

Structure Factor Check

1ZRT

Title: RHODOBACTER CAPSULATUS CYTOCHROME BC1 COMPLEX WITH STIGMATELLIN BOUND
 Date: 22-MAY-05
 PDB code: 1ZRT

Crystal

Cell parameters:
 a: 95.63 A b: 154.36 A c: 103.06 A
 α : 90.00 β : 113.57 γ : 90.00
 Space group: P 1 21 1
 Number of NCS-operators: 1
 NC-symmetry only for information

Structure Factors

Input

Nominal resolution range: 59.8 – 3.51 A
 Reflections in file: 33265
 Unique reflections above 0: 33265
 above 1 σ : 33129
 above 3 σ : 22313

SFCHECK

Nominal resolution range: 59.8 – 3.51 A
\05max. from input data, min. from author\05
 Used reflections: 33265
 Completeness: 96.5 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.069
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.7830 0.3458 1.0000
 B_{overall} (by Patterson): 65.A²
 Optical resolution: 2.53 A
 Expected opt. resol. for complete data set: 2.53 A
 Estimated minimal error: 0.149 A

Model

13366 atoms
 Number of chains: 16
 Volume not occupied by model: 58.9 %
 $\langle B \rangle$ (for atomic model): 84.6 A²
 $\sigma(B)$: 21.27 A²
 Matthews coefficient: 3.73
 Corresponding solvent % : 66.73

Model vs. Structure Factors

R-factor for all reflections: 0.354
 Correlation factor: 0.776
 R-factor: 0.358
 for $F > 2.0\sigma$
 nom. resolution range: 59.39 – 3.50A
 reflections used: 33130
 Rfree: 0.404
 Nfree: 1654
 R-factor without free-refl.: 0.355
 Non free-reflections: 31476
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.812 A
 Estimated maximal error: 0.691 A
 DPI: 0.805 A

Scaling

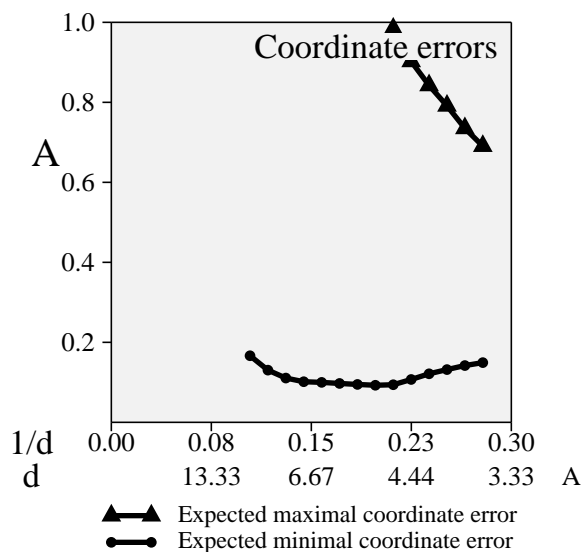
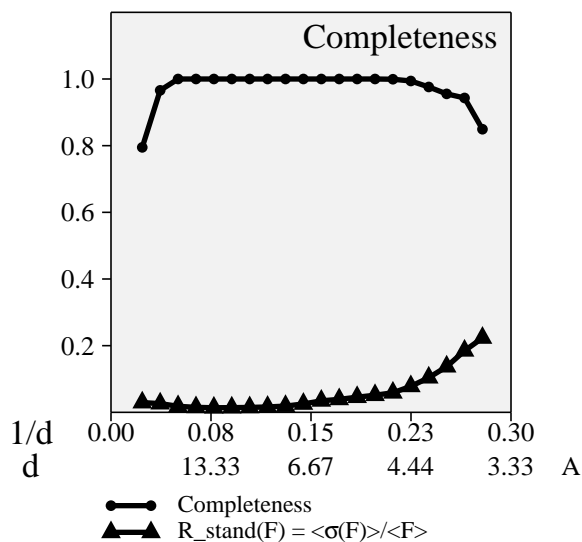
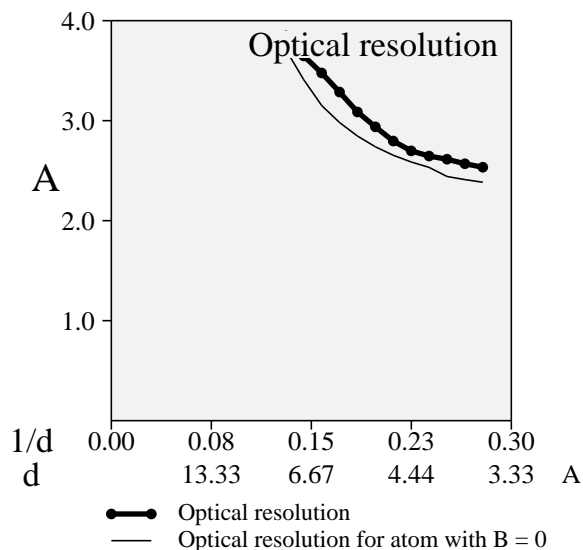
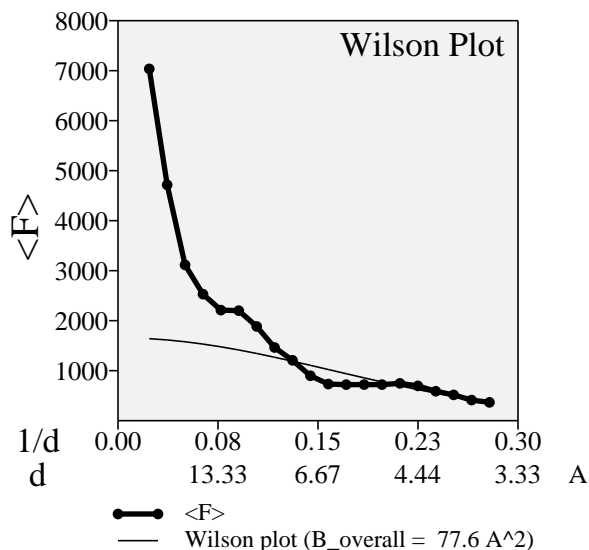
Scale: 1.359
 Bdiff: -8.36
 Anisothermal Scaling (Beta):
 -0.1989 27.4726 -4.4128 0.0000 4.5029 0.0000
 Solvent correction – Ks,Bs: 0.463 250.539

Refinement

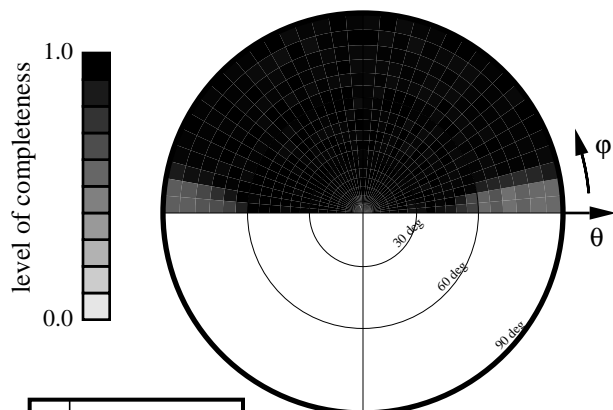
Program: CNS 1.1
 Nominal resolution range: 59.4 – 3.50 A
 Reported R-factor: 0.300
 Number of reflections used: 33265
 Reported Rfree: 0.36
 Sigma cut-off: N.A.

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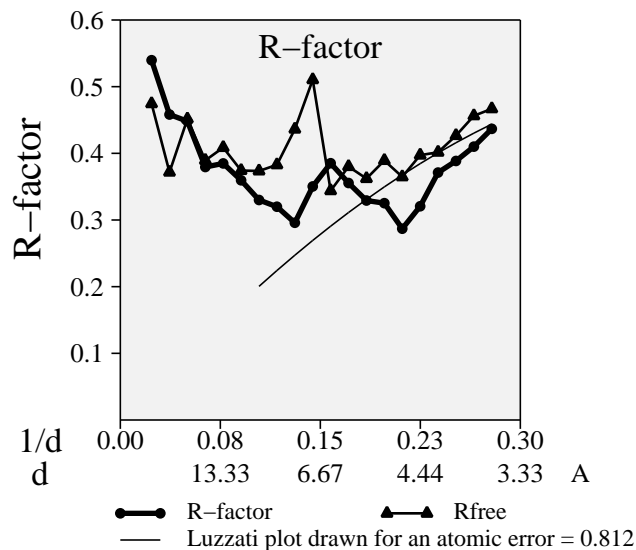


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	66.43	0.00
k	90.00	90.00
l	0.00	0.00

