

Structure Factor Check

4YSZ

Title: CRYSTAL STRUCTURE OF MITOCHONDRIAL RHODOQUINOL-FUMARATE REDU
 ASCARIS SUUM WITH 2-IODO-N-[3-(051-METHYLETHOXY(05PHENYL)BENZAM
 Date: 17-MAR-15
 PDB code: 4YSZ

Crystal

Cell parameters:

a: 123.93 A b: 126.97 A c: 219.34 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Number of NCS-operators: 2
 NC-symmetry only for information

Structure Factors

Input

Nominal resolution range: 29.8 – 3.30 A
 Reflections in file: 52775
 Unique reflections above 0: 51443
 above 1 σ : 50561
 above 3 σ : 37715
 Reflections > 0: 1332

SFCHECK

Nominal resolution range: 29.8 – 3.30 A
\05max. from input data, min. from author\05
 Used reflections: 51430
 Reflections out of resolution: 13
 Completeness: 97.5 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.068
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.9350 0.9202 1.0000
 B_{overall} (by Patterson): 52. A²
 Optical resolution: 2.33 A
 Expected opt. resol. for complete data set: 2.33 A
 Estimated minimal error: 0.072 A

Model

18361 atoms (15 water molecules)
 Number of chains: 30
 Volume not occupied by model: 54.7 %
 $\langle B \rangle$ (for atomic model): 61.4 A²
 $\sigma(B)$: 14.60 A²
 Matthews coefficient: 3.36
 Corresponding solvent % : 63.07

Model vs. Structure Factors

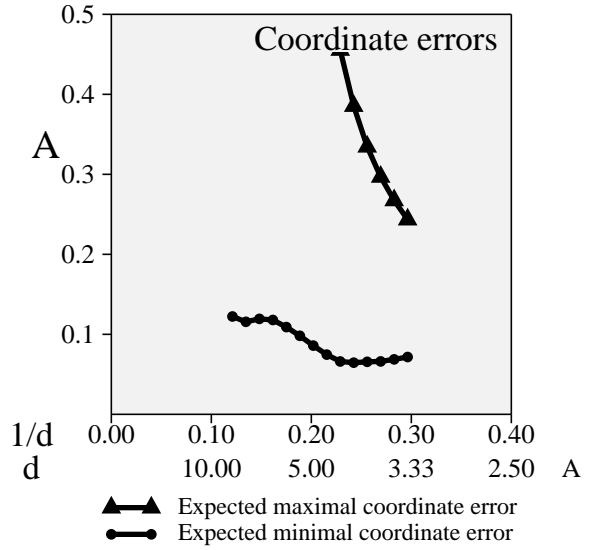
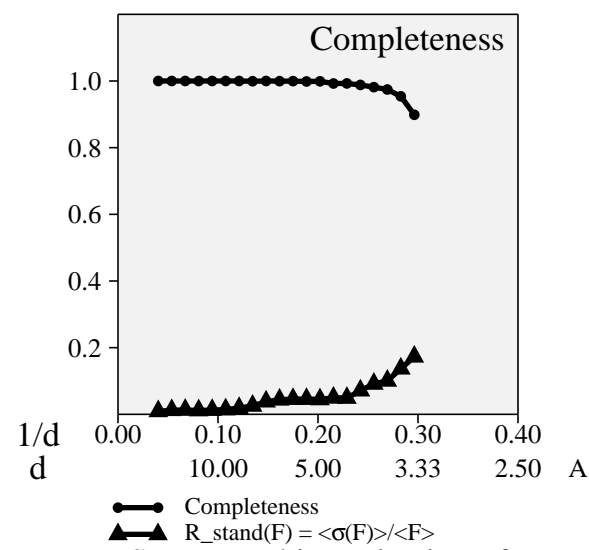
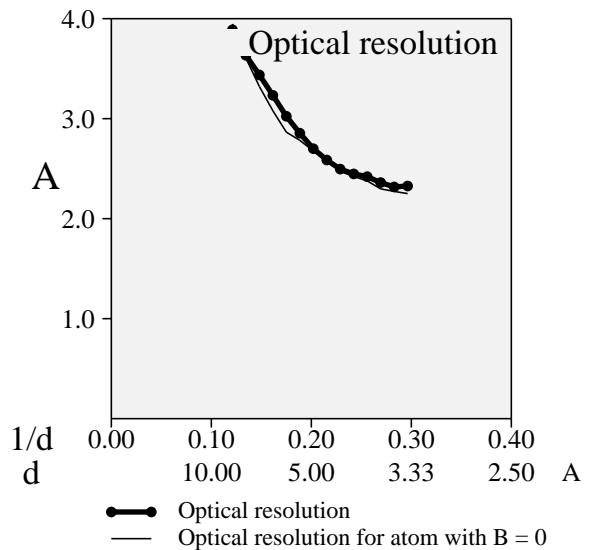
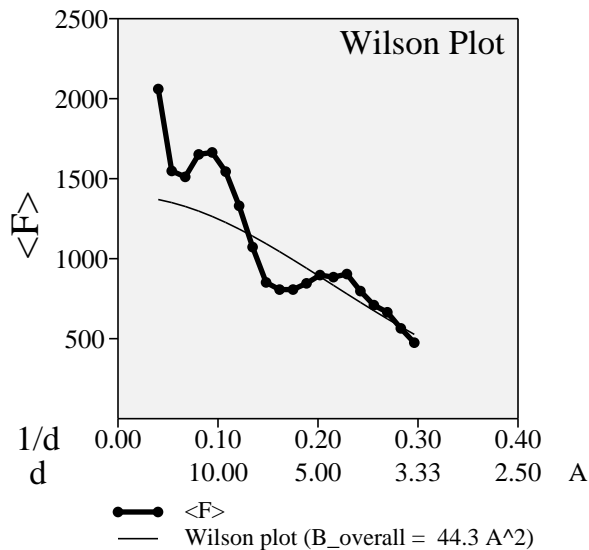
R-factor for all reflections: 0.240
 Correlation factor: 0.844
 R-factor: 0.250
 for $F > 2.0\sigma$
 nom. resolution range: 29.82 – 3.30A
 reflections used: 50549
 Rfree: 0.304
 Nfree: 2580
 R-factor without free-refl.: 0.247
 Non free-reflections: 47969
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.496 A
 Estimated maximal error: 0.243 A
 DPI: 0.497 A
Scaling
 Scale: 0.897
 Bdiff: -3.72
 Anisothermal Scaling (Beta):
 -2.7378 -2.7590 -2.5170 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.521 249.824

Refinement

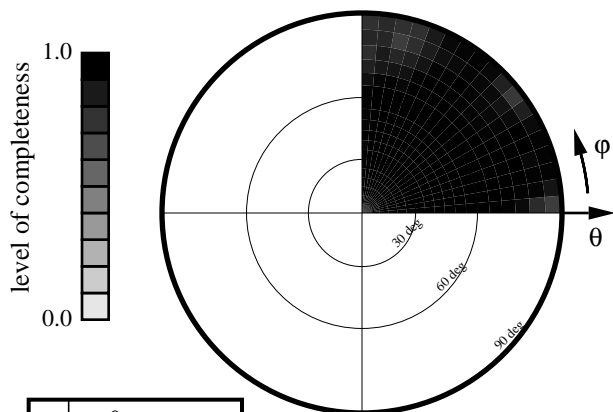
Program: REFMAC 5.7.0029
 Nominal resolution range: 29.8 – 3.30 A
 Reported R-factor: 0.179
 Number of reflections used: 48822
 Reported Rfree: 0.25
 Sigma cut-off: N.A.

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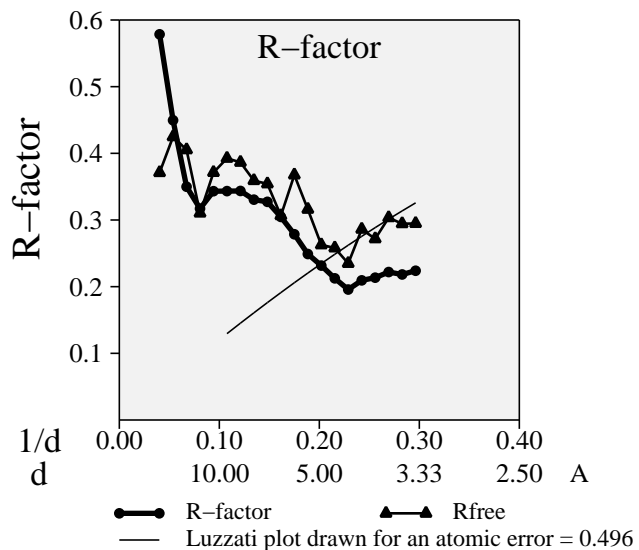


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

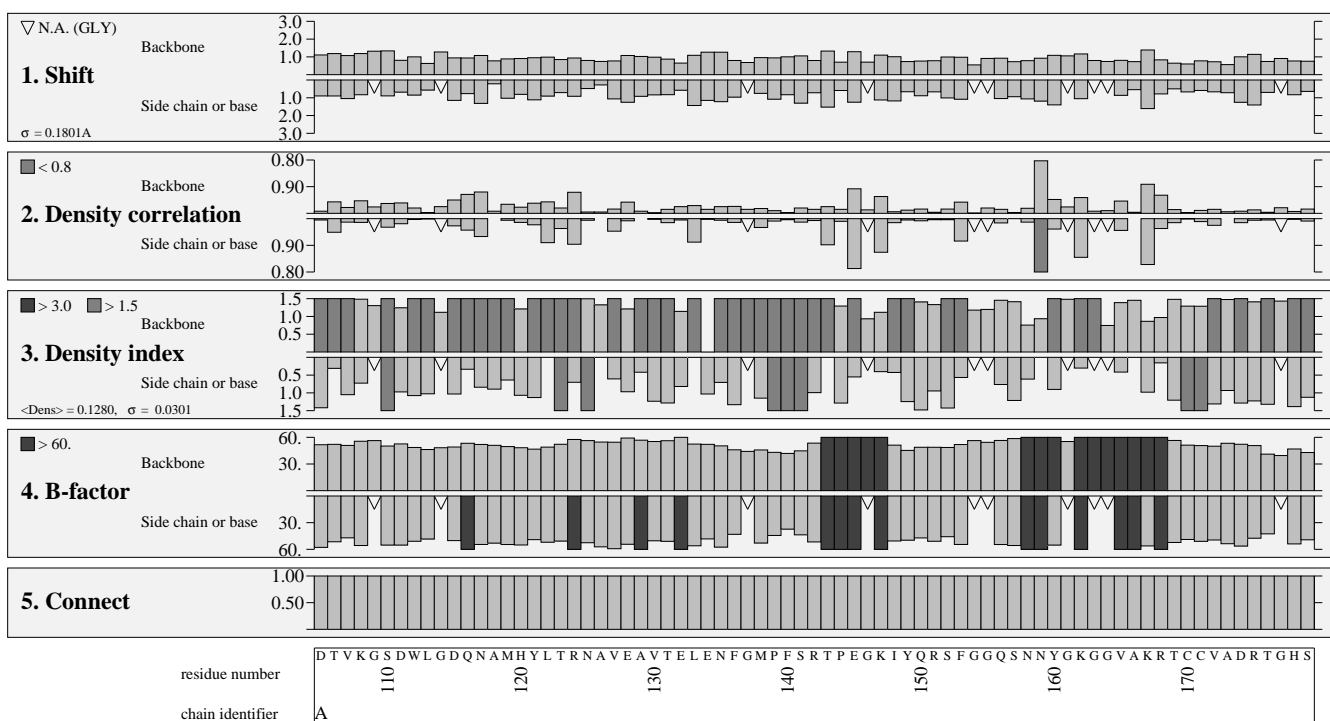
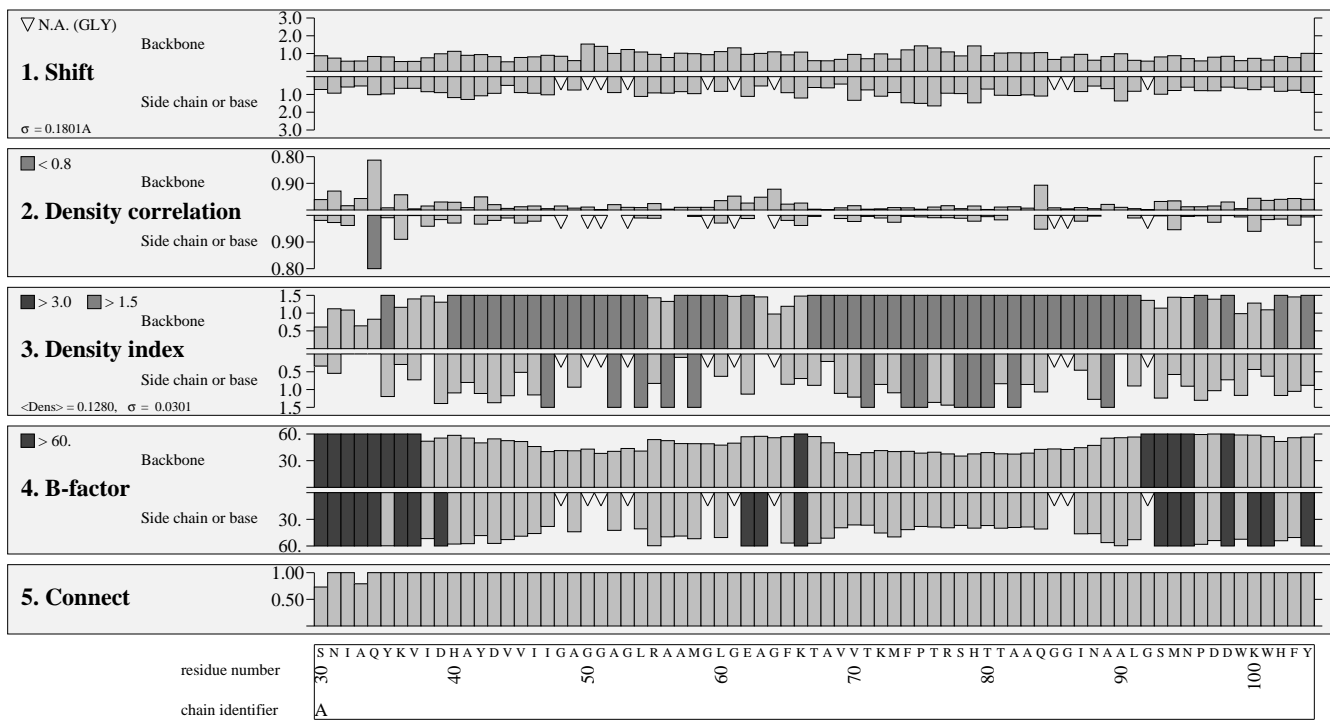
polar coordinates of the crystallographical axes



