

Structure Factor Check

3CX5

Title: STRUCTURE OF COMPLEX III WITH BOUND CYTOCHROME C IN REDUCED STATE AND DEFINITION OF A MINIMAL CORE INTERFACE FOR ELECTRON TRANSFER.
 Date: 23-APR-08
 PDB code: 3CX5

Crystal

Cell parameters:
 a: 145.12 A b: 165.09 A c: 194.37 A
 α : 90.00 β : 104.09 γ : 90.00
 Space group: P 1 21 1

Model

38020 atoms (1648 water molecules)
 Number of chains: 51
 Volume not occupied by model: 63.6 %
 $\langle B \rangle$ (for atomic model): 45.6 A²
 $\sigma(B)$: 18.83 A²
 Matthews coefficient: 4.24
 Corresponding solvent % : 70.78

Refinement

Program: CNS 1.1
 Nominal resolution range: 19.0 – 1.90 A
 Reported R-factor: 0.245
 Number of reflections used: 660107
 Reported Rfree: 0.26
 Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 19.0 – 1.90 A
 Reflections in file: 660107
 Unique reflections above 0: 660107
 above 1 σ : 655005
 above 3 σ : 351728

SFCHECK

Nominal resolution range: 19.0 – 1.90 A
\05max. from input data, min. from author\05
 Used reflections: 660107
 Completeness: 95.0 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.090
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.6921 0.7006
 B_{overall} (by Patterson): 33.A²
 Optical resolution: 1.60 A
 Expected opt. resol. for complete data set: 1.60 A
 Estimated minimal error: 0.040 A

Model vs. Structure Factors

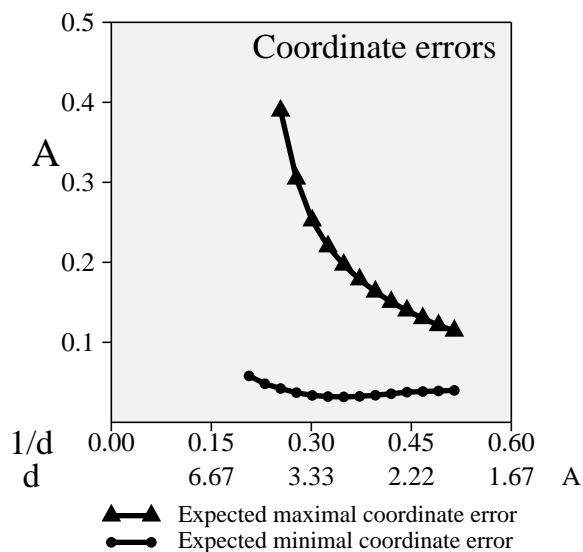
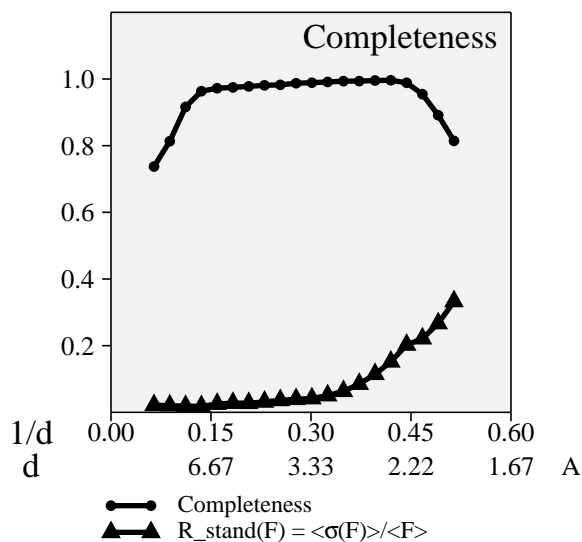
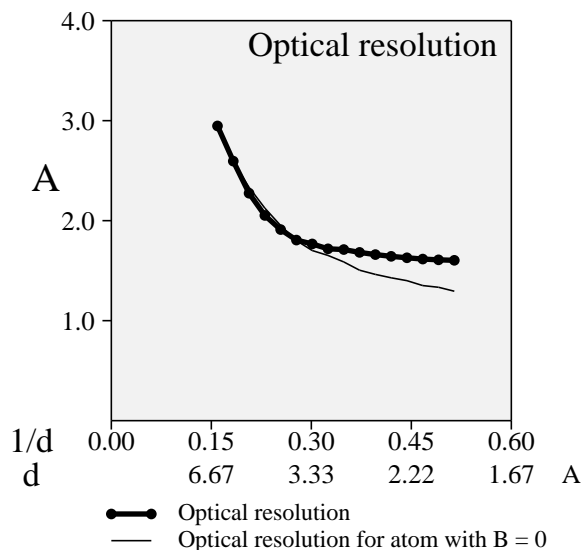
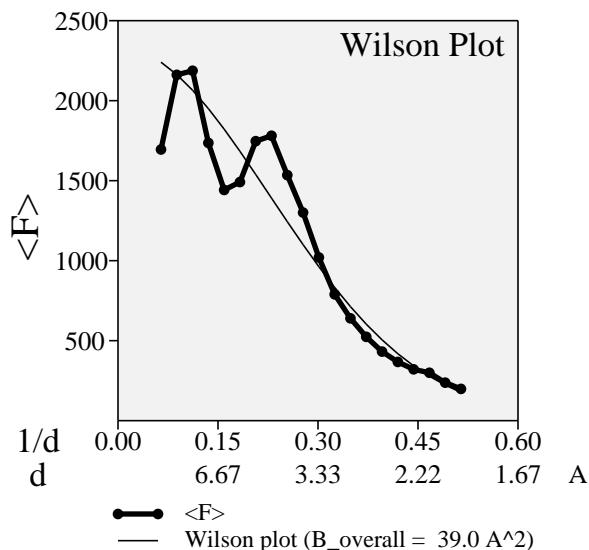
R-factor for all reflections: 0.263
 Correlation factor: 0.921
 R-factor: 0.265
 for $F > 2.0\sigma$
 nom. resolution range: 18.99 – 1.90A
 reflections used: 655013
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.309 A
 Estimated maximal error: 0.114 A
 DPI: 0.122 A

Scaling

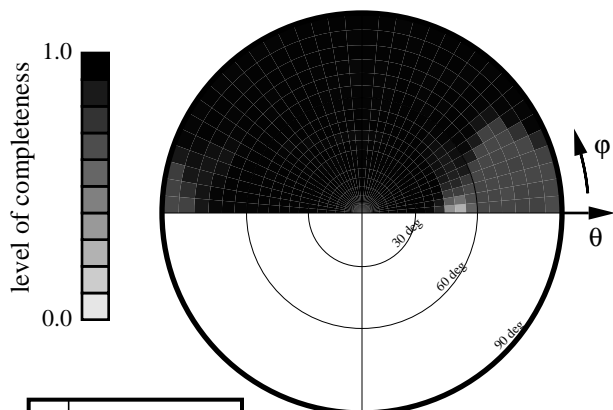
Scale: 1.472
 Bdiff: -5.31
 Anisothermal Scaling (Beta):
 3.8736 -0.2216 0.1231 0.0000 0.2758 0.0000
 Solvent correction – Ks,Bs: 0.746 250.016

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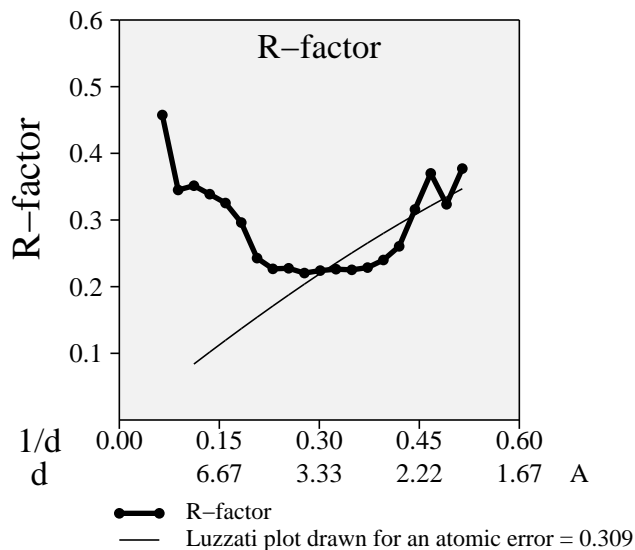


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	75.91	0.00
k	90.00	90.00
l	0.00	0.00

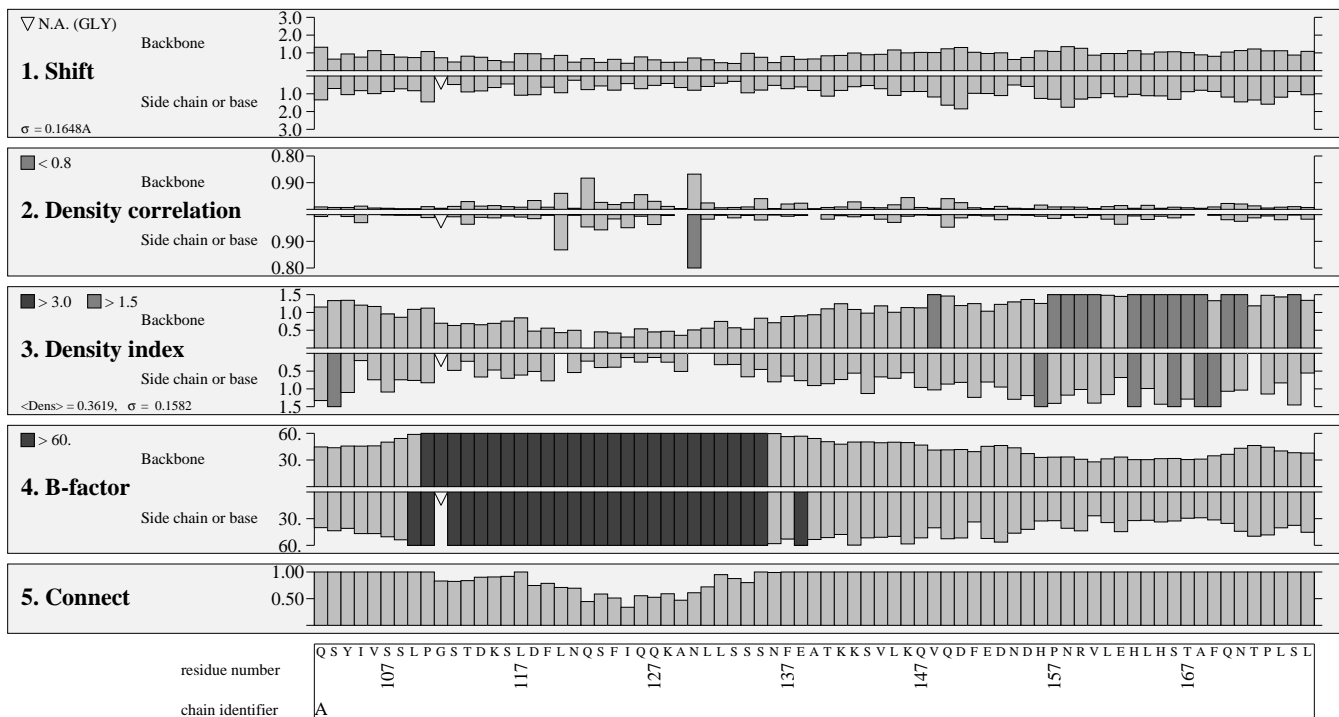
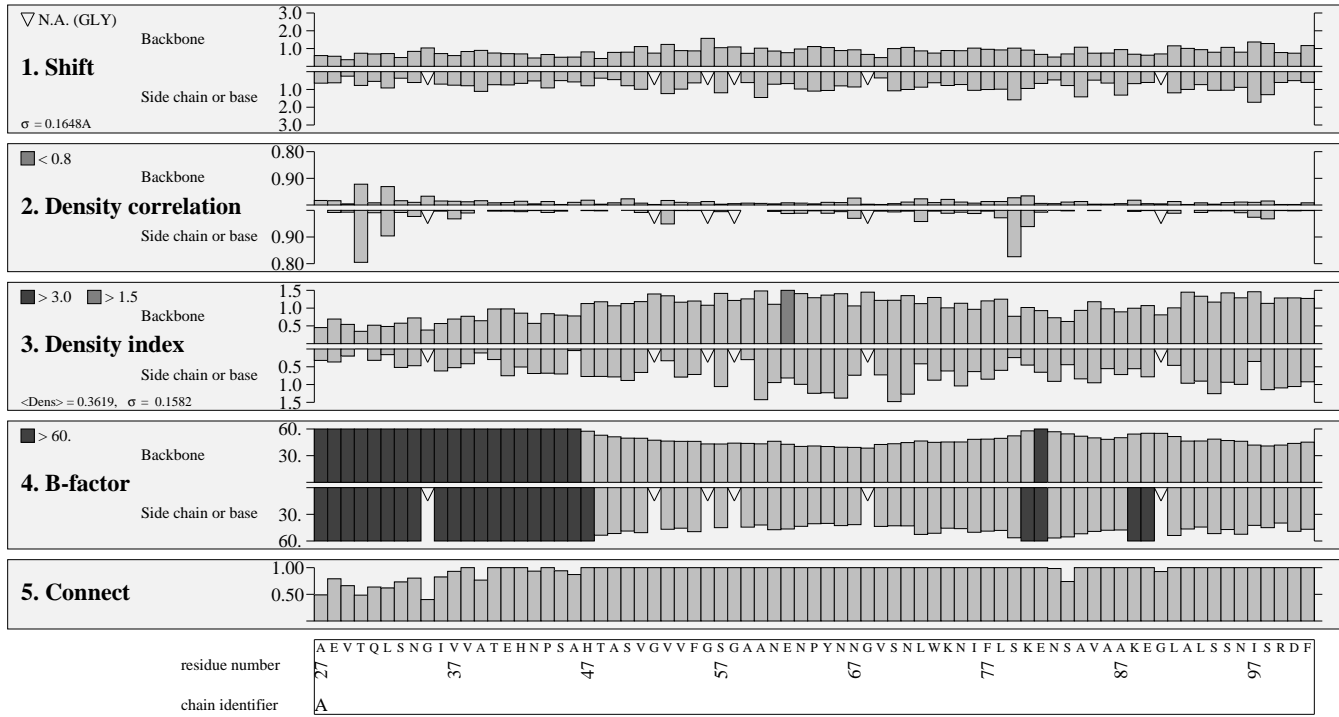
polar coordinates of the crystallographical axes



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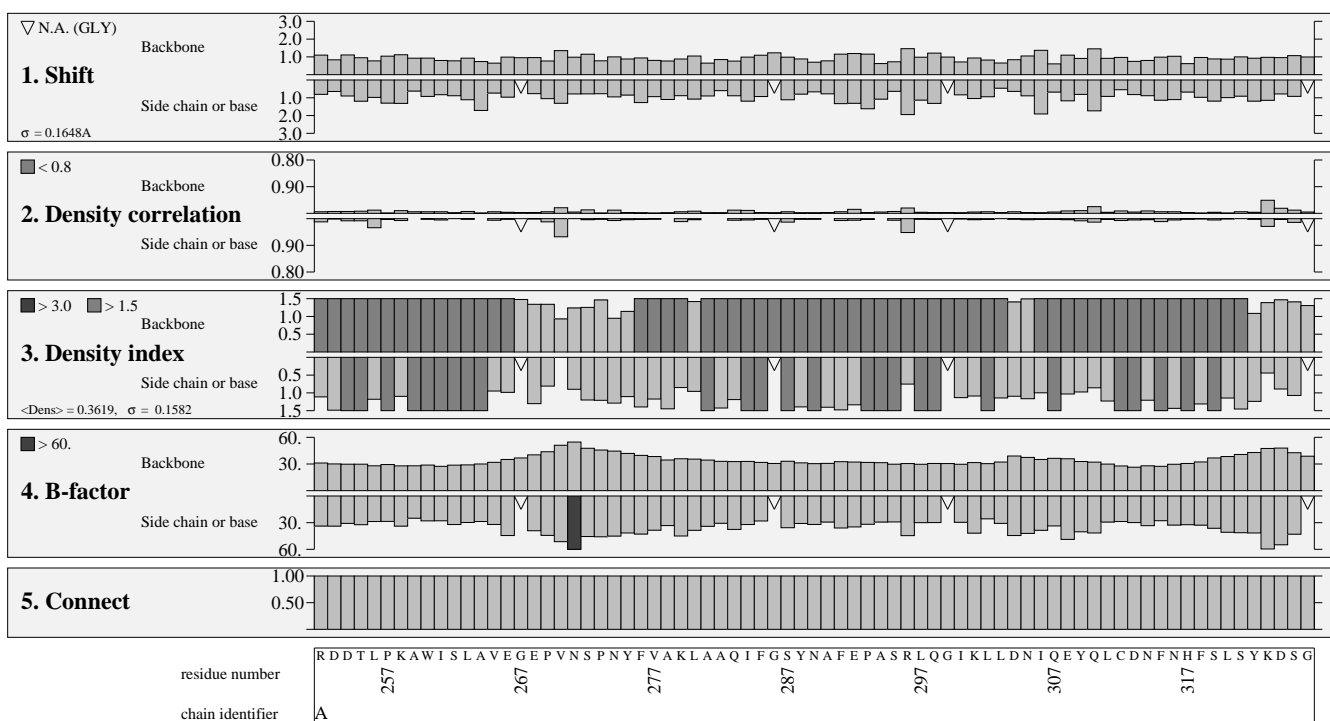
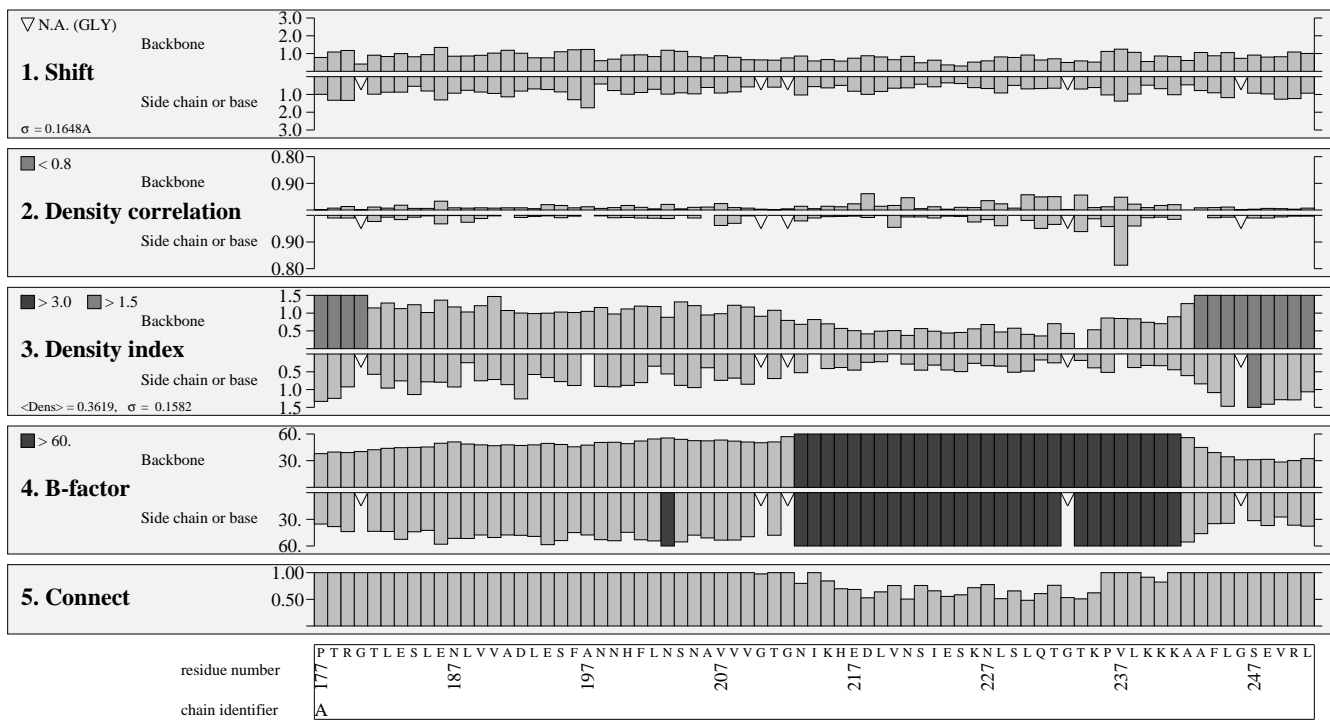
Local estimation [N_omit = 2]



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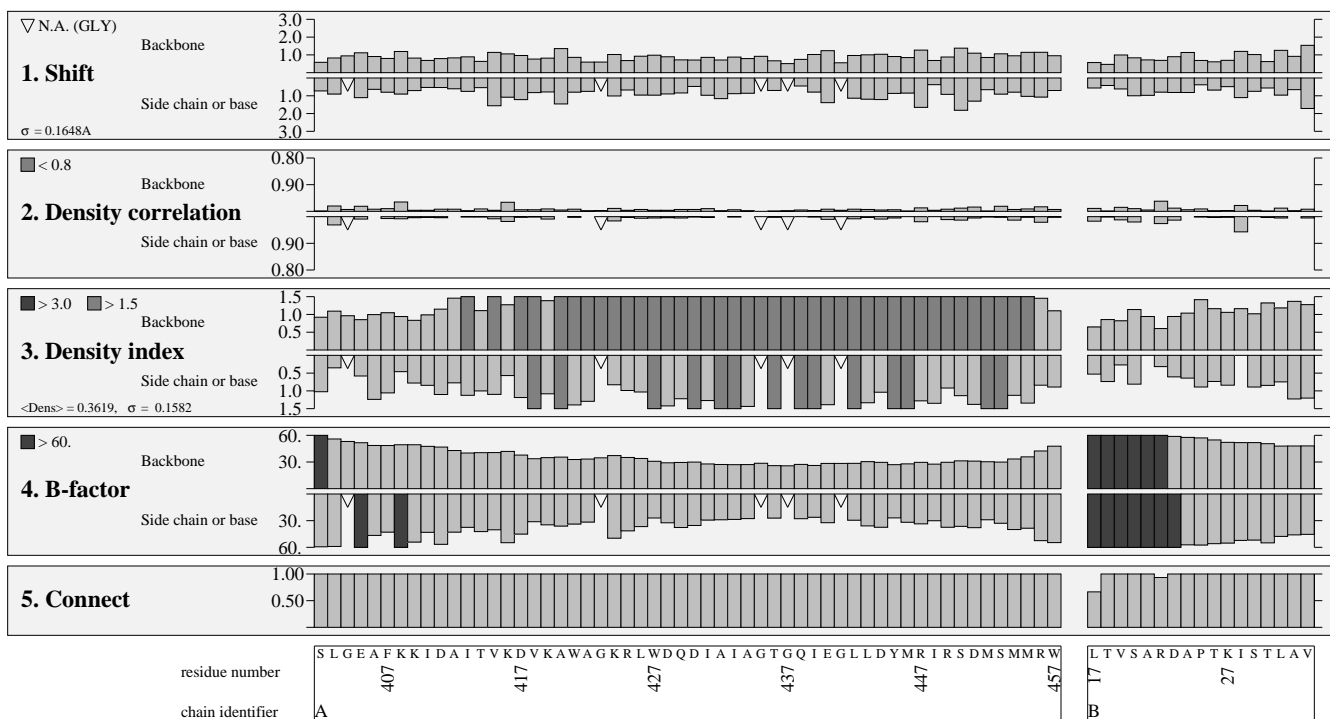
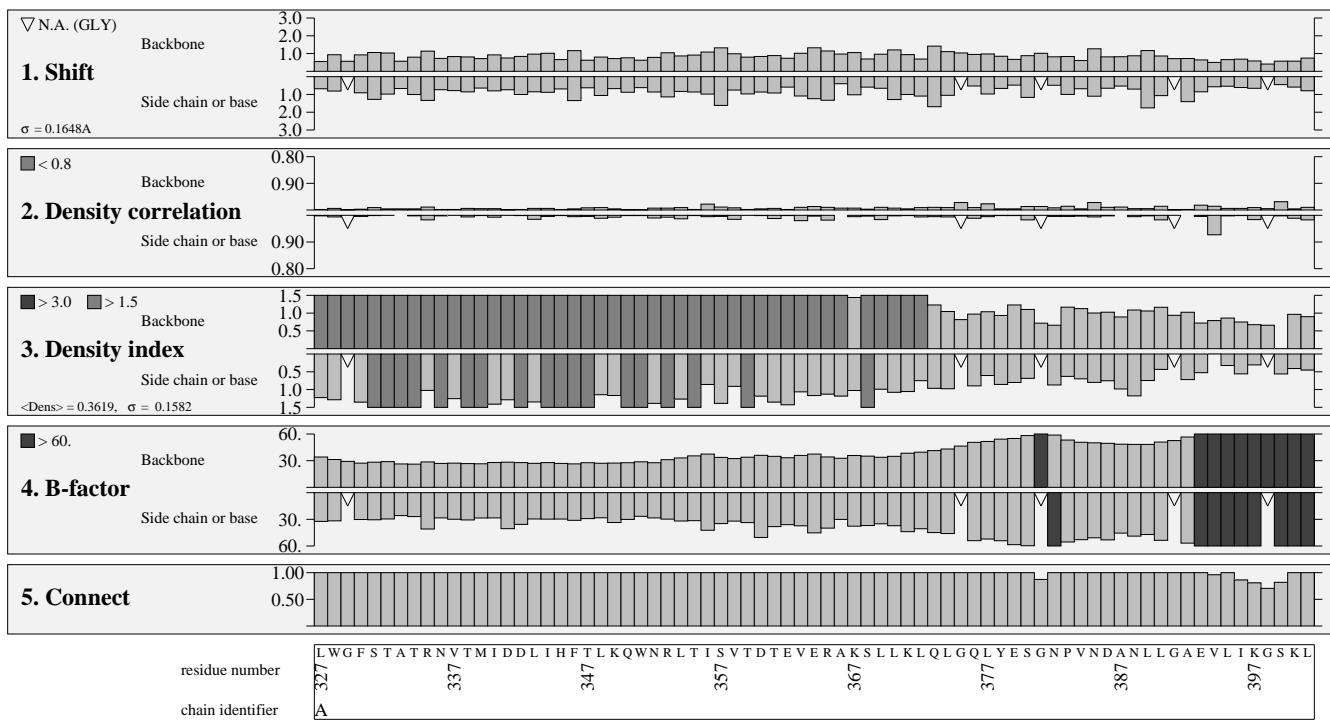
Local estimation (2) [N_omit = 2]



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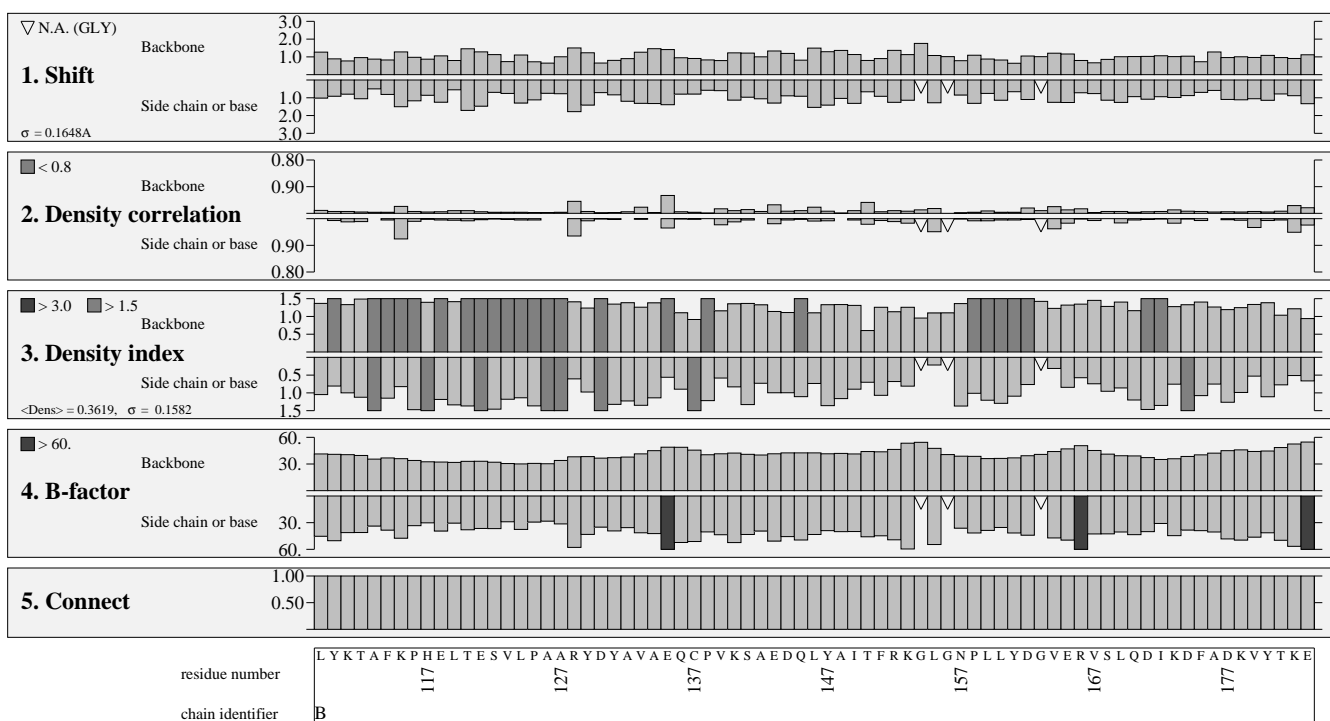
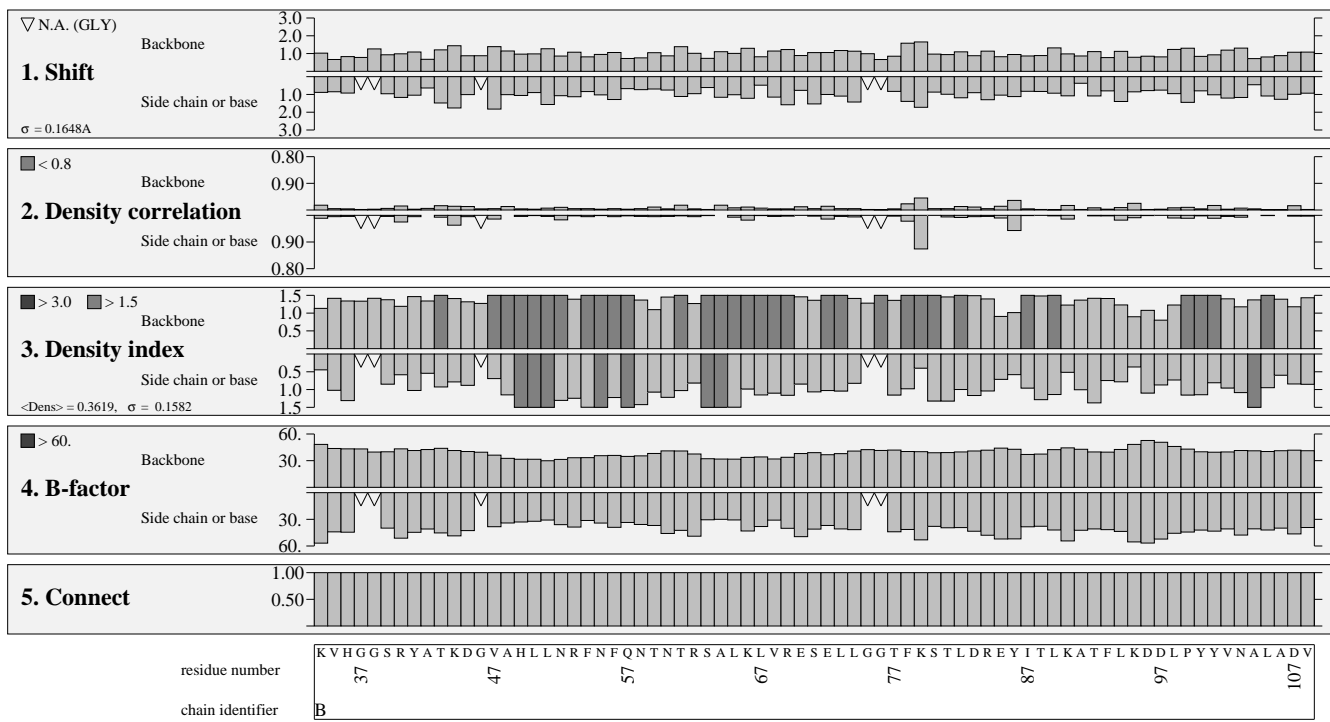
Local estimation (3) [N_omit = 2]