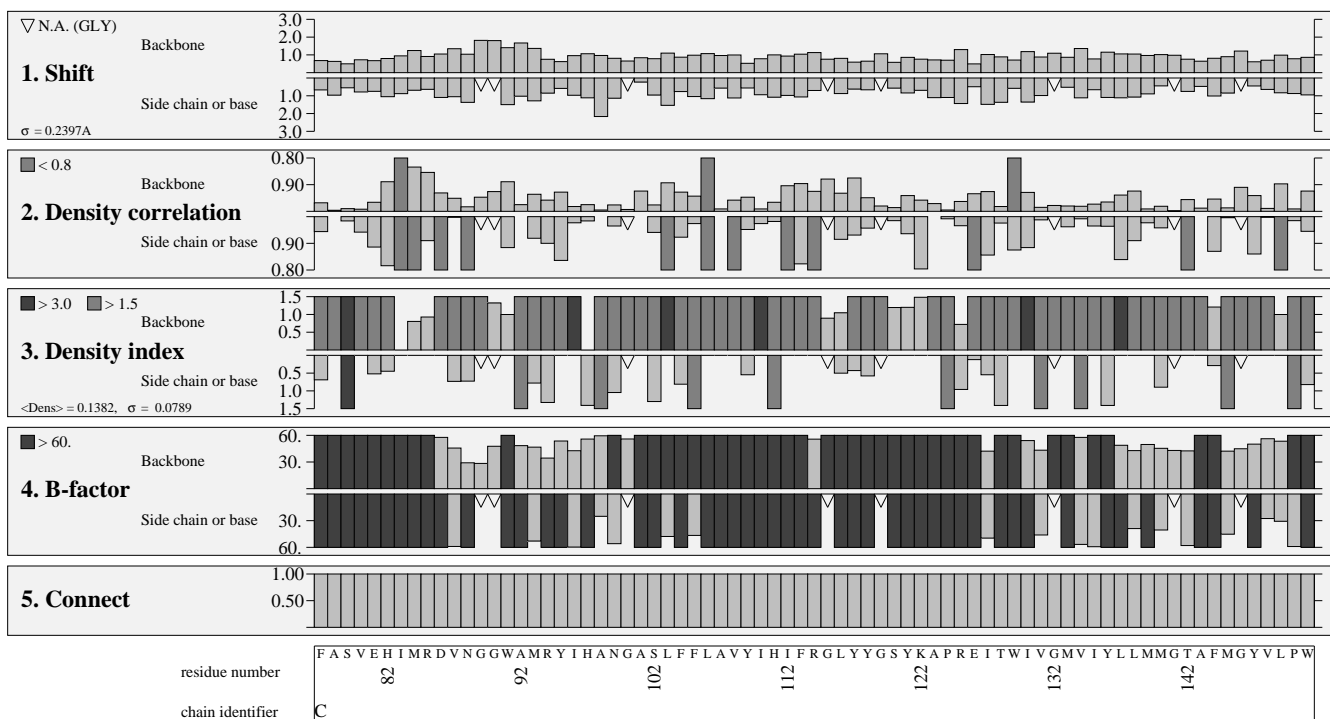
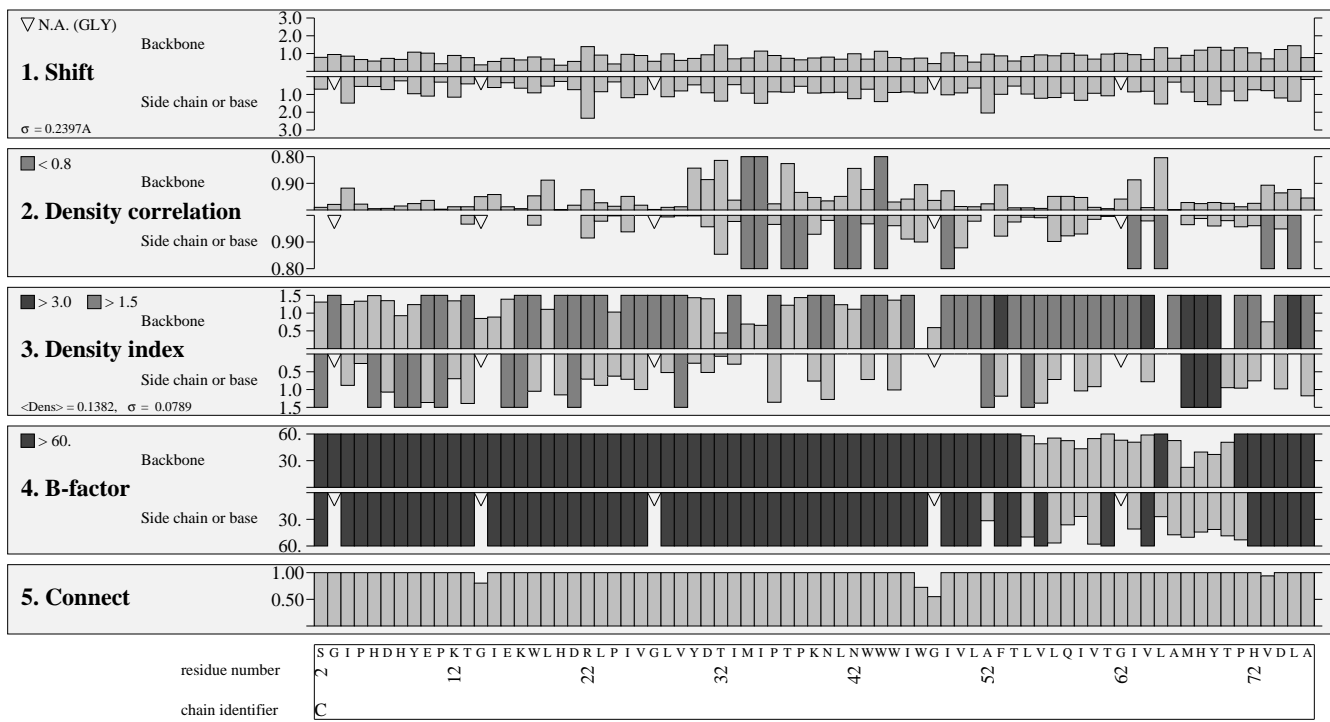
polar coordinates of the crystallographical axes



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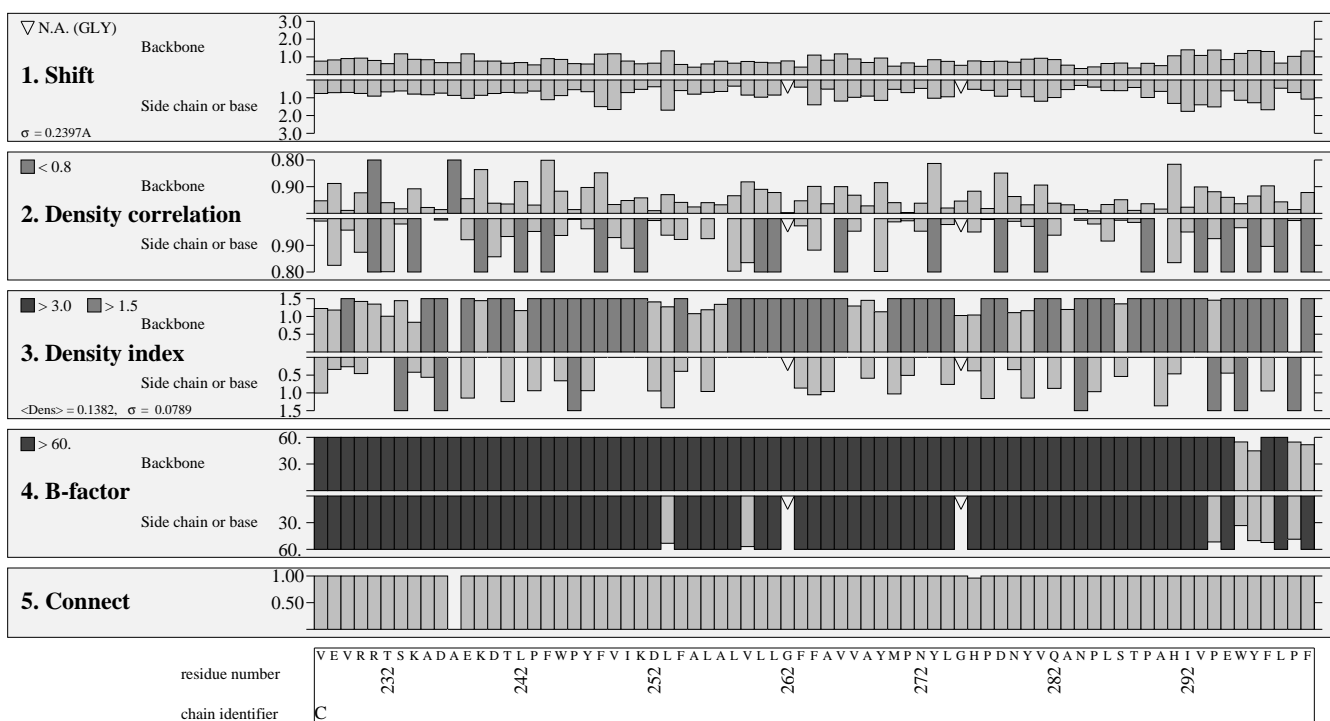
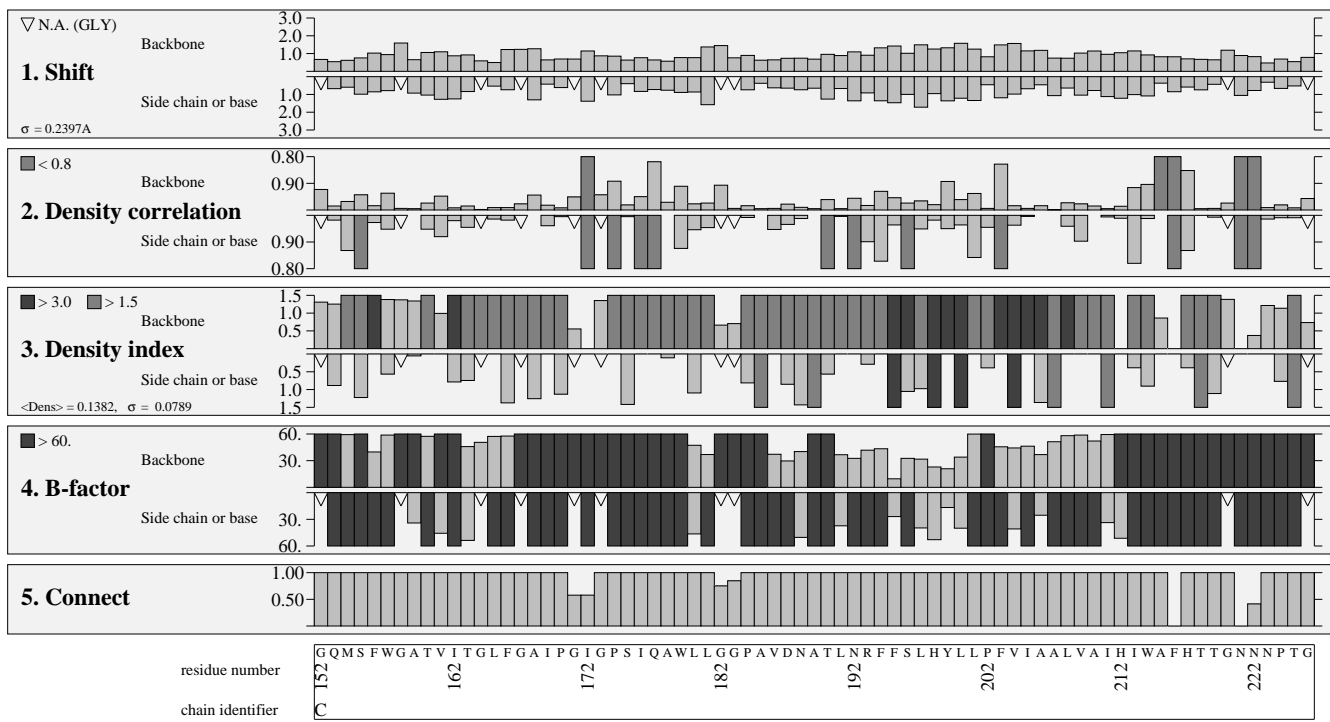
Local estimation



