"Judge not, that you be not judged" Bible, Matthew, ch.7

Structure Factor Check

2H89

Title:	AVIAN RESPIRATORY COMPLEX II WITH MALONATE BOUND
Date:	06−JUN−06
PDB code:	2H89

Crystal

Cell parameters:

a: 70.52 A	b: 84.12 A	c: 292.21 A
α: 90.00	β: 90.00	γ: 90.00

Space group: P 21 21 21

Model

9302 atoms (580 water molecules)

Number of chains:	51
Volume not occupied by model:	52.6 %
<B> (for atomic model):	59.5 A^2
σ(B):	15.13 A^2
Matthews coefficient:	3.33
Corresponding solvent % :	62.75

Refinement

Program:	CNS 1.1
Nominal resolution range:	50.7 − 2.40 A
Reported R−factor:	0.226
Number of reflections used:	59635
Reported Rfree:	0.28
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		50.7 − 2.29 A
Reflections in file:		63071
Unique reflections	above 0:	63071
	above 1σ:	62361
	above 3σ:	43380

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Nominal resolution range:	50.7 − 2.40 A
\05max. from input data, min. from author\05	
Used reflections:	59635
Reflections out of resolution:	3436
Completeness:	86.3 %
R_stand(F) = <σ(F)>/<F> :	0.092
Anisotropic distribution of Structure Factors	
ratio of eigen values:	0.9882 1.0000 0.7279
B_overall (by Patterson):	44.A^2
Optical resolution:	1.93 A
Expected opt. resol. for complete data set:	1.93 A
Estimated minimal error:	0.039 A

Model vs. Structure Factors

R−factor for all reflections:	0.244
Correlation factor:	0.917
R−factor:	0.251
for F > 2.0 σ	
nom. resolution range:	50.74 − 2.40A
reflections used:	59044
Rfree:	0.300
Nfree:	2886
R−factor without free−refl.:	0.248
Non free−reflections:	56158
<u> (error in coords by Luzzati plot):	0.363 A
Estimated maximal error:	0.116 A
DPI:	0.258 A

Scaling

Scale:	0.872
Bdiff:	−2.45

Anisothermal Scaling (Beta):
3.3086 3.3590 −1.6387 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.495 250.062

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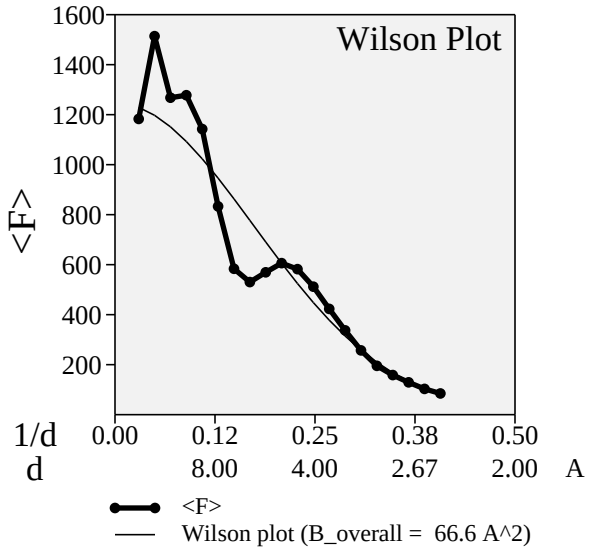
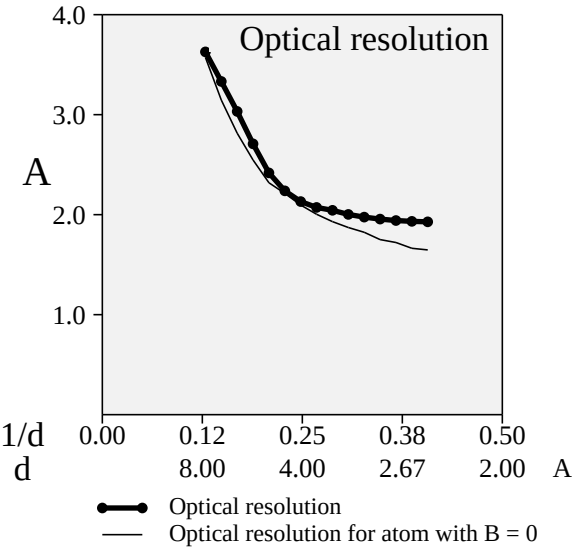
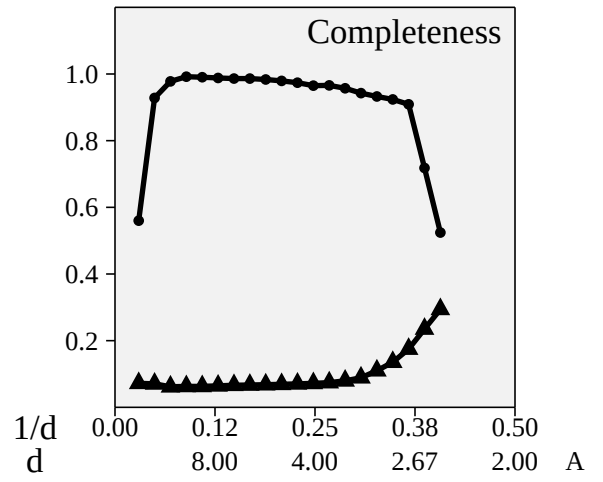


