

Structure Factor Check

3H1H

Title: CYTOCHROME BC1 COMPLEX FROM CHICKEN
 Date: 12-APR-09
 PDB code: 3H1H

Crystal

Cell parameters:

a: 169.59 A b: 182.52 A c: 240.57 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 69.3 – 3.16 A
 Reflections in file: 123804
 Unique reflections above 0: 123804
 above 1 σ : 122044
 above 3 σ : 92275

SFCHECK

Nominal resolution range: 69.3 – 3.16 A
\05max. from input data, min. from author\05
 Used reflections: 123804
 Completeness: 96.8 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.064
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.3725 0.3752
 B_{overall} (by Patterson): 52. A²
 Optical resolution: 2.28 A
 Expected opt. resol. for complete data set: 2.28 A
 Estimated minimal error: 0.090 A

Model

32608 atoms (19 water molecules)

Number of chains: 51
 Volume not occupied by model: 61.7 %
 $\langle B \rangle$ (for atomic model): 75.7 A²
 $\sigma(B)$: 19.83 A²
 Matthews coefficient: 4.08
 Corresponding solvent % : 69.60

Model vs. Structure Factors

R-factor for all reflections: 0.296
 Correlation factor: 0.848
 R-factor: 0.301
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 – 3.16A
 reflections used: 121877

Rfree: 0.331
 Nfree: 2419
 R-factor without free-refl.: 0.301
 Non free-reflections: 119458
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.594 A
 Estimated maximal error: 0.476 A
 DPI: 0.477 A

Scaling

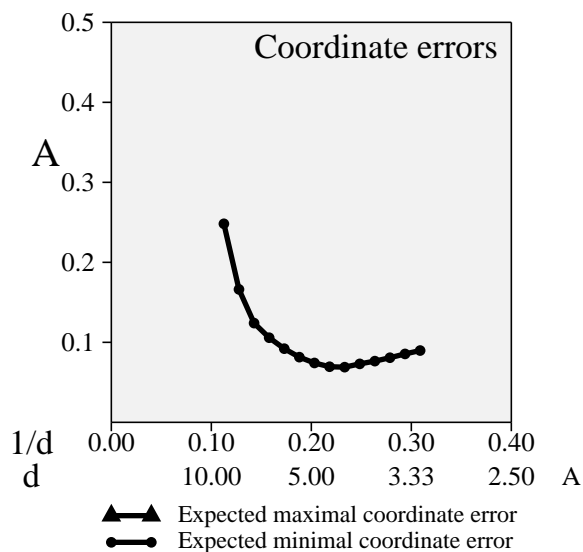
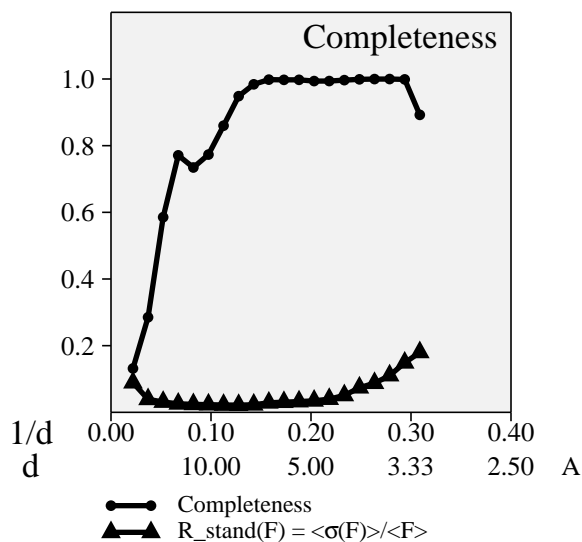
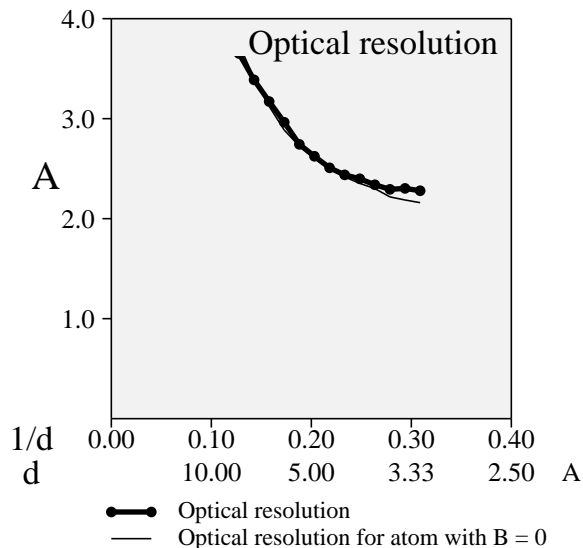
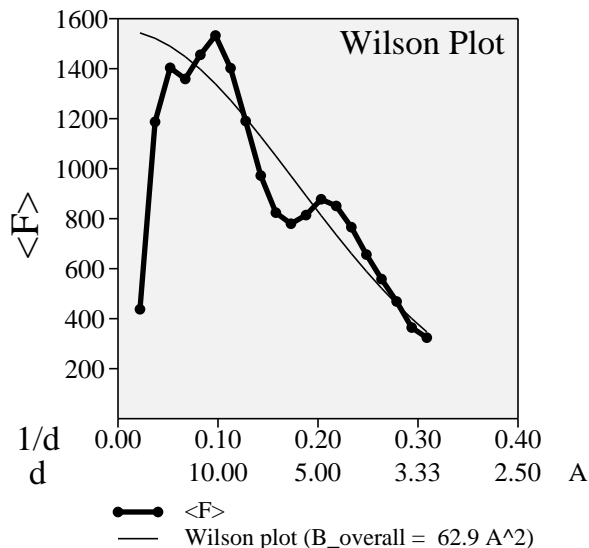
Scale: 0.685
 Bdiff: -7.62
 Anisothermal Scaling (Beta):
 17.8193 -1.4625 -1.0967 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.844 250.356

Refinement

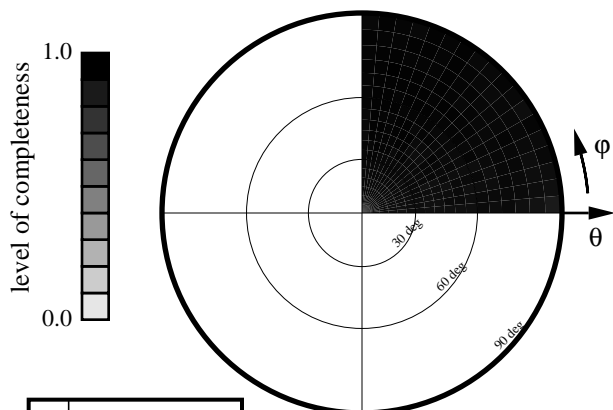
Program: CNS 1.1
 Nominal resolution range: 20.0 – 3.16 A
 Reported nominal resolution: 3.00 A
 Reported R-factor: 0.253
 Number of reflections used: 123634
 Reported Rfree: 0.29
 Sigma cut-off: N.A.

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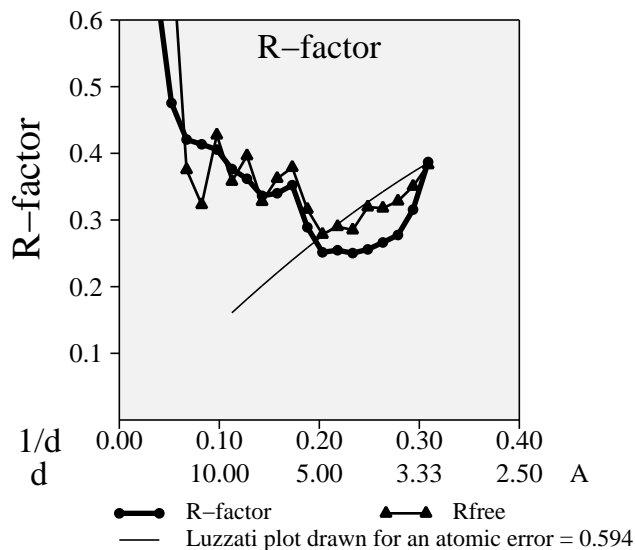


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

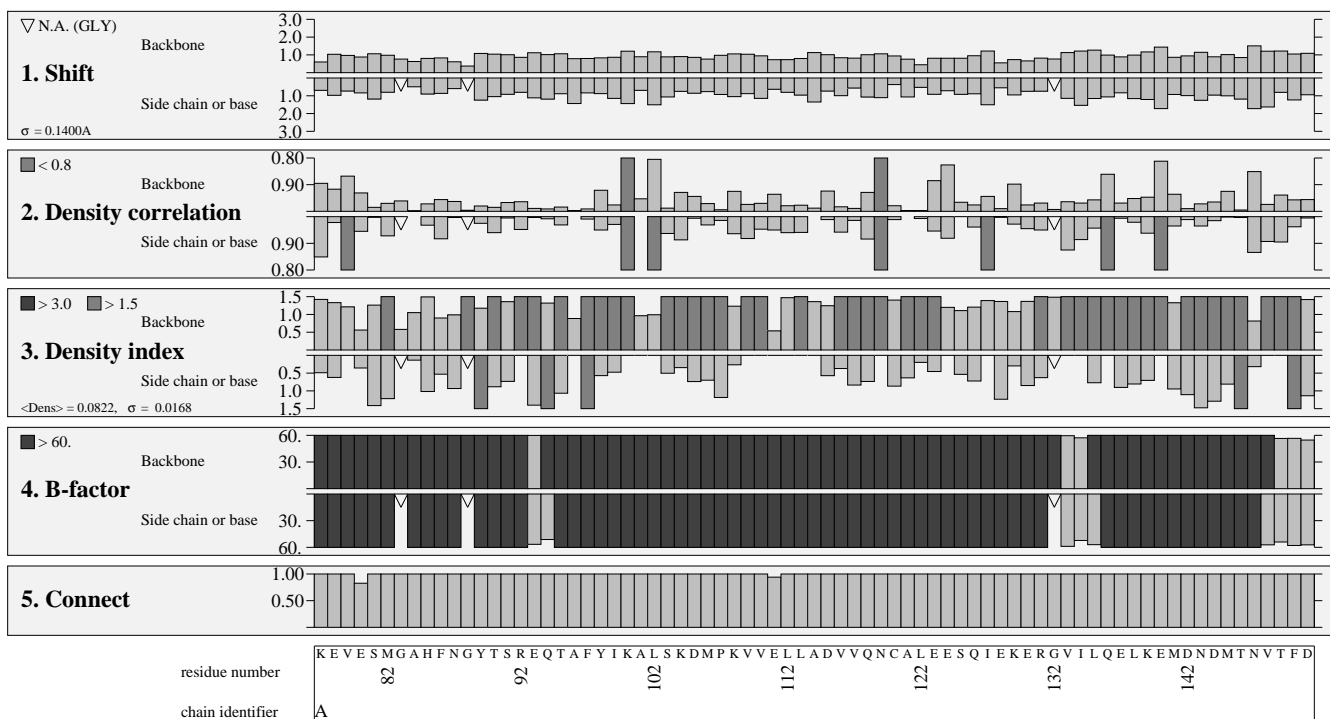
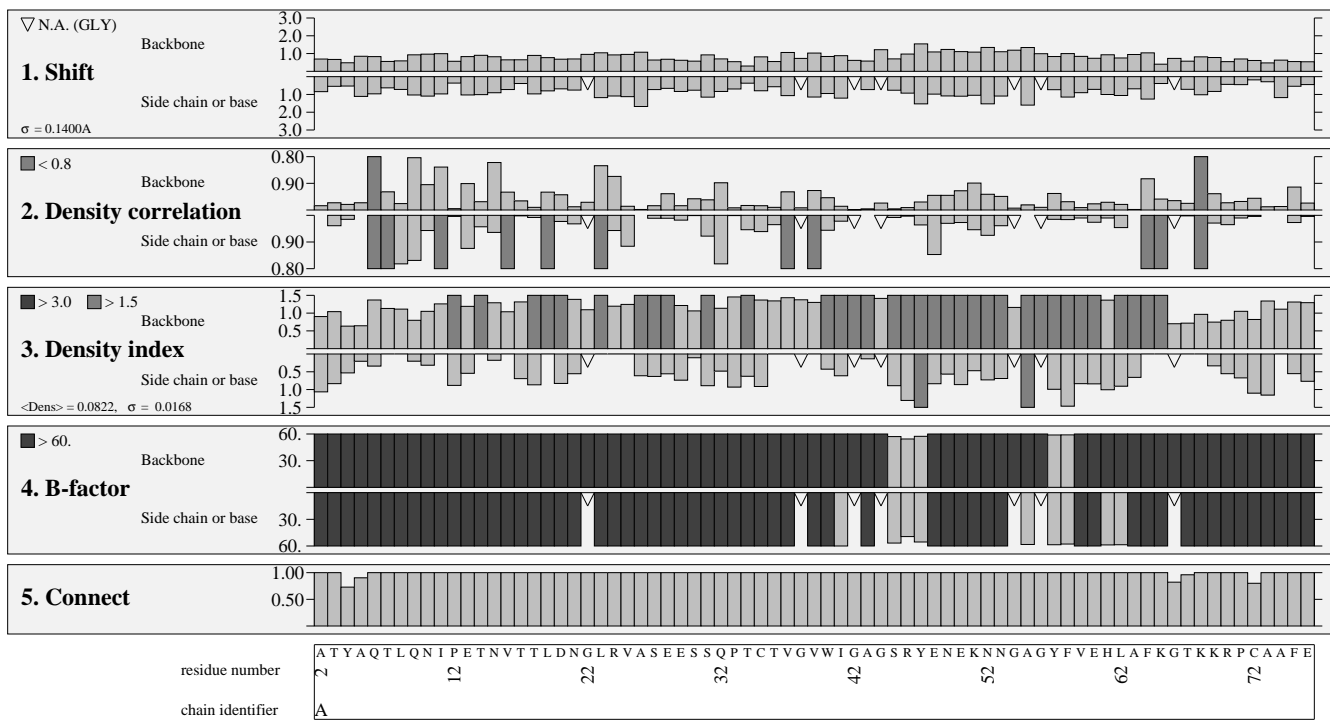
polar coordinates of the crystallographical axes



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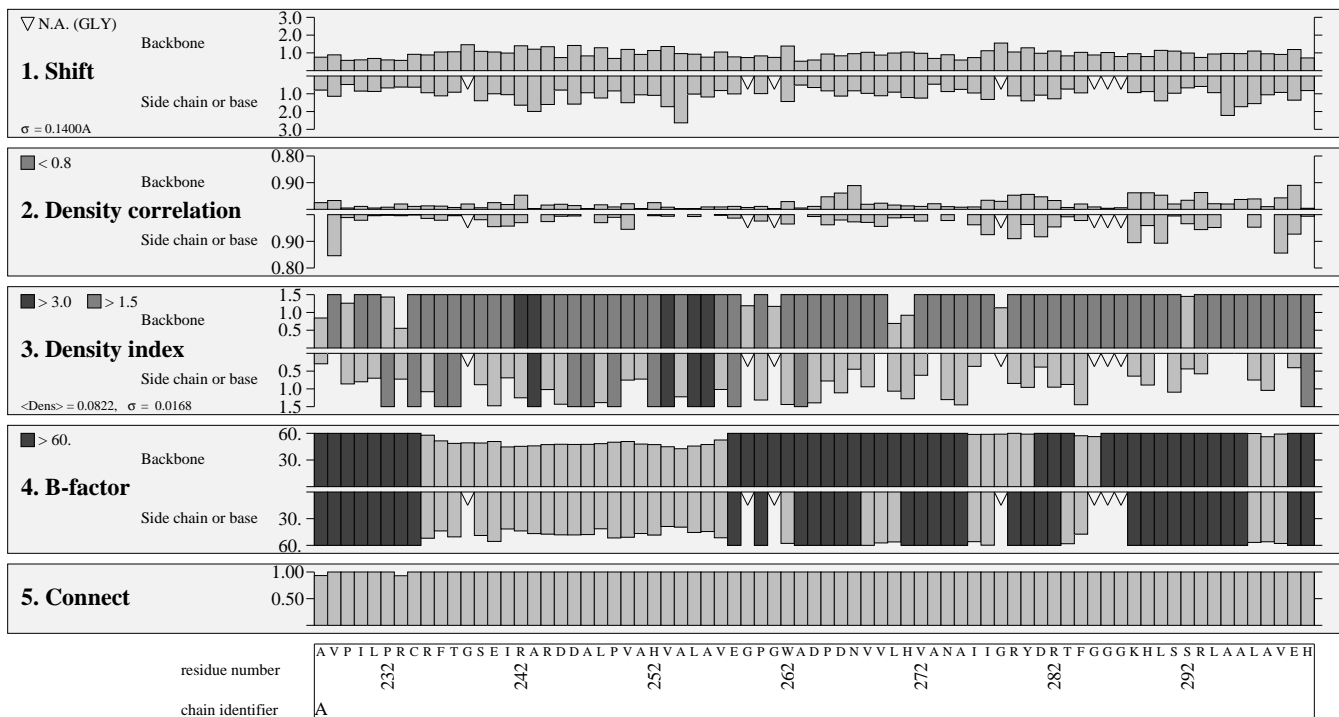
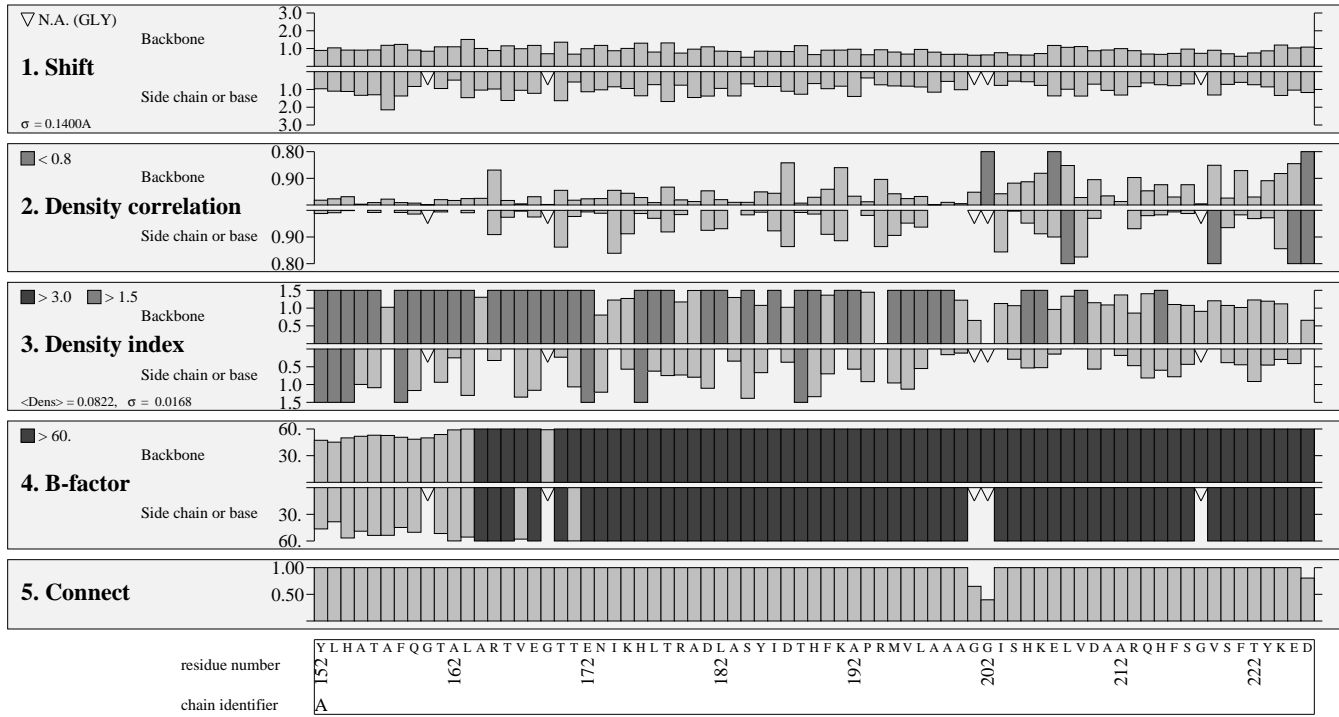
Local estimation