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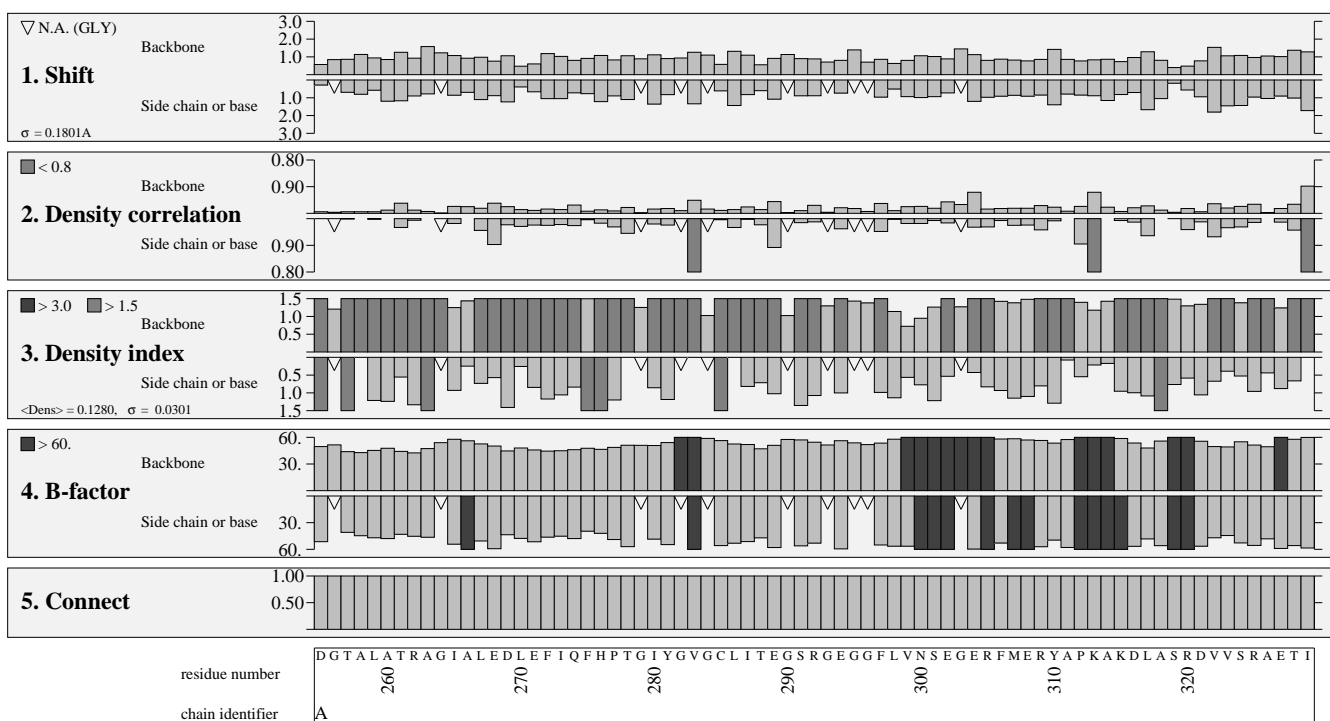
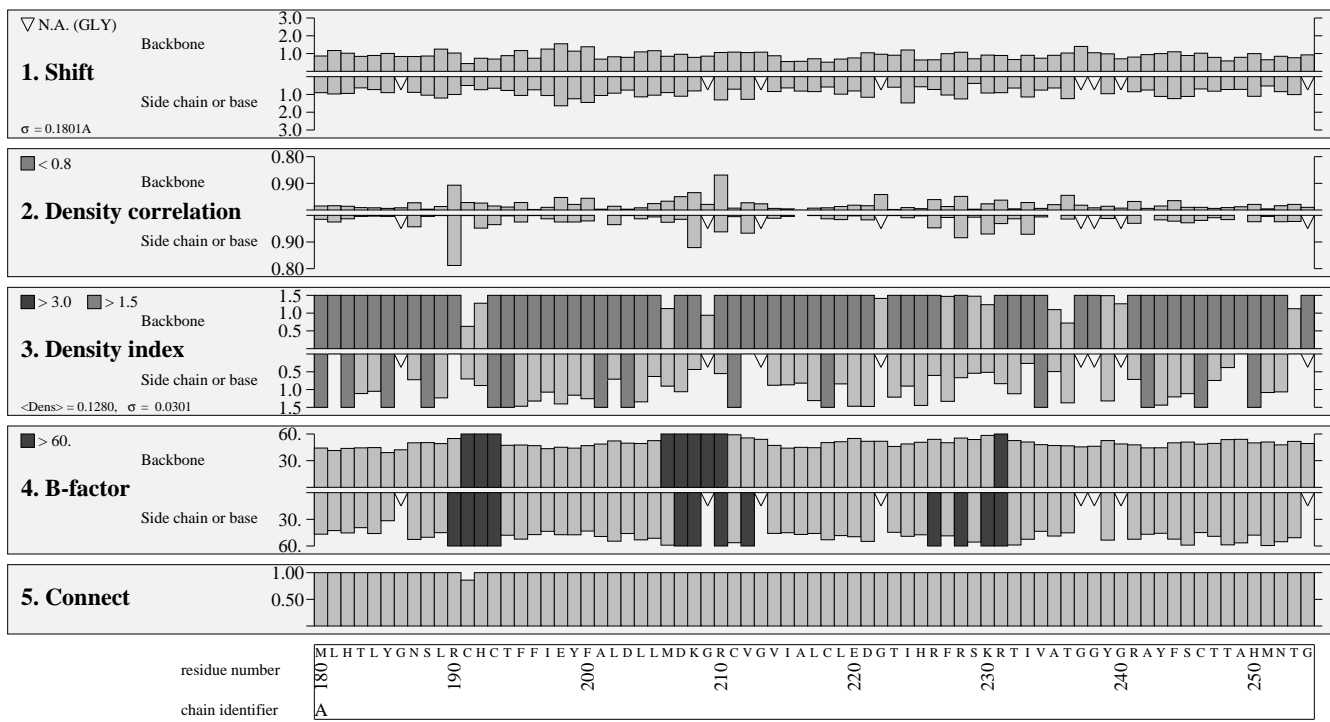
Local estimation