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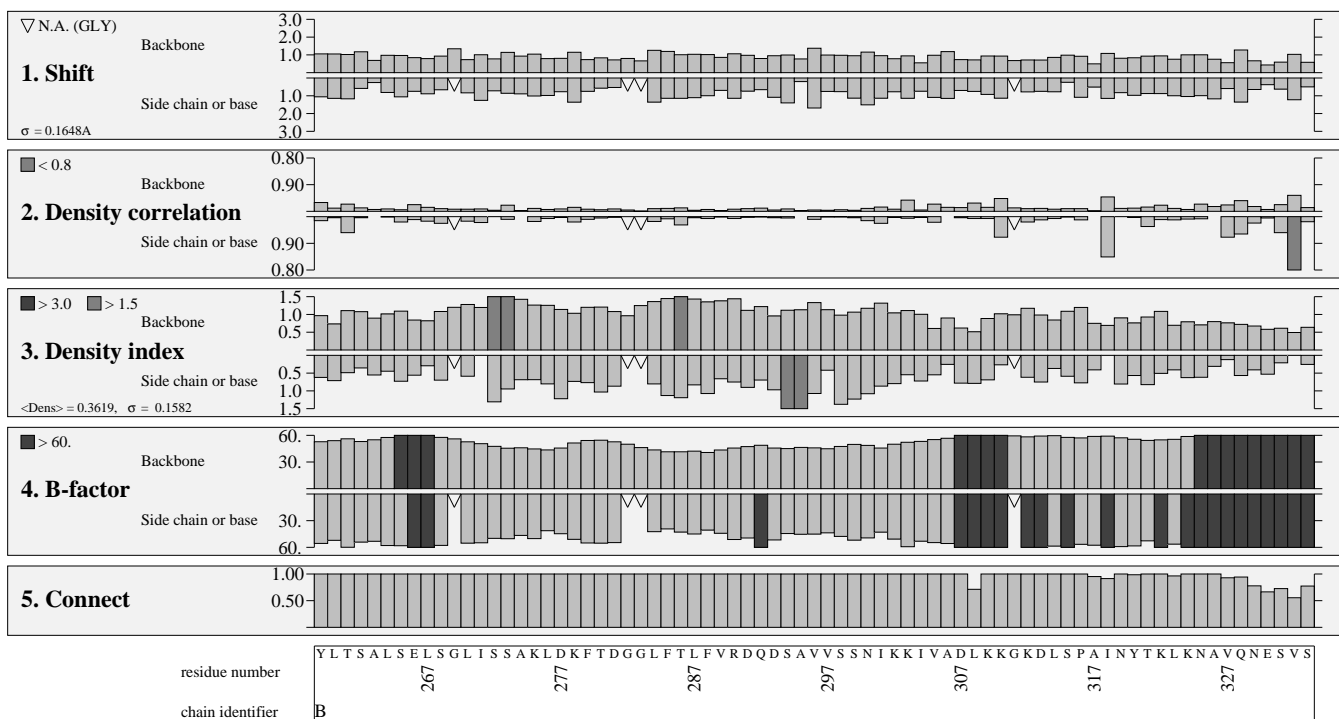
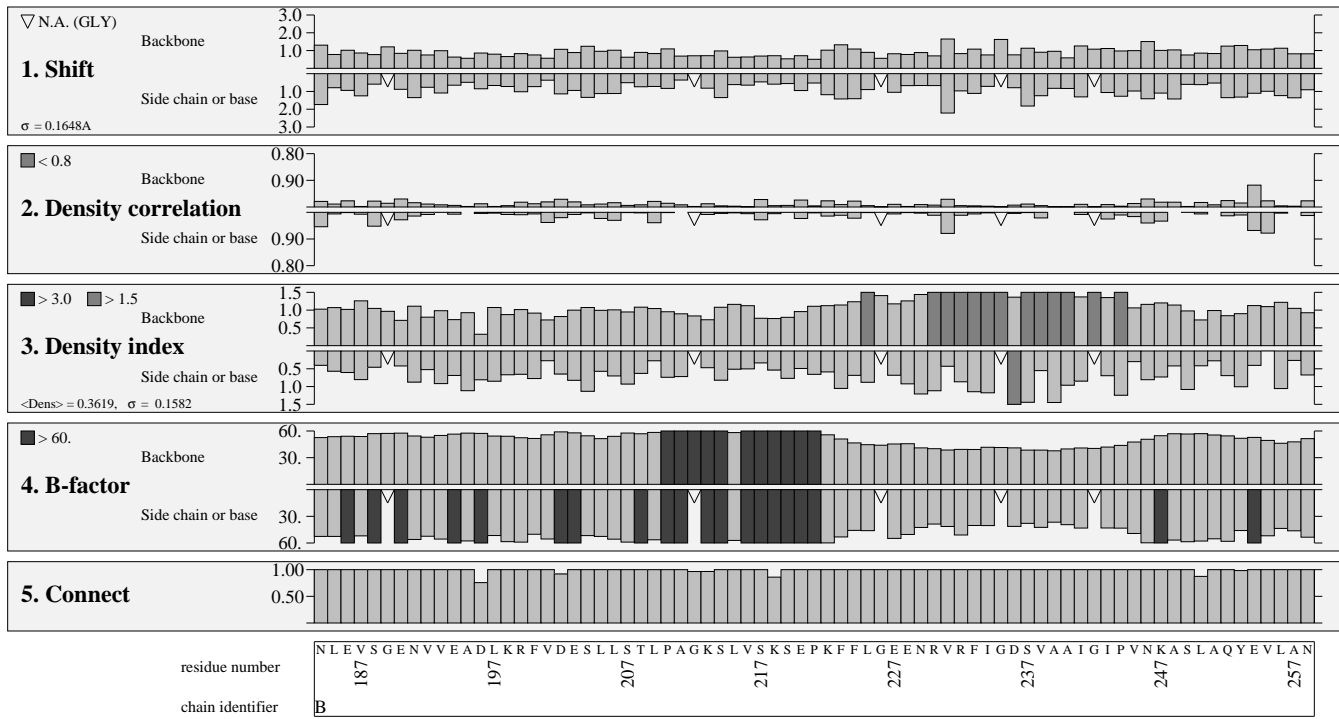
Local estimation (4) [N_omit = 2]



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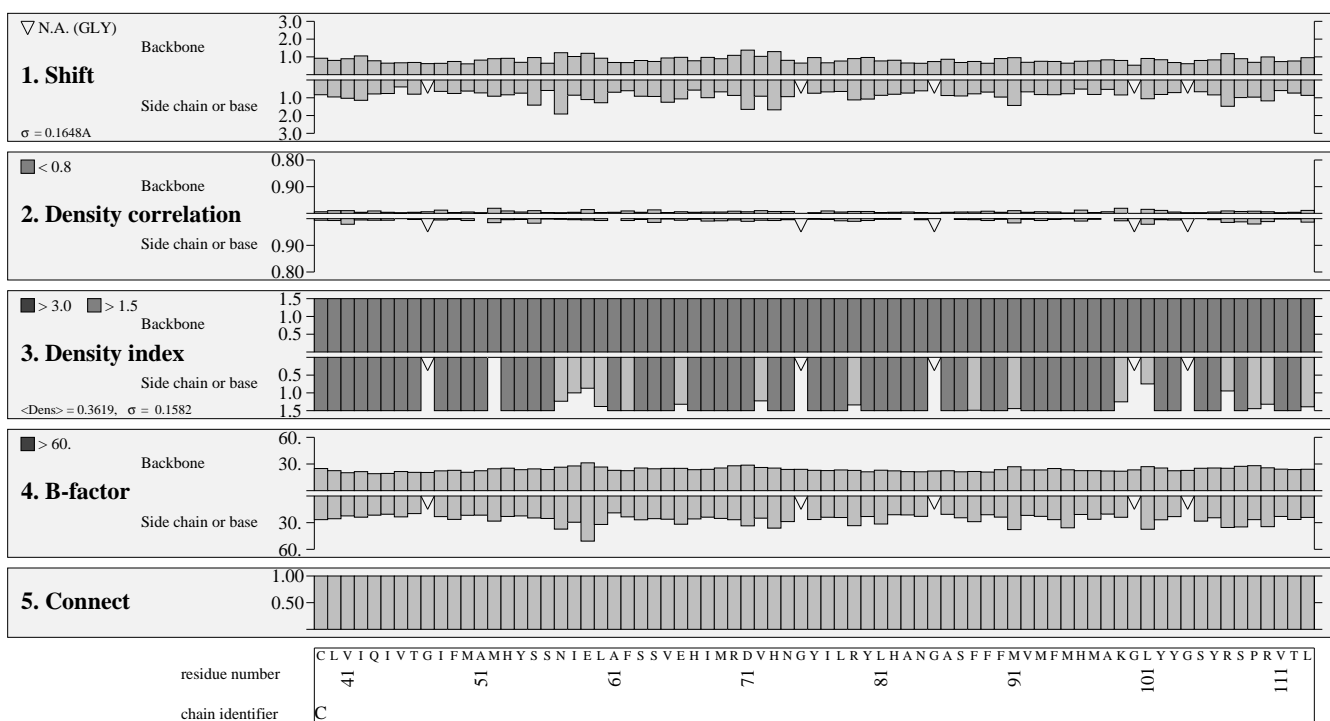
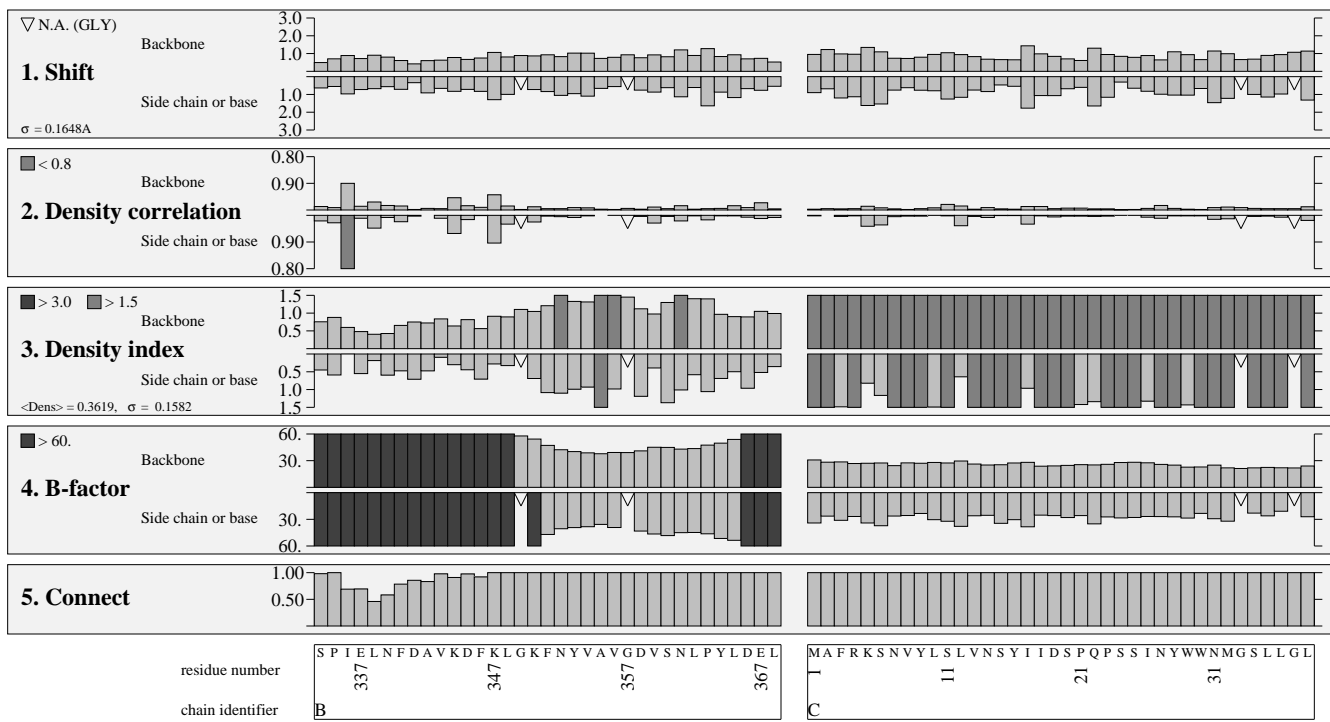
Local estimation (5) [N_omit = 2]



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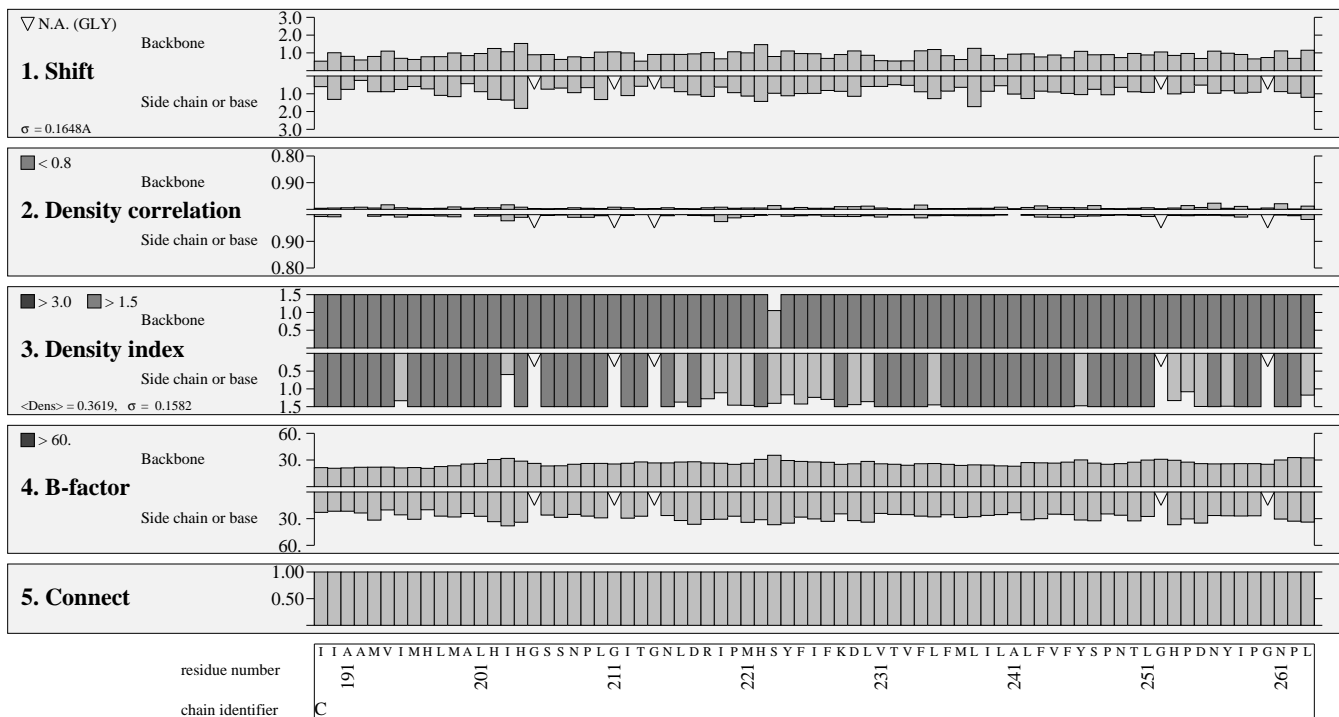
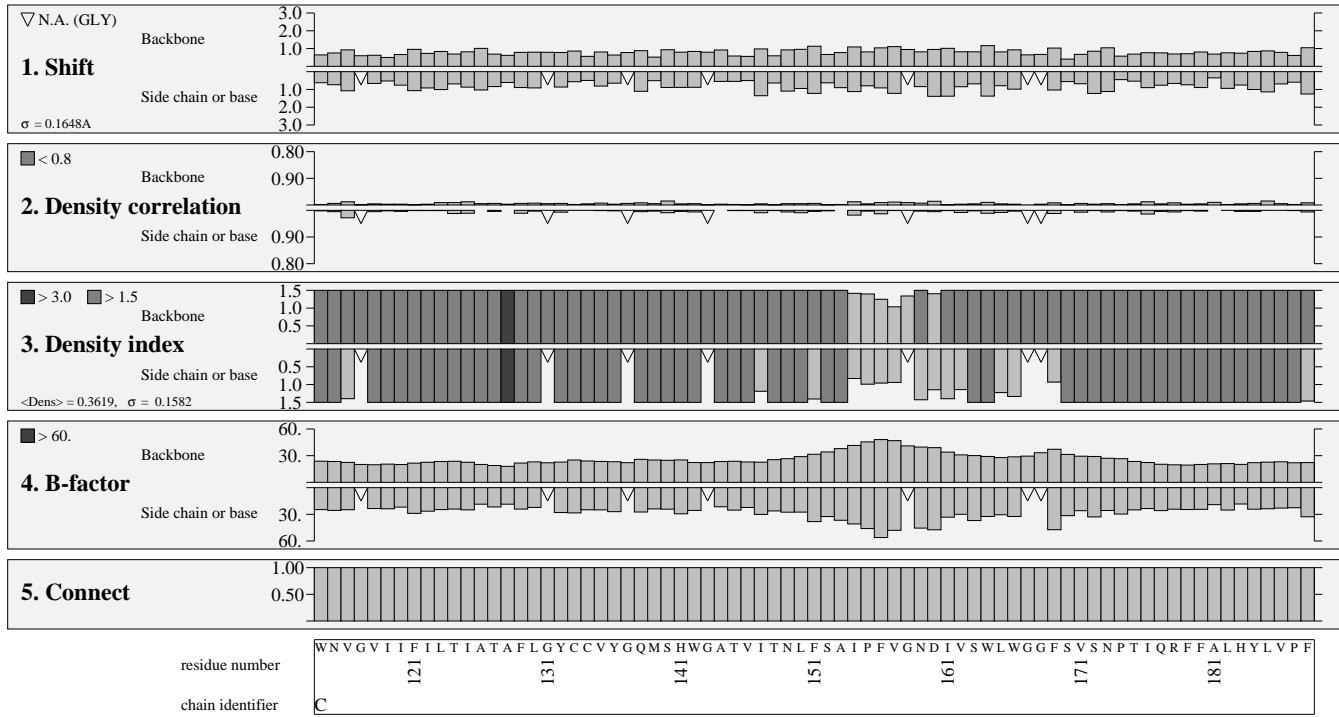
Local estimation (6) [N_omit = 2]



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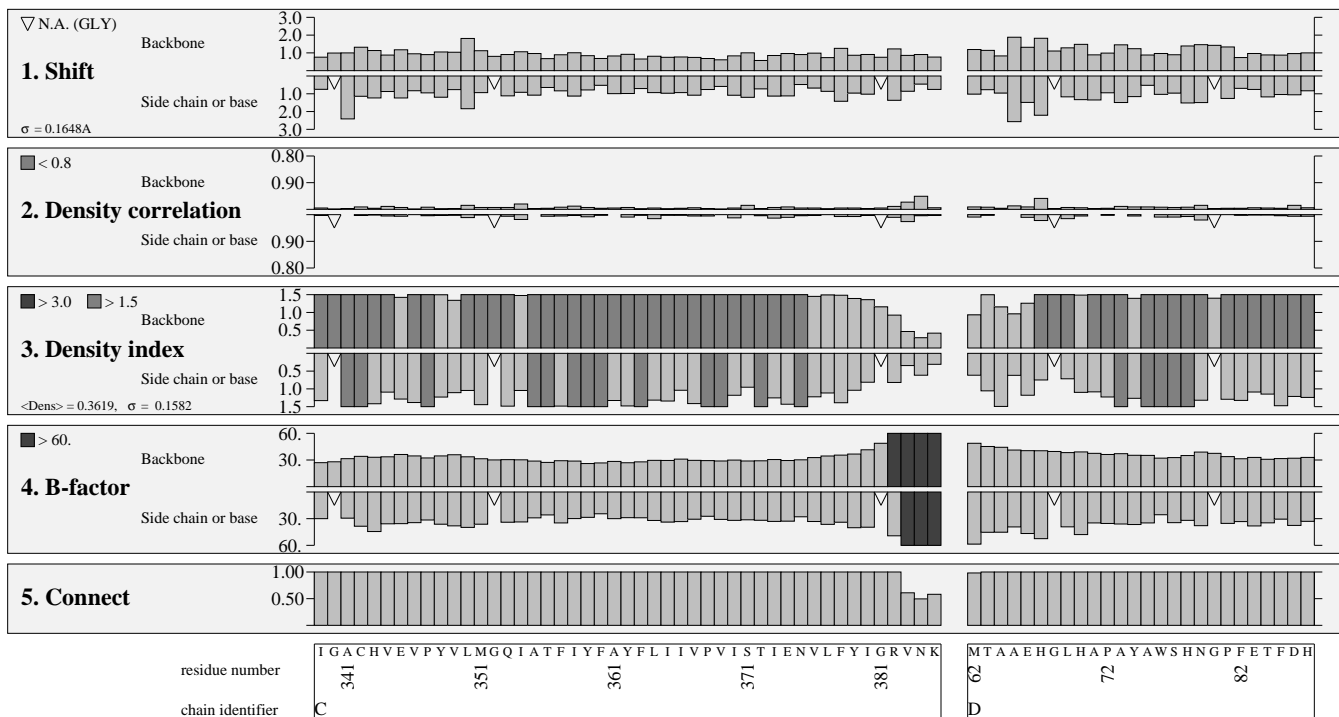
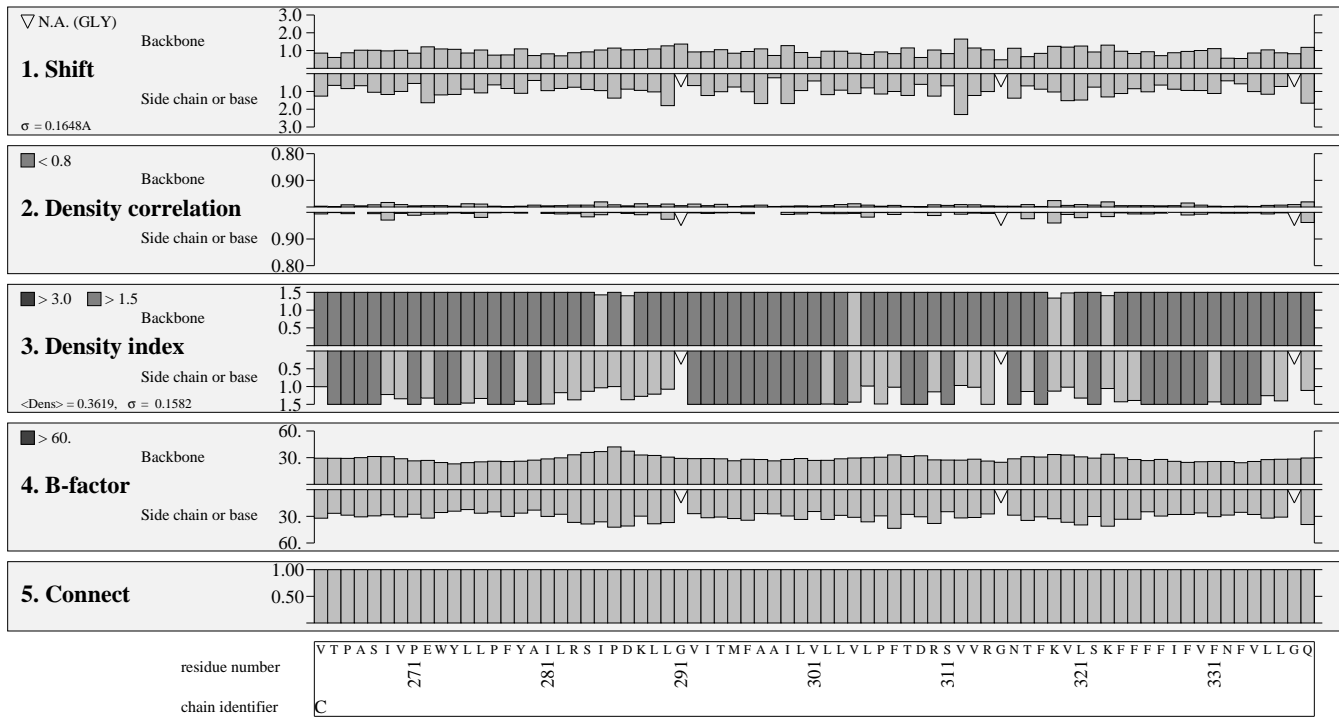
Local estimation (7) [N_omit = 2]



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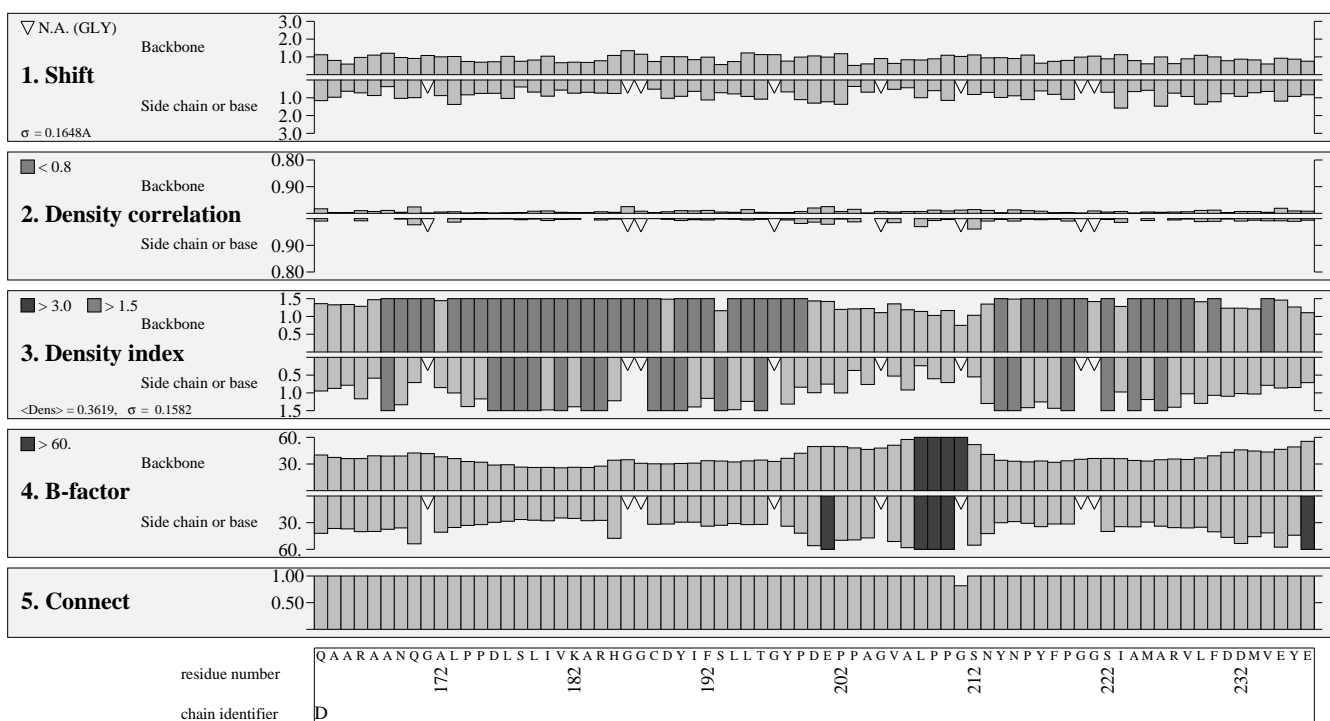
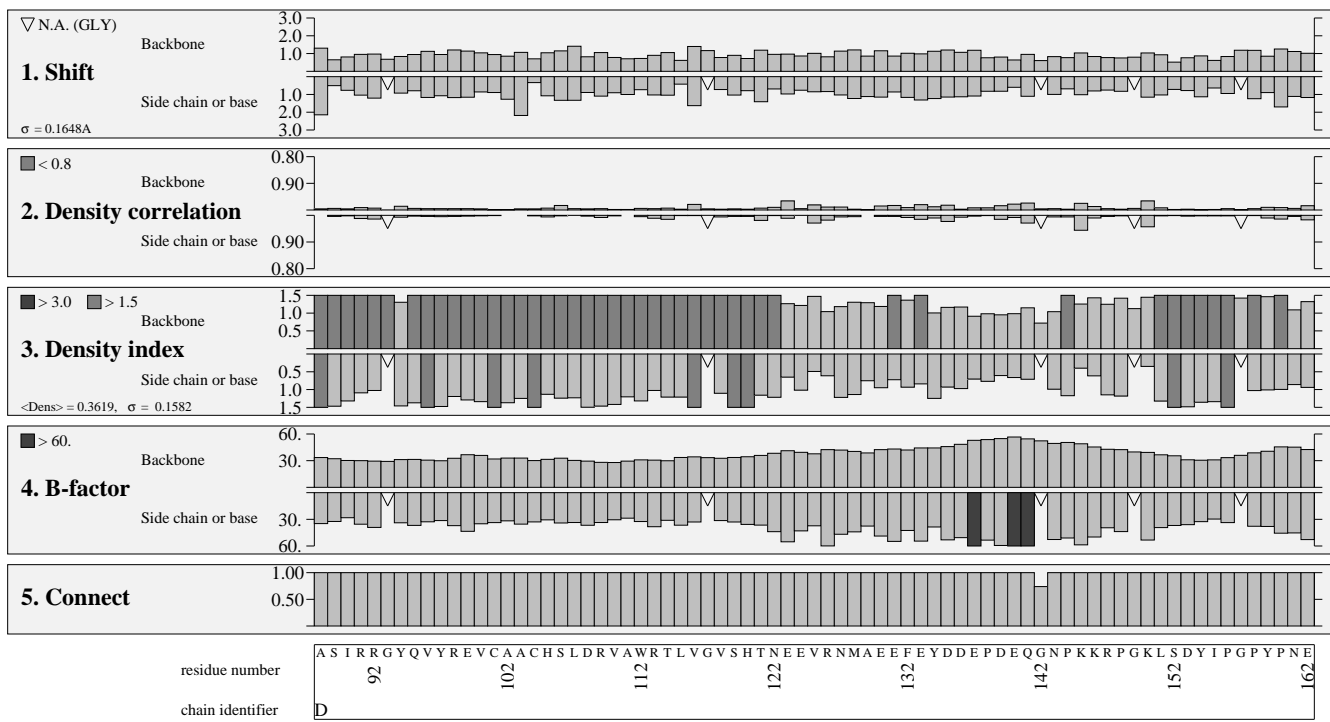
Local estimation (8) [N_omit = 2]