Structure Factor Check

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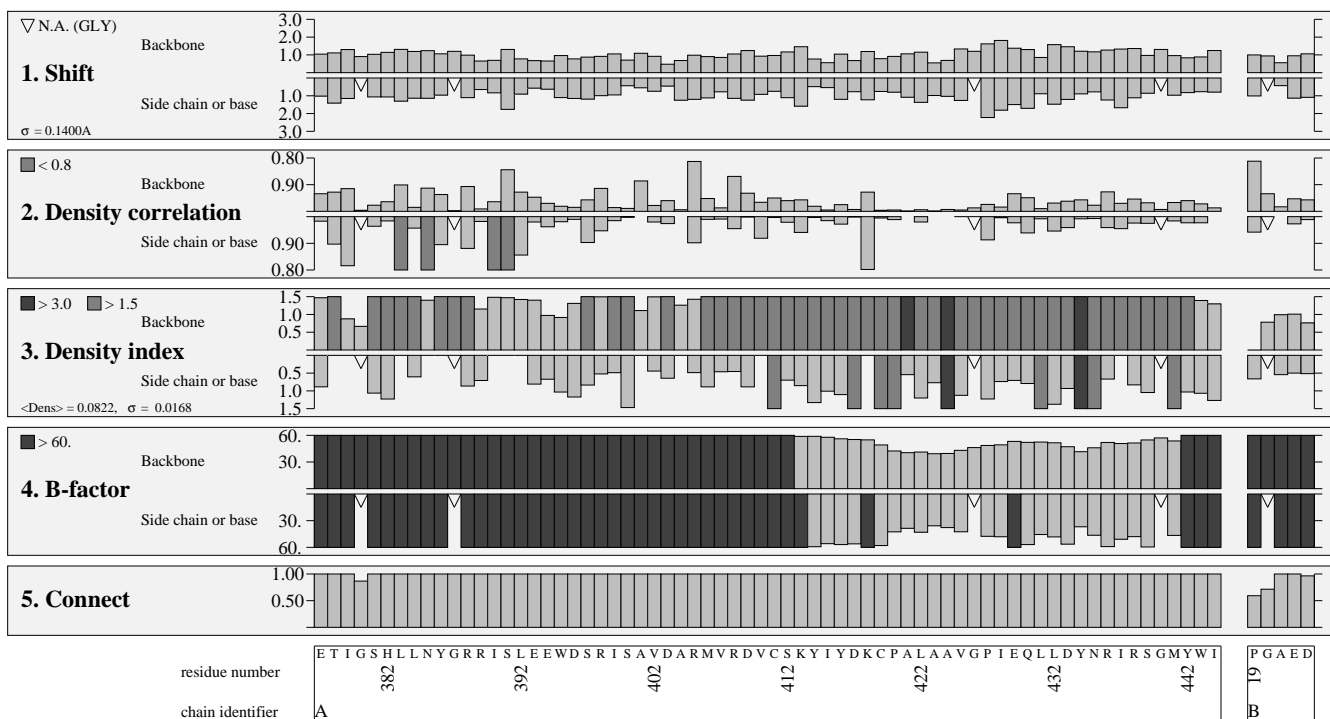
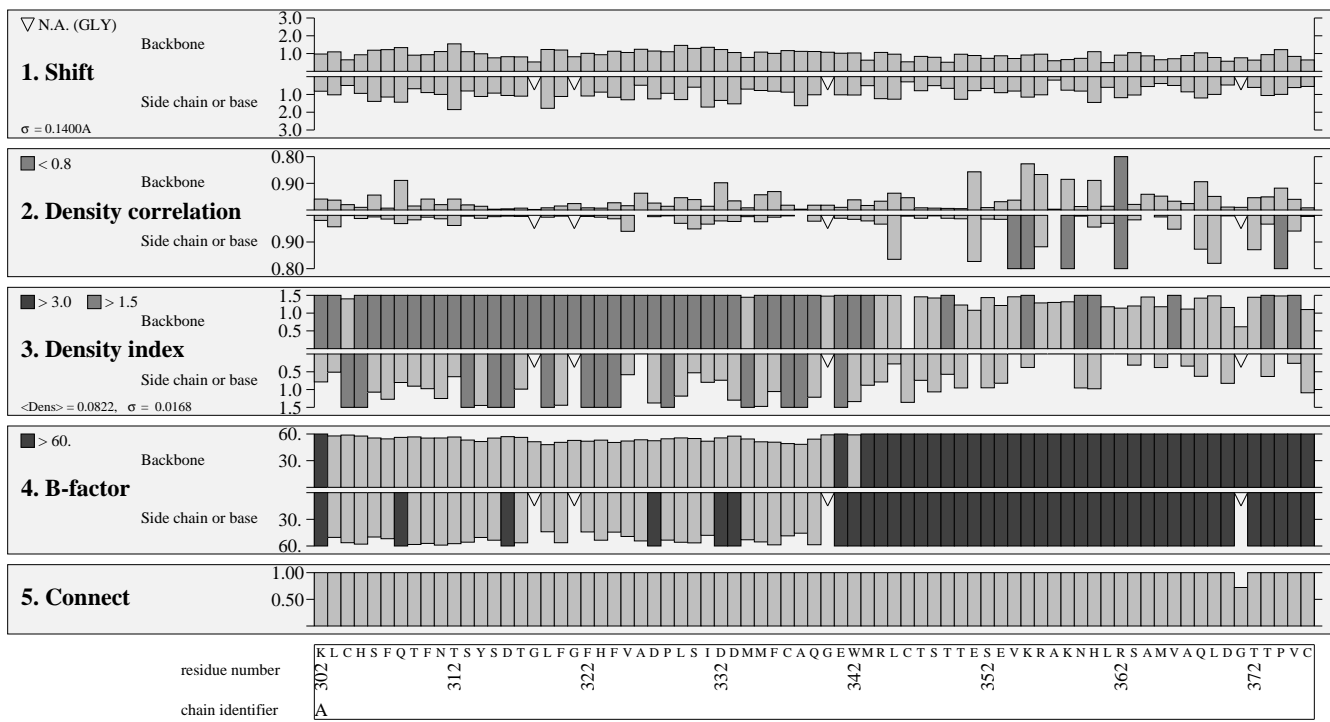
Local estimation (2)



Structure Factor Check

3H1H

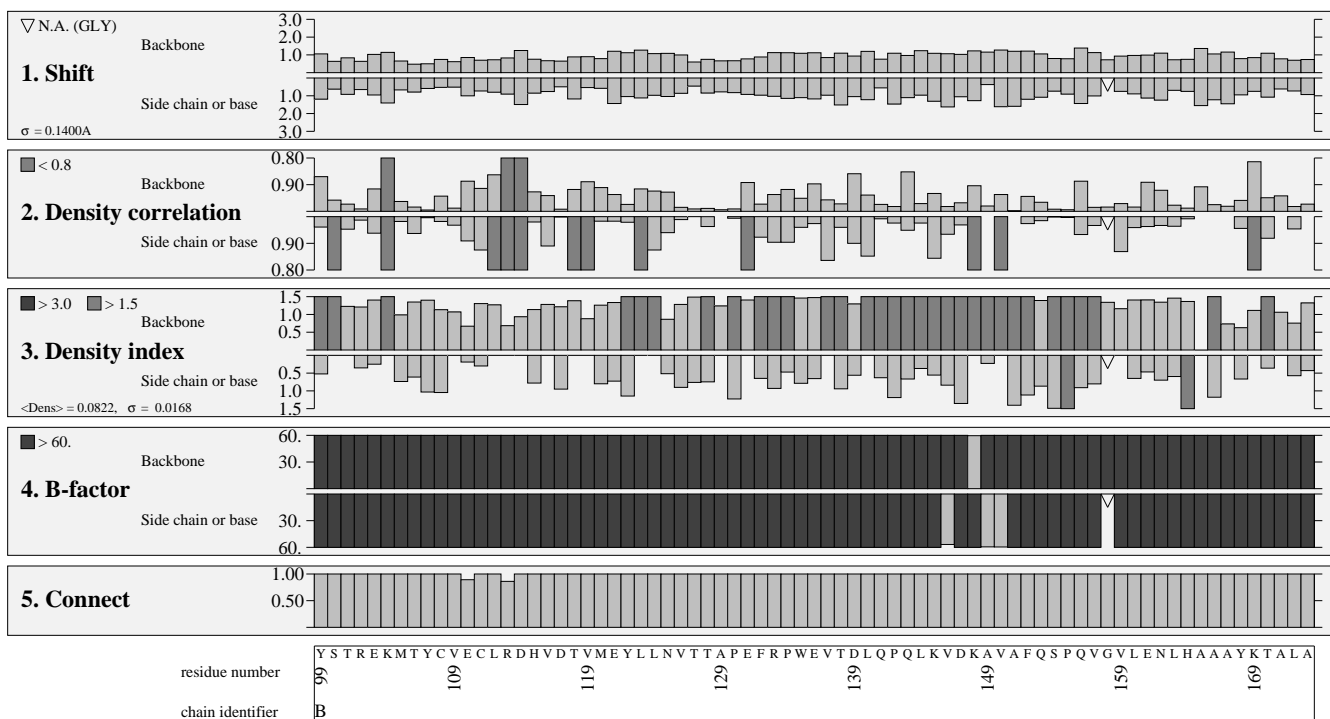
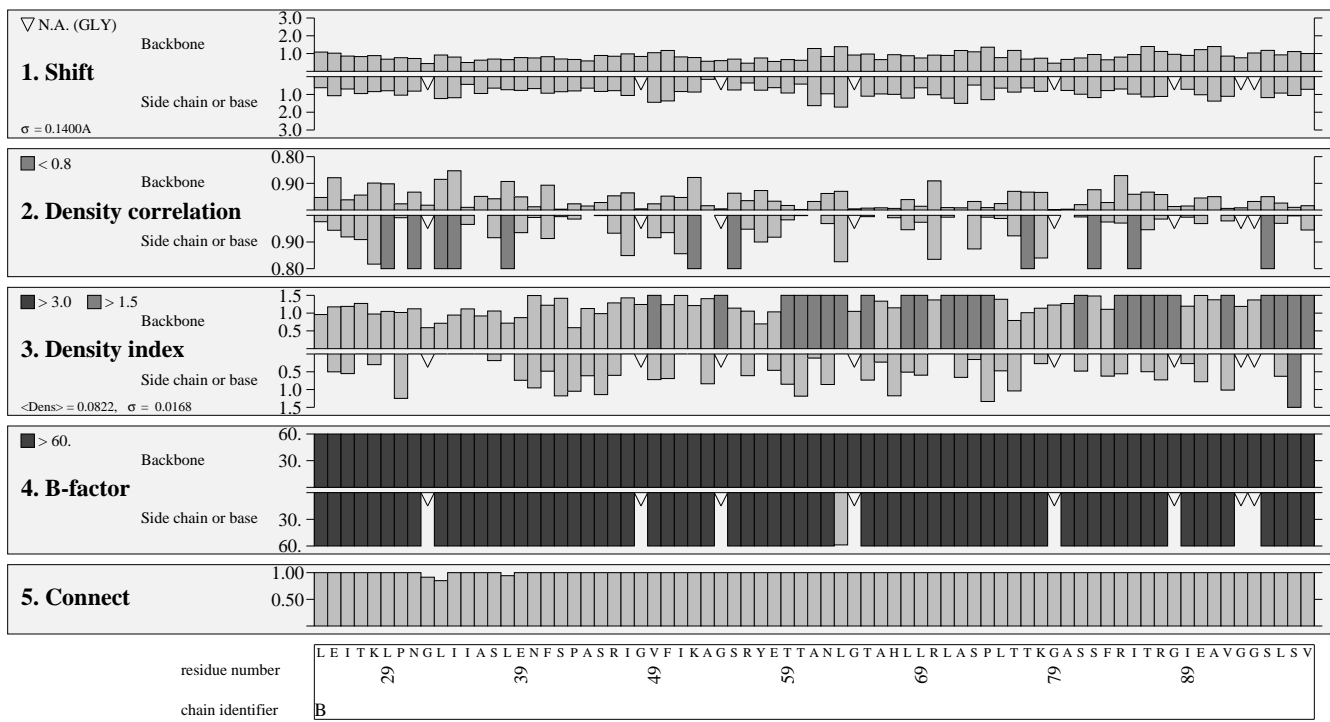
Local estimation (3)



Structure Factor Check

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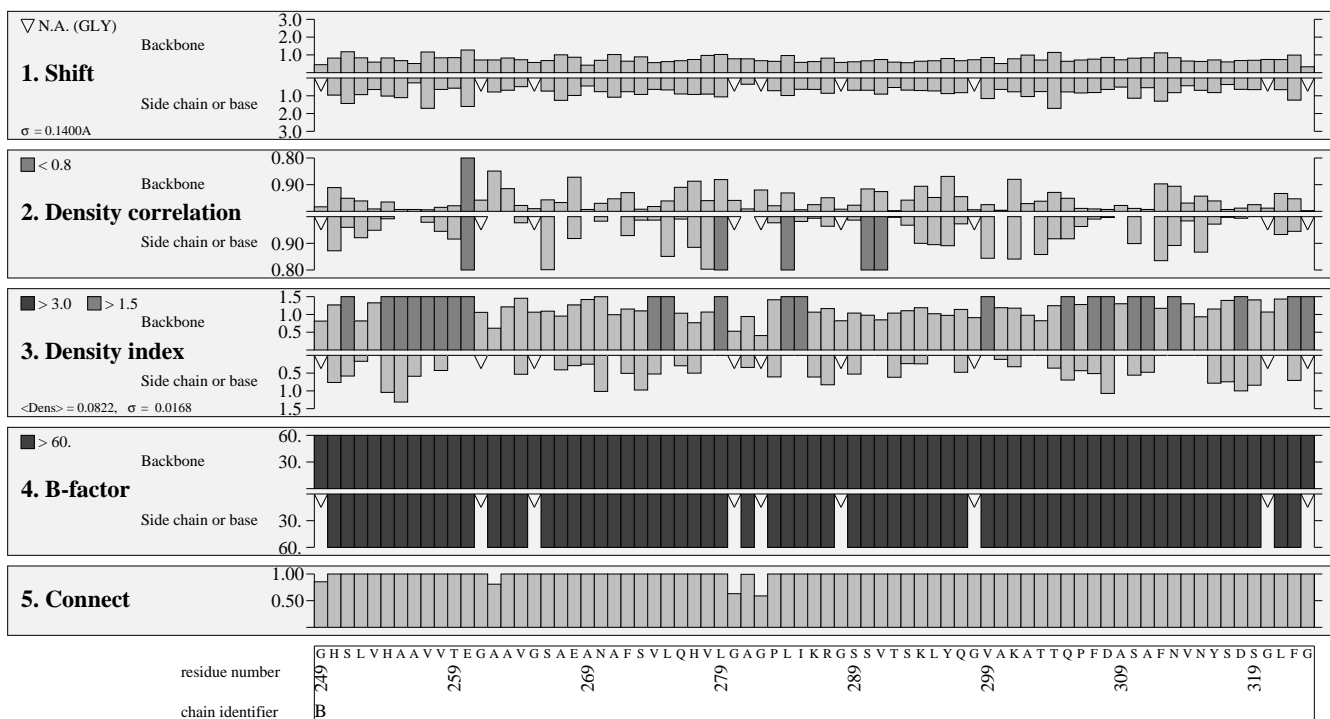
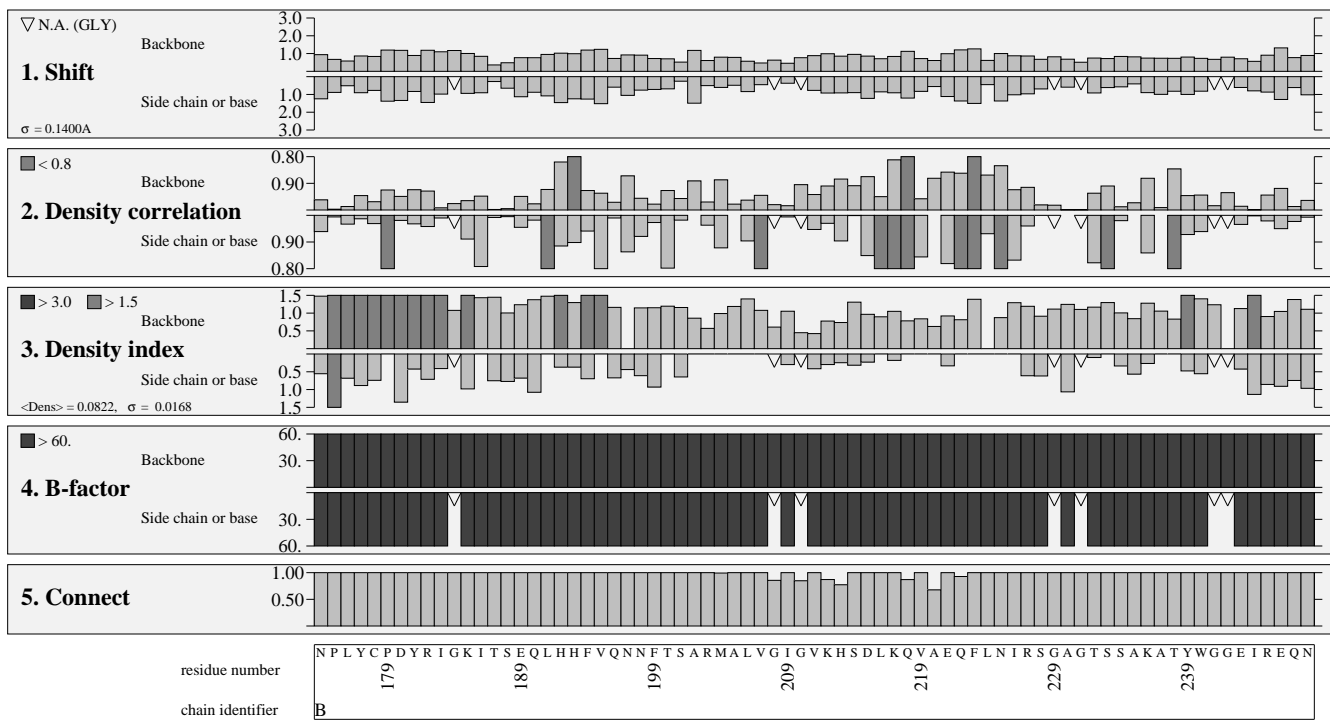
Local estimation (4)



Structure Factor Check

3H1H

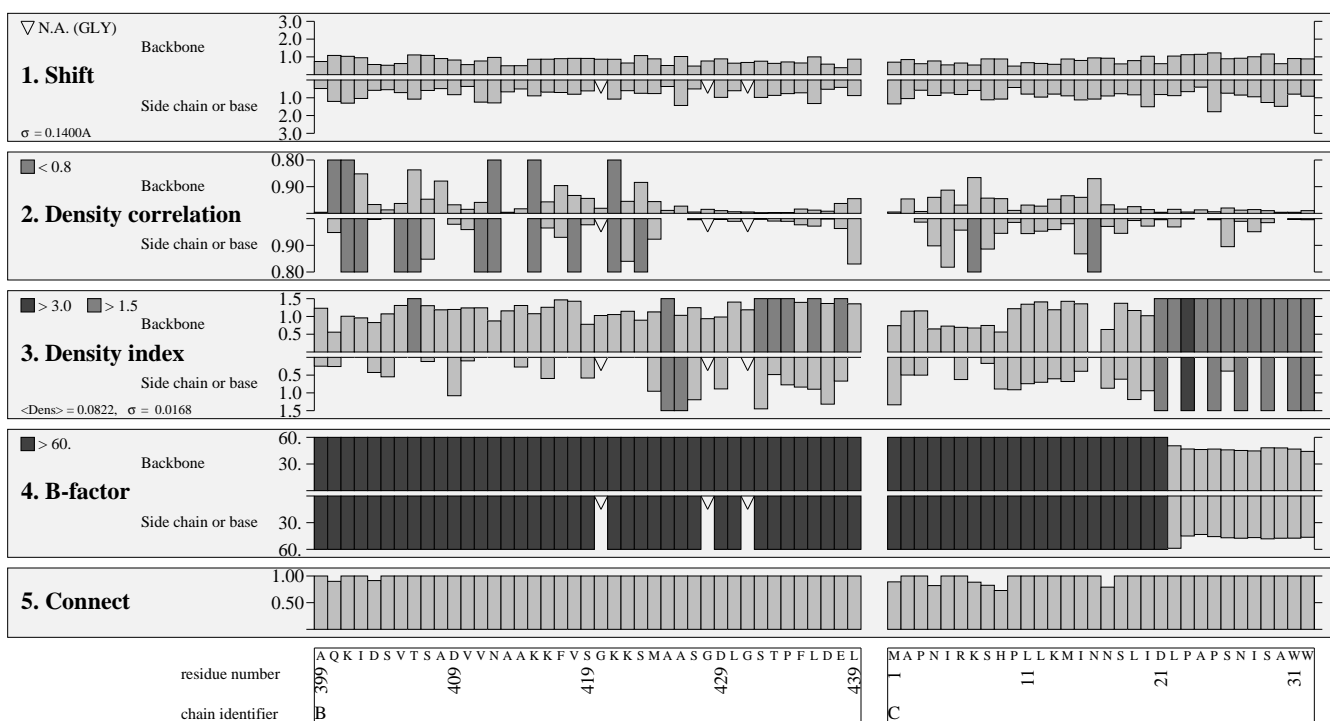
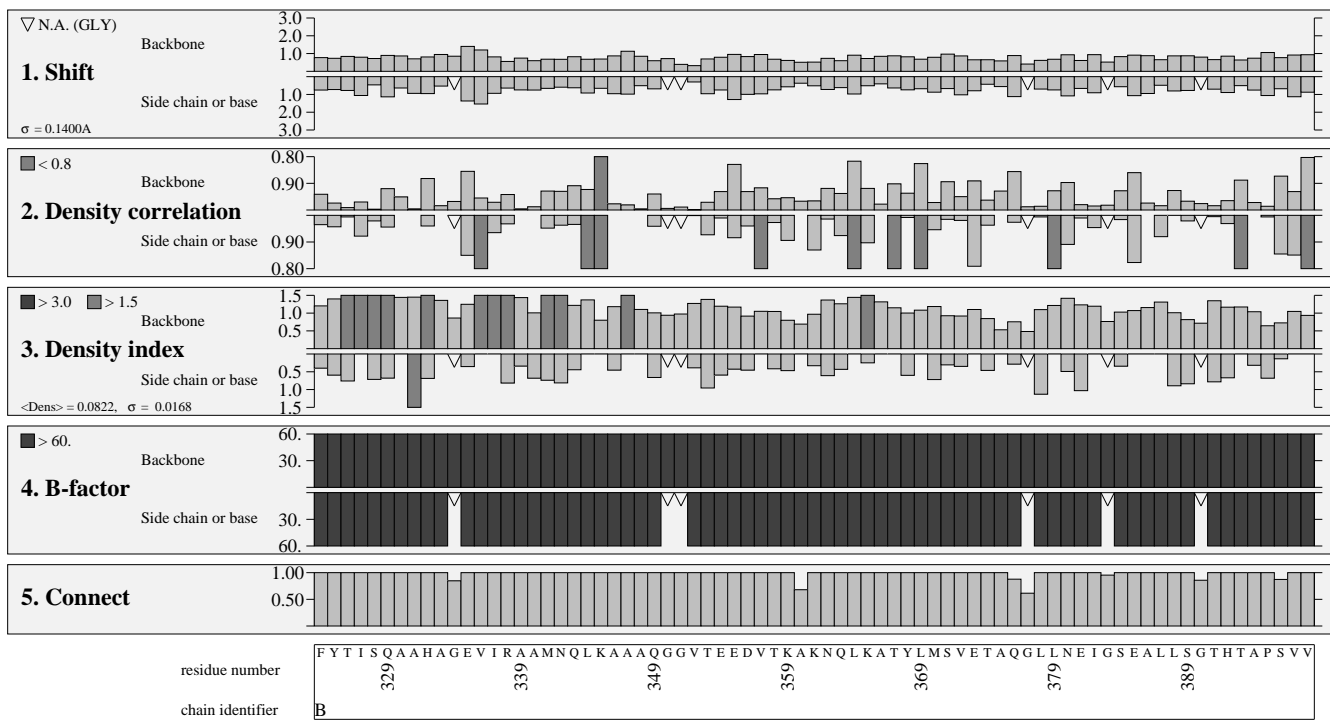
Local estimation (5)