Structure Factor Check

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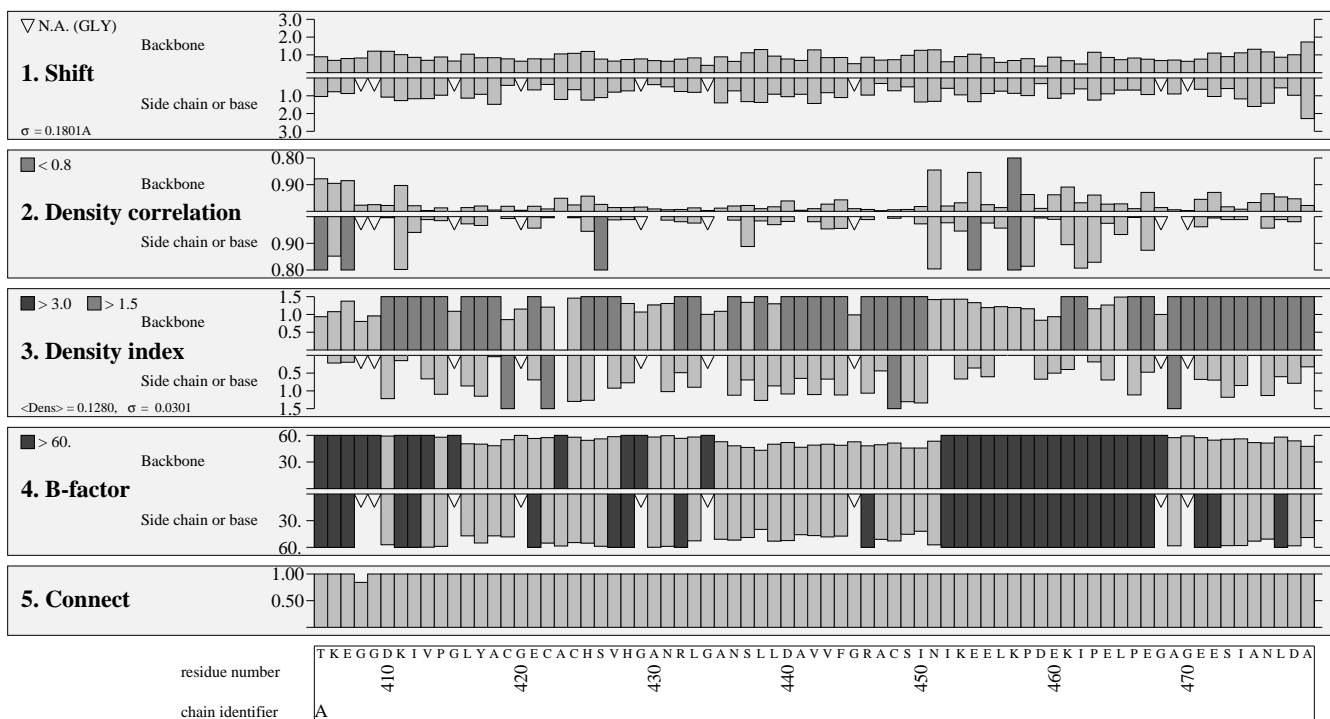
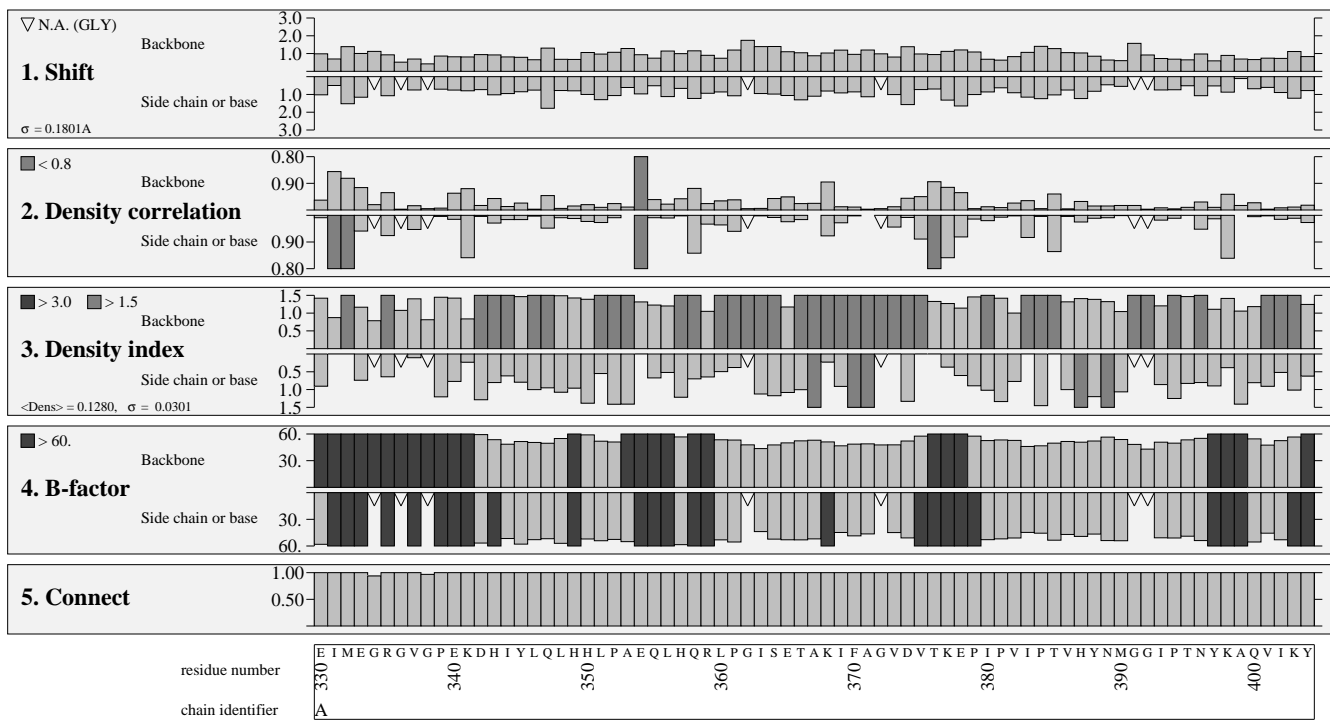
Local estimation (2)



Structure Factor Check

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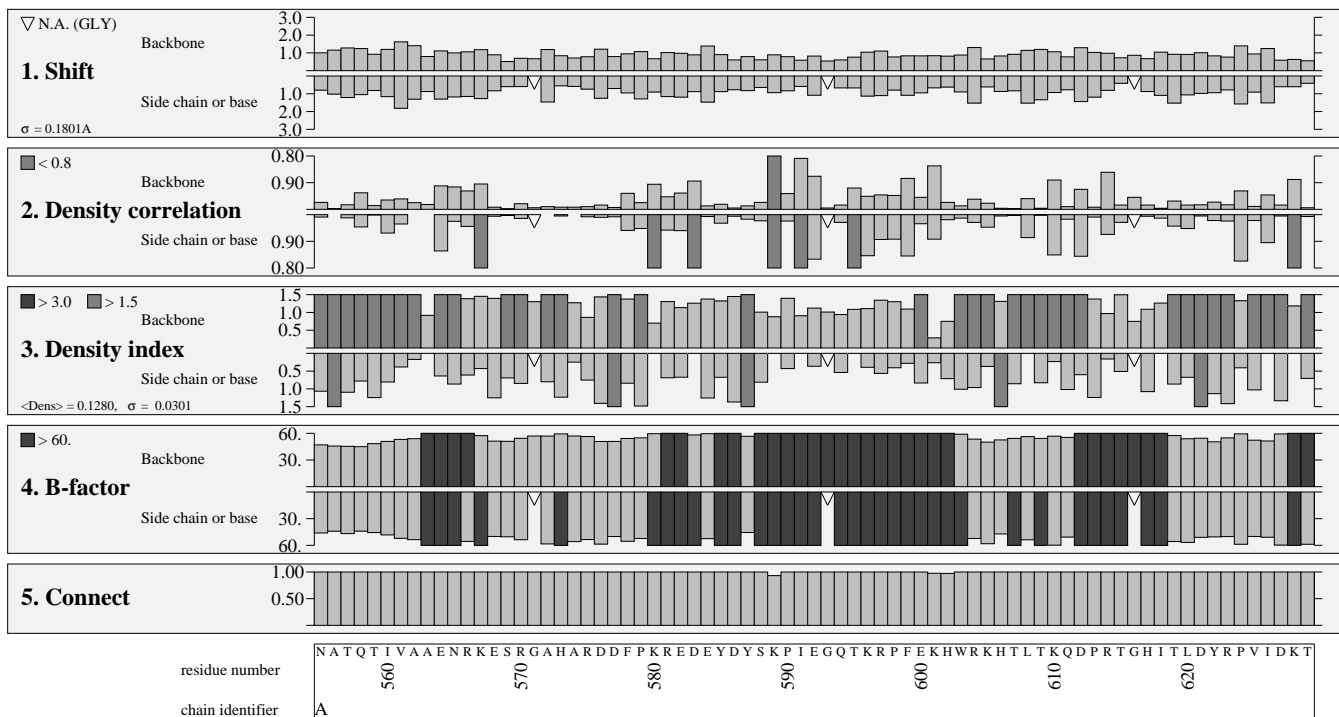
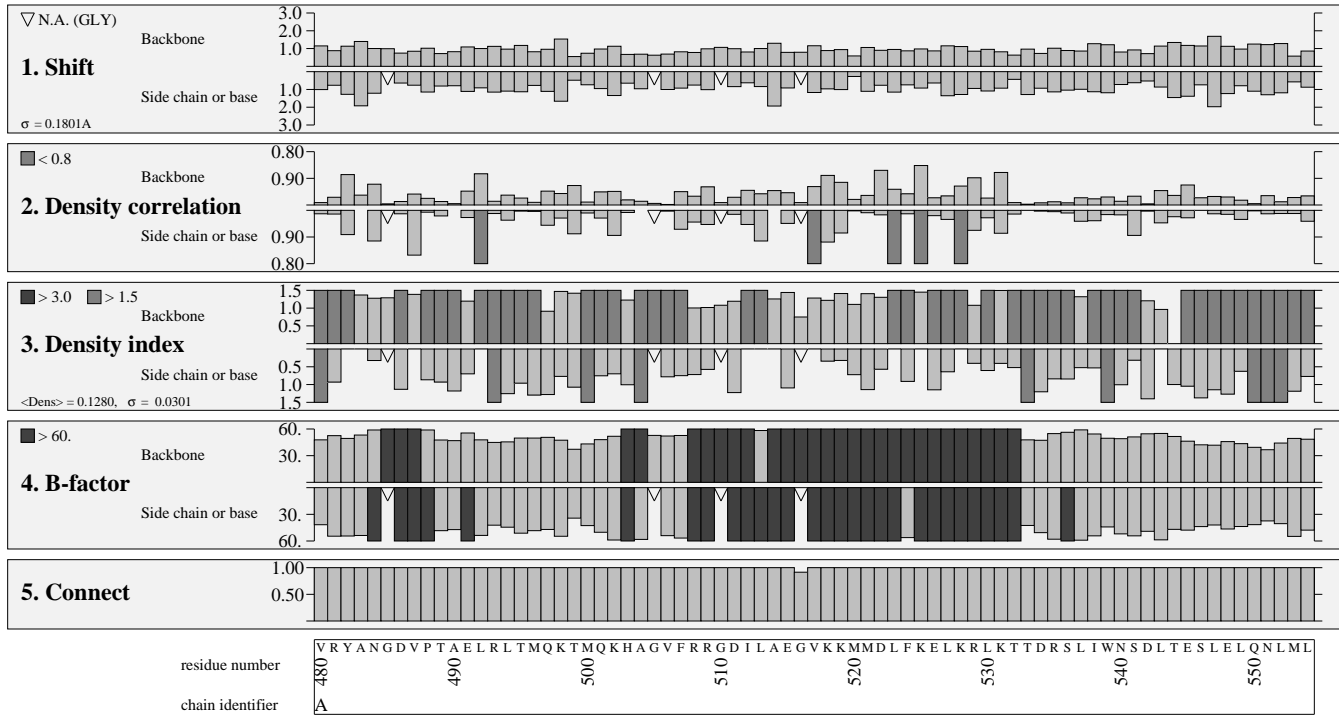
Local estimation (3)