Structure Factor Check

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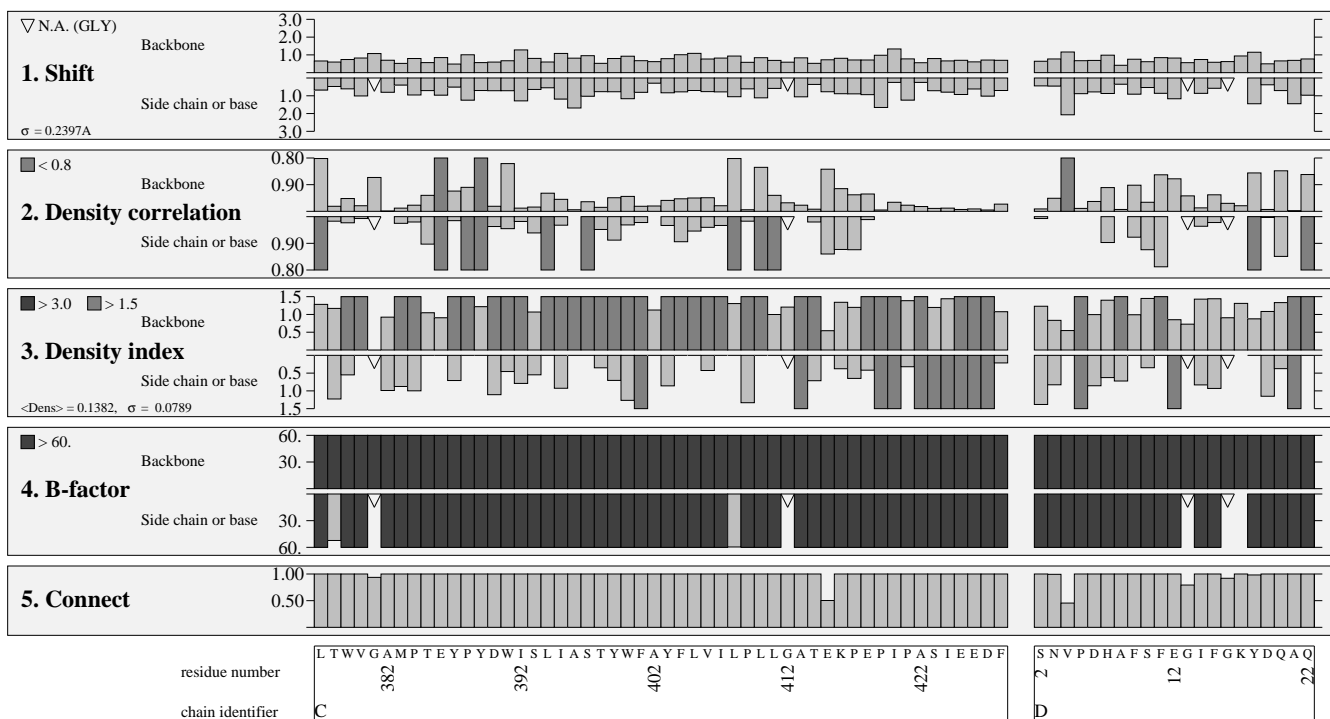
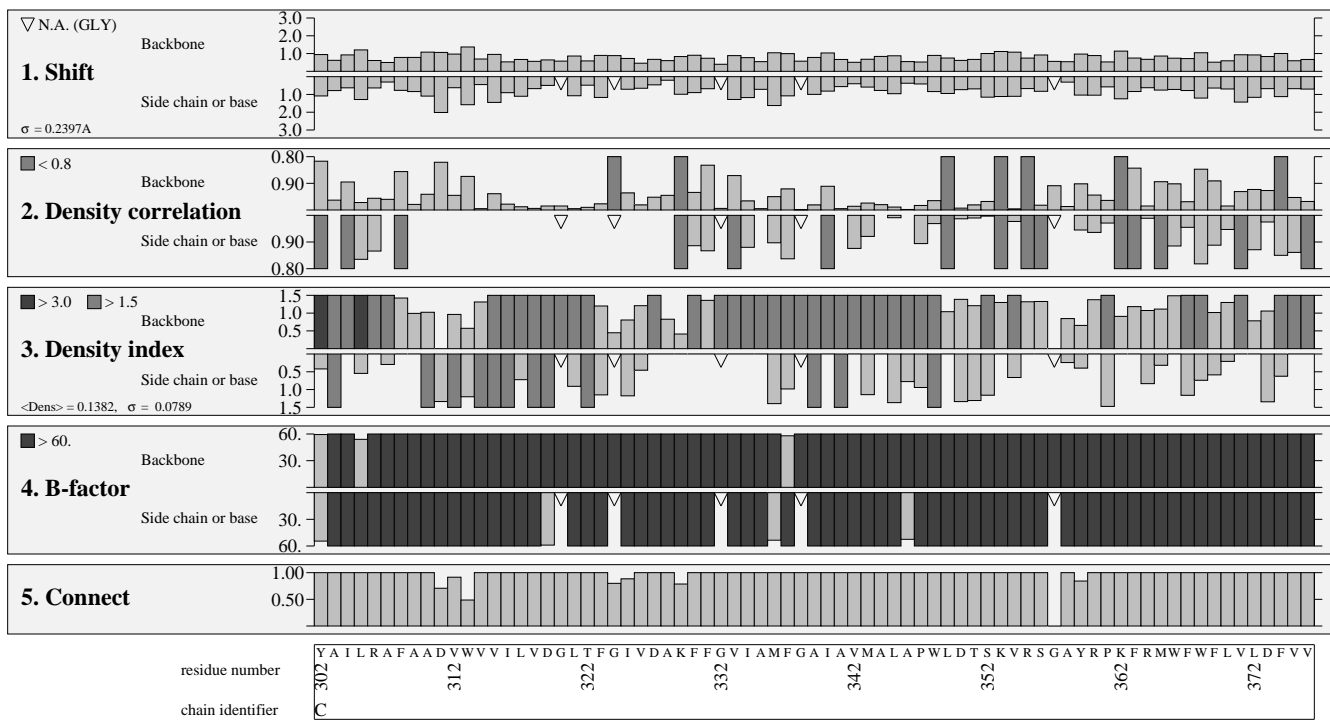
Local estimation (2)