Structure Factor Check

3H1H

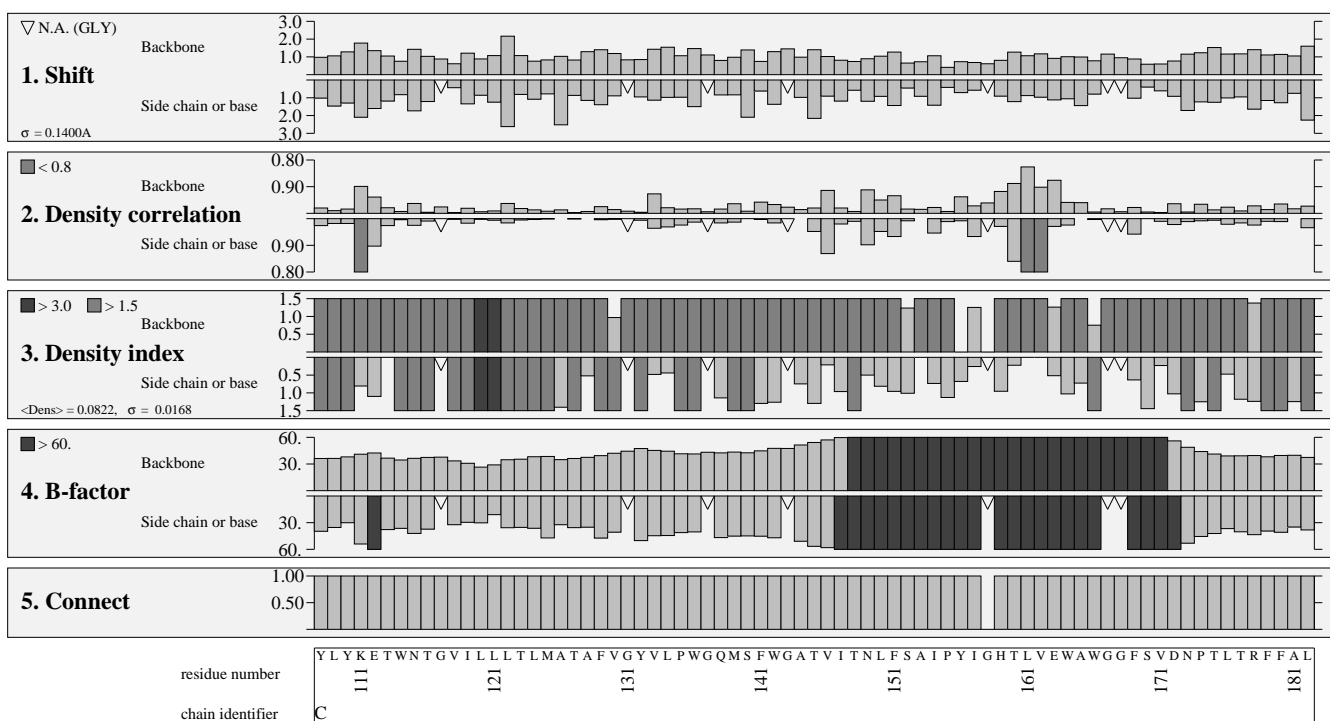
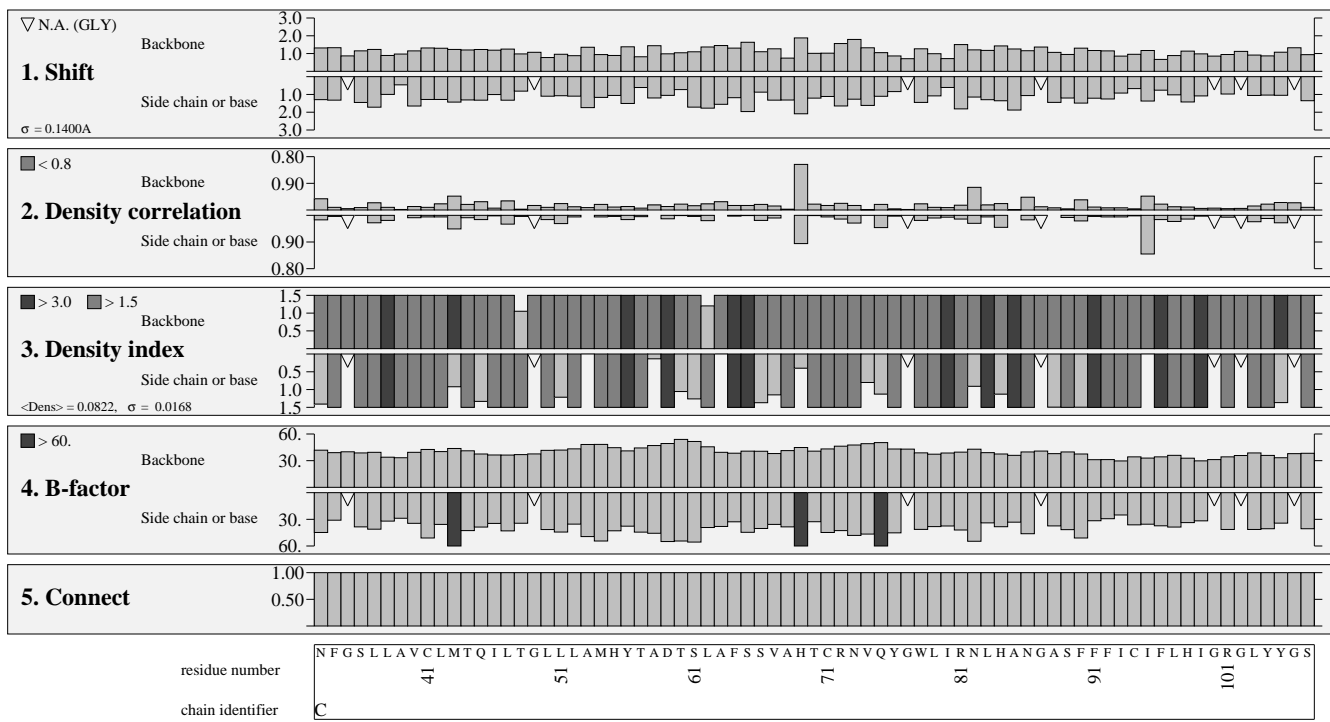
Local estimation (6)



Structure Factor Check

3H1H

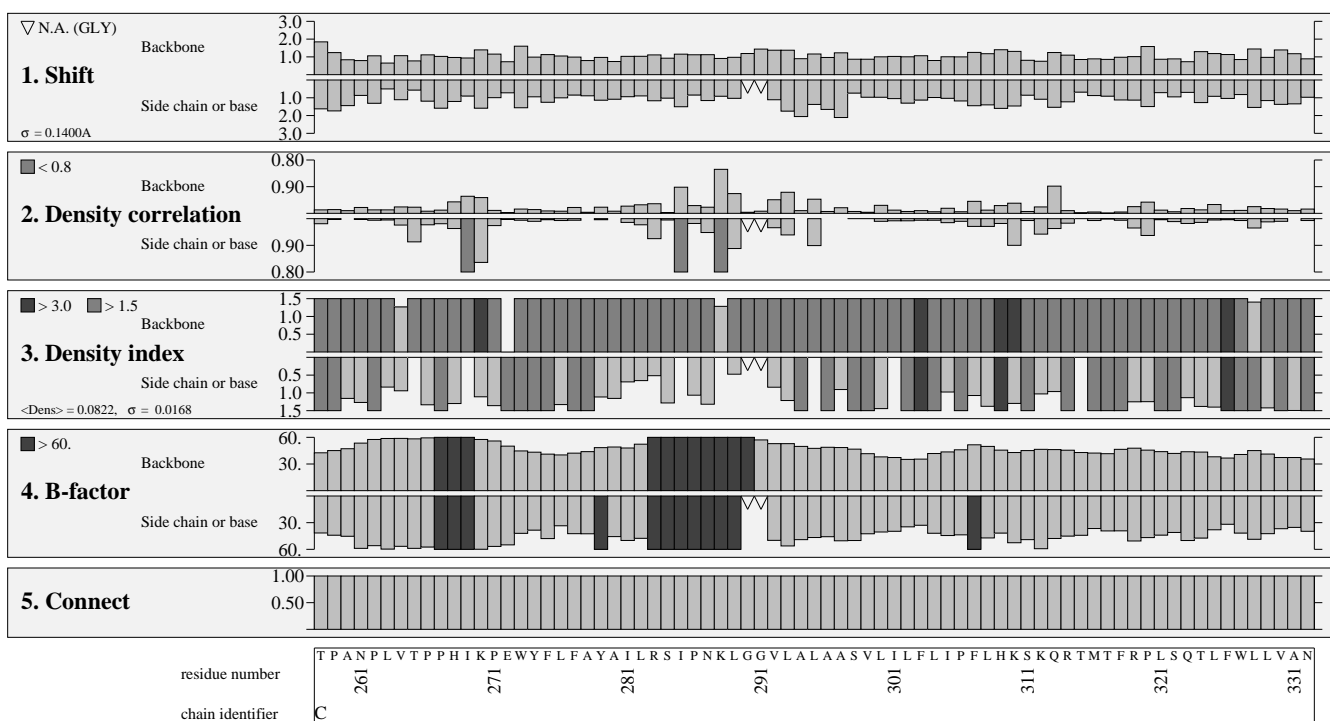
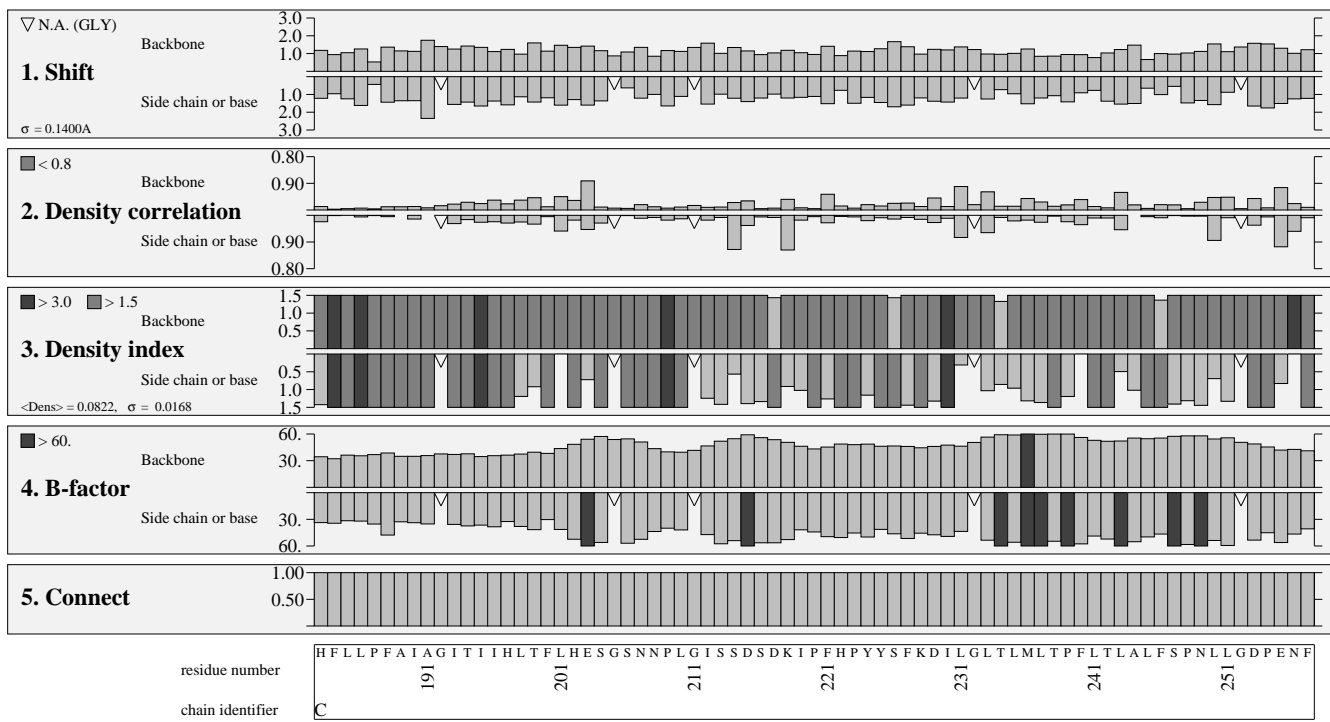
Local estimation (7)



Structure Factor Check

3H1H

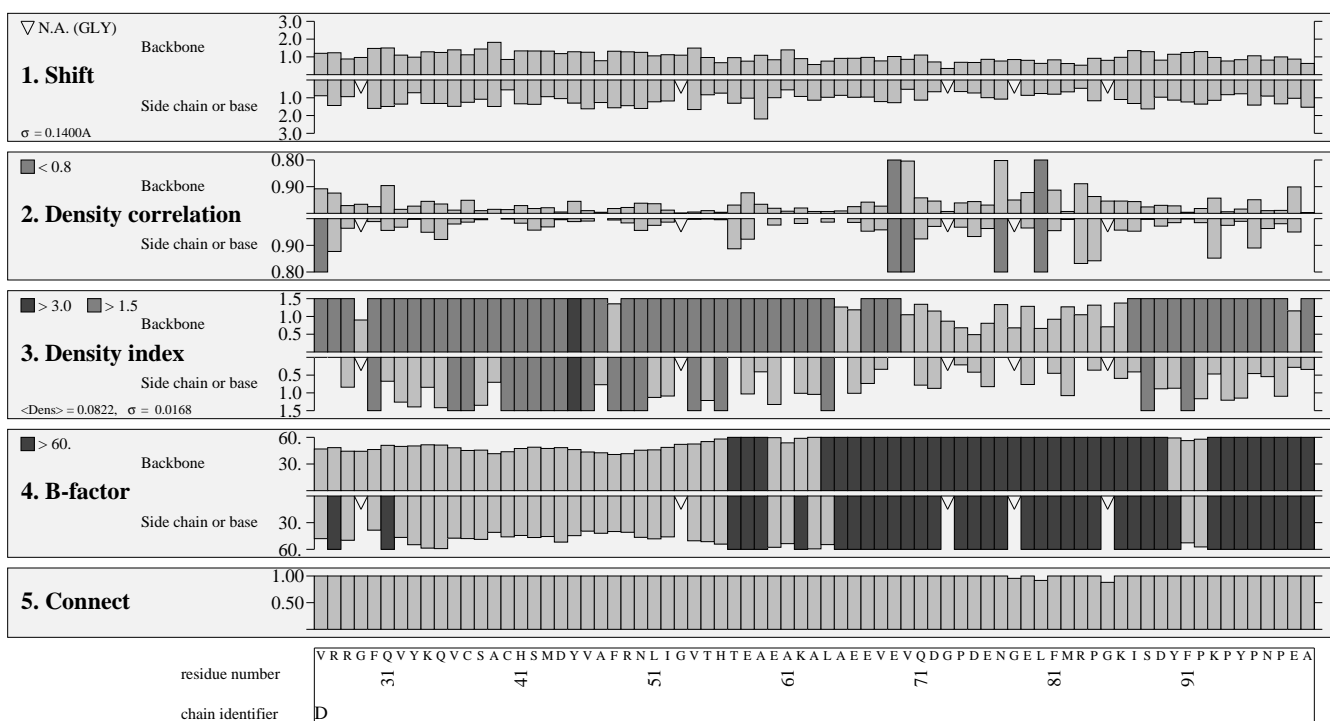
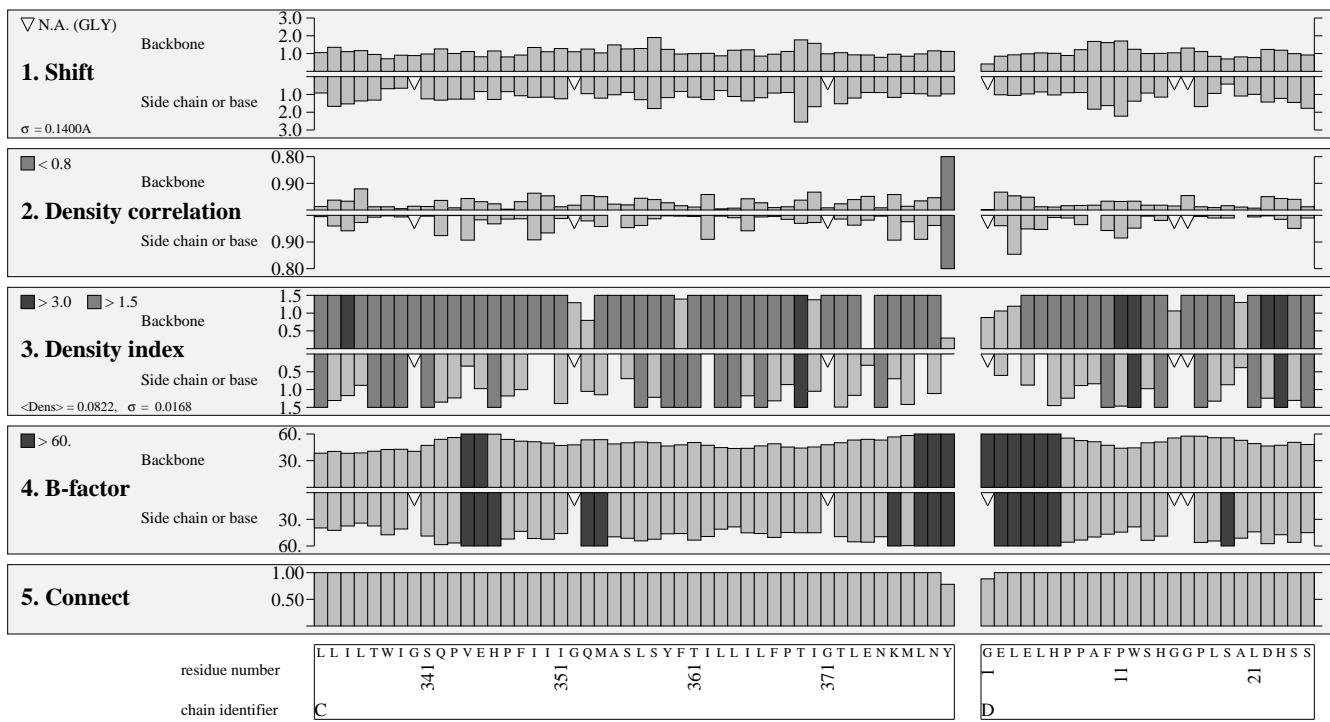
Local estimation (8)



Structure Factor Check

3H1H

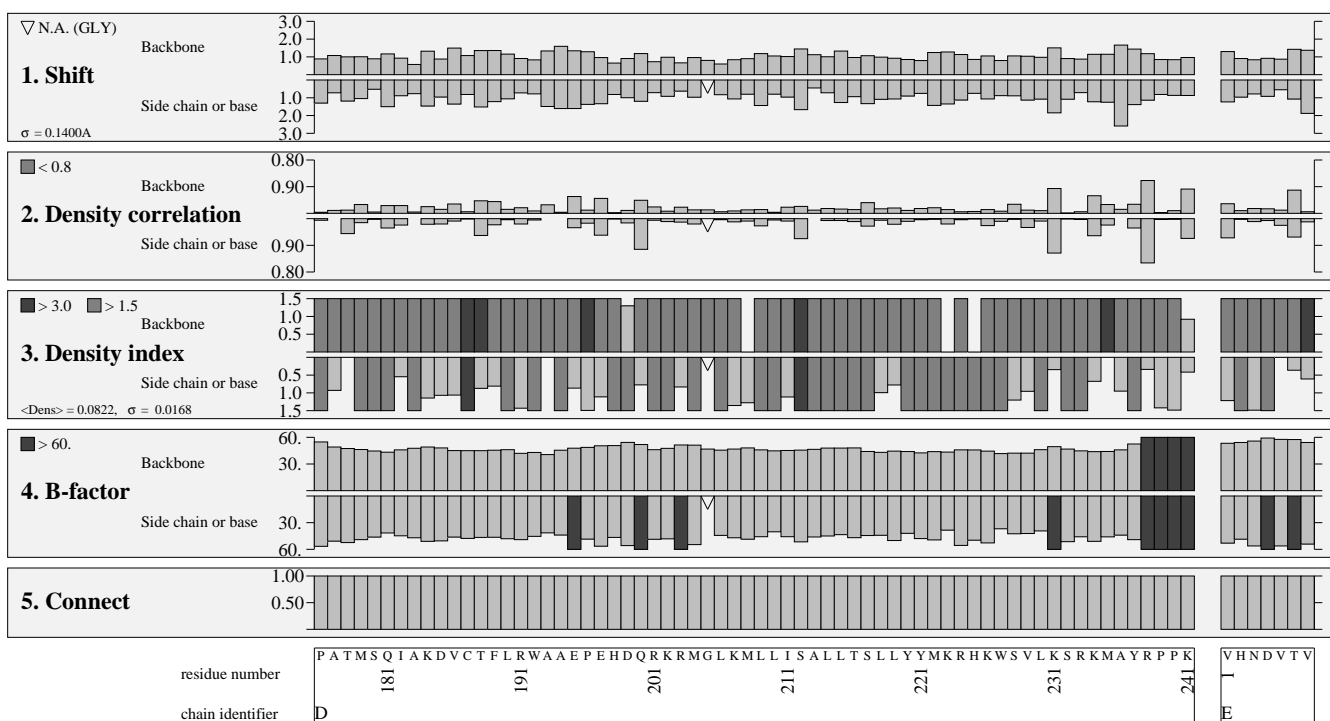
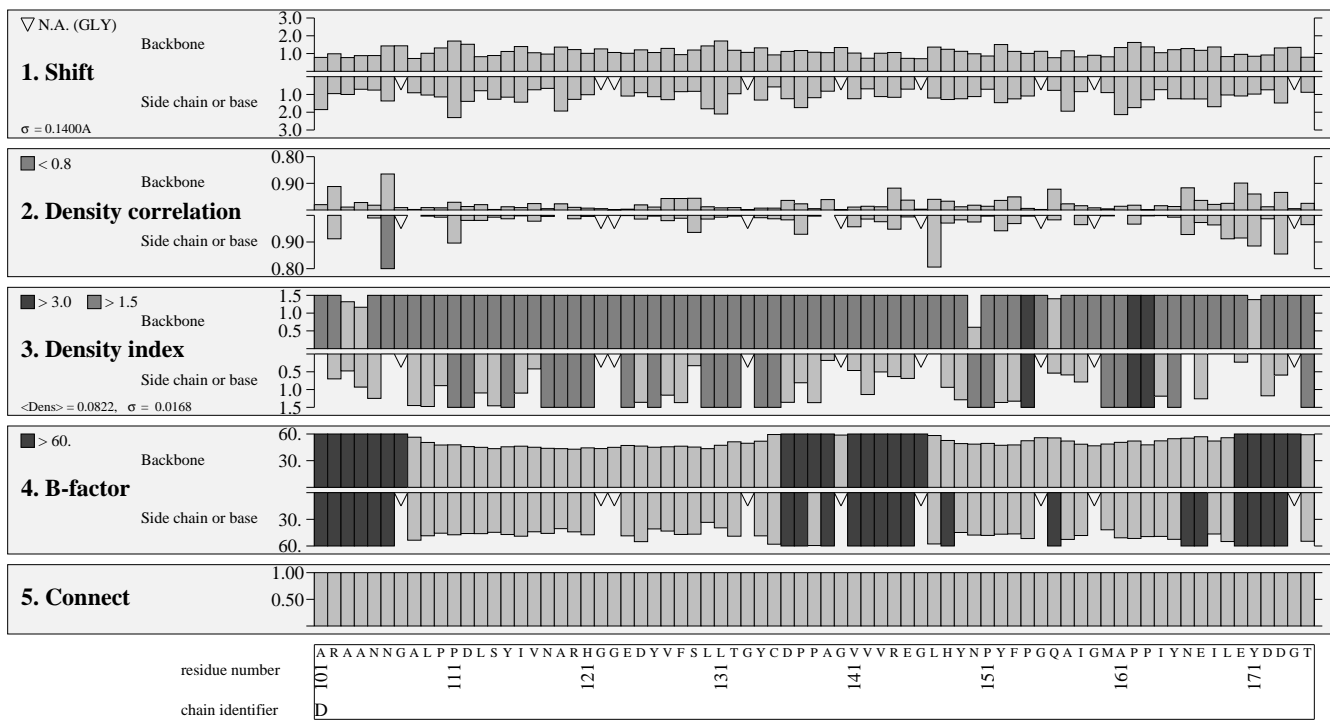
Local estimation (9)