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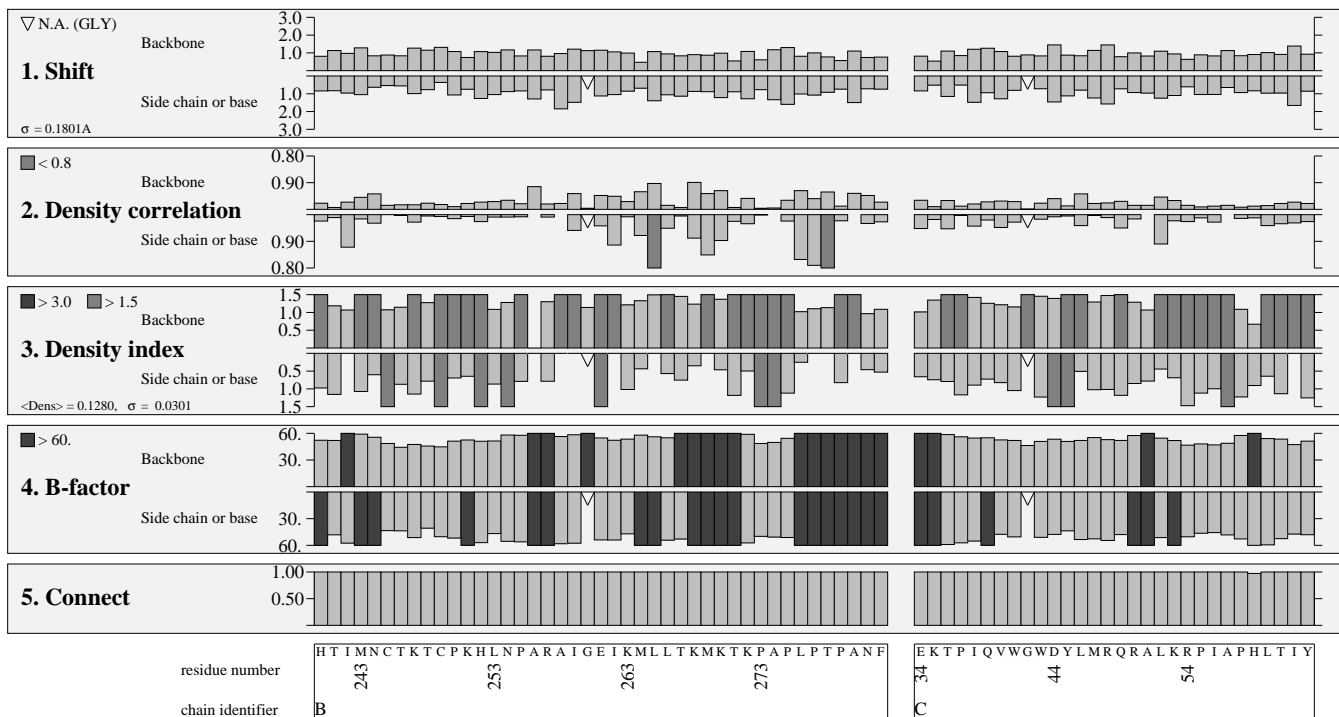
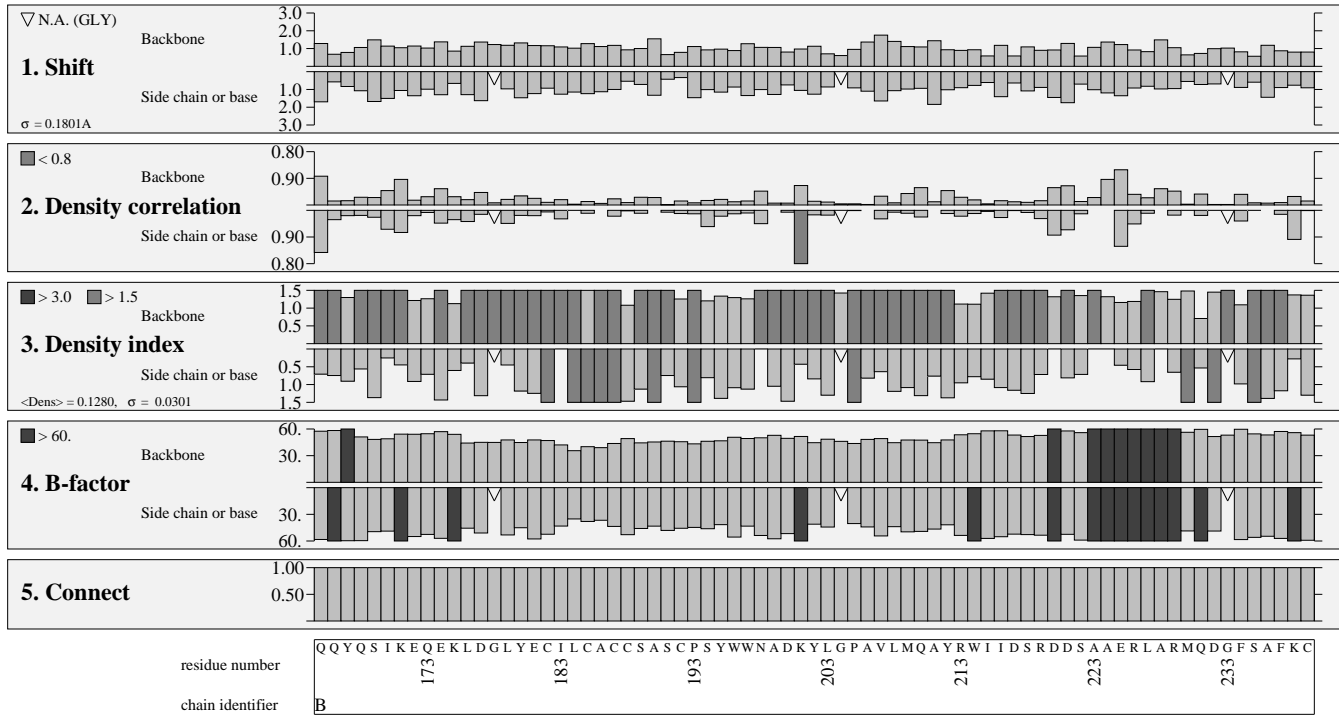
Local estimation (4)



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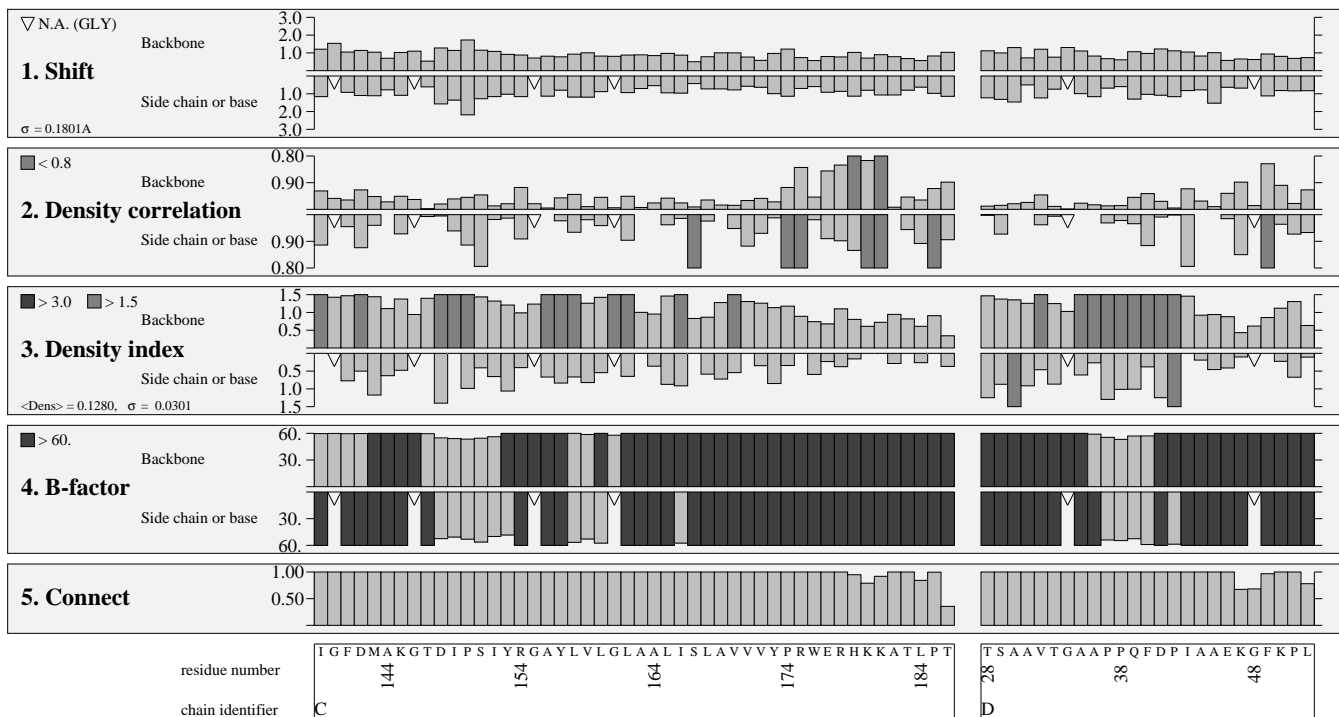
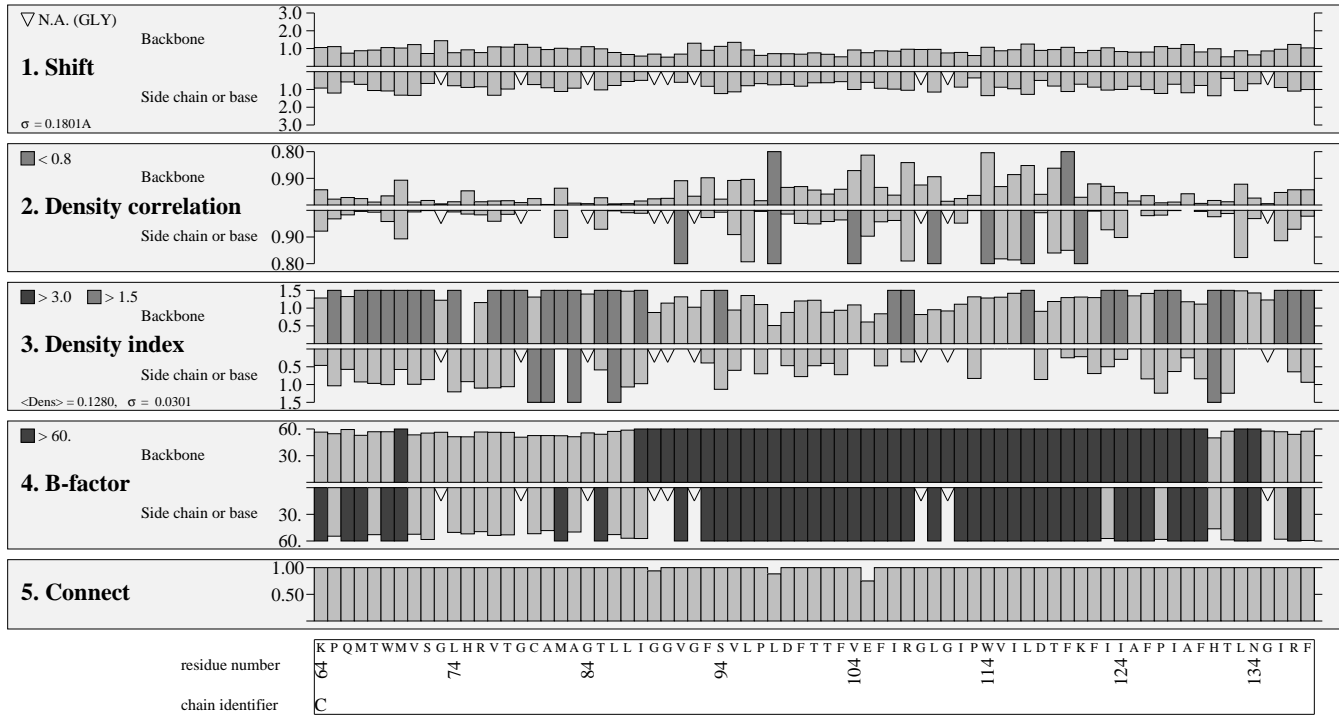
Local estimation (6)