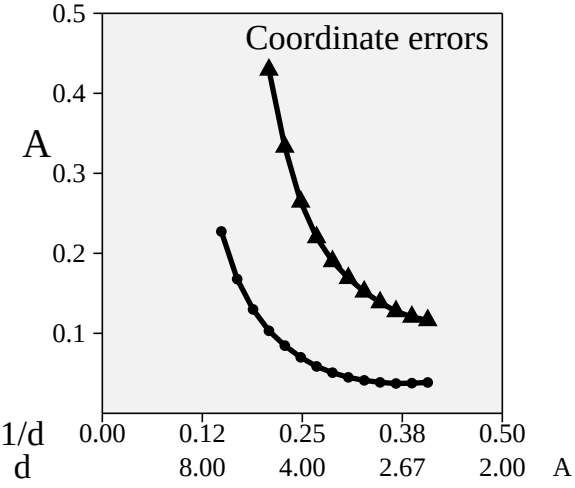
<F>
Wilson plot (B_overall = 66.6 A^2)



Optical resolution
Optical resolution for atom with B = 0

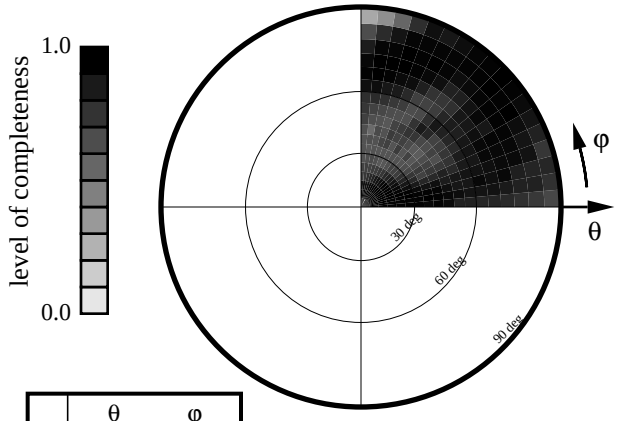


Completeness
R_stand(F) = <σ(F)>/<F>



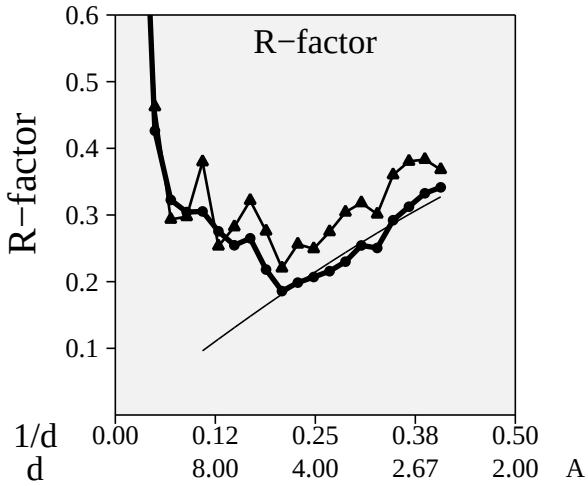
Expected maximal coordinate error
Expected minimal coordinate error

