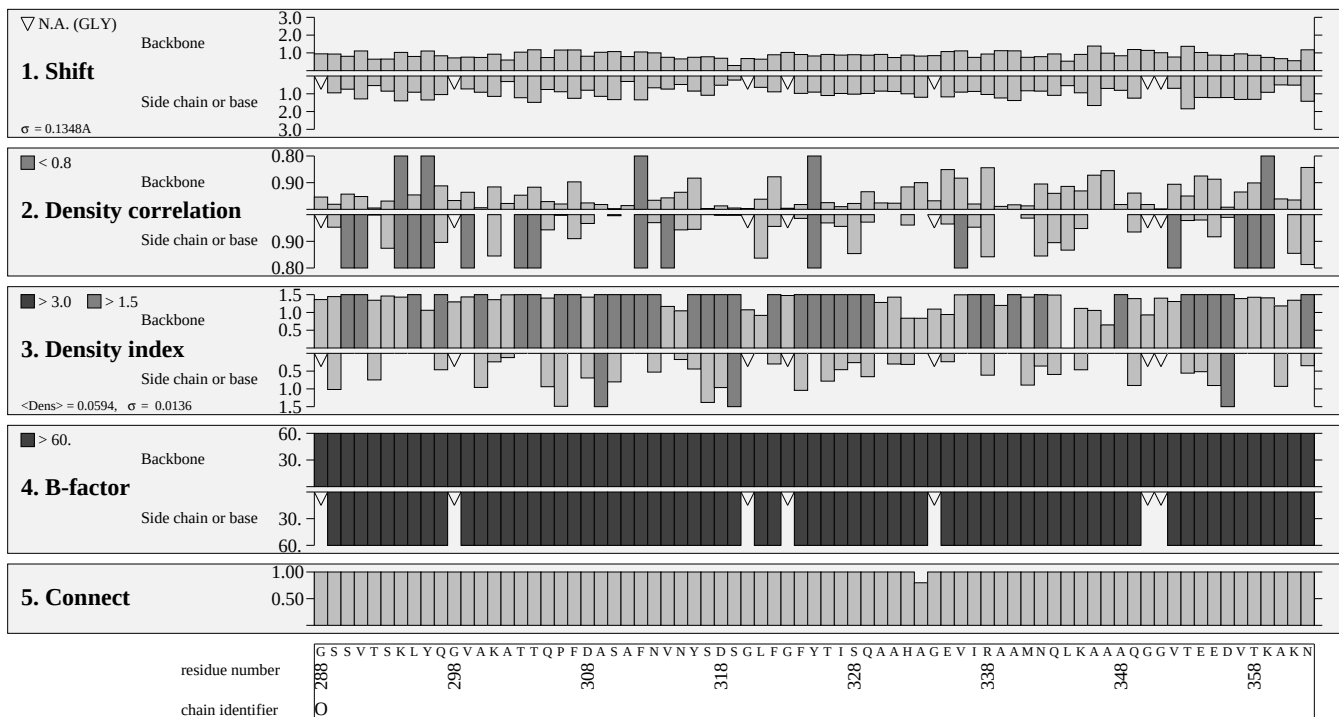
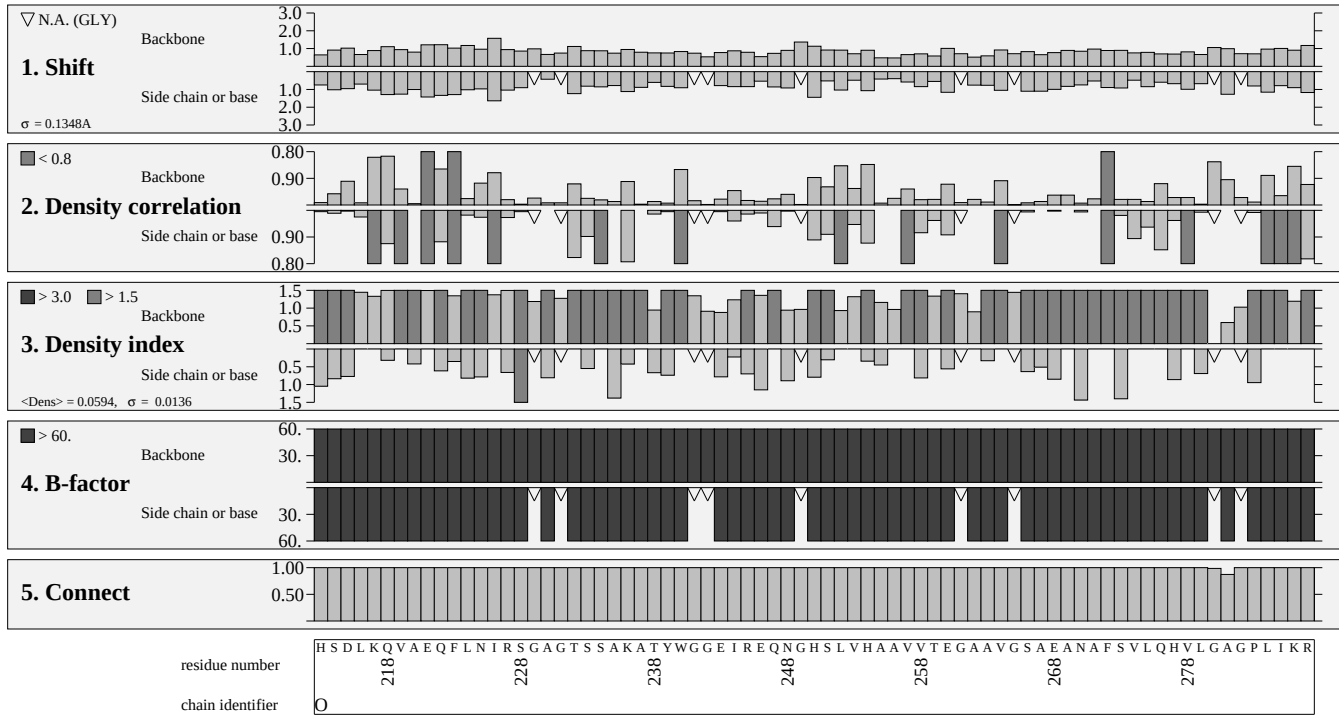
Local estimation (18)