Structure Factor Check

3H1H

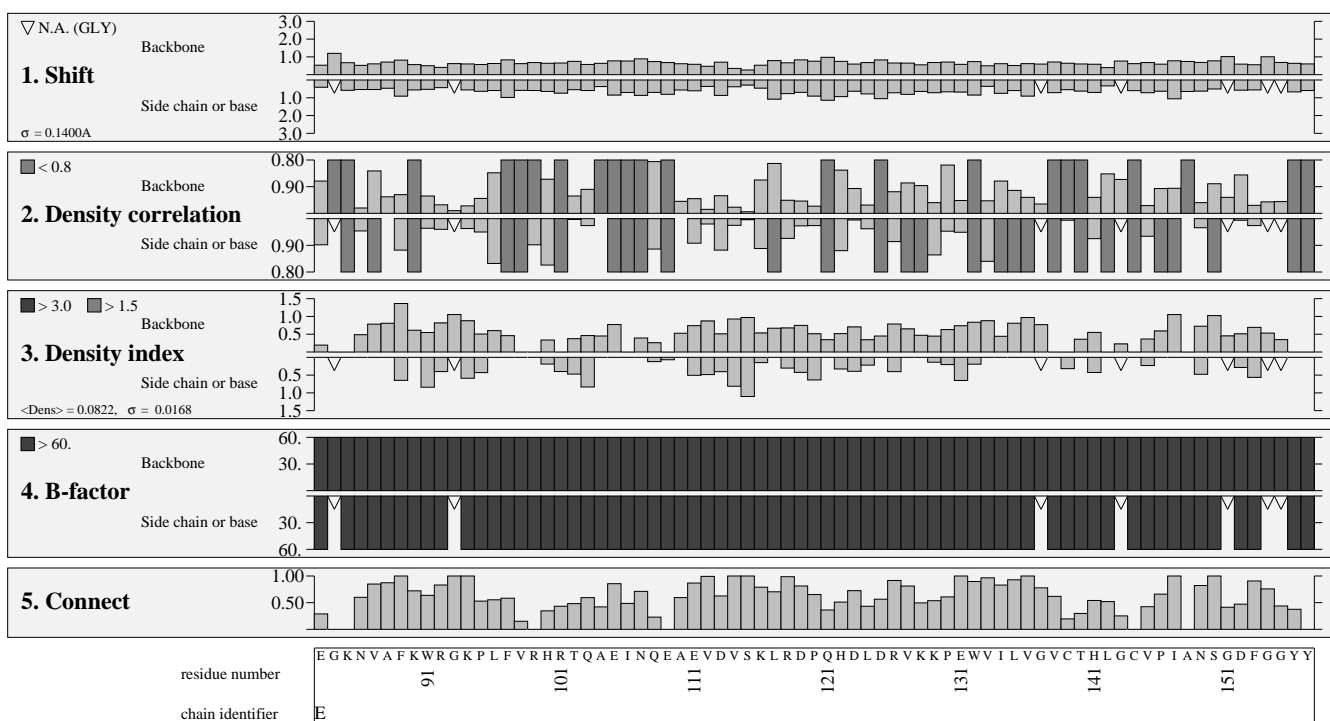
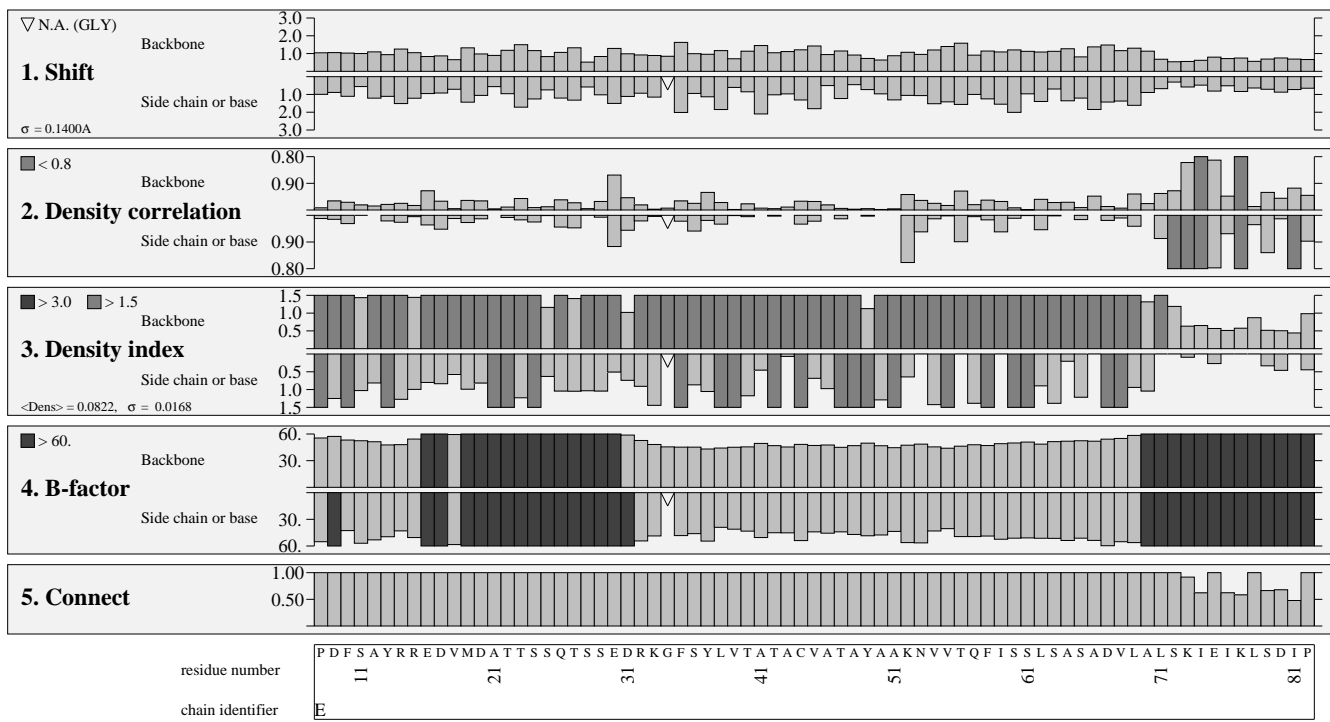
Local estimation (10)



Structure Factor Check

3H1H

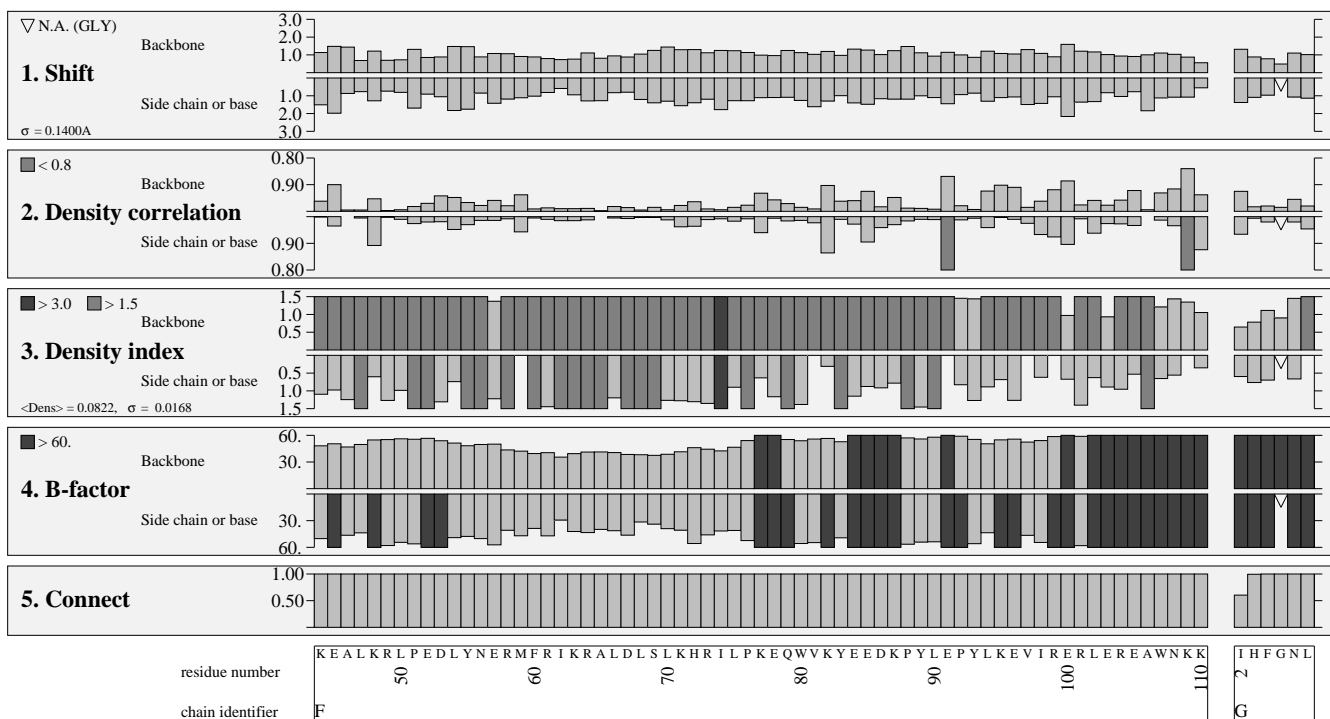
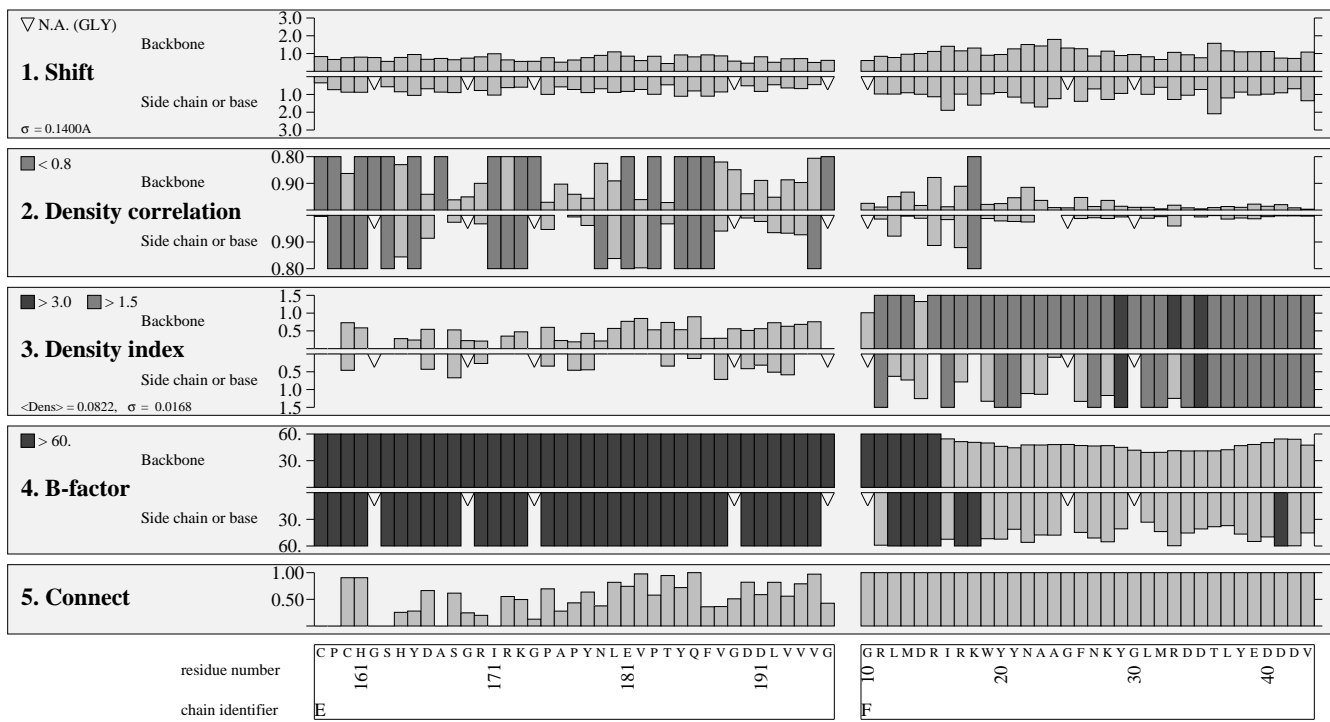
Local estimation (11)



Structure Factor Check

3H1H

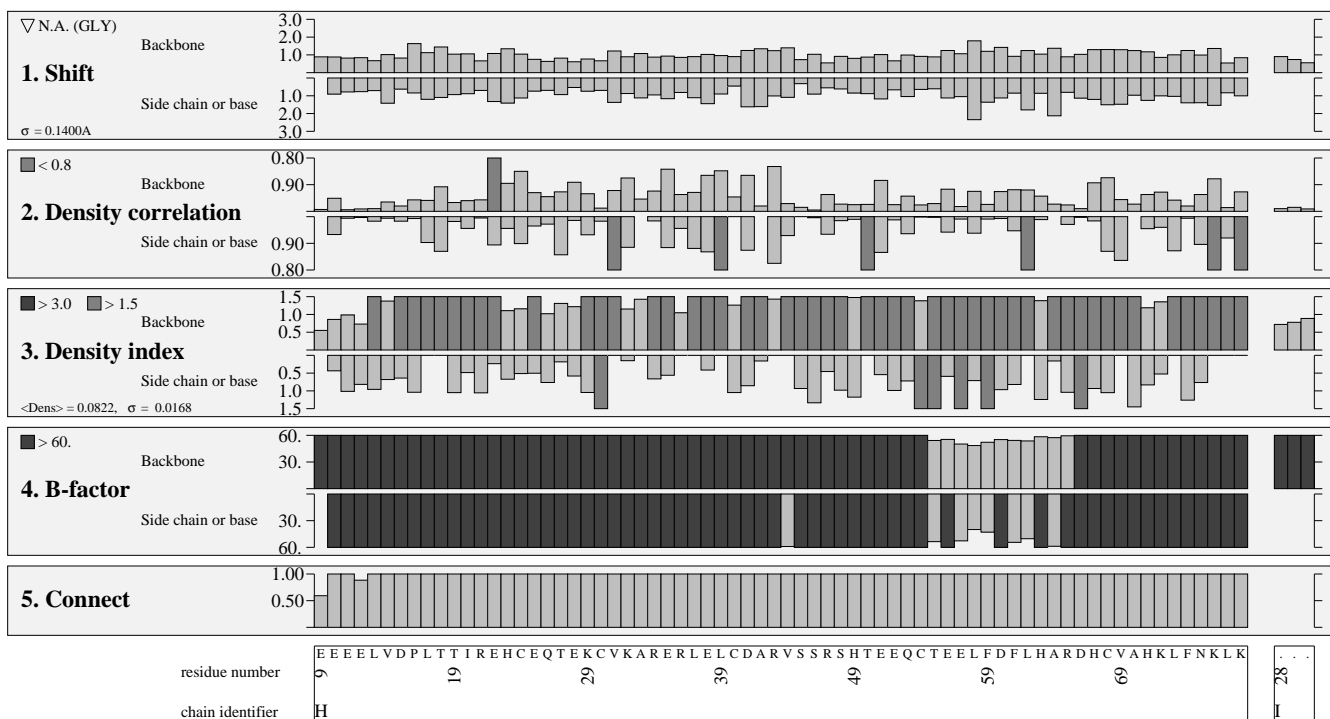
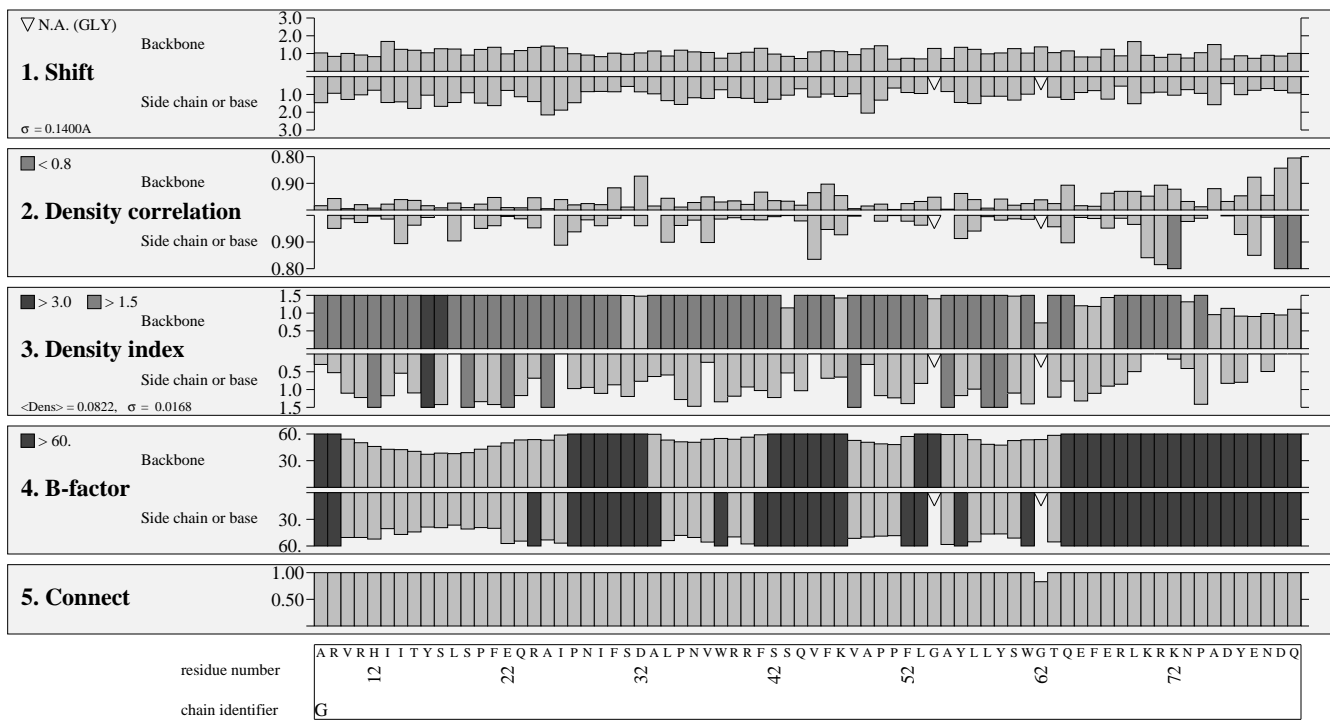
Local estimation (12)



