

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 A b: 182.45 A c: 241.33 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 42.7 – 3.00 A
 Reflections in file: 141717
 Unique reflections above 0: 141717
 above 1 σ : 138899
 above 3 σ : 81483

SFCHECK

Nominal resolution range: 42.7 – 3.00 A
\05max. from input data, min. from author\05
 Used reflections: 141716
 Reflections out of resolution: 1
 Completeness: 92.6 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.106
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.5954 0.6935
 B_{overall} (by Patterson): 53. A²
 Optical resolution: 2.23 A
 Expected opt. resol. for complete data set: 2.23 A
 Estimated minimal error: 0.106 A

Model

32679 atoms (14 water molecules)

Number of chains: 51
 Volume not occupied by model: 63.4 %
 $\langle B \rangle$ (for atomic model): 77.3 A²
 $\sigma(B)$: 17.81 A²
 Matthews coefficient: 4.17
 Corresponding solvent % : 70.30

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 – 3.00A
 reflections used: 138910
 Rfree: 0.321
 Nfree: 2736
 R-factor without free-refl.: 0.295
 Non free-reflections: 136174
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.476 A
 Estimated maximal error: 0.290 A
 DPI: 0.409 A

Scaling

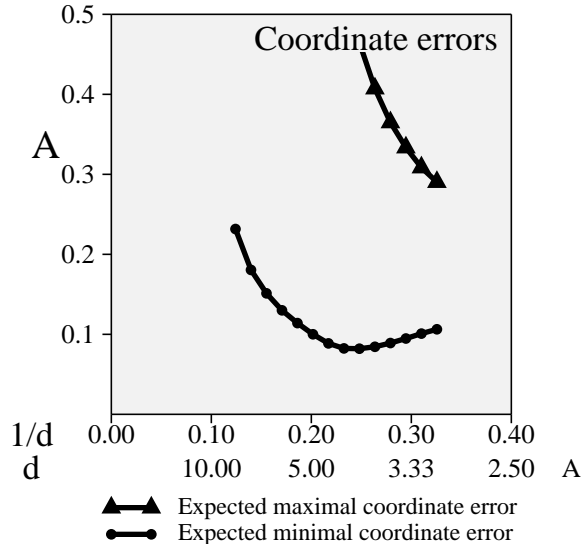
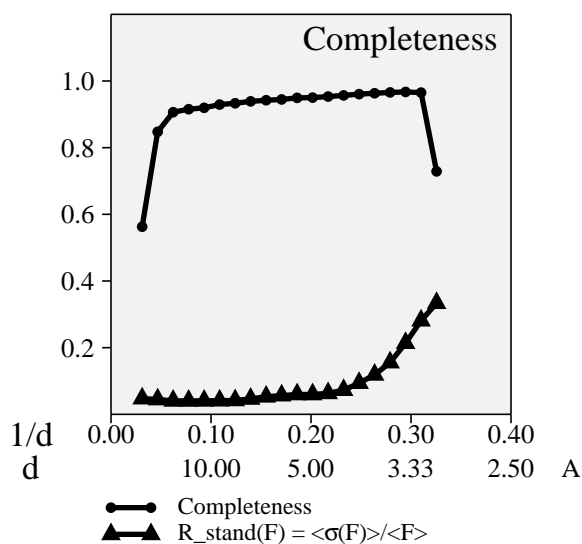
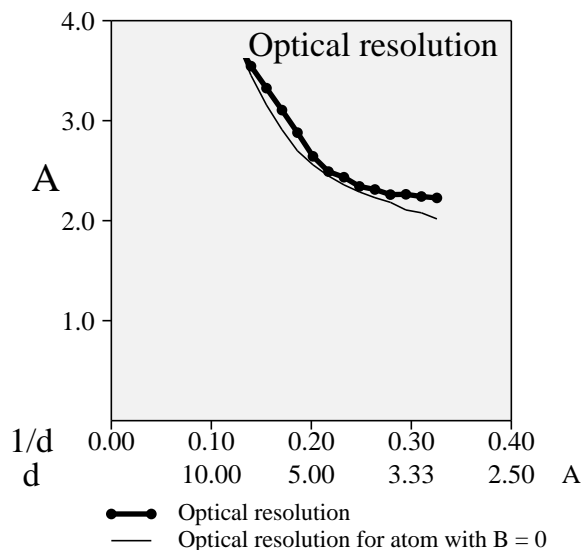
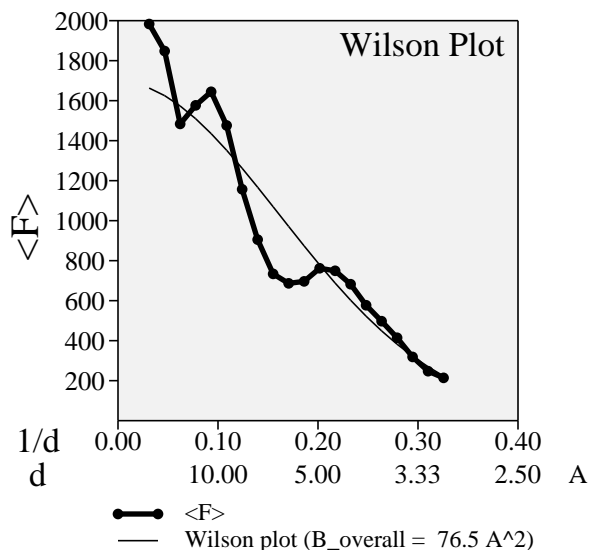
Scale: 0.602
 Bdiff: -9.31
 Anisothermal Scaling (Beta):
 7.7362 -2.3363 1.2298 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.642 250.136

Refinement

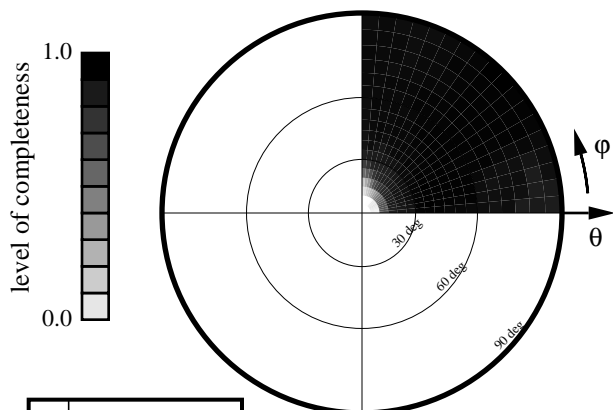
Program: CNS 1.1
 Nominal resolution range: 42.7 – 3.00 A
 Reported R-factor: 0.243
 Number of reflections used: 141718
 Reported Rfree: 0.28
 Sigma cut-off: N.A.

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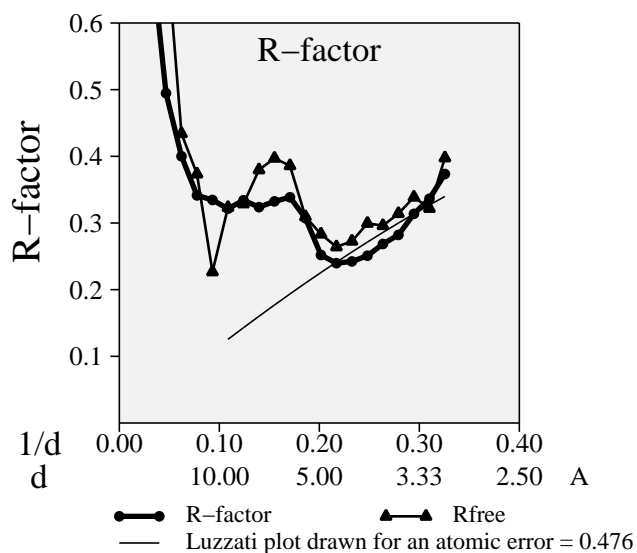


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

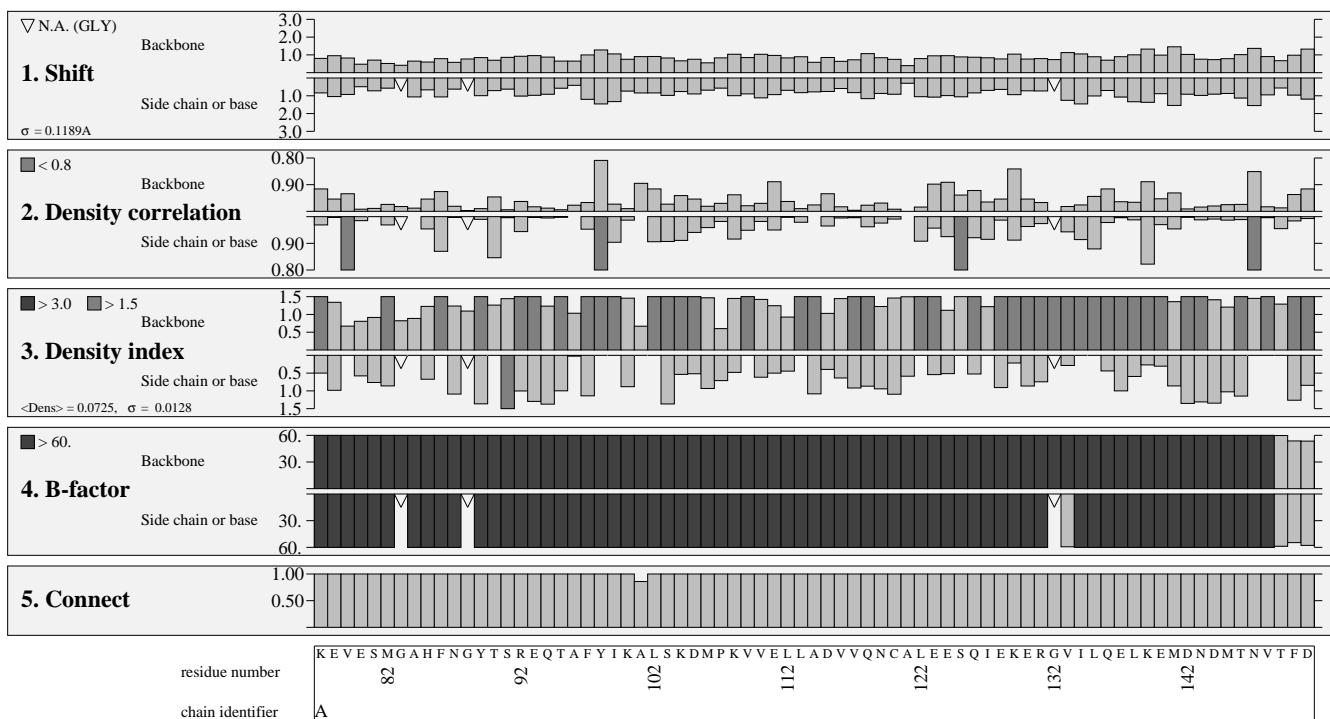
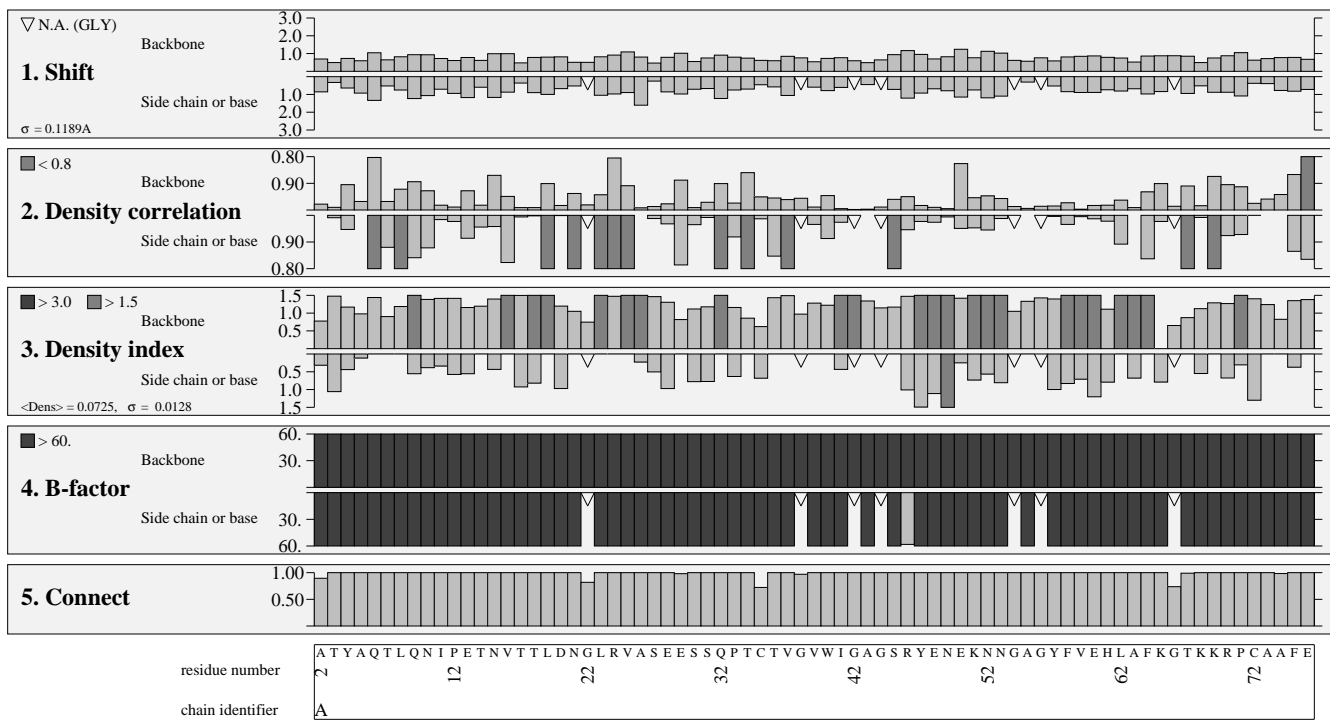
polar coordinates of the crystallographical axes



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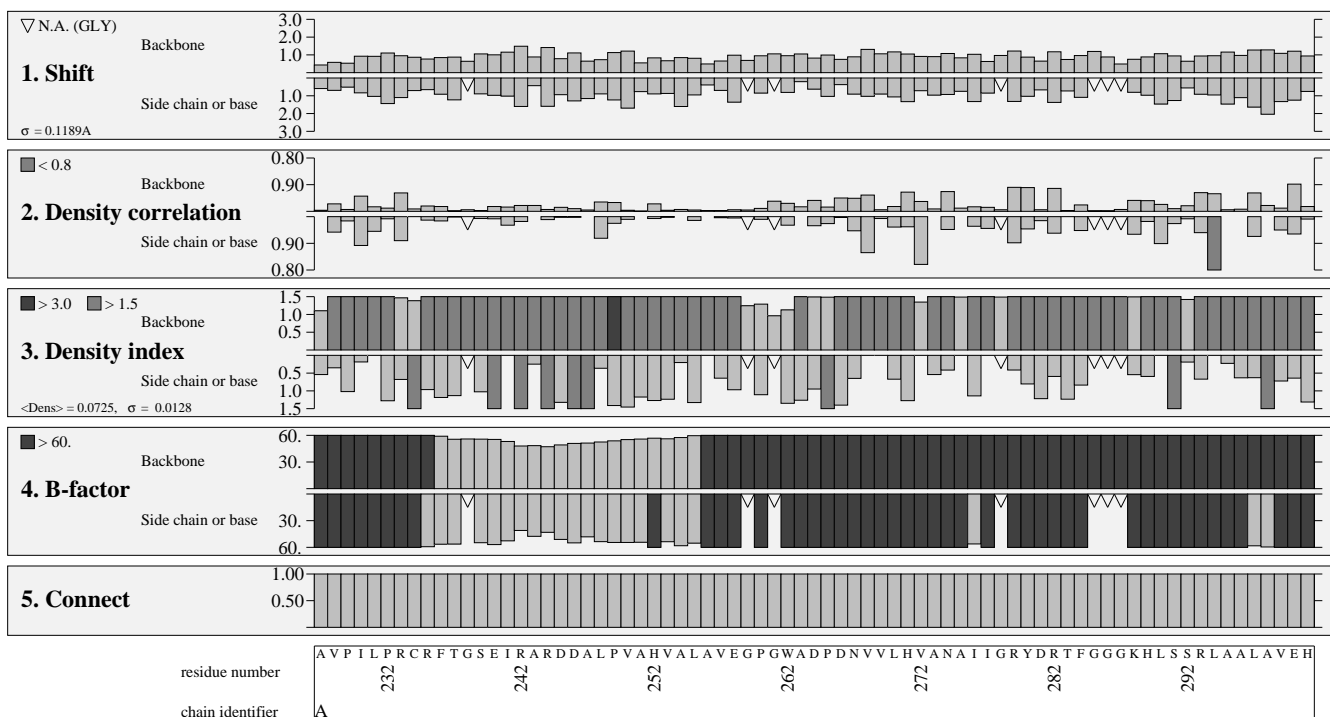
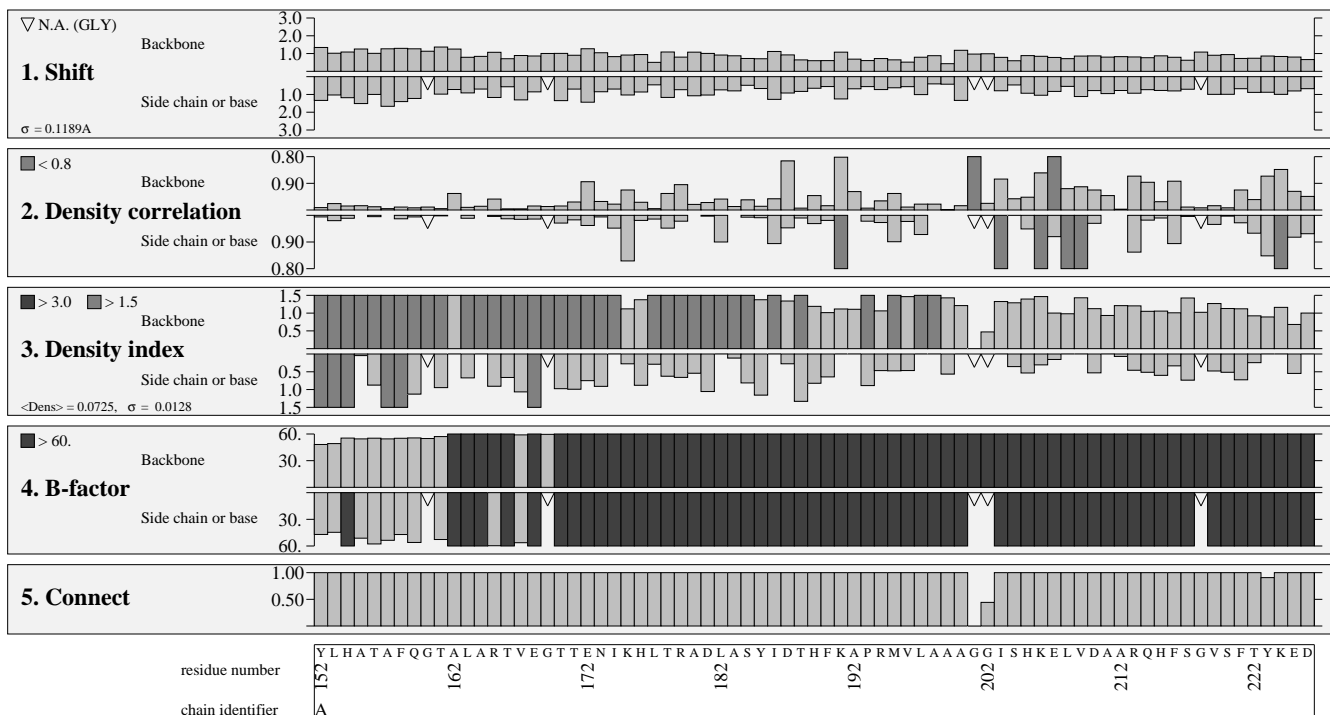
Local estimation