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



R−factor
Rfree
Luzzati plot drawn for an atomic error = 0.363

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Structure Factor Check

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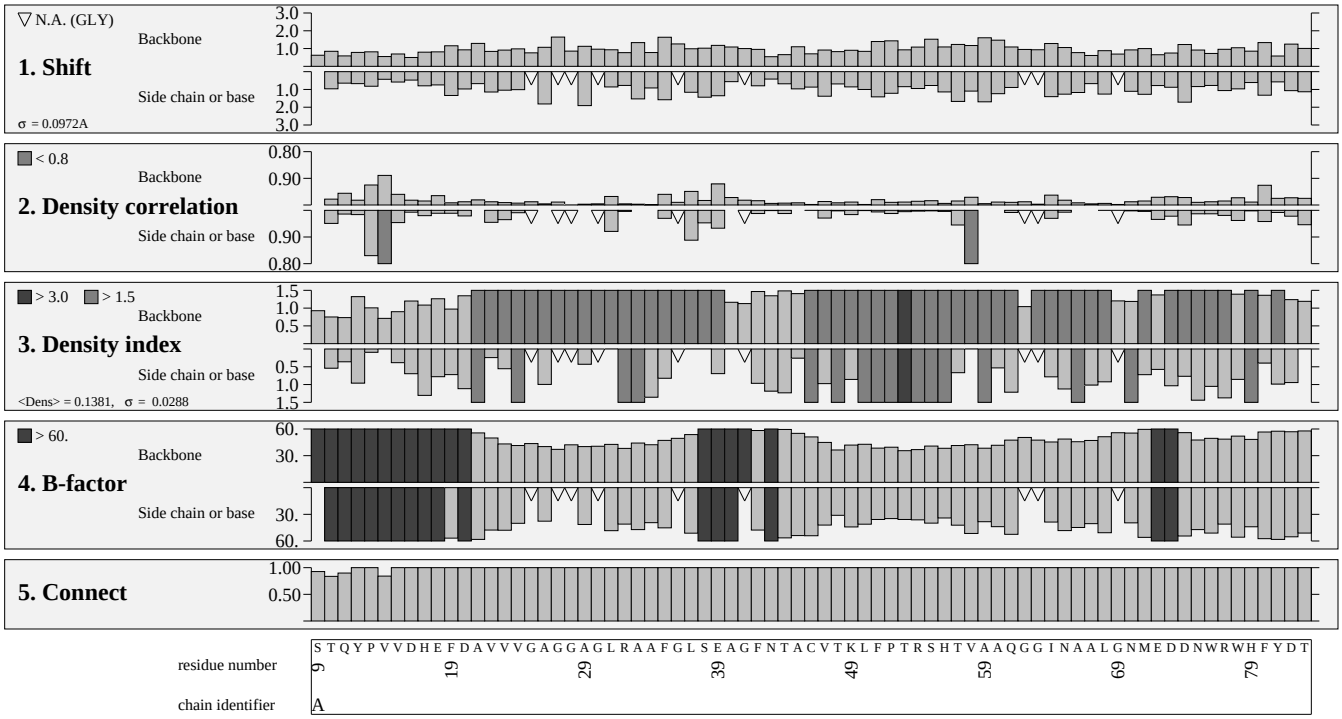
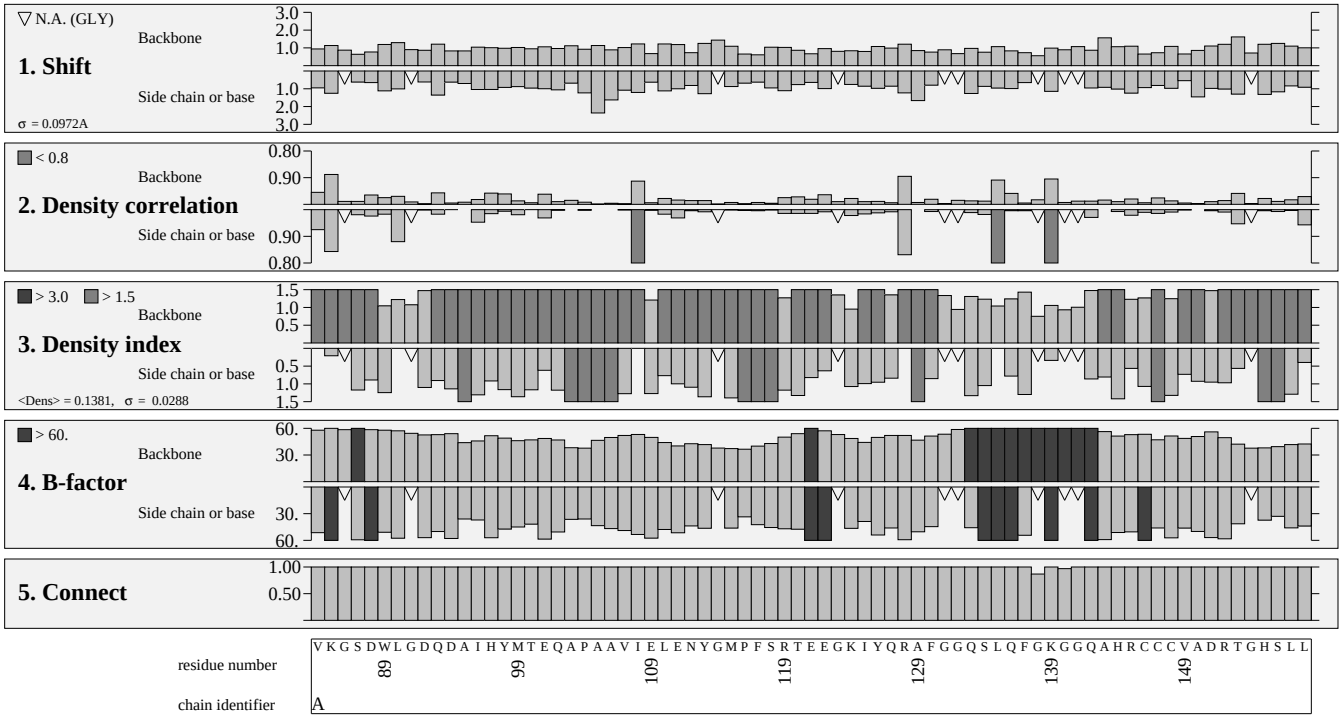
Local estimation