Structure Factor Check

3H1H

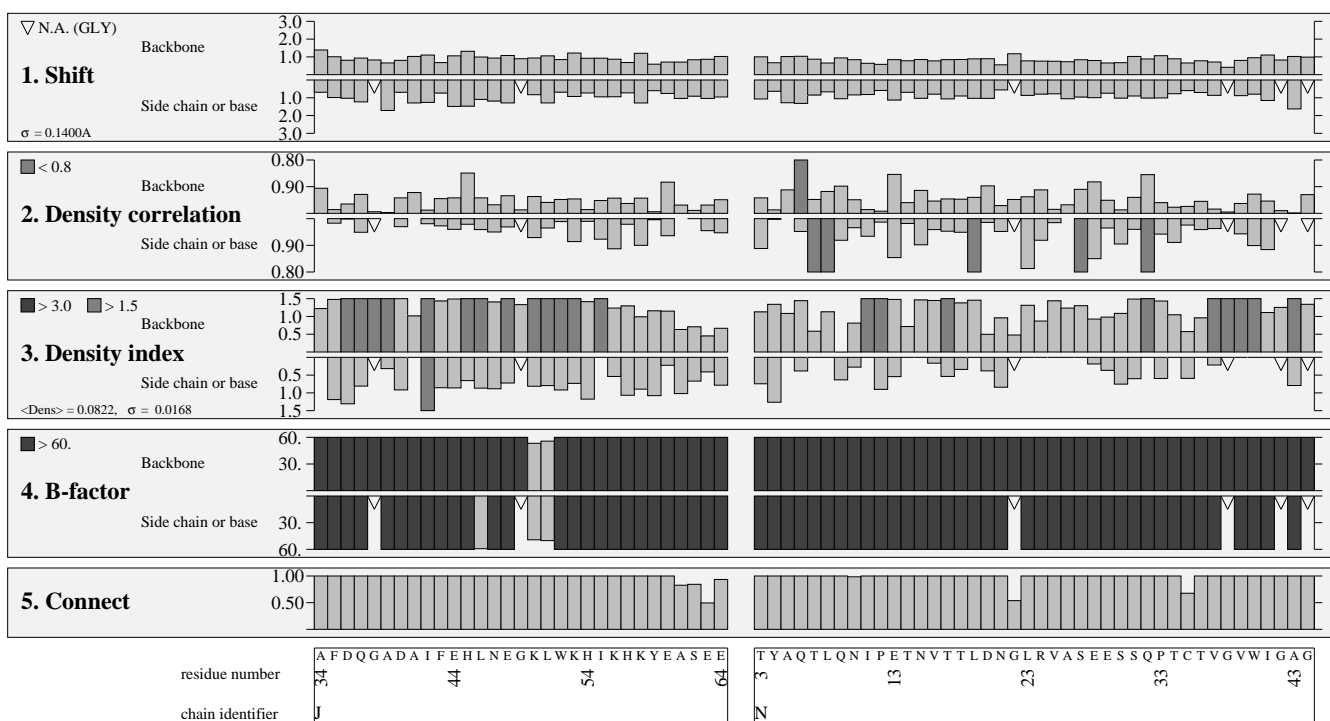
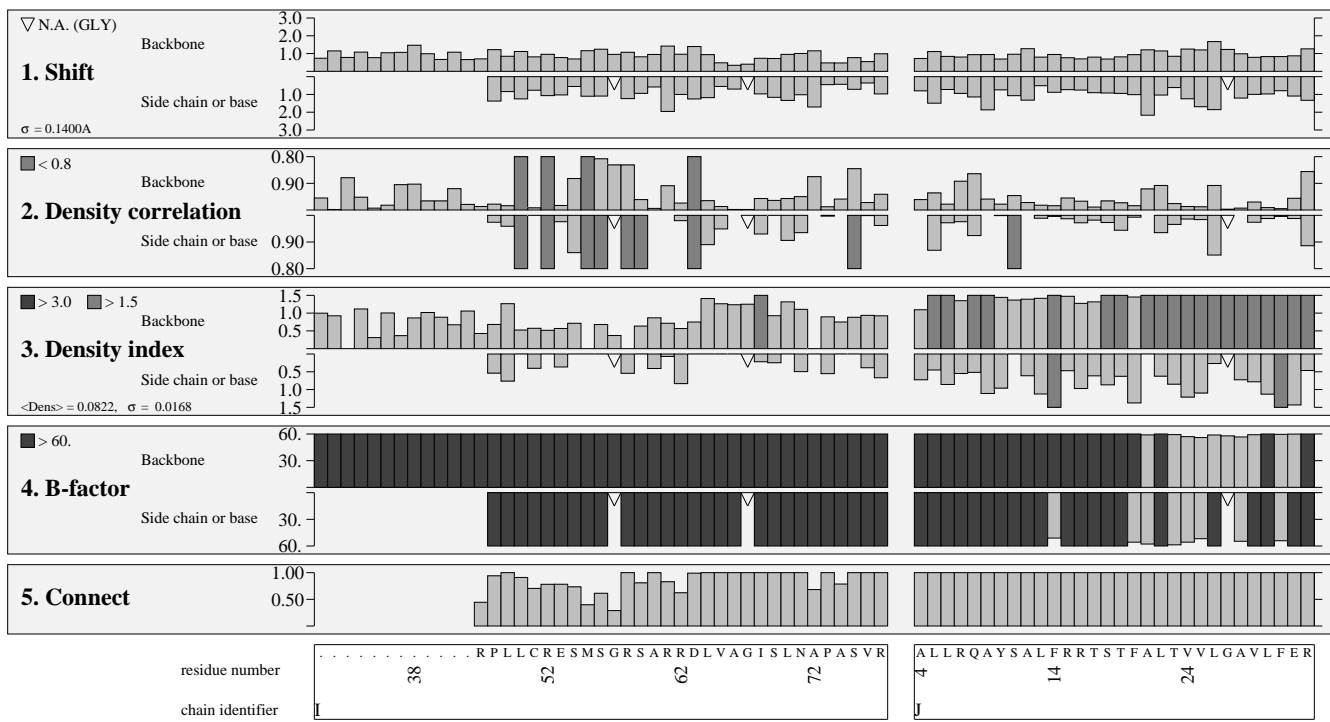
Local estimation (13)



Structure Factor Check

3H1H

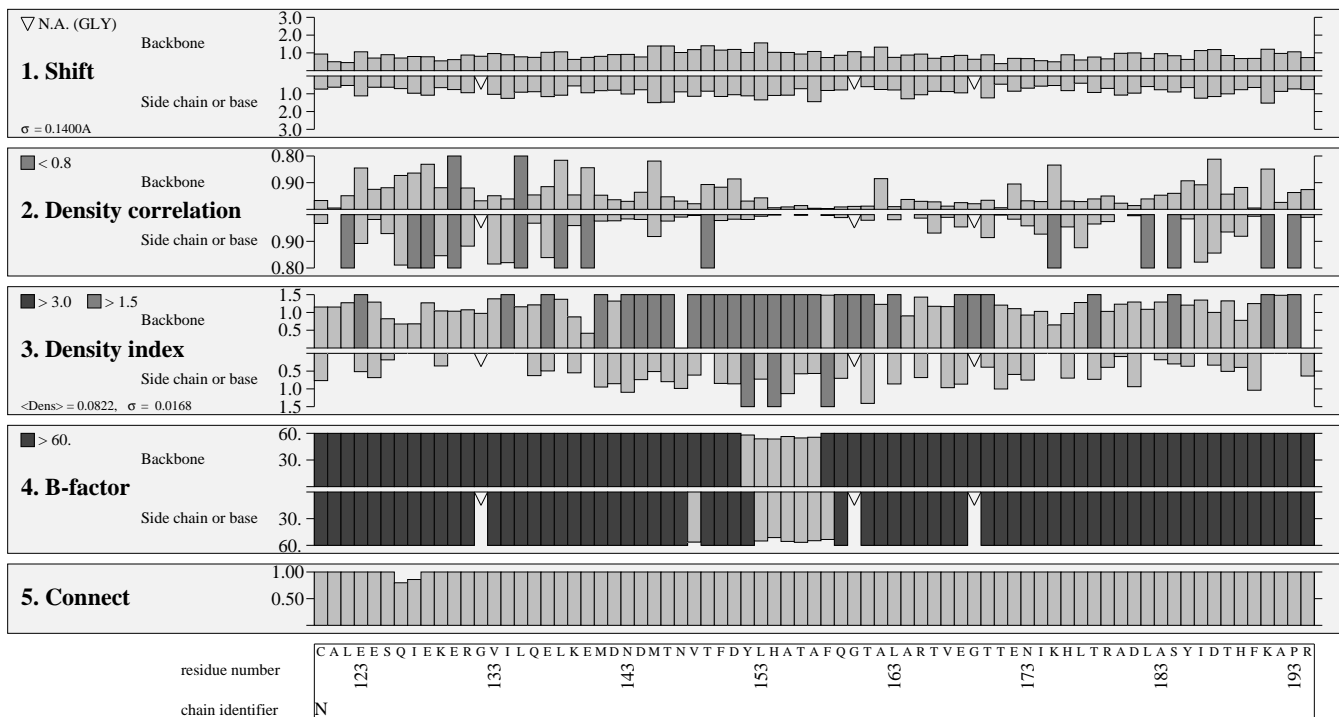
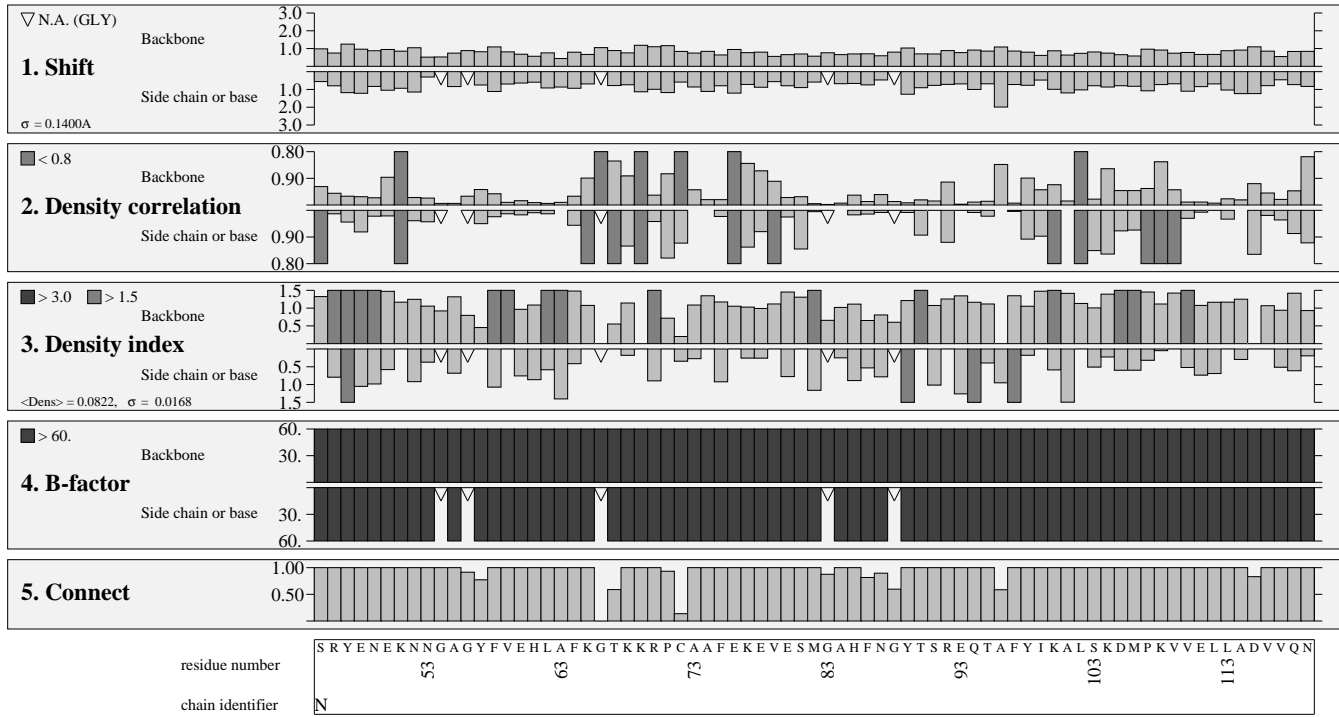
Local estimation (14)



Structure Factor Check

3H1H

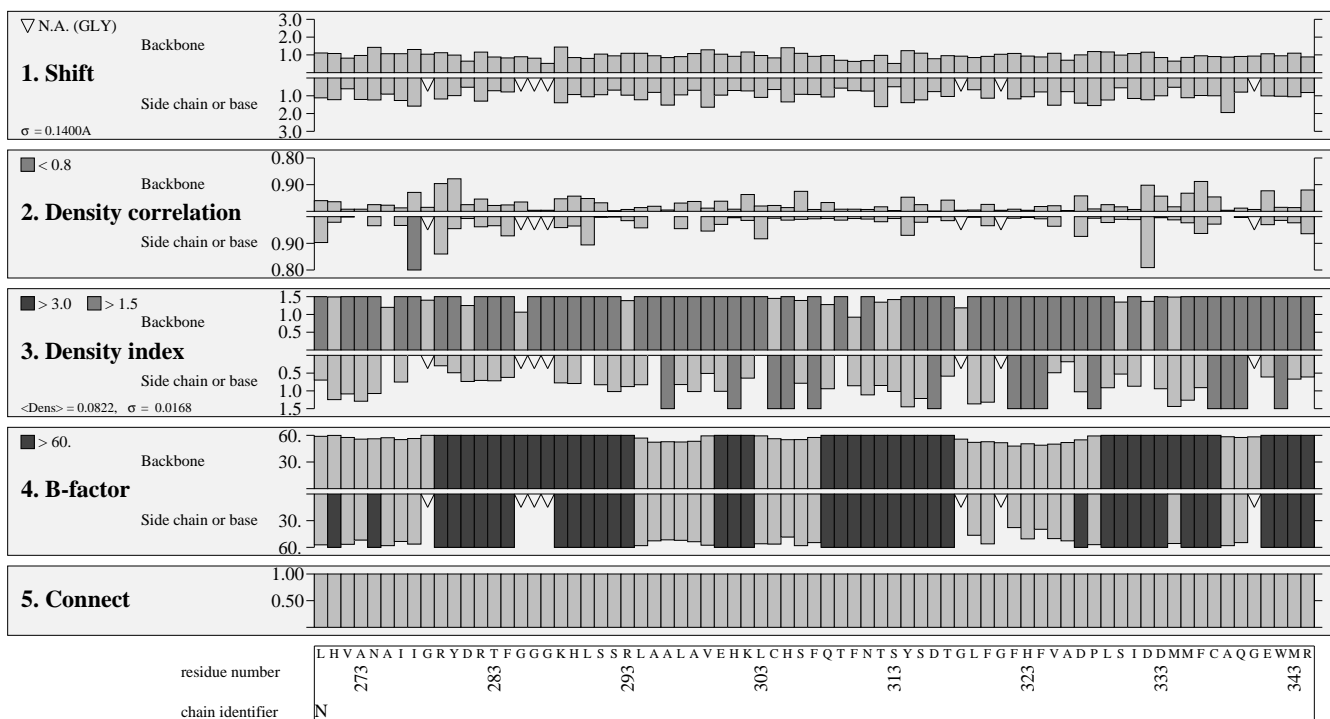
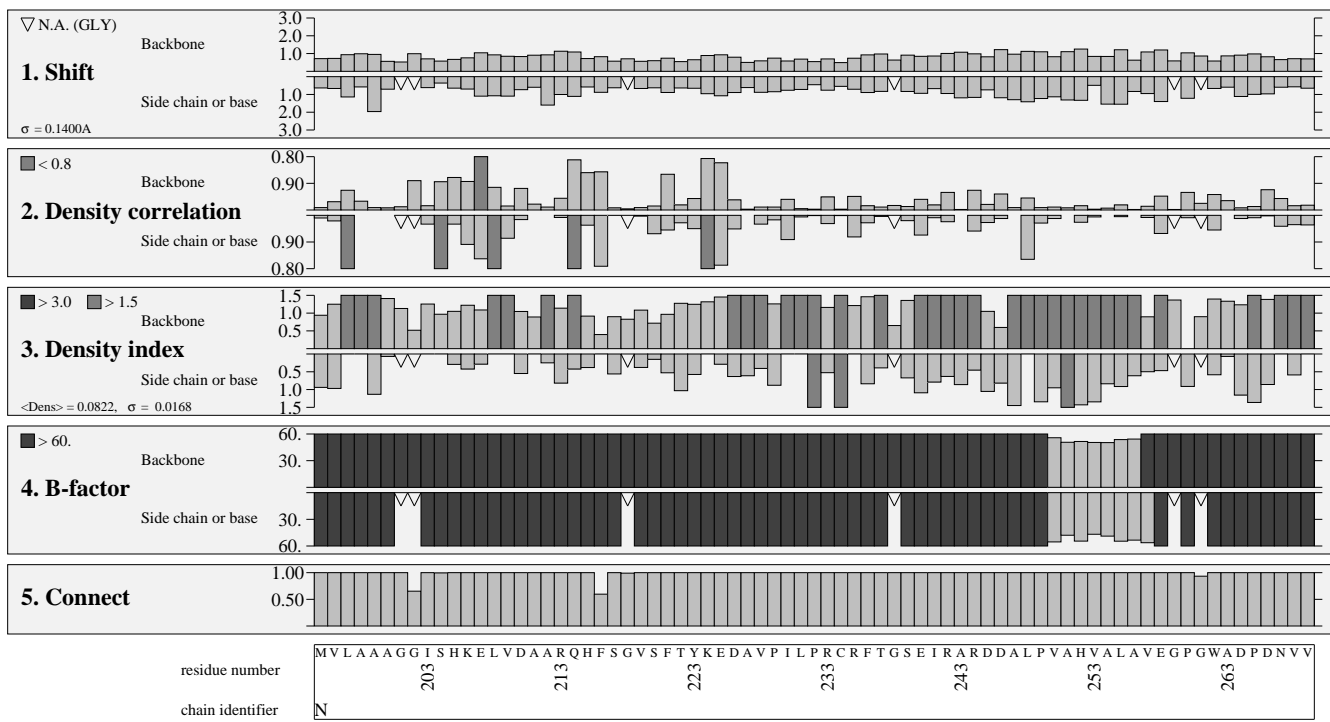
Local estimation (15)



Structure Factor Check

3H1H

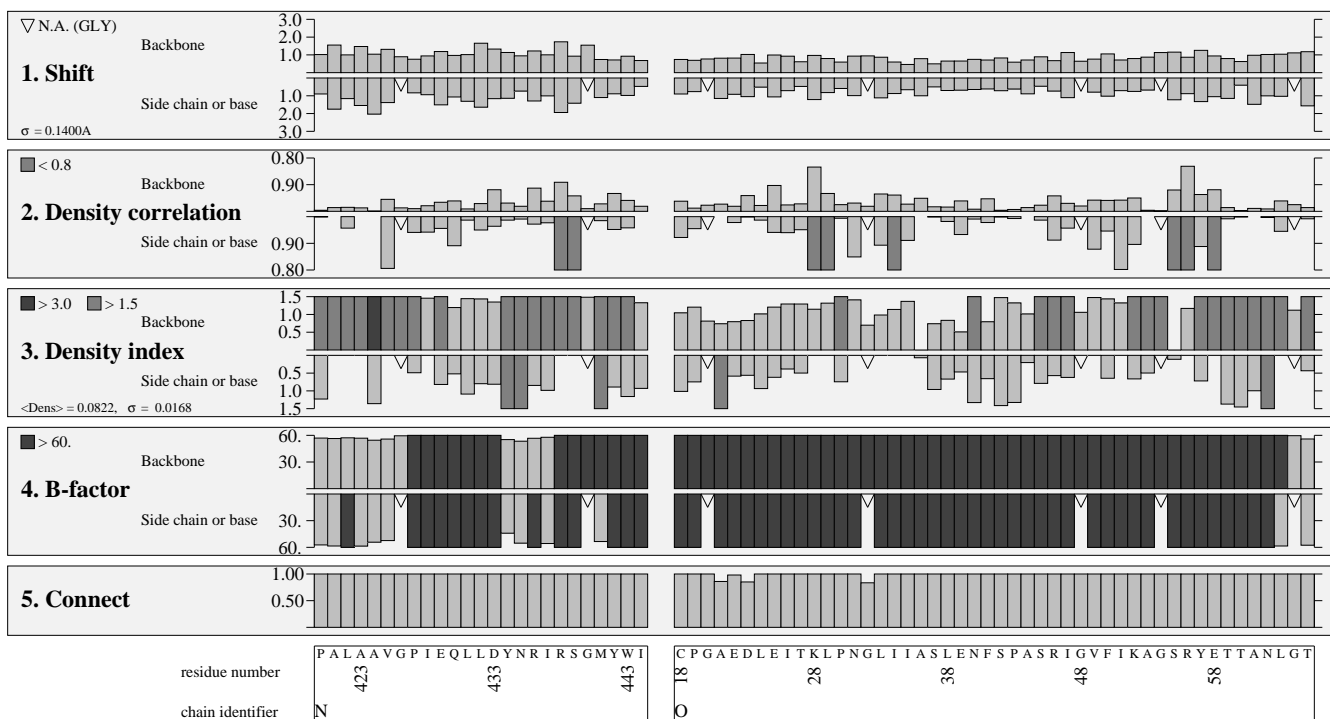
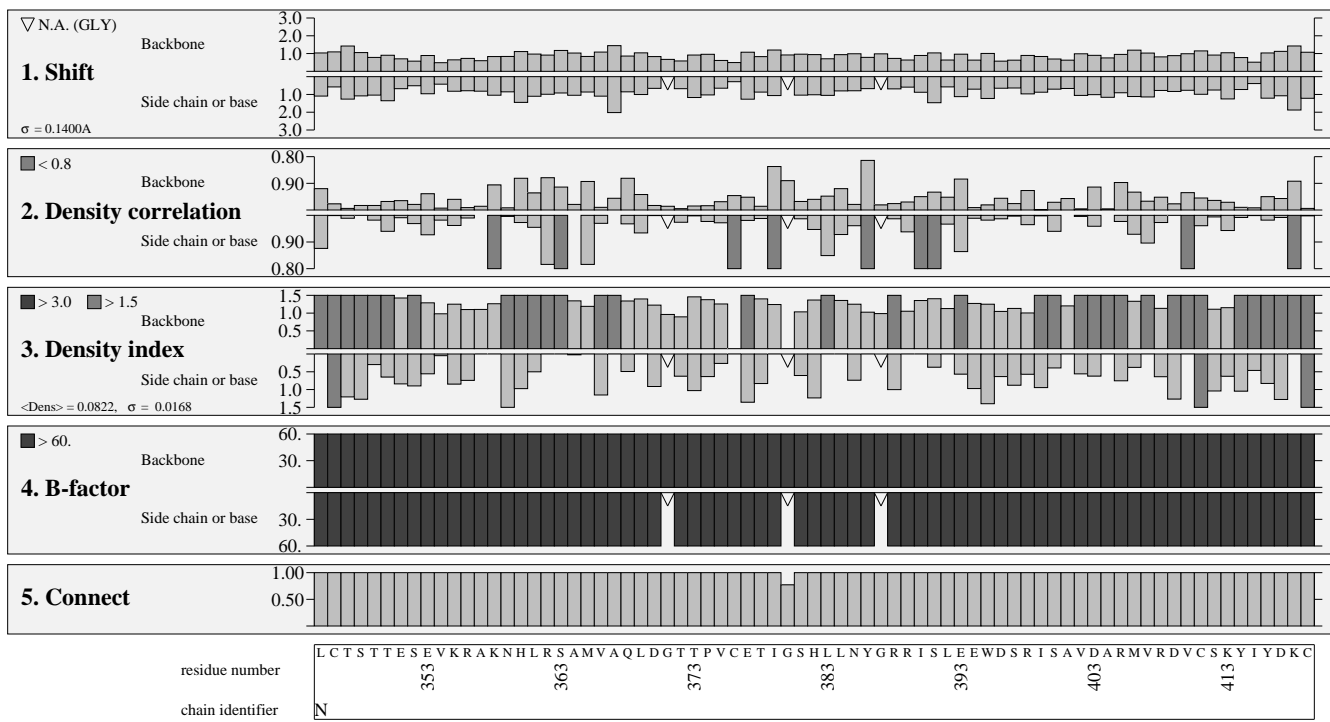
Local estimation (16)