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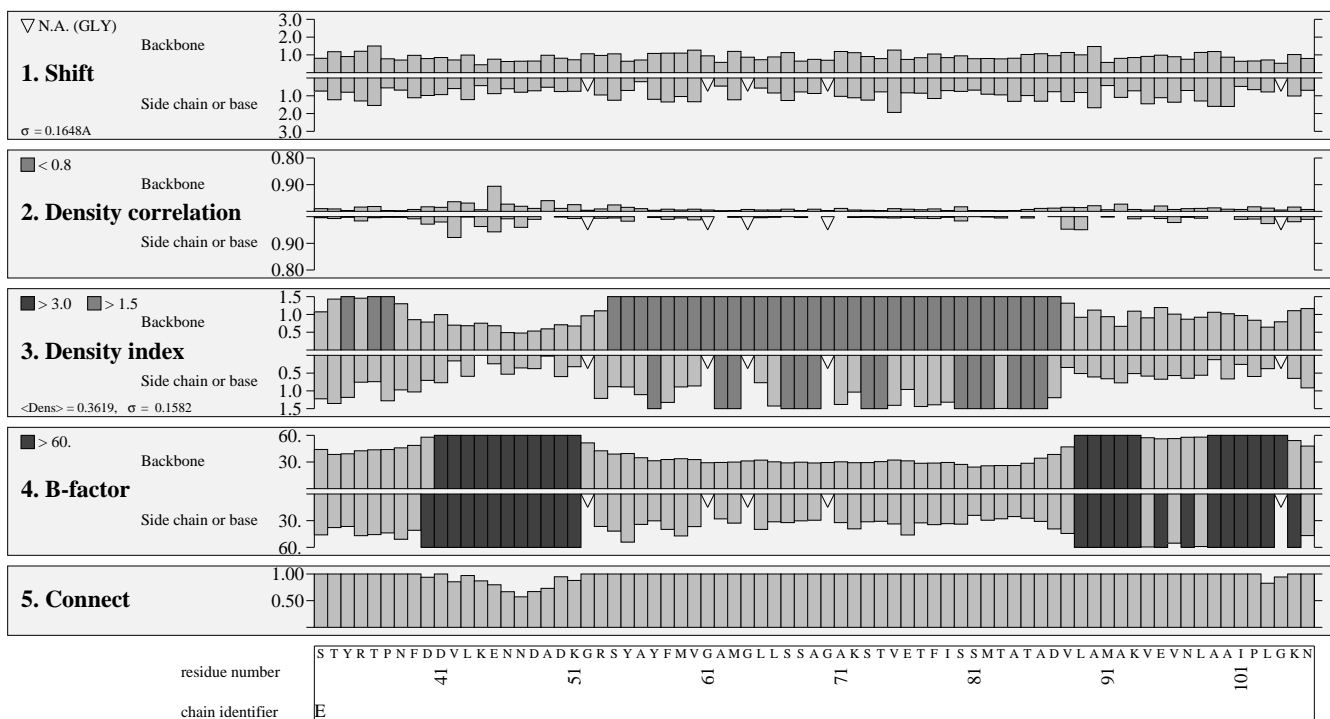
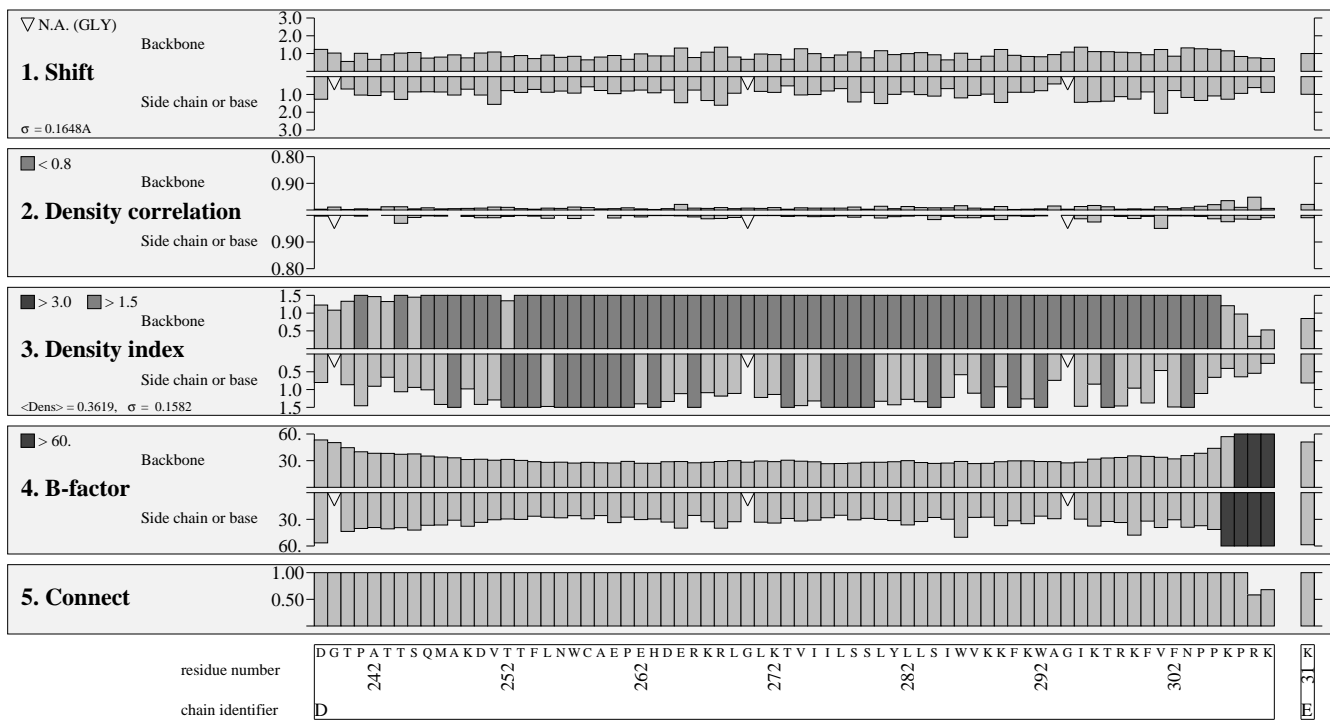
Local estimation (9) [N_omit = 2]



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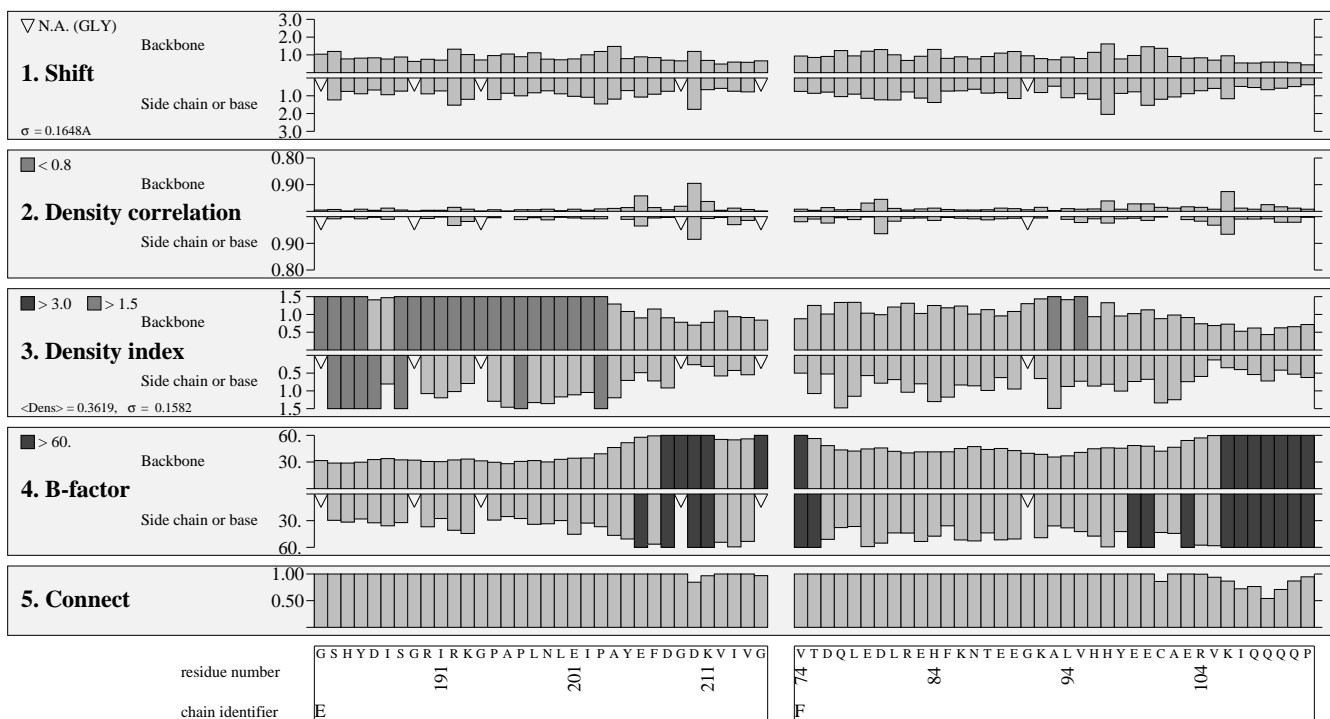
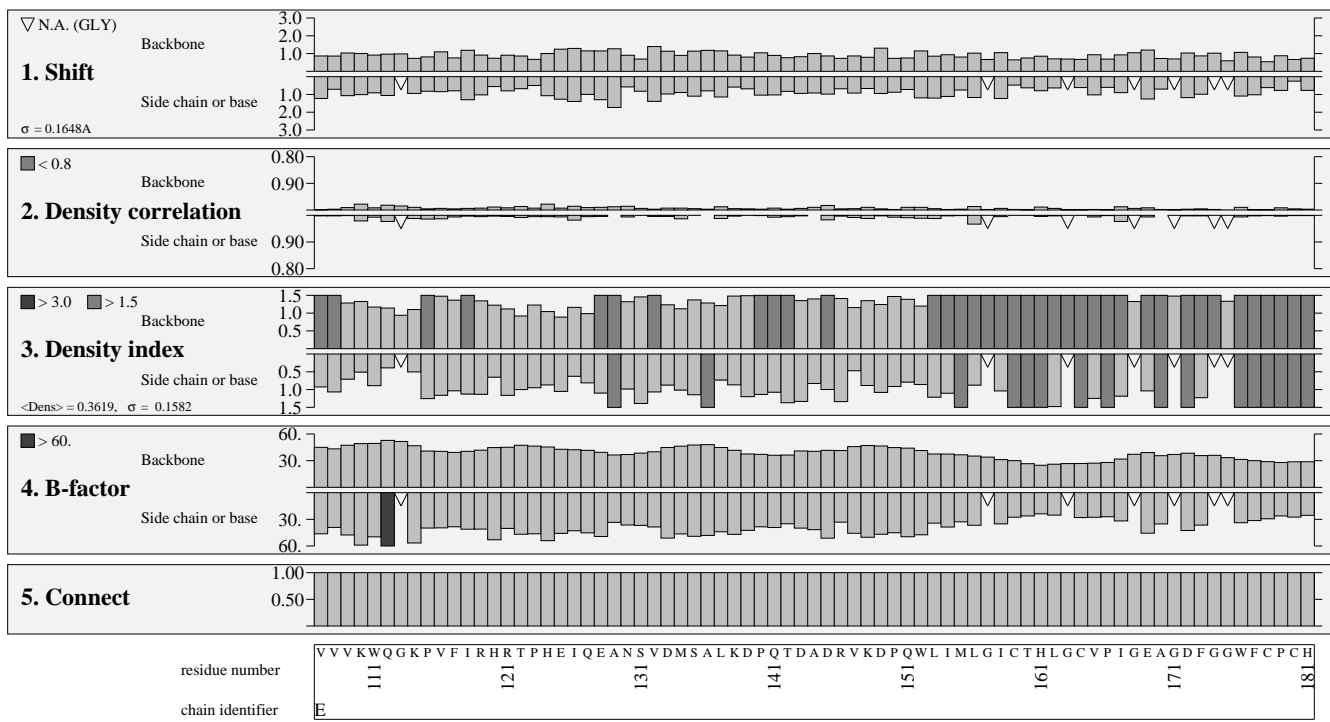
Local estimation (10) [N_omit = 2]



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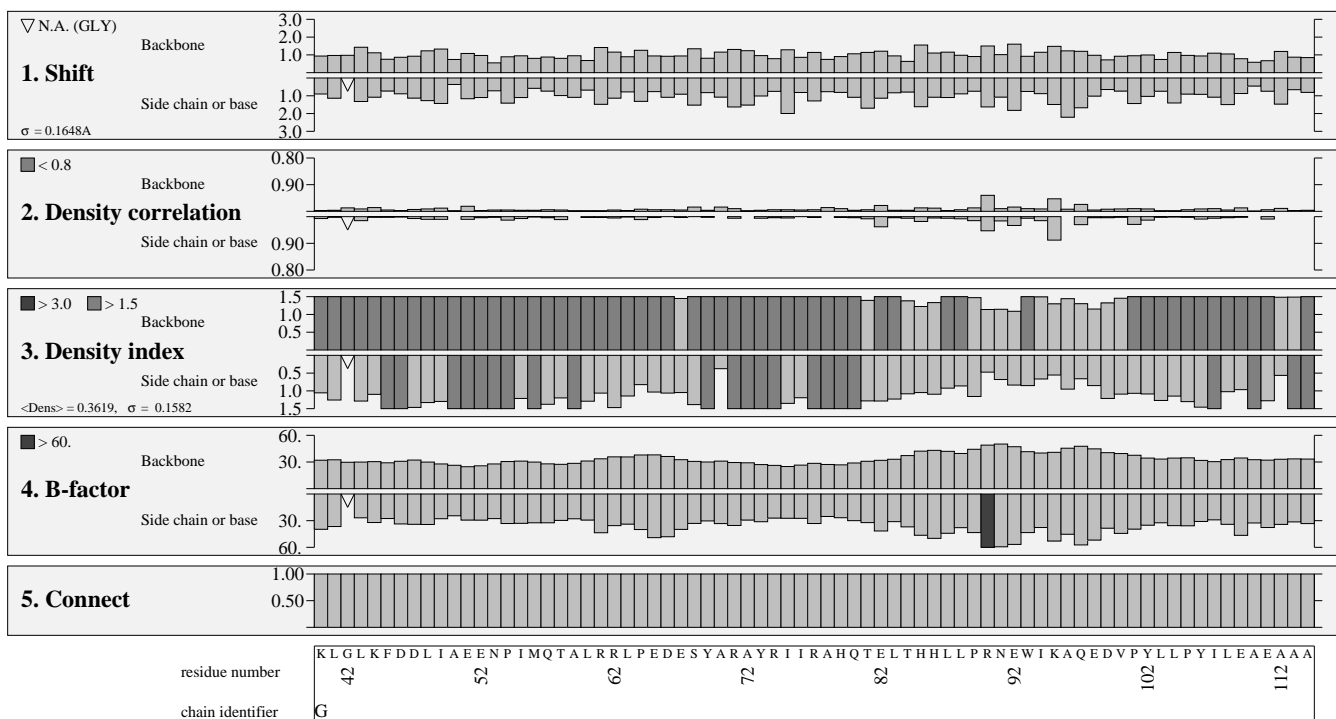
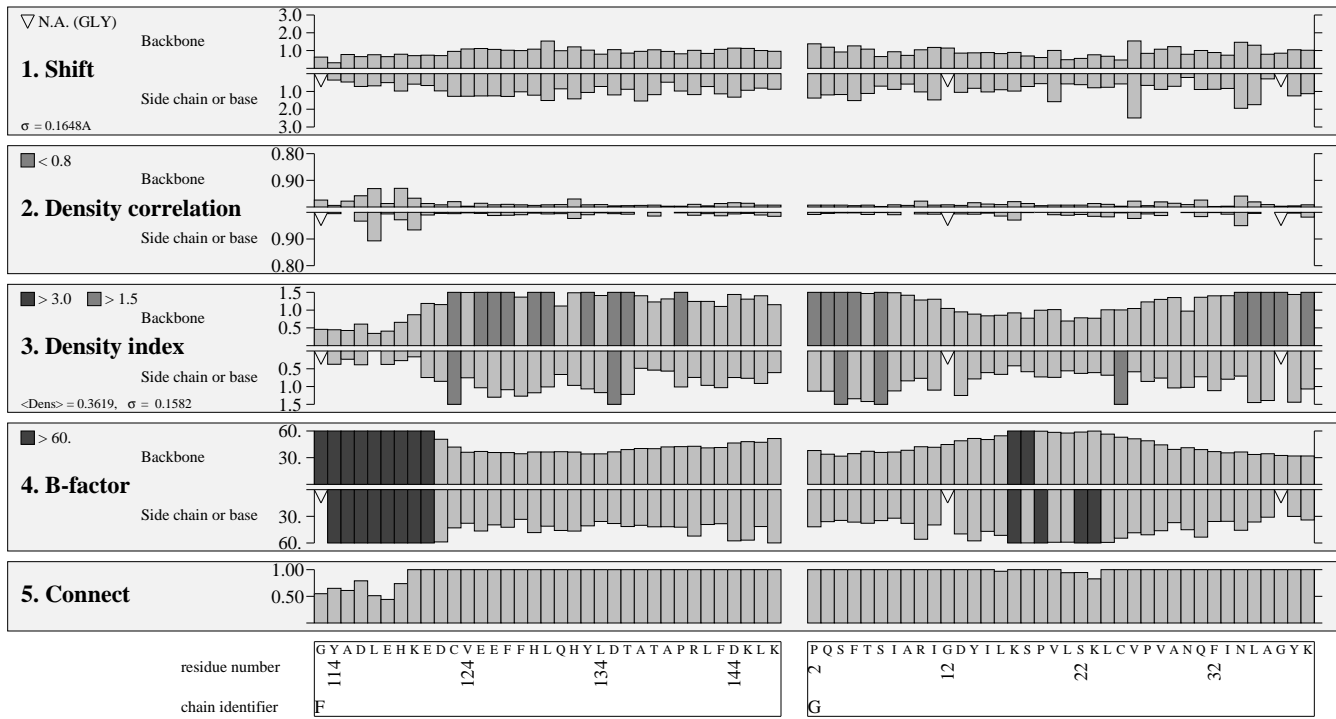
Local estimation (11) [N_omit = 2]



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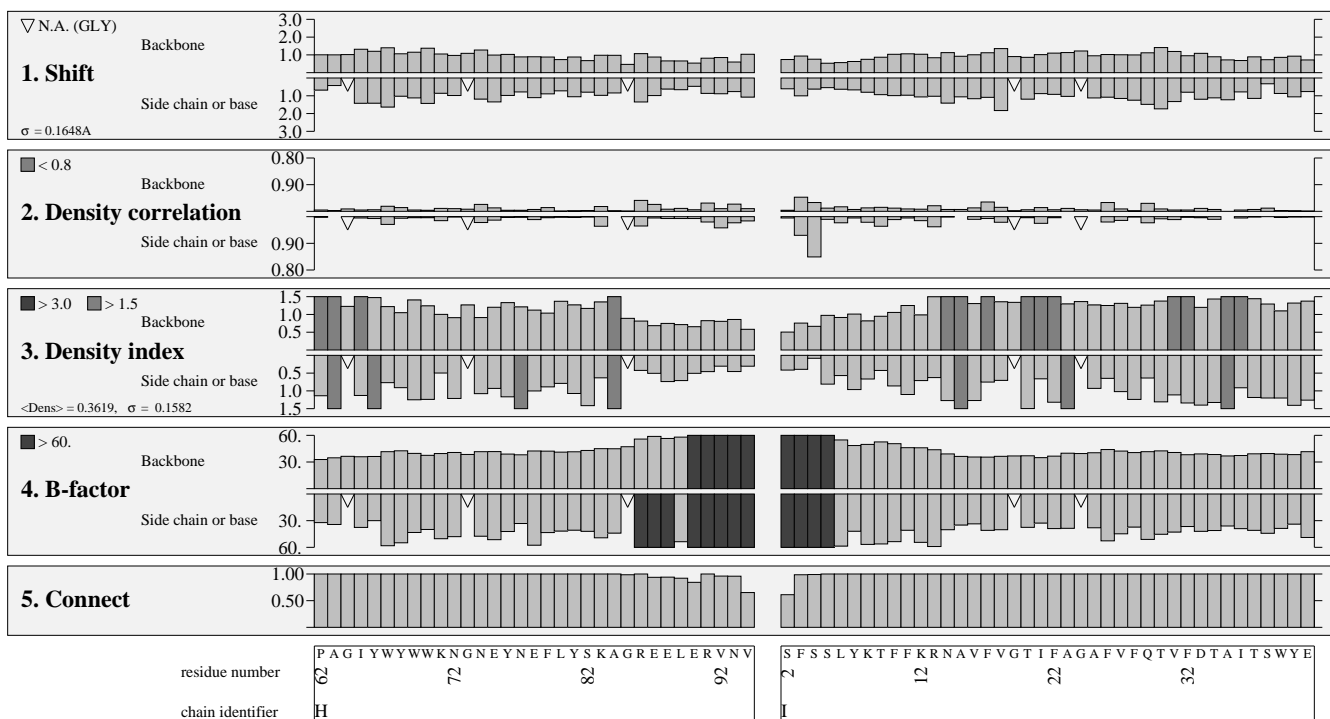
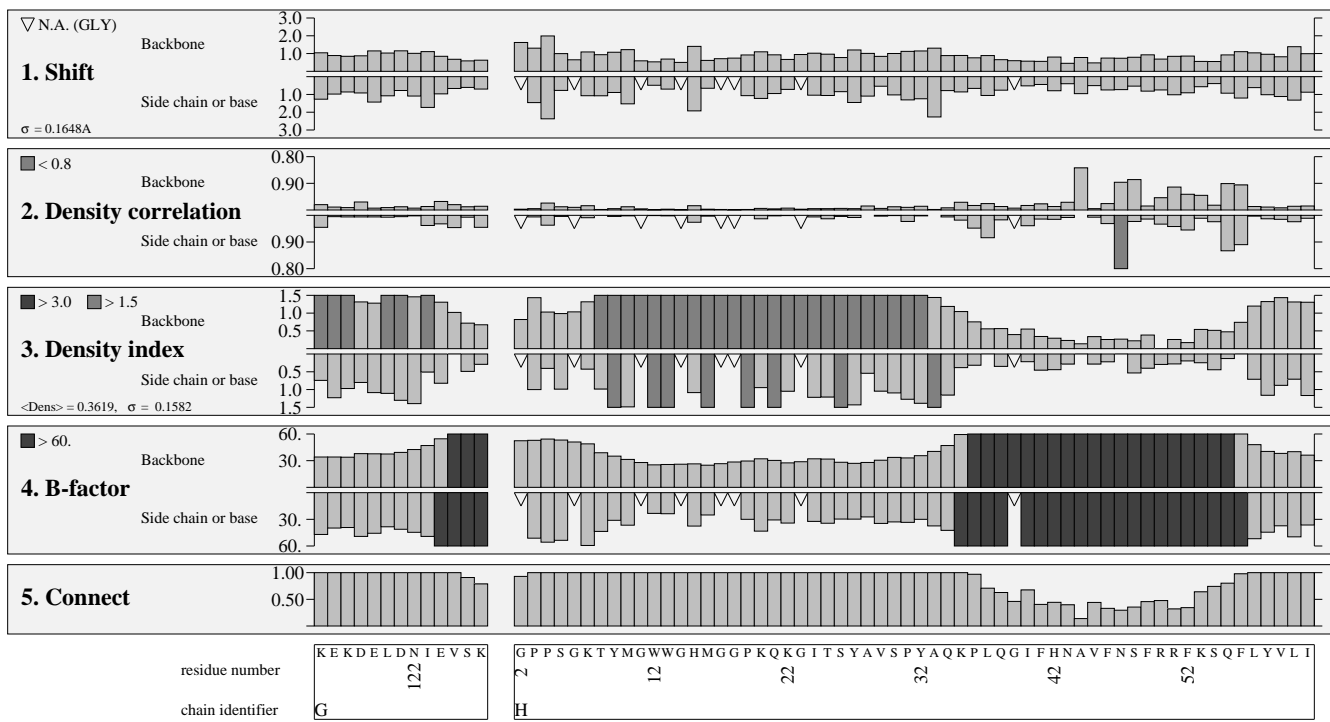
Local estimation (12) [N_omit = 2]



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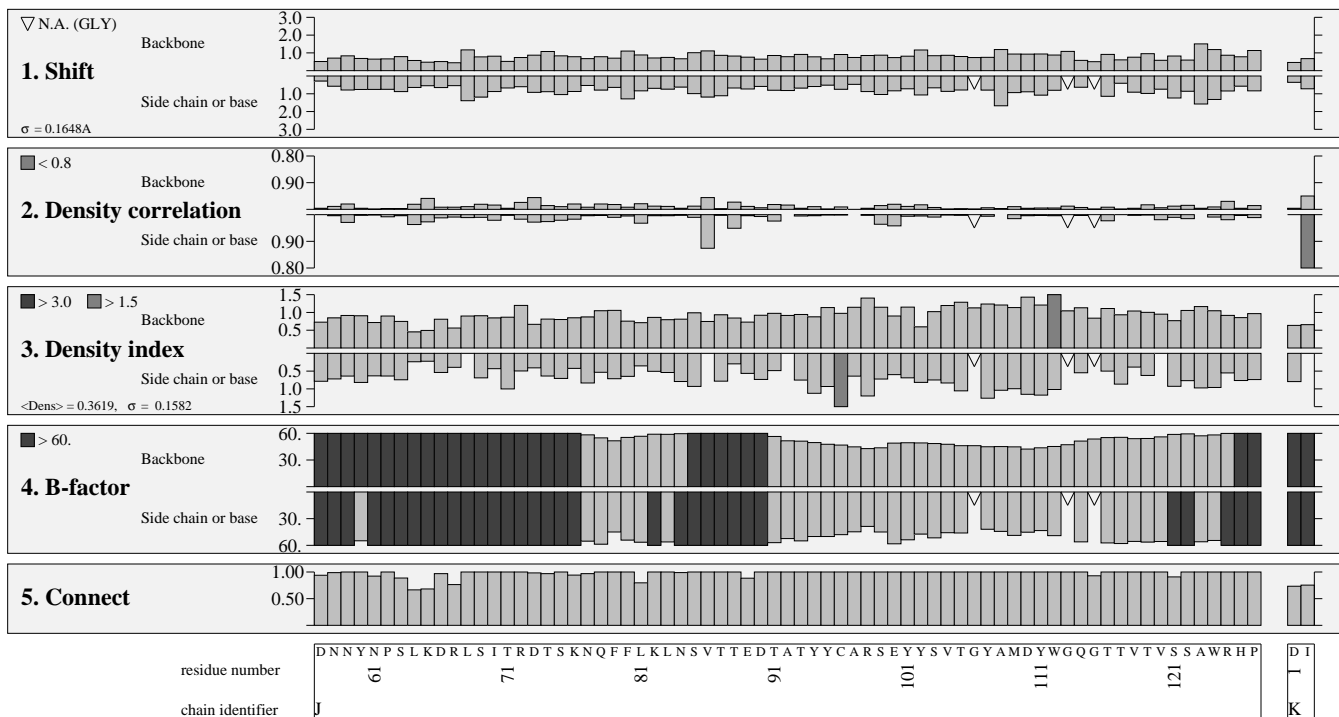
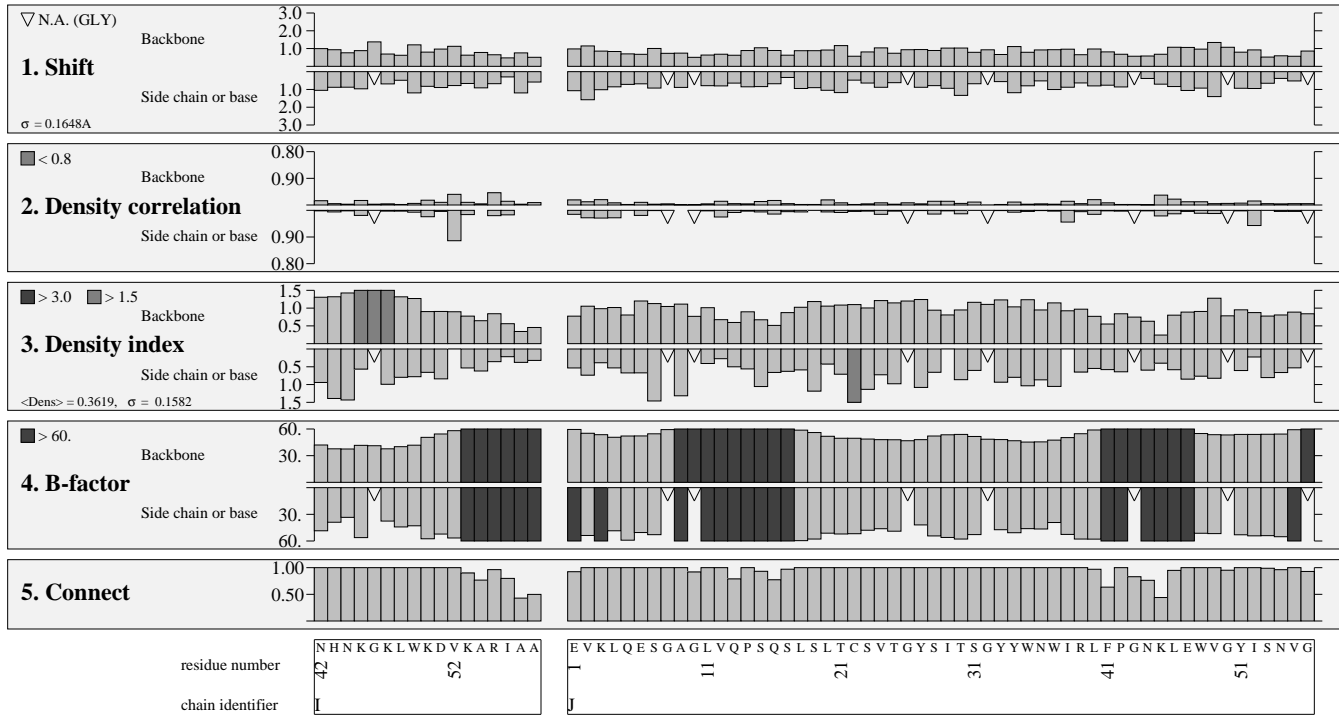
Local estimation (13) [N_omit = 2]