Structure Factor Check

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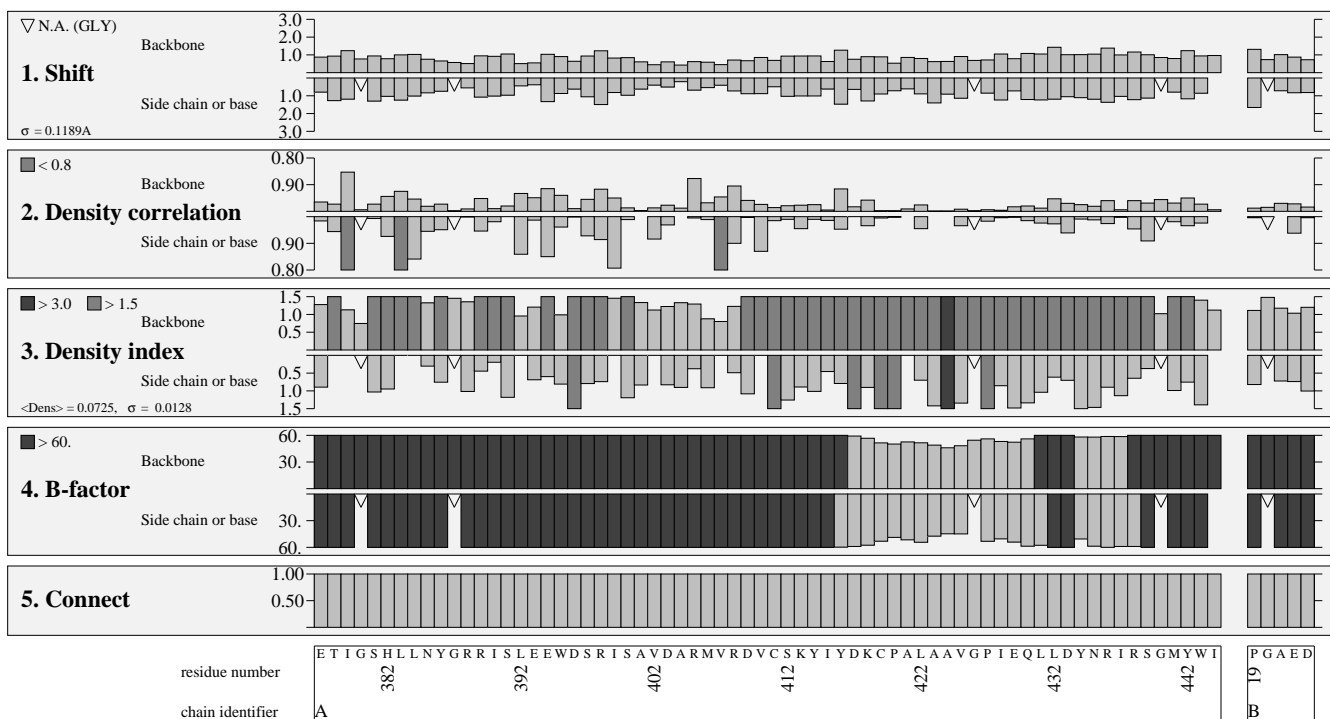
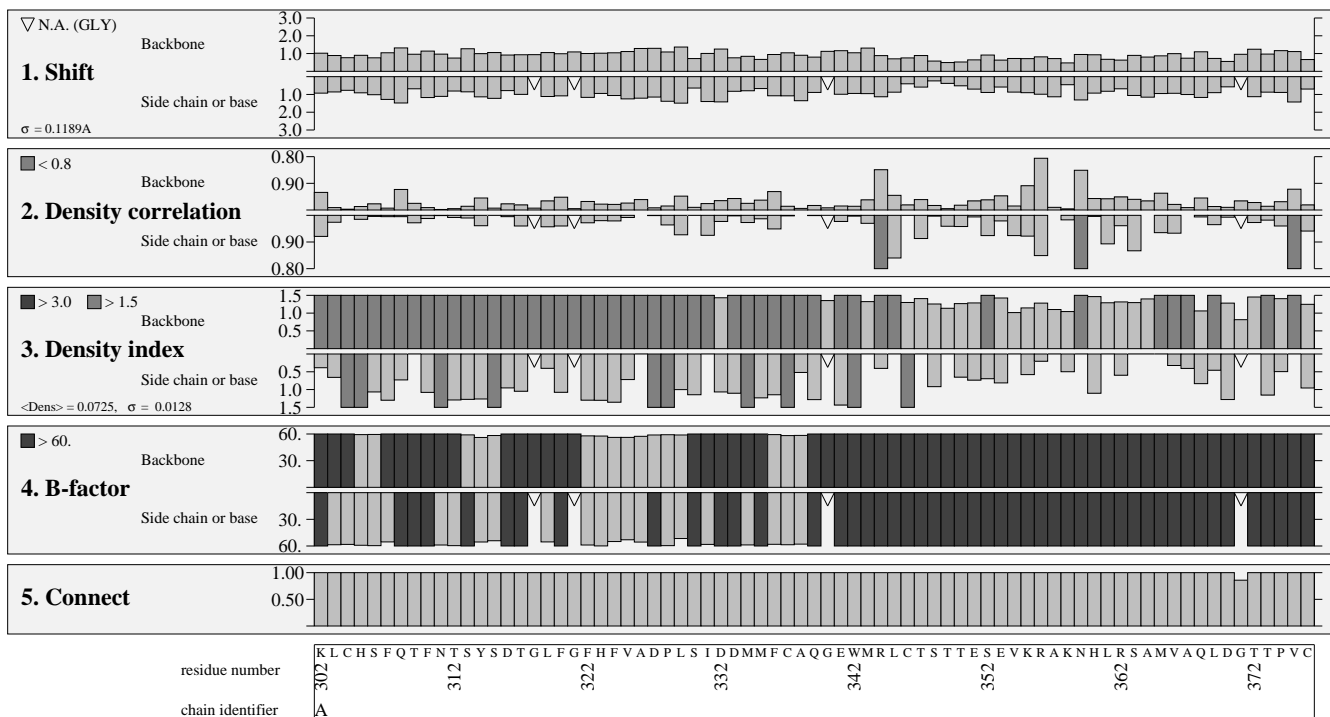
Local estimation (2)



Structure Factor Check

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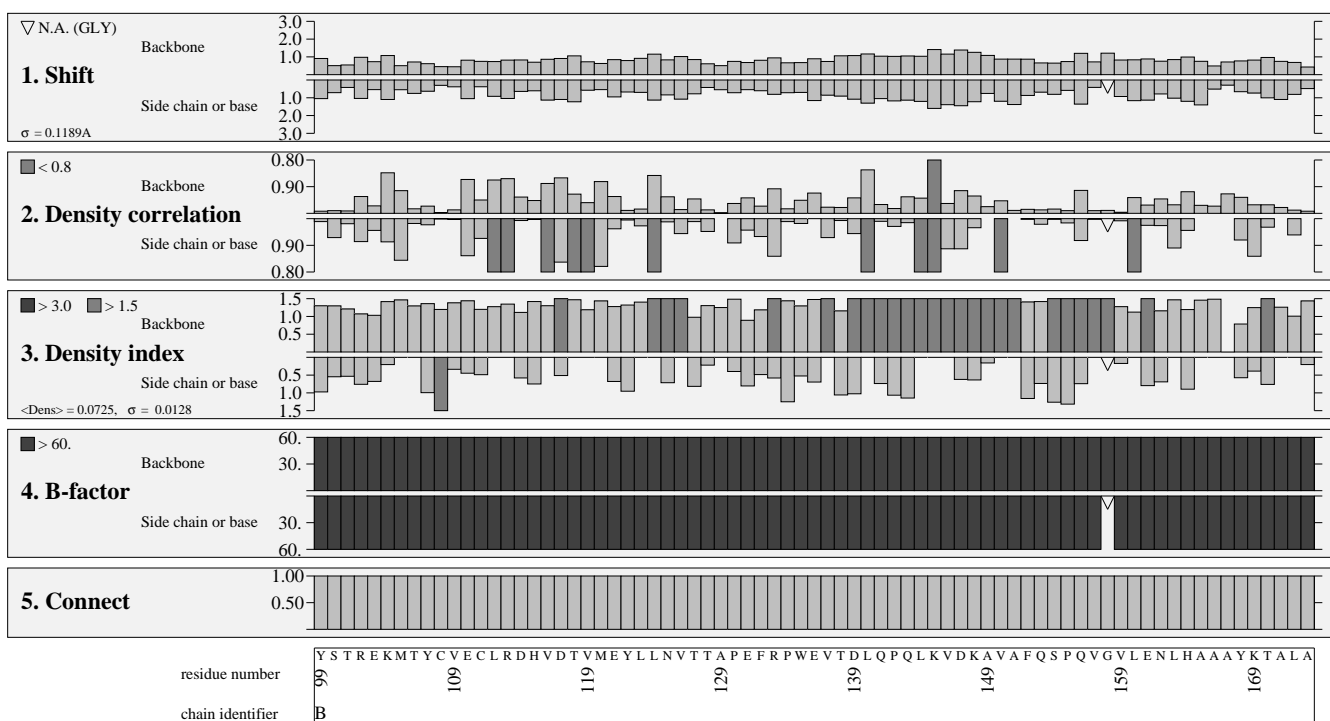
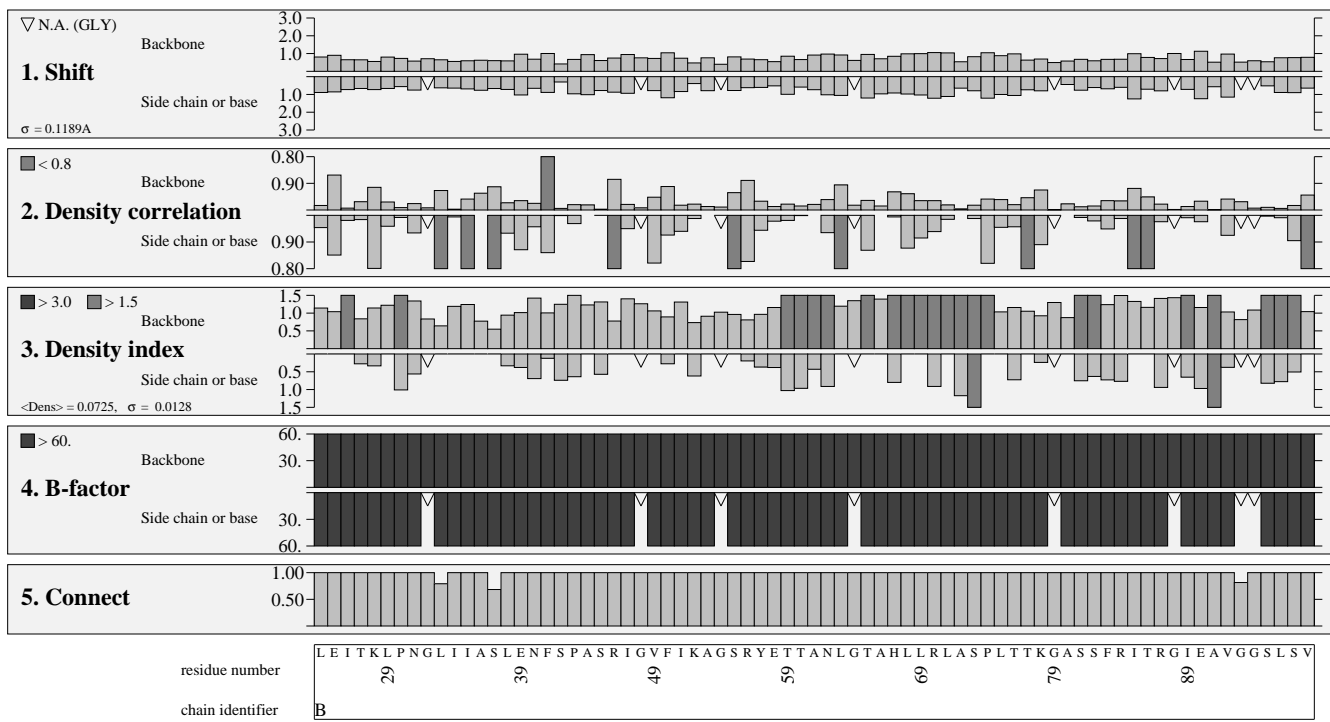
Local estimation (3)



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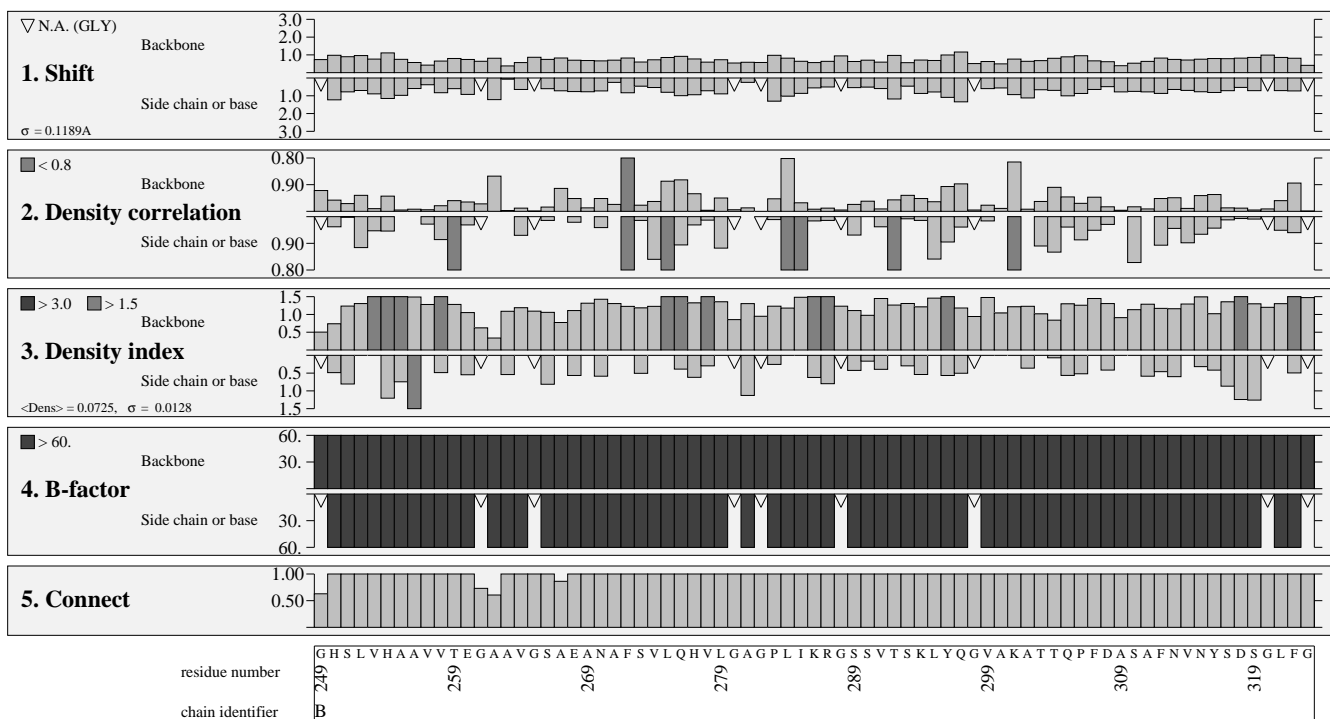
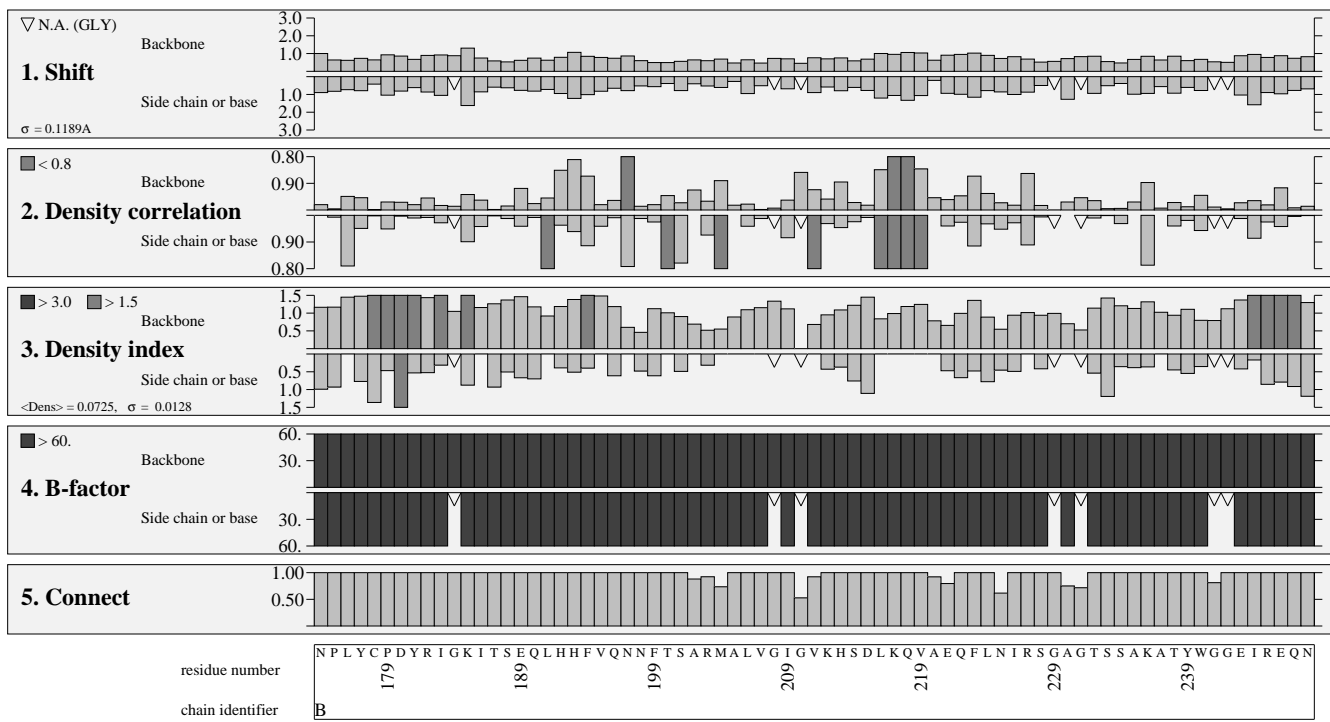
Local estimation (4)



Structure Factor Check

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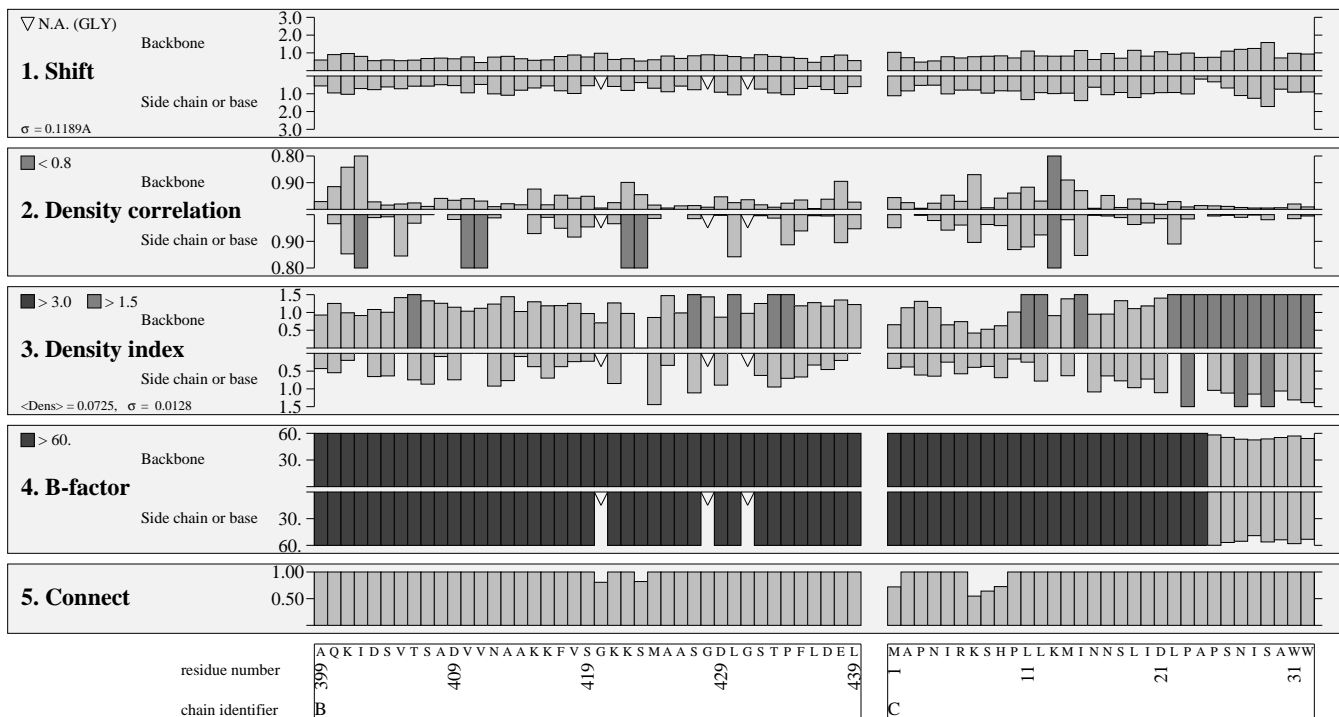
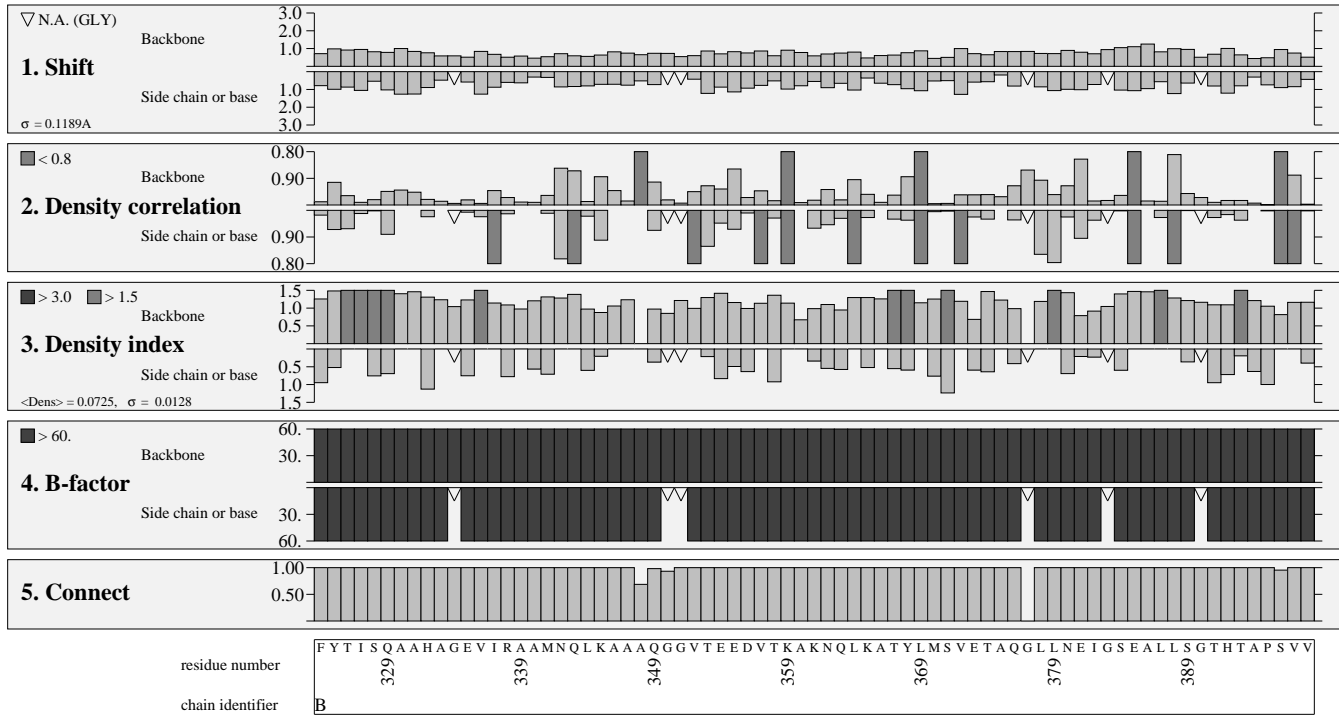
Local estimation (5)