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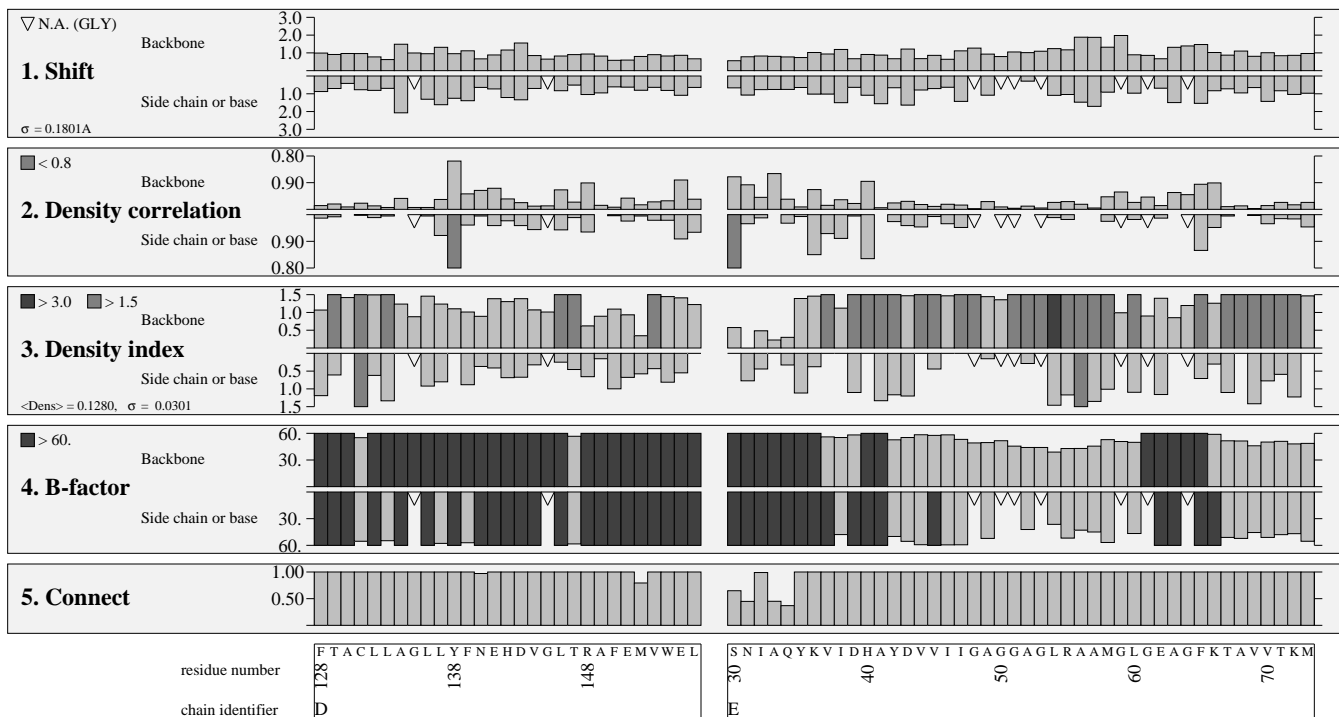
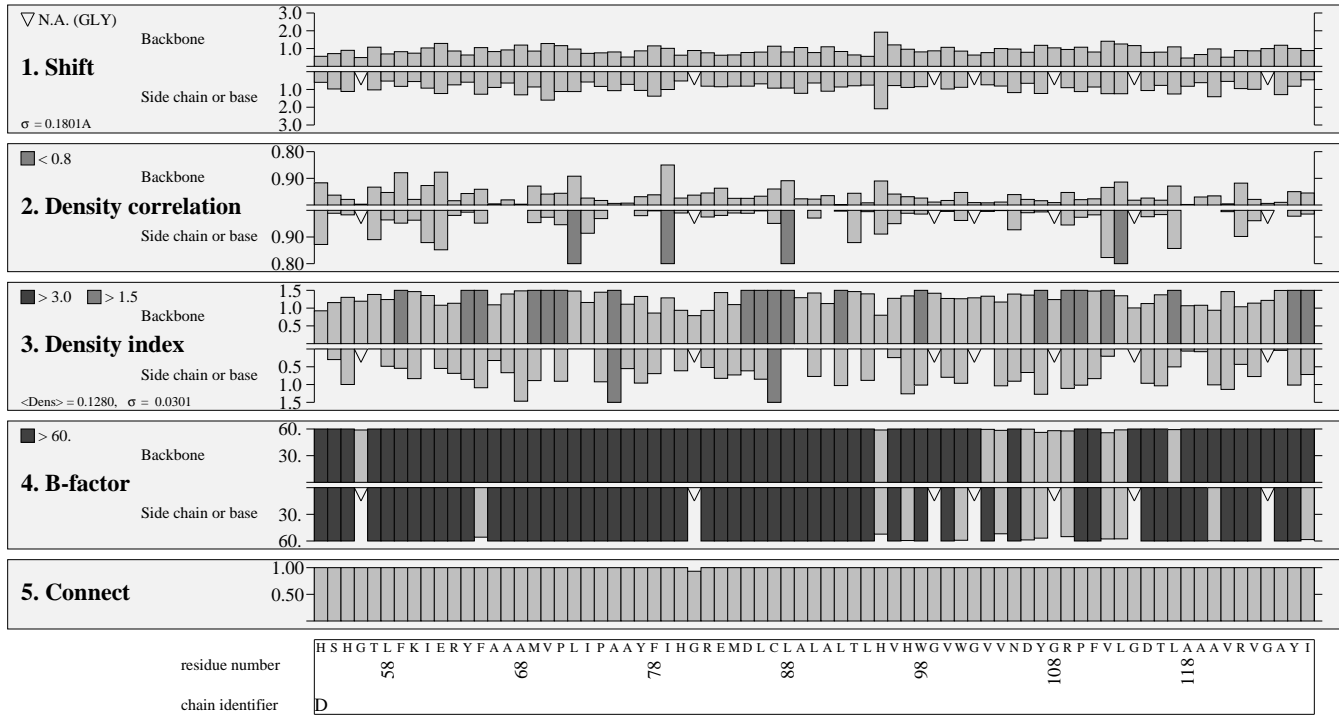
Local estimation (7)



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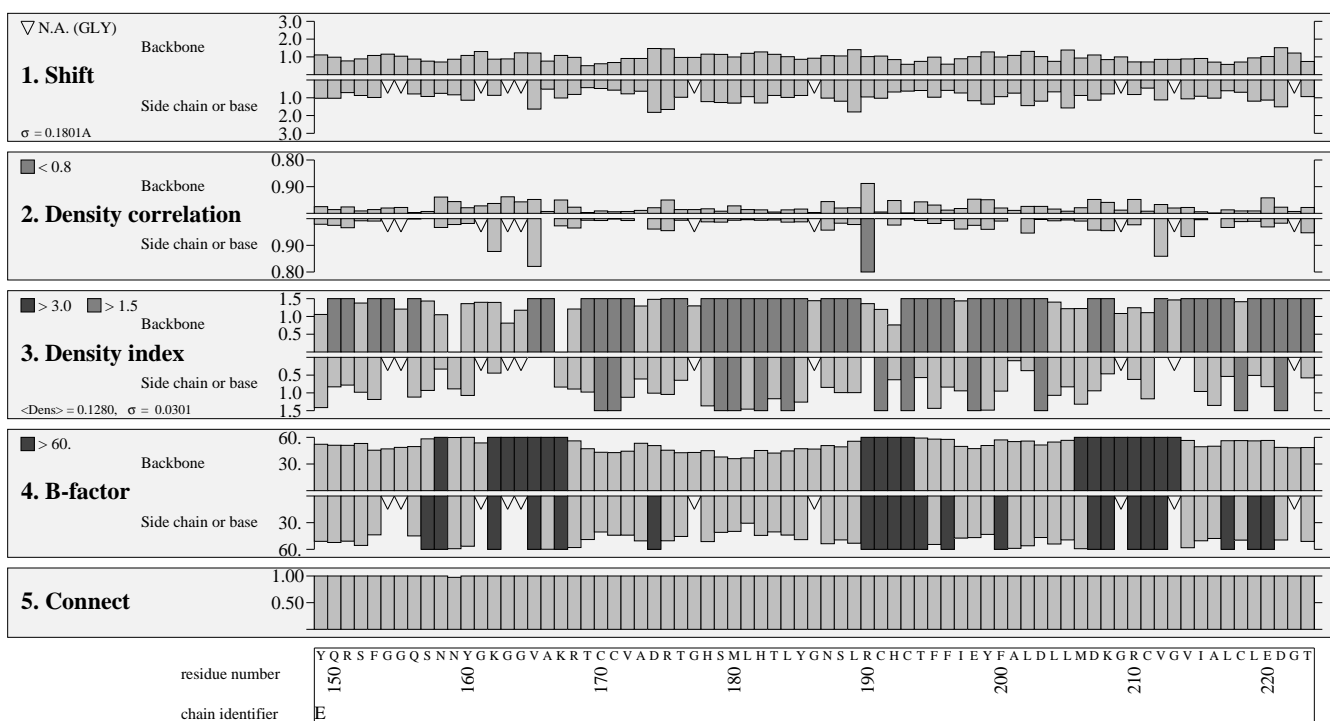
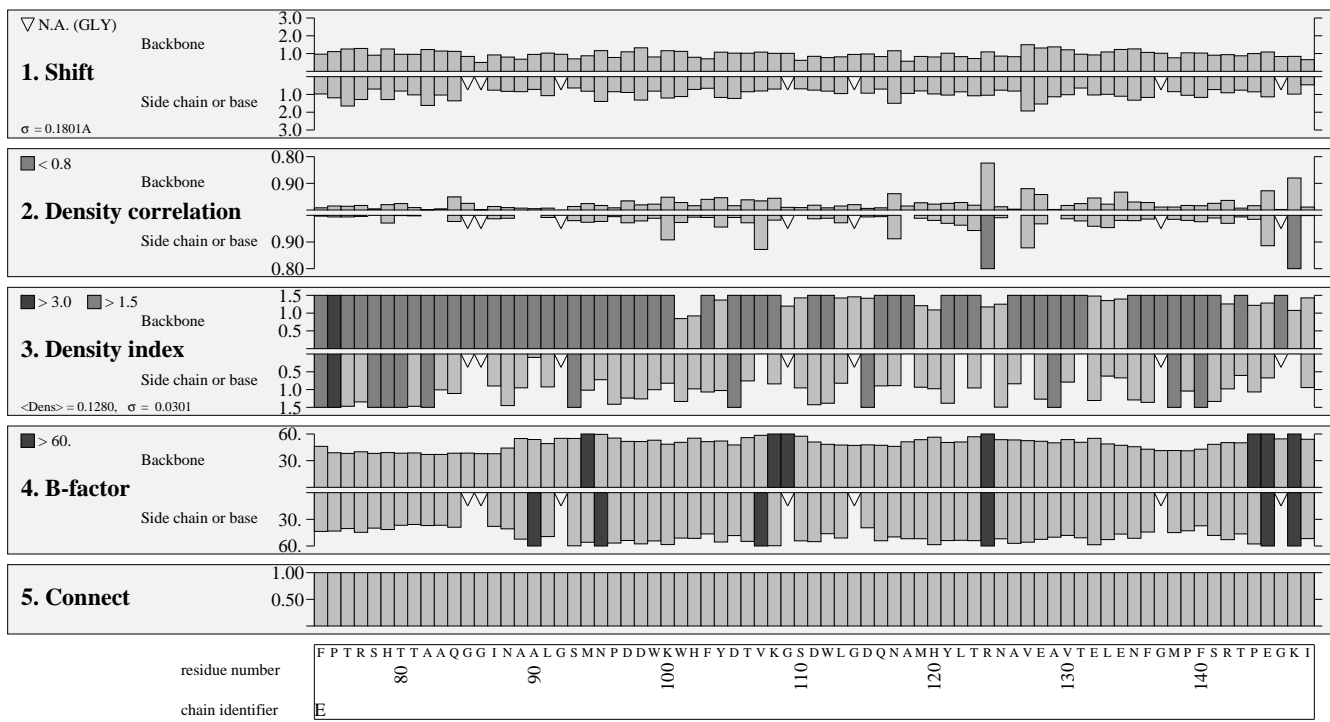
Local estimation (8)