Structure Factor Check

3H1K

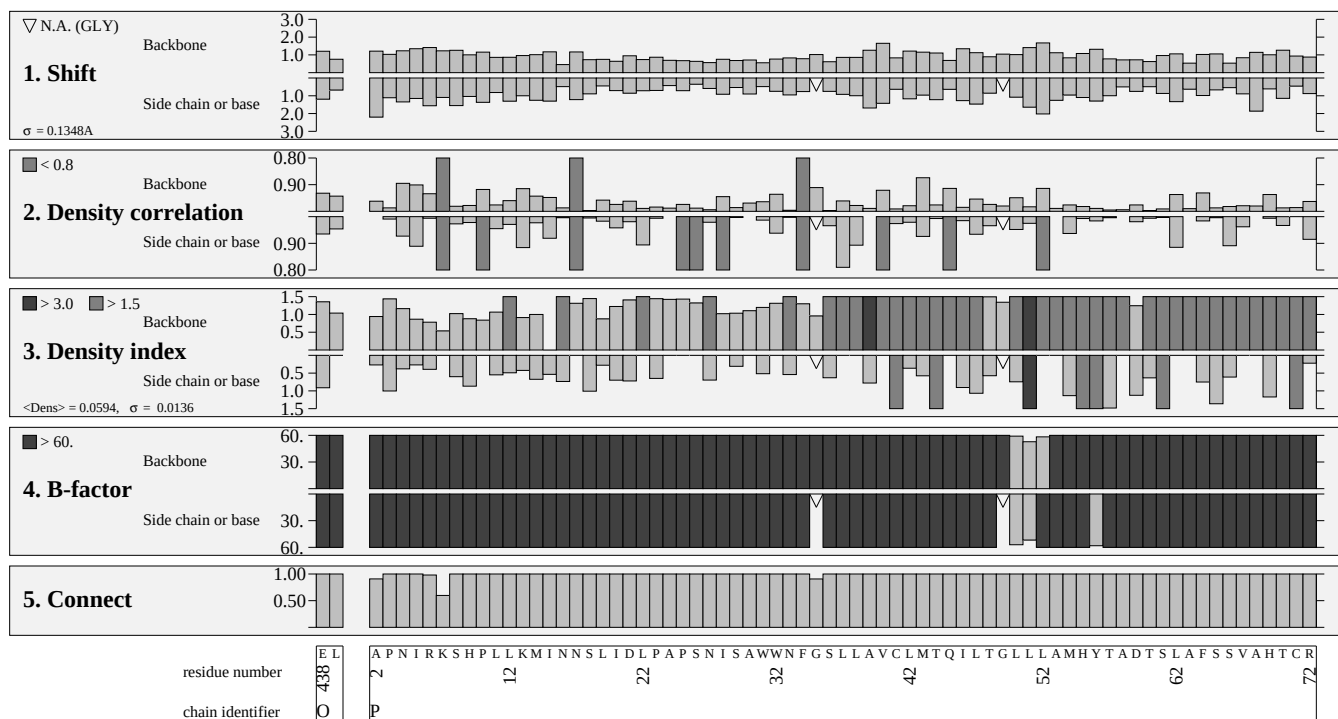
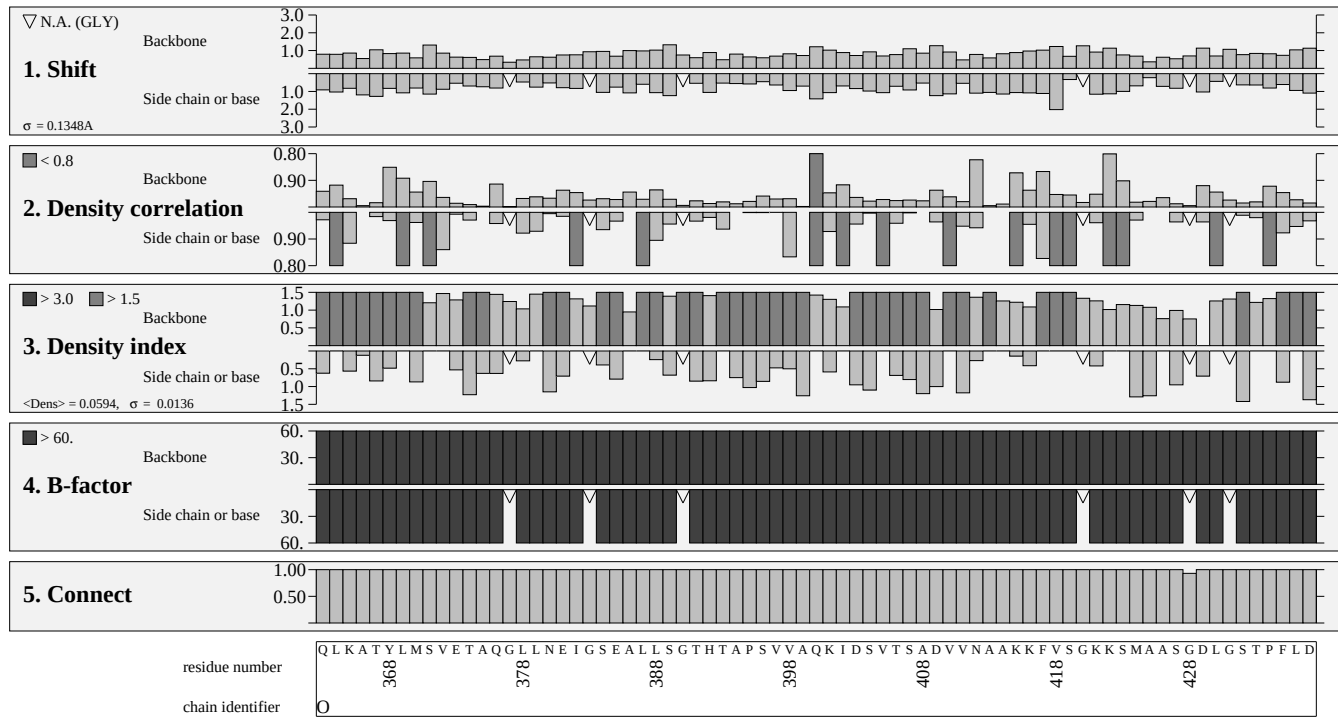
Local estimation (19)



Structure Factor Check

3H1K

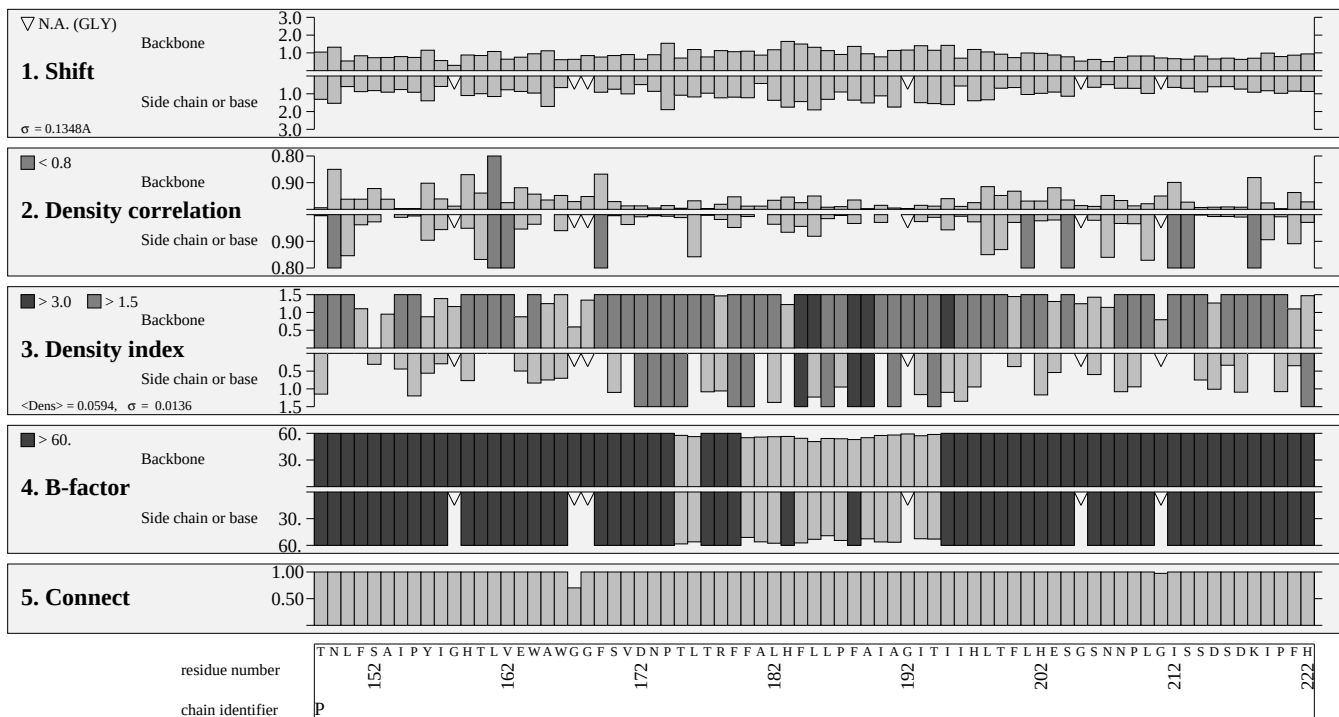
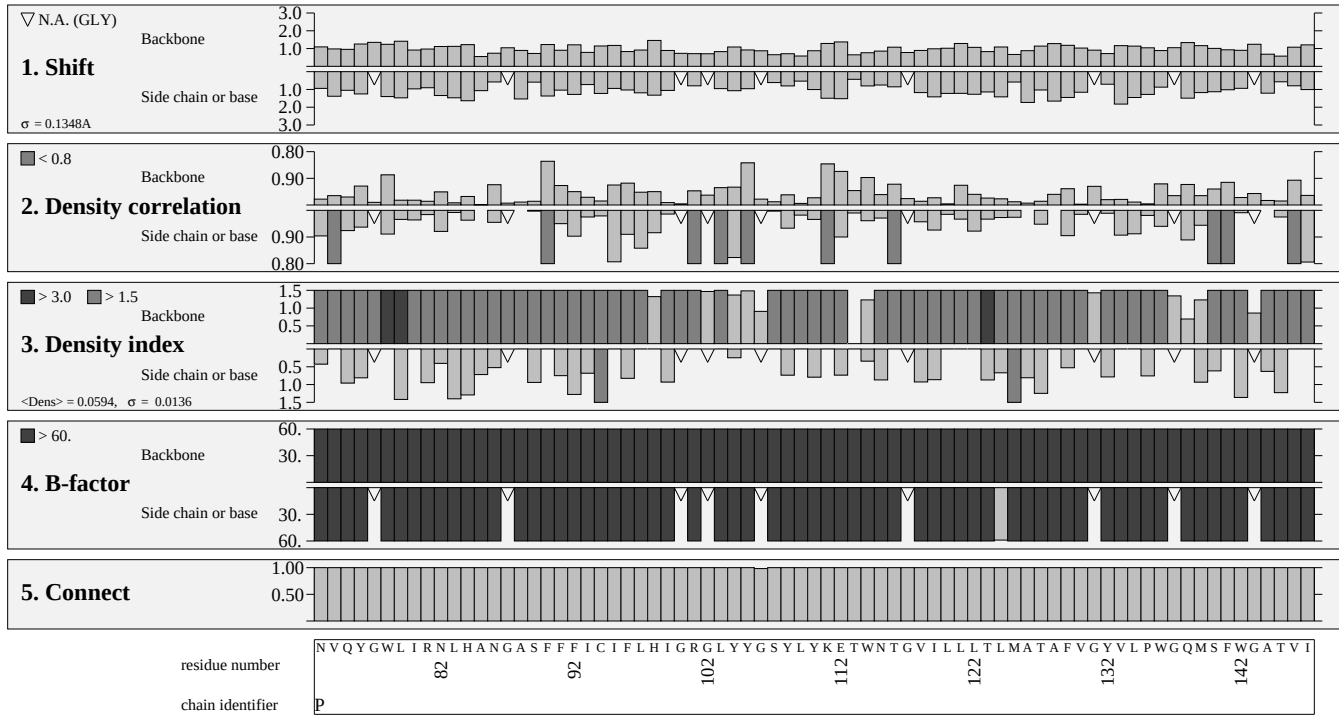
Local estimation (20)