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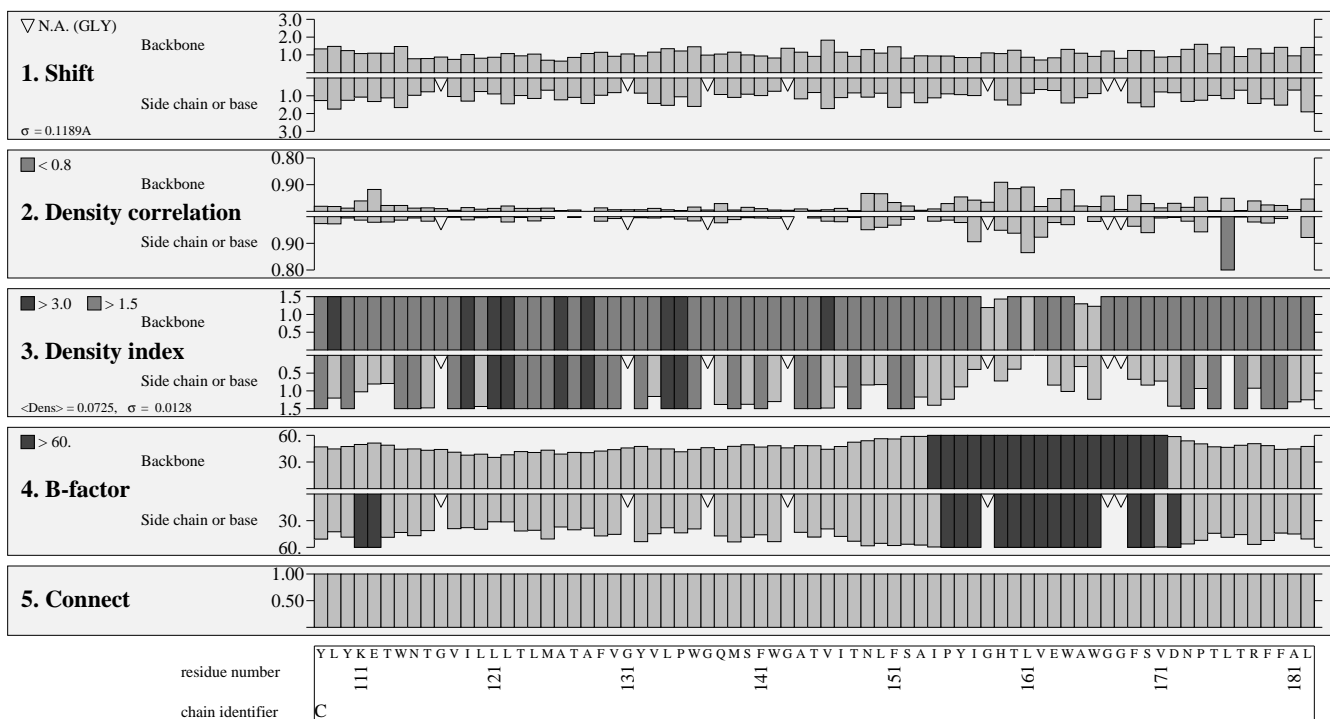
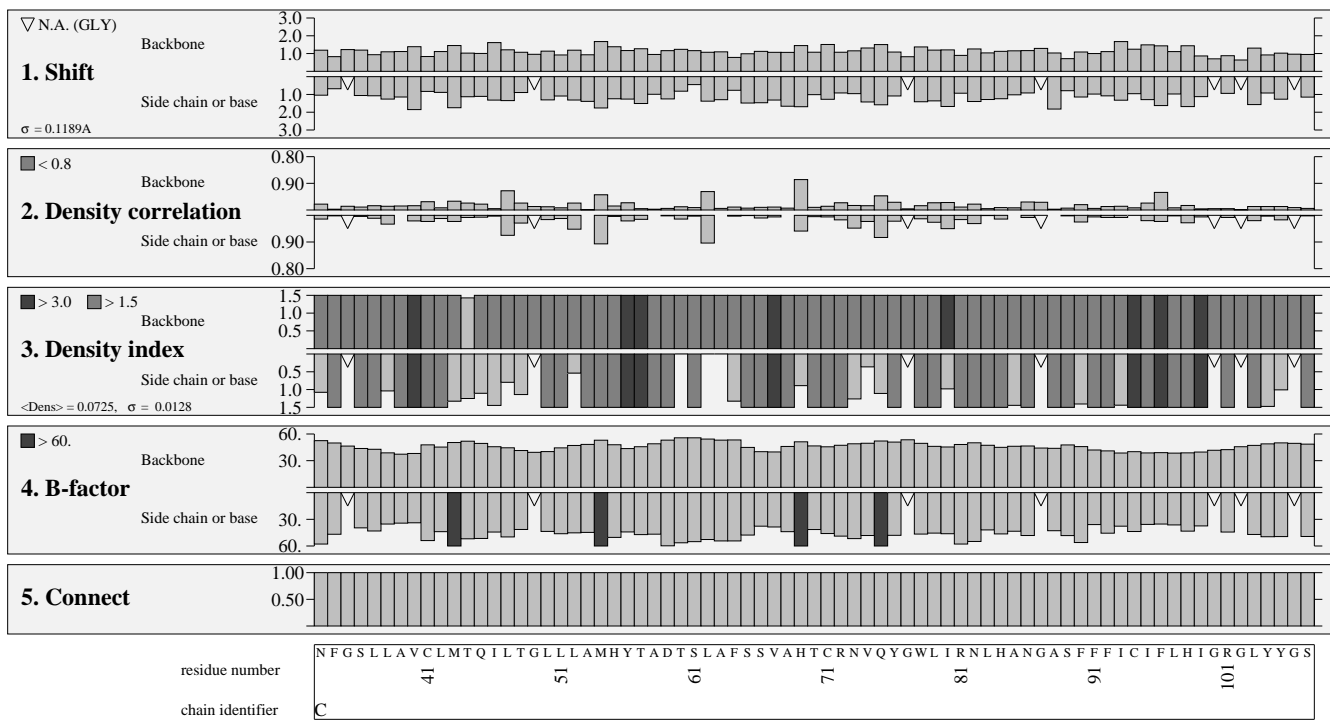
Local estimation (6)



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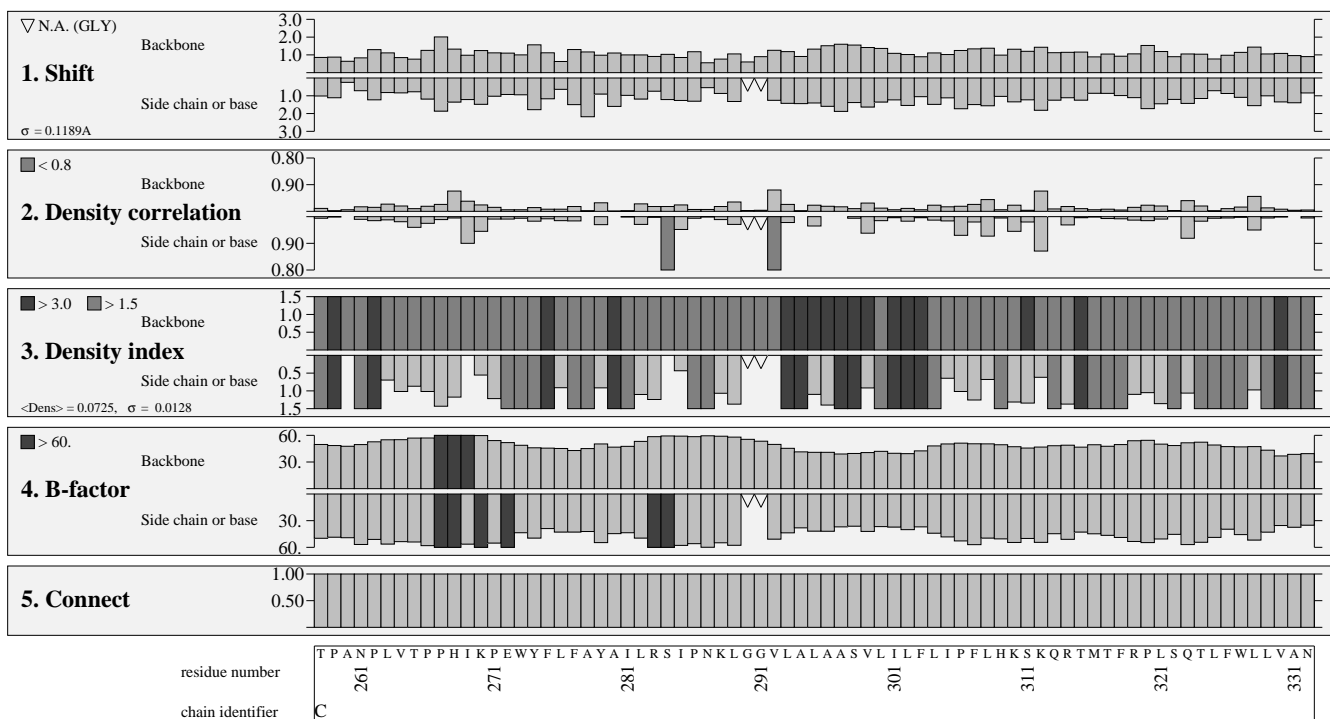
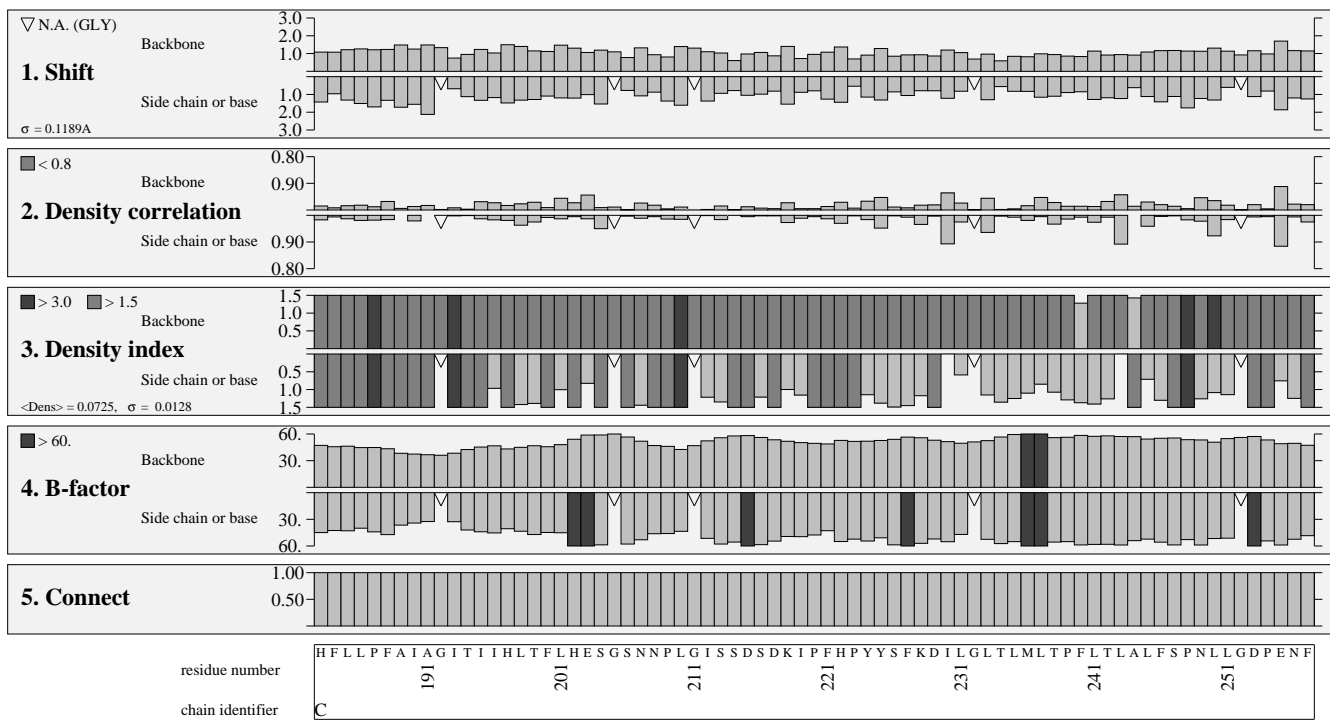
Local estimation (7)



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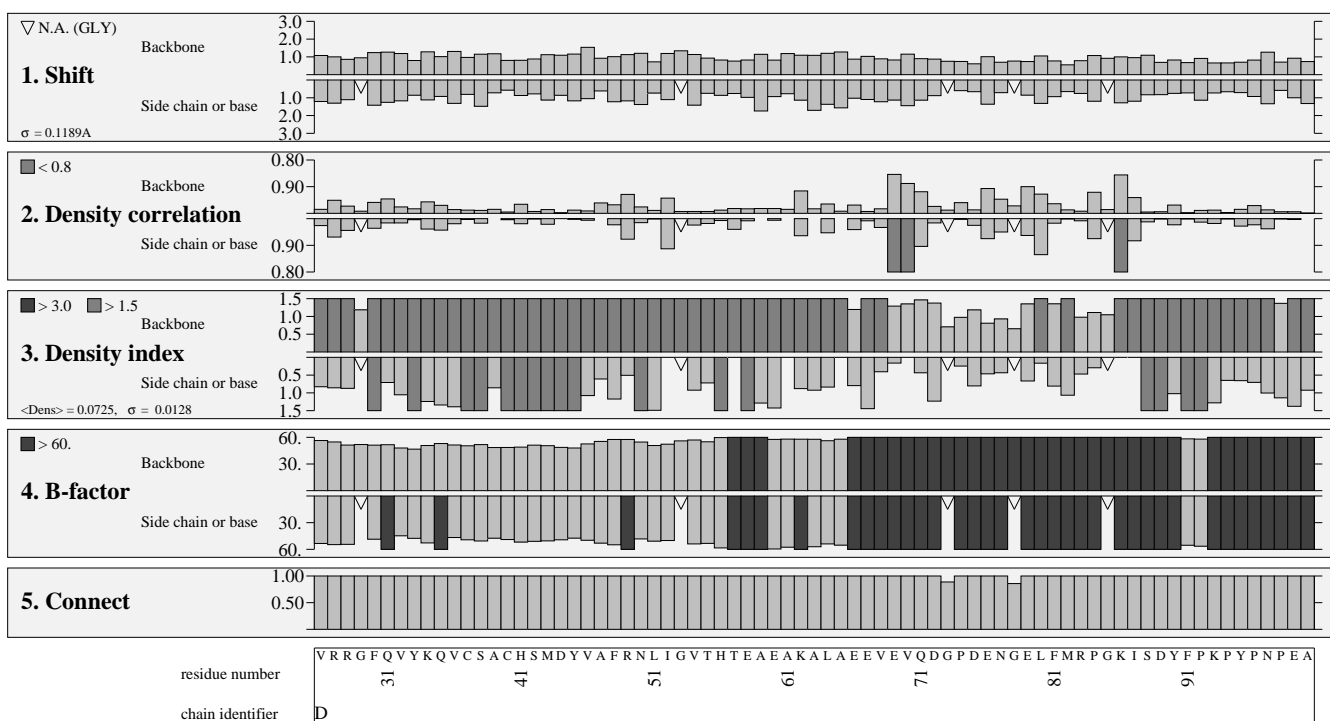
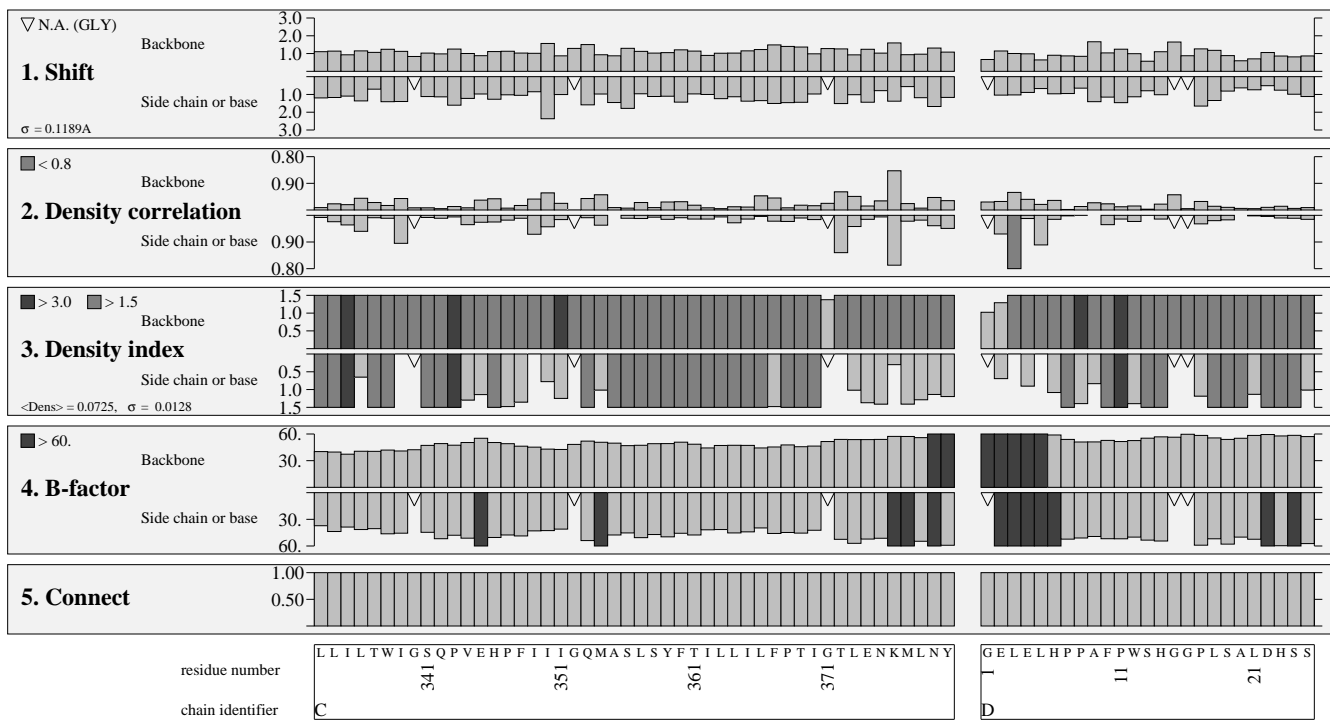
Local estimation (8)



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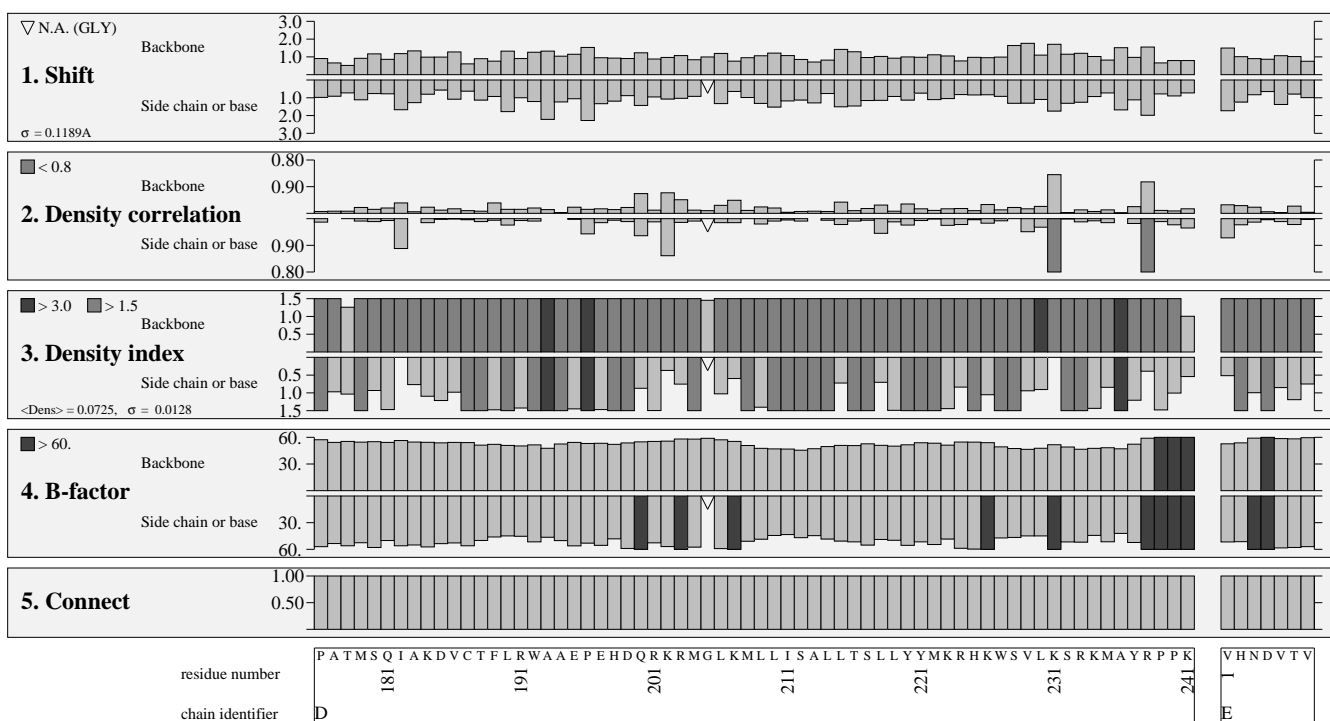
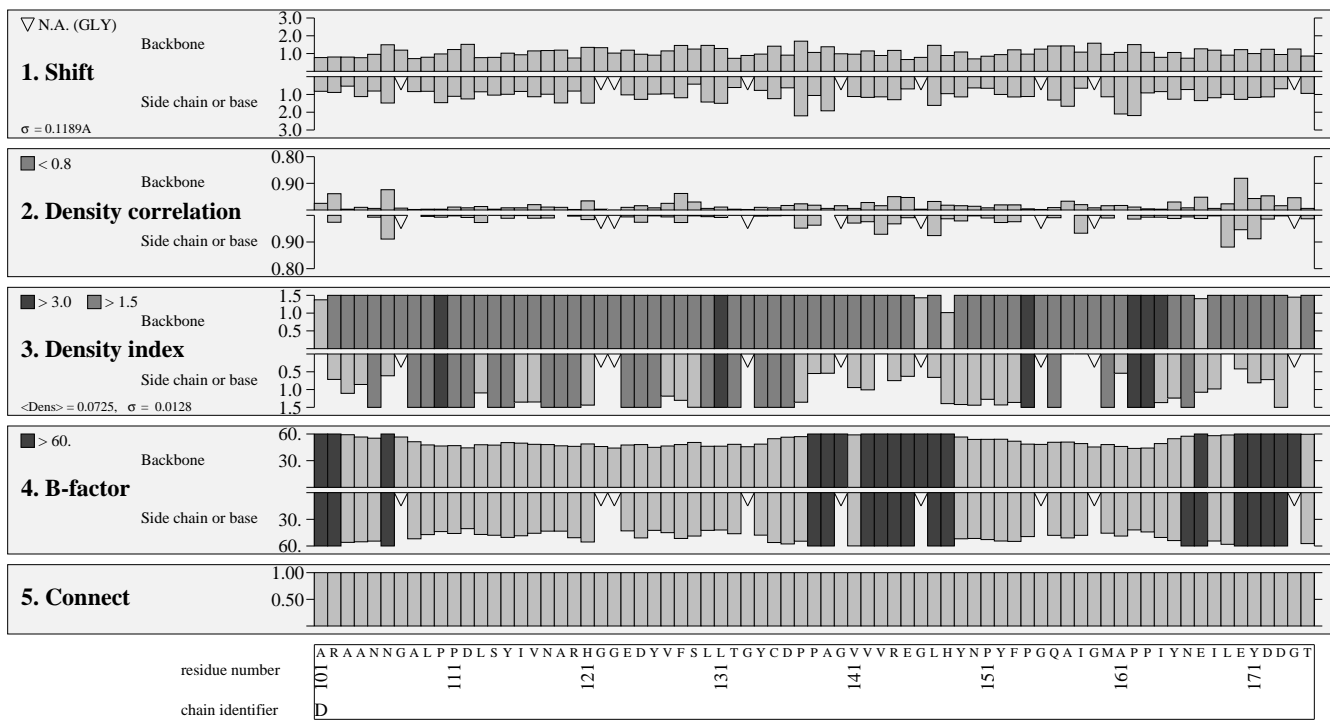
Local estimation (9)