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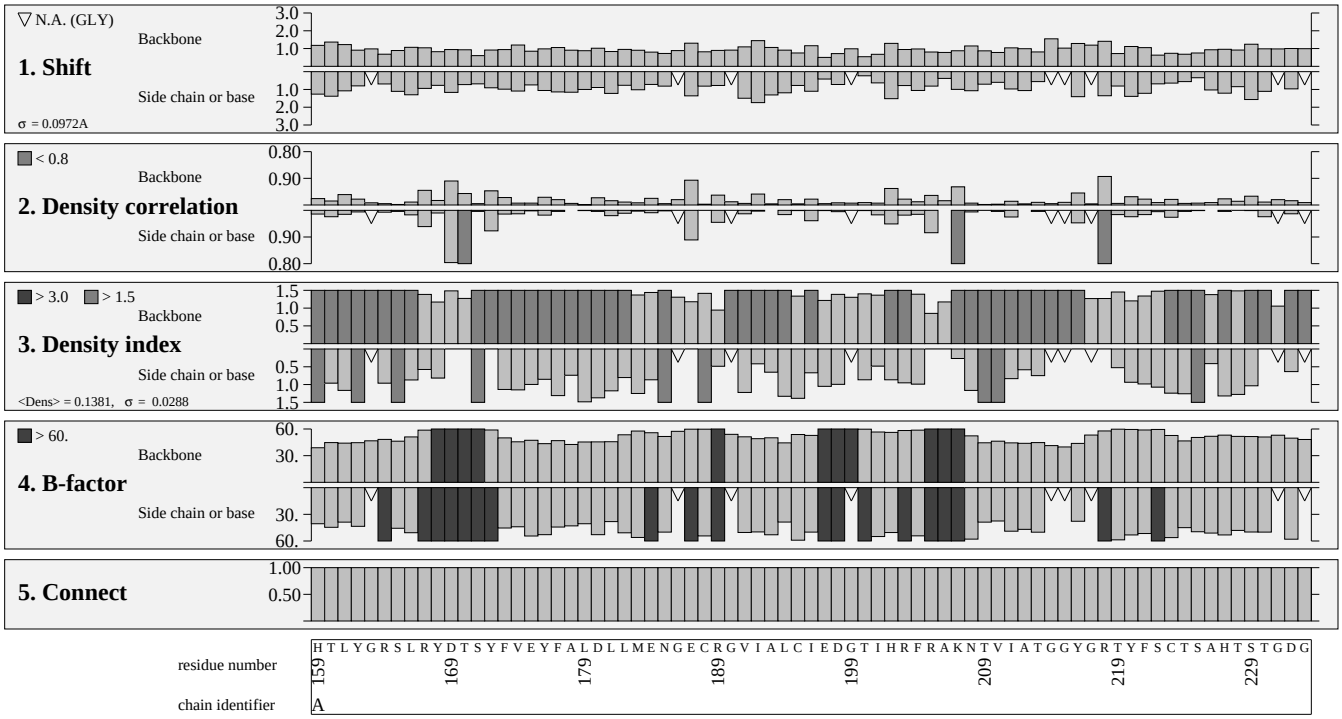
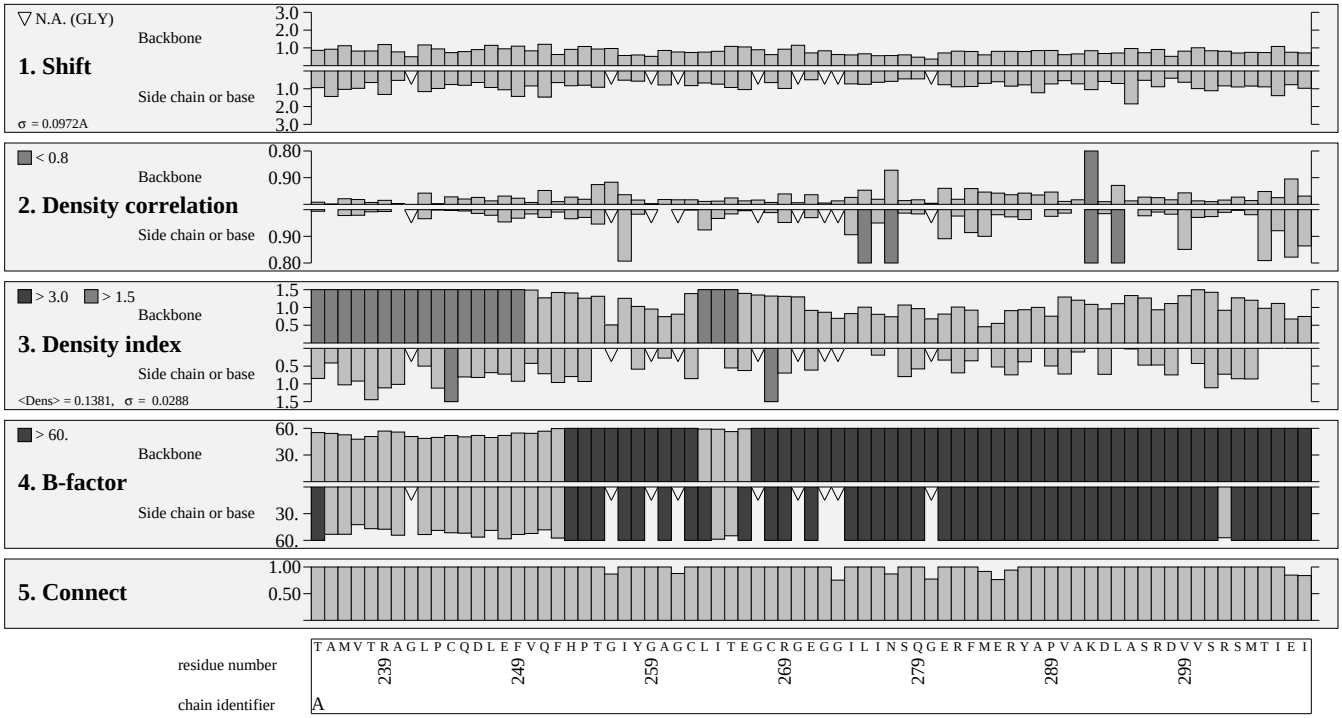
Structure Factor Check

2H89

Local estimation (2)