Structure Factor Check

3H1H

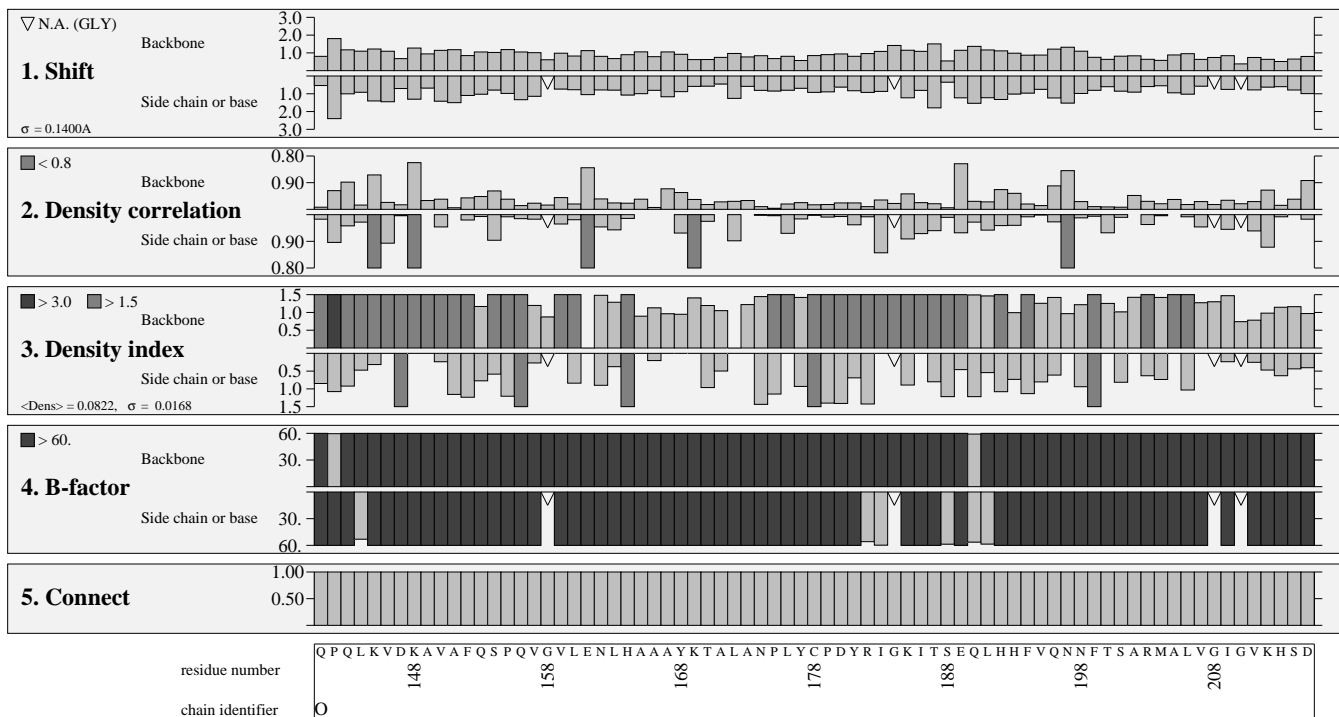
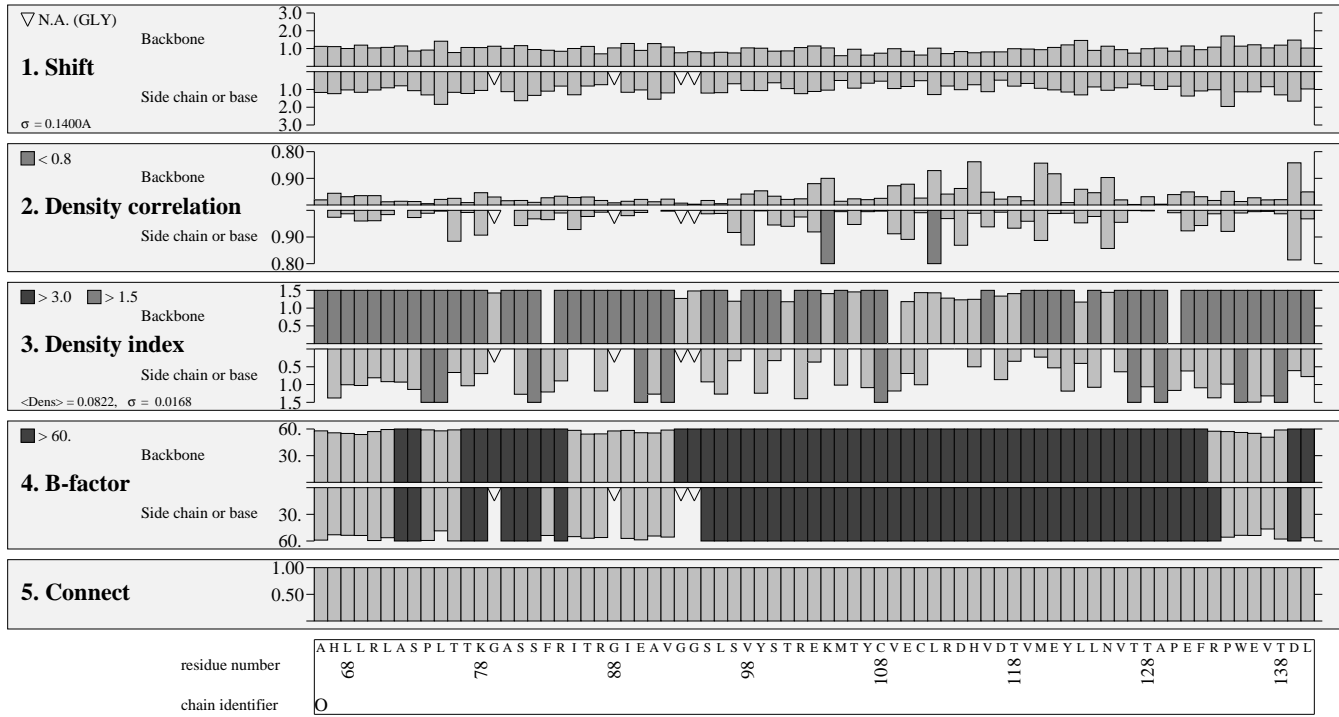
Local estimation (17)



Structure Factor Check

3H1H

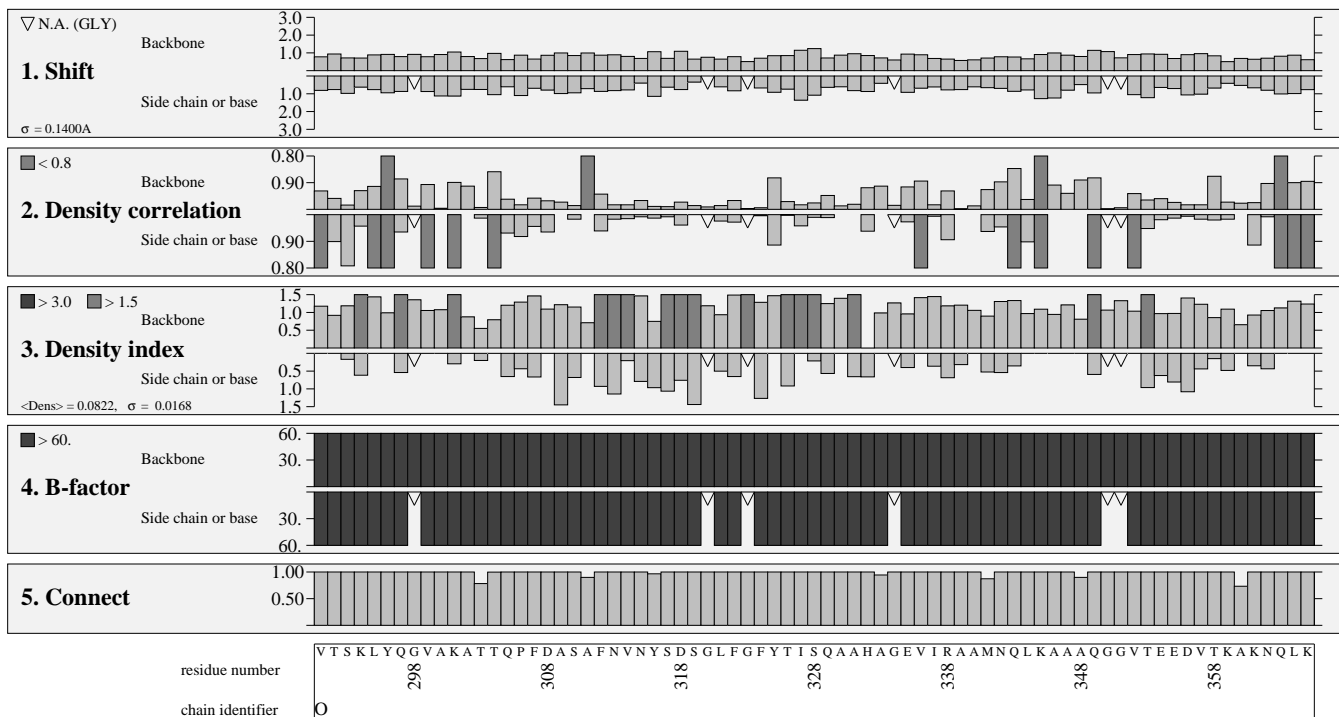
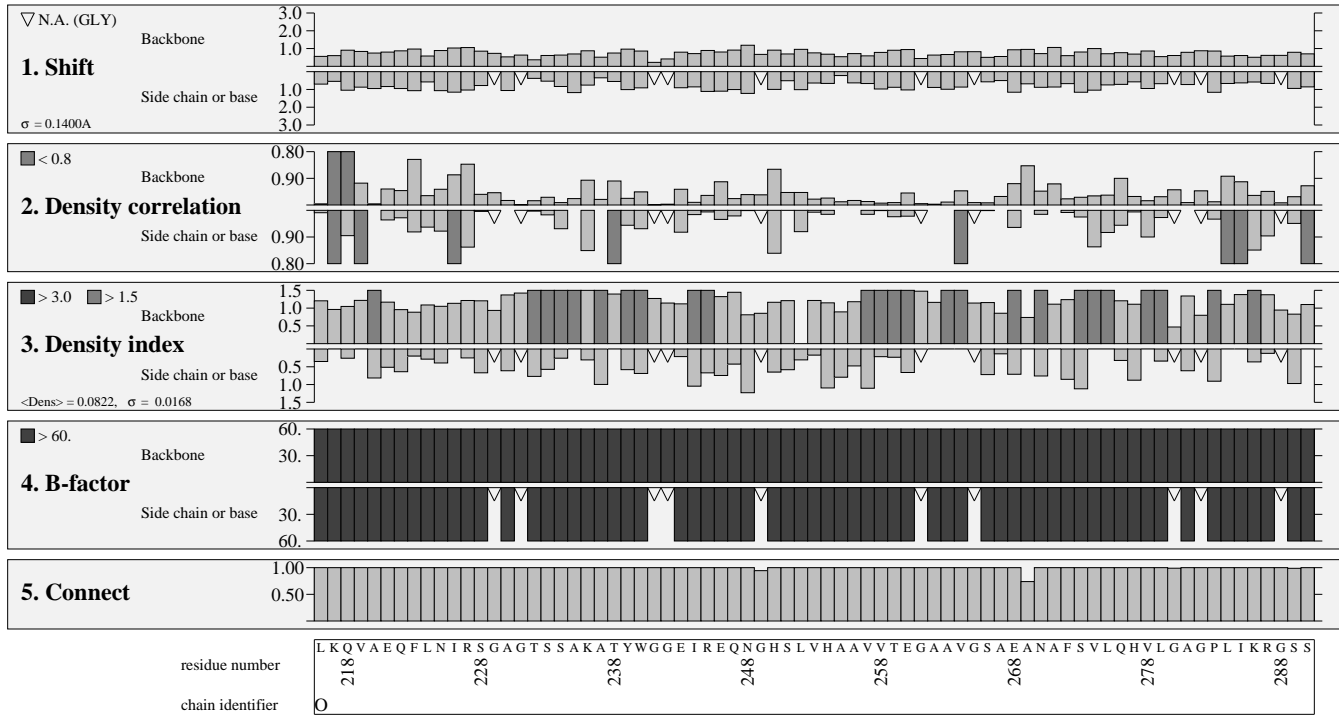
Local estimation (18)



Structure Factor Check

3H1H

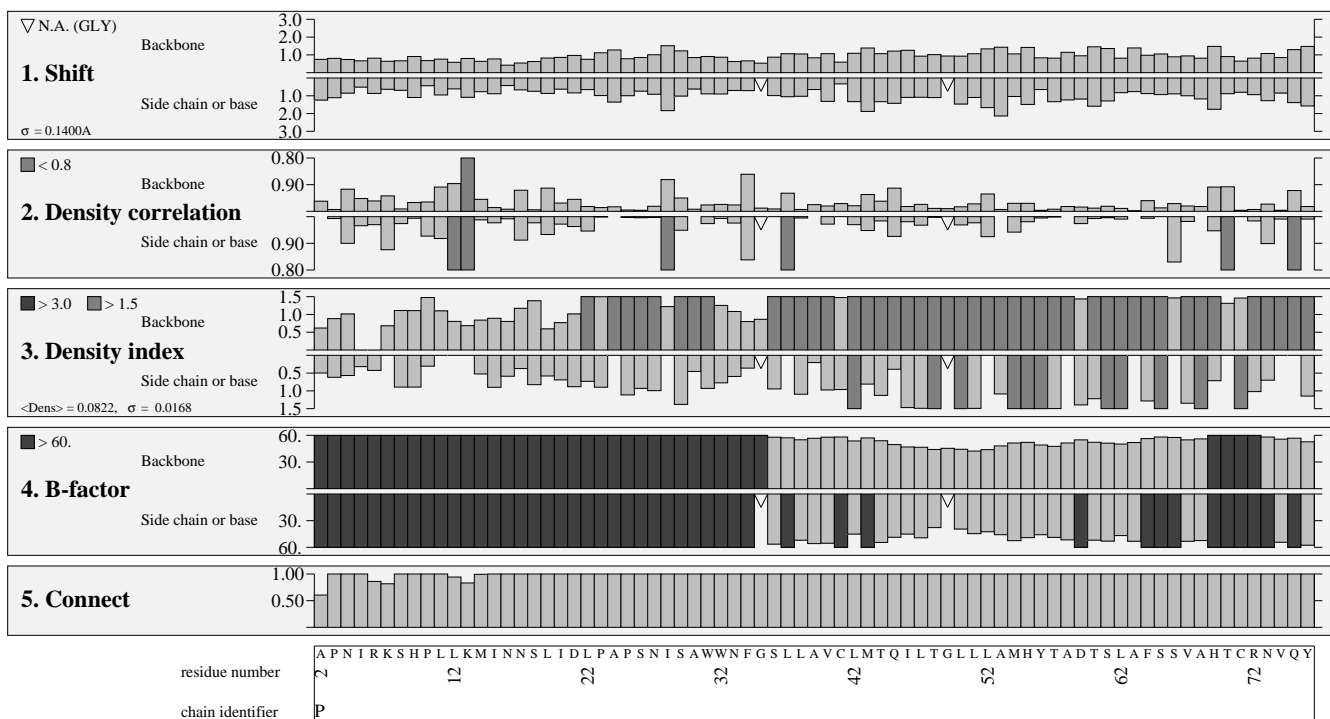
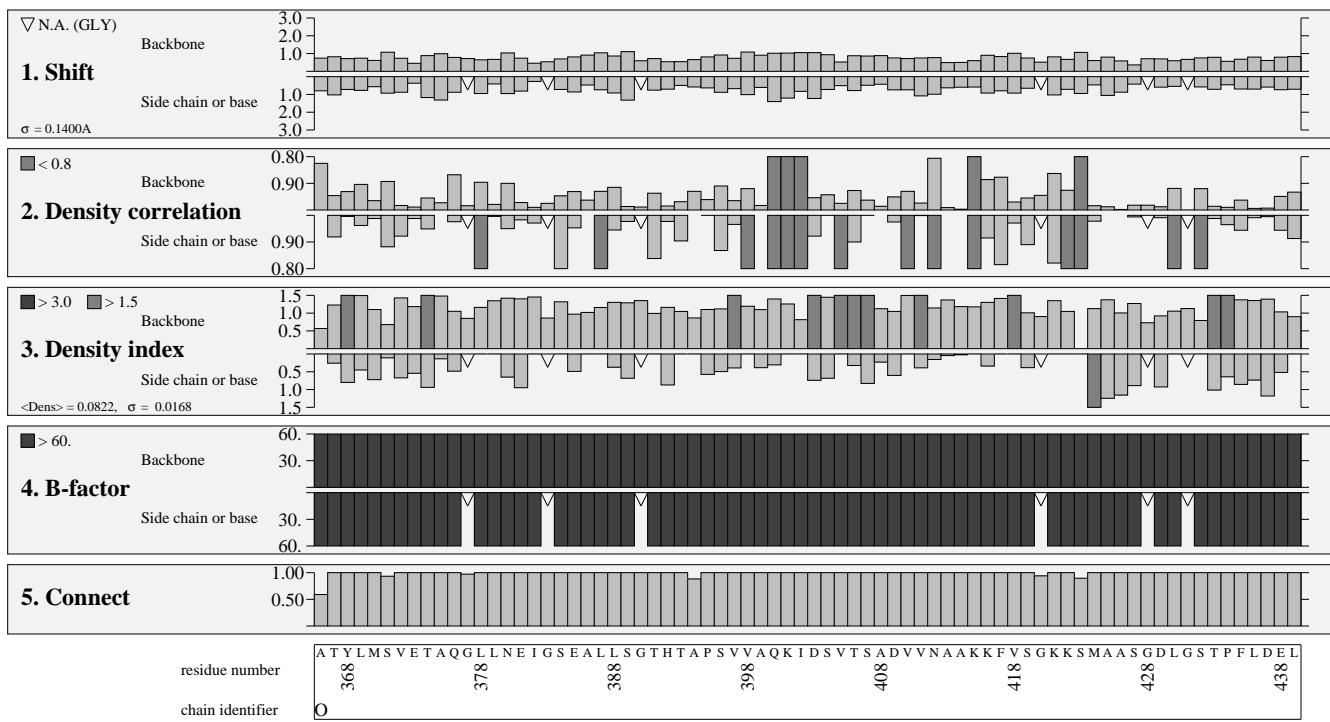
Local estimation (19)



Structure Factor Check

3H1H

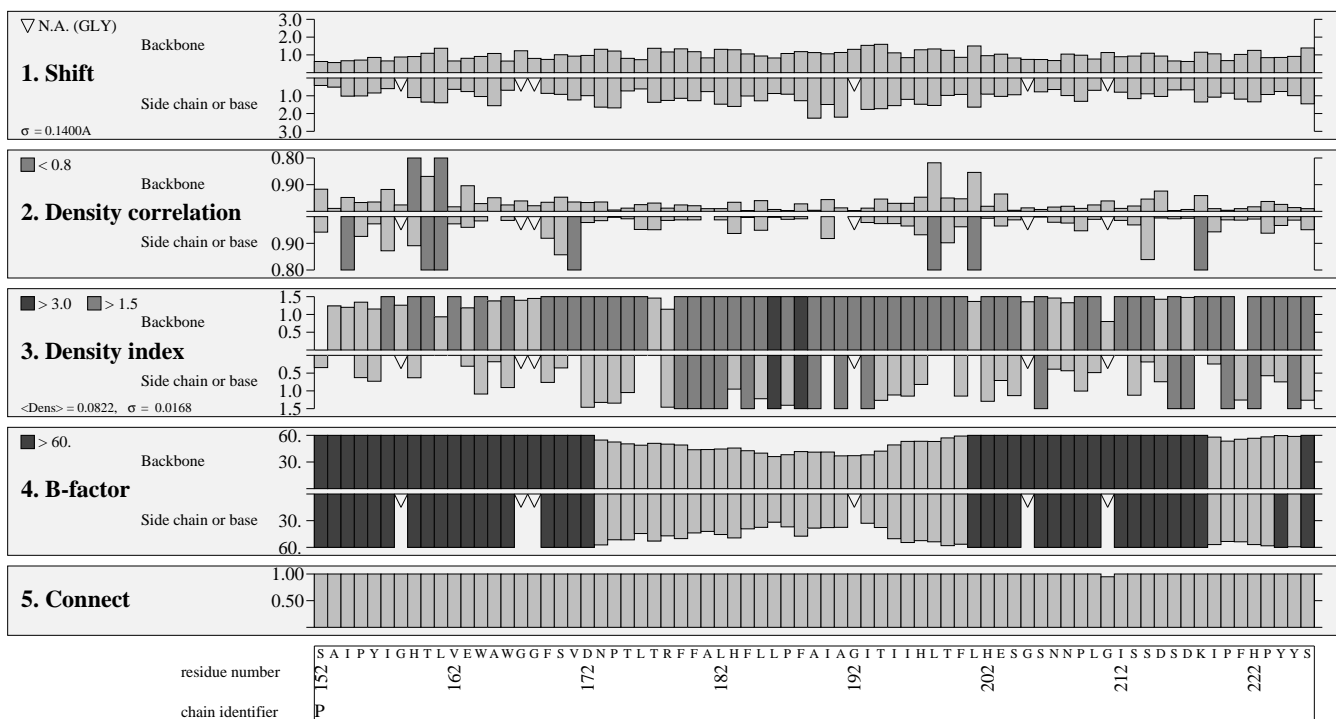
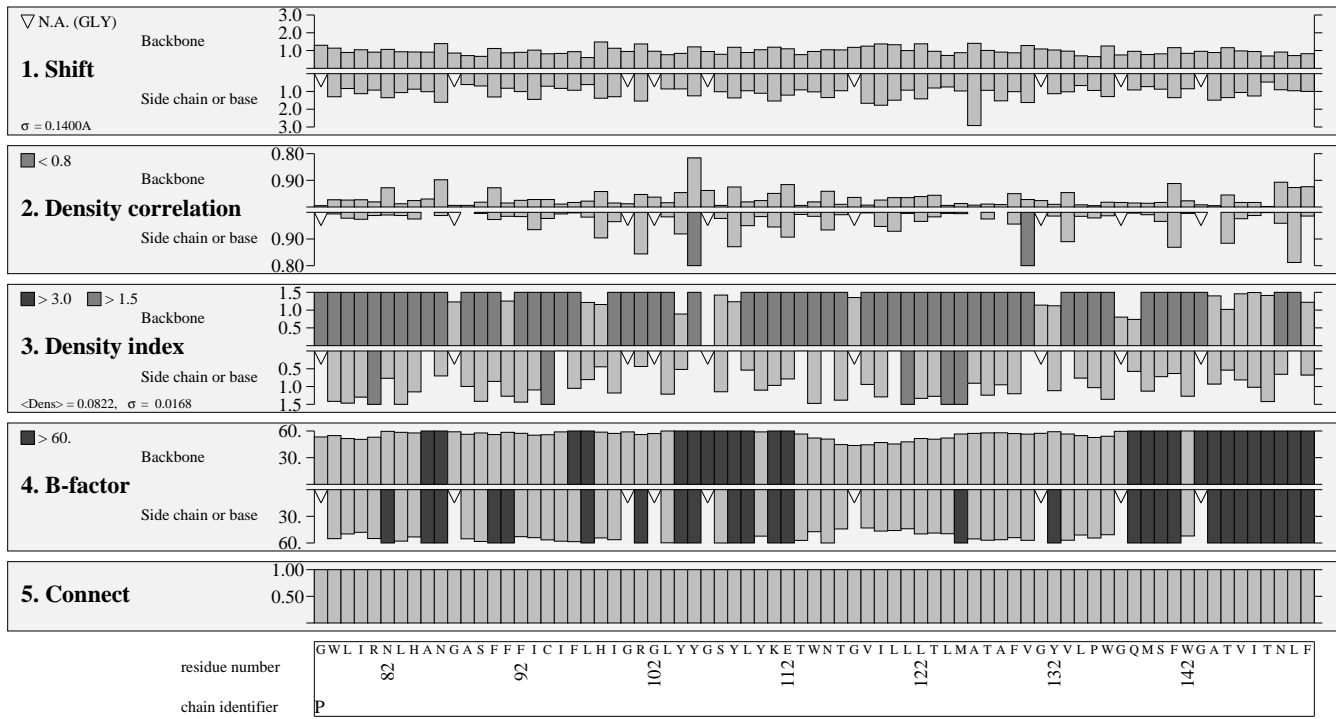
Local estimation (20)