Structure Factor Check

3H1K

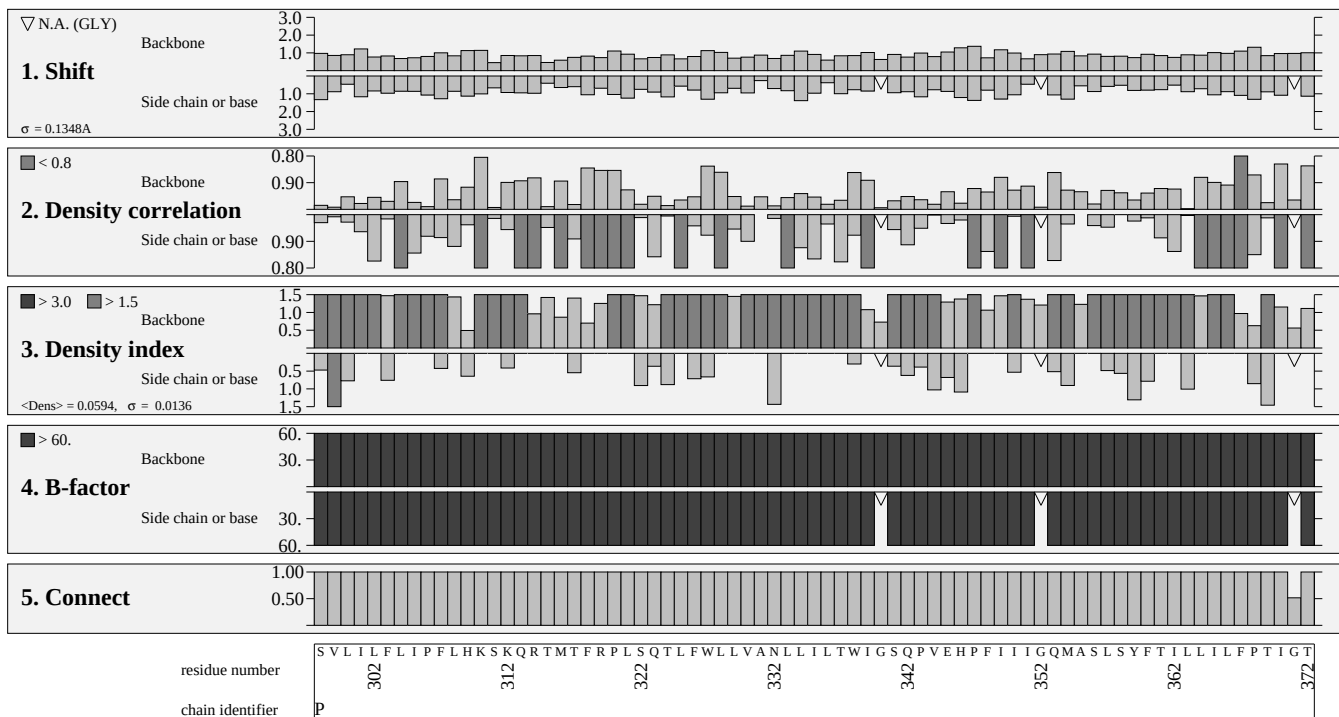
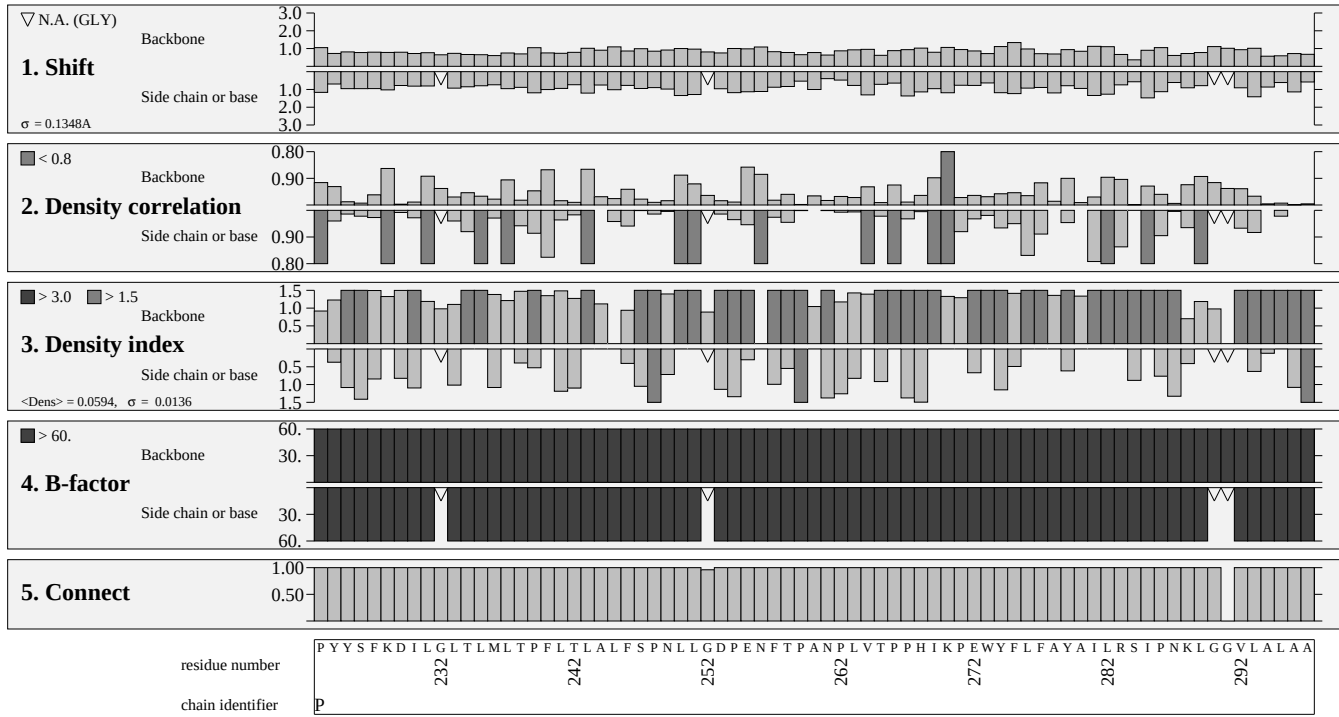
Local estimation (21)