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Structure Factor Check

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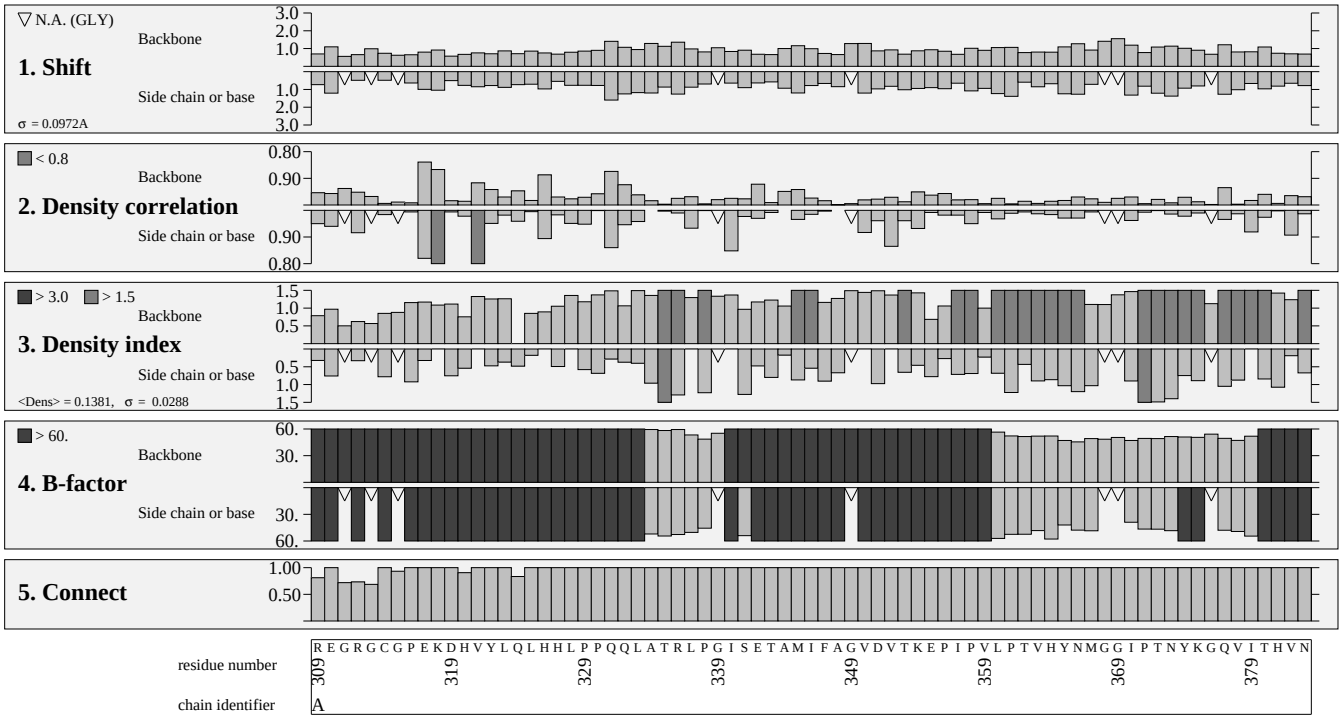
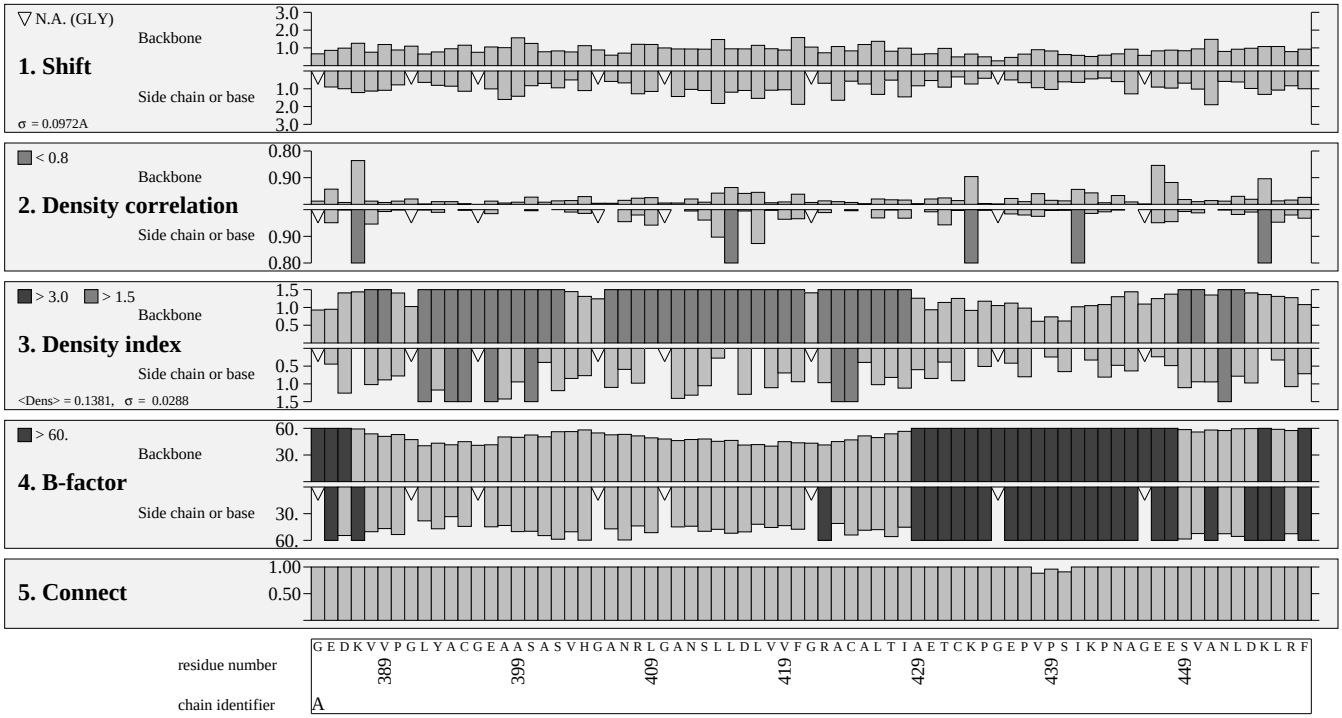
Local estimation (3)