Structure Factor Check

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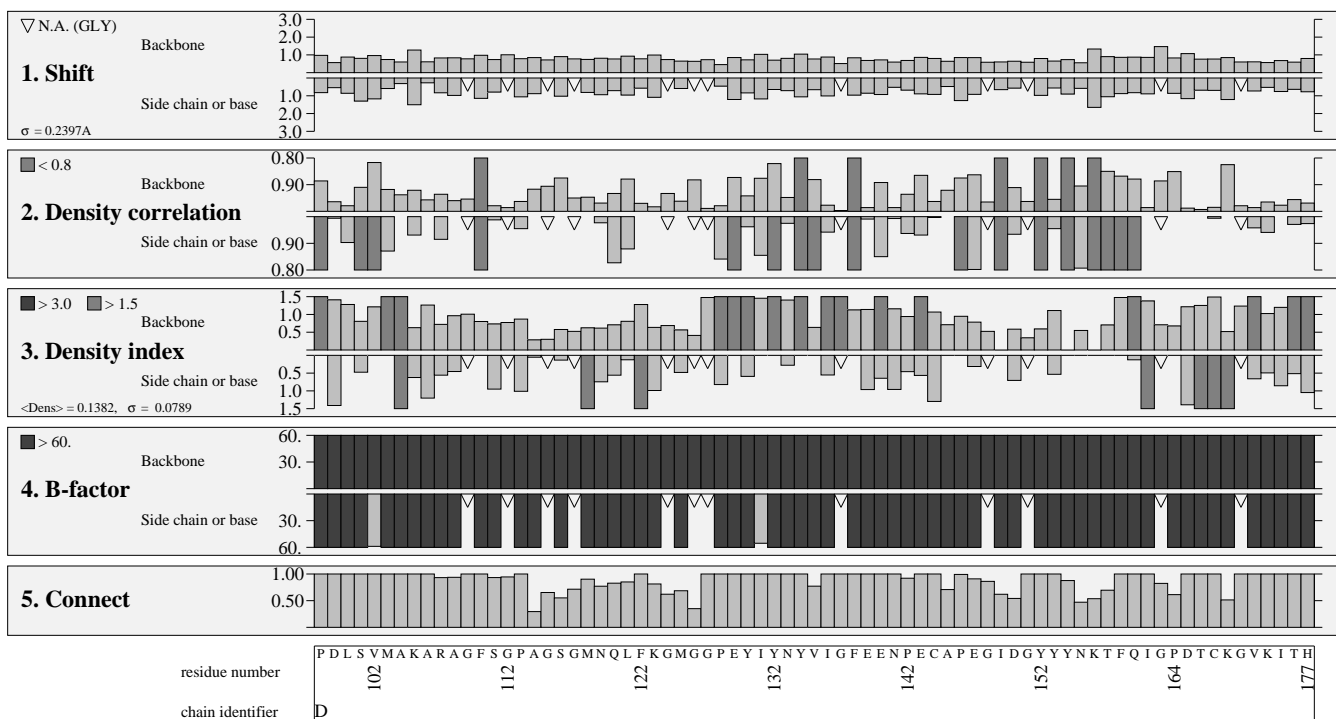
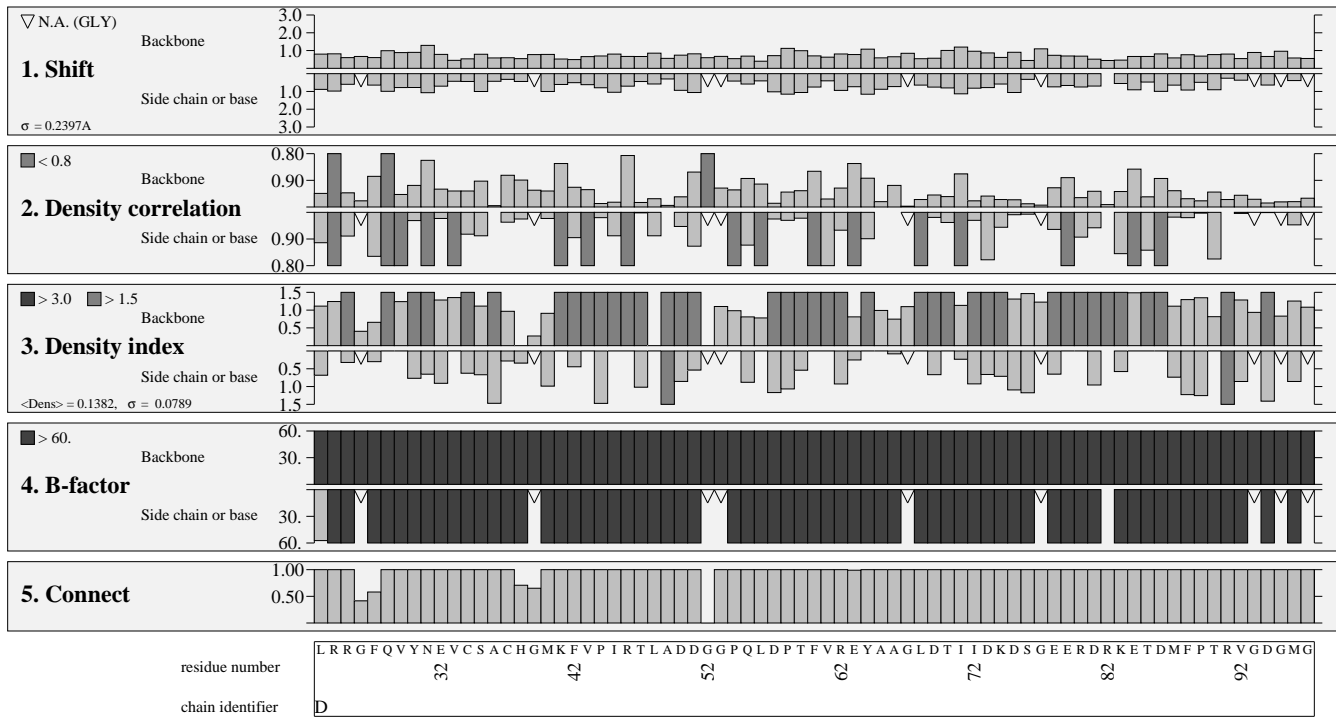
Local estimation (3)



Structure Factor Check

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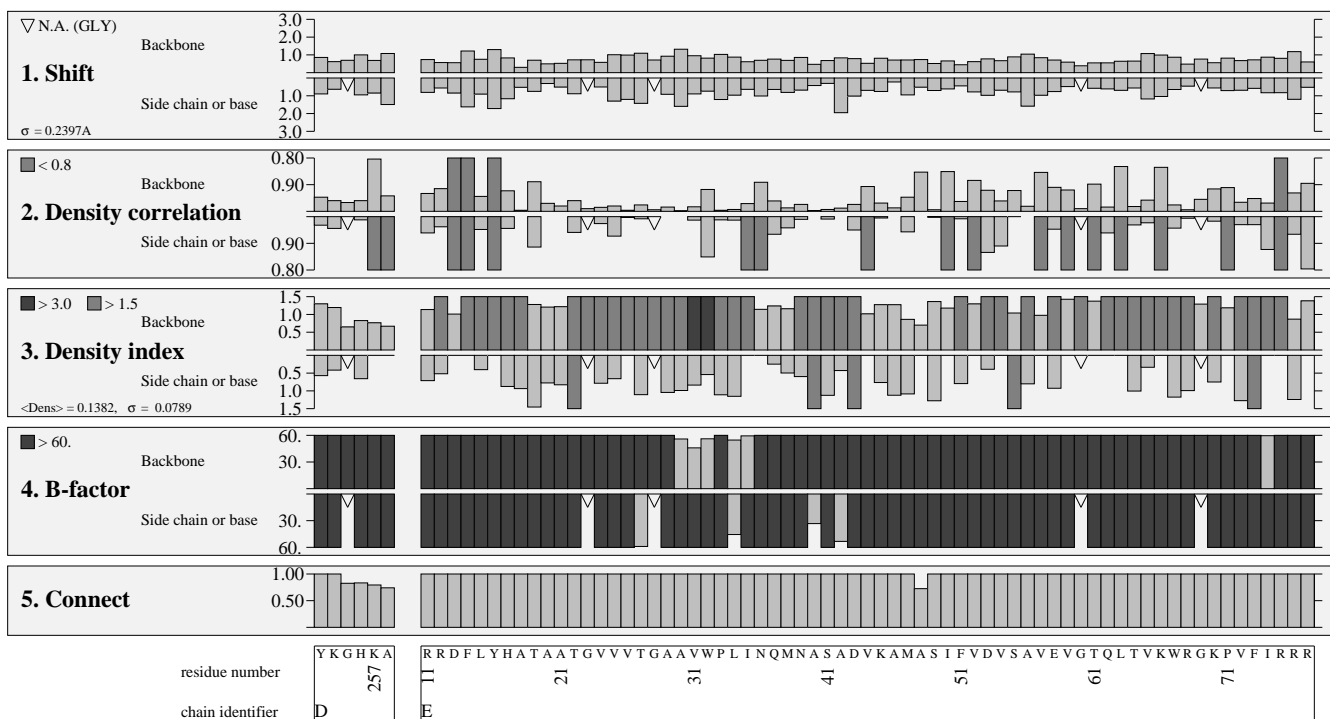
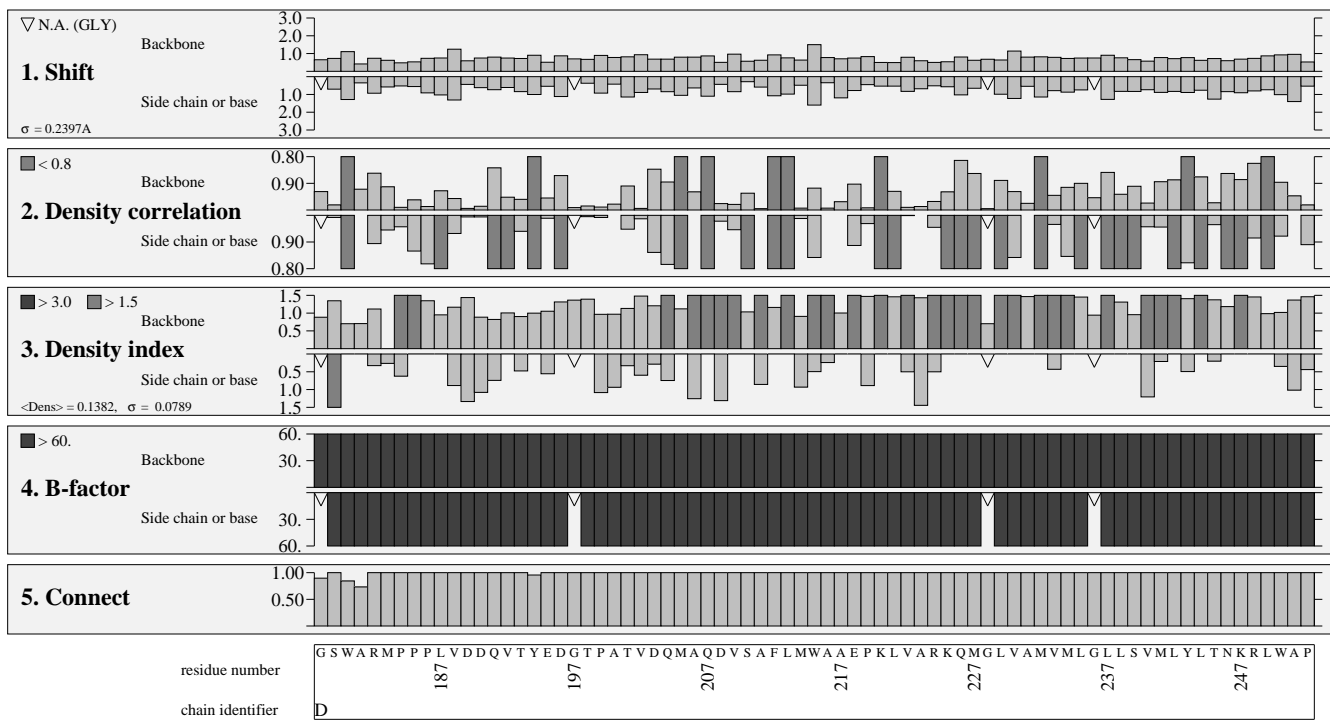
Local estimation (4)