Structure Factor Check

3H1K

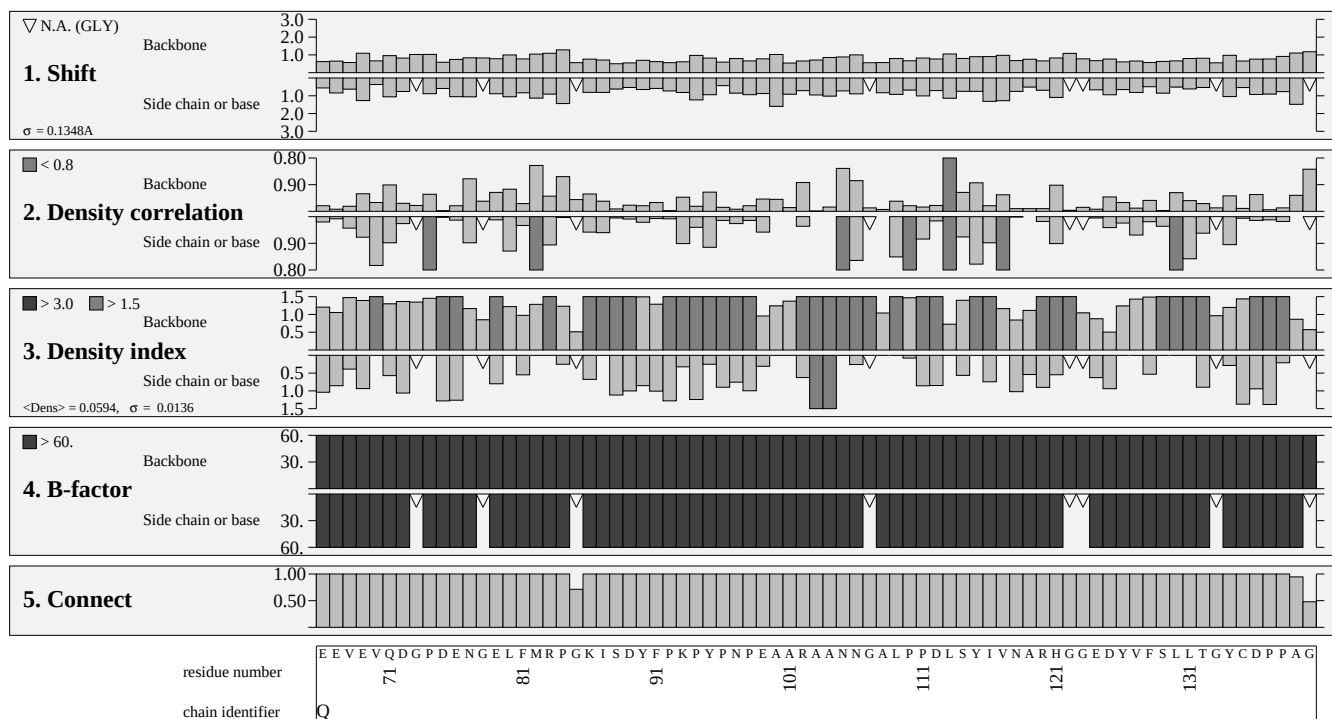
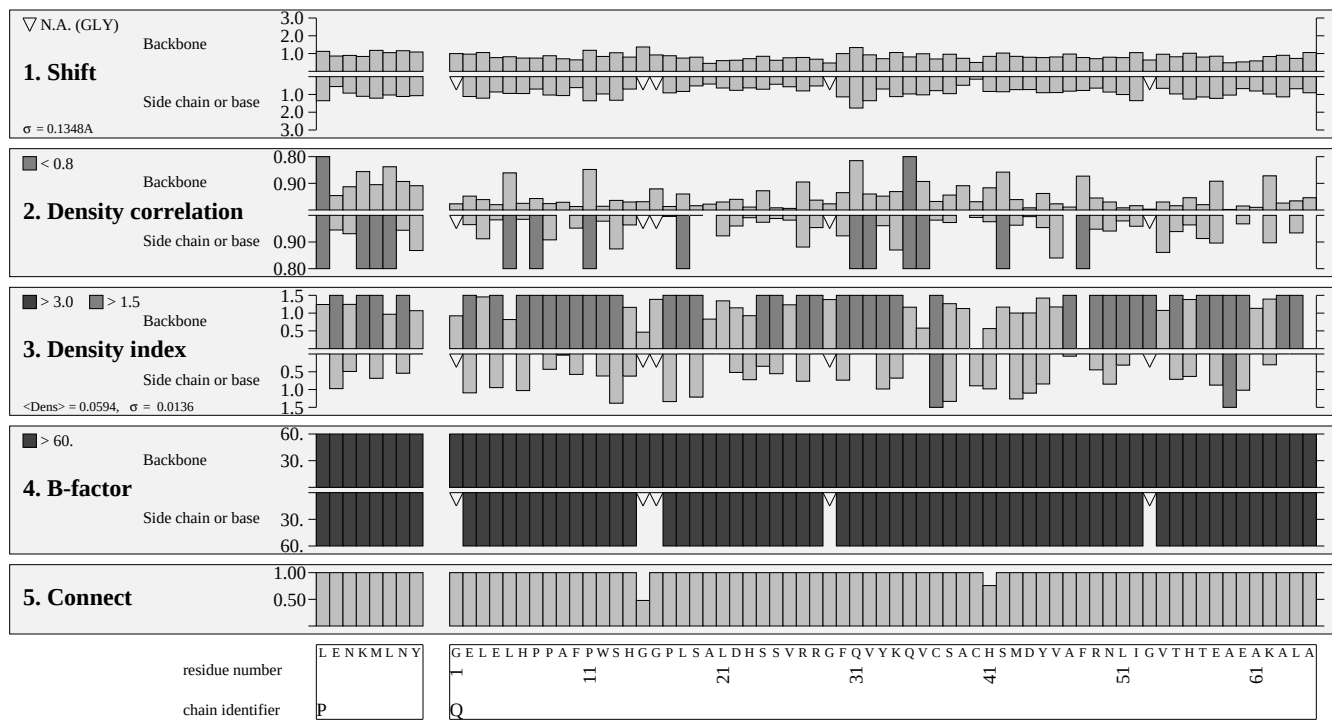
Local estimation (22)