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Structure Factor Check

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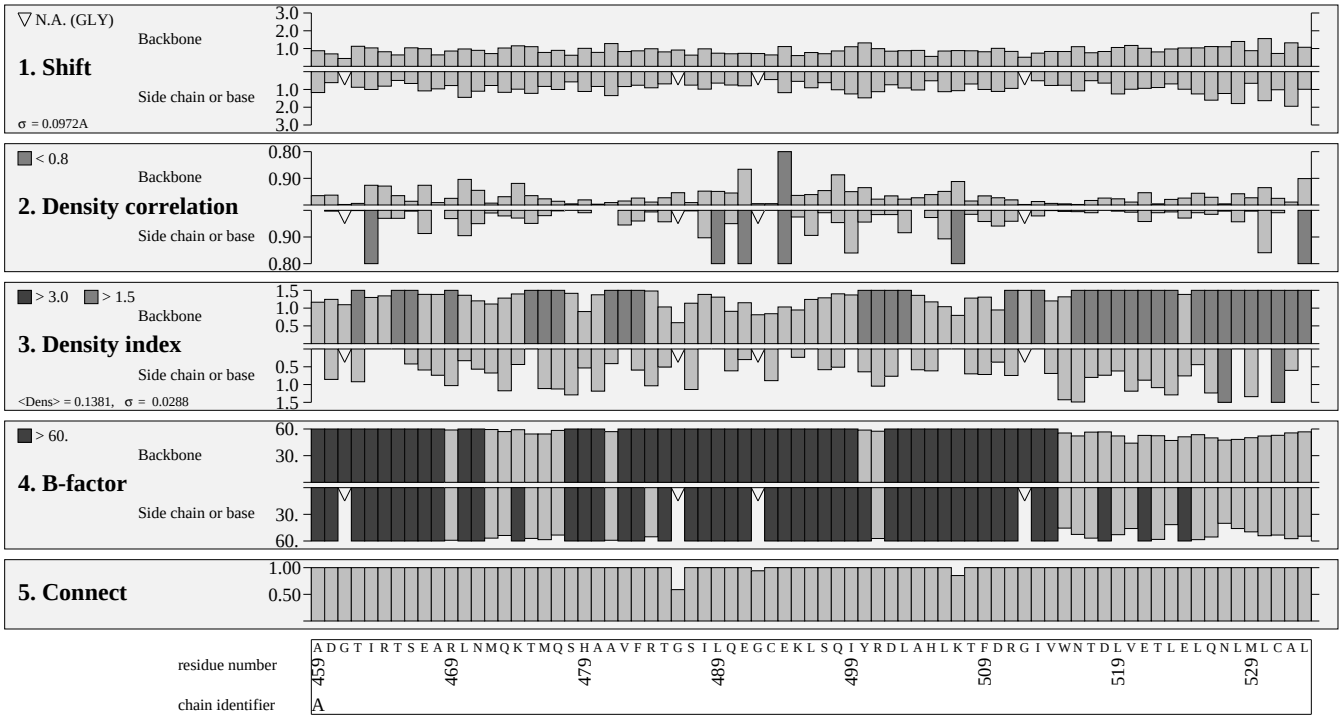
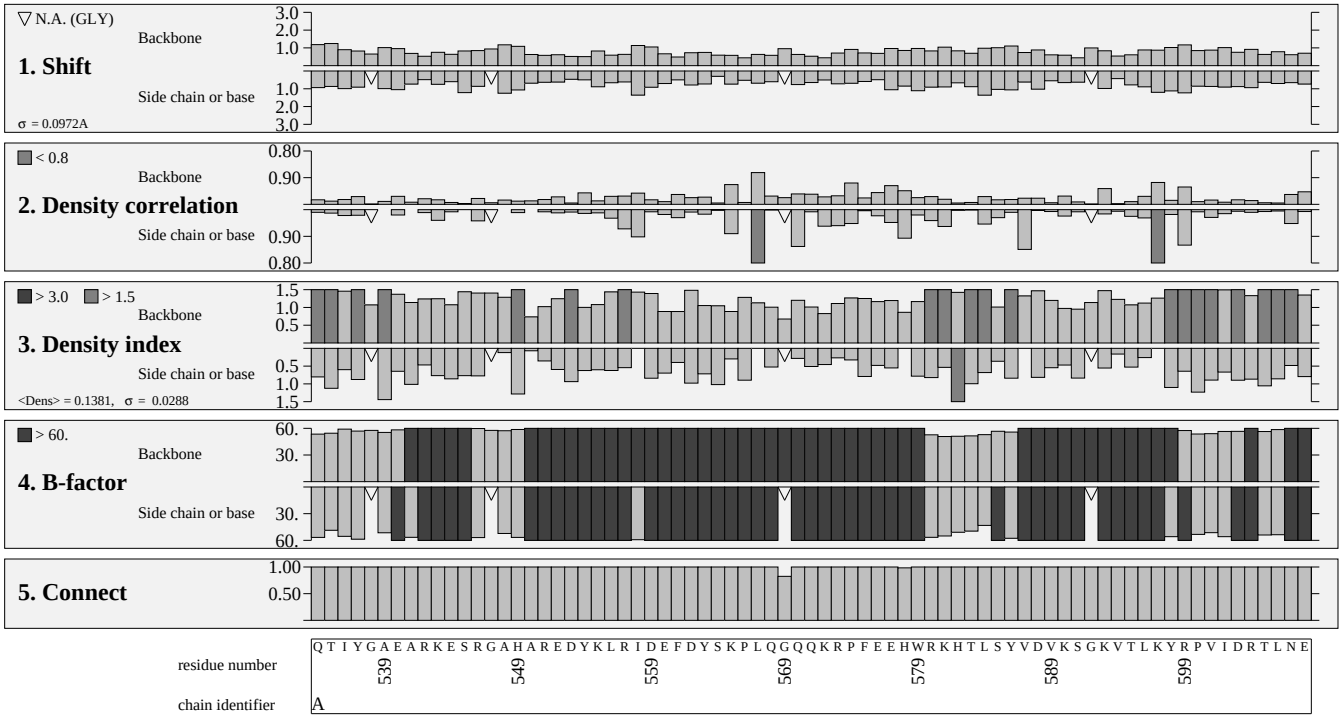
Local estimation (4)