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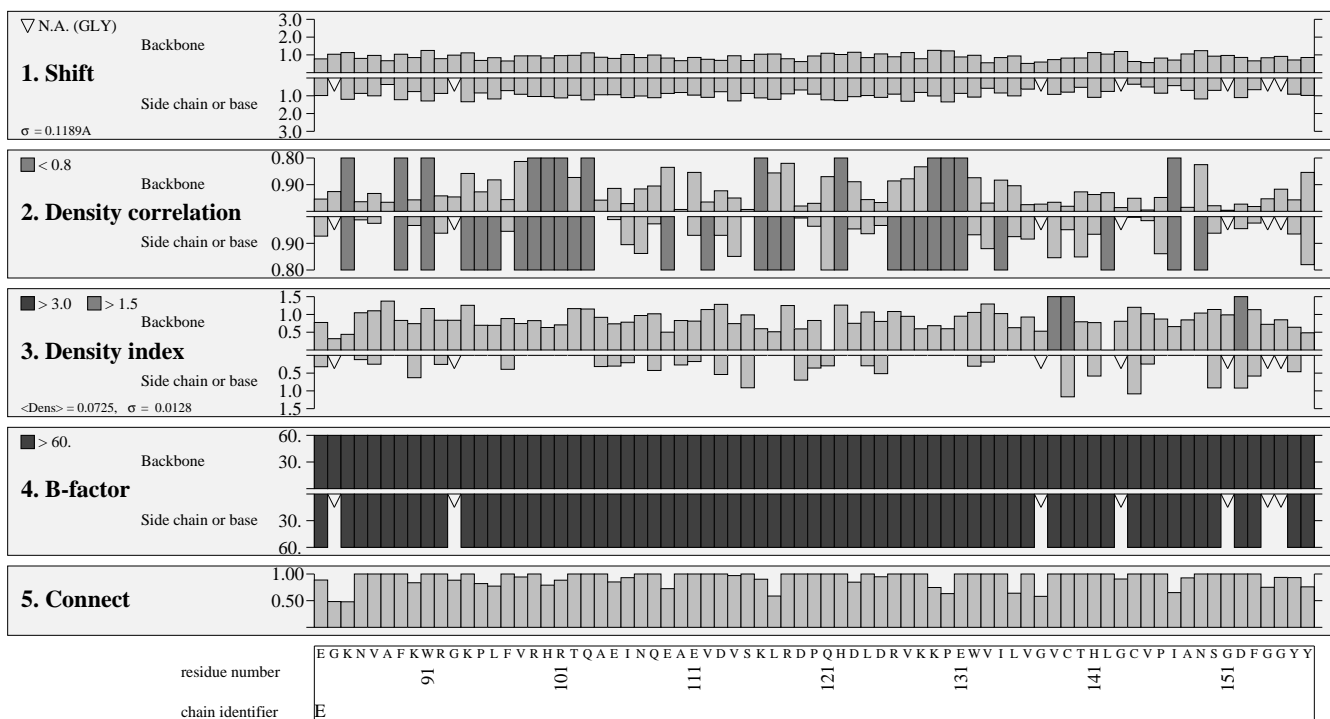
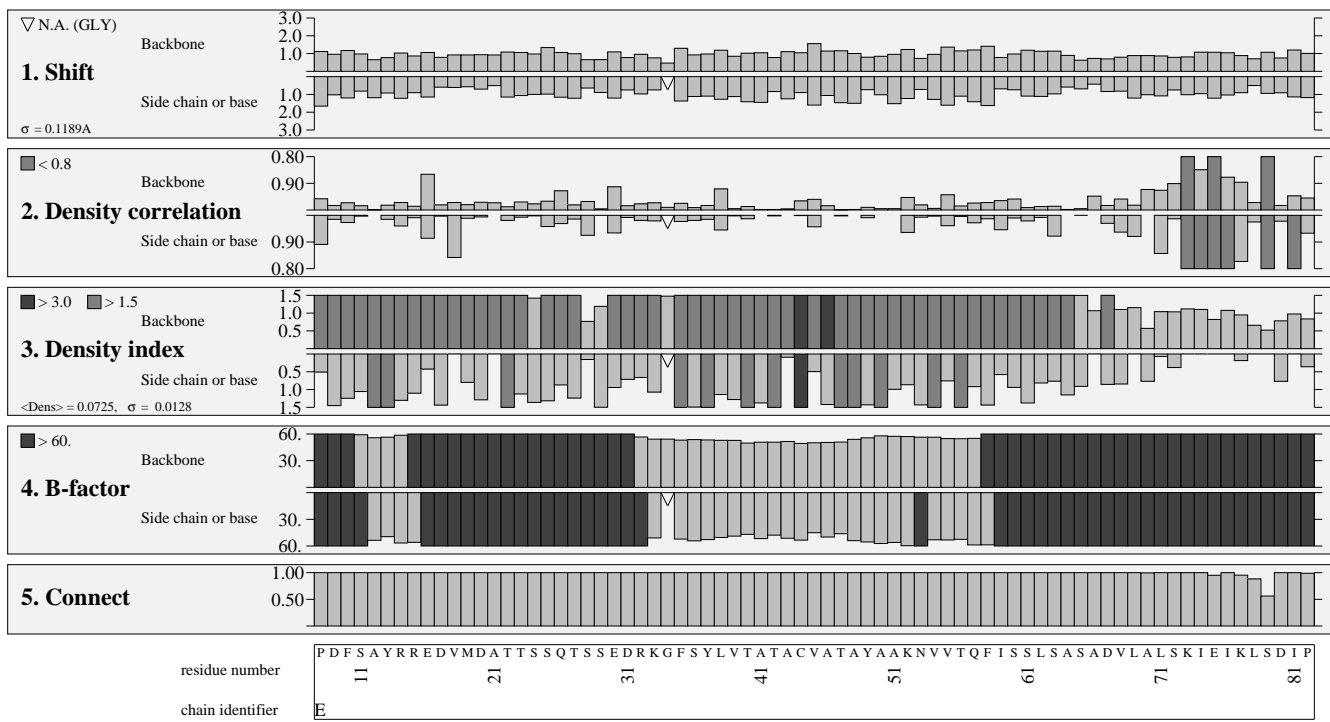
Local estimation (10)



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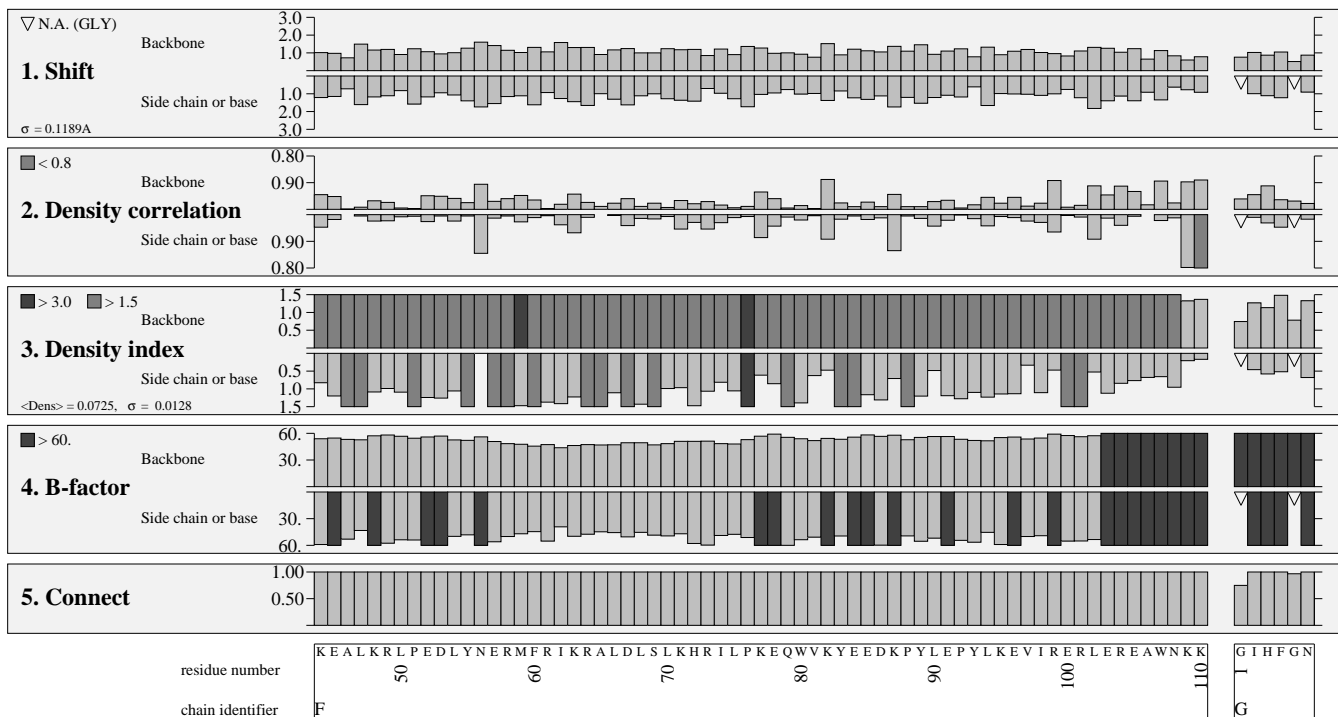
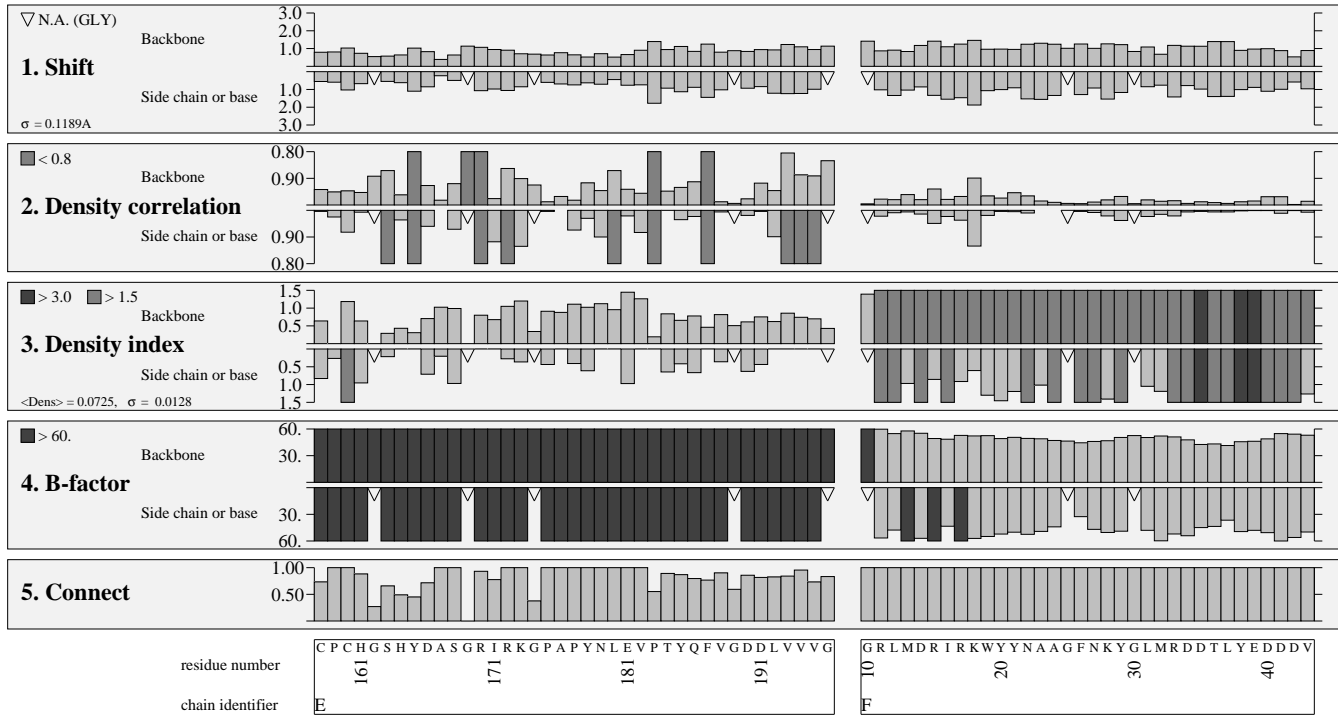
Local estimation (11)



Structure Factor Check

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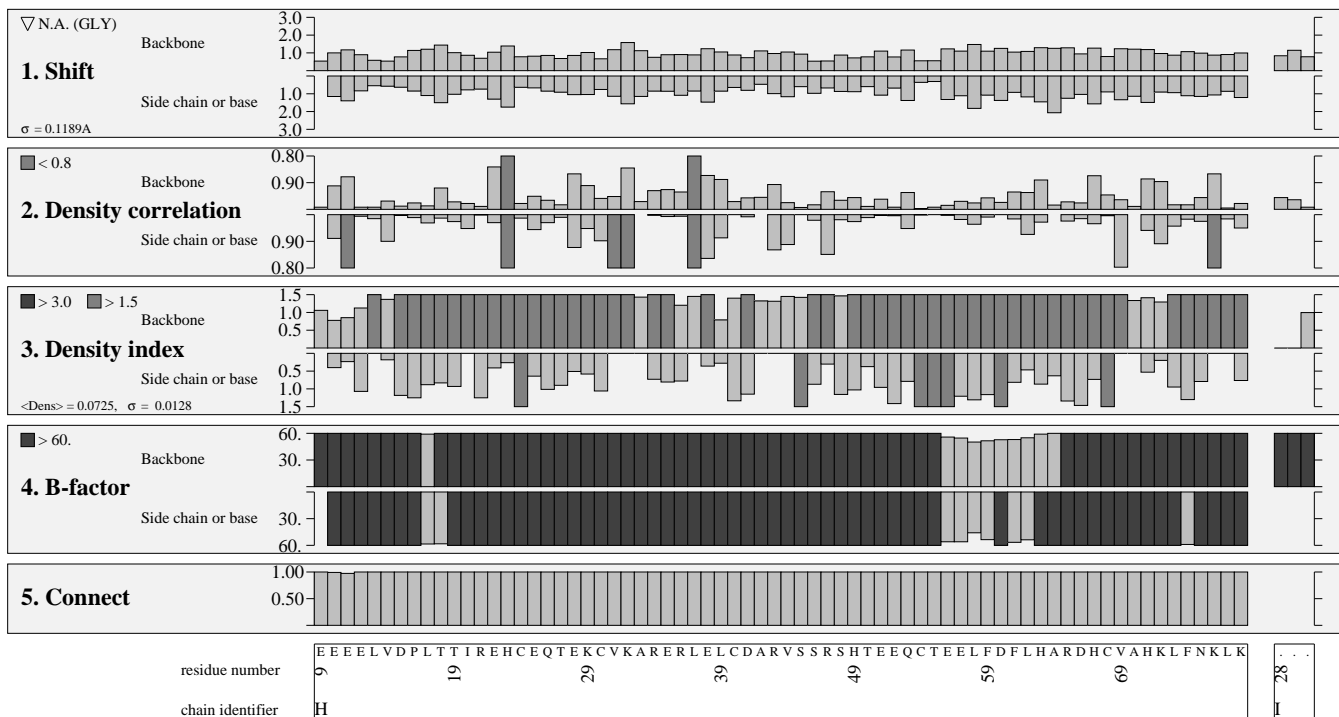
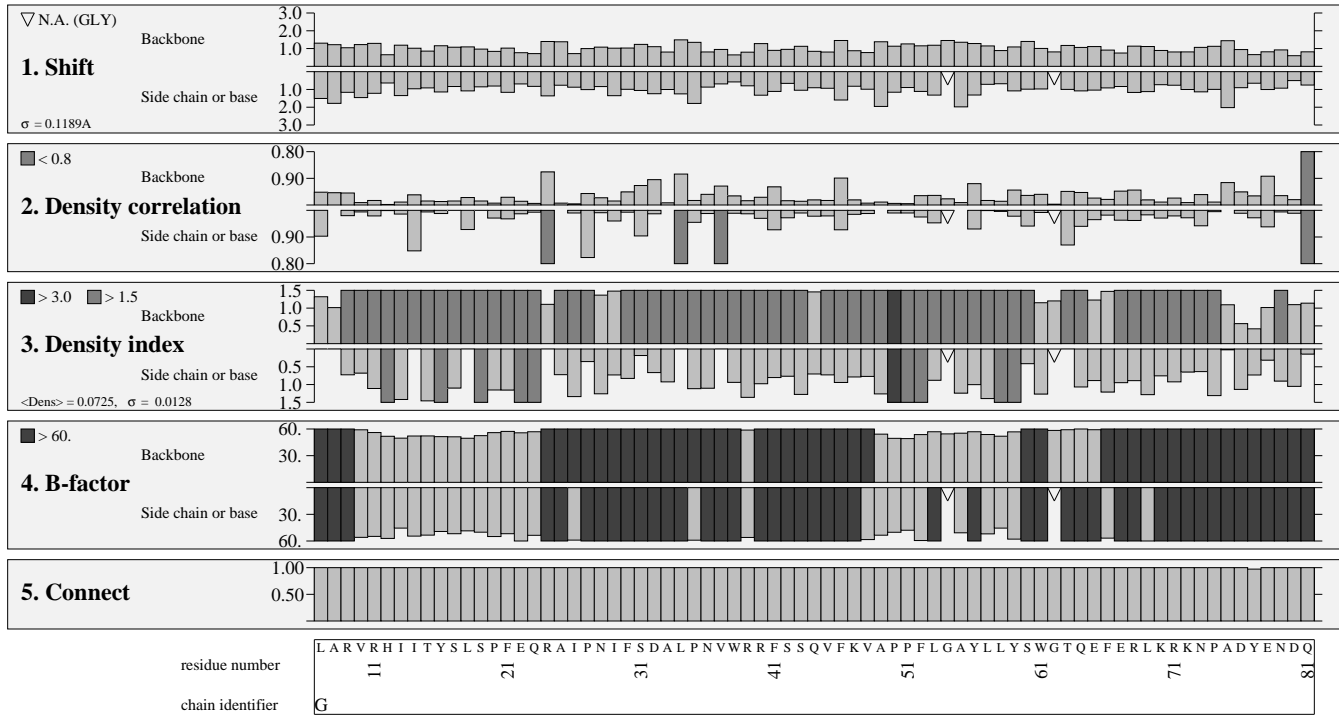
Local estimation (12)