Structure Factor Check

3H1K

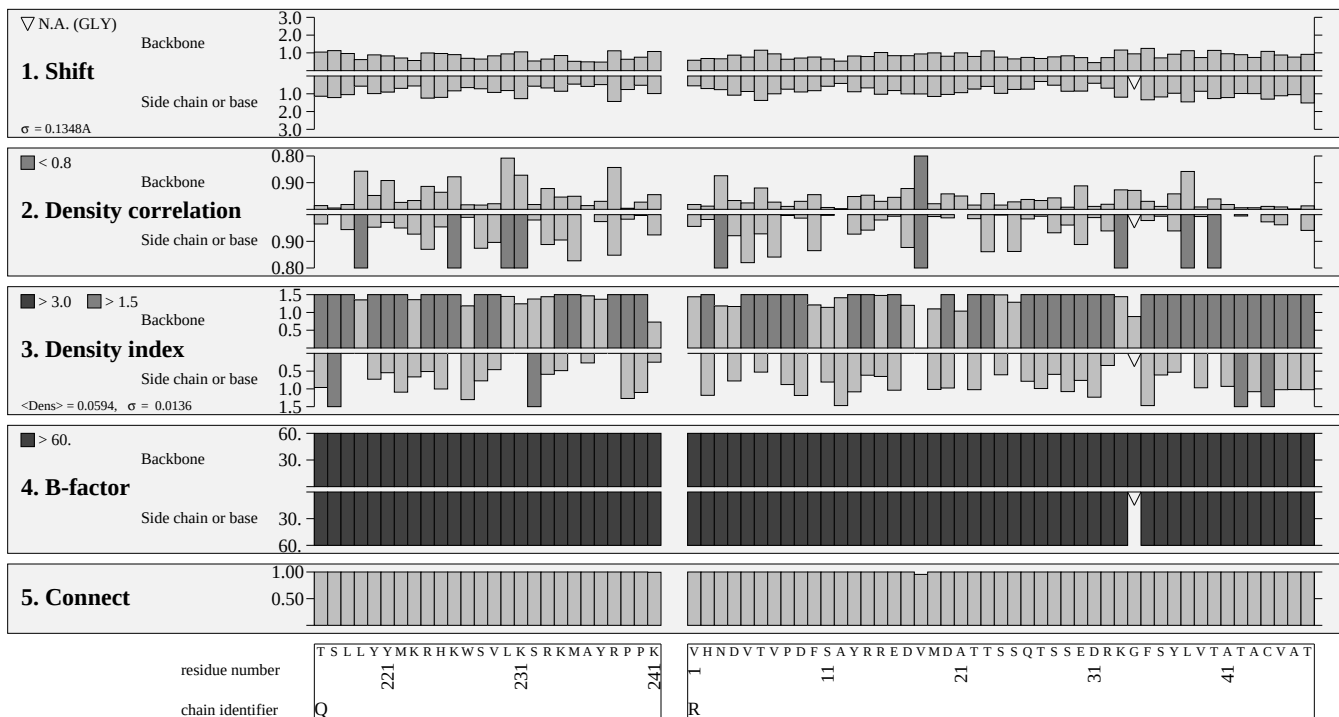
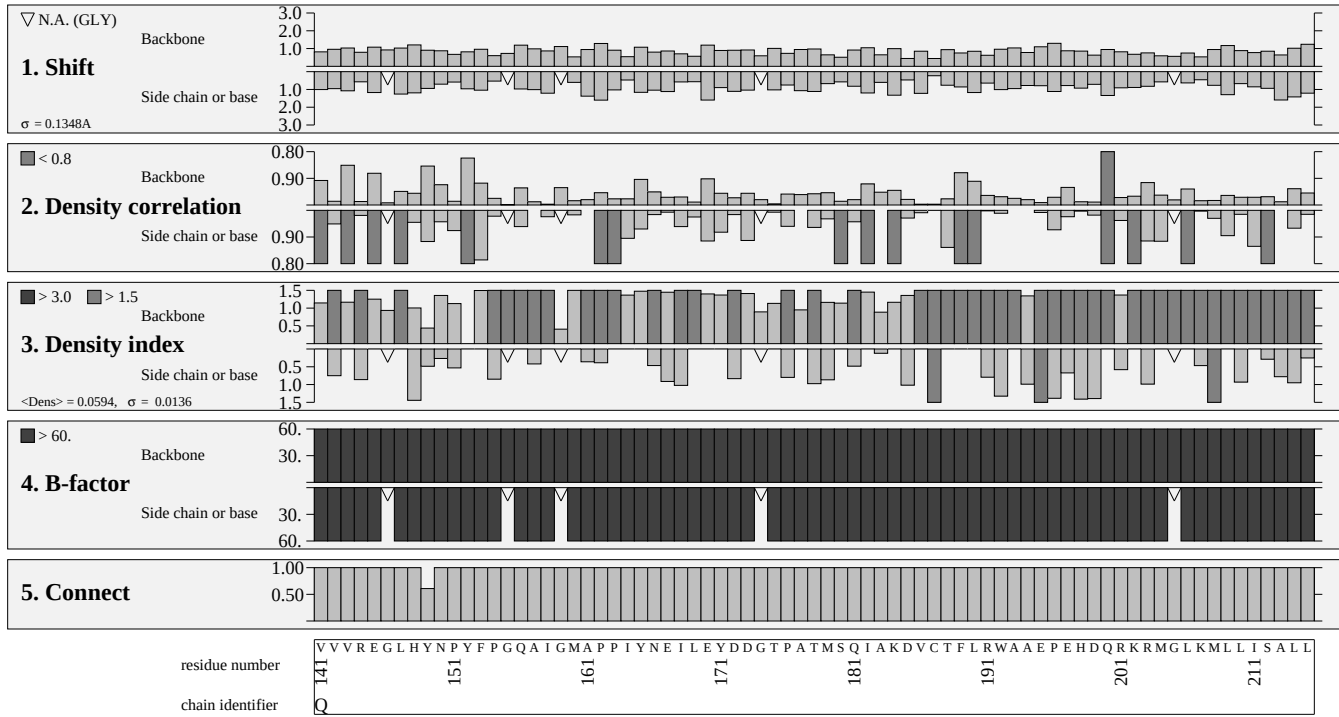
Local estimation (23)



Structure Factor Check

3H1K

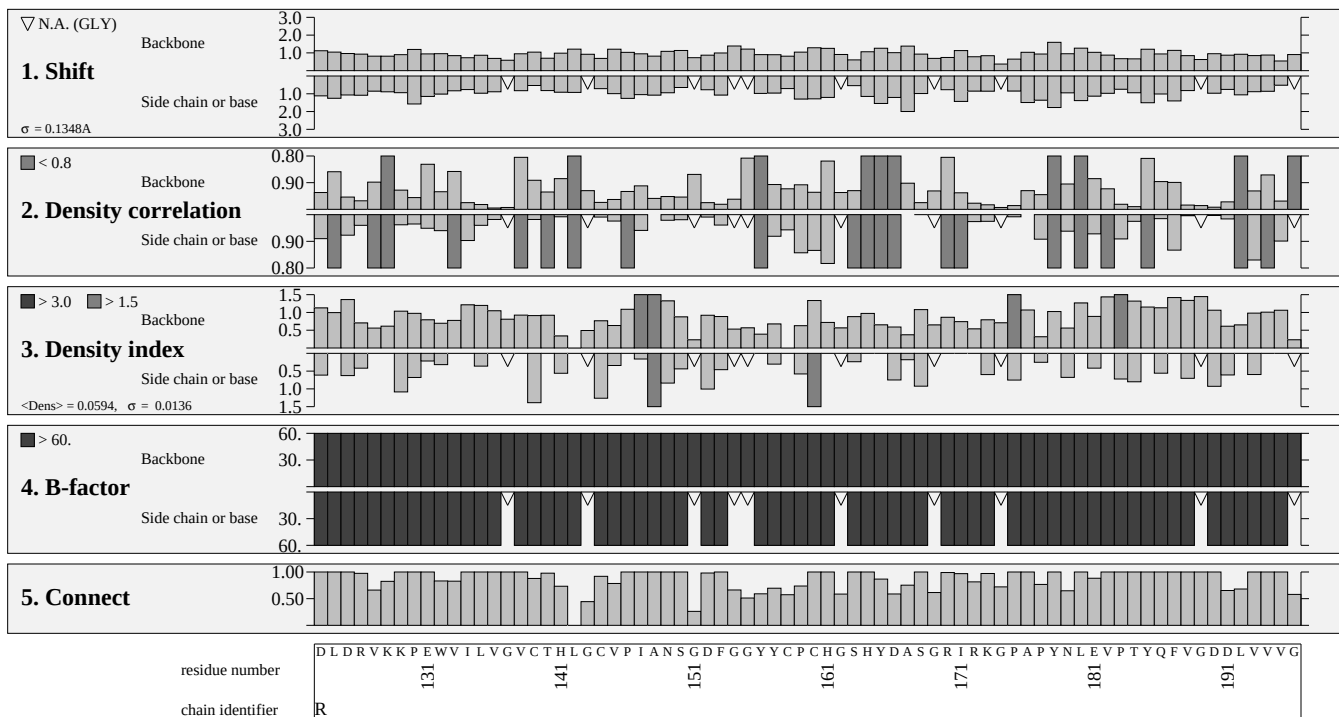
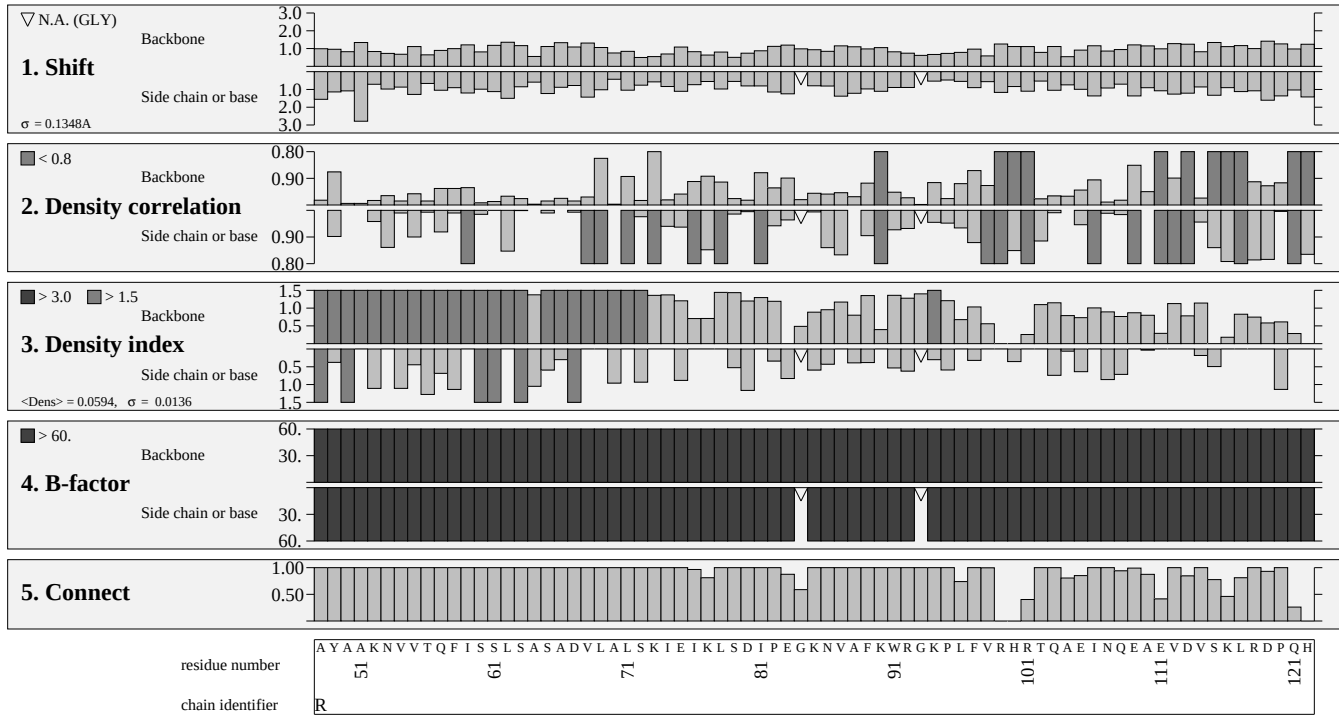
Local estimation (24)