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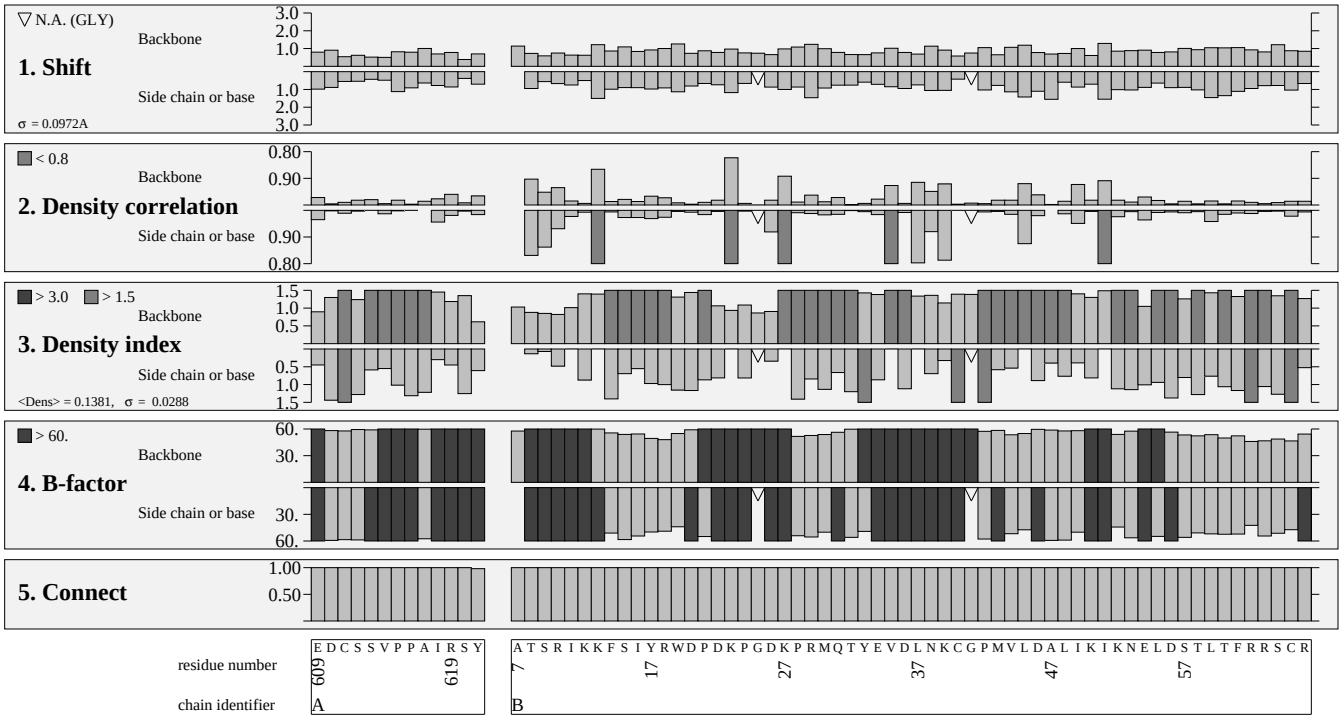
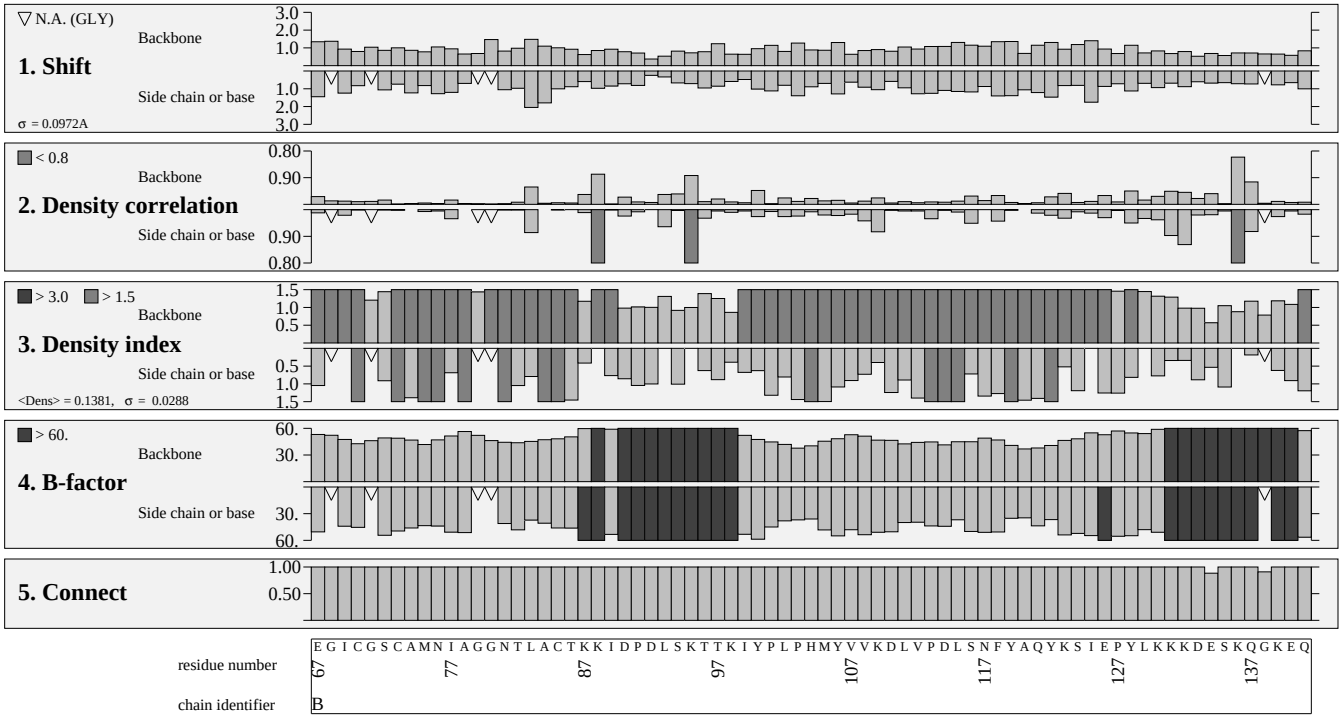
Structure Factor Check

2H89

Local estimation (5)