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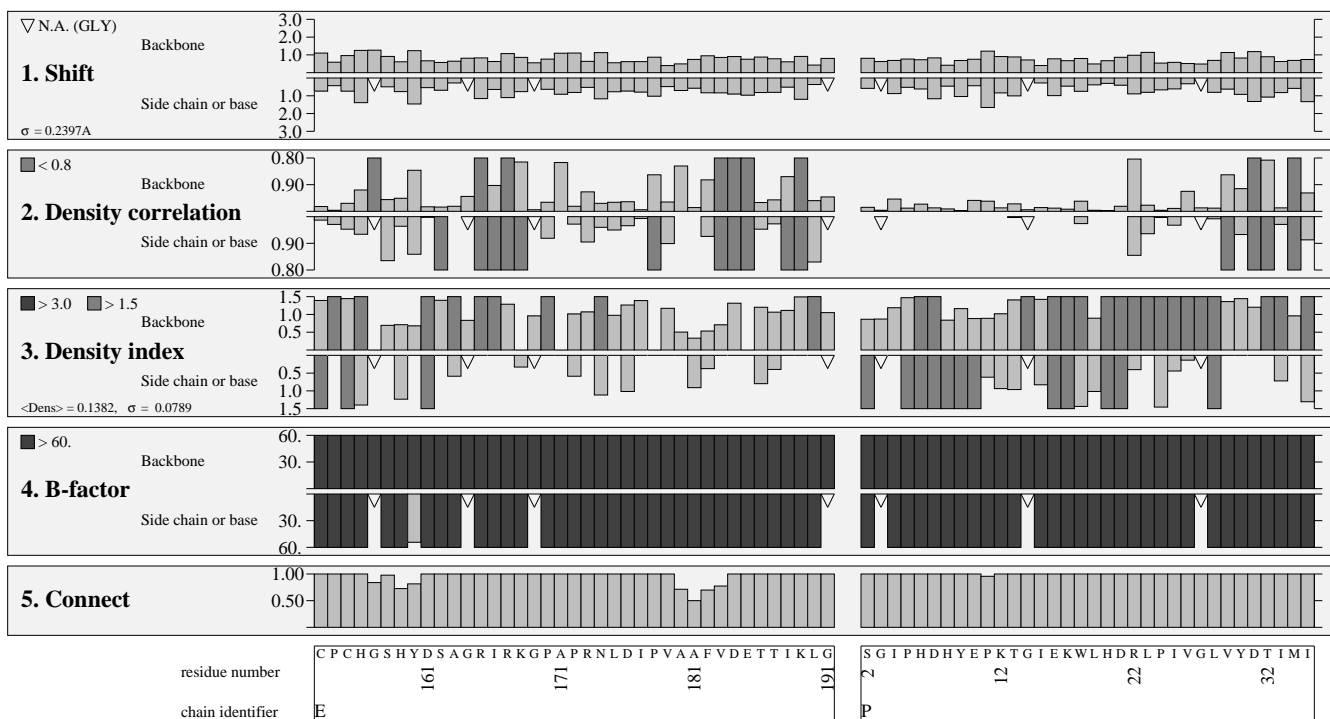
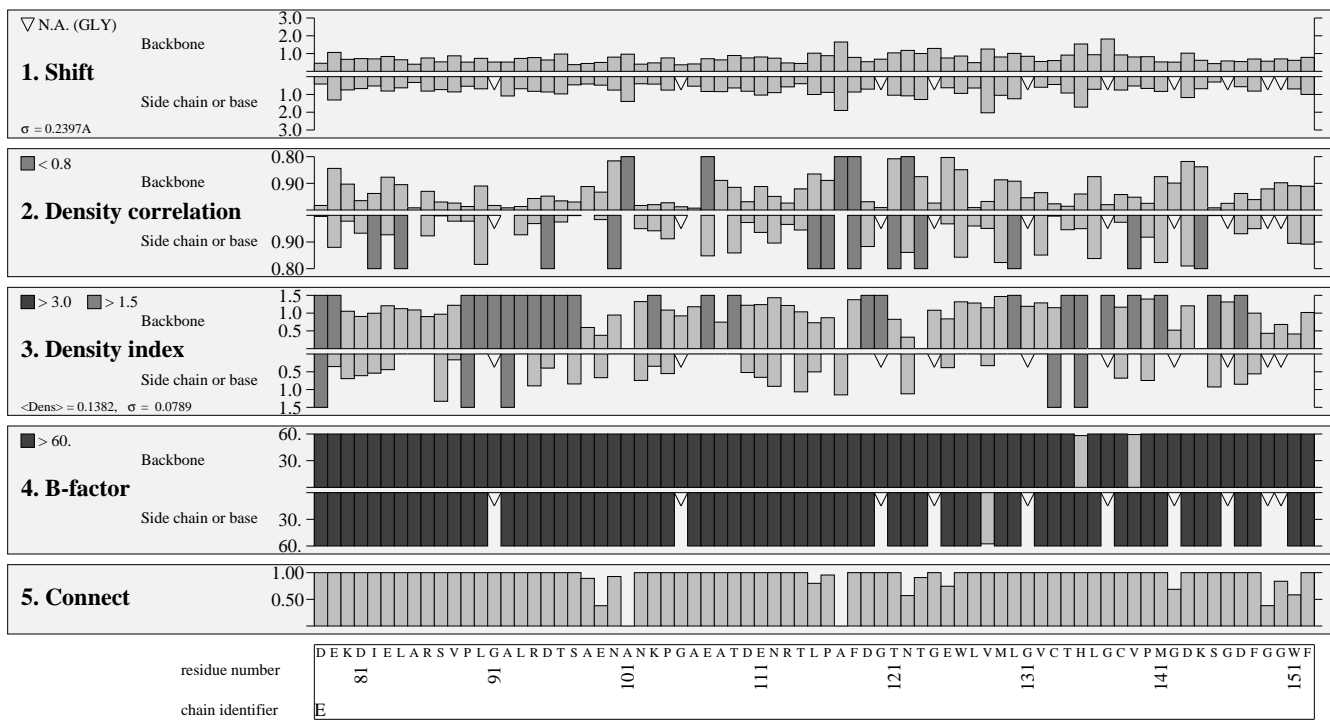
Local estimation (5)