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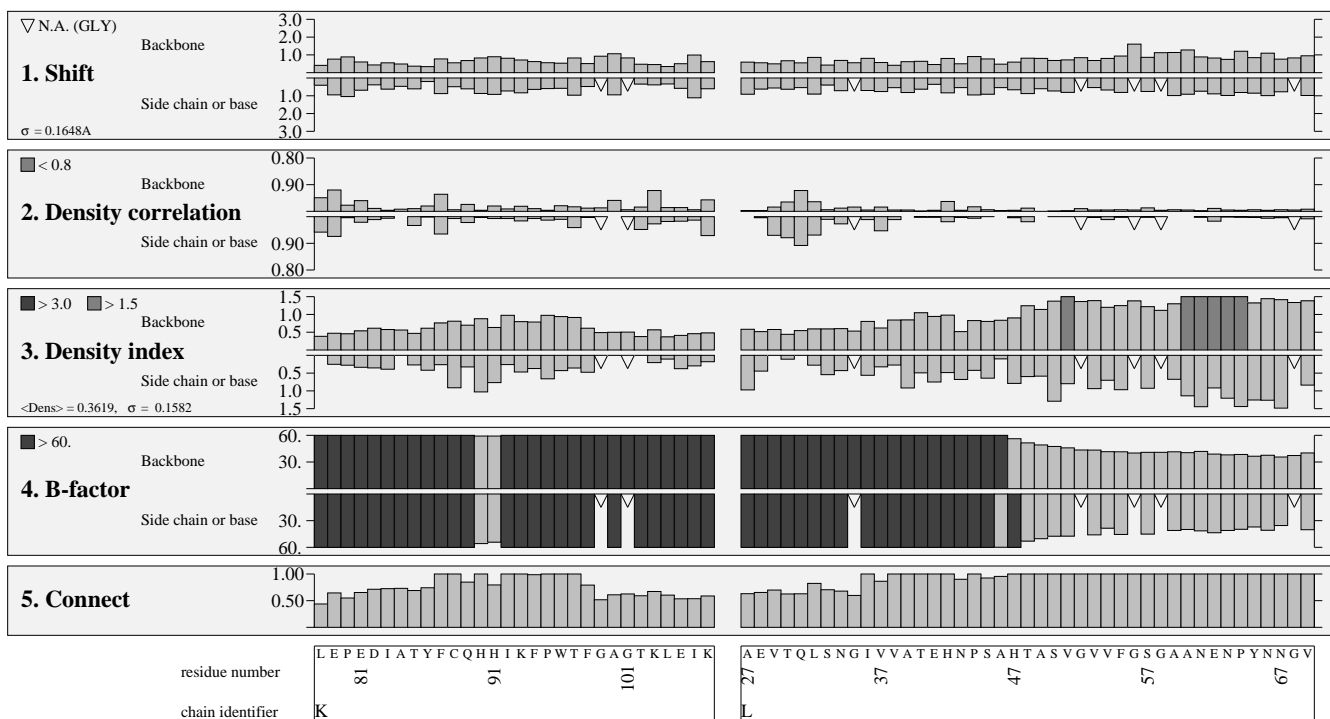
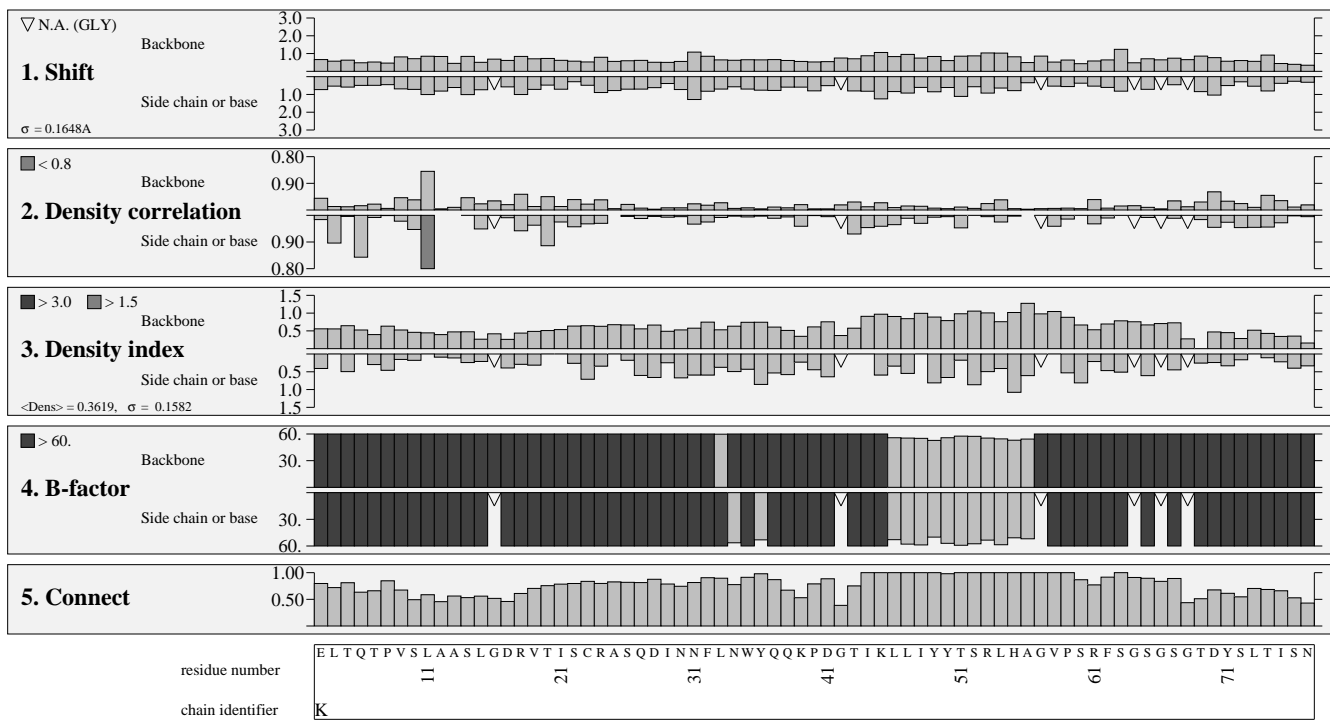
Local estimation (14) [N_omit = 2]



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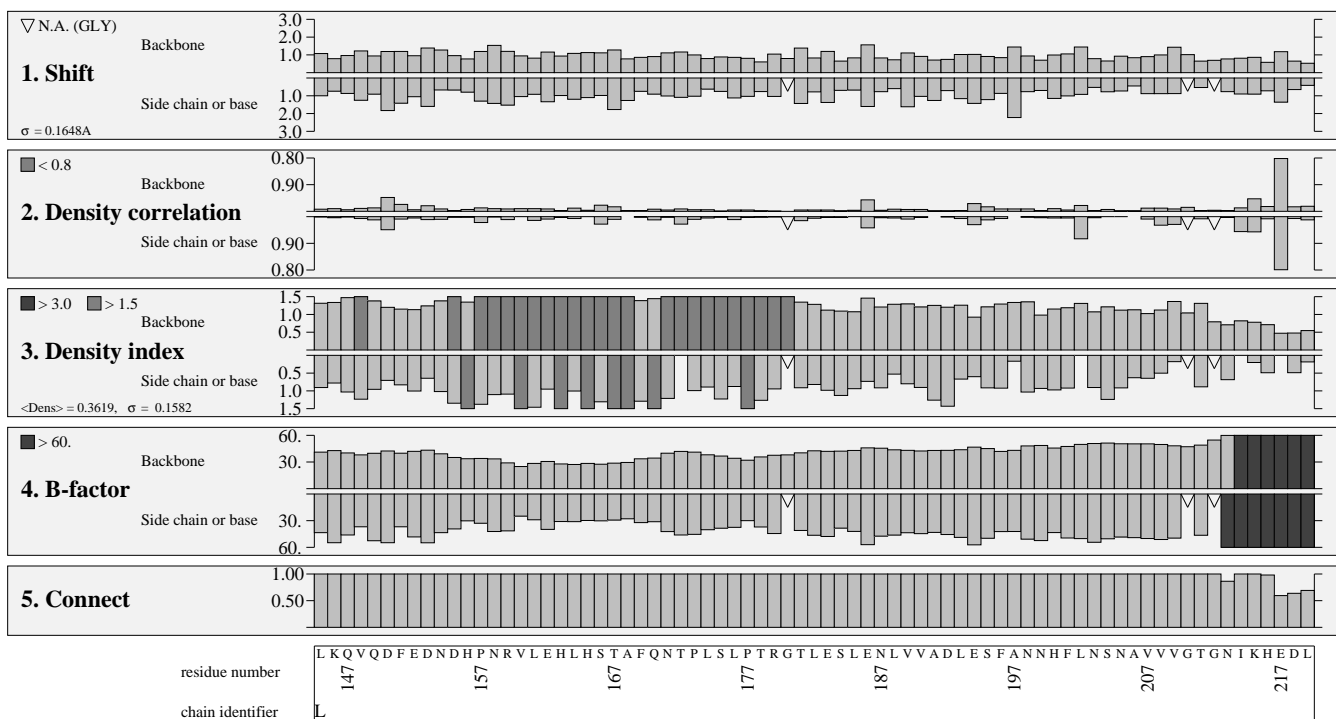
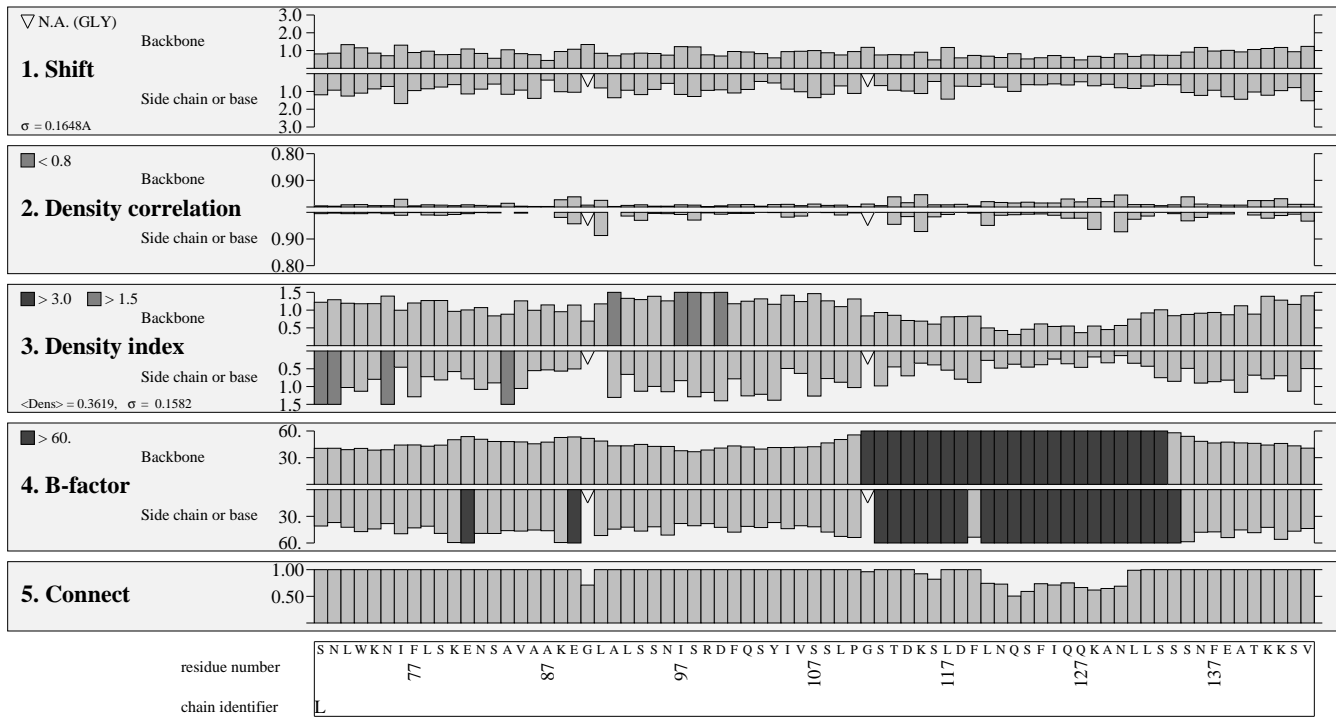
Local estimation (15) [N_omit = 2]



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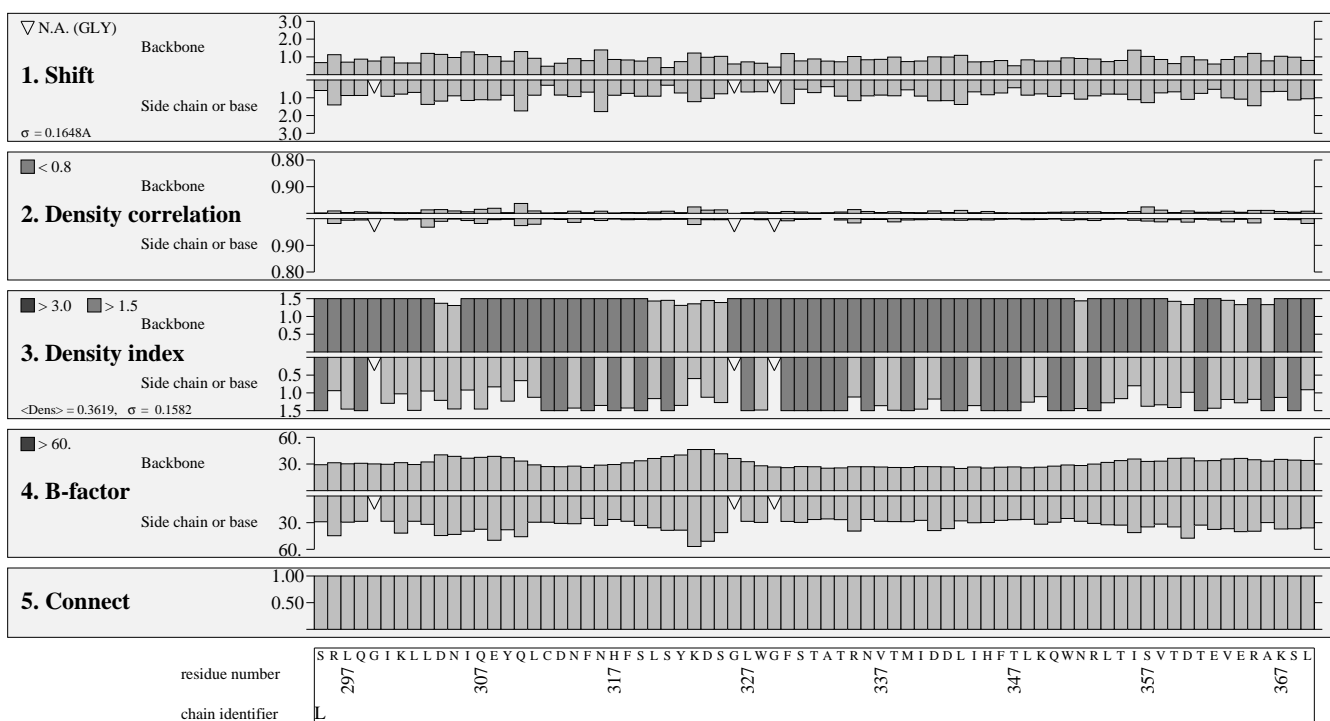
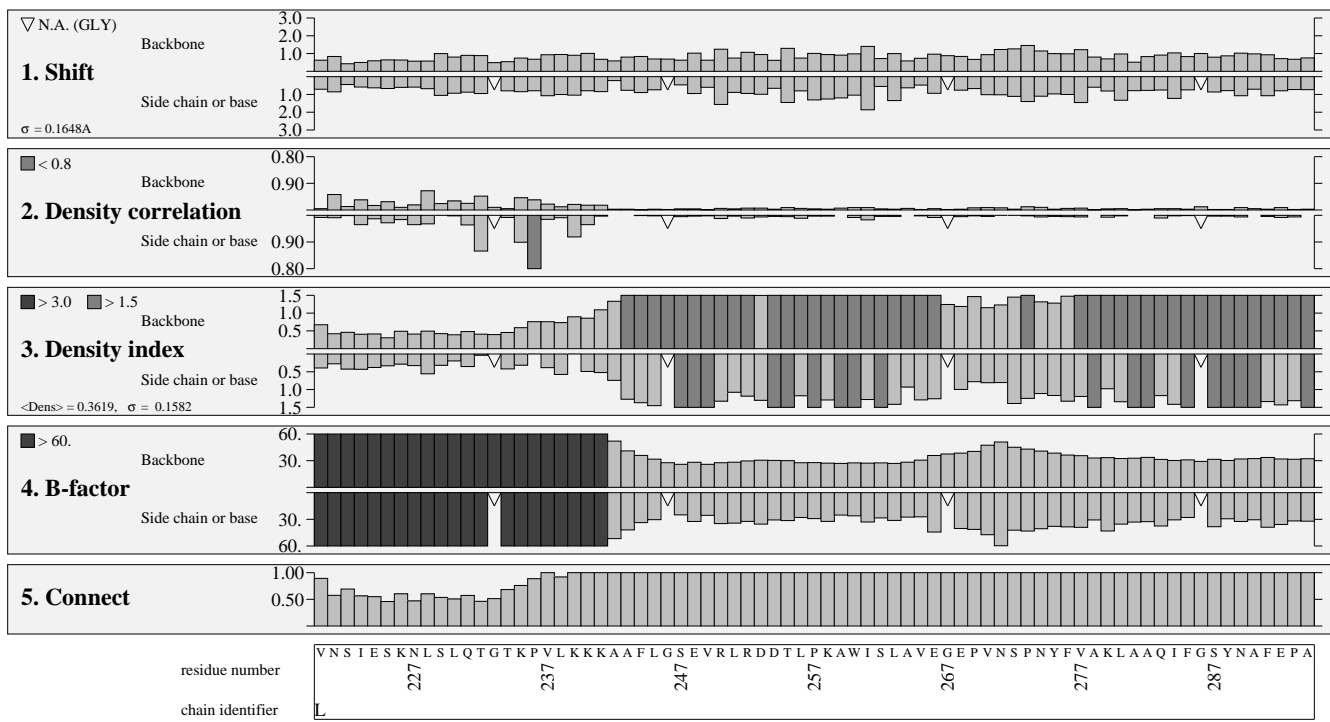
Local estimation (16) [N_omit = 2]



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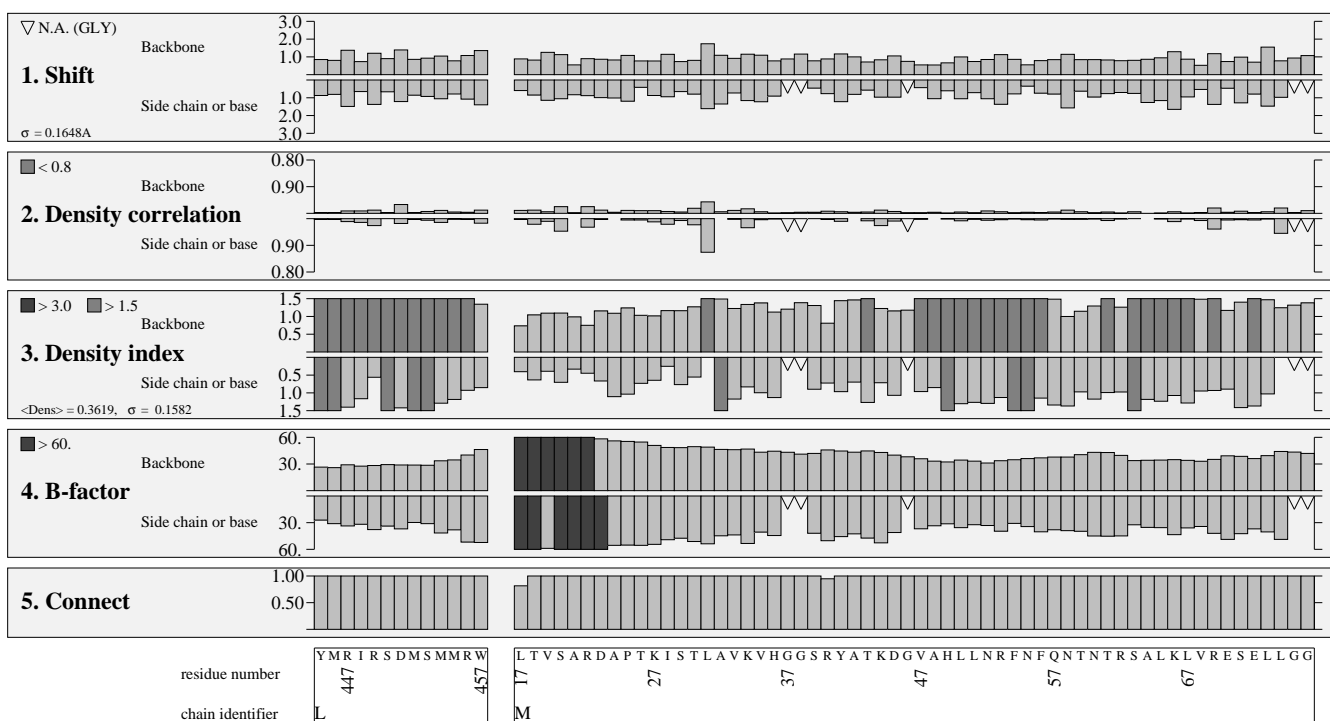
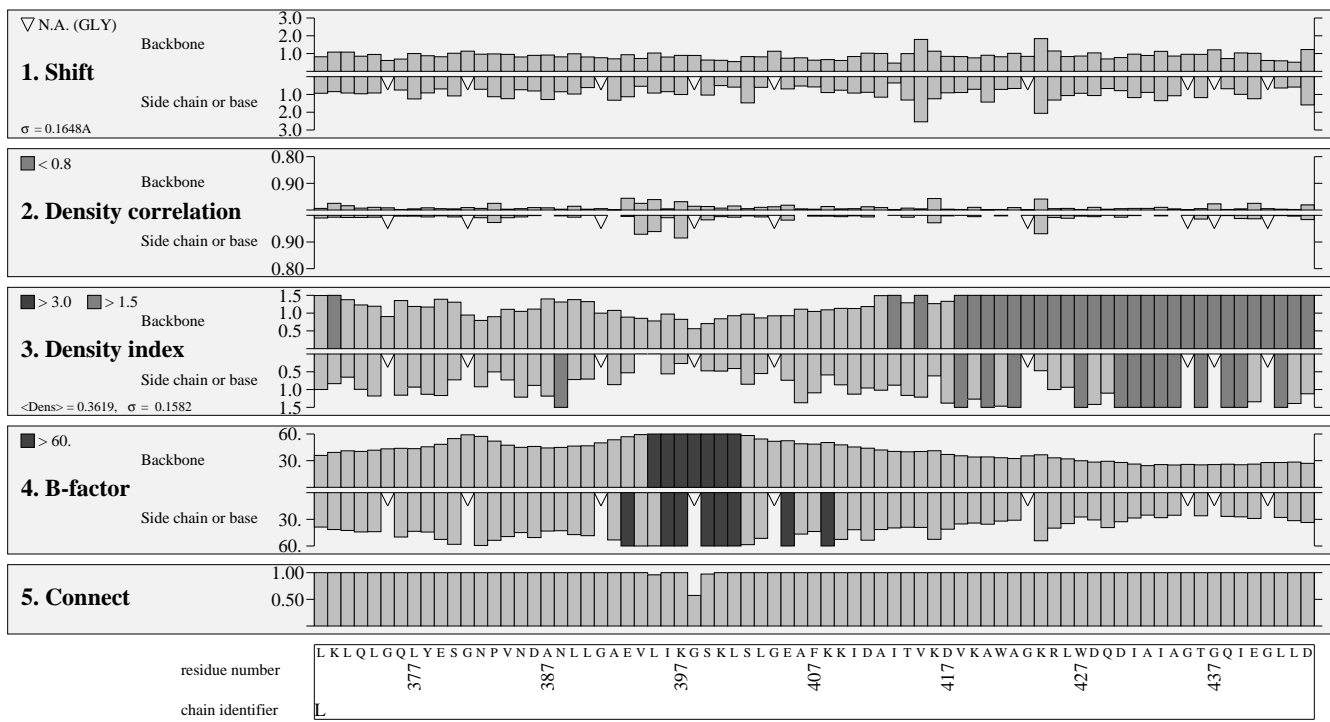
Local estimation (17) [N_omit = 2]



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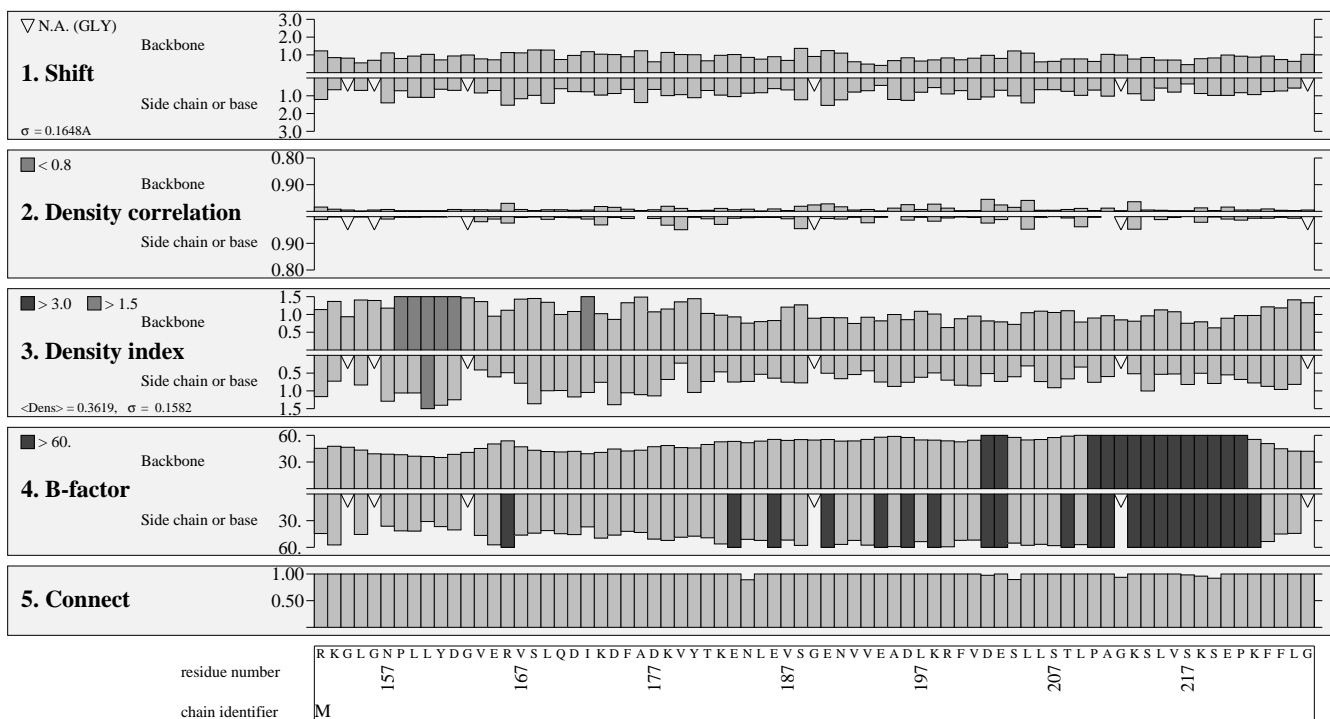
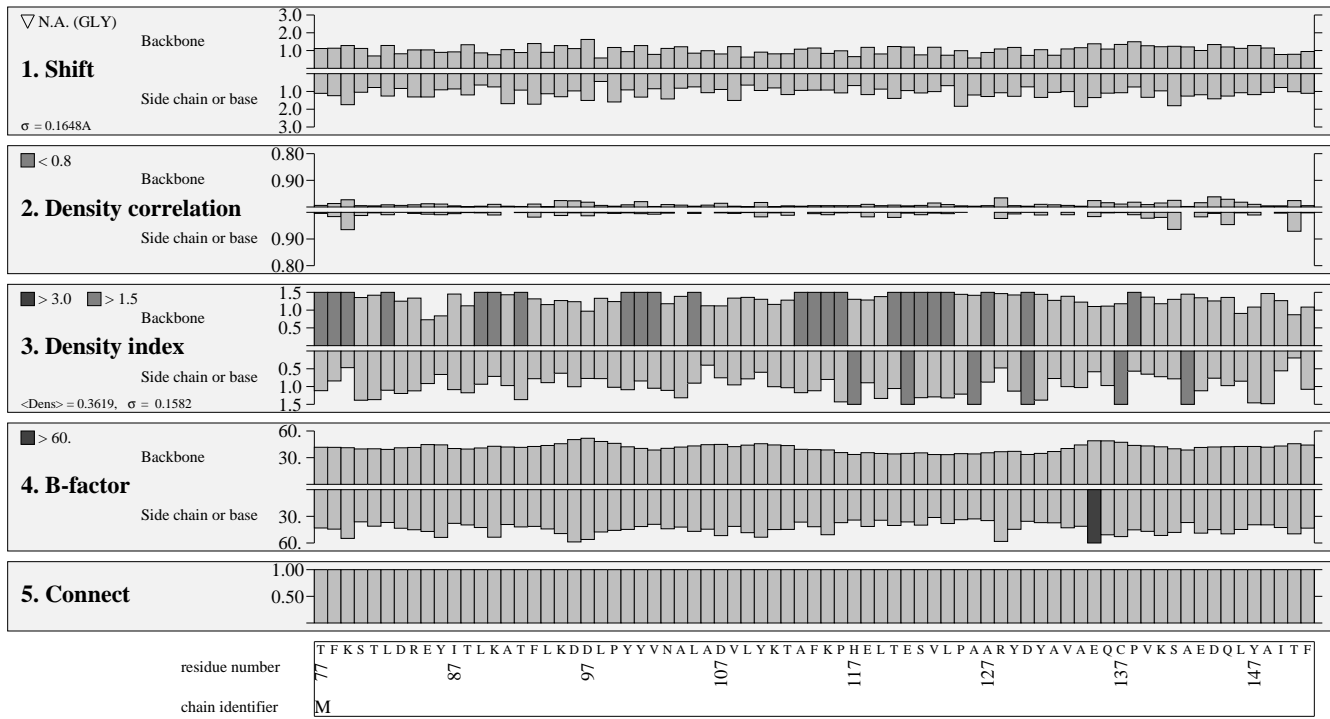
Local estimation (18) [N_omit = 2]



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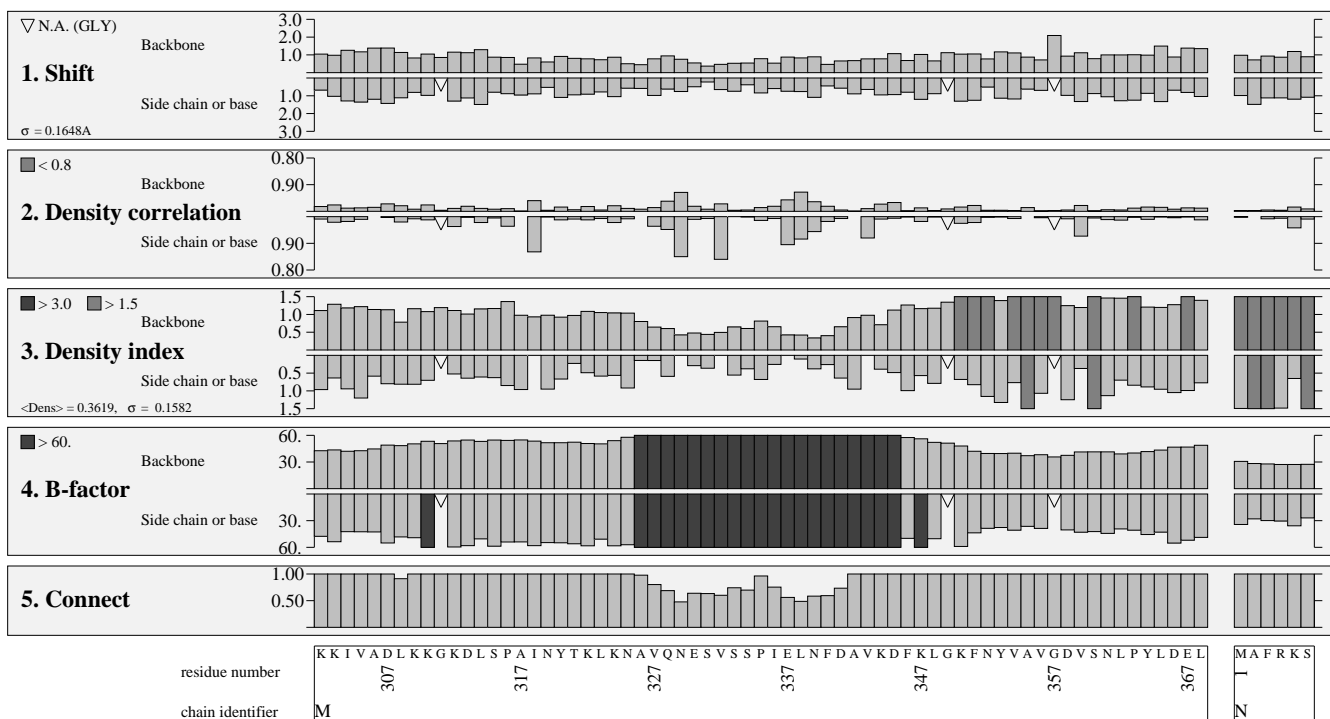
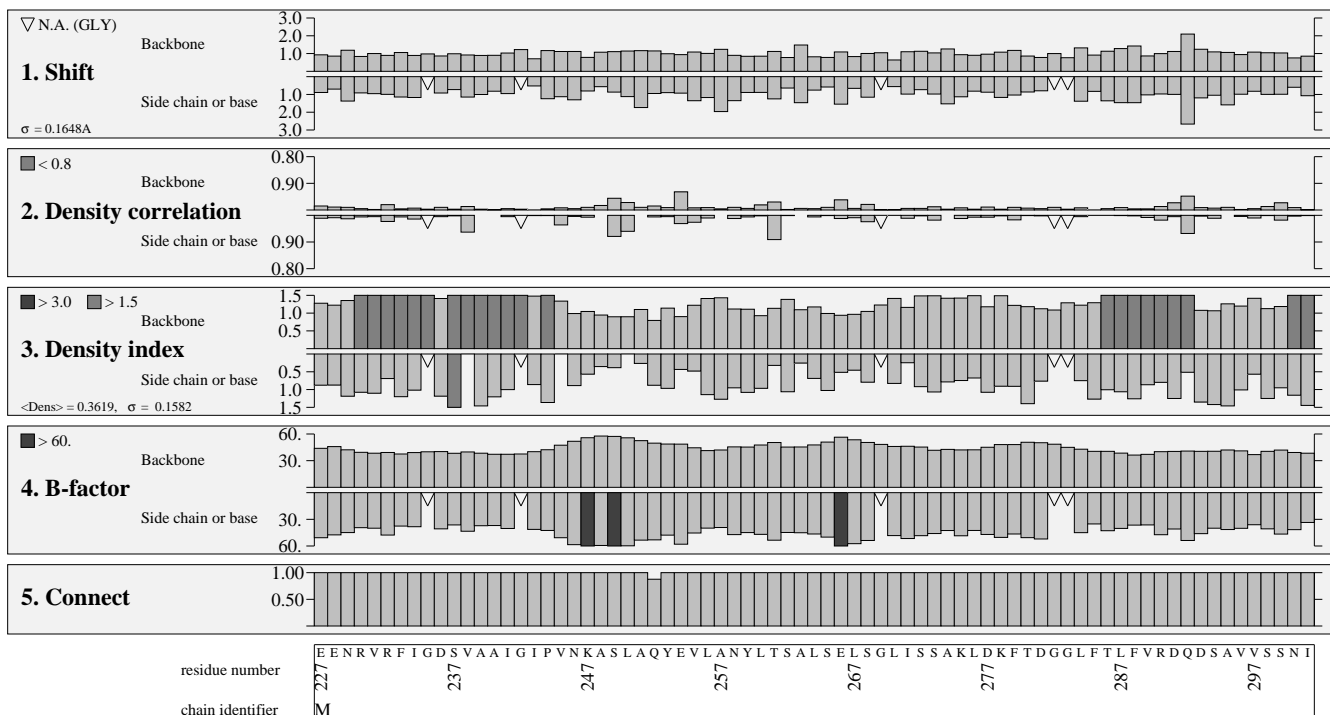
Local estimation (19) [N_omit = 2]