Structure Factor Check

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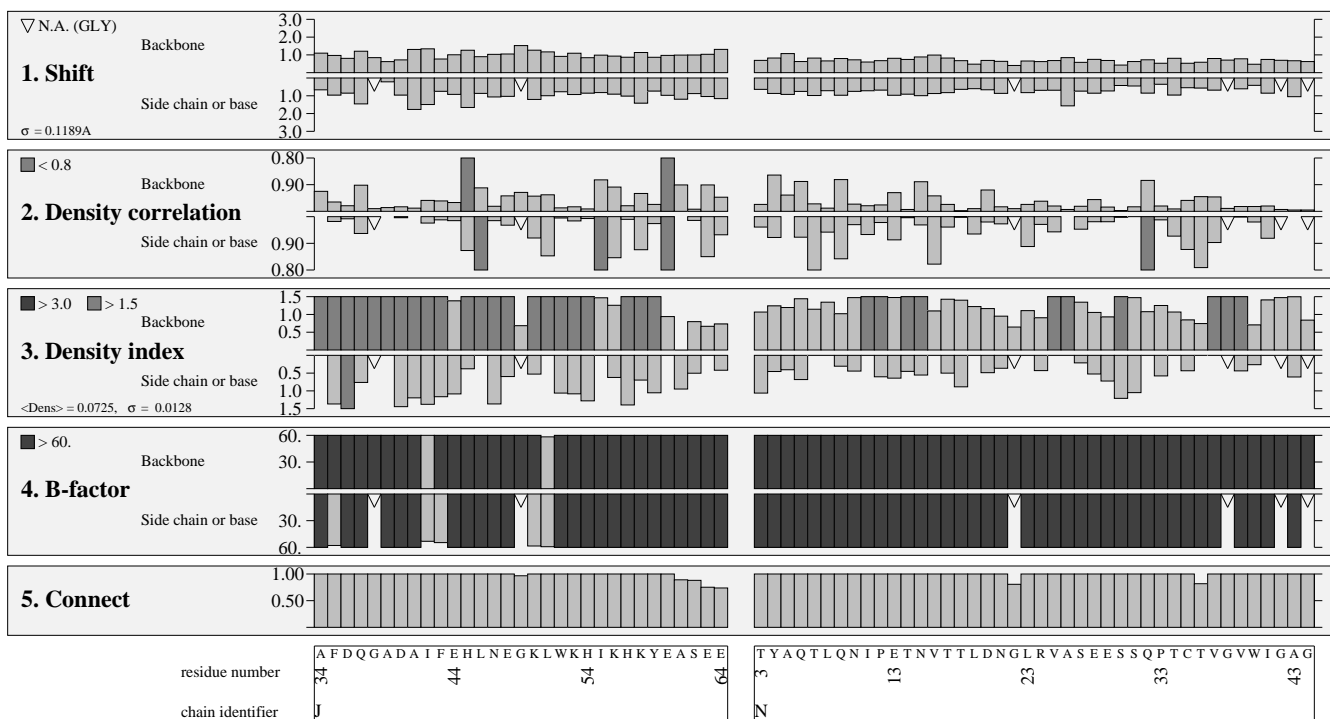
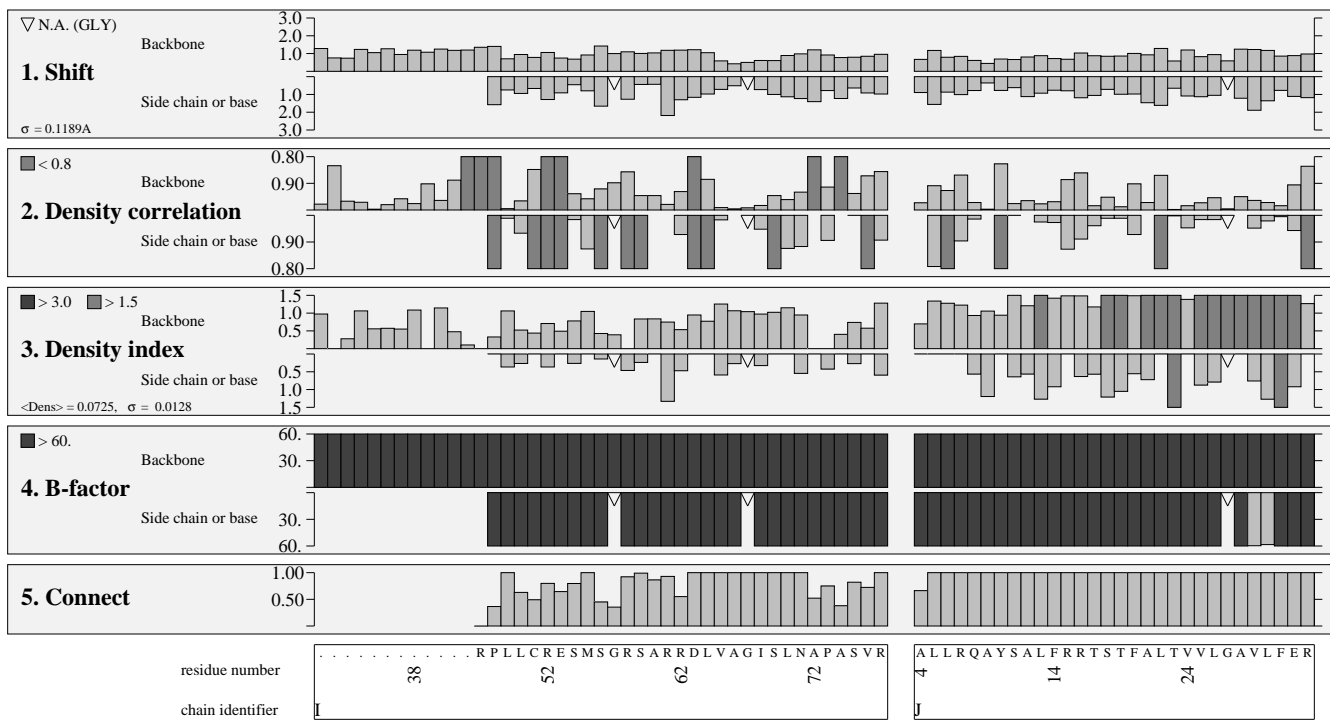
Local estimation (13)



Structure Factor Check

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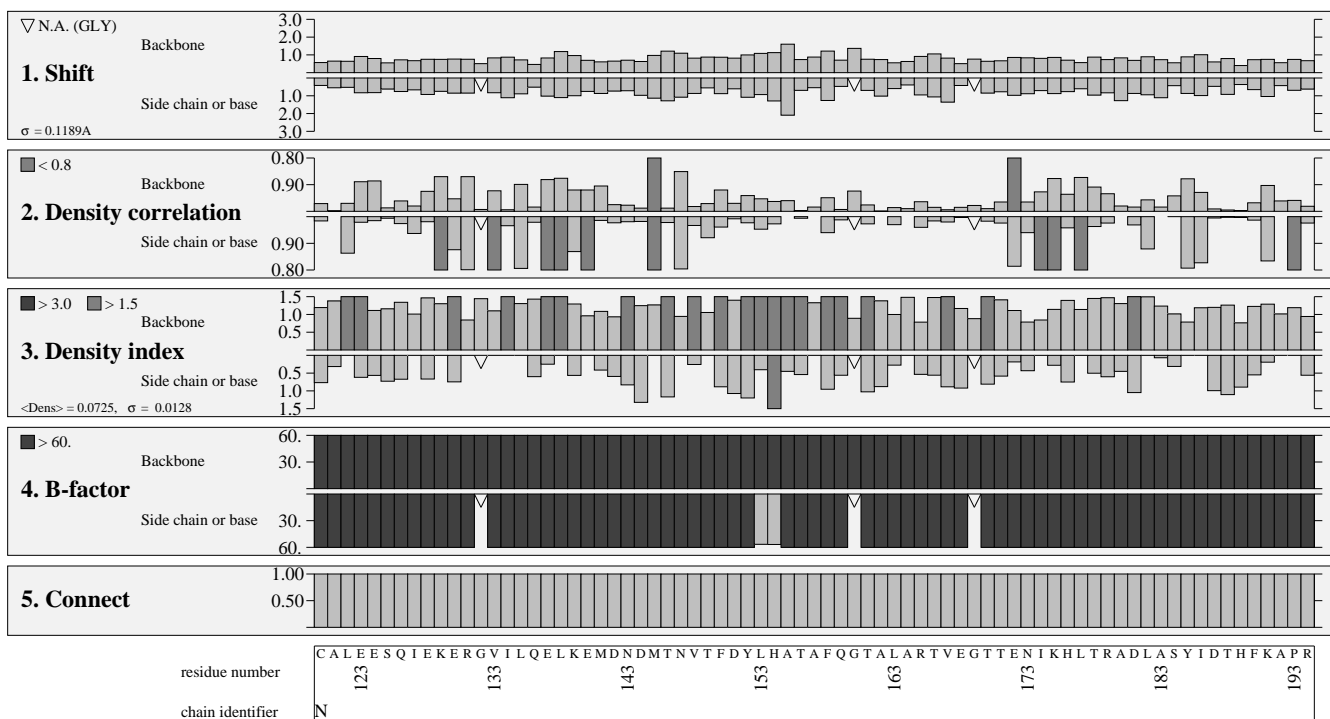
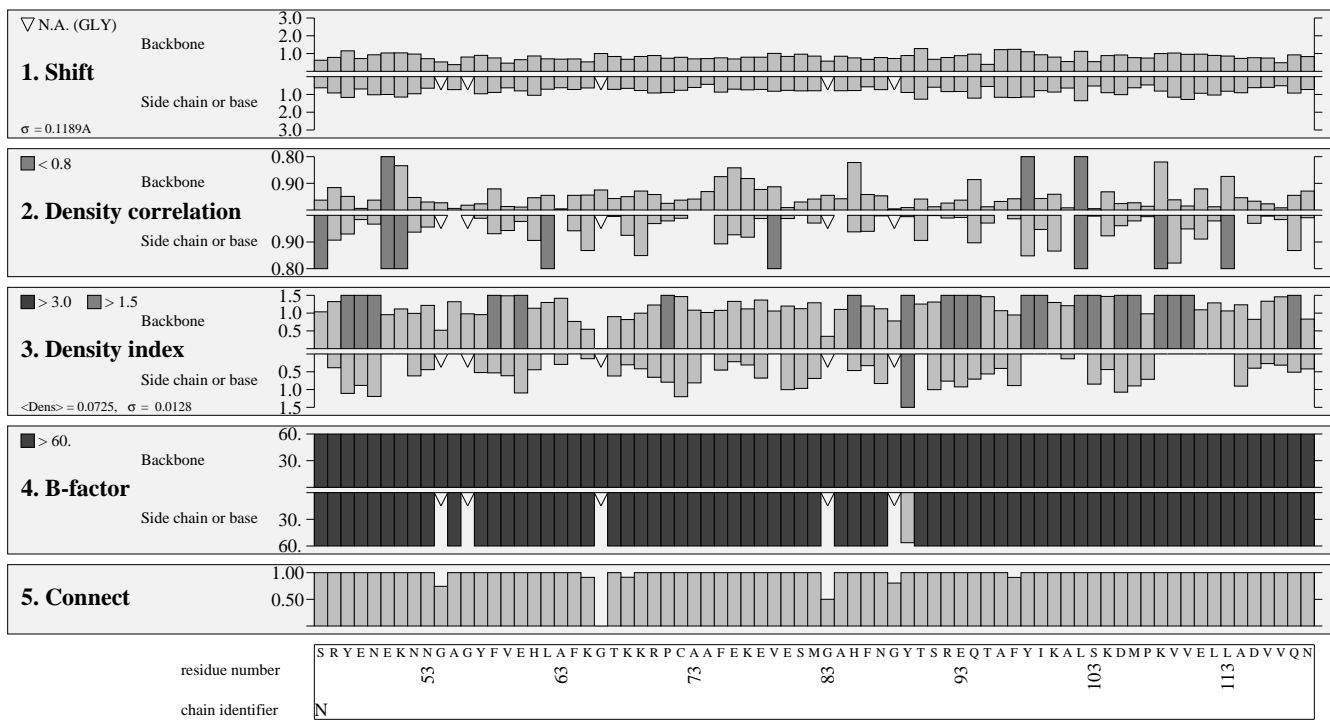
Local estimation (14)



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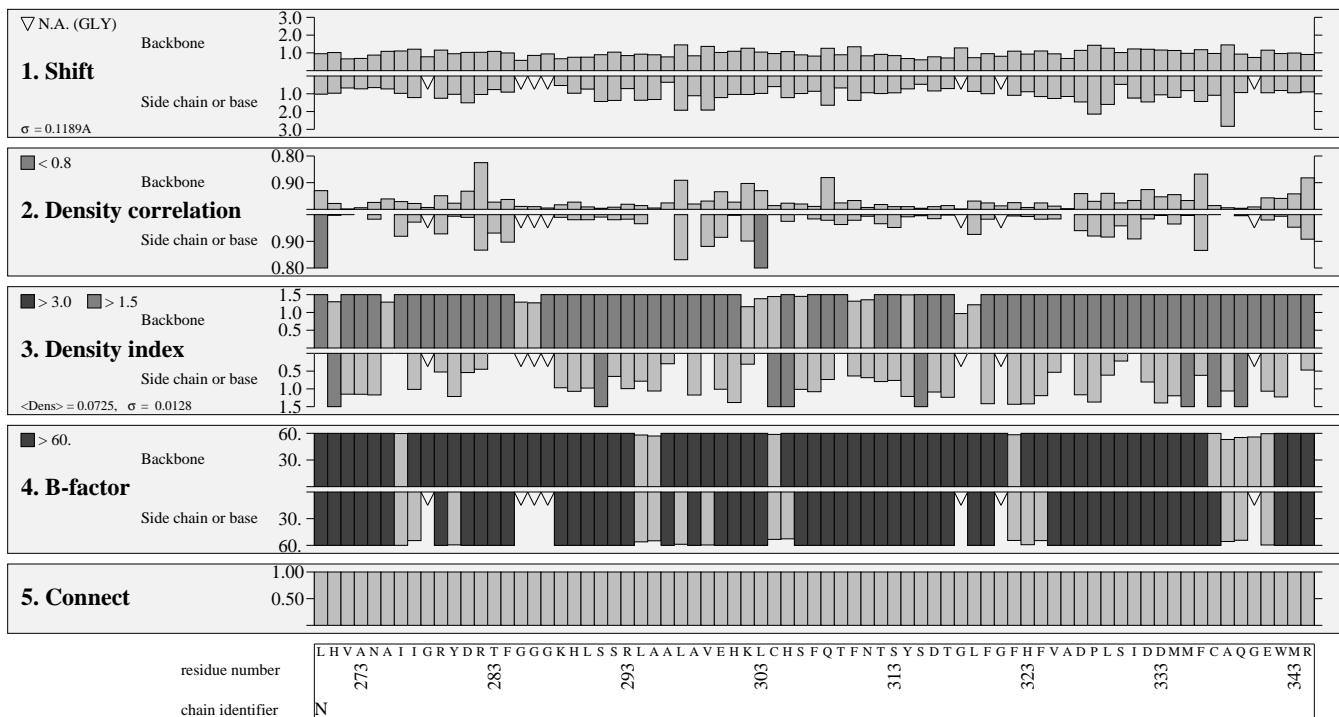
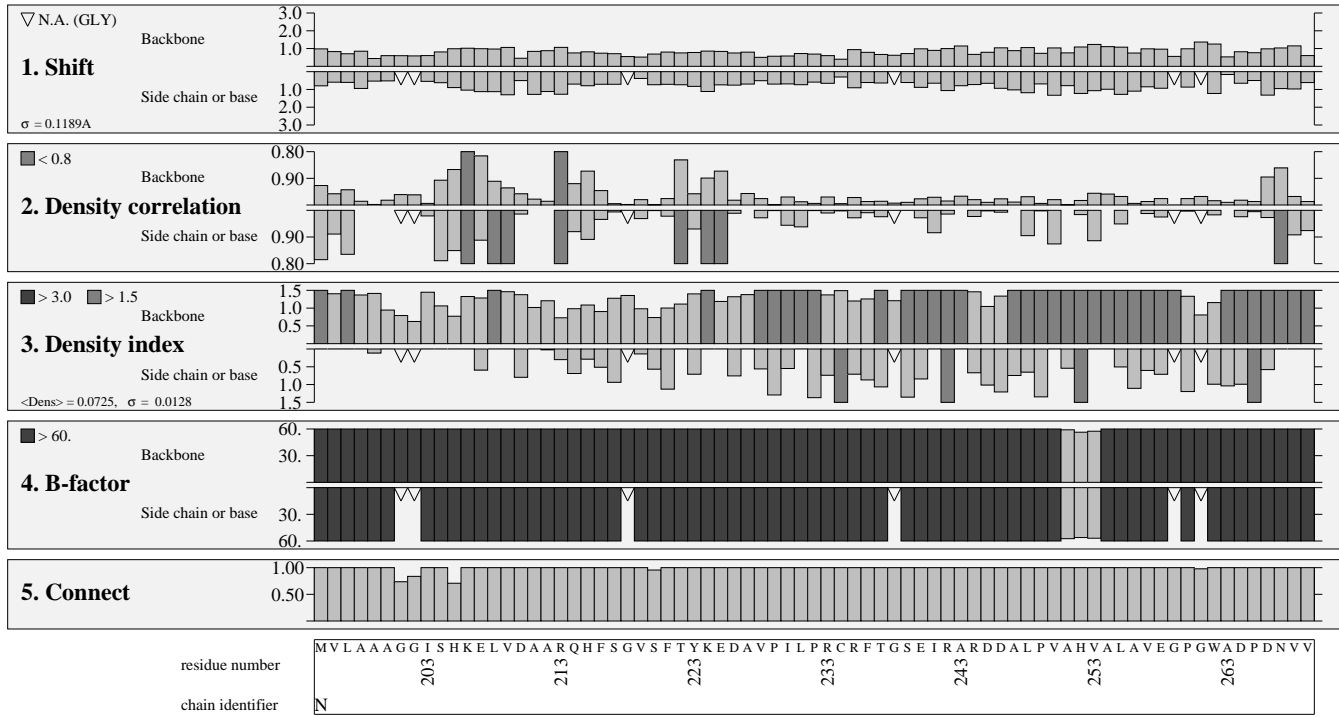
Local estimation (15)



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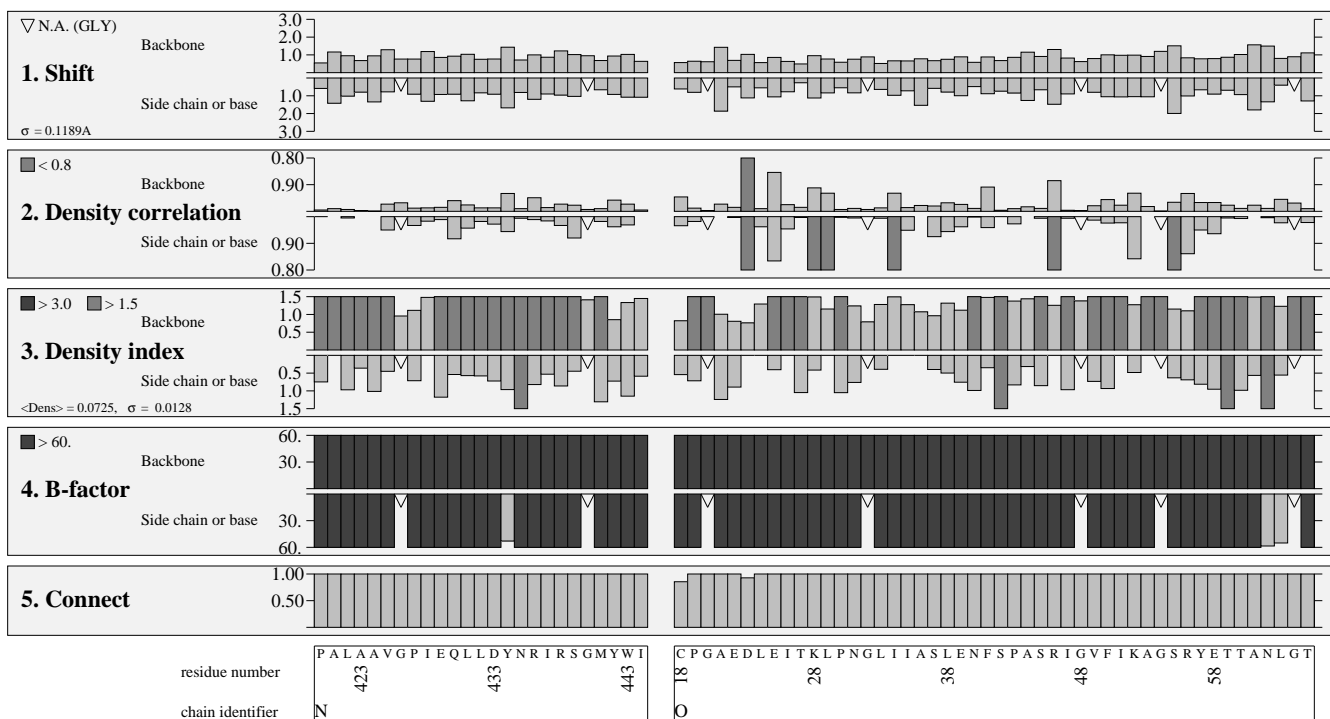
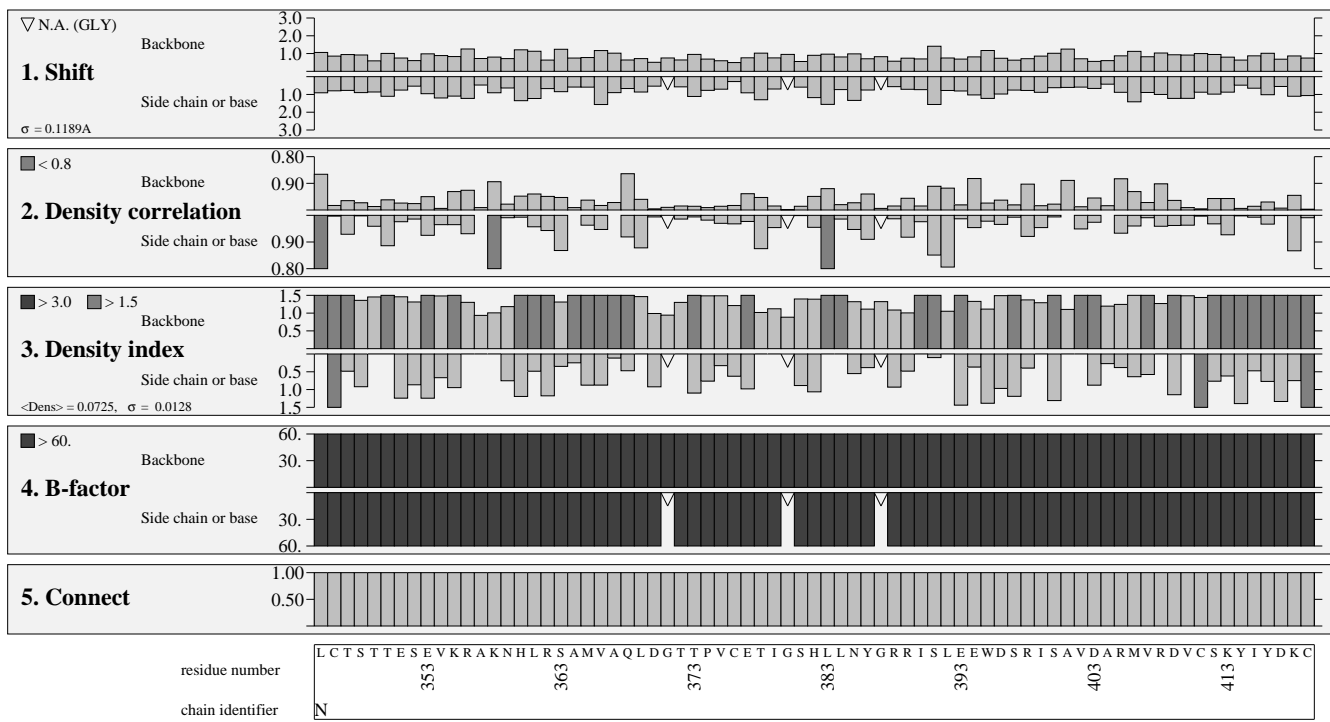
Local estimation (16)