Structure Factor Check

3H1H

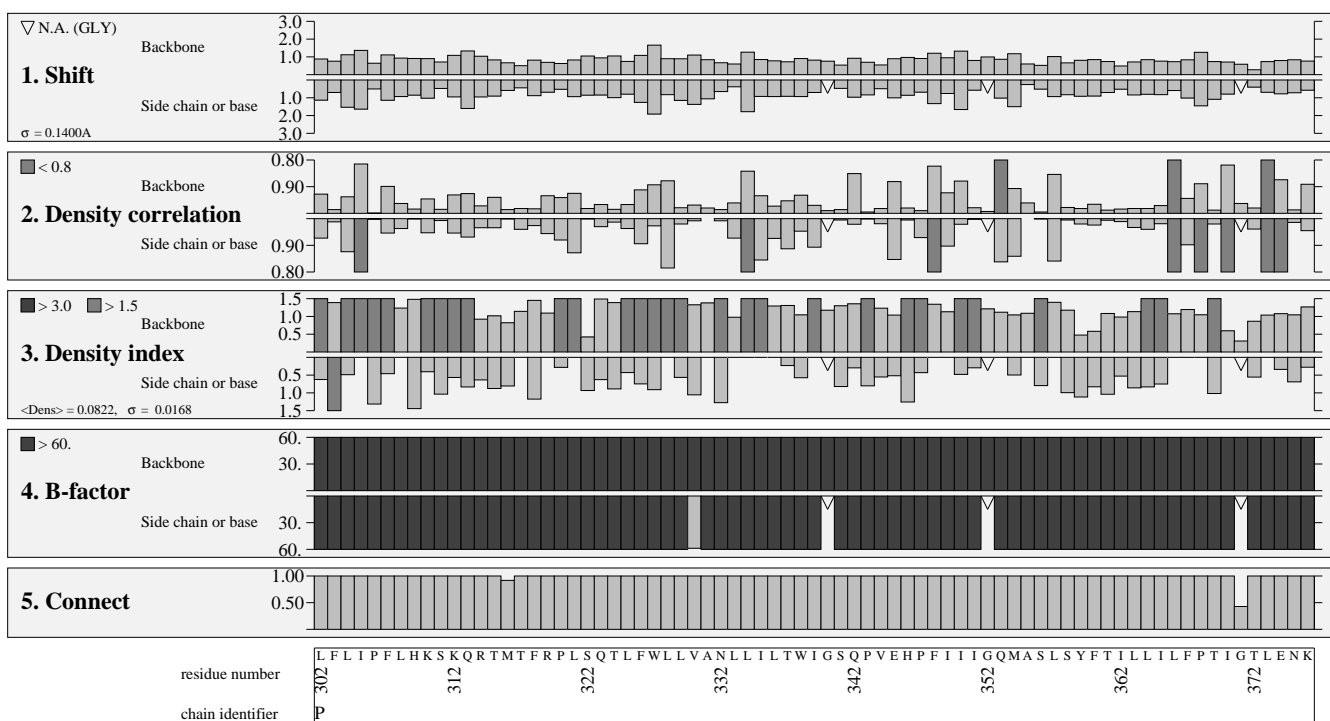
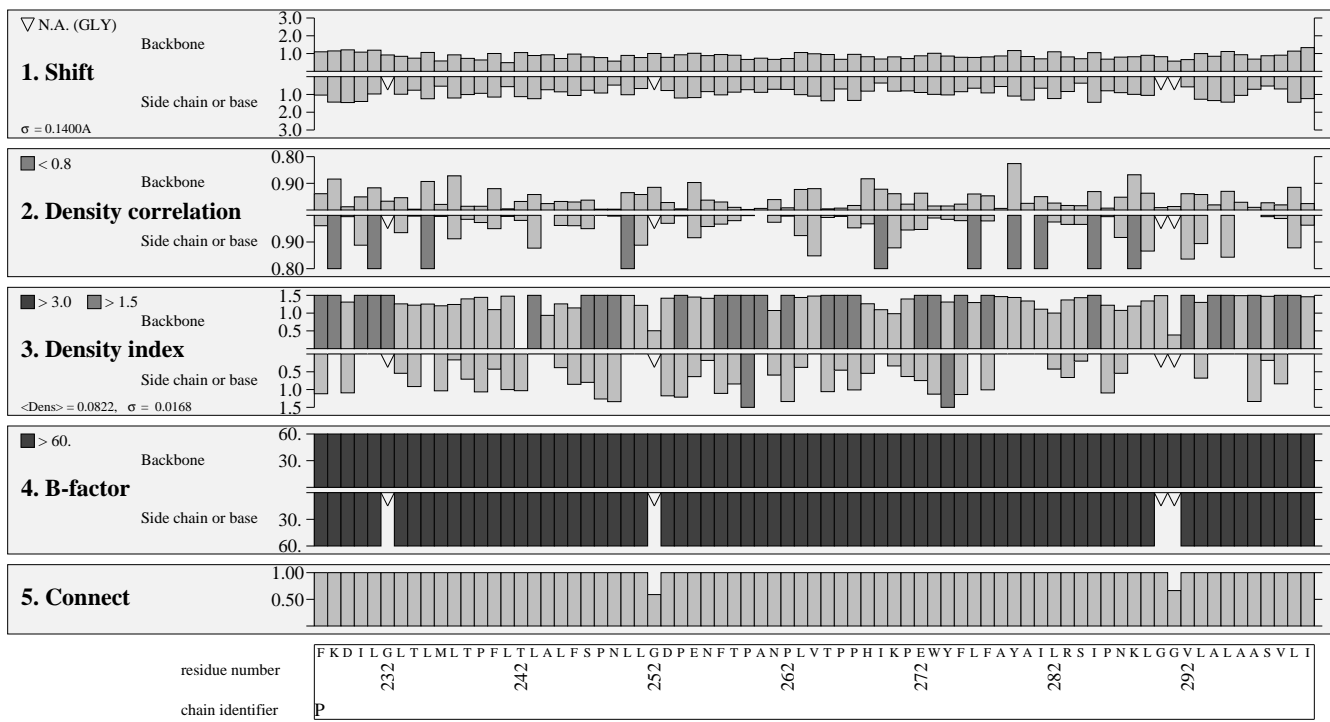
Local estimation (21)



Structure Factor Check

3H1H

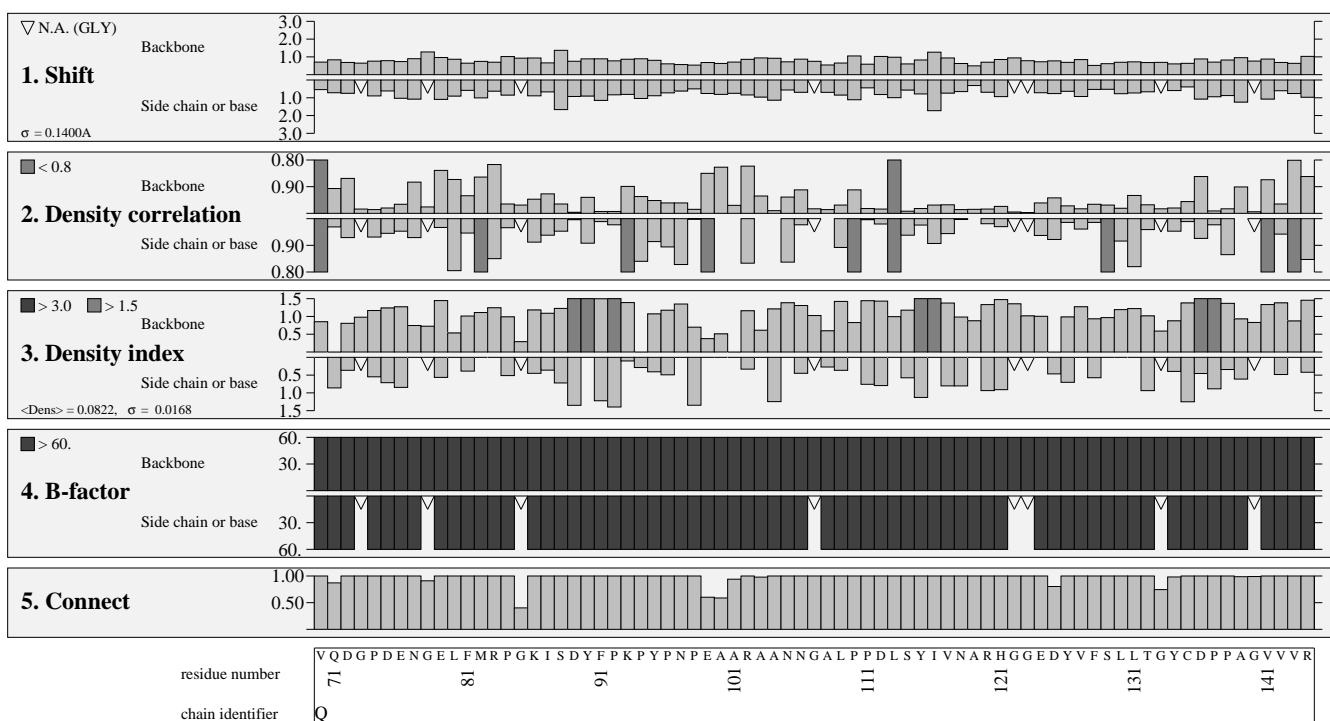
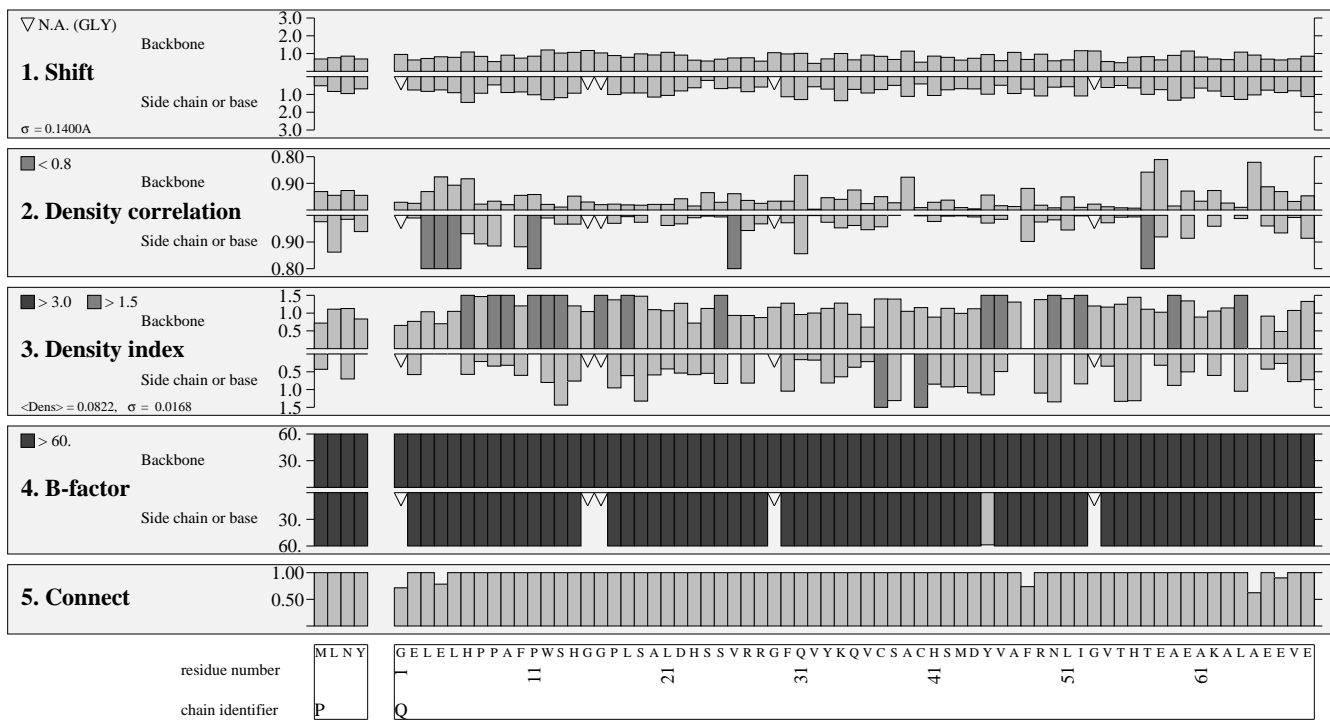
Local estimation (22)



Structure Factor Check

3H1H

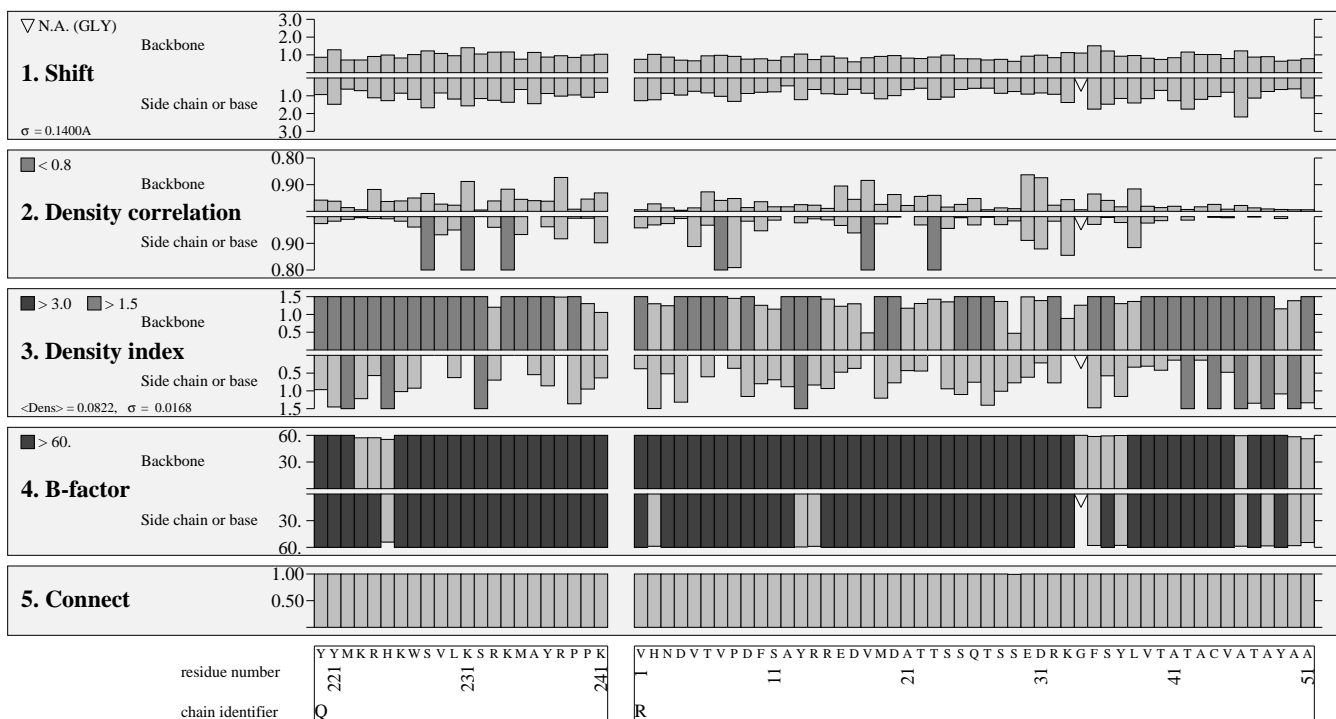
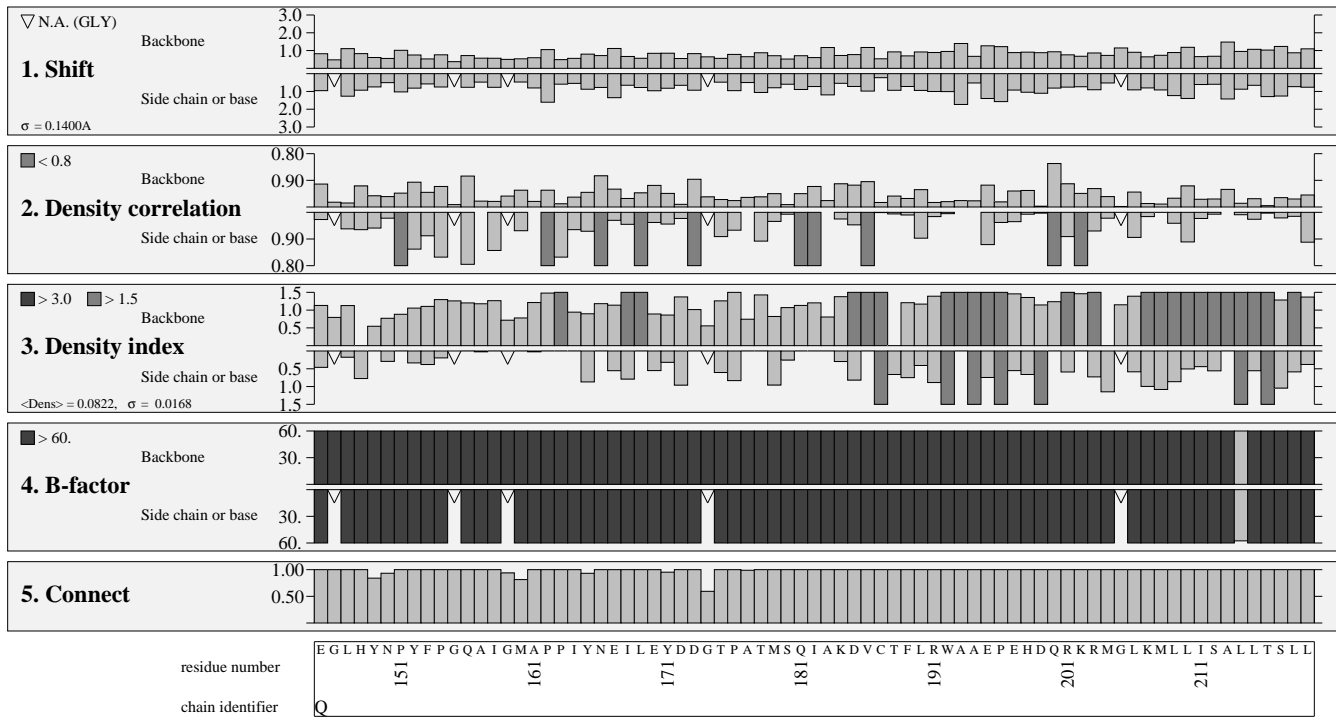
Local estimation (23)