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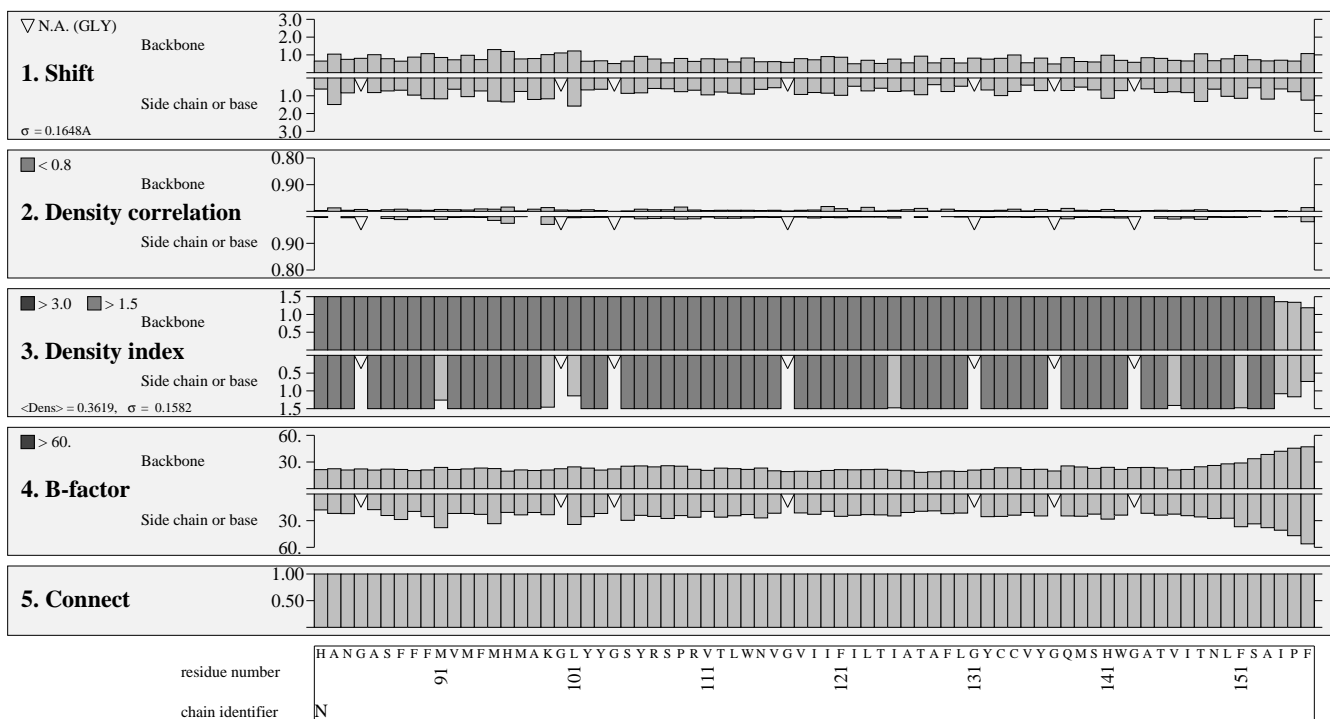
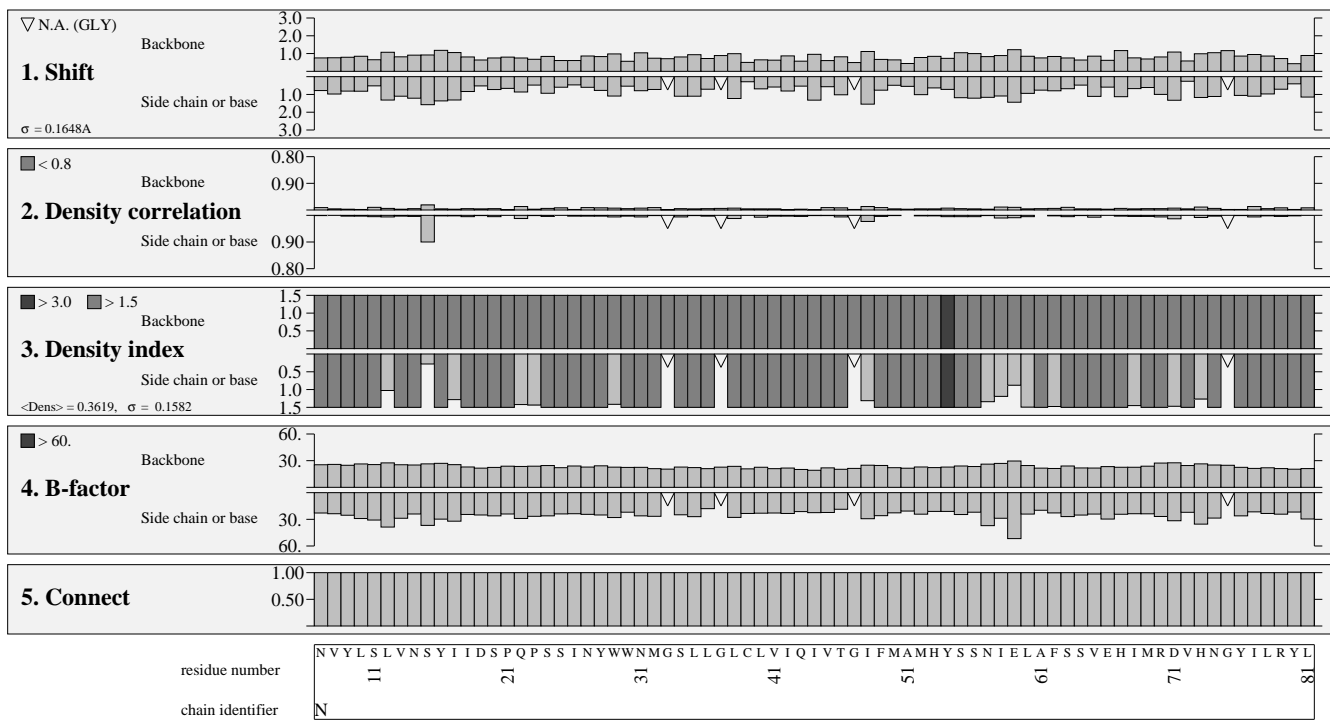
Local estimation (20) [N_omit = 2]



Structure Factor Check

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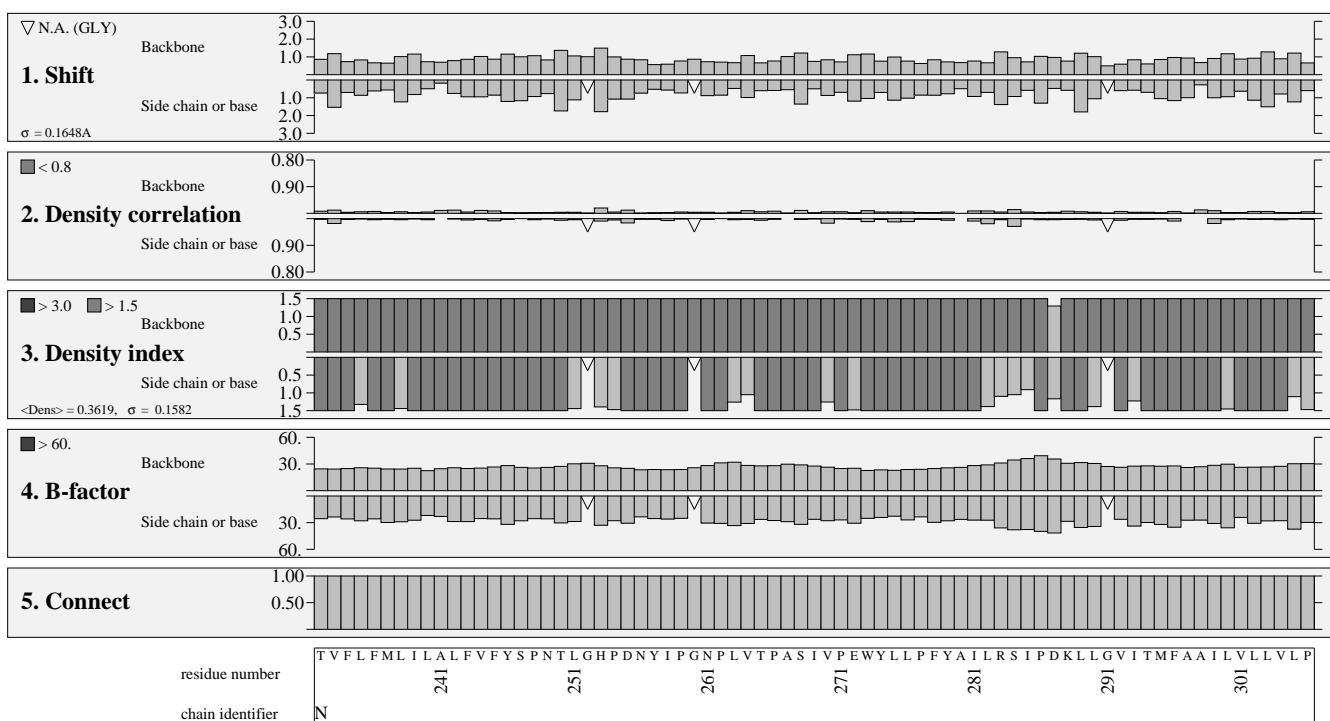
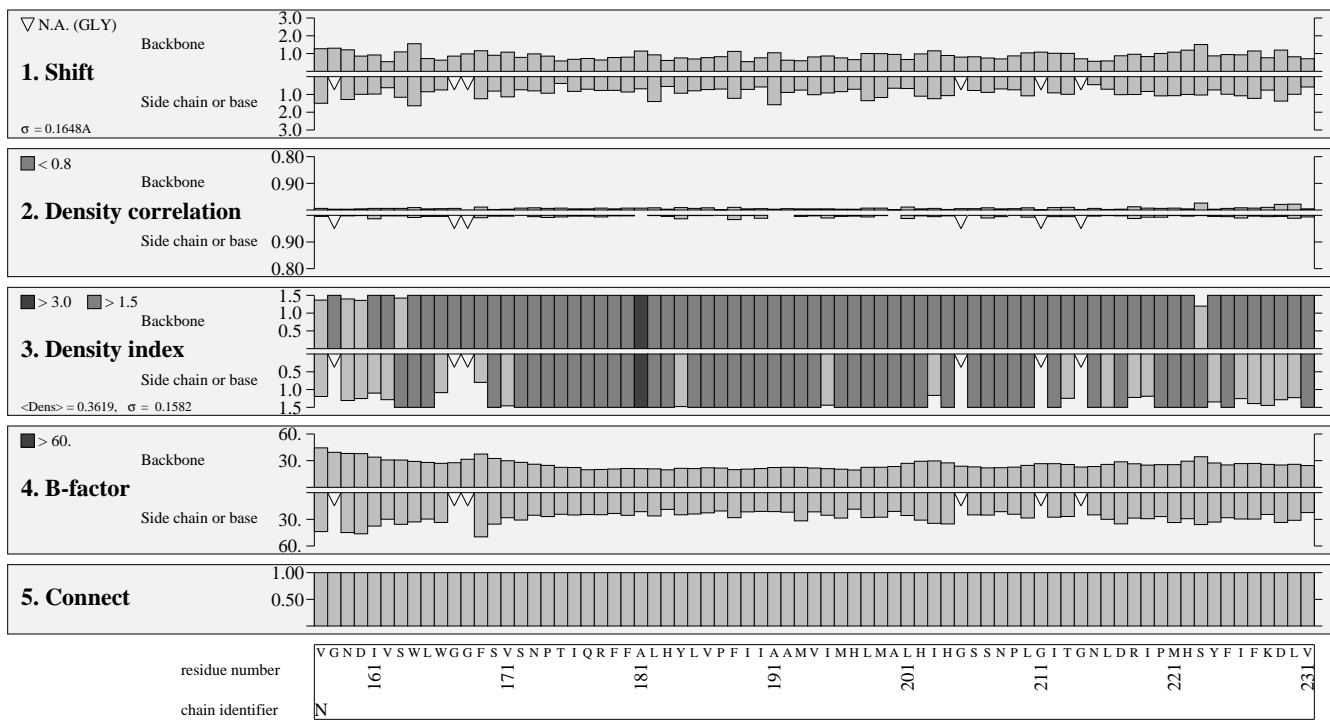
Local estimation (21) [N_omit = 2]



Structure Factor Check

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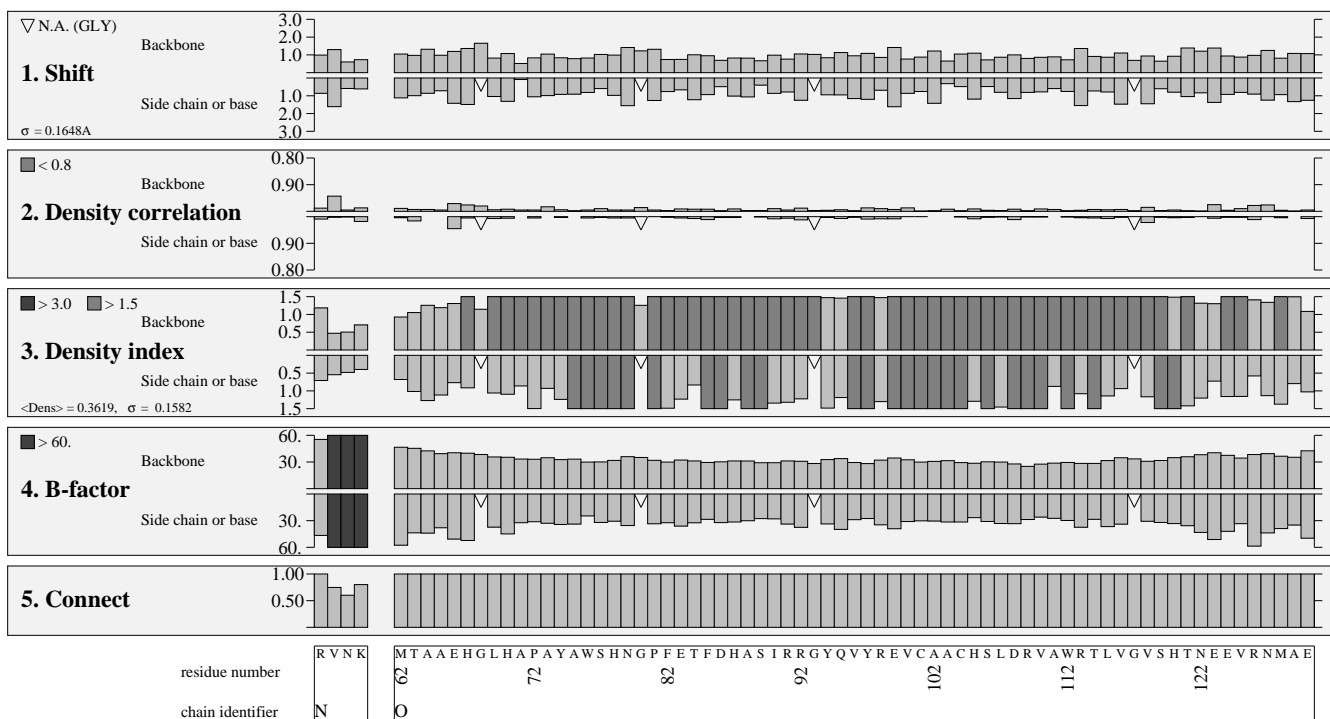
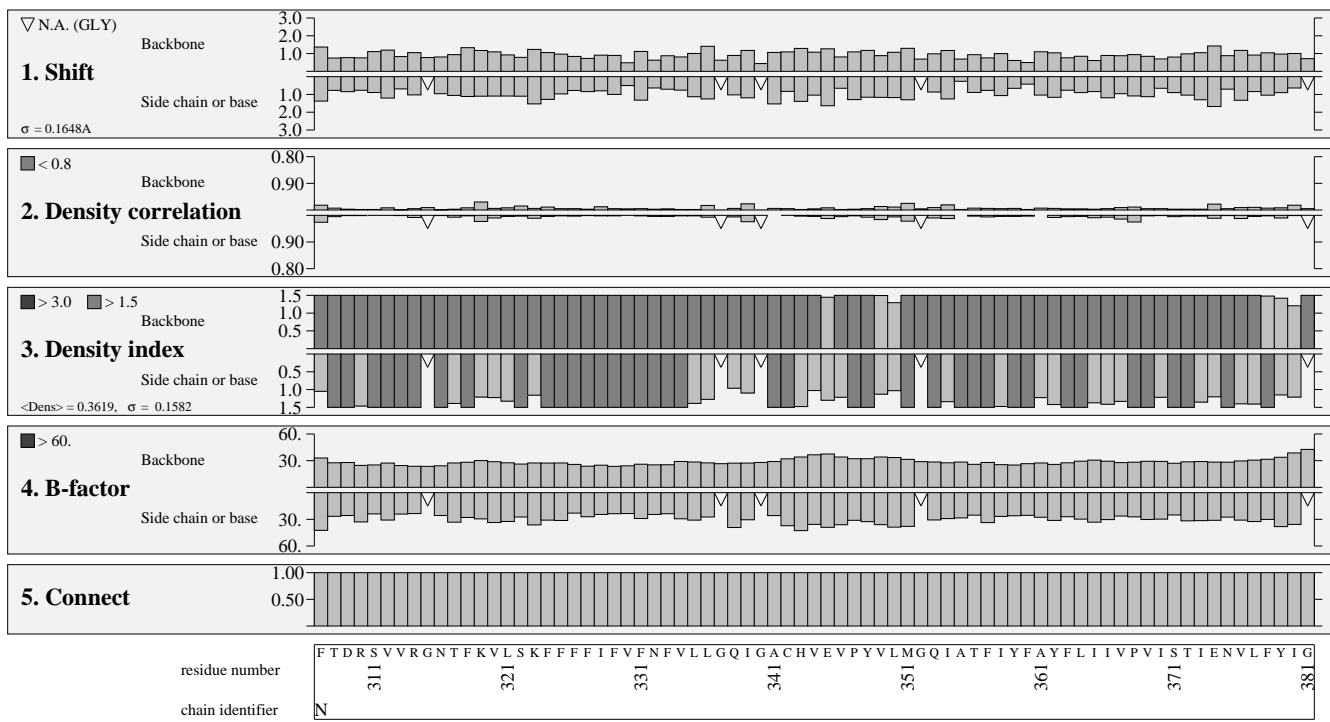
Local estimation (22) [N_omit = 2]



Structure Factor Check

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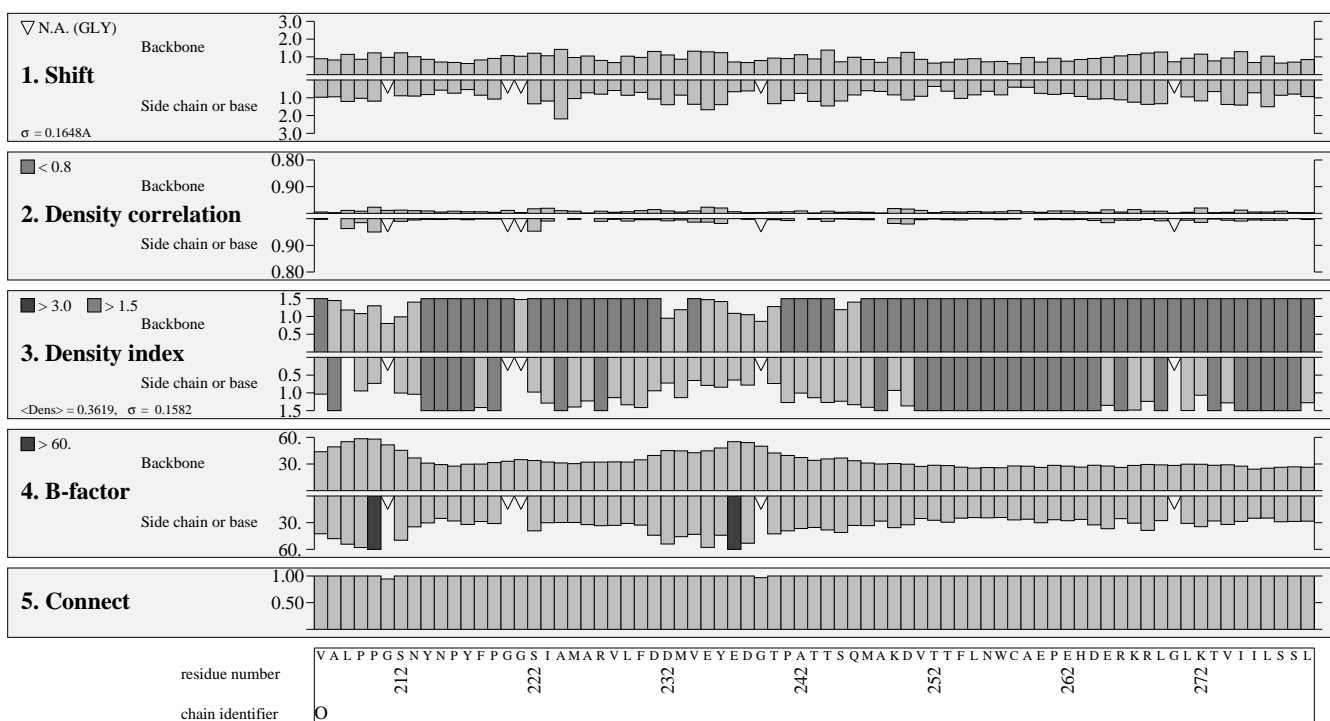
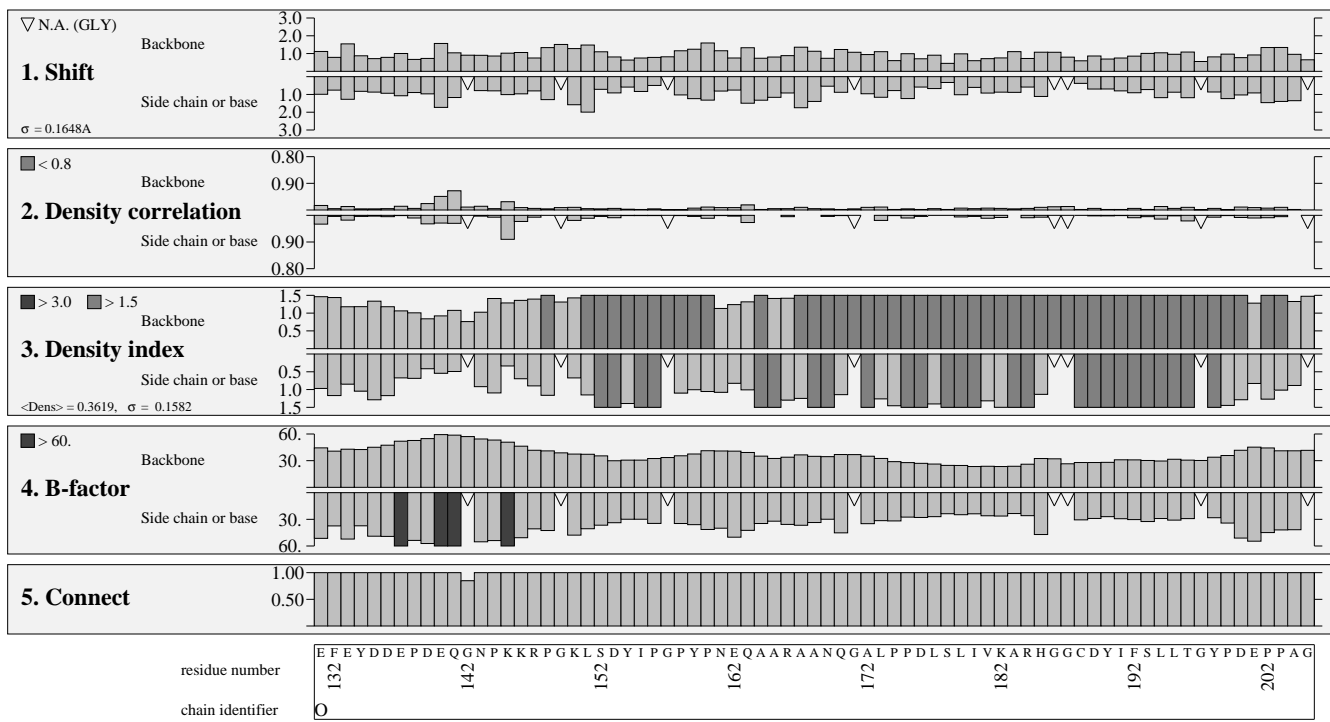
Local estimation (23) [N_omit = 2]



Structure Factor Check

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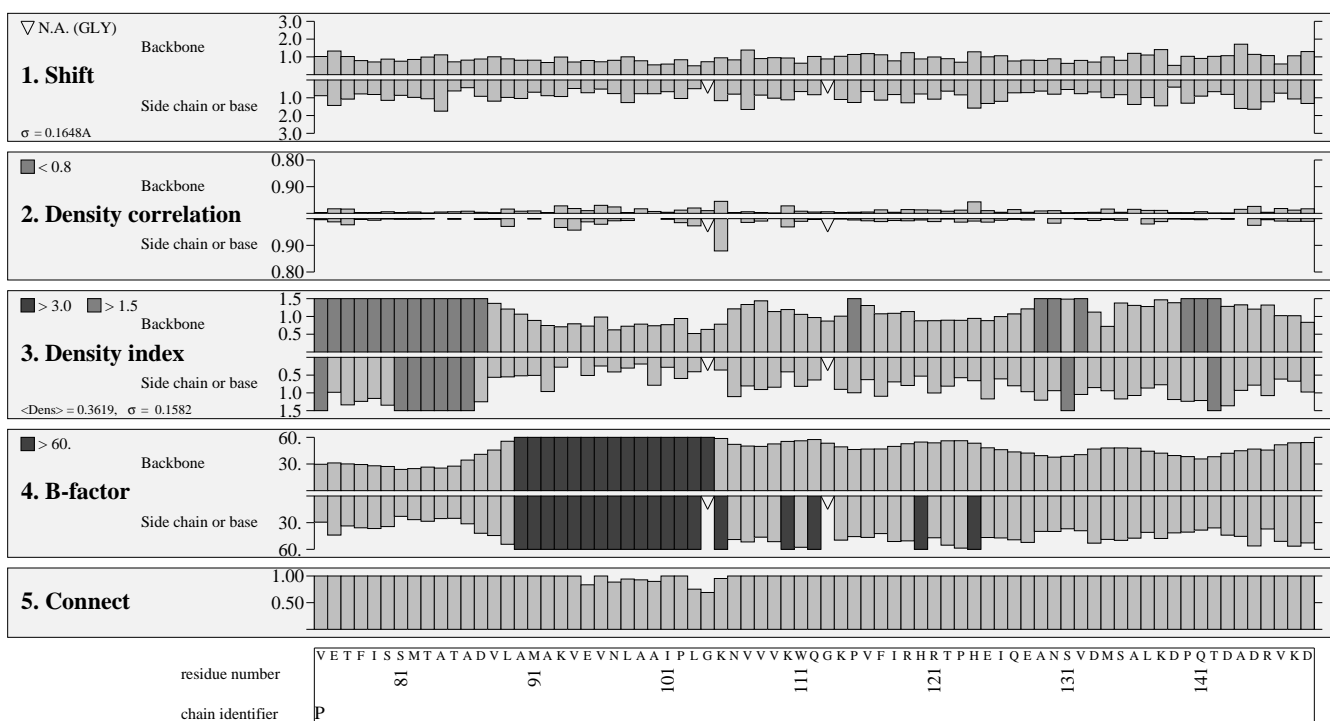
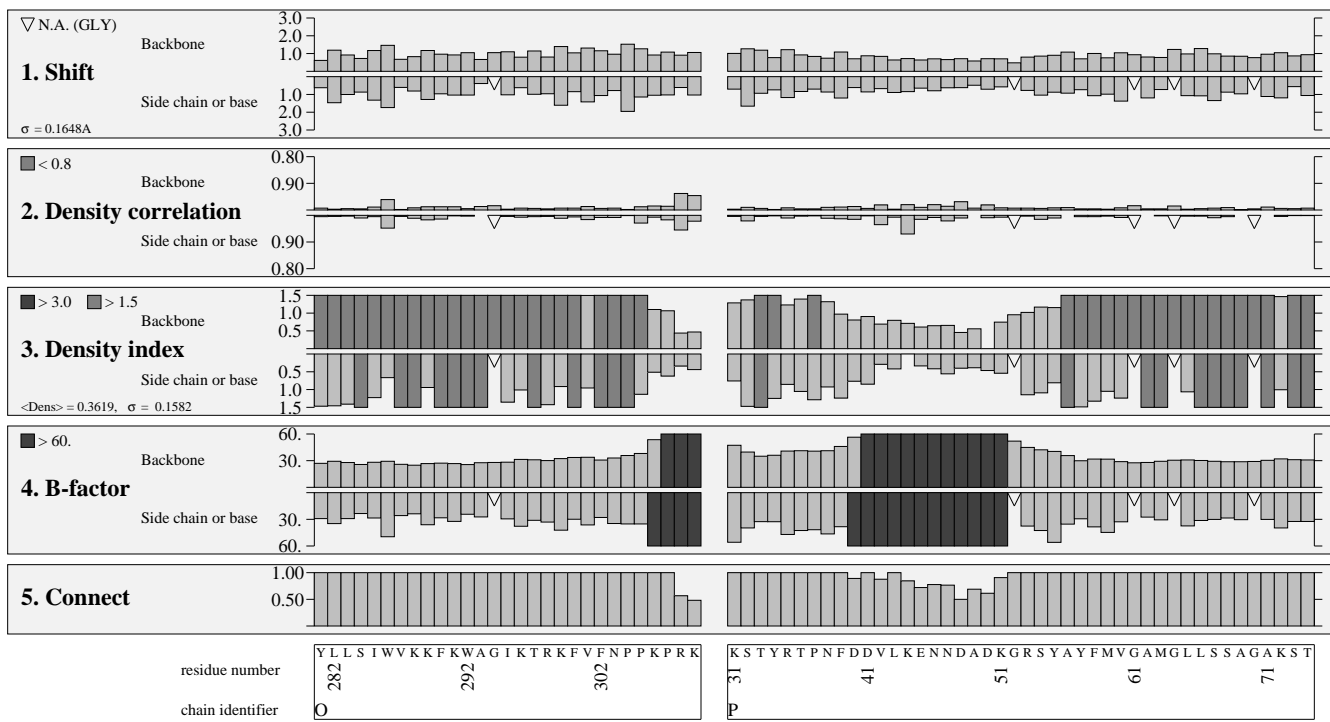
Local estimation (24) [N_omit = 2]