Structure Factor Check

3H1K

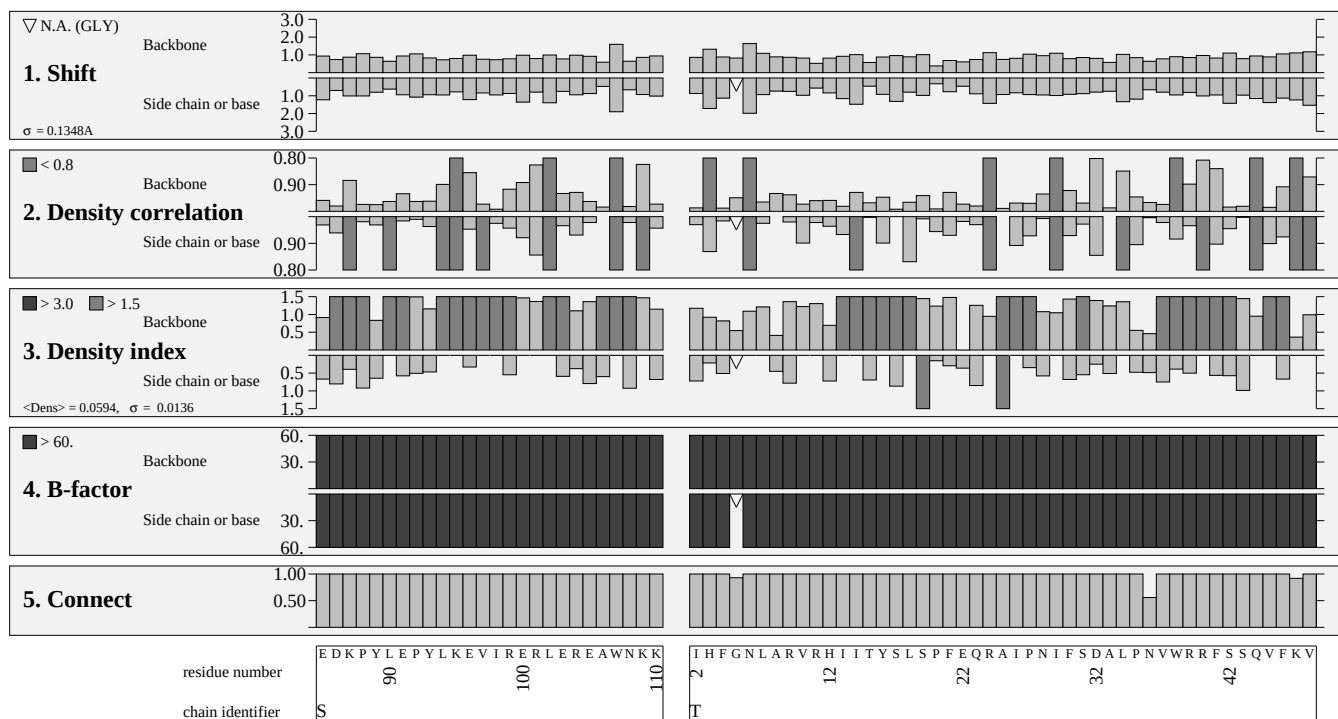
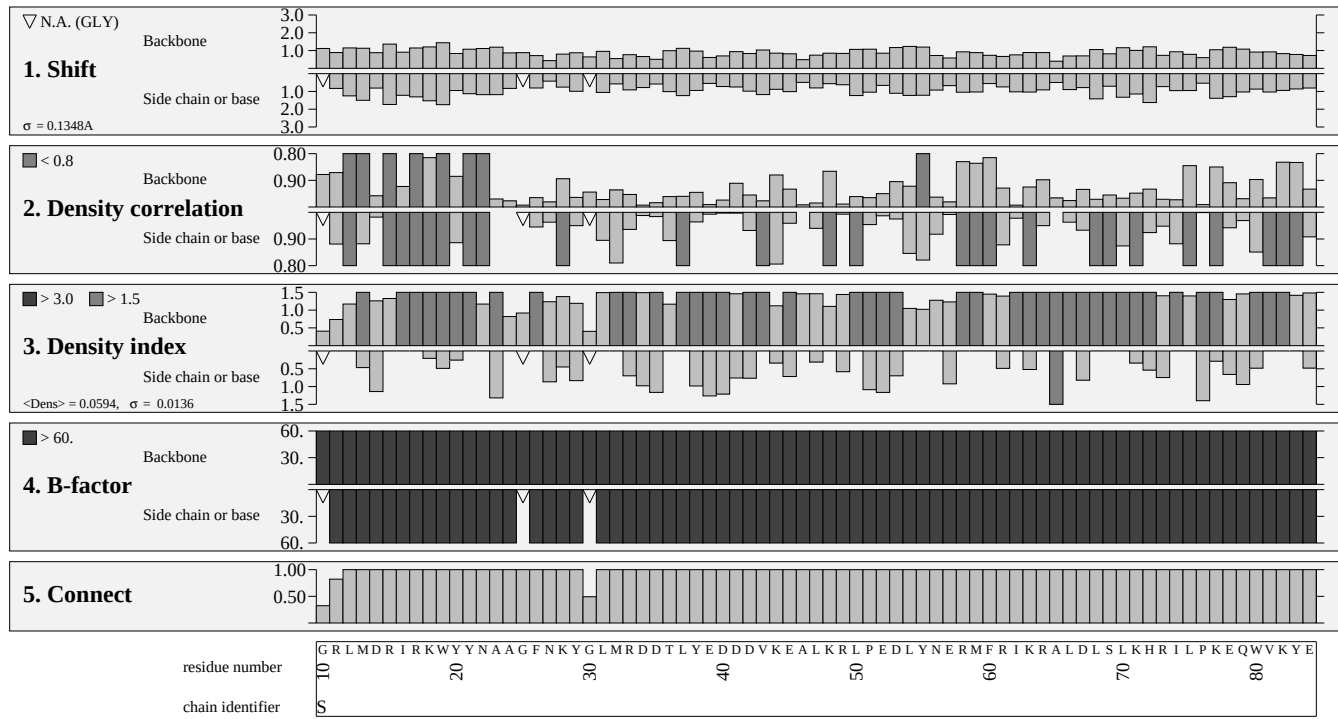
Local estimation (25)