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Structure Factor Check

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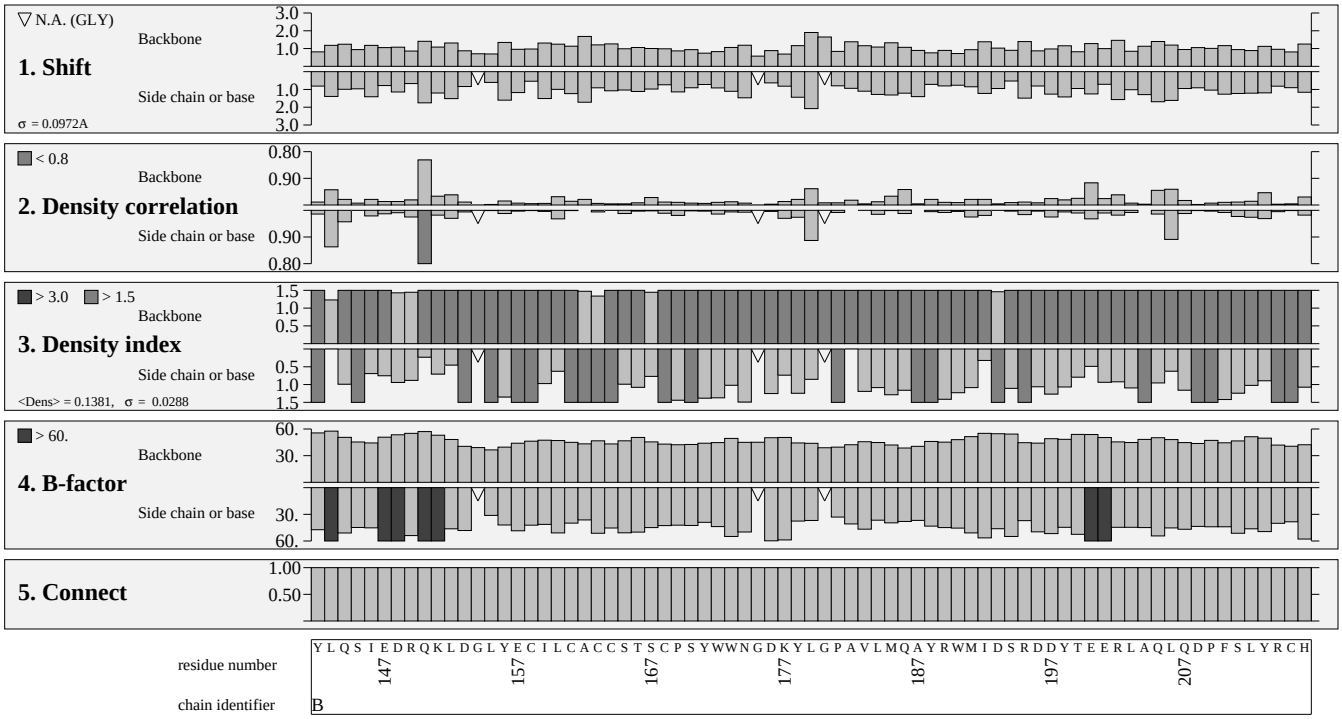
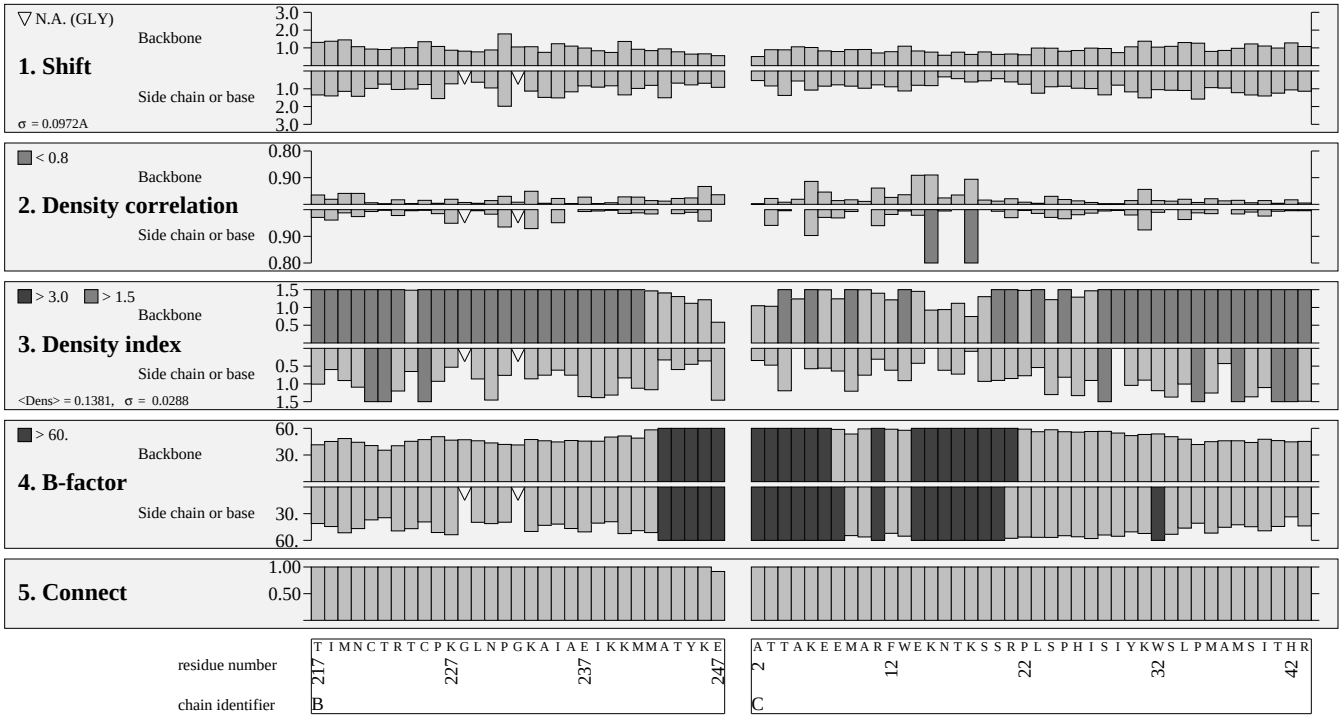
Local estimation (6)





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Structure Factor Check

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