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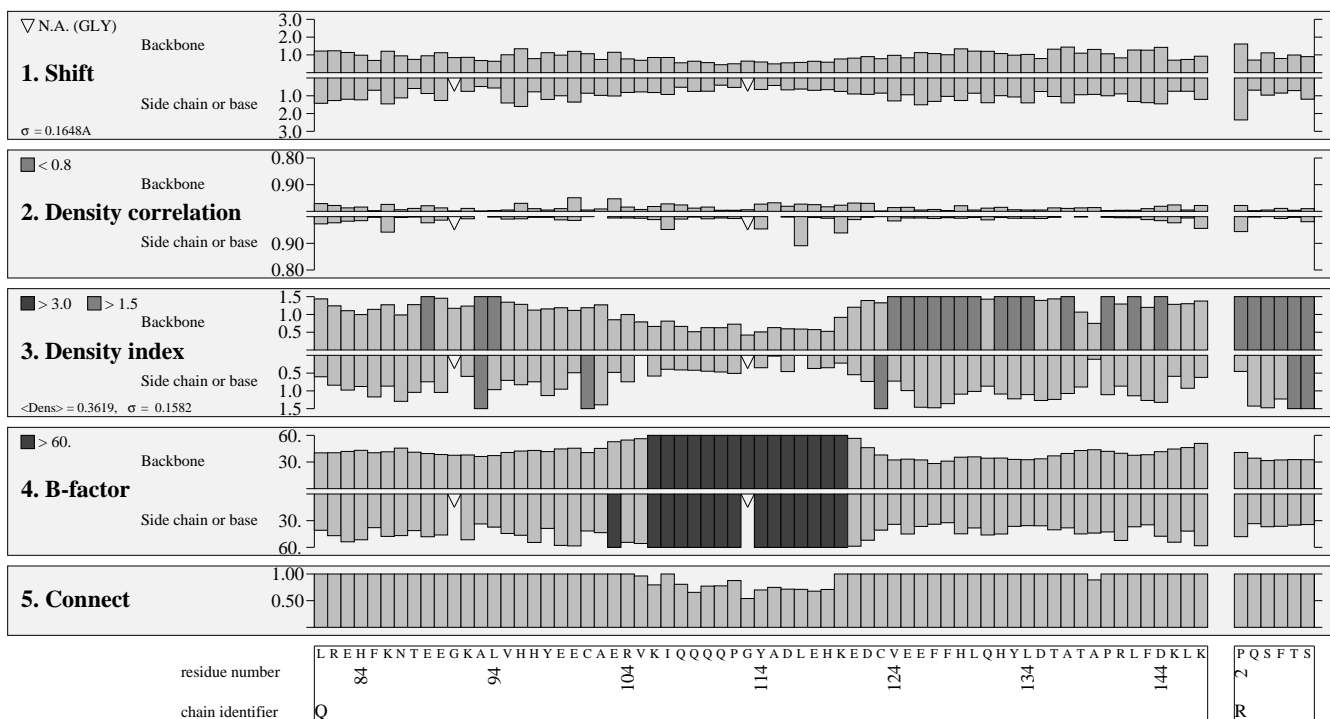
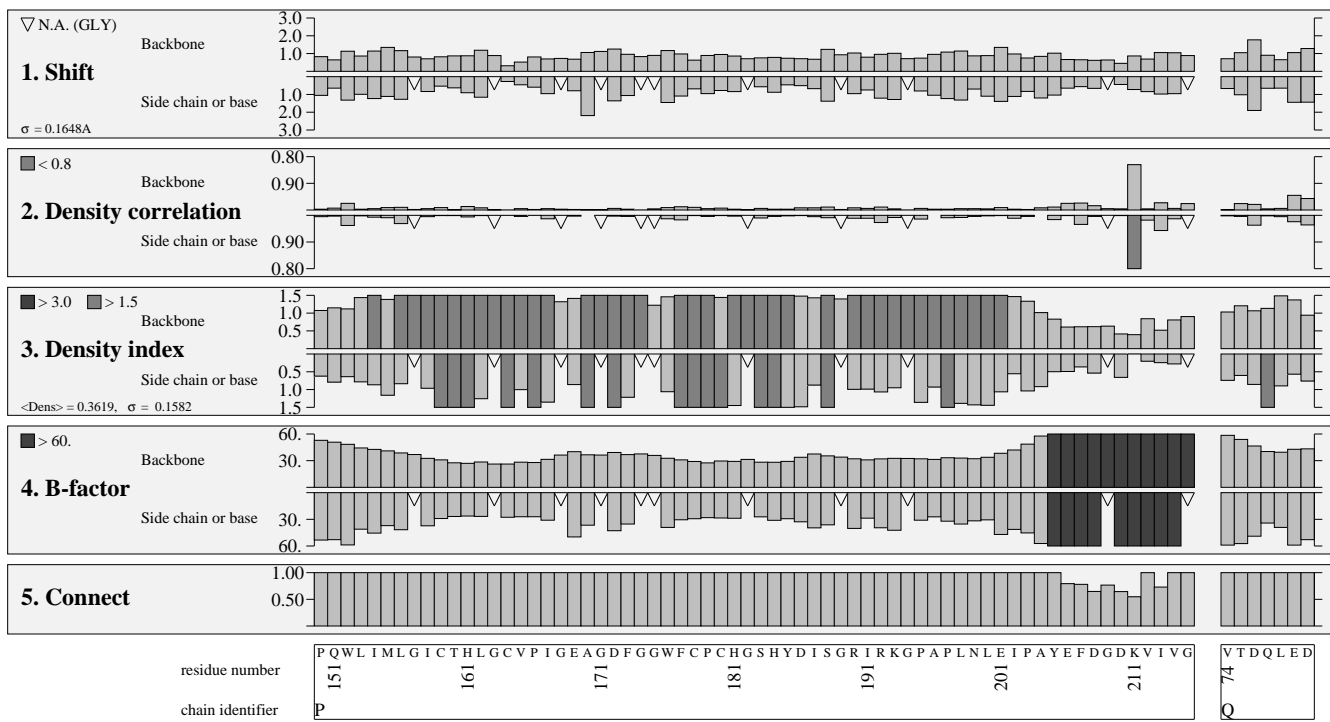
Local estimation (25) [N_omit = 2]



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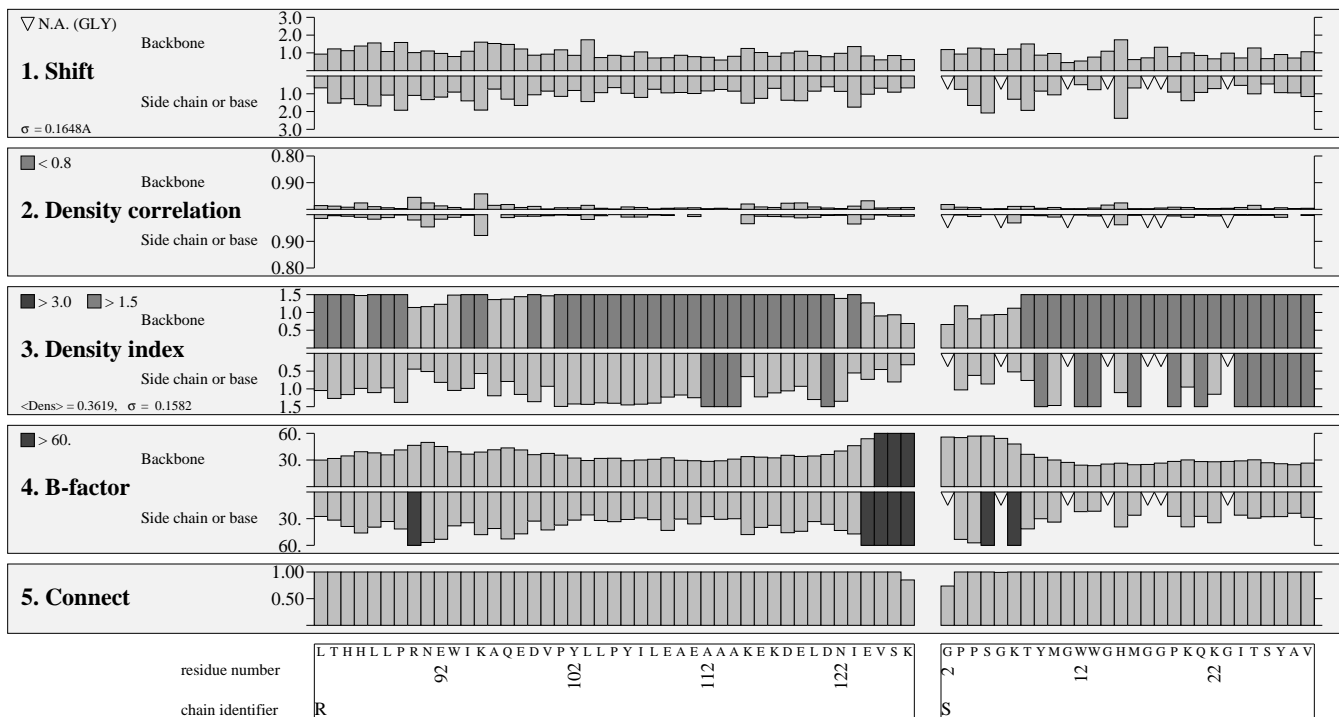
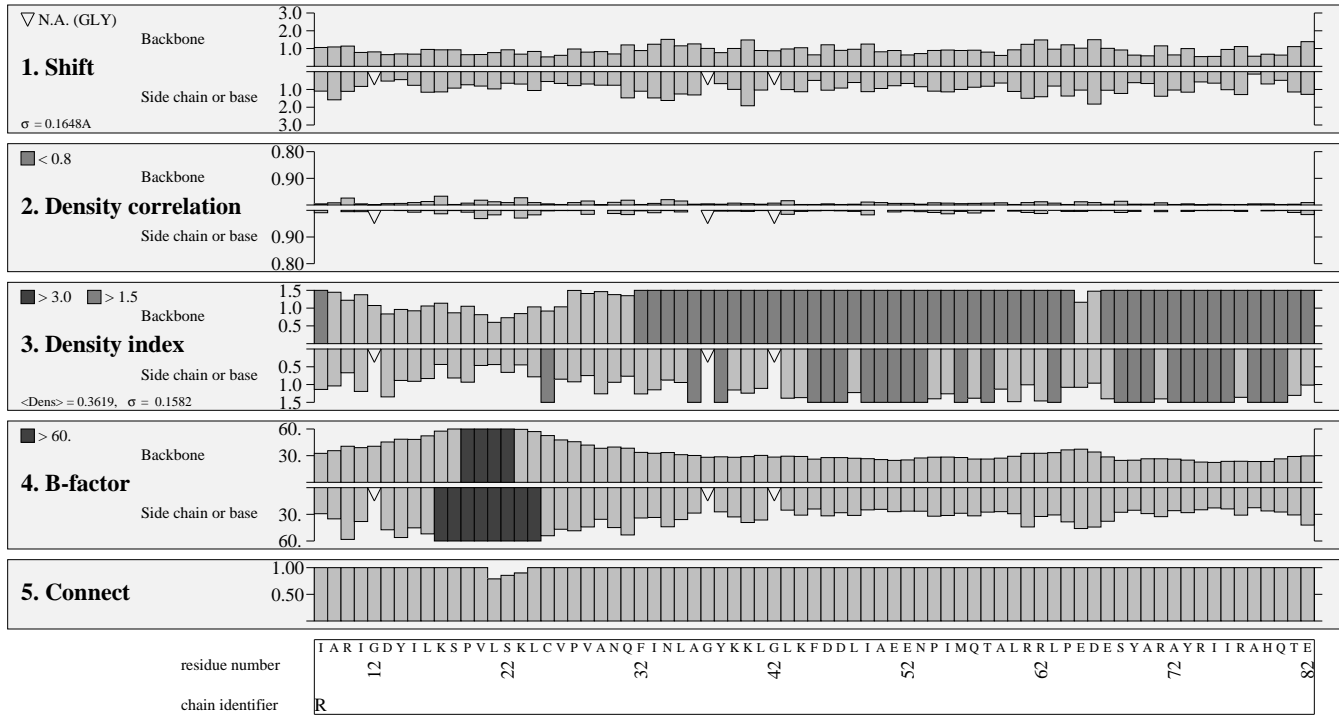
Local estimation (26) [N_omit = 2]



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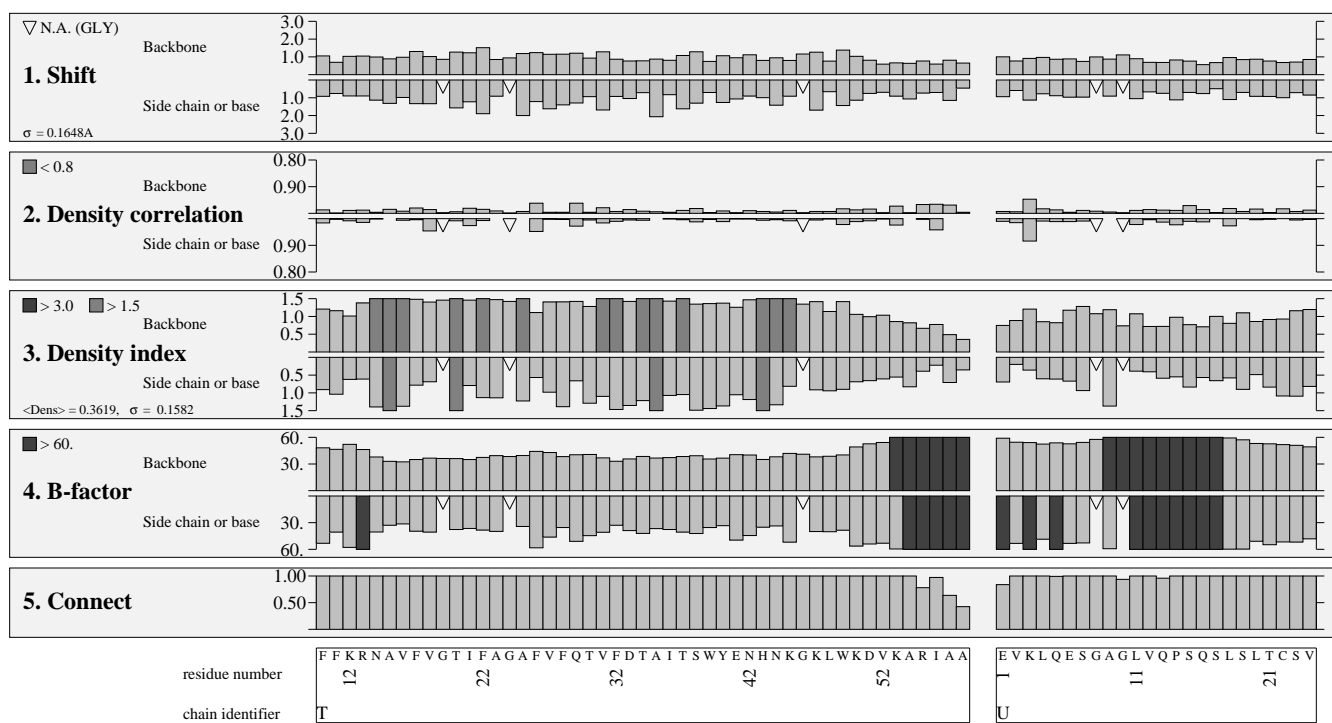
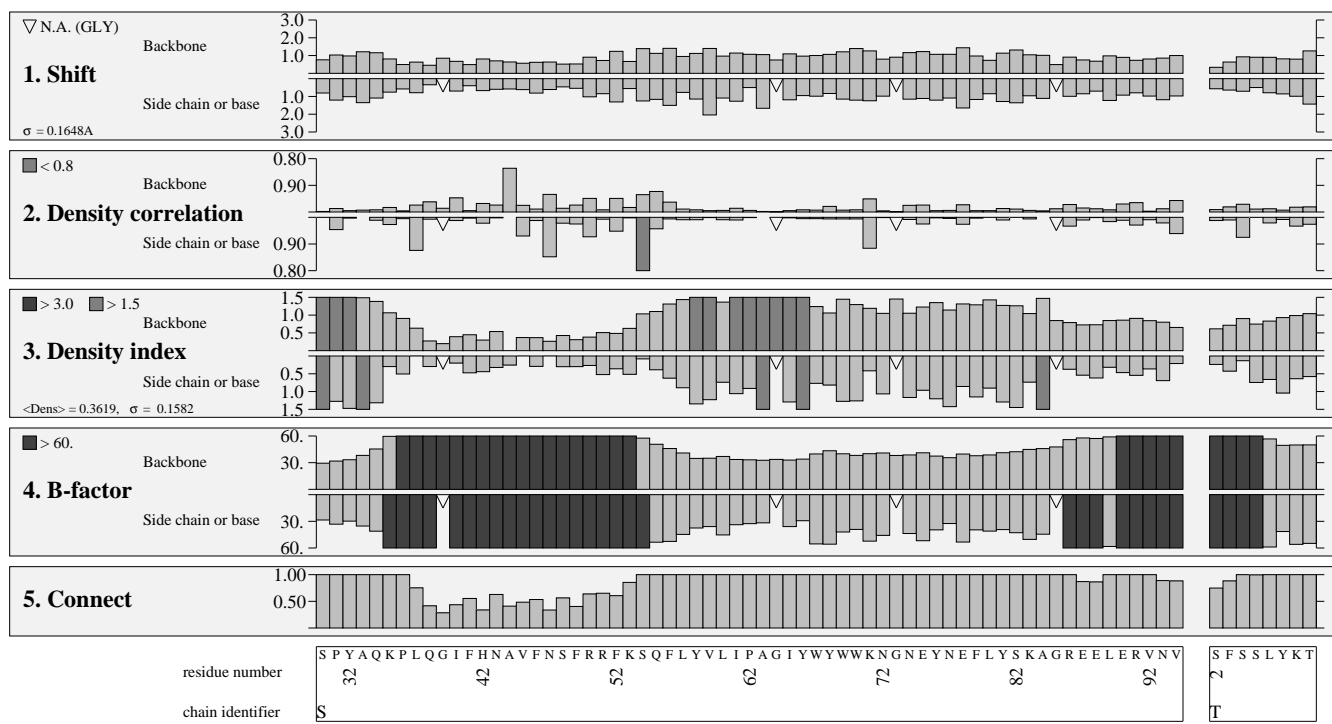
Local estimation (27) [N_omit = 2]



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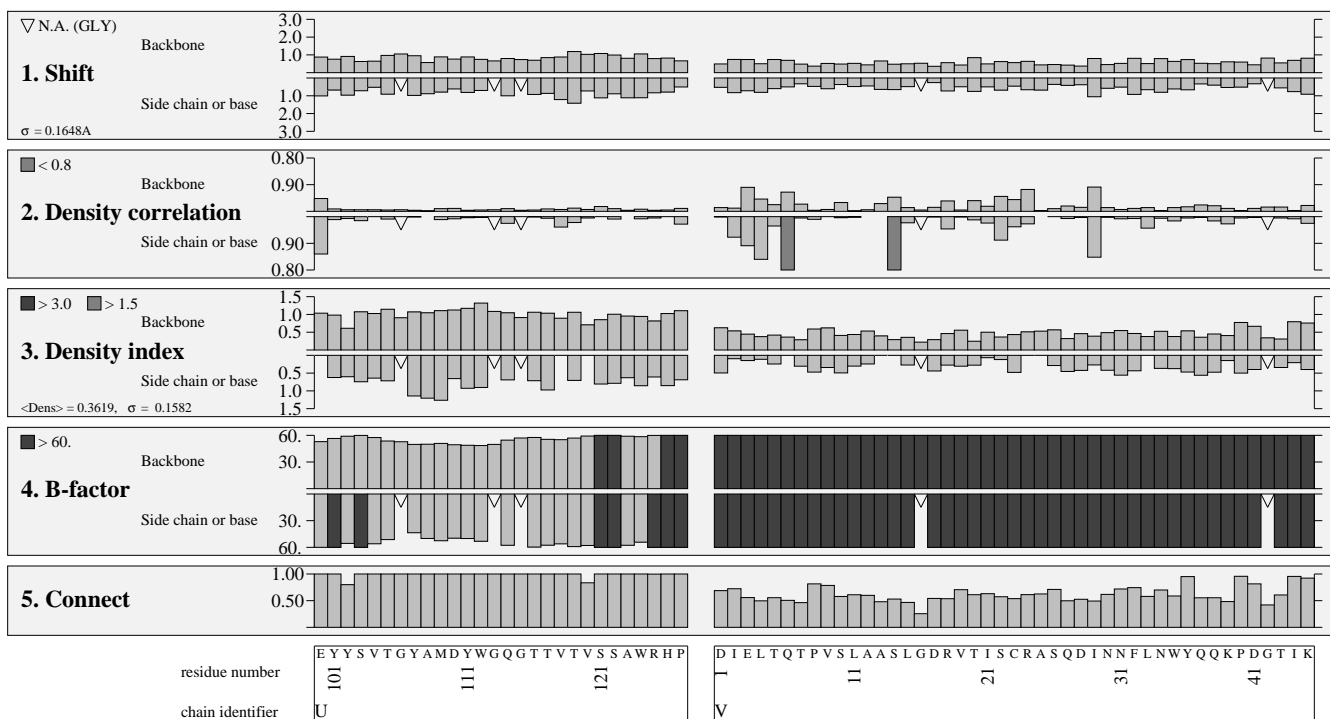
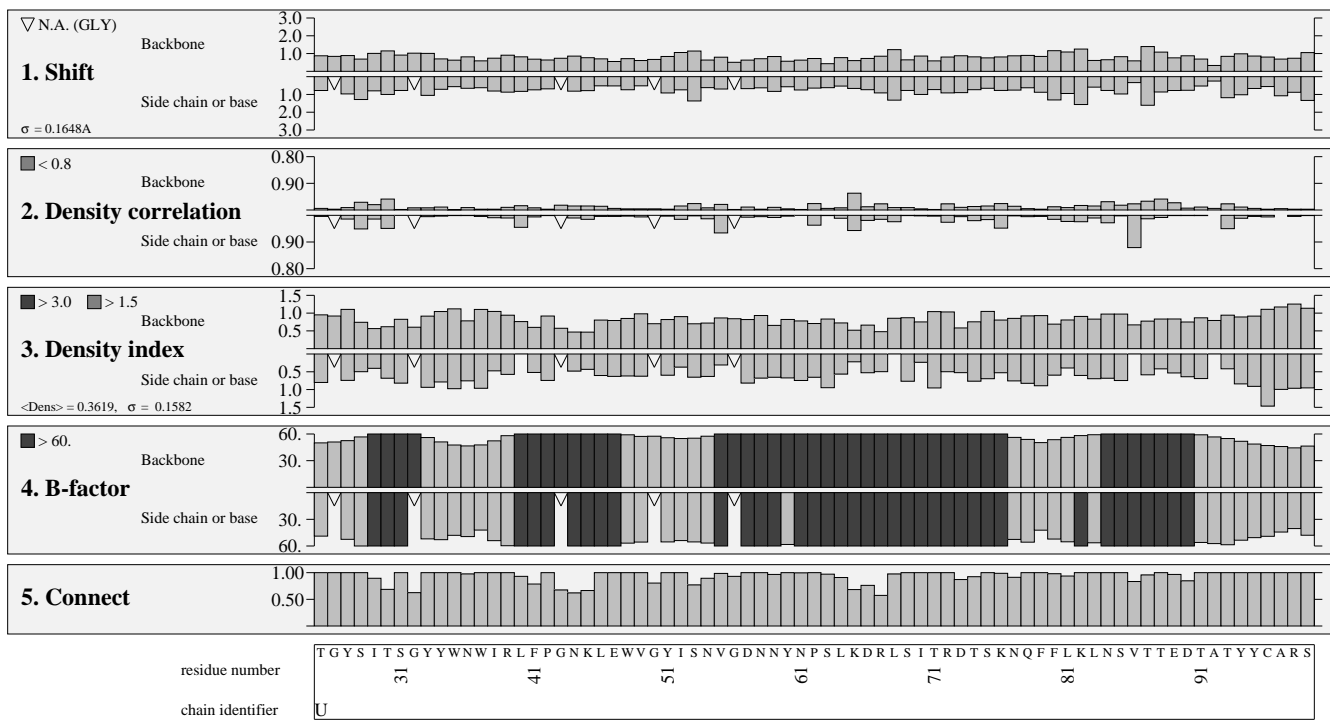
Local estimation (28) [N_omit = 2]



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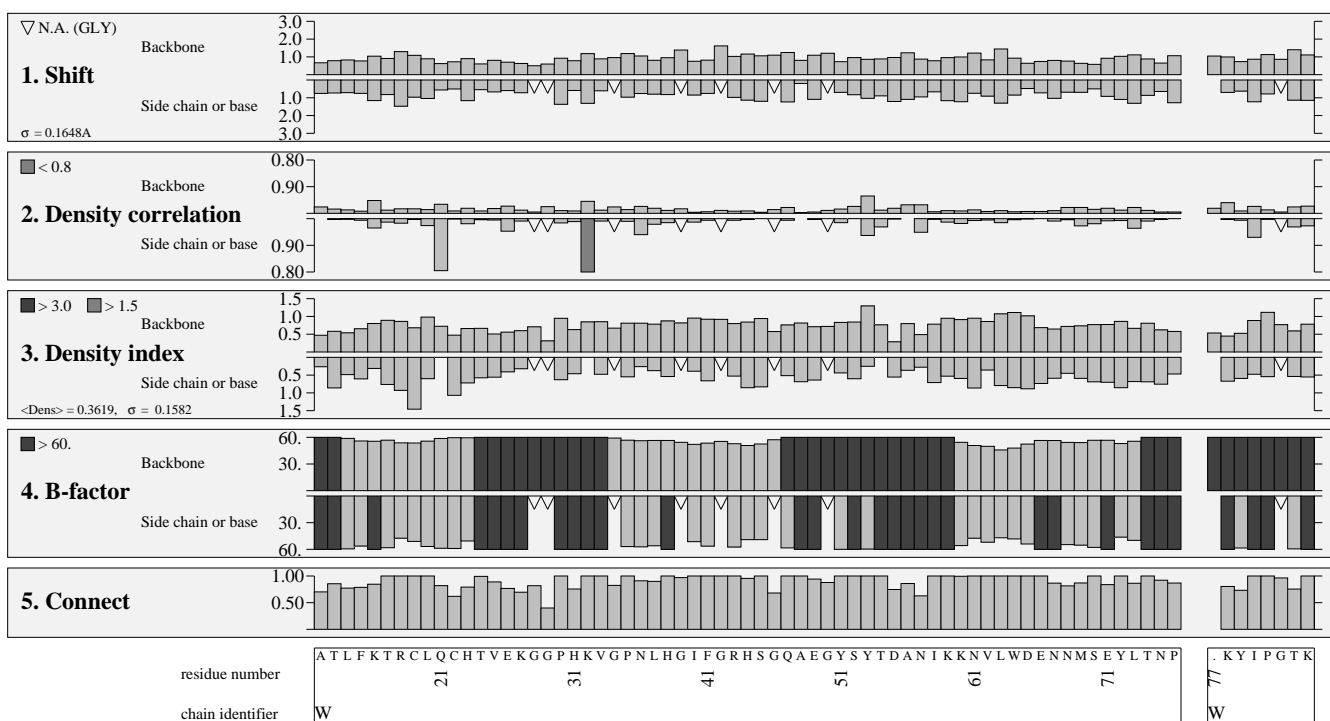
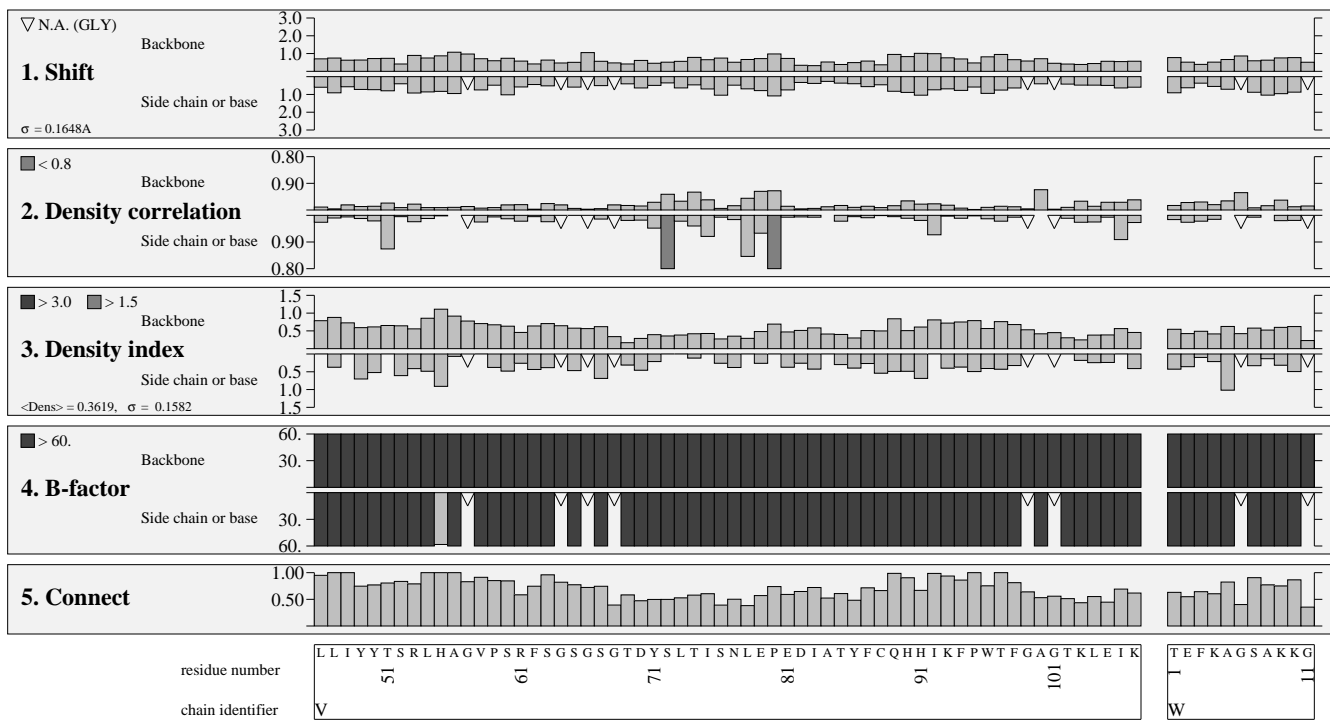
Local estimation (29) [N_omit = 2]



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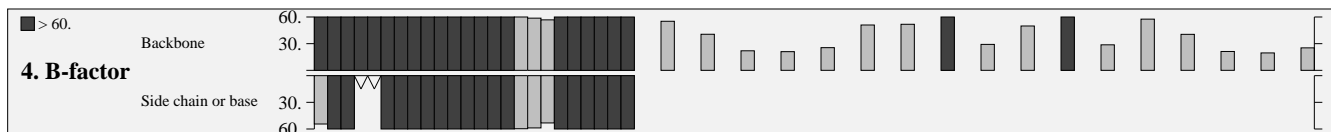
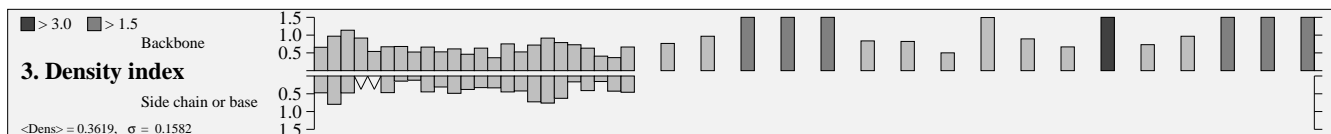
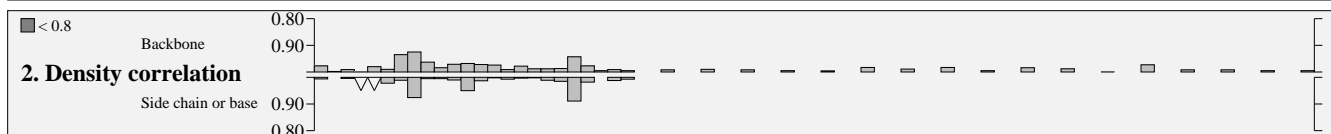
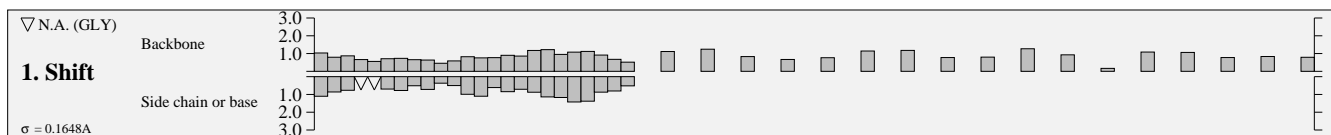
Local estimation (30) [N_omit = 2]



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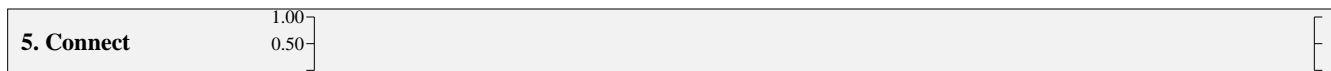
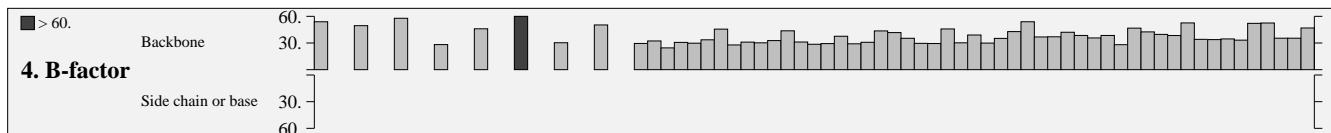
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Local estimation (31) [N_omit = 2]



residue number	M A F G G L K K E K D R N D L I T Y L K K A C E
chain identifier	W

Z_4013. Z_402. Z_4001. Z_4002. Z_4005. Z_4010. Z_4011. Z_4033. Z_4003. Z_4014. Z_4031. Z_4004. Z_4113. Z_412. Z_4021. Z_4022. Z_4025.