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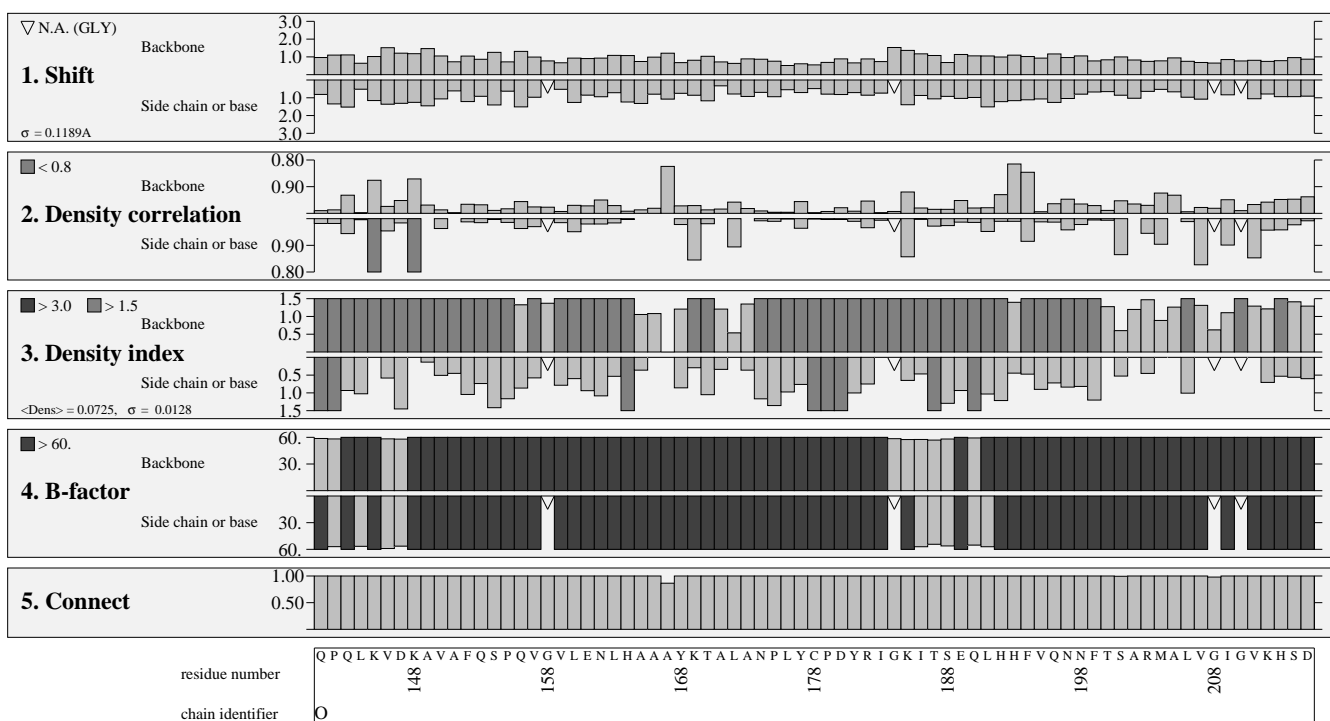
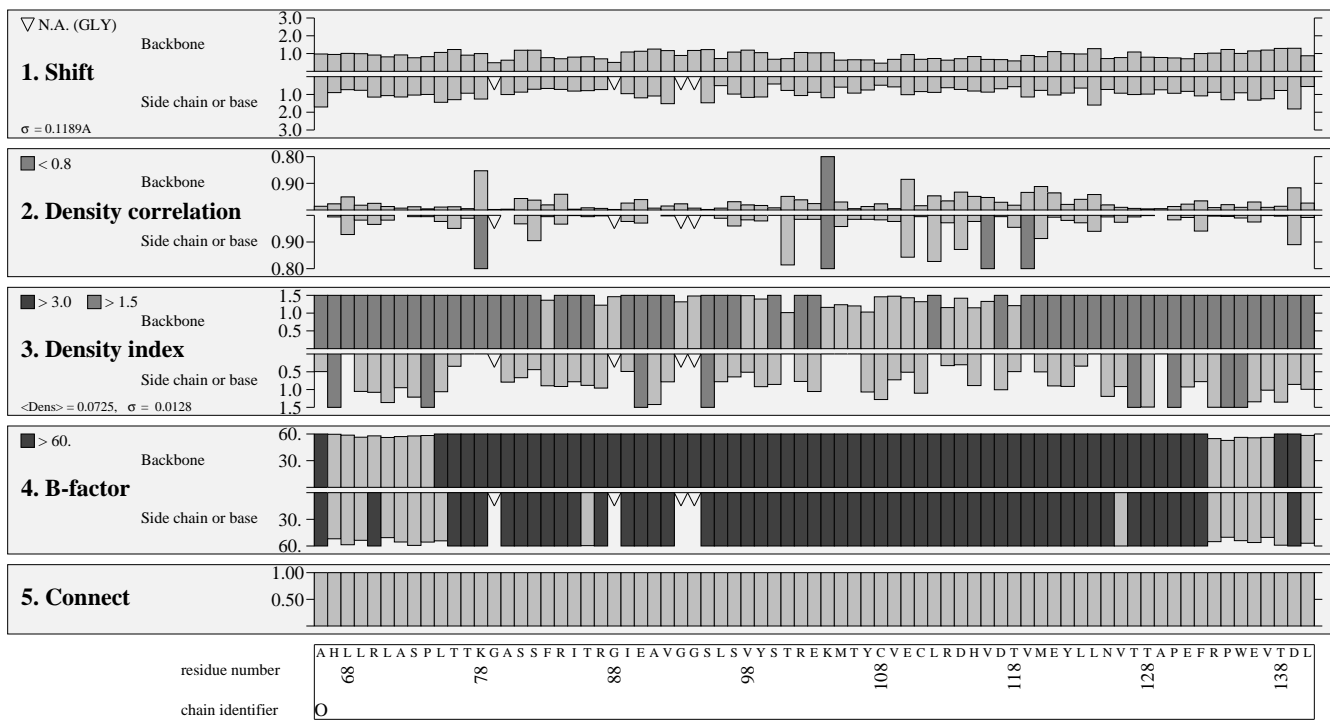
Local estimation (17)



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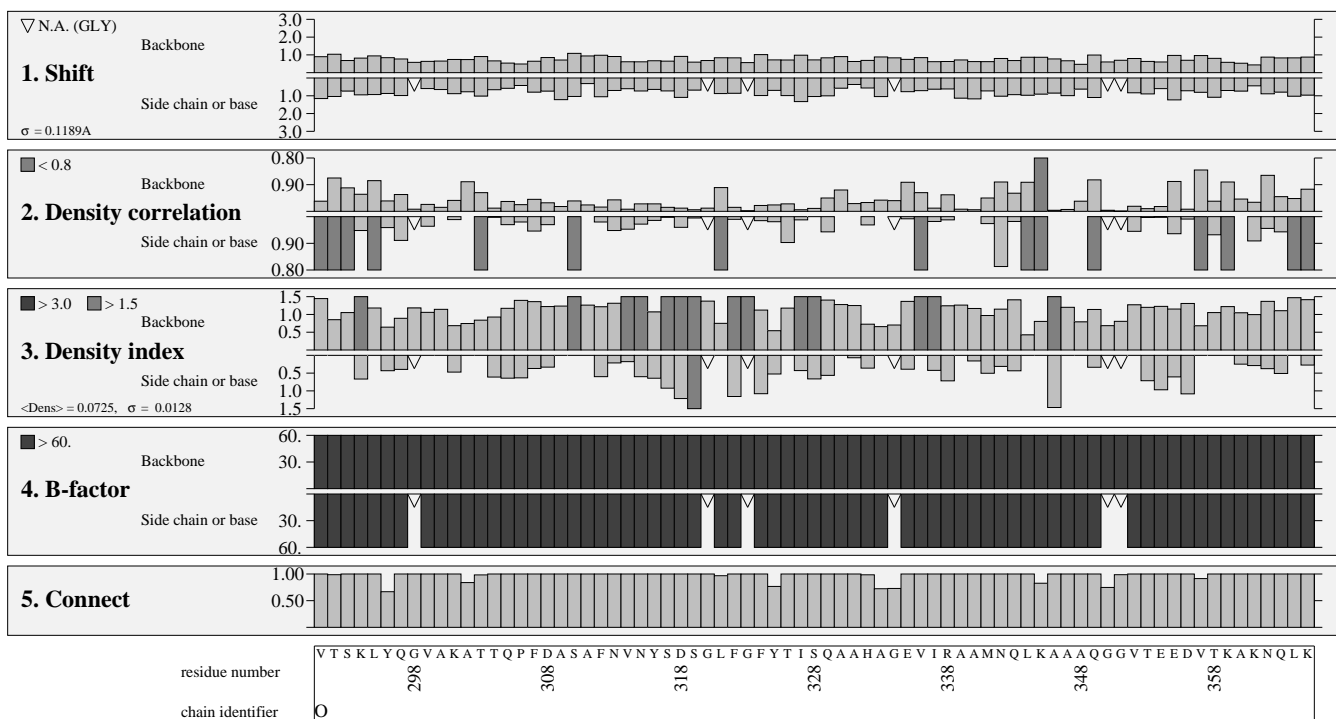
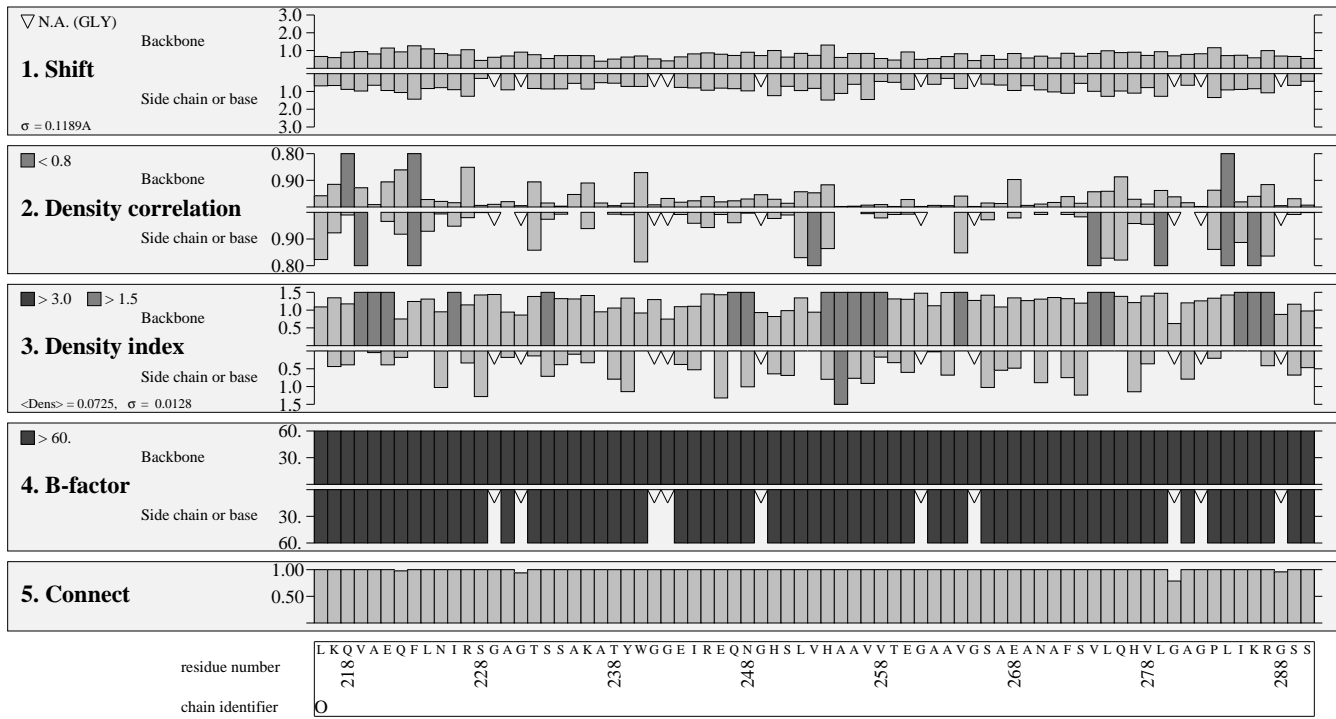
Local estimation (18)



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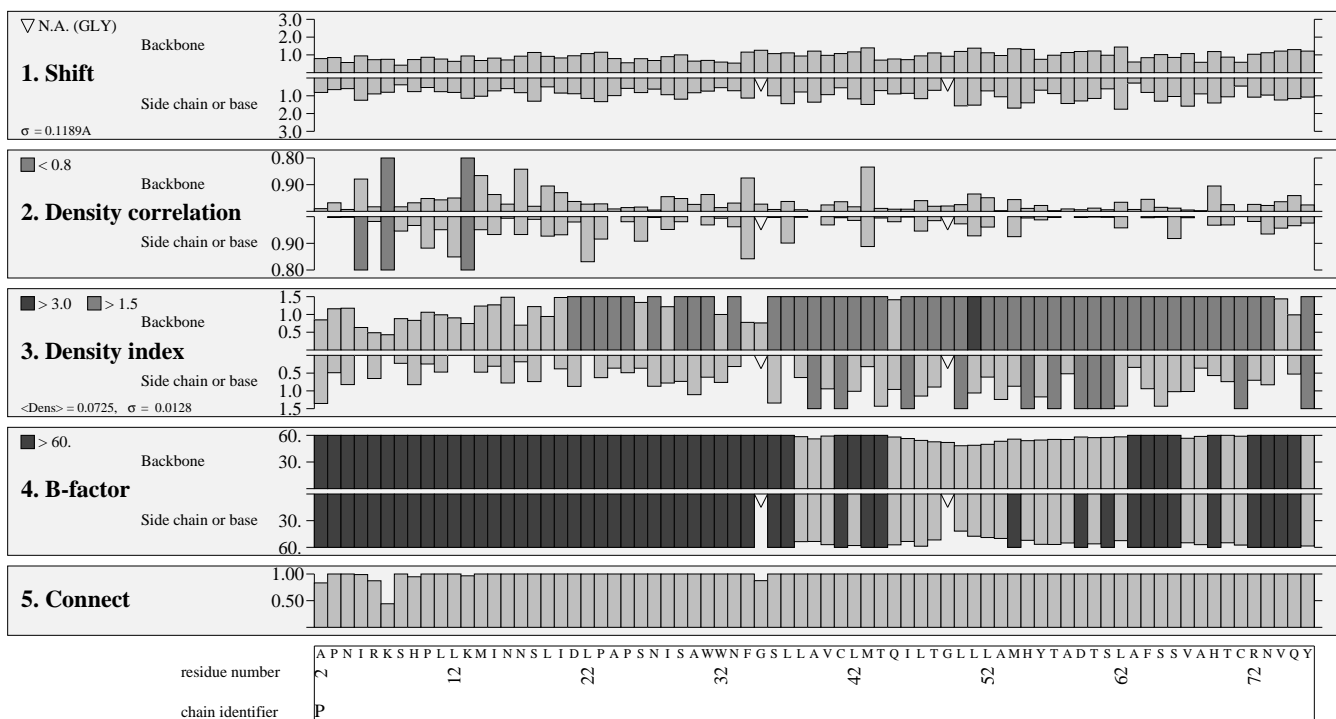
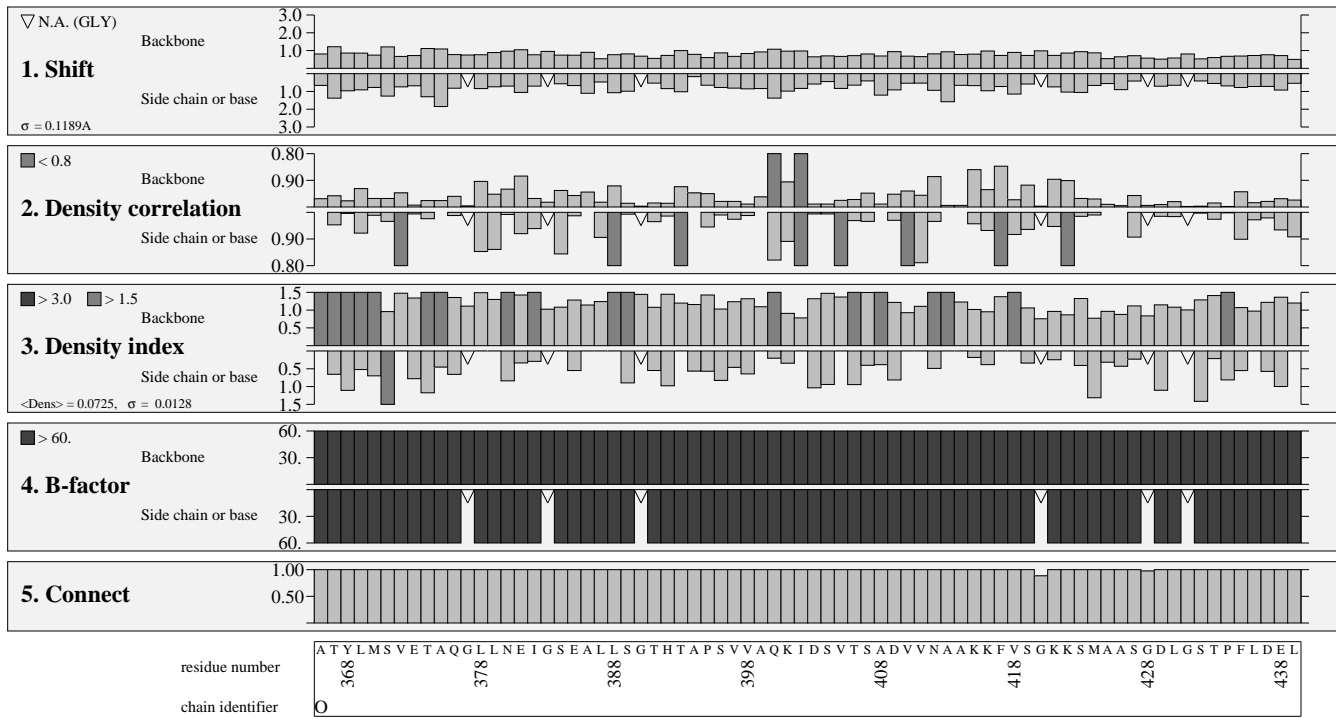
Local estimation (19)



Structure Factor Check

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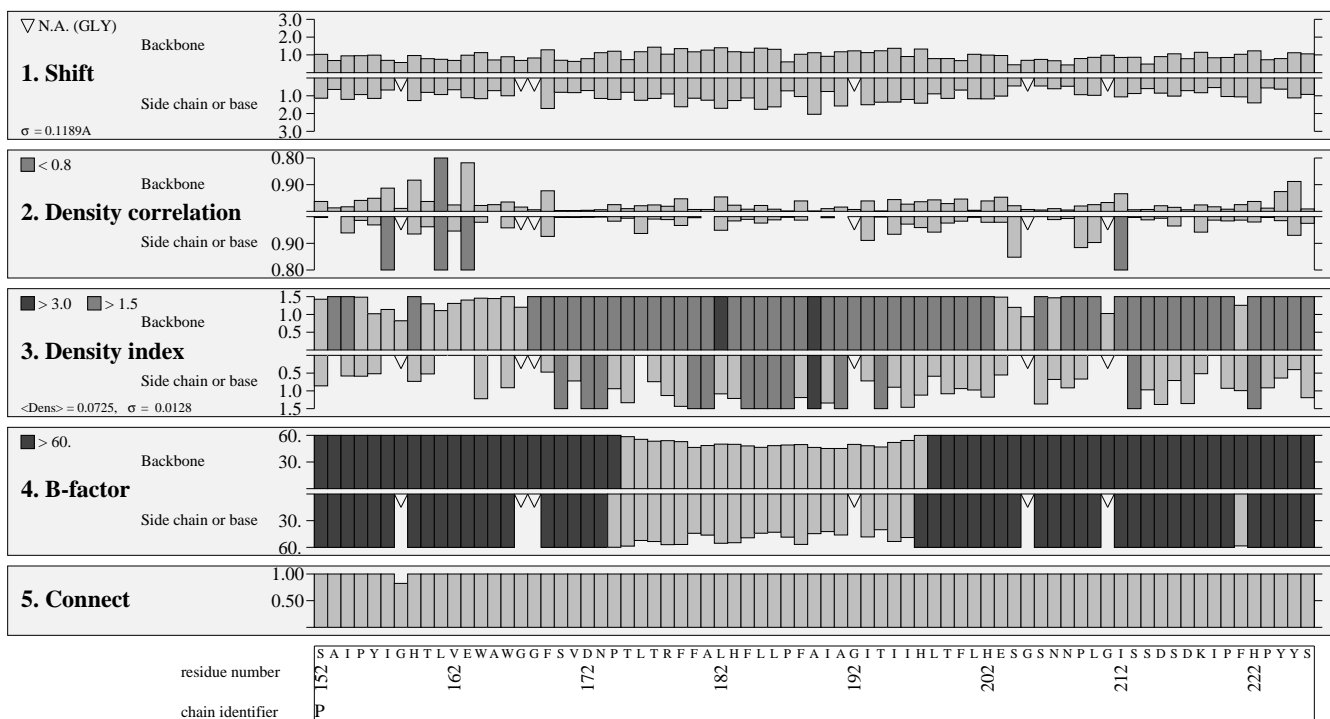
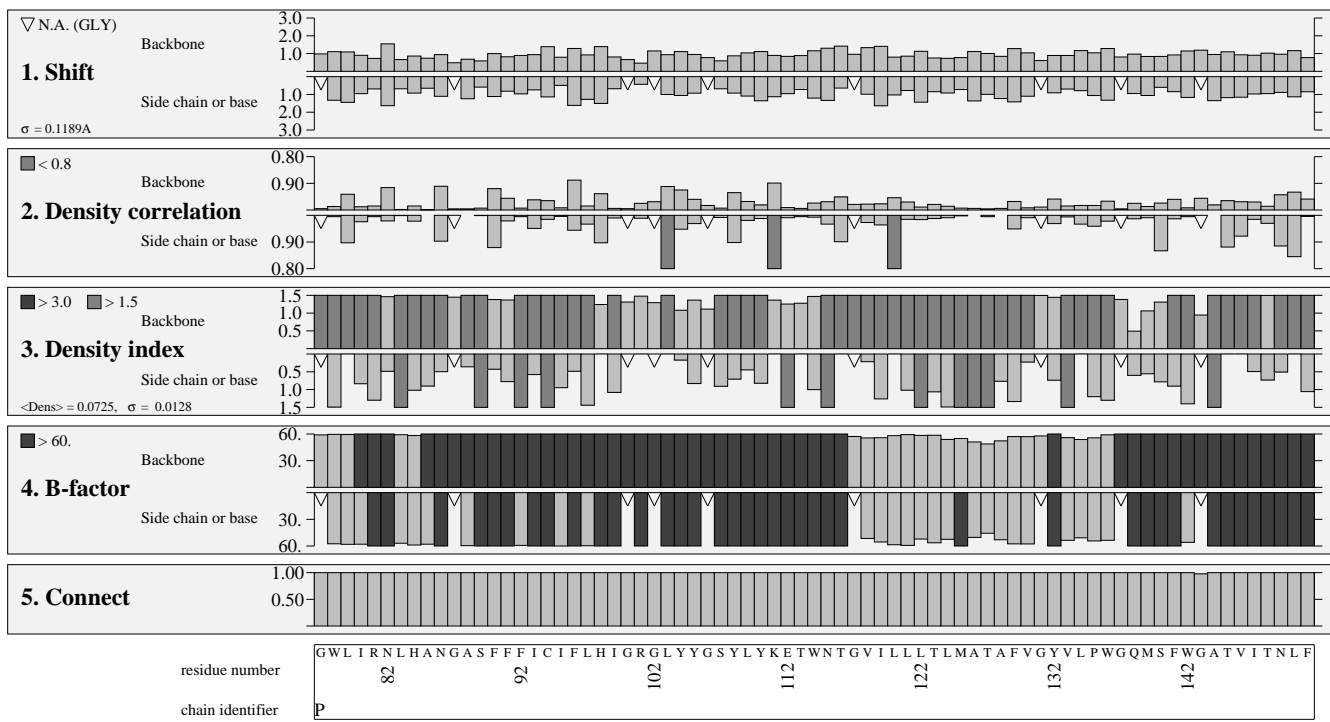
Local estimation (20)