Structure Factor Check

3H1H

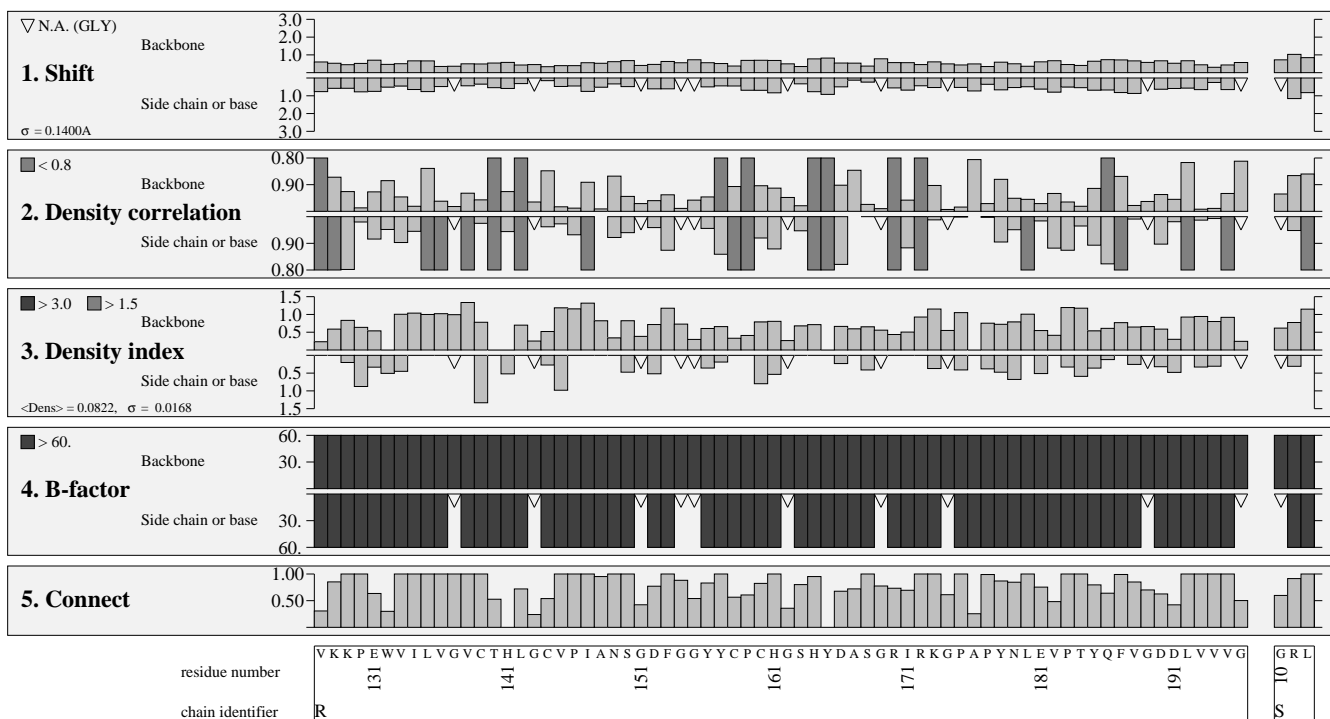
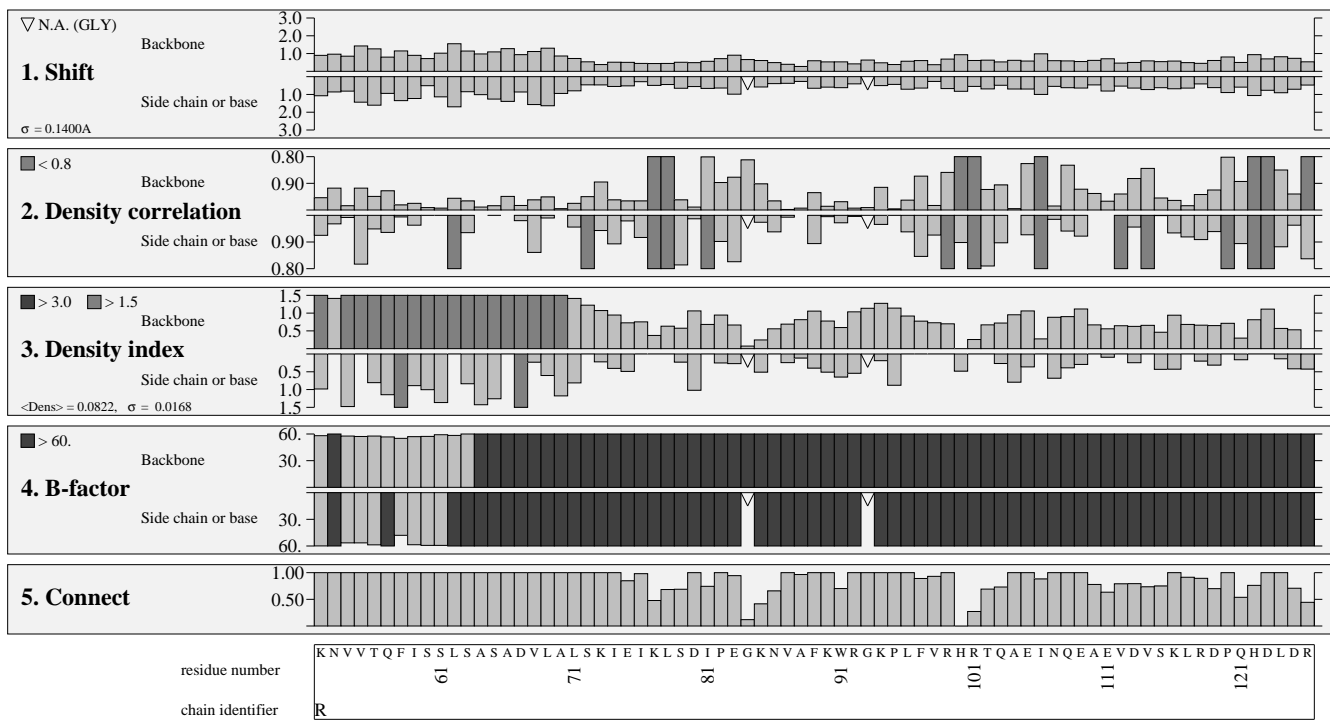
Local estimation (24)



Structure Factor Check

3H1H

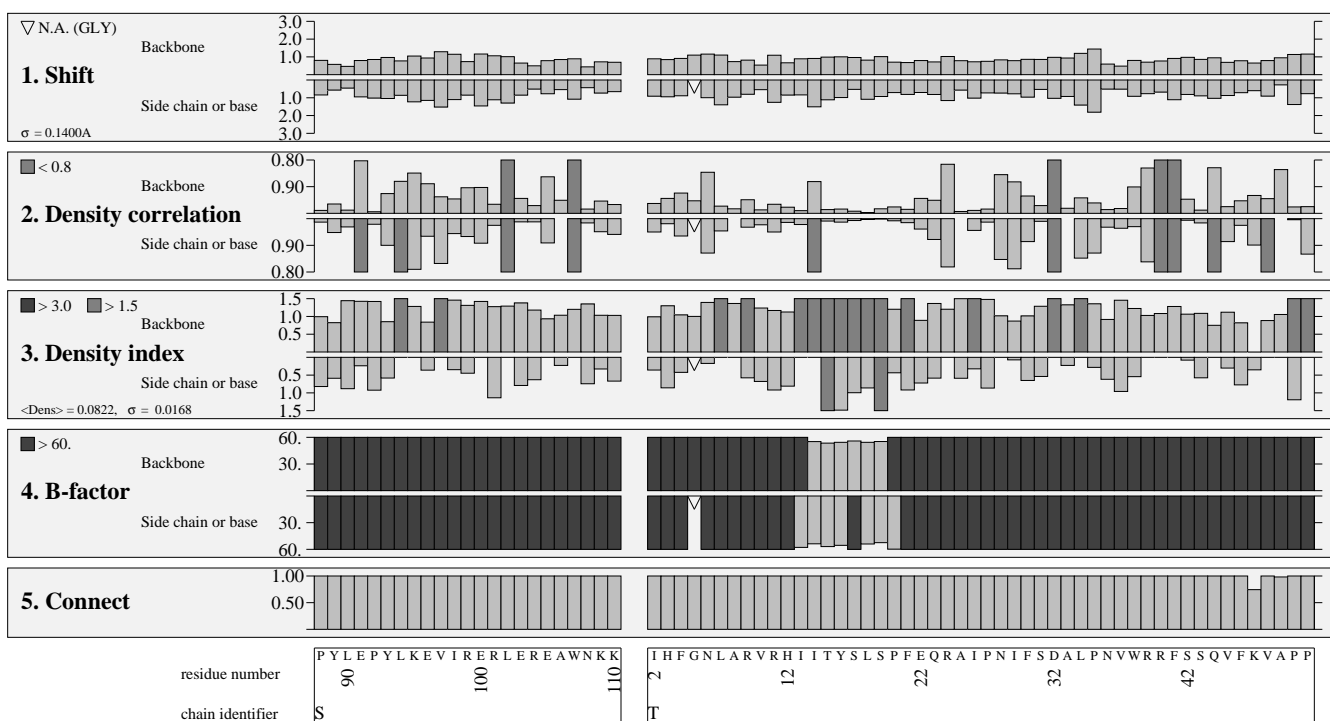
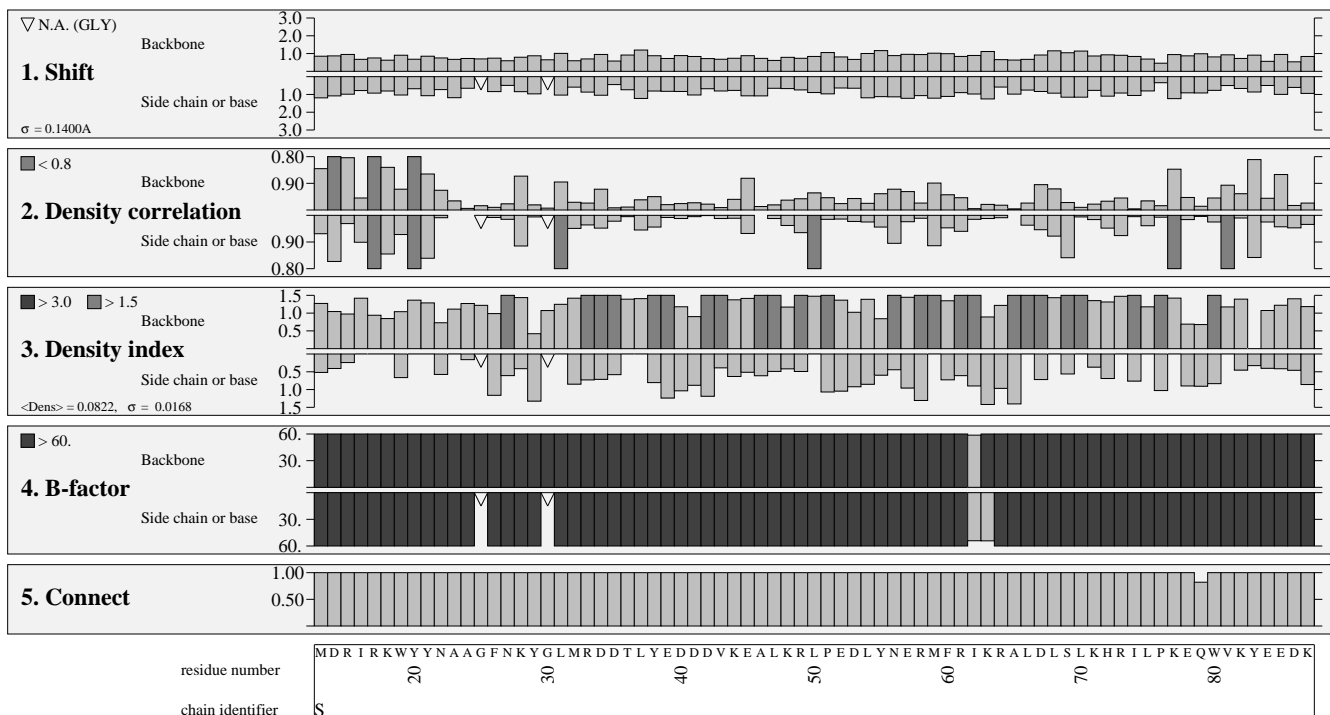
Local estimation (25)



Structure Factor Check

3H1H

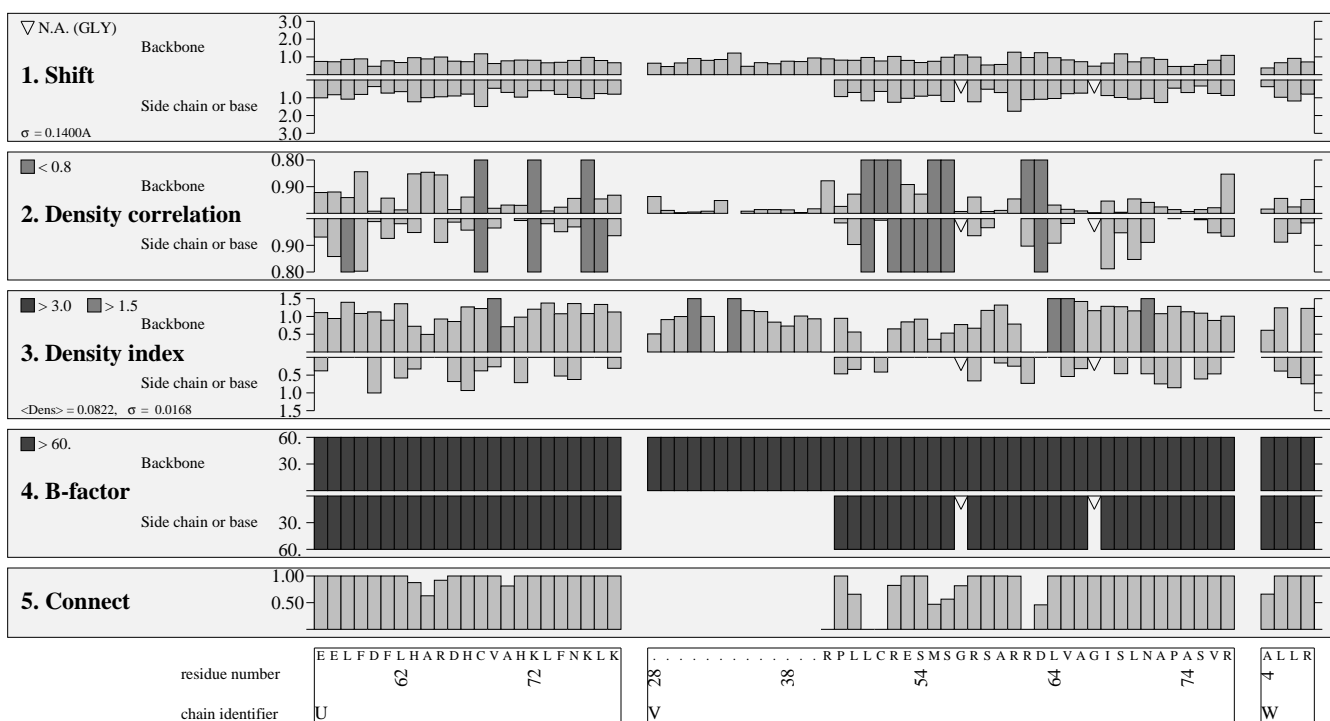
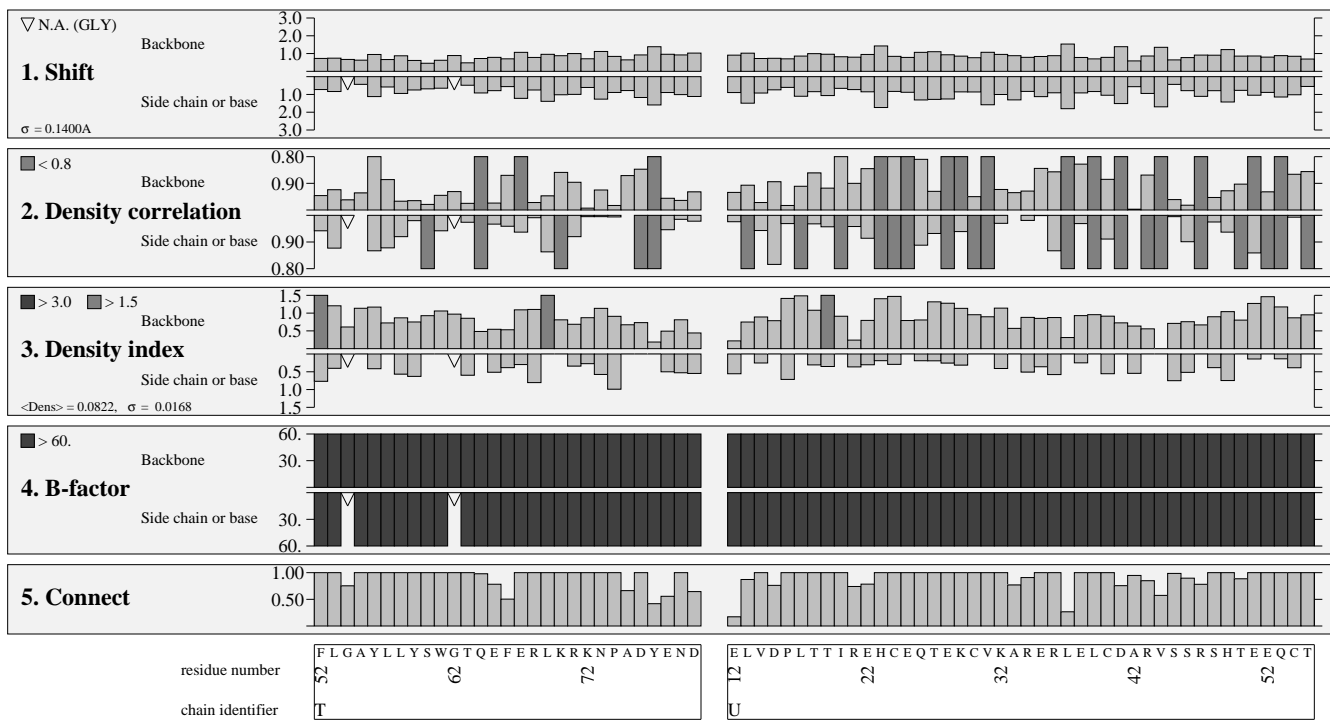
Local estimation (26)



Structure Factor Check

3H1H

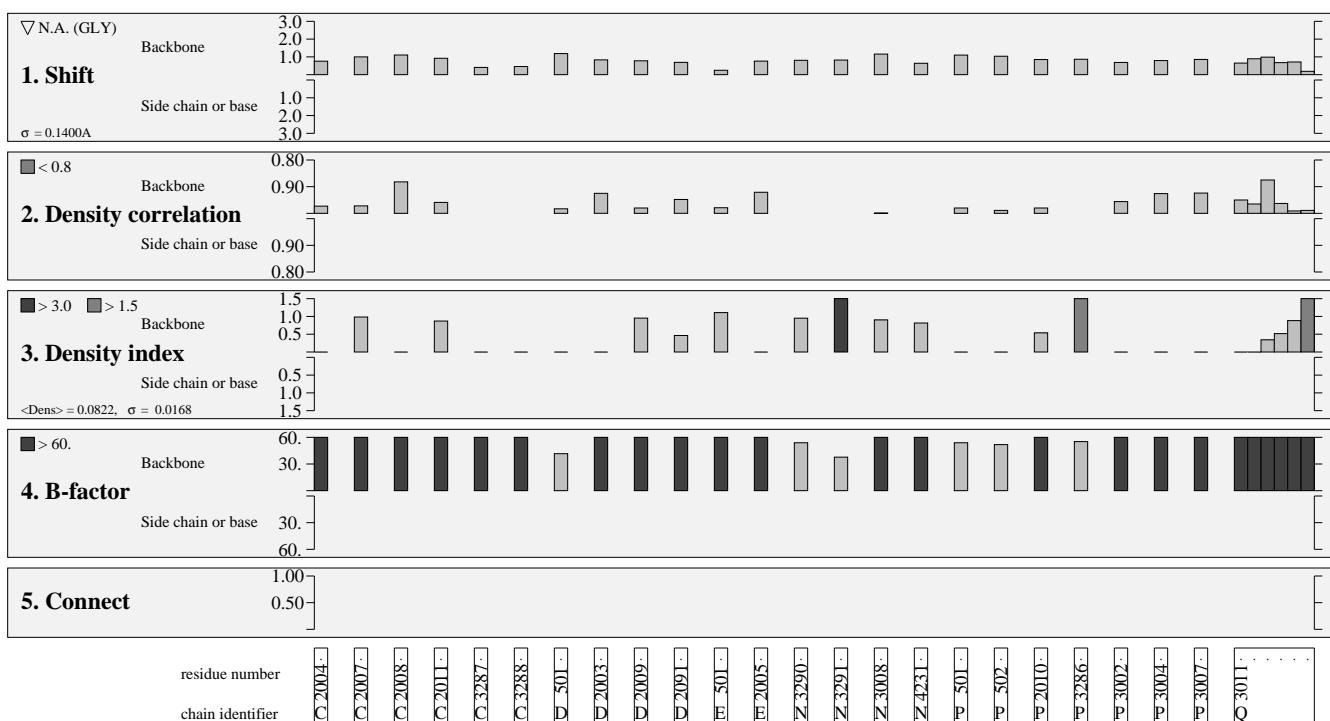
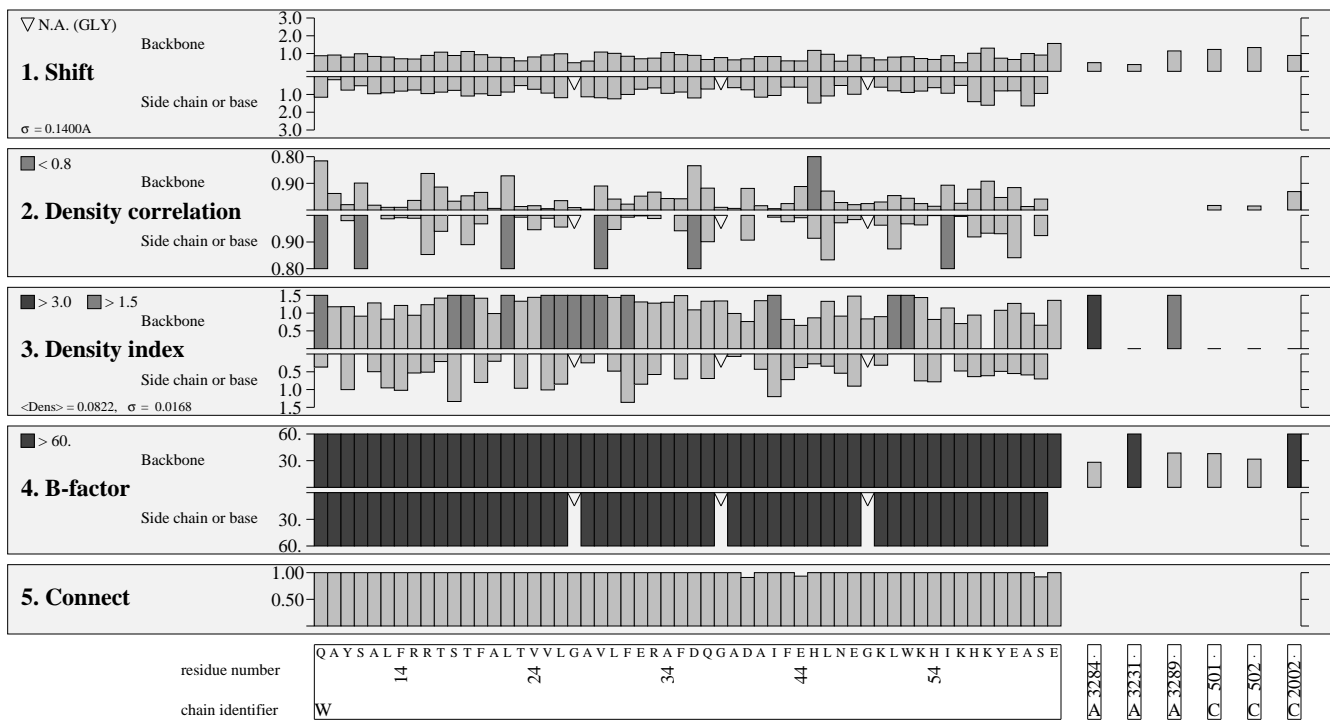
Local estimation (27)



Structure Factor Check

3H1H

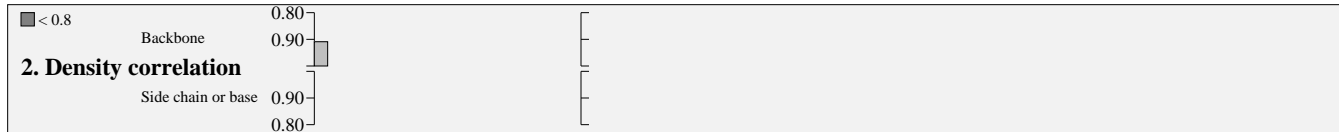
Local estimation (28)



Structure Factor Check

3H1H

Local estimation (29)



residue number	Backbone	Side chain or base
384	0.75	0.75
385	0.75	0.75

chain identifier Q