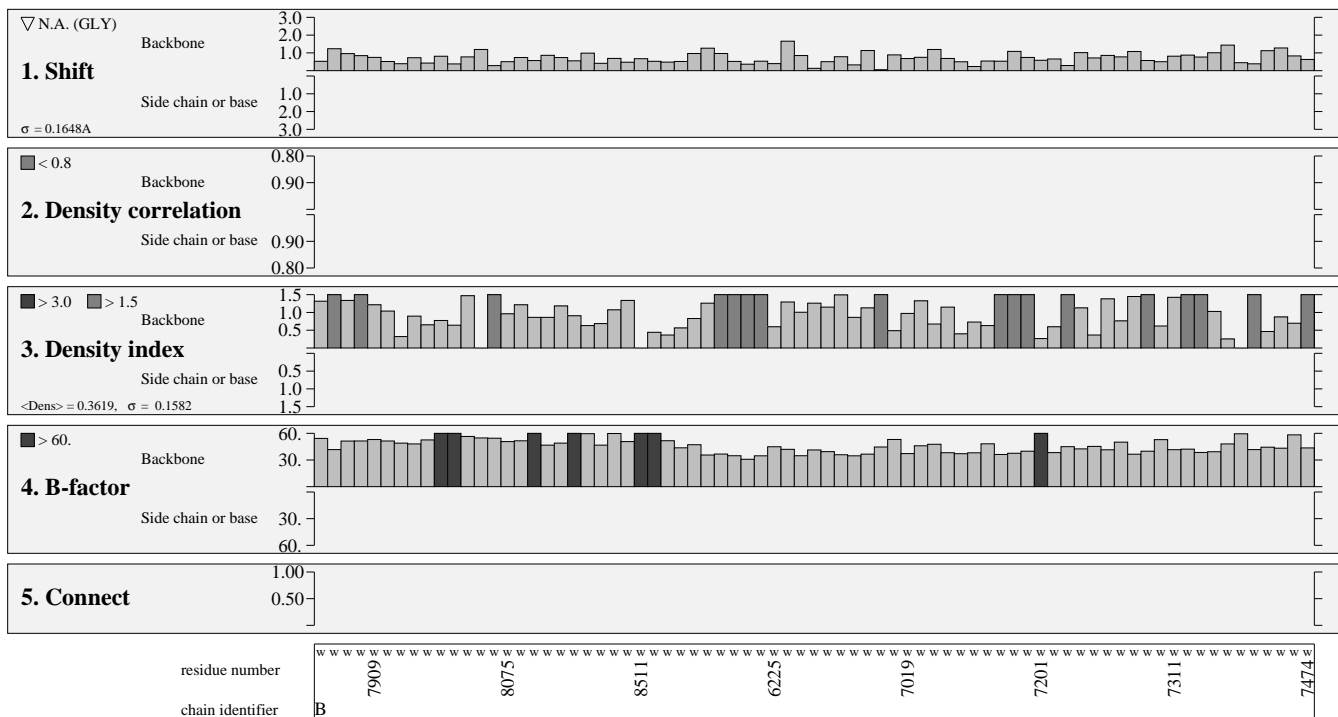
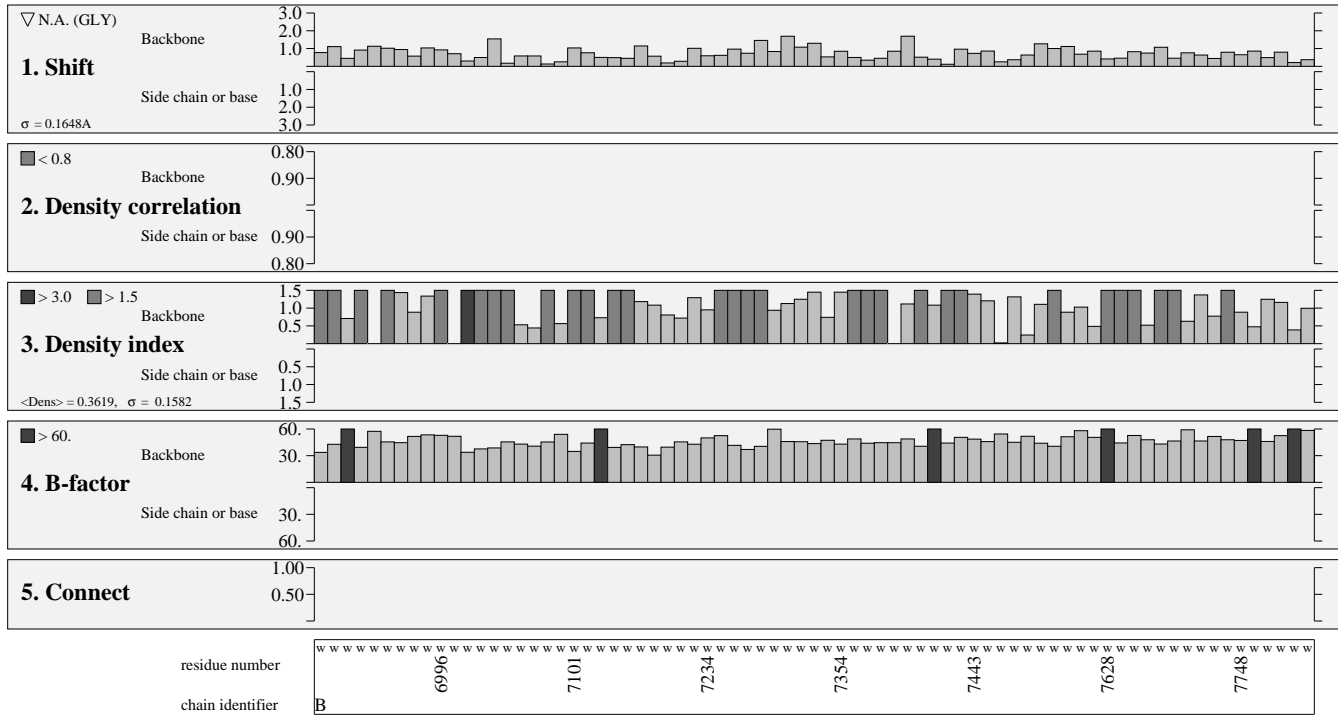


residue number	Z_4110. Z_4111. Z_4131. Z_4023. Z_4114. Z_4146. Z_4024. Z_4026.
chain identifier	Z_5006 Z_5096 Z_5168 Z_6252 Z_6496 Z_6650

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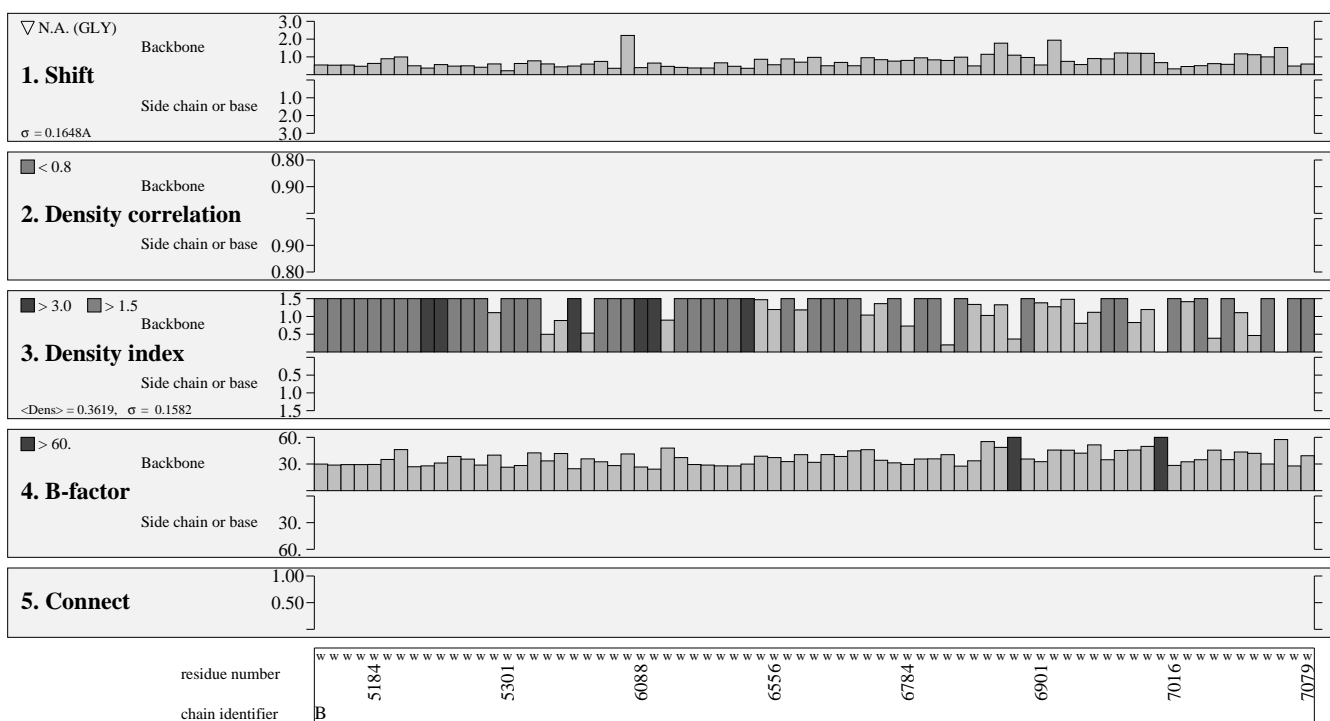
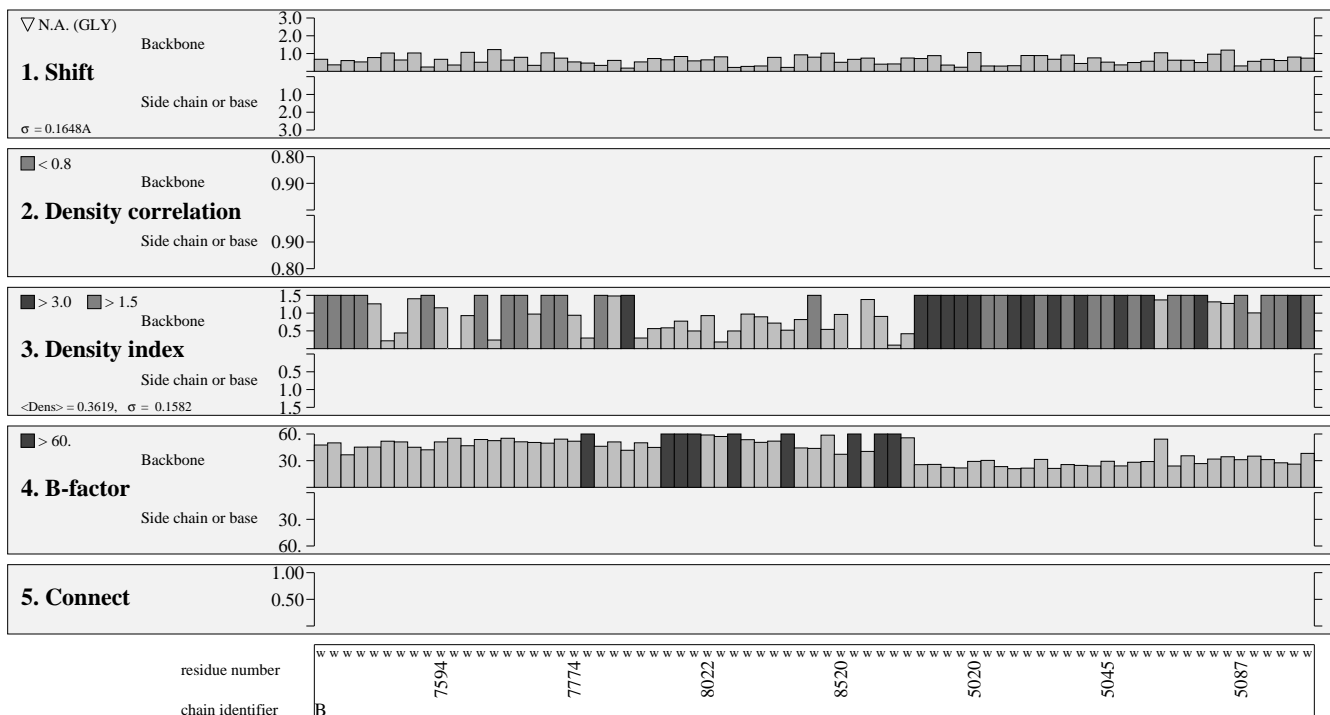
Local estimation (32) [N_omit = 2]



Structure Factor Check

3CX5

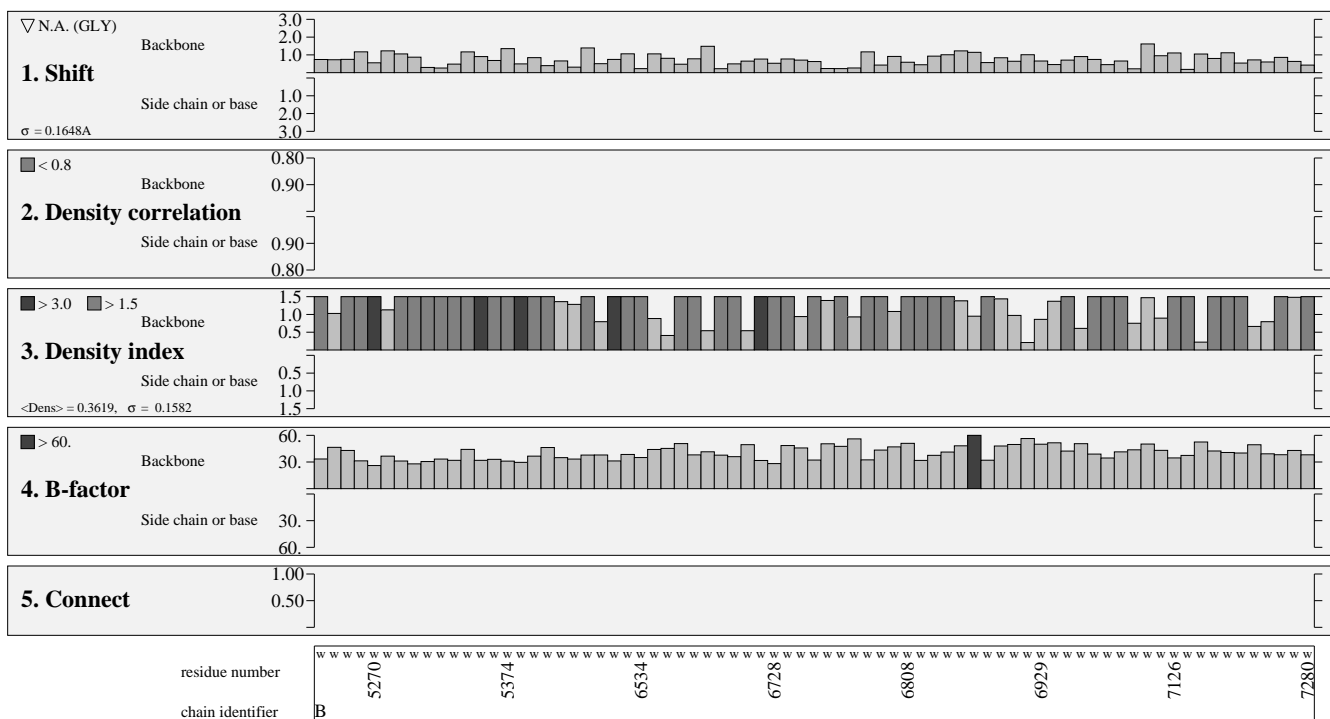
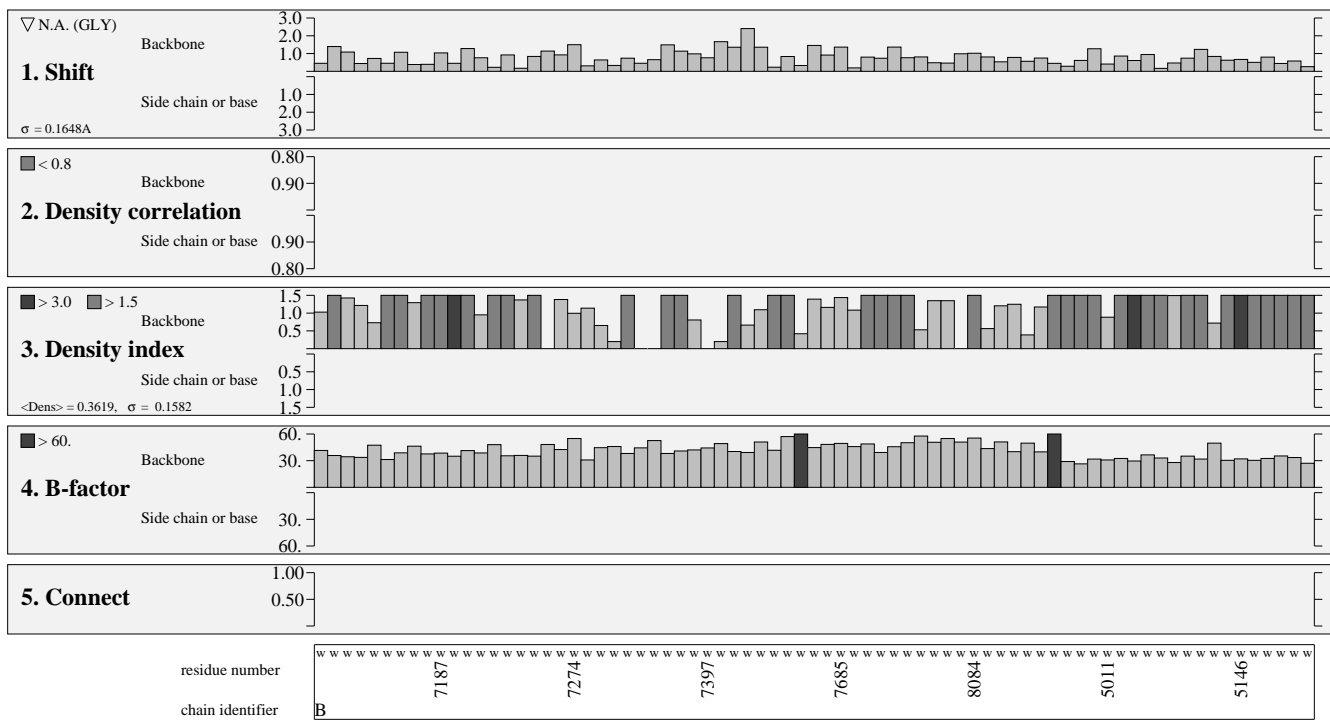
Local estimation (33) [N_omit = 2]



Structure Factor Check

3CX5

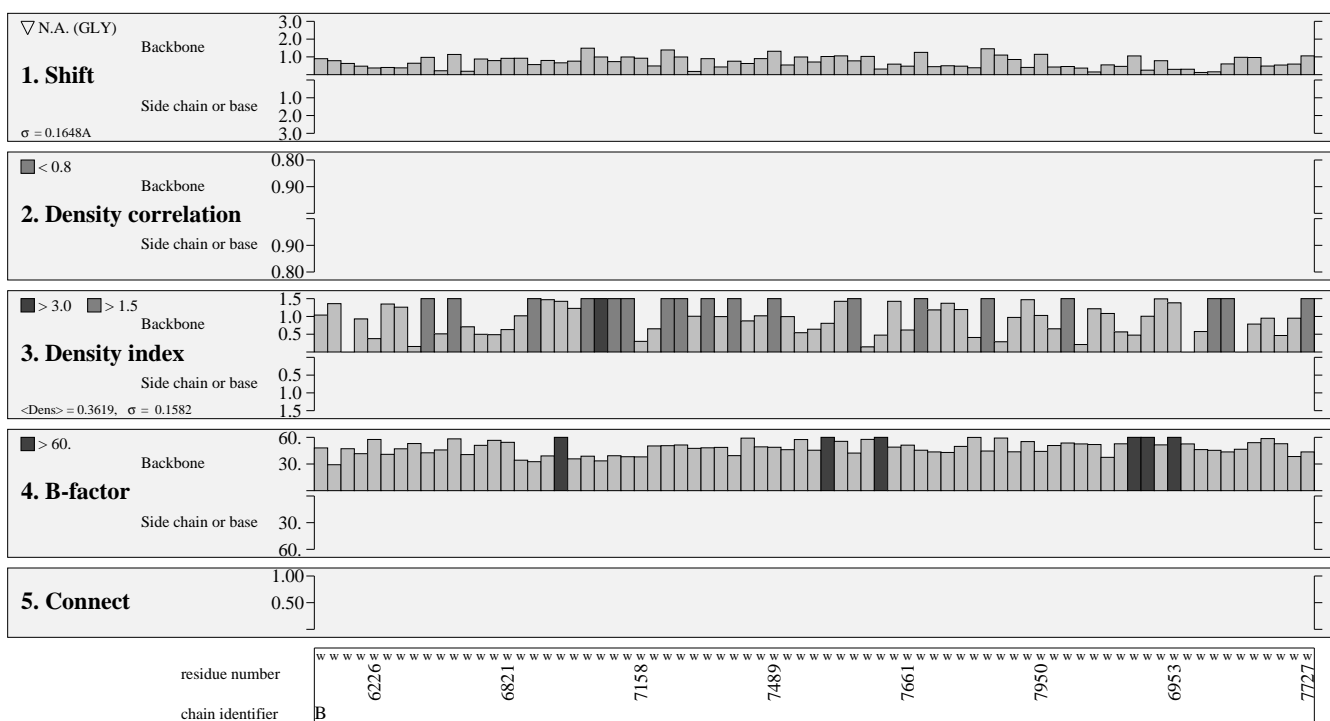
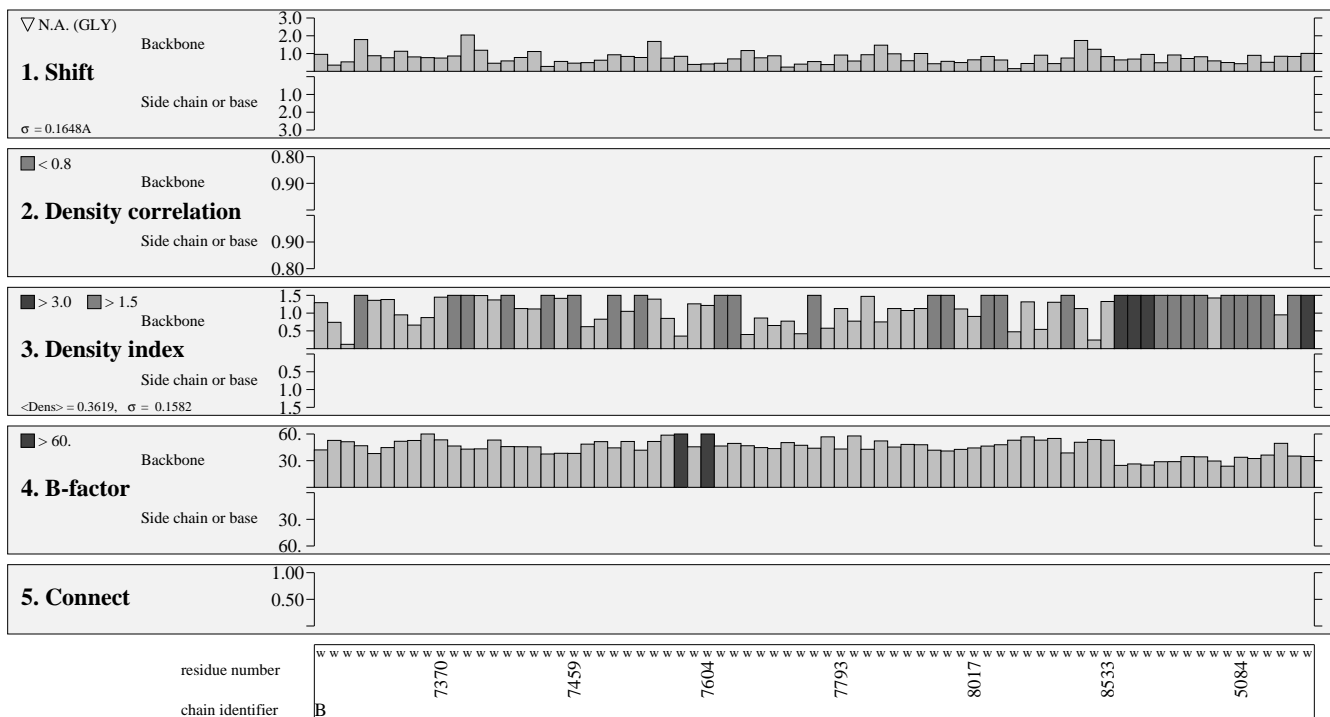
Local estimation (34) [N_omit = 2]



Structure Factor Check

3CX5

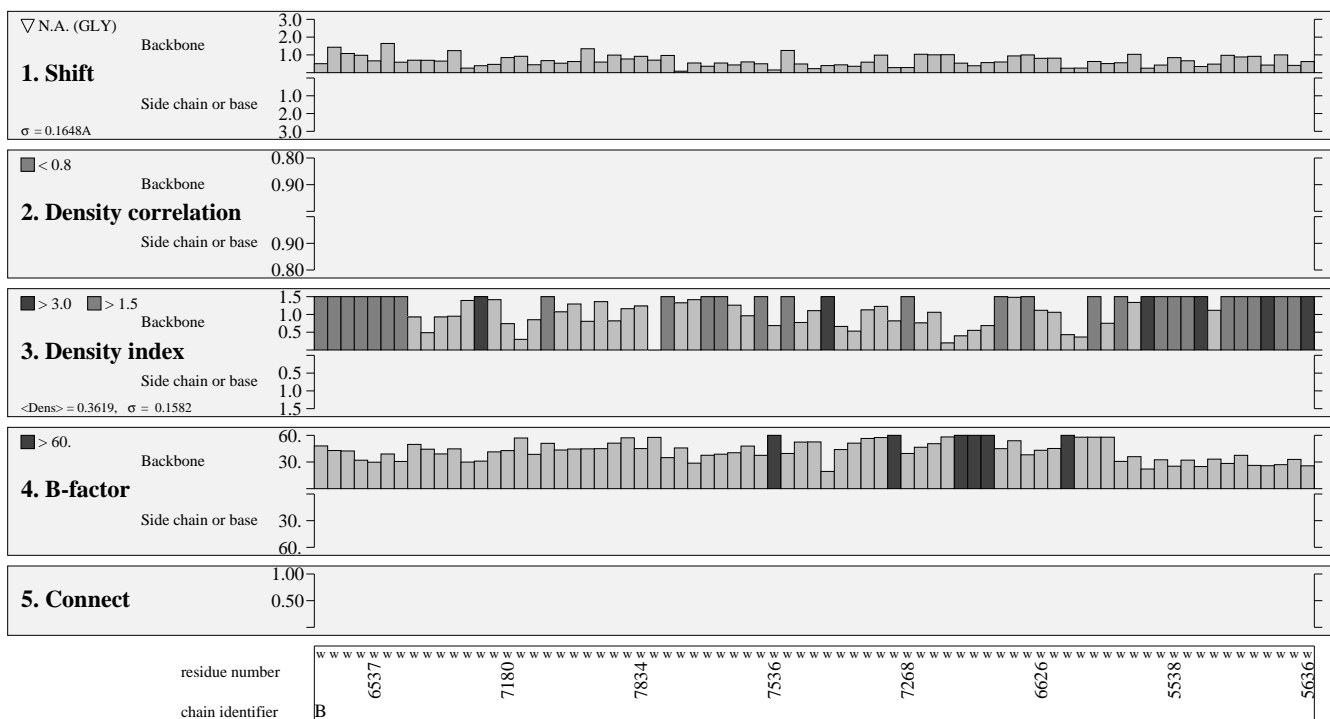
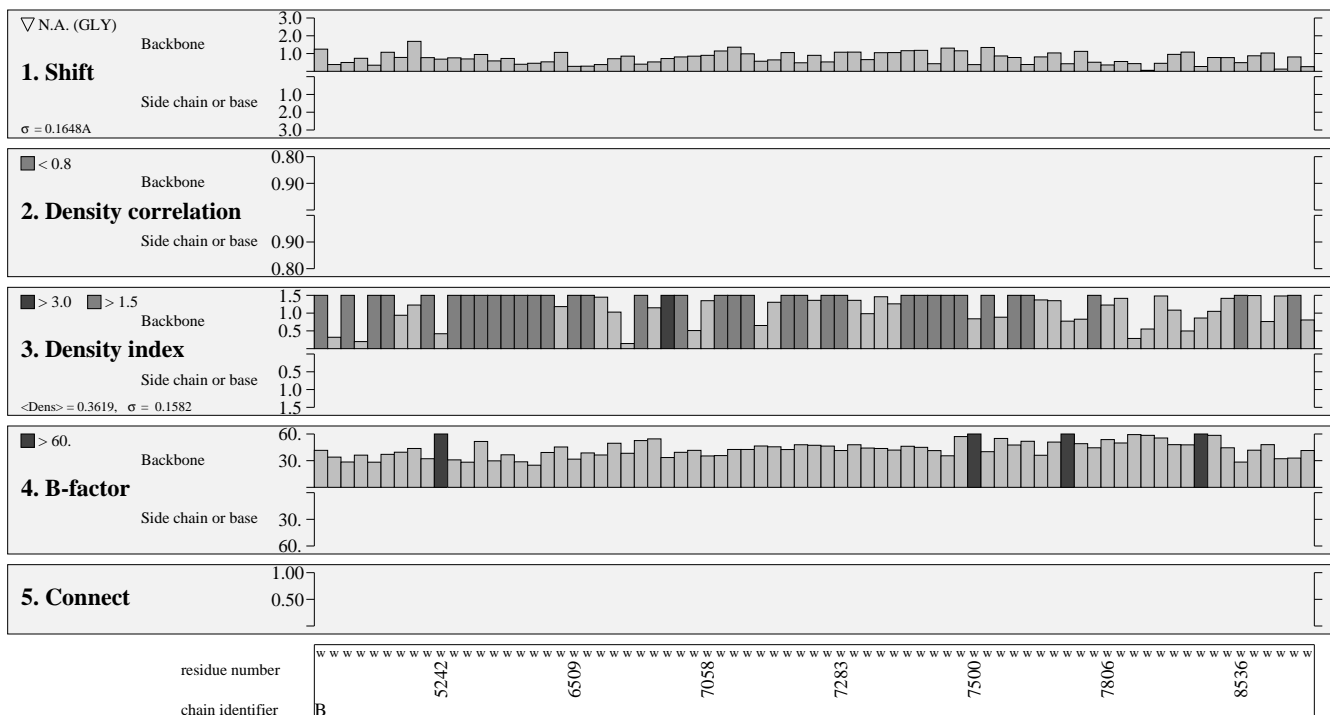
Local estimation (35) [N_omit = 2]



Structure Factor Check

3CX5

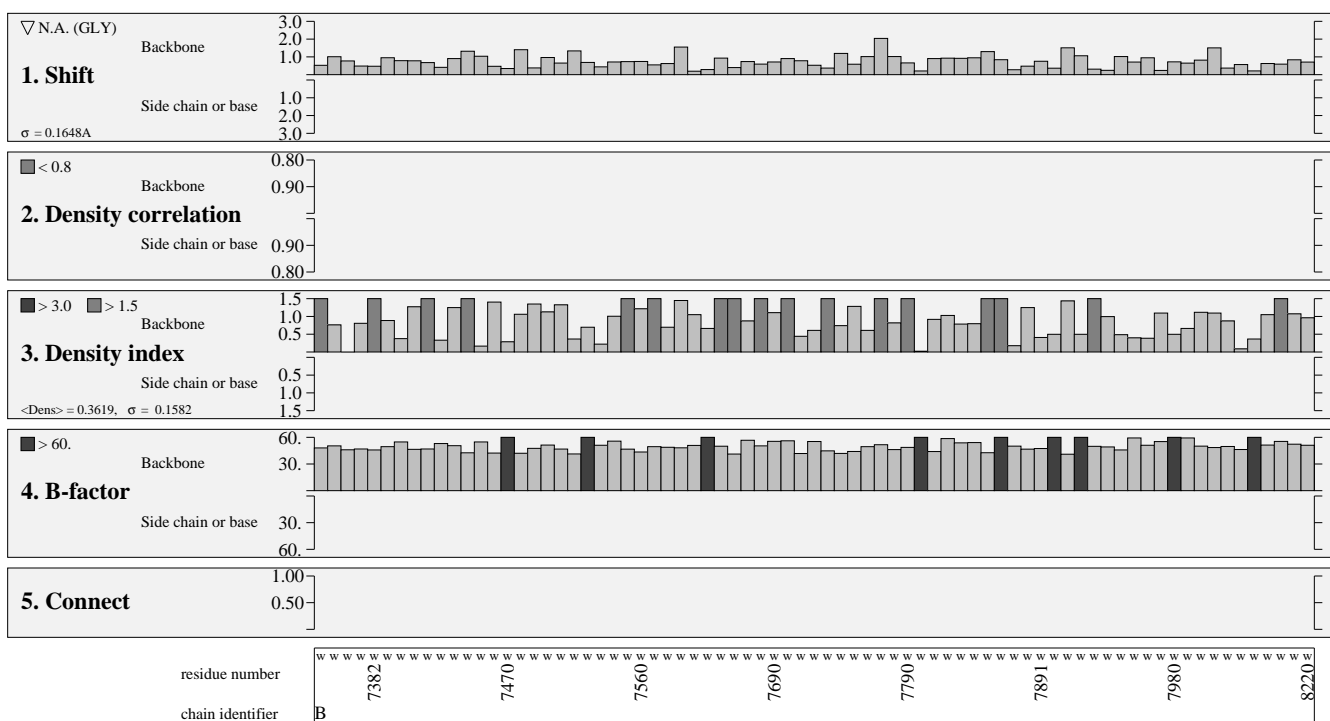
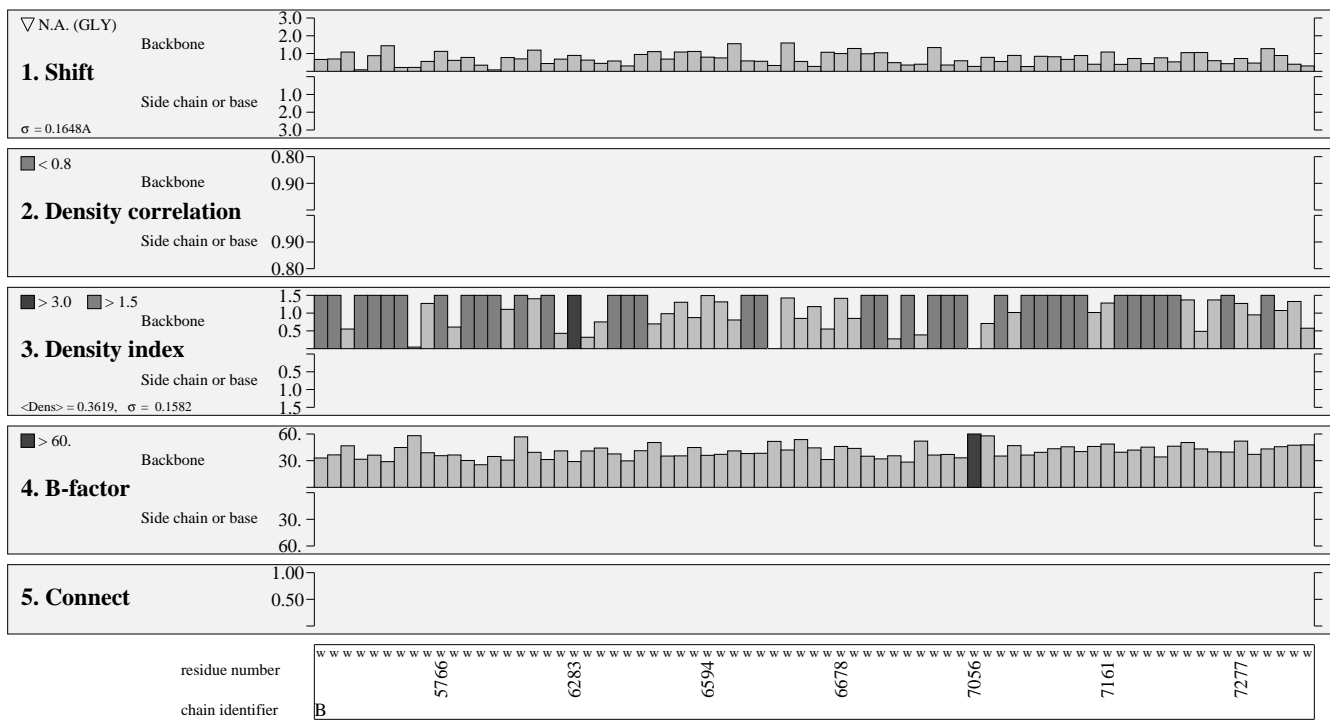
Local estimation (36) [N_omit = 2]



Structure Factor Check

3CX5

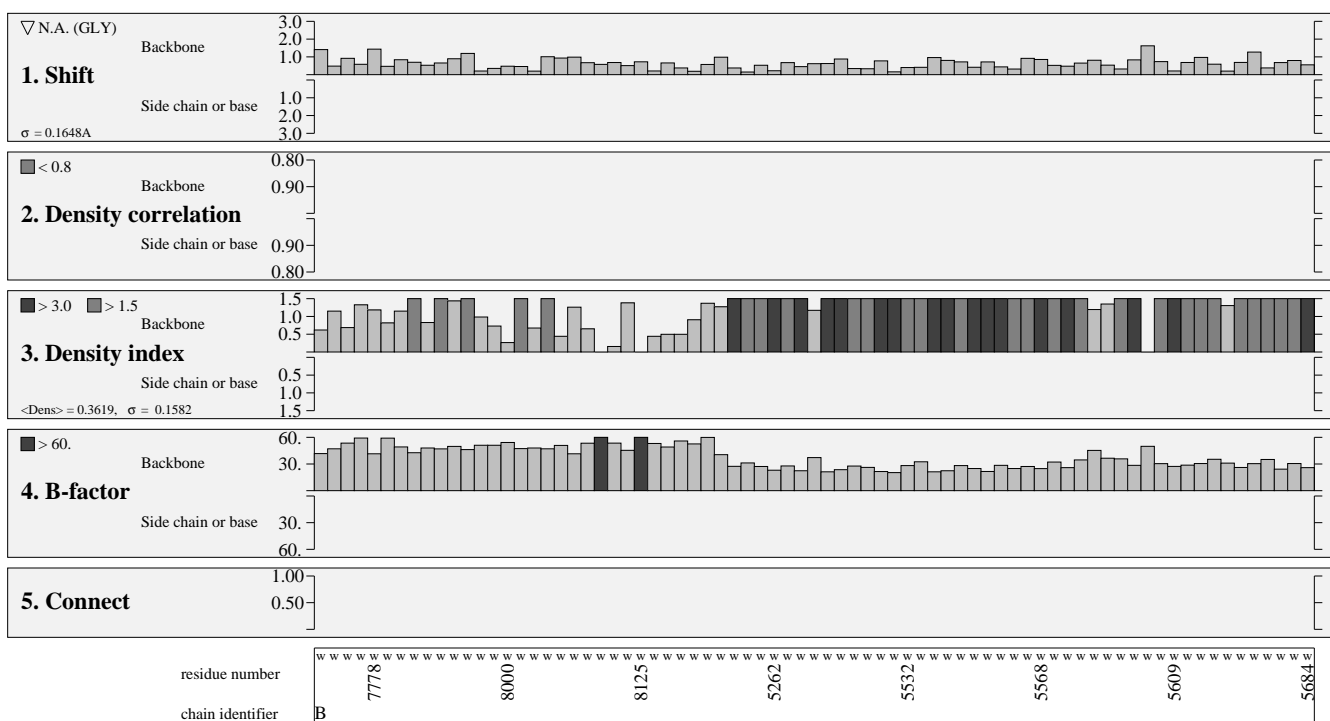
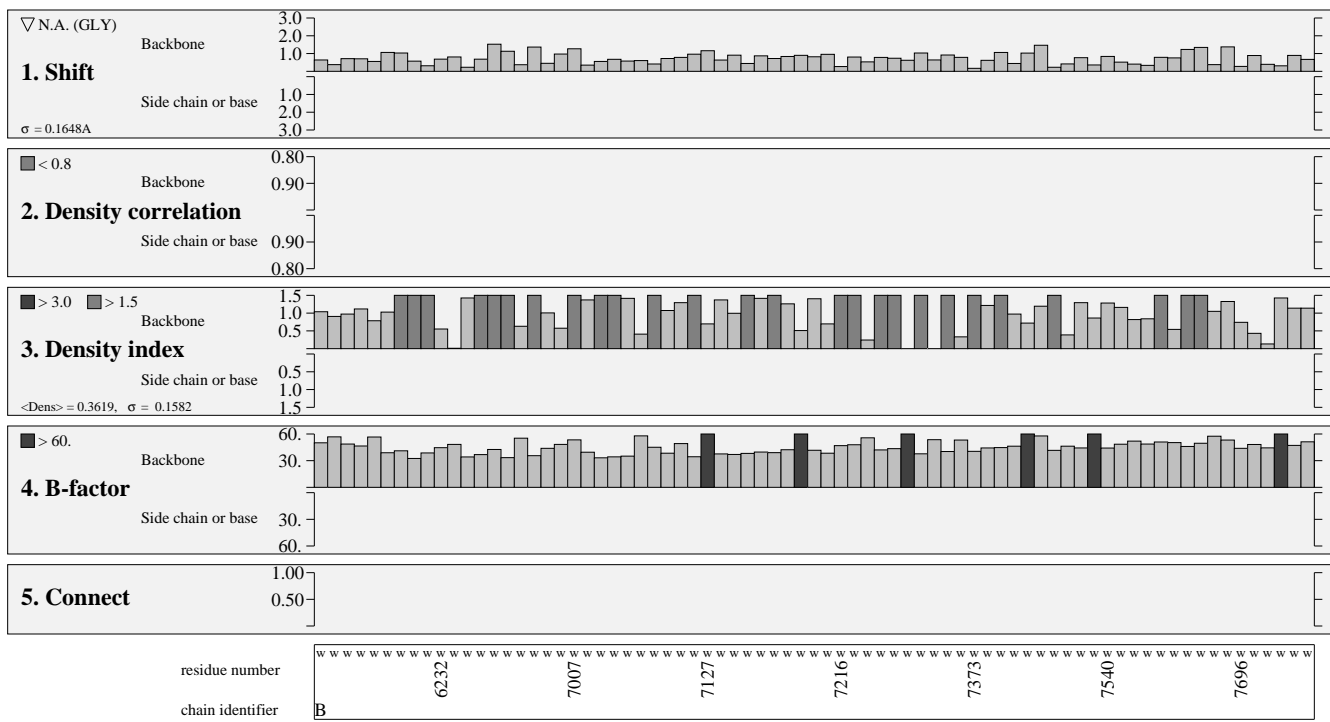
Local estimation (37) [N_omit = 2]



Structure Factor Check

3CX5

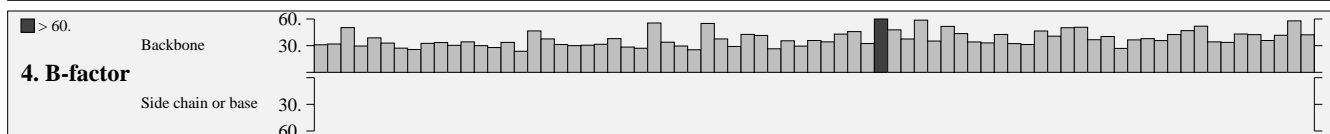
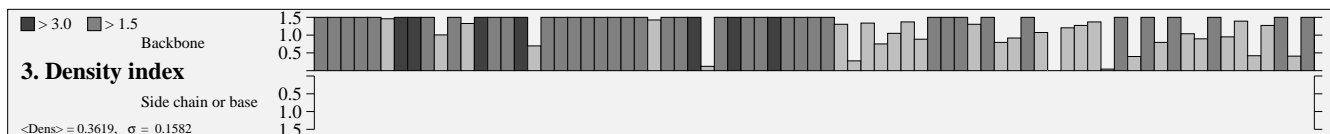
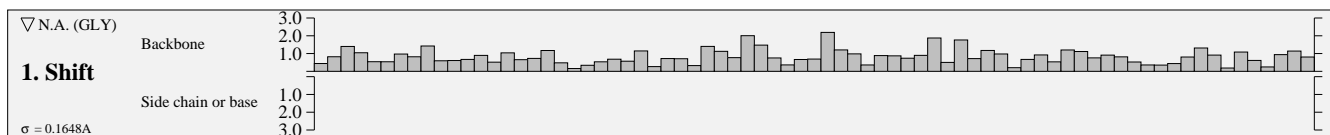
Local estimation (38) [N_omit = 2]



Structure Factor Check

3CX5

Local estimation (39) [N_omit = 2]

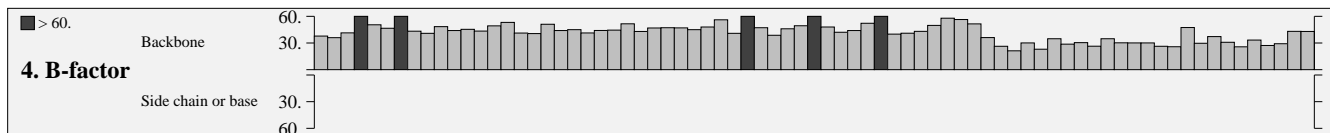
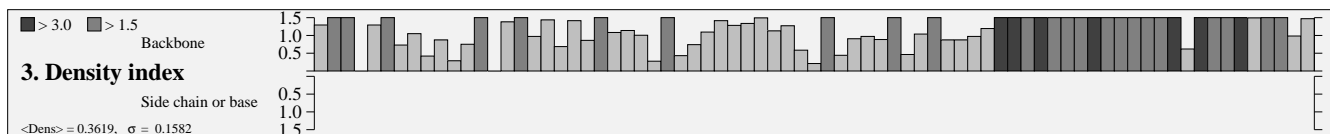
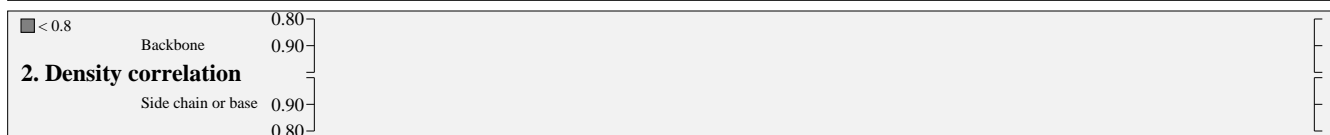
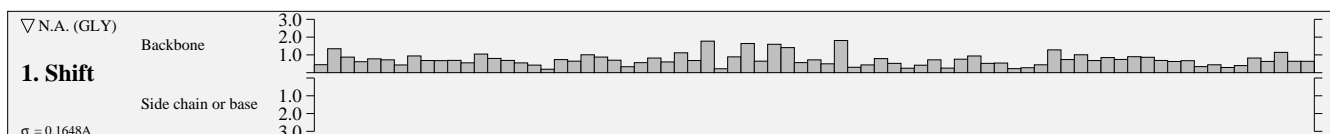


residue number

chain identifier

B

5761 5860 6544 6675 6955 6971 7196



residue number

chain identifier

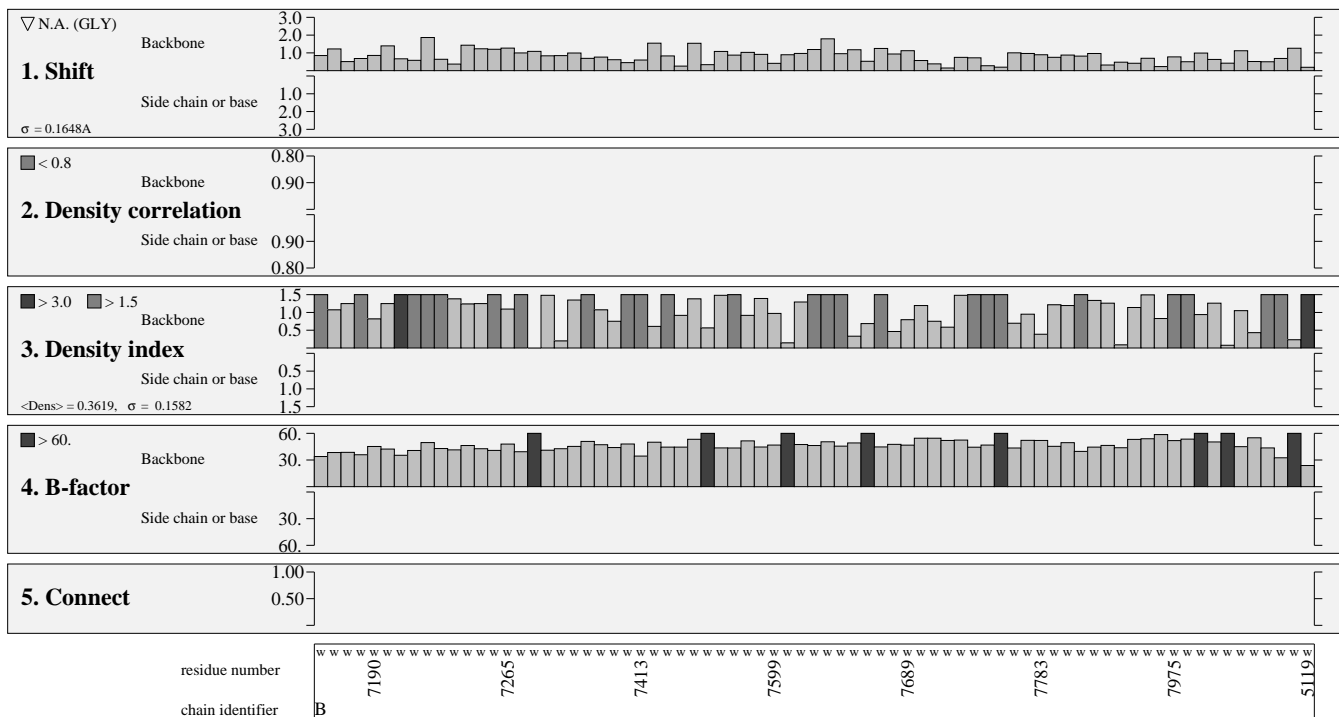
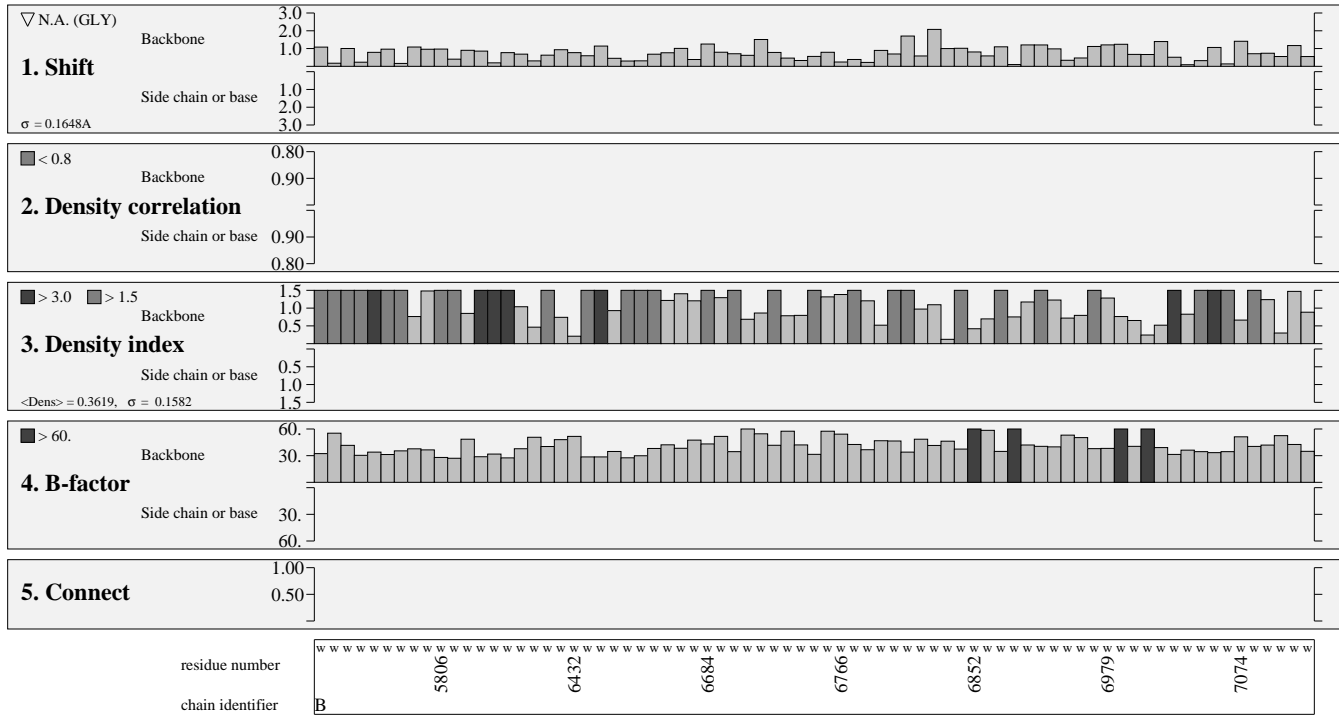
B

7341 7523 7680 7861 8078 5511 5612 5697

Structure Factor Check

3CX5

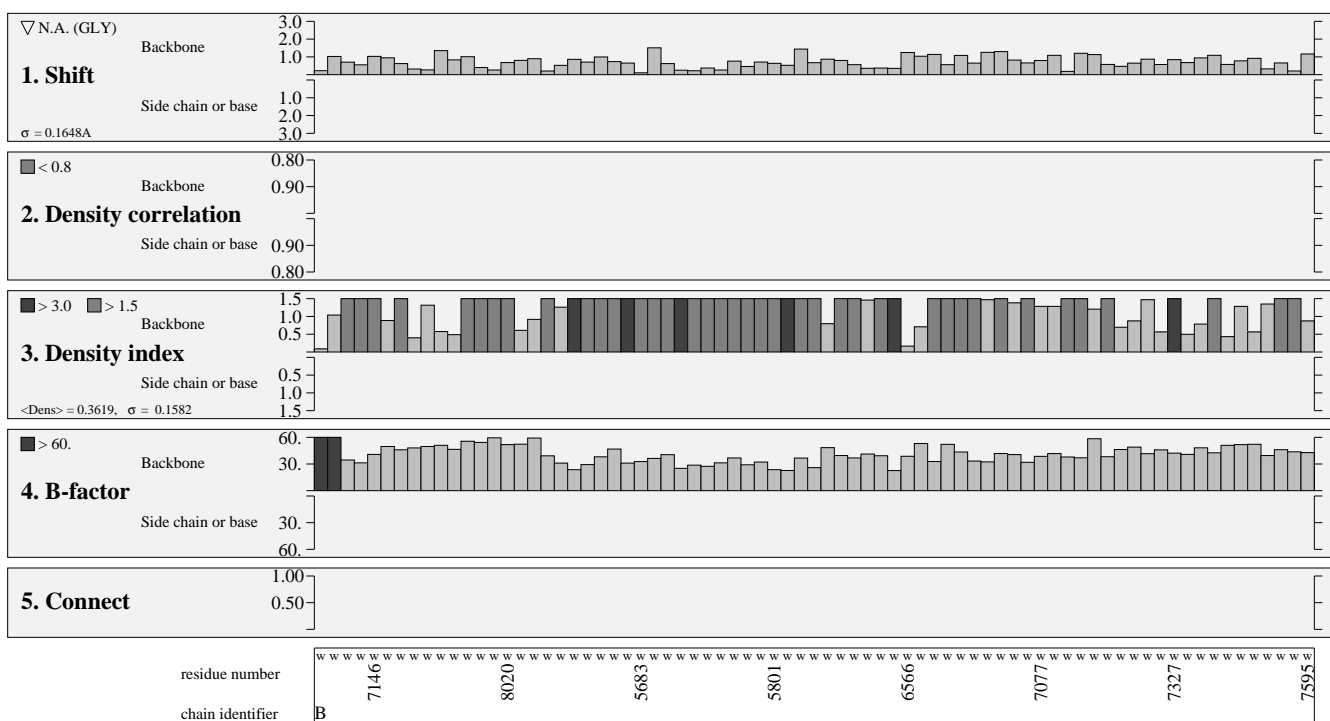
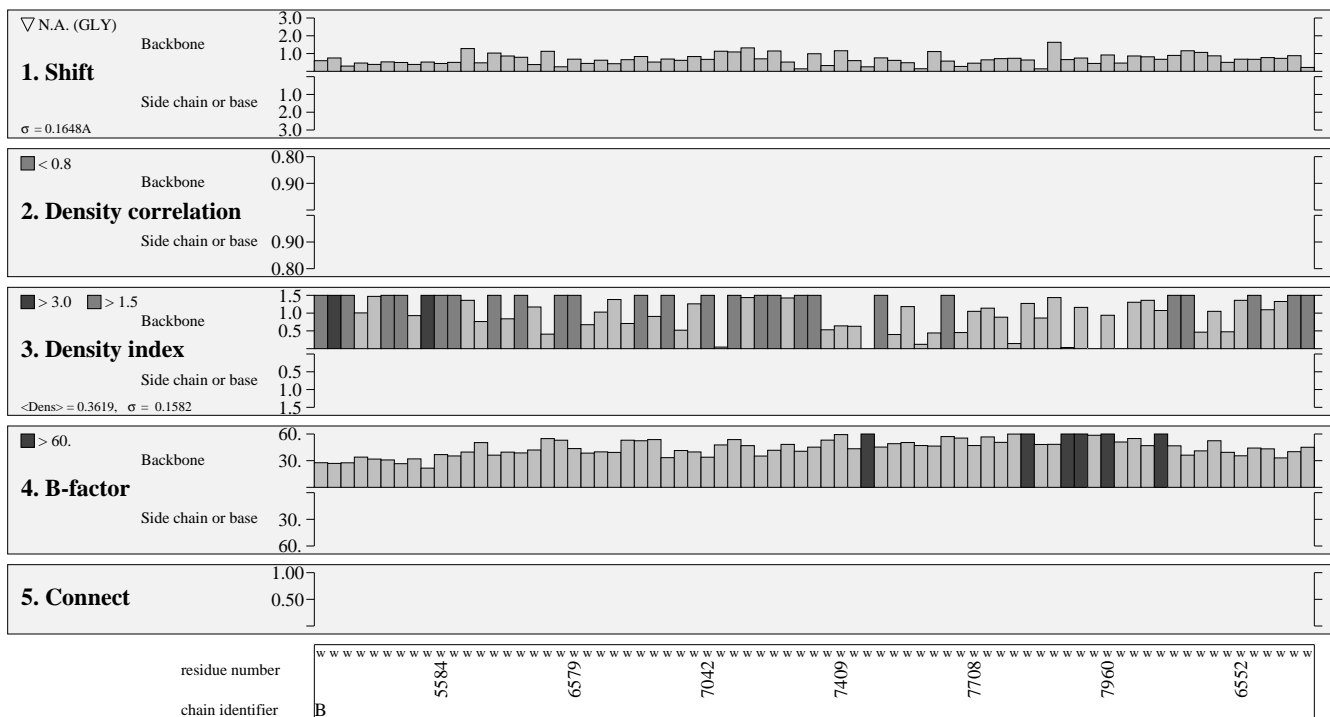
Local estimation (40) [N_omit = 2]



Structure Factor Check

3CX5

Local estimation (41) [N_omit = 2]



Structure Factor Check

3CX5

Local estimation (42) [N_omit = 2]