Structure Factor Check

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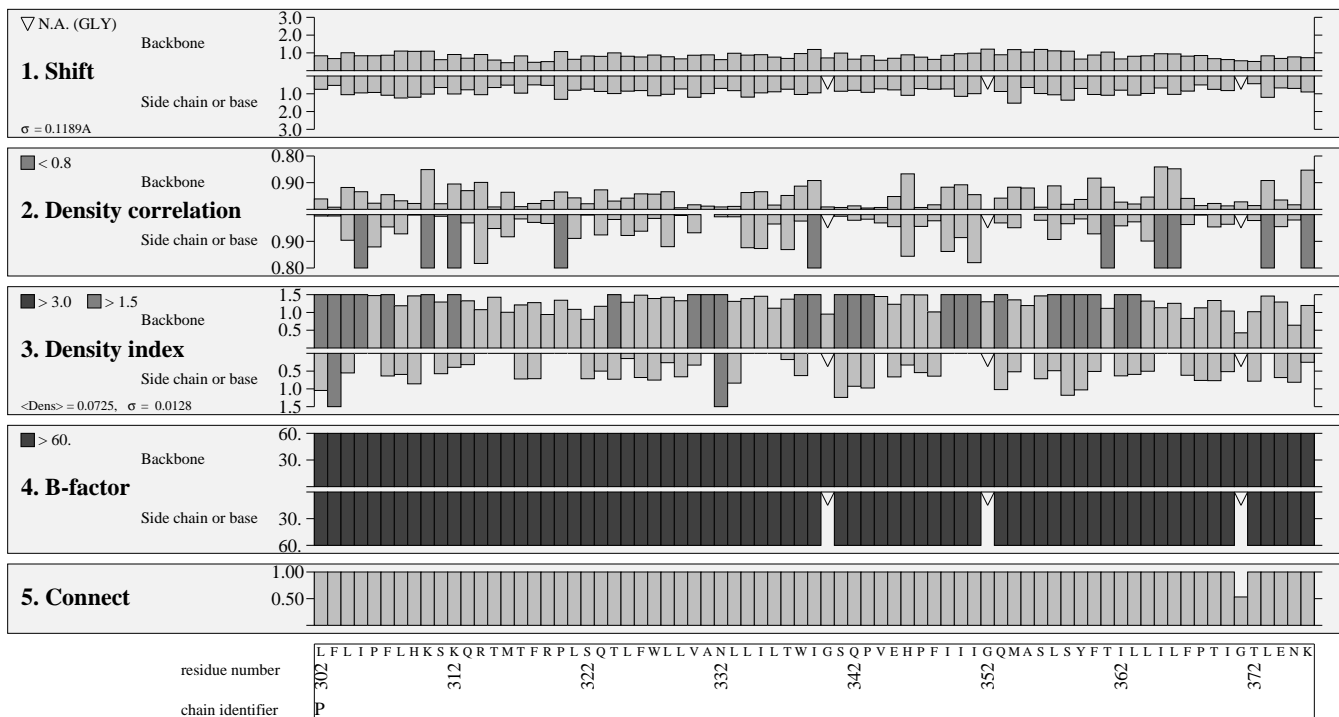
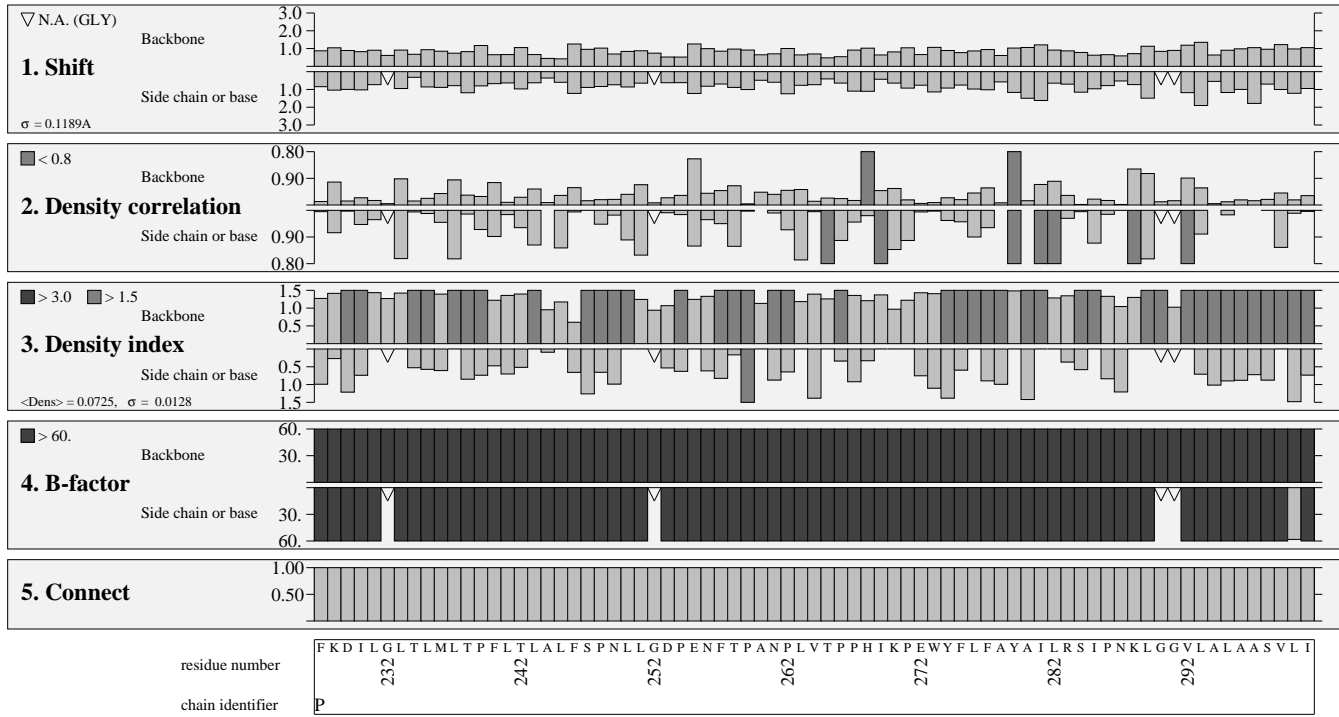
Local estimation (21)



Structure Factor Check

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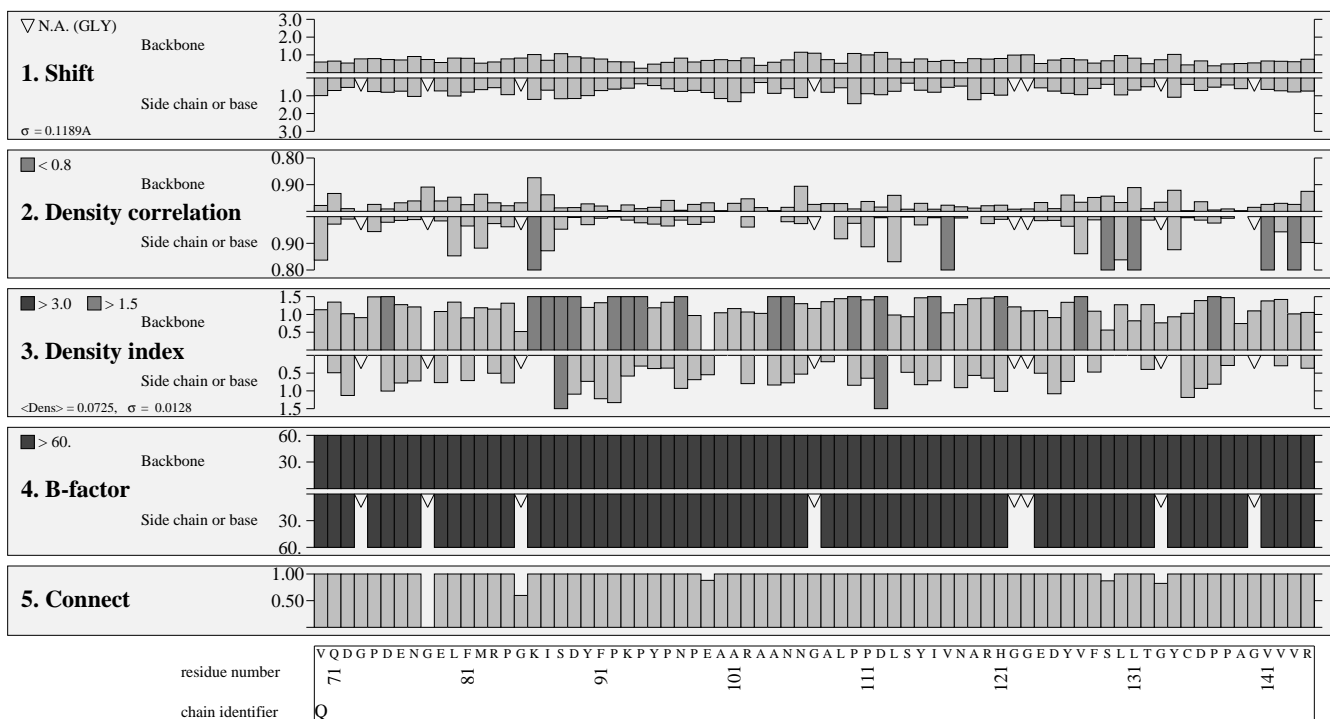
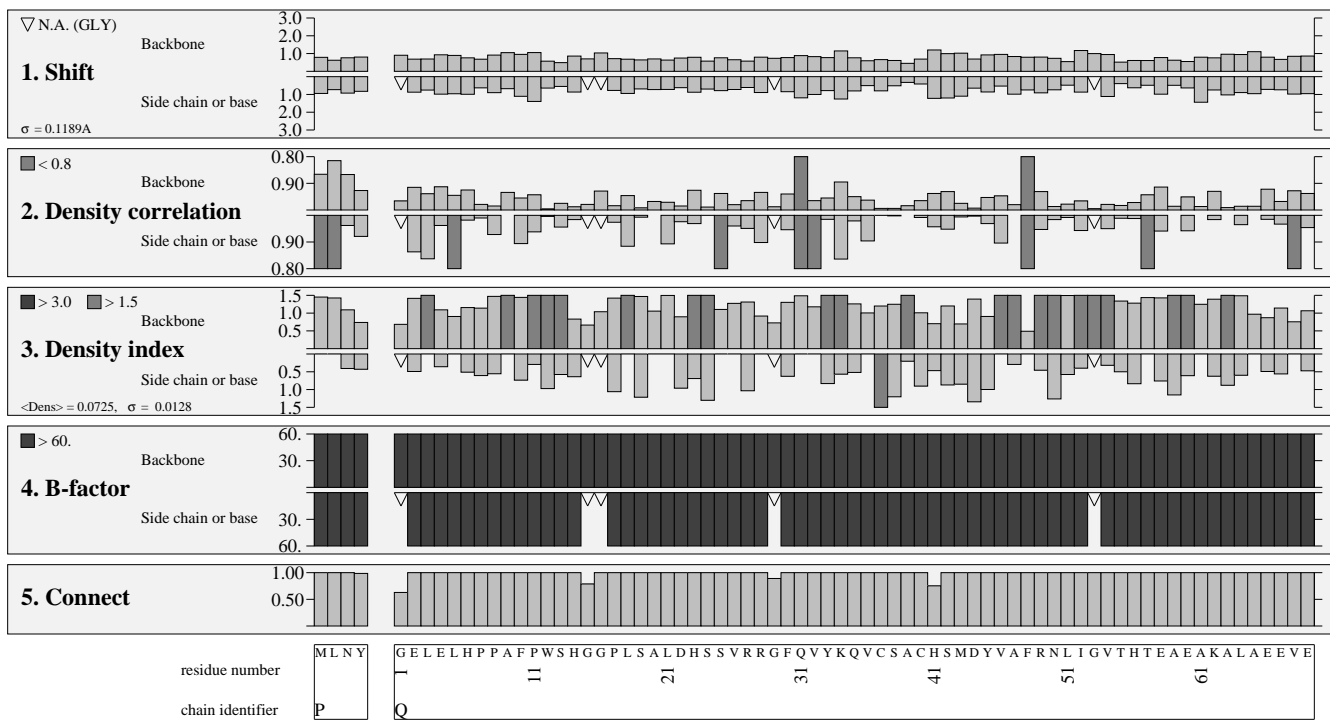
Local estimation (22)



Structure Factor Check

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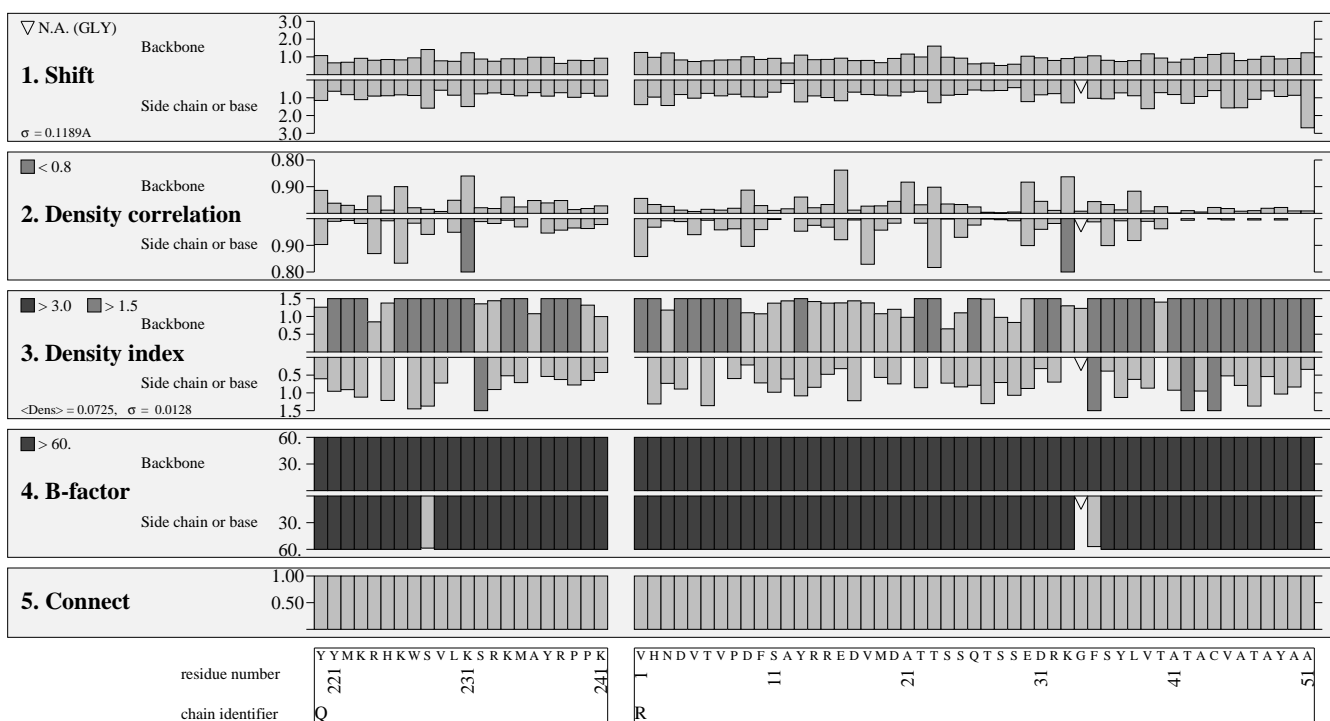
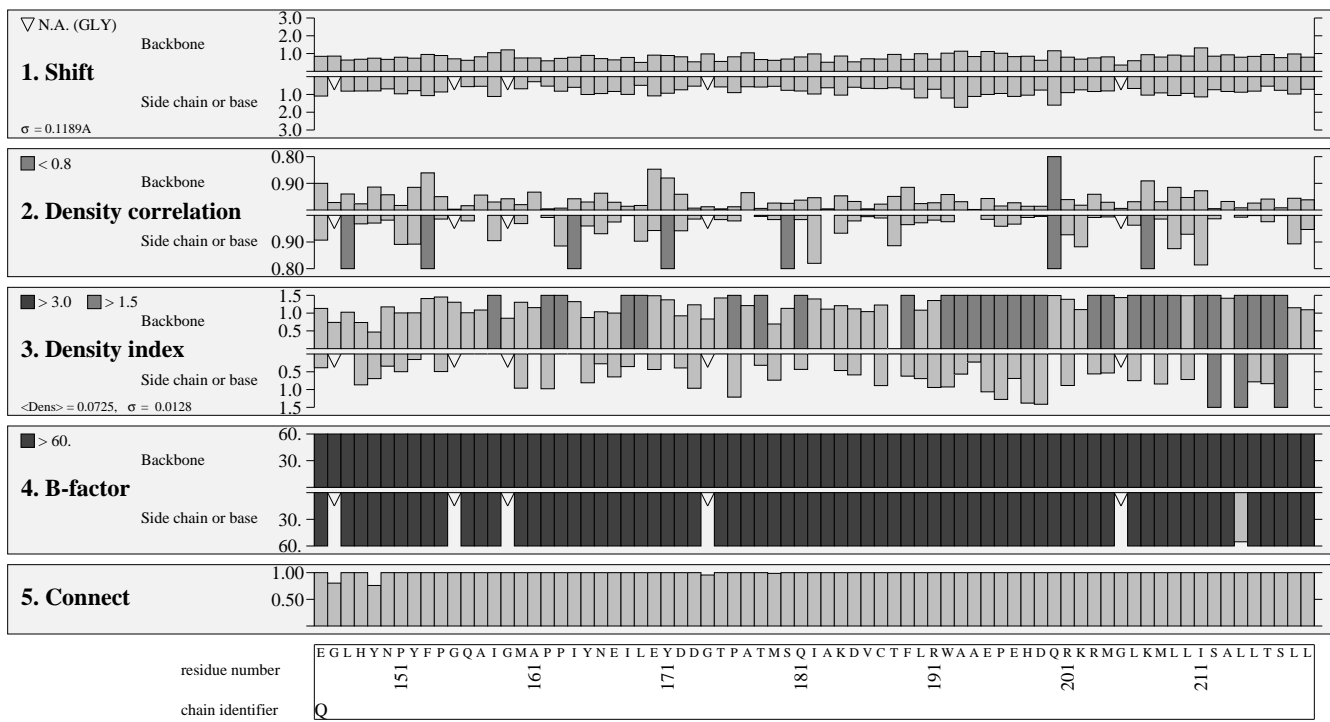
Local estimation (23)