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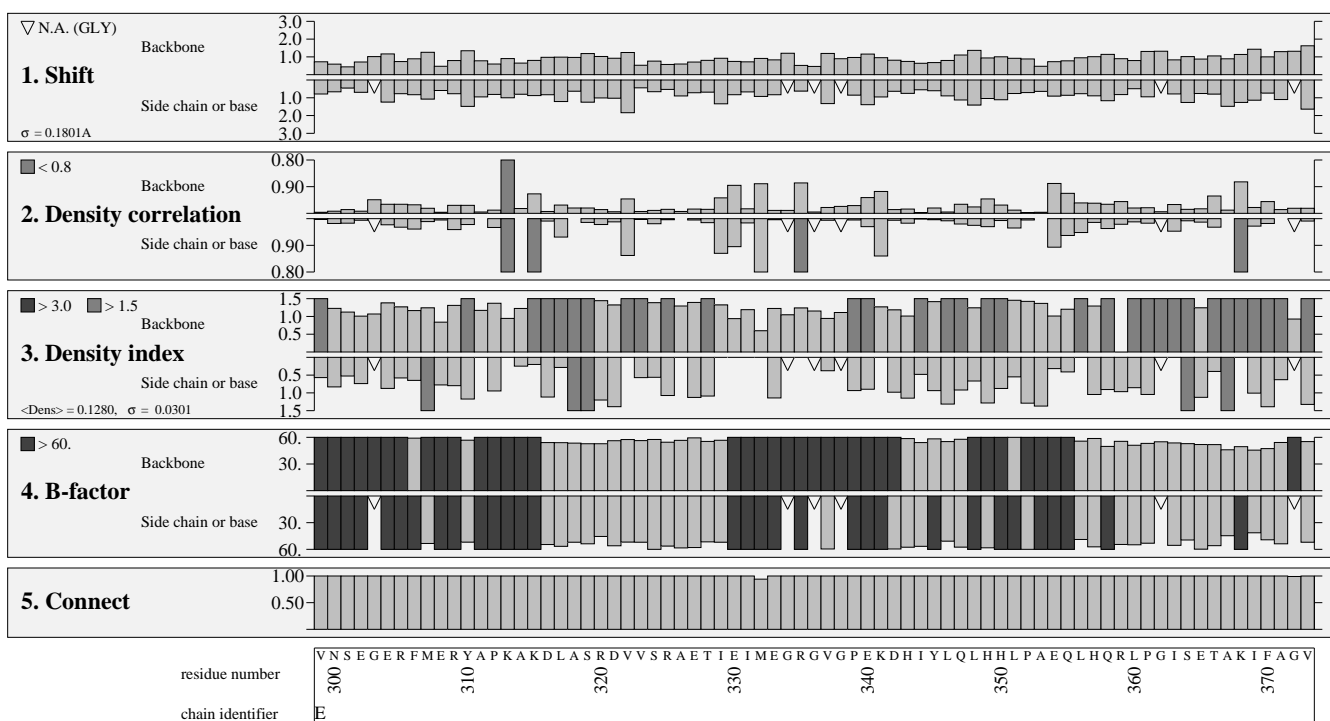
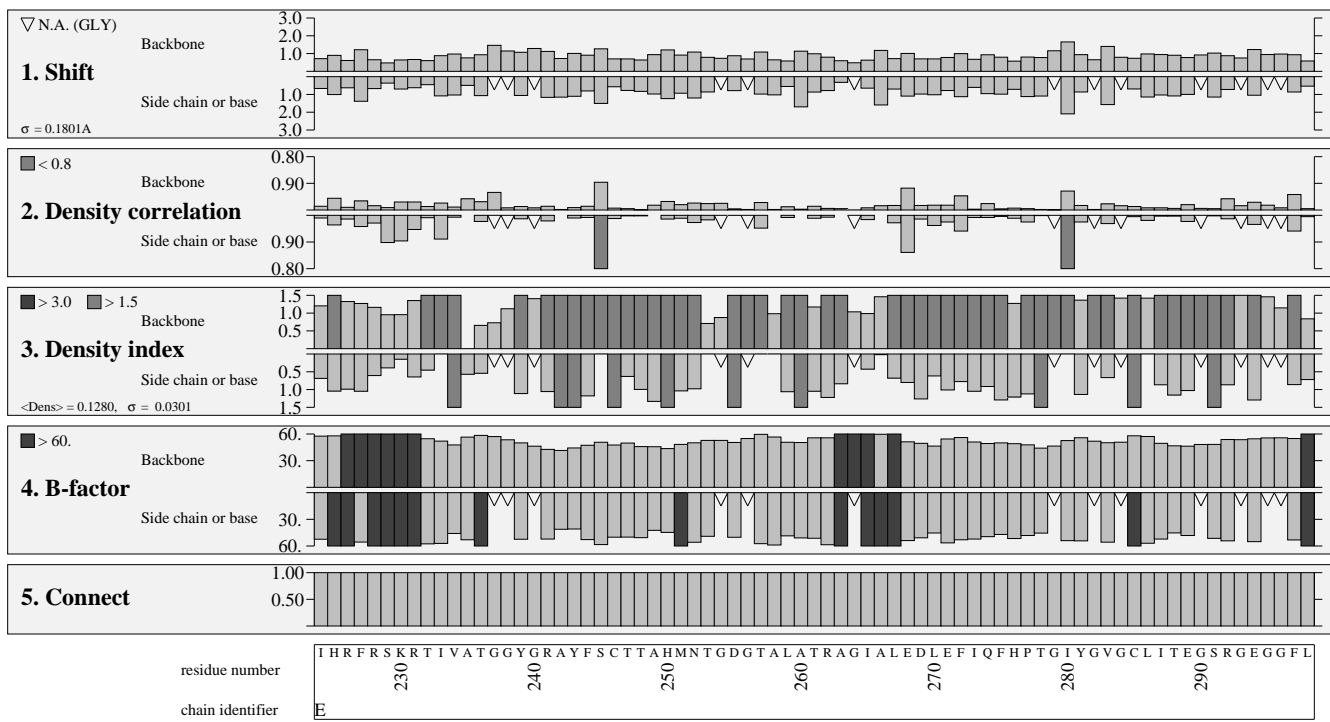
Local estimation (9)



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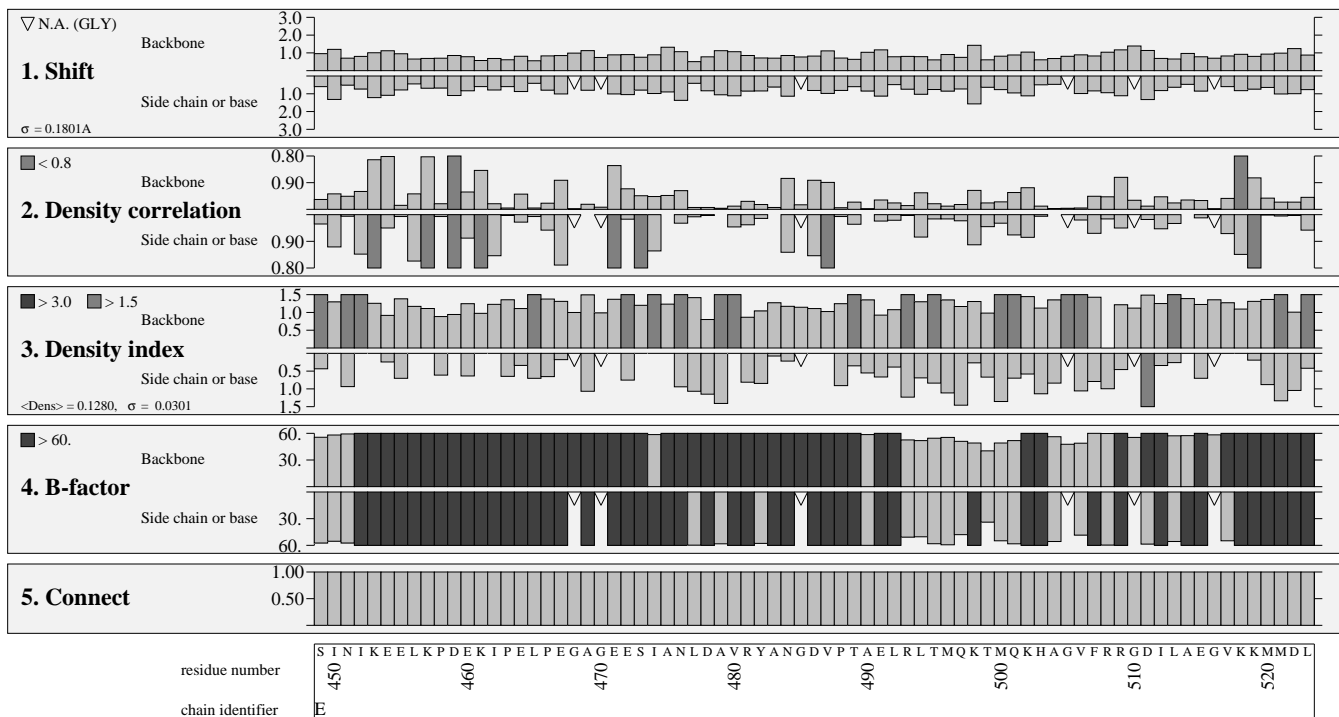
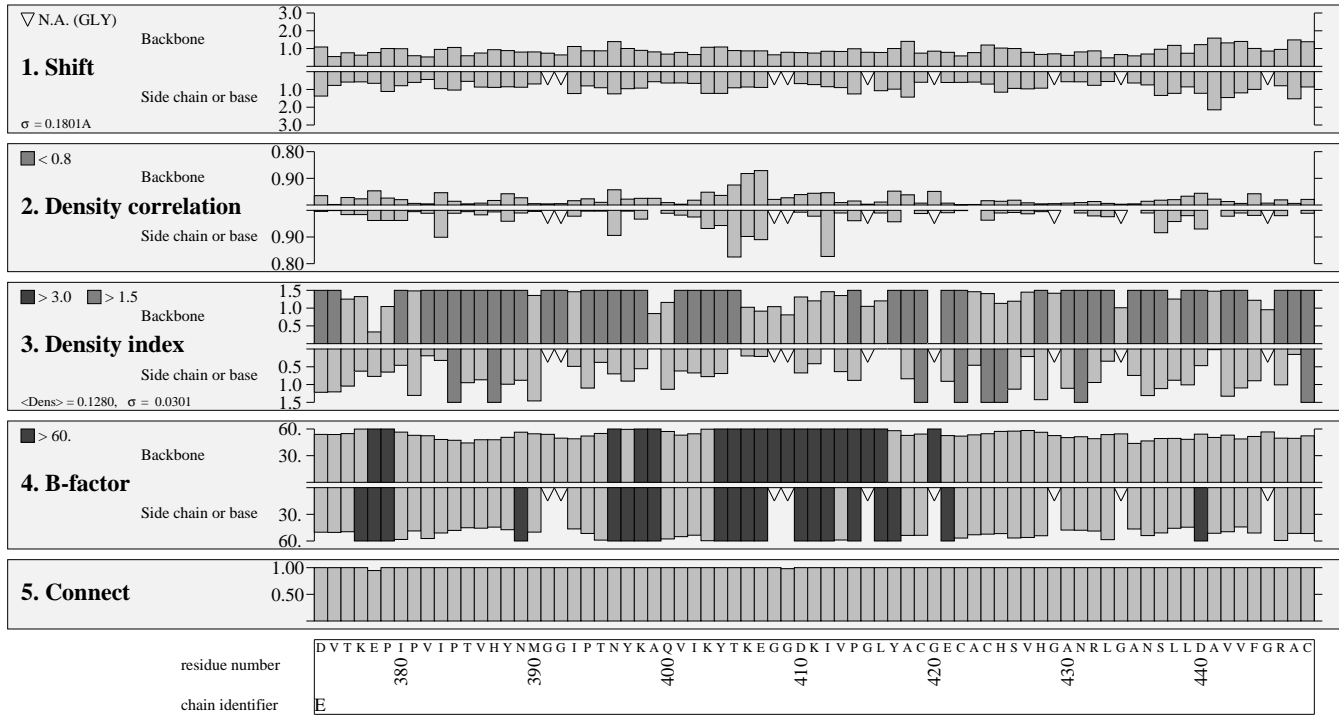
Local estimation (10)