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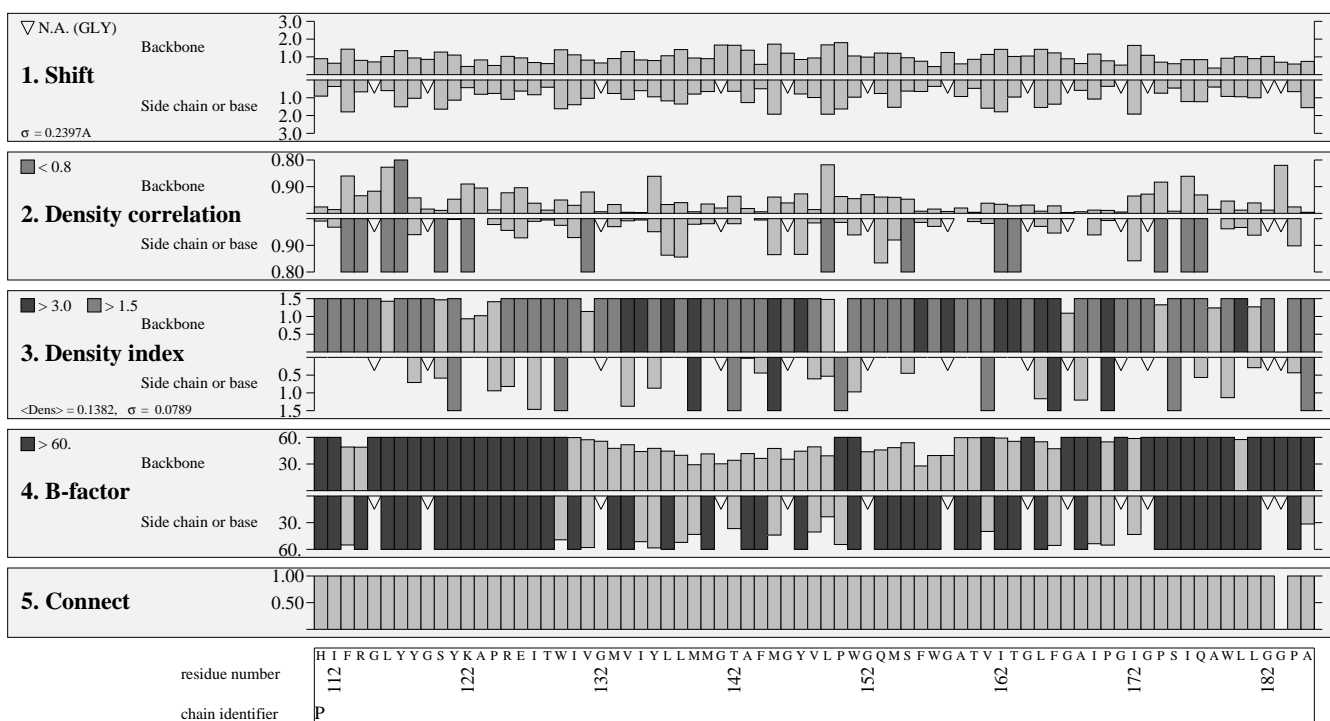
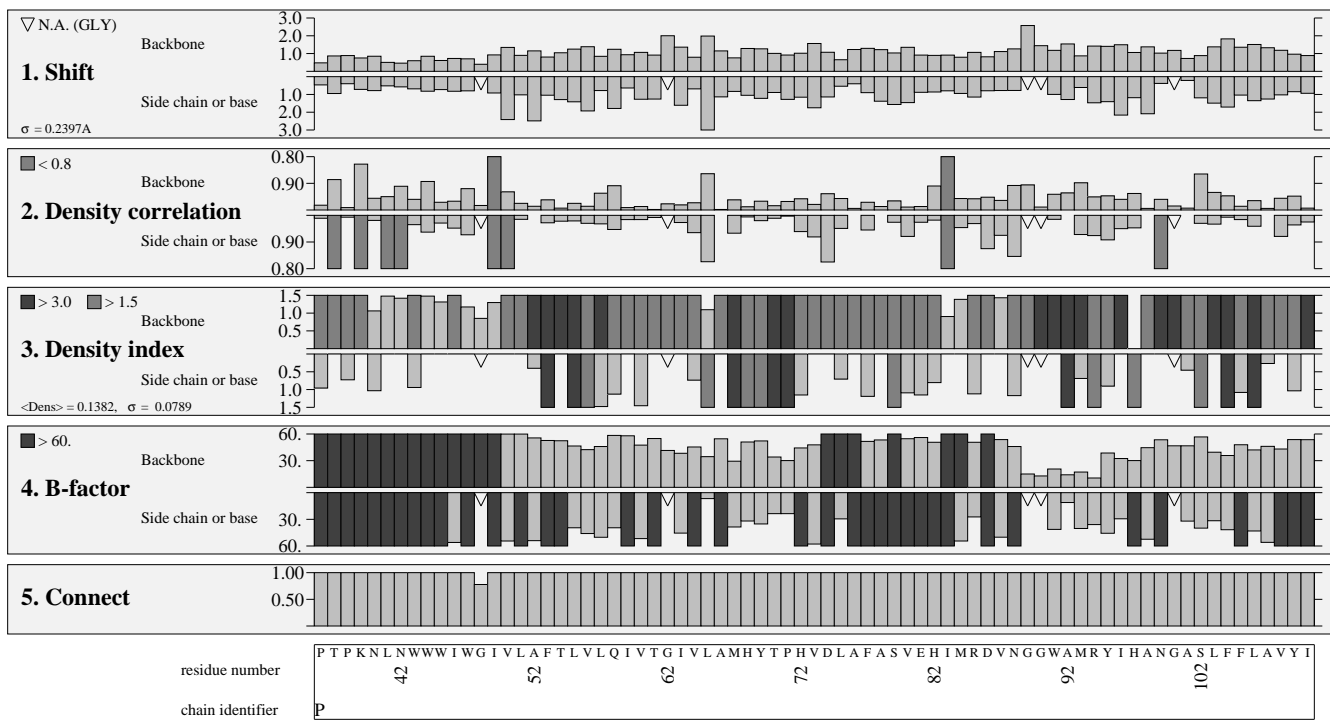
Local estimation (6)



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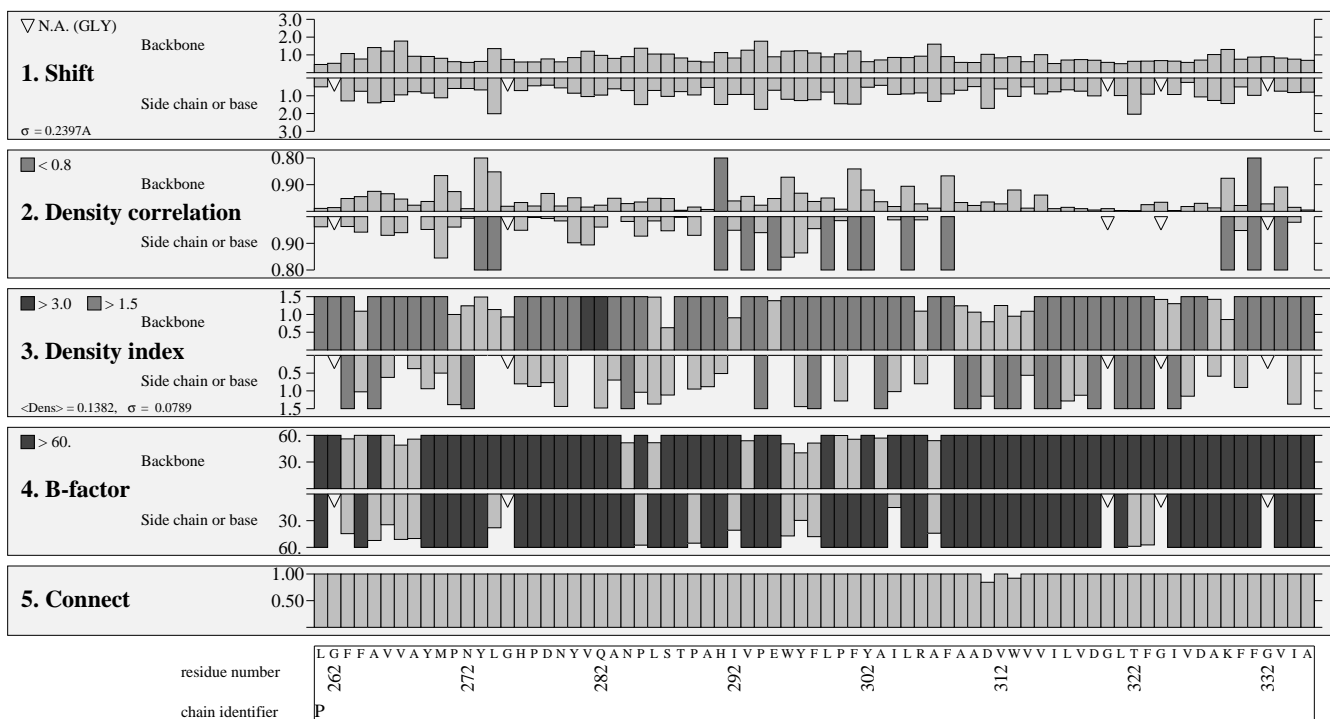
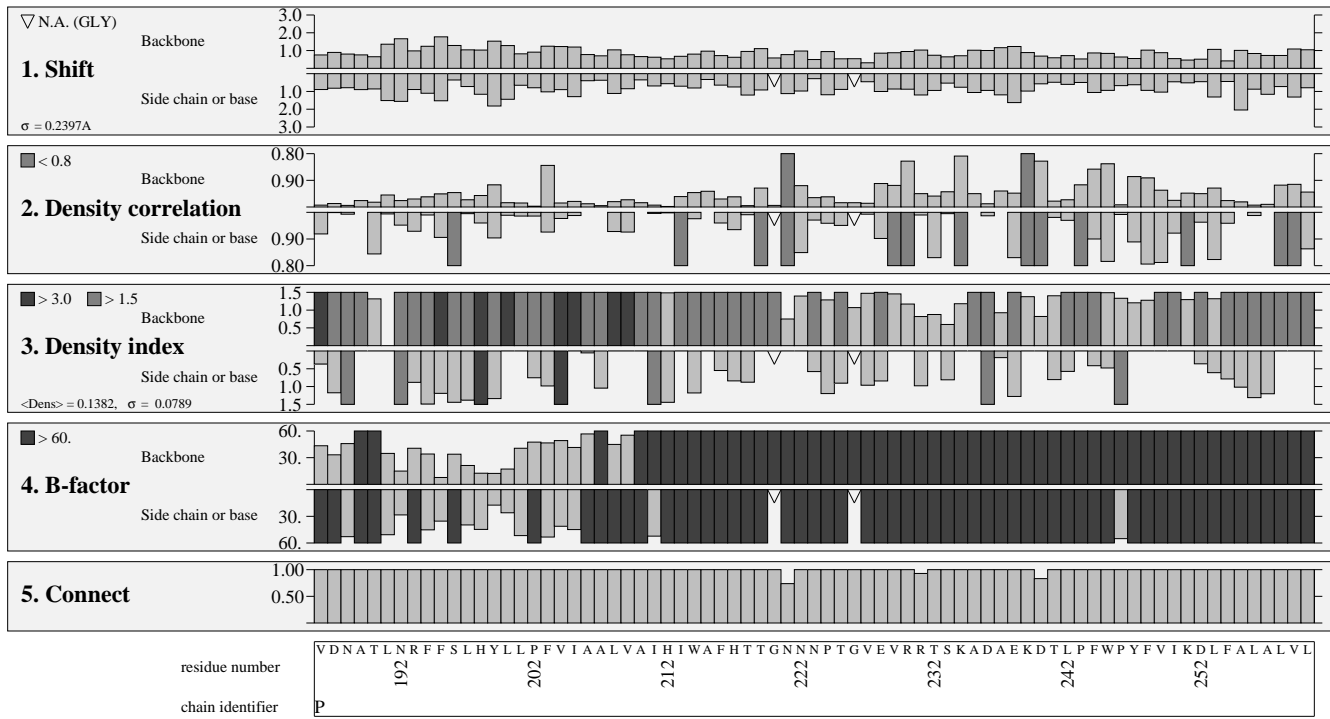
Local estimation (7)