Structure Factor Check

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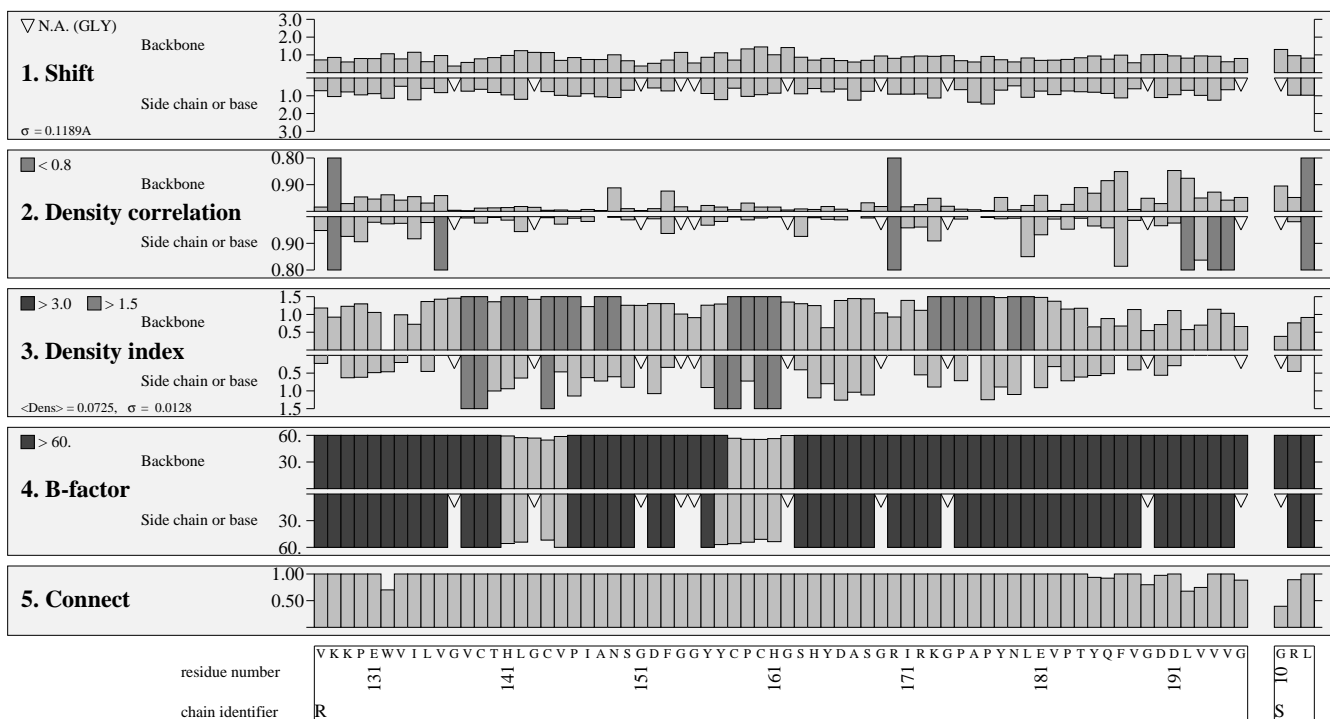
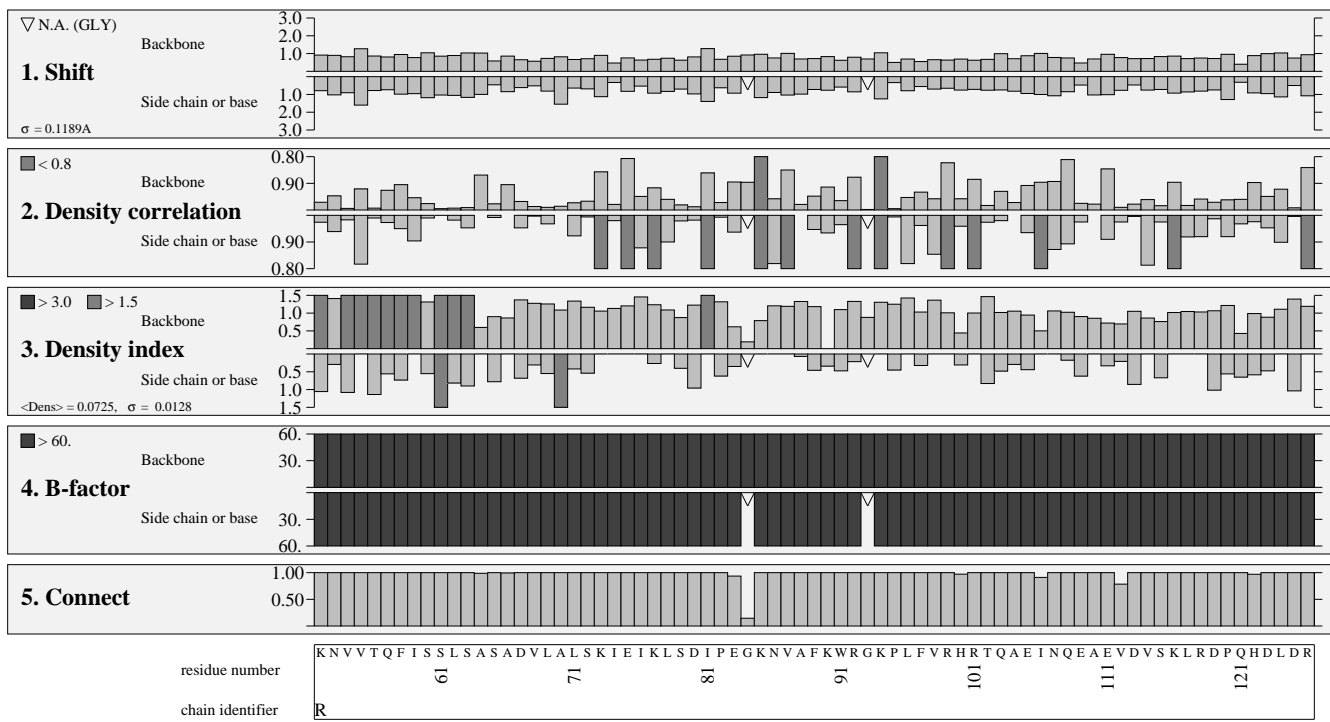
Local estimation (24)



Structure Factor Check

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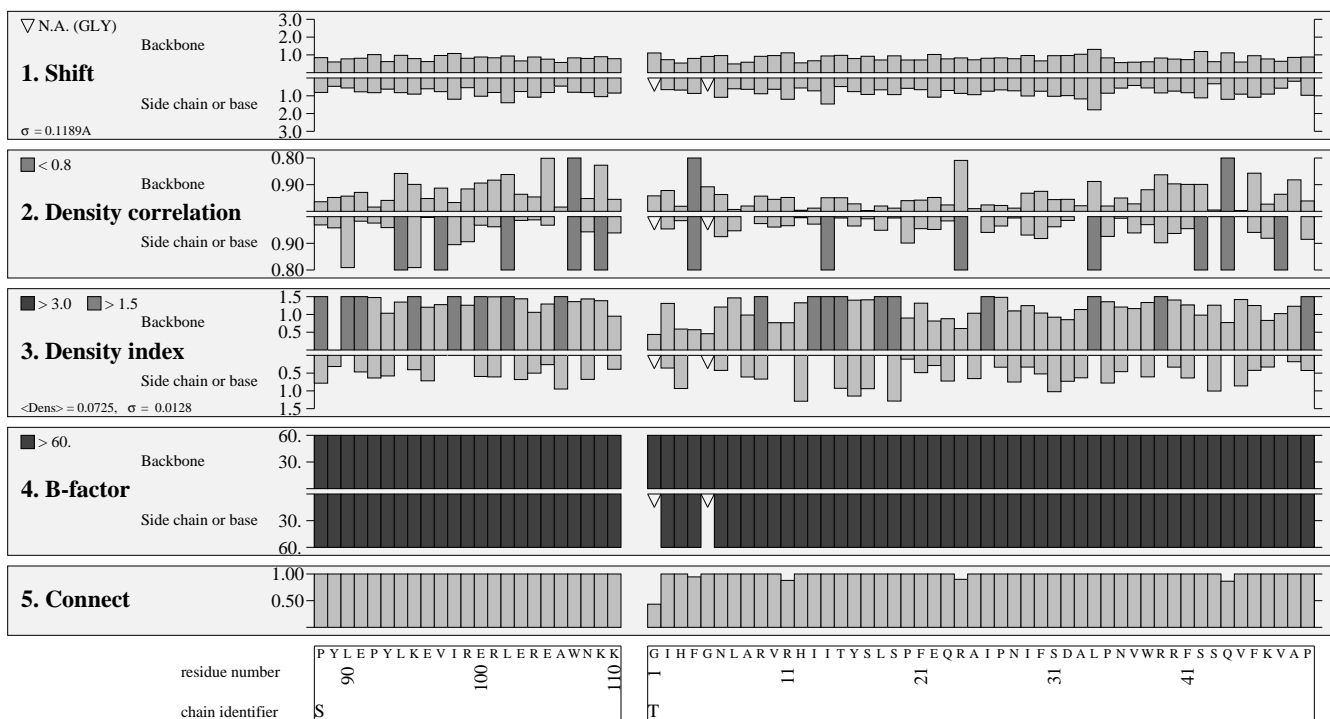
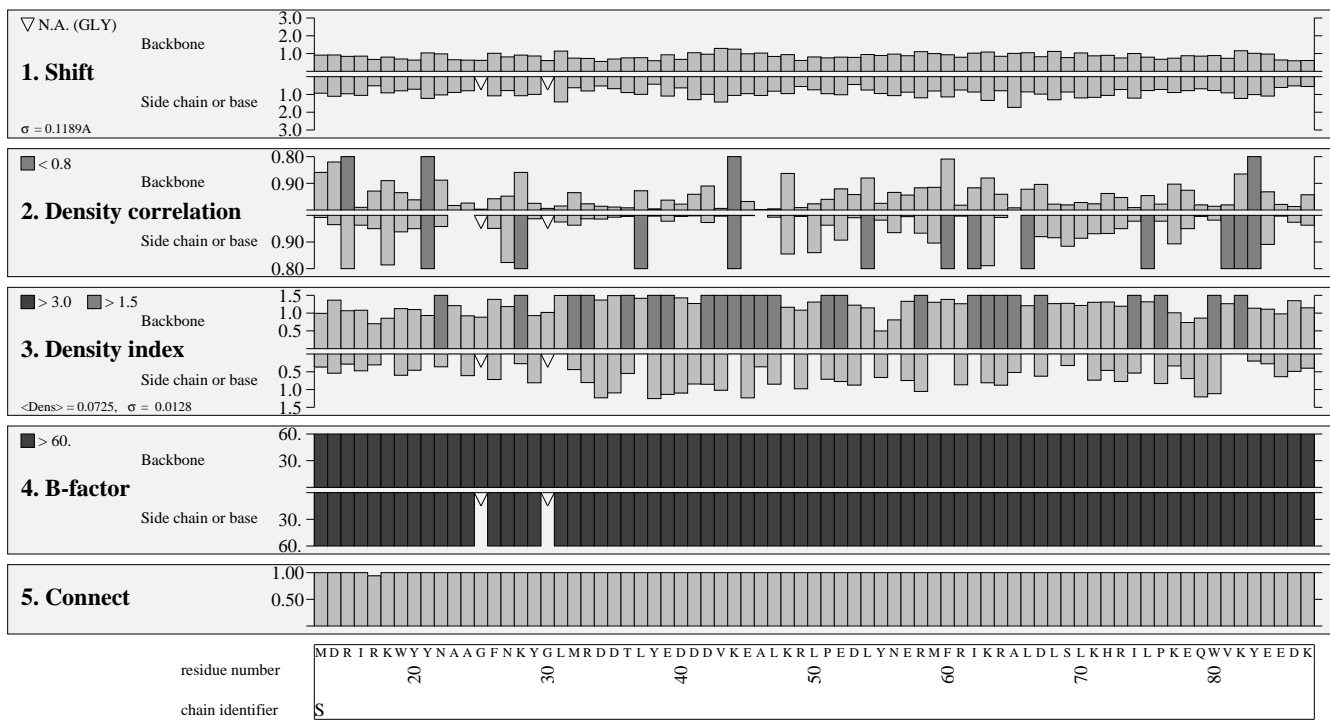
Local estimation (25)



Structure Factor Check

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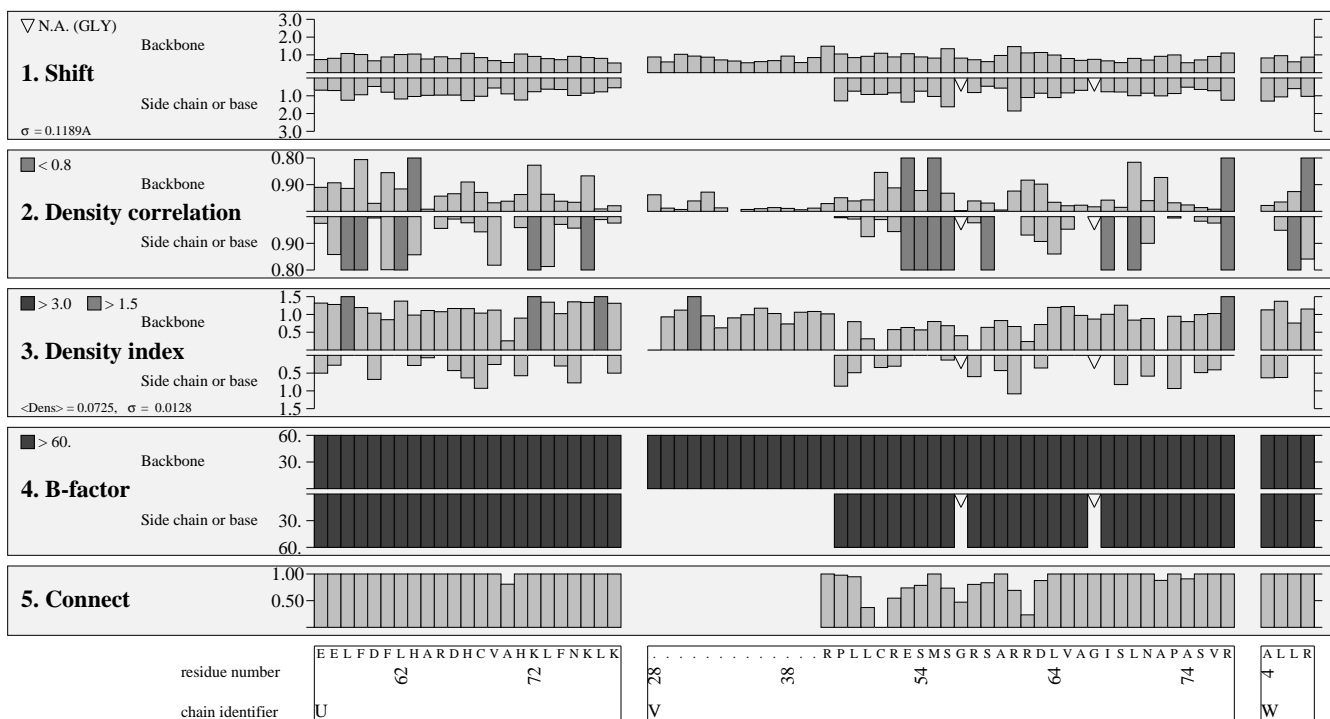
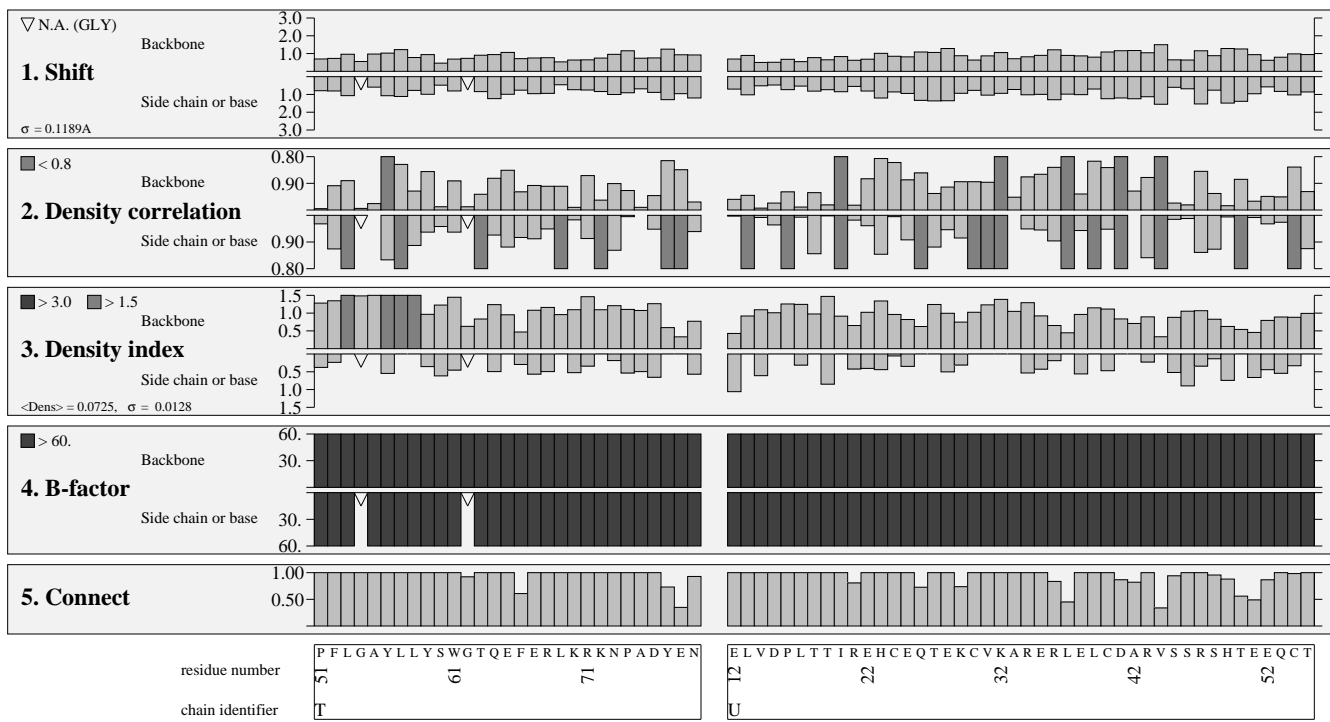
Local estimation (26)



Structure Factor Check

3H1J

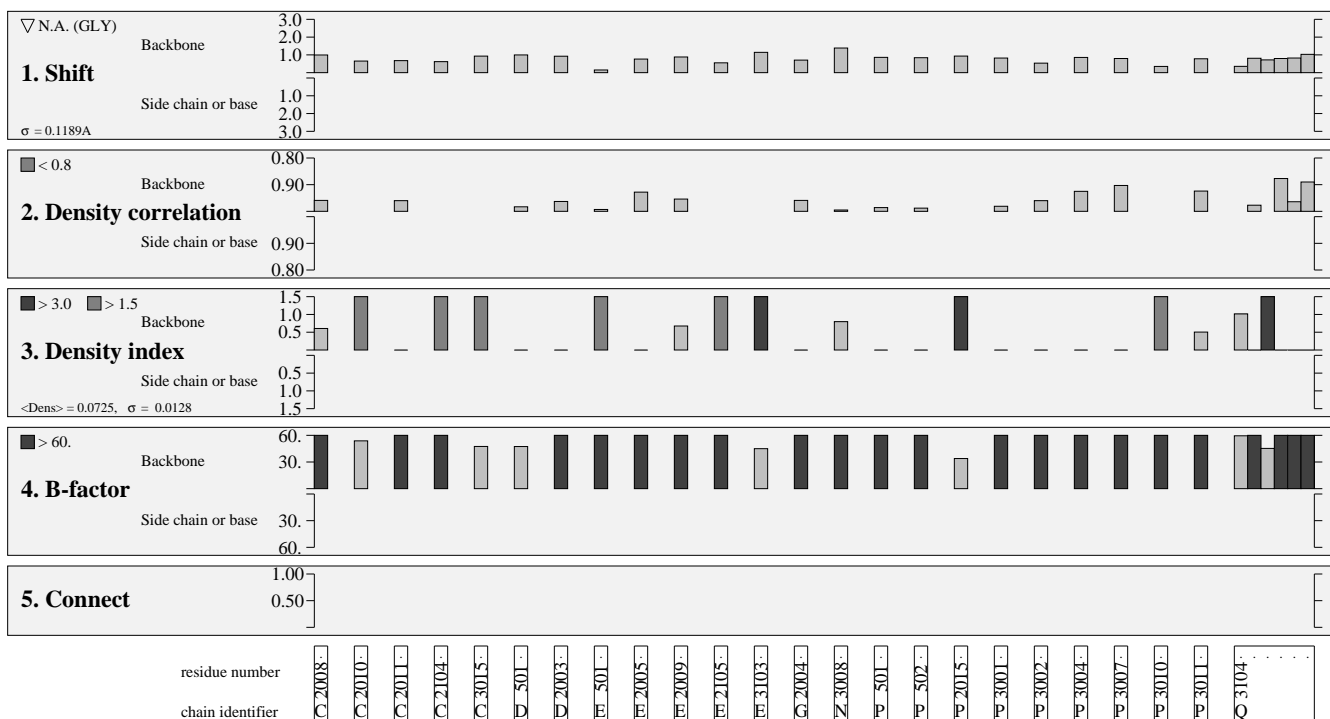
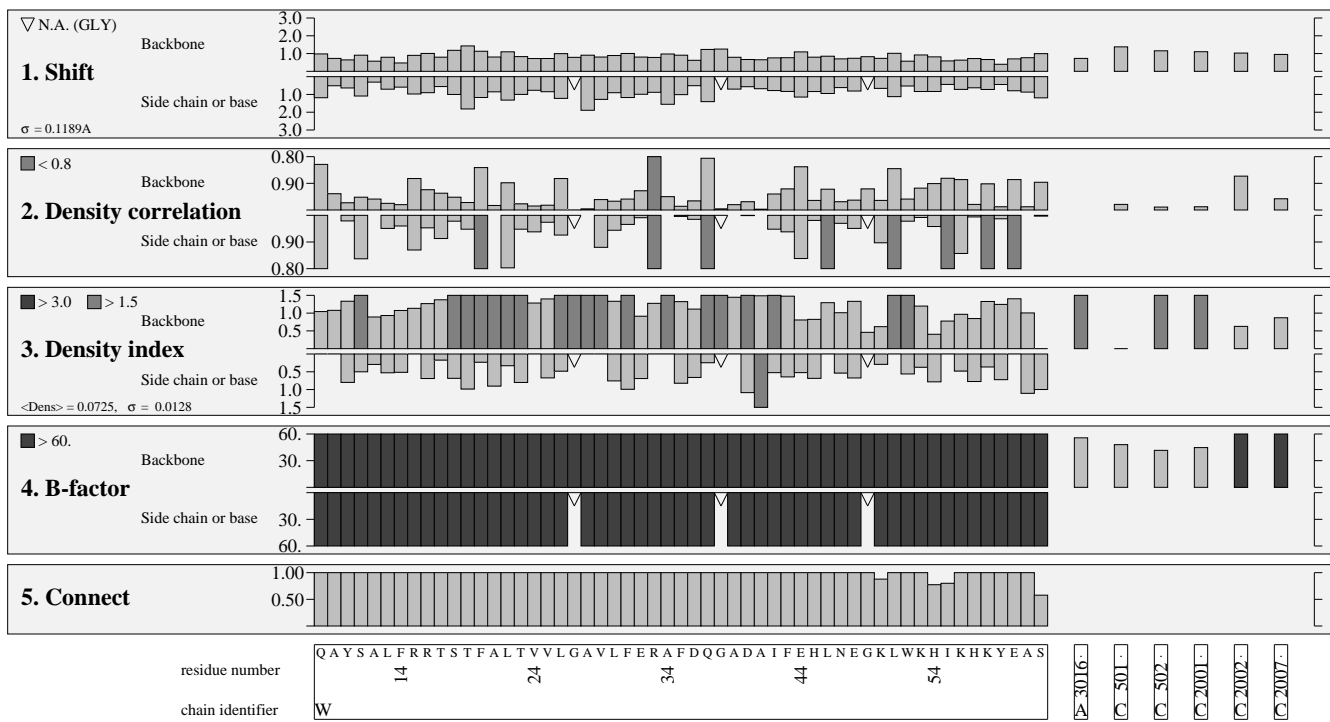
Local estimation (27)



Structure Factor Check

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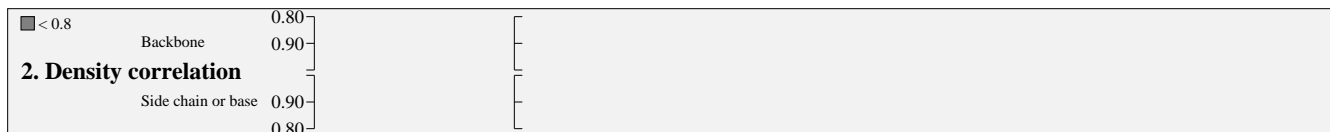
Local estimation (28)



Structure Factor Check

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Local estimation (29)



residue number	wwwwwwwwwwwwwwww
	384
chain identifier	Q
	1233