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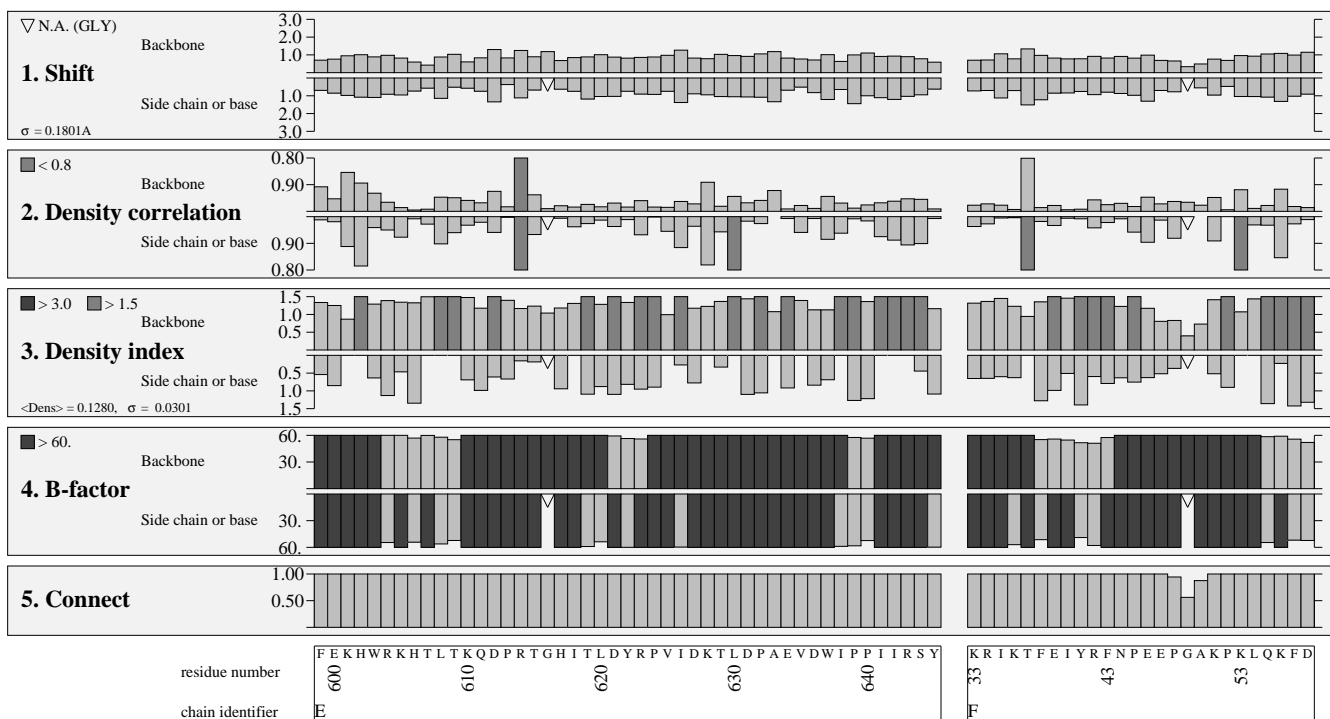
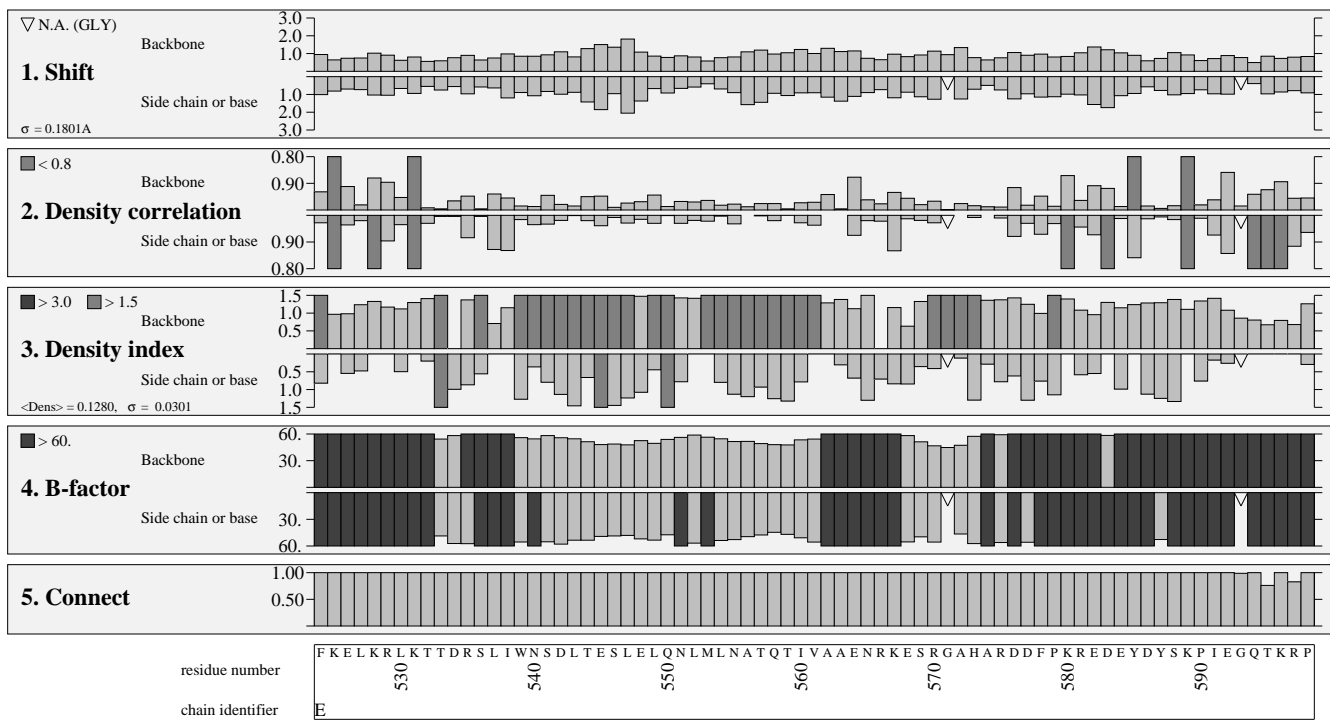
Local estimation (11)



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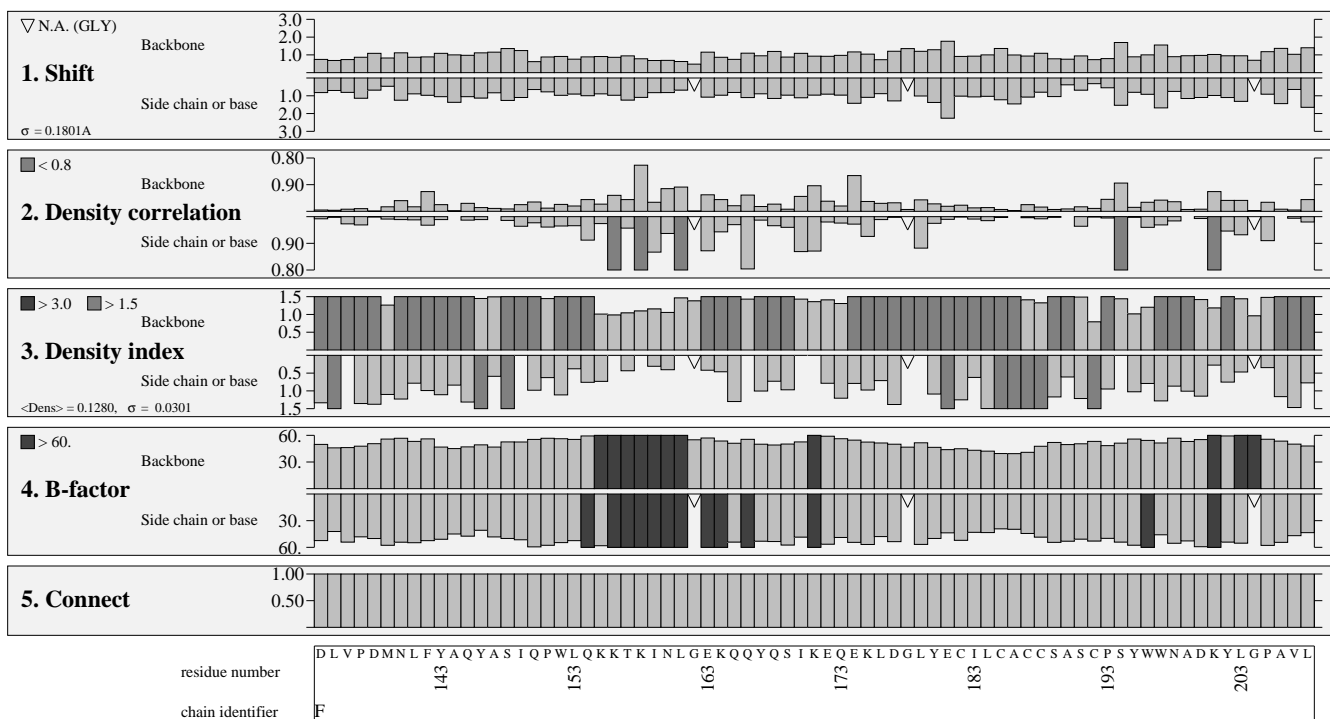
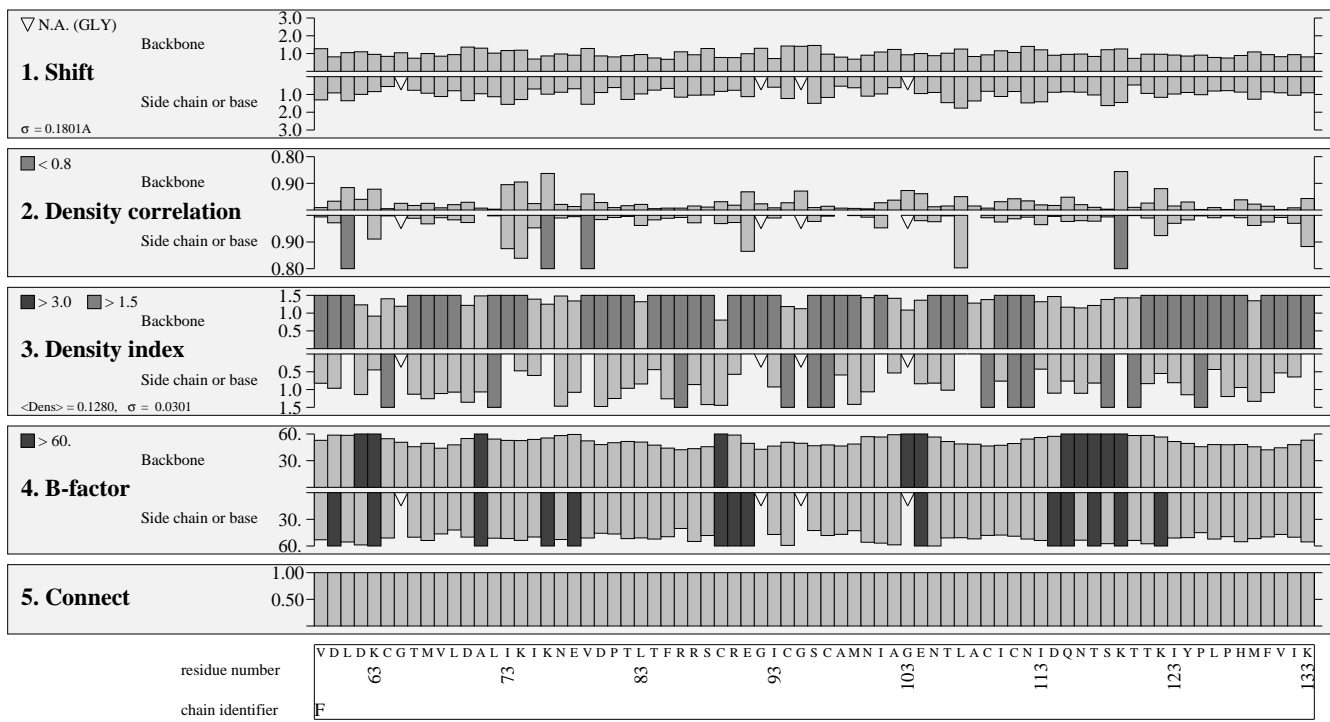
Local estimation (12)