Structure Factor Check

3H1K

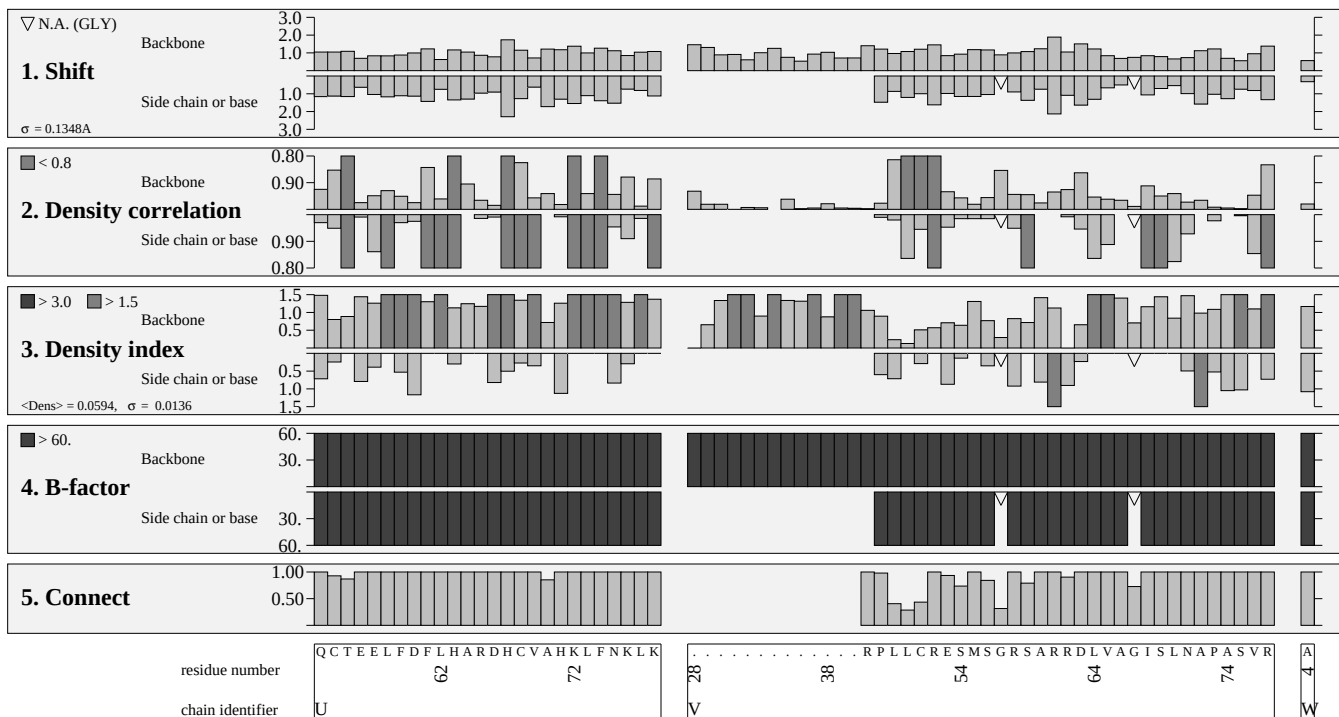
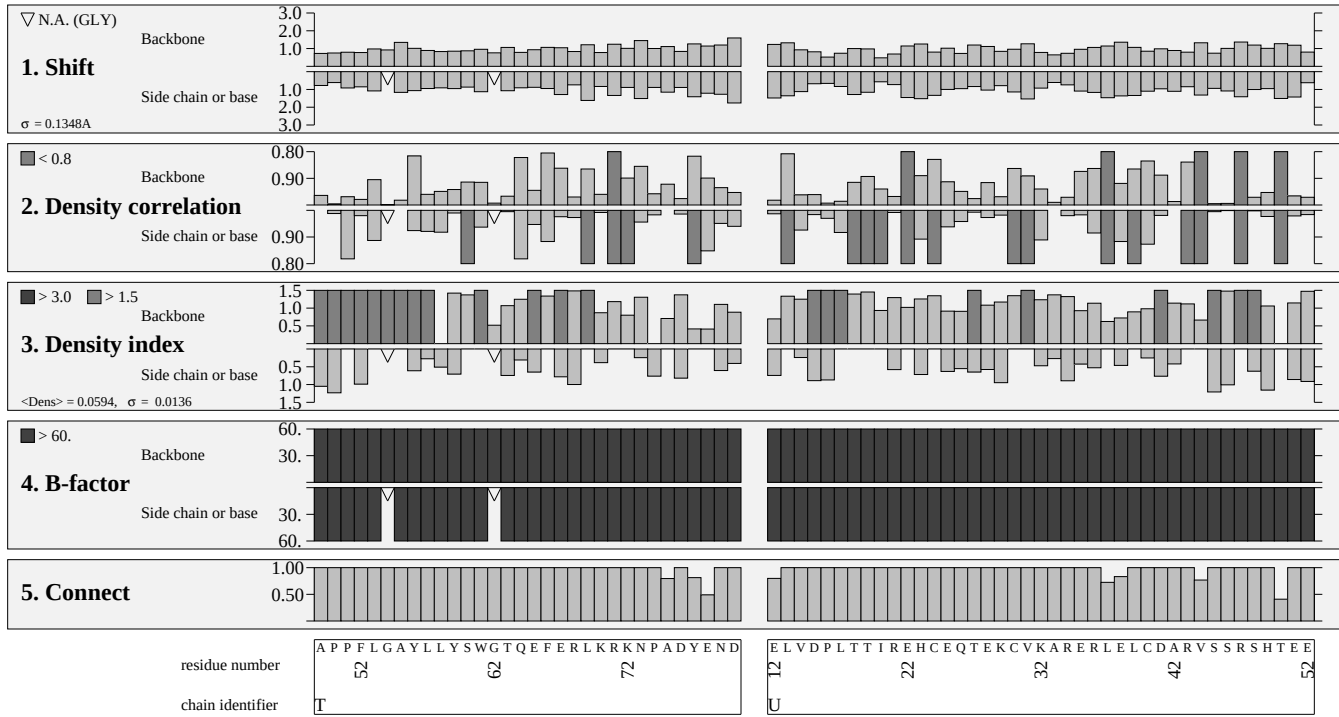
Local estimation (26)