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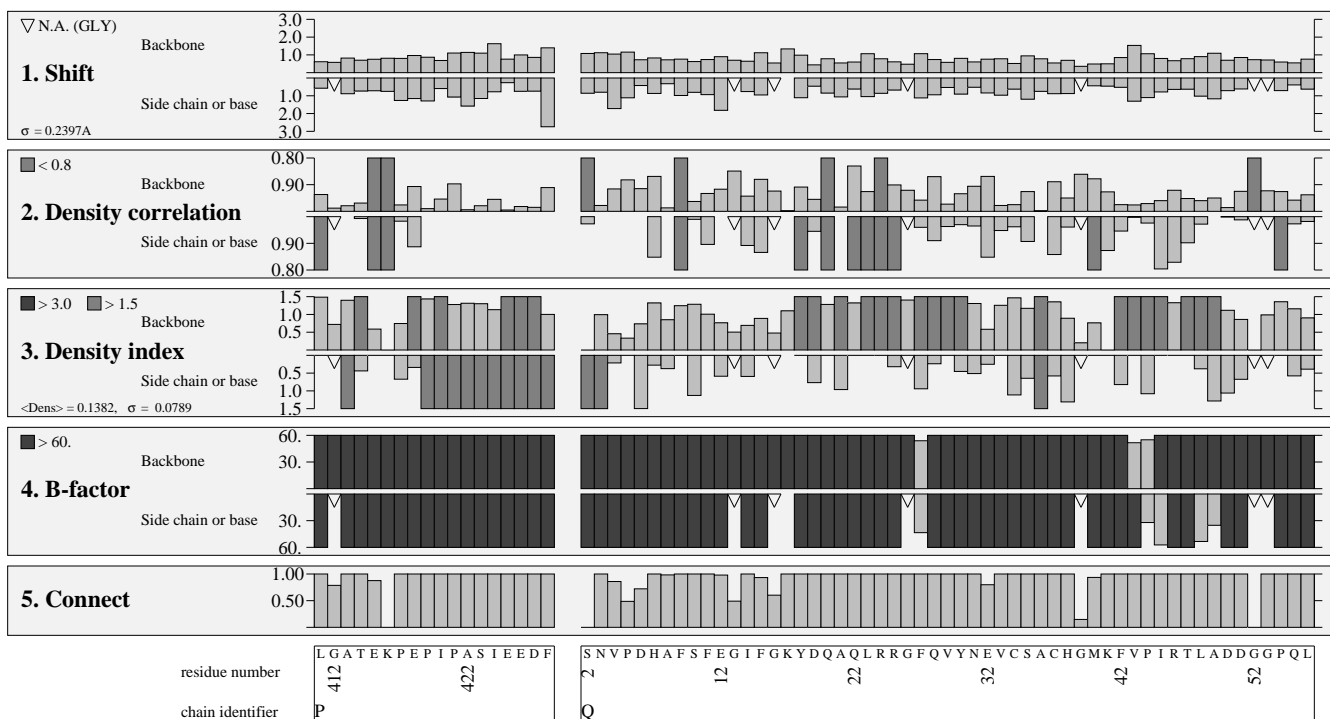
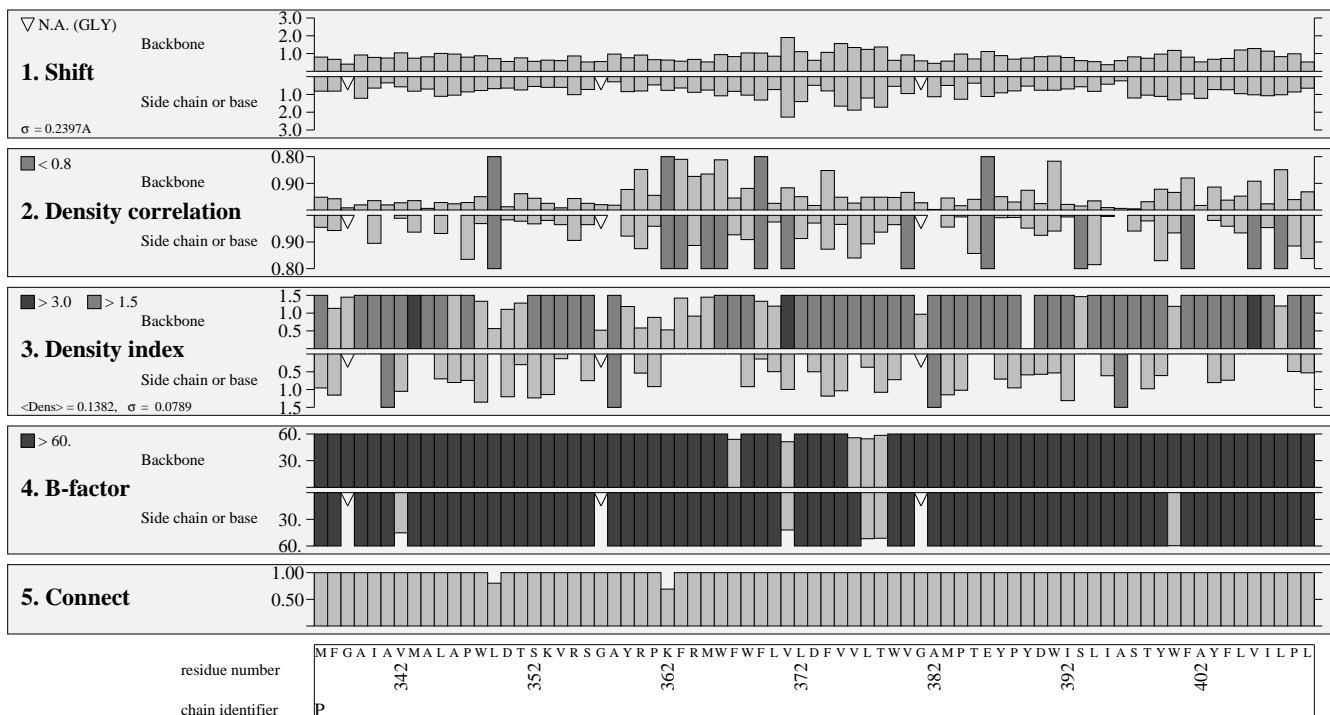
Local estimation (8)