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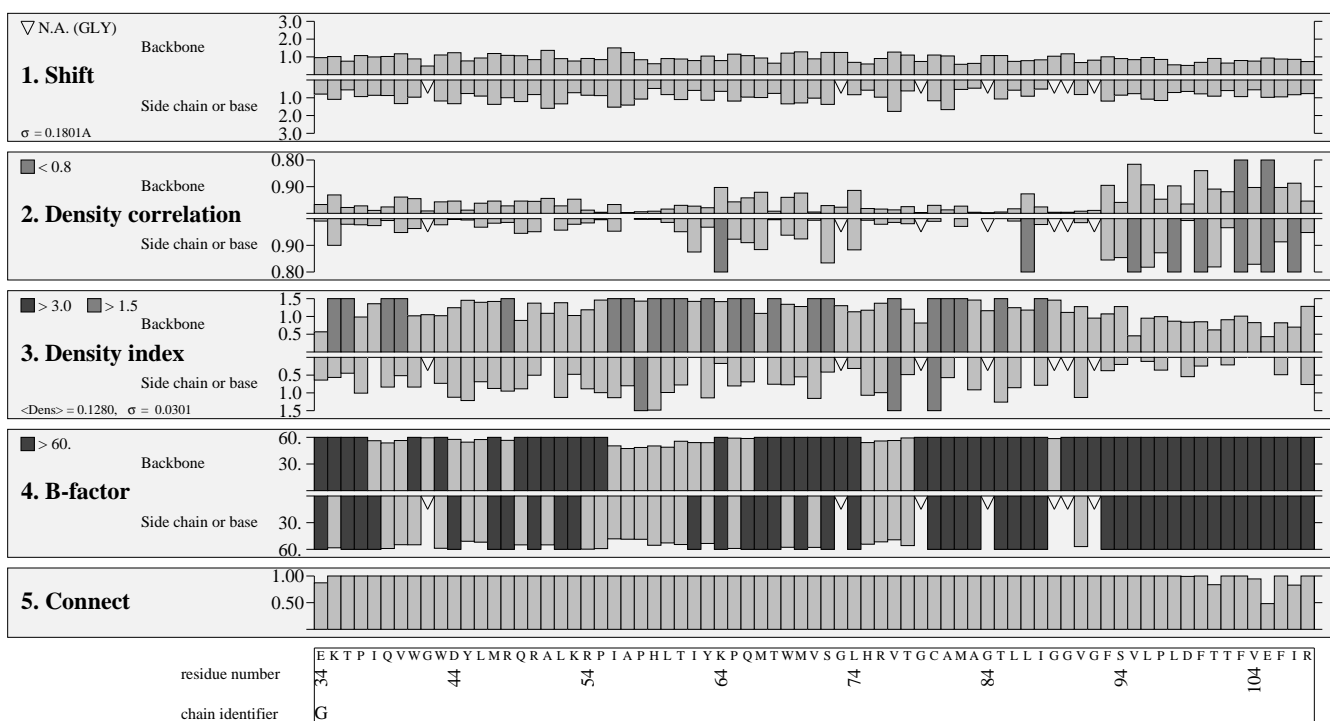
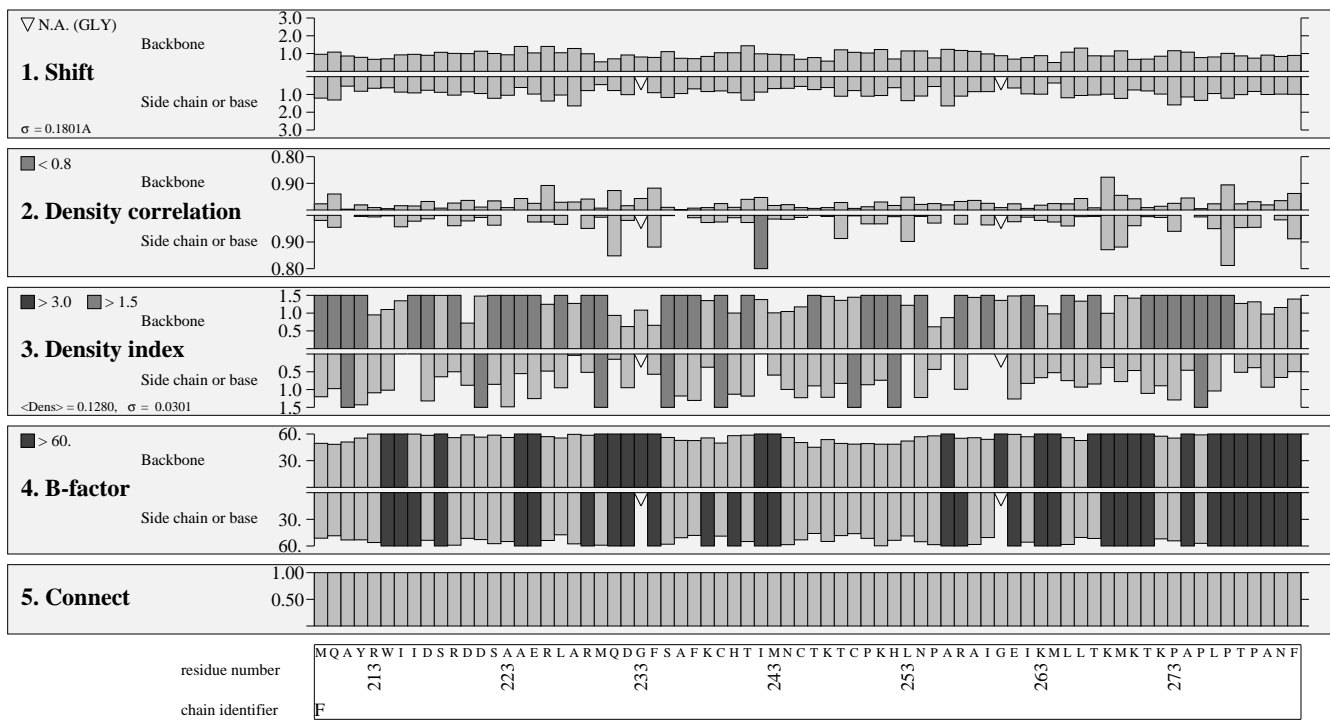
Local estimation (13)



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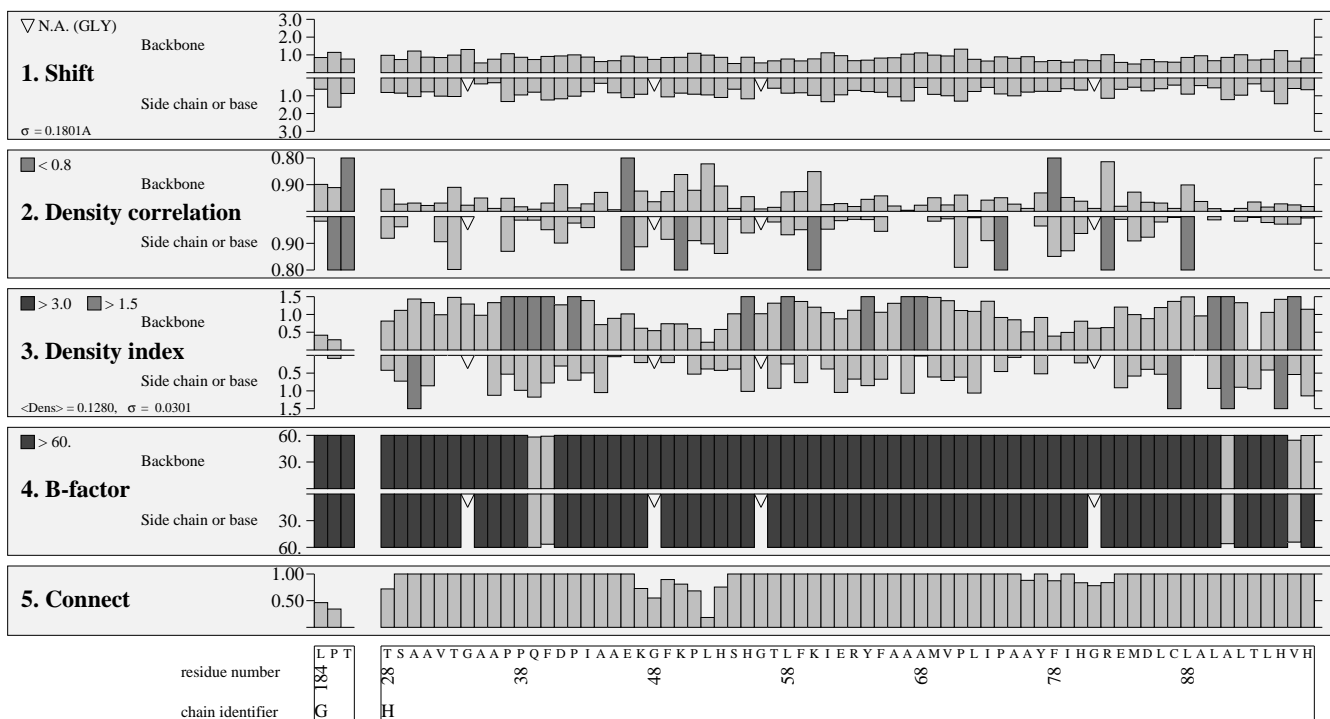
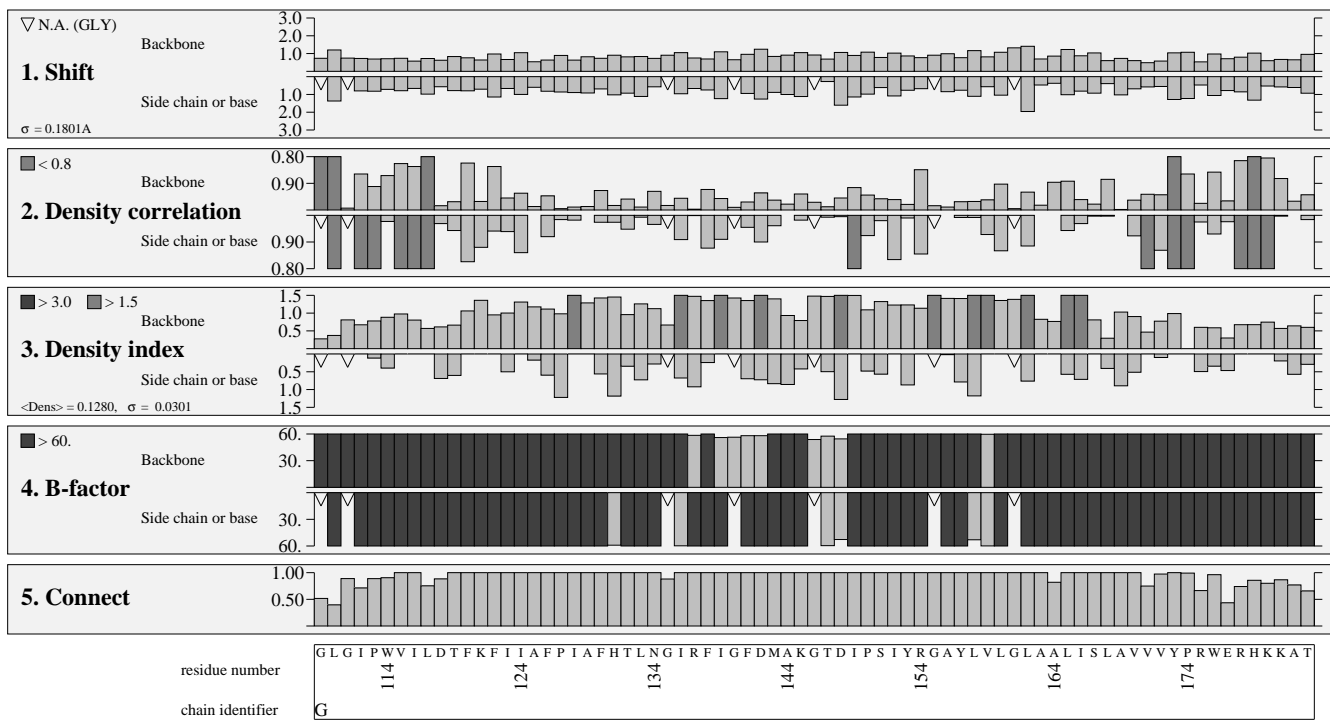
Local estimation (14)



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Local estimation (15)



Structure Factor Check

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Local estimation (16)