Structure Factor Check

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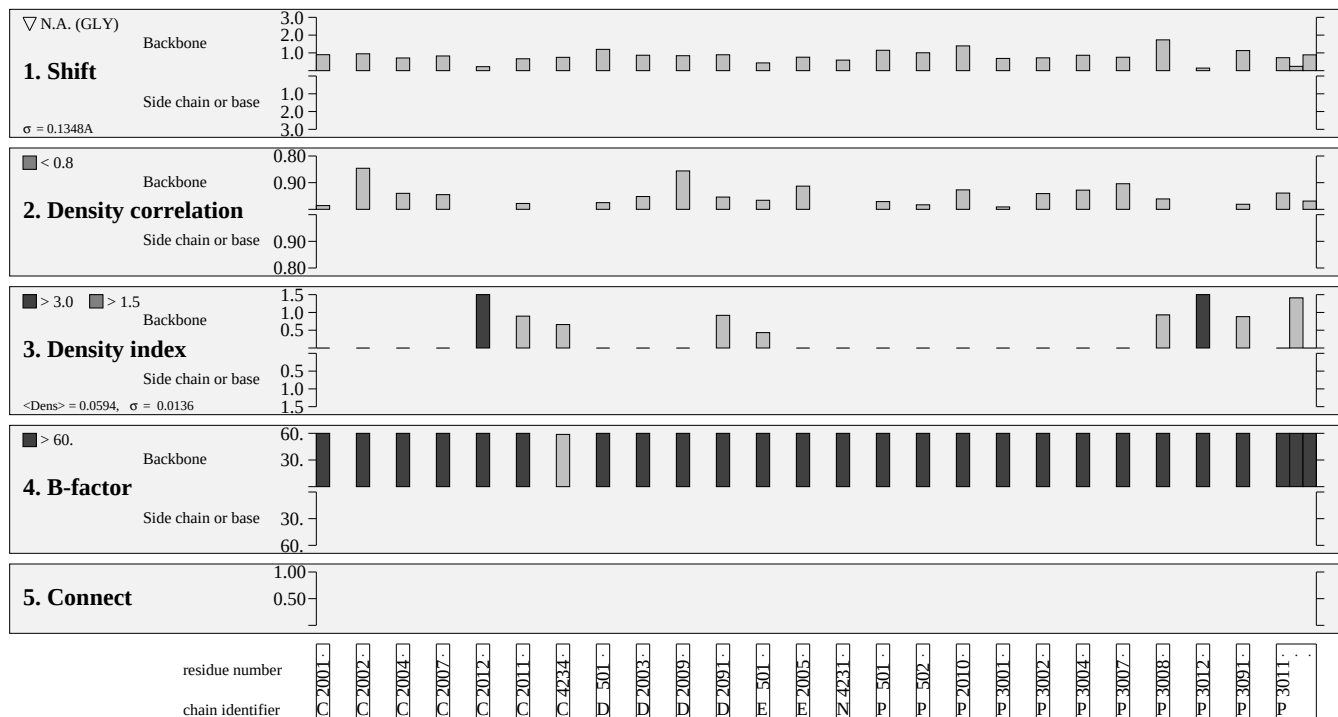
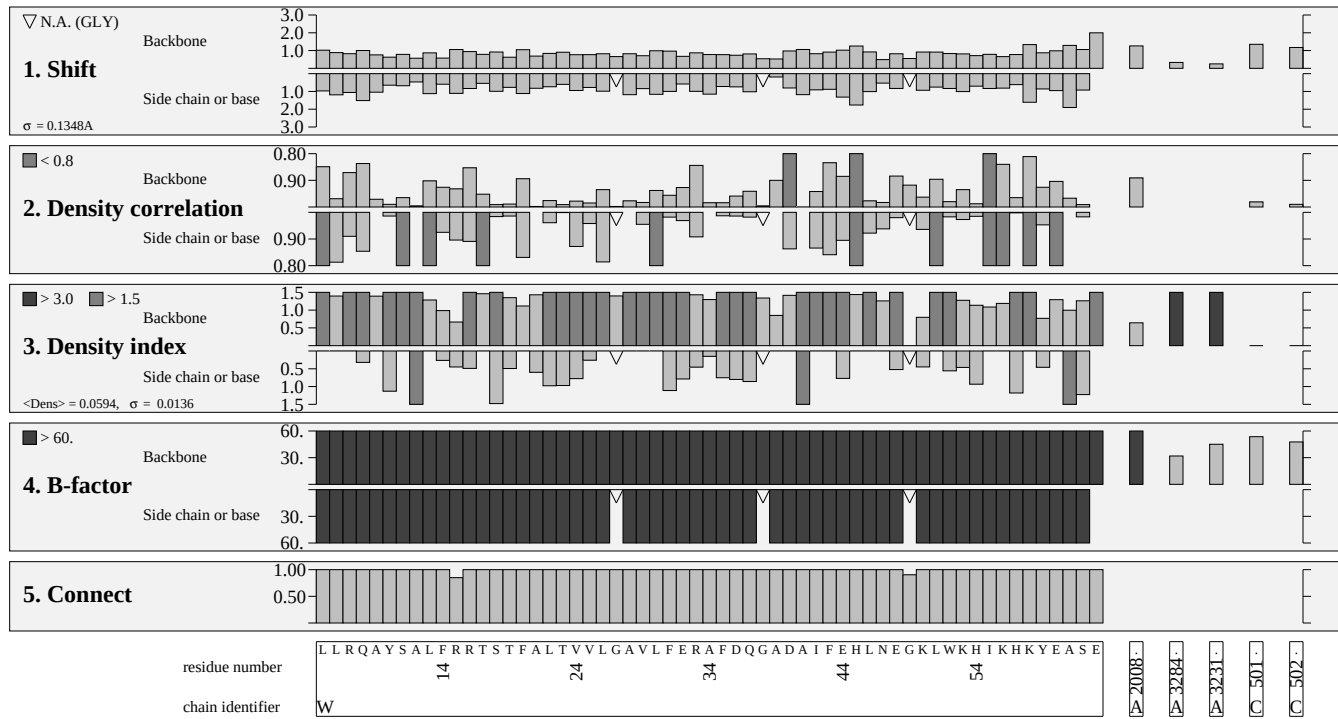
Local estimation (27)



Structure Factor Check

3H1K

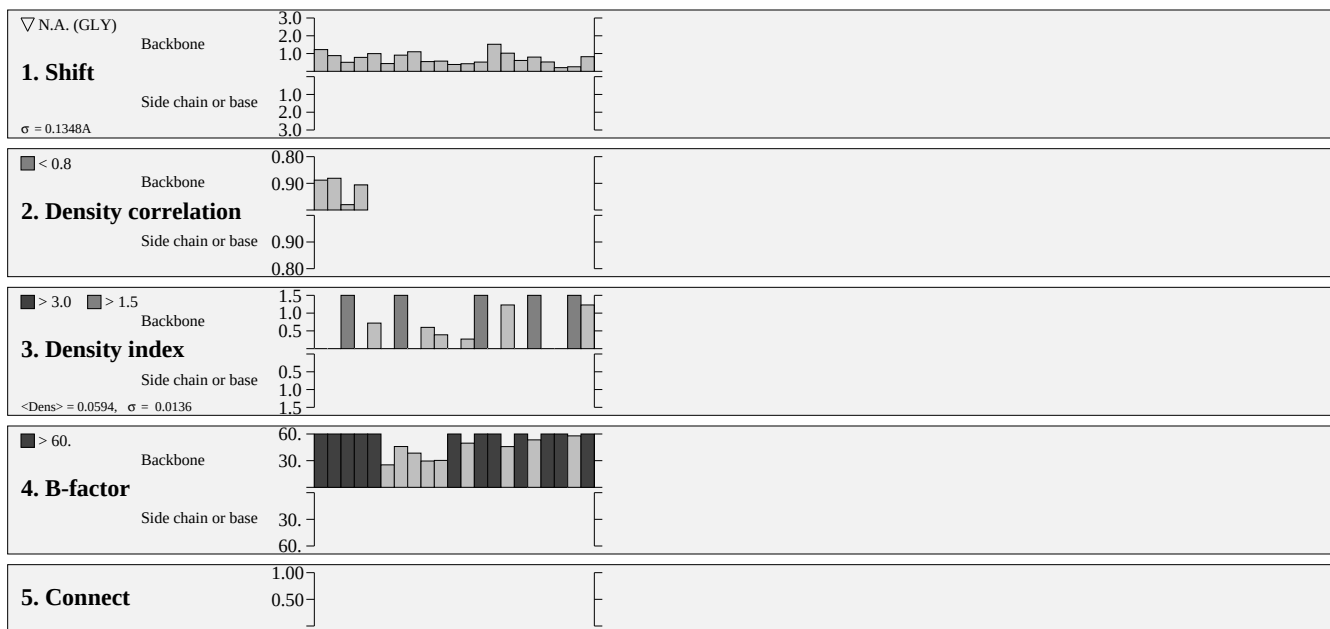
Local estimation (28)



Structure Factor Check

3H1K

Local estimation (29)



residue number	. . . w w w w w w w w w w w w w w w w
chain identifier	P