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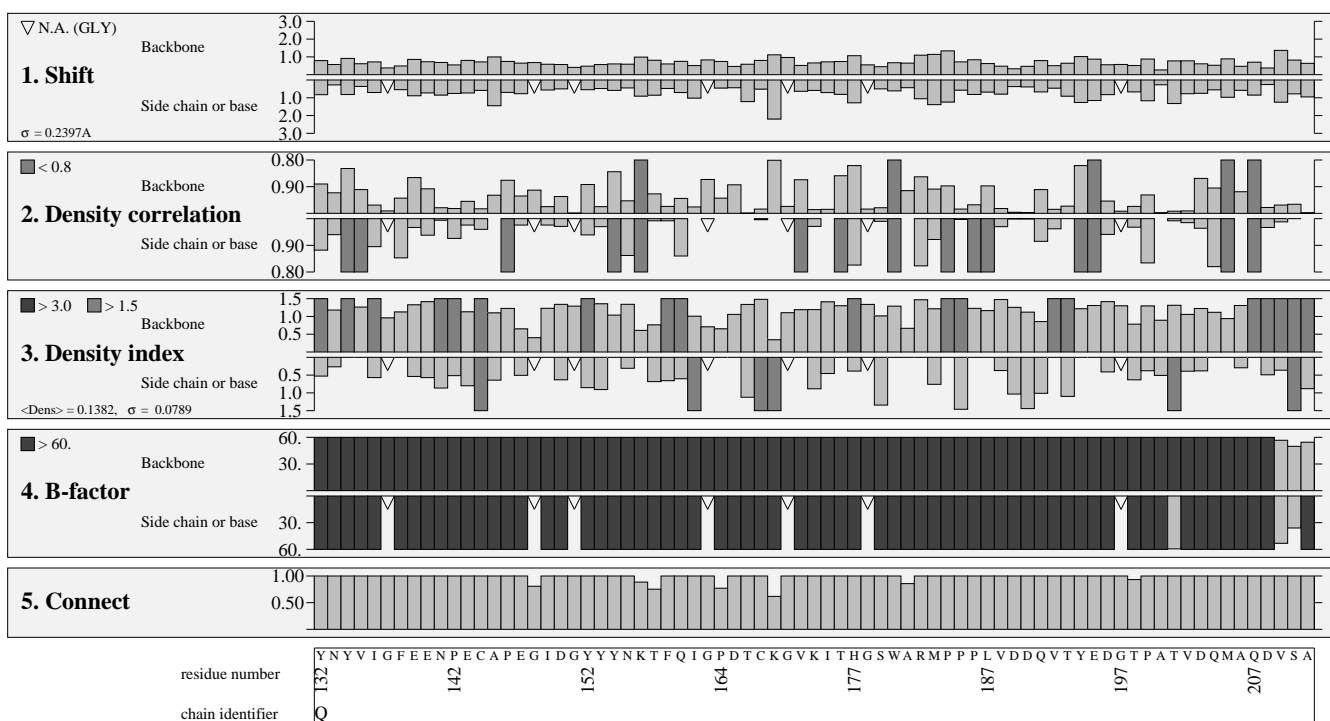
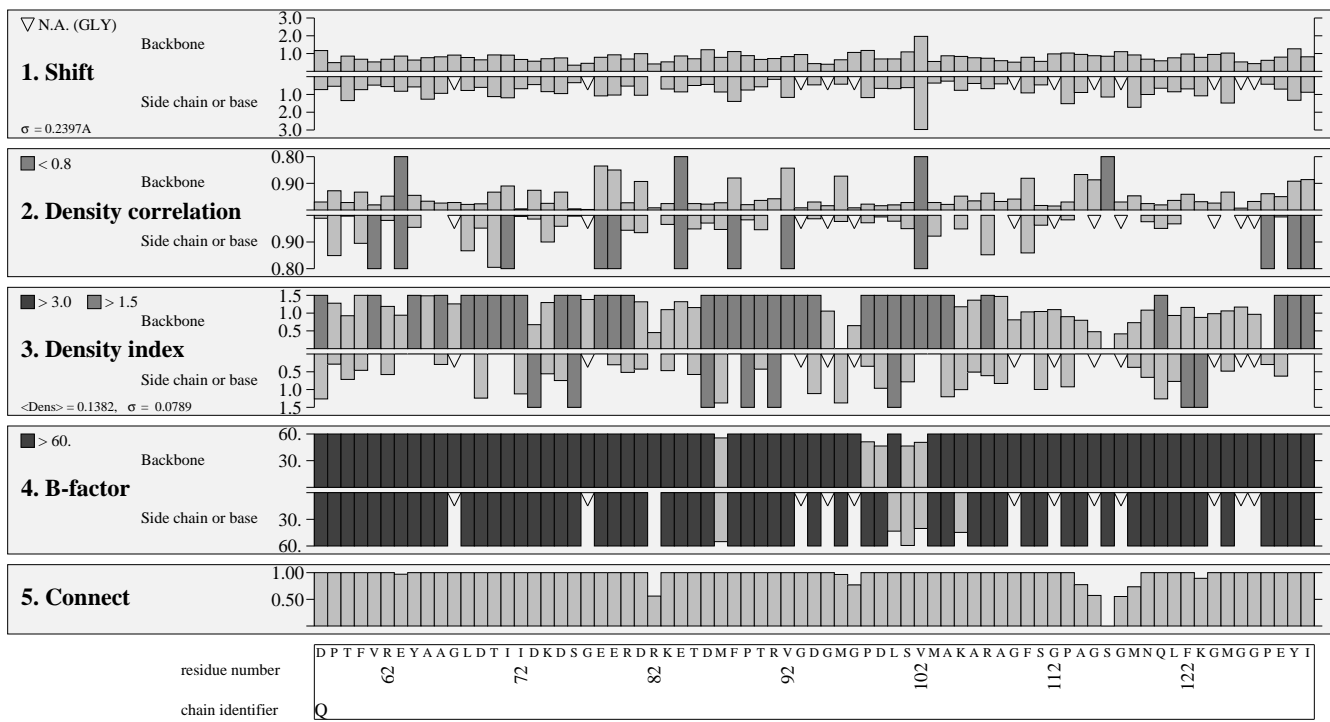
Local estimation (9)



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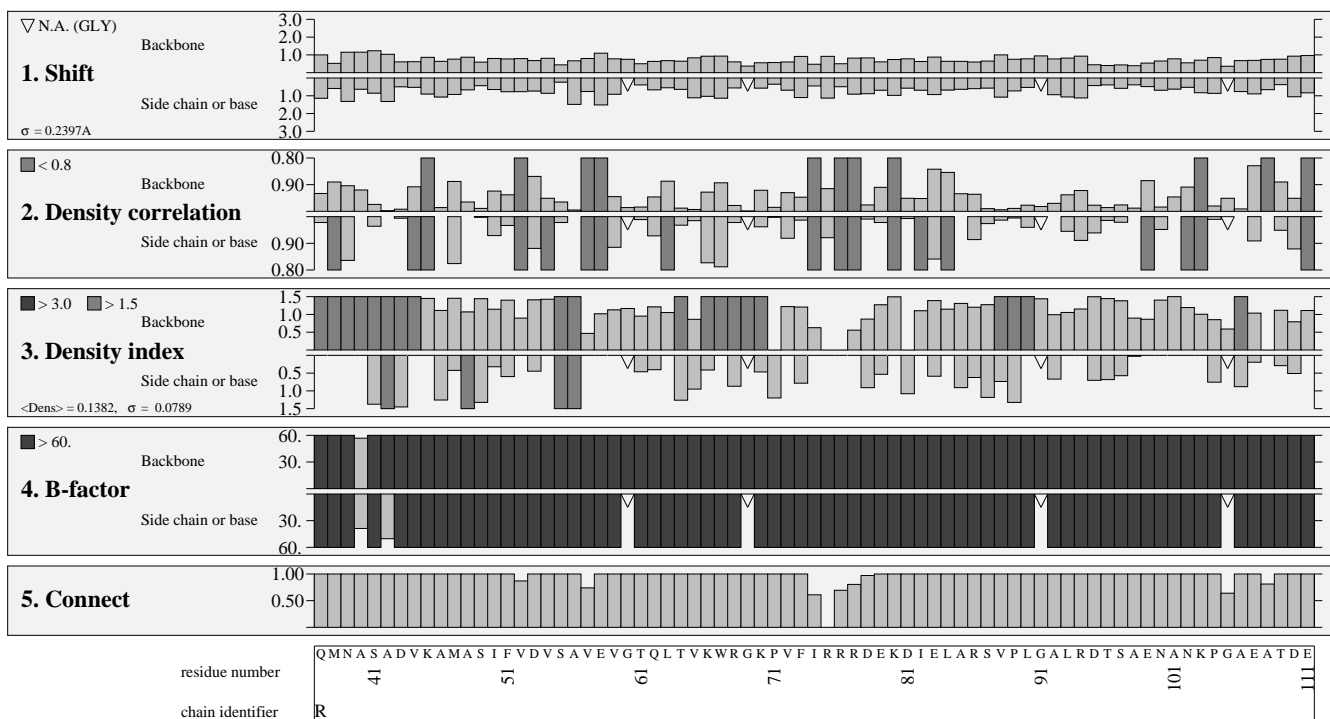
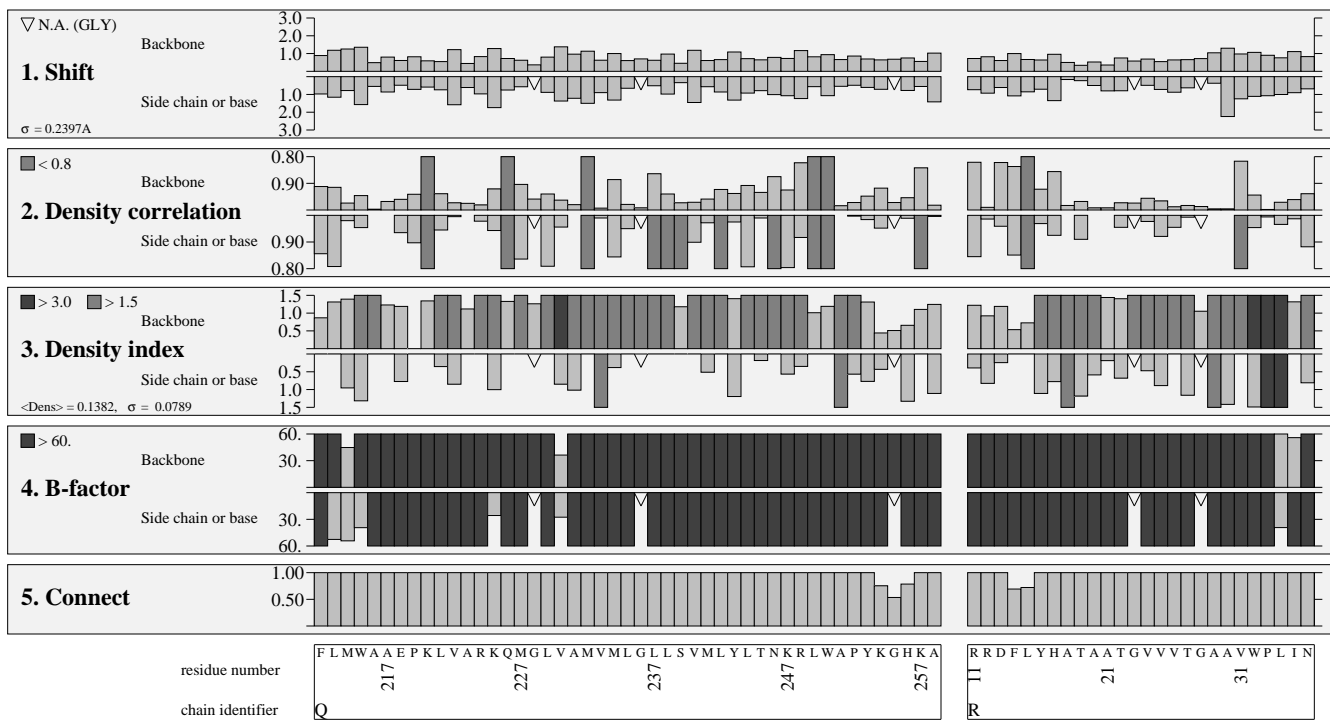
Local estimation (10)



Structure Factor Check

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Local estimation (11)



Structure Factor Check

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Local estimation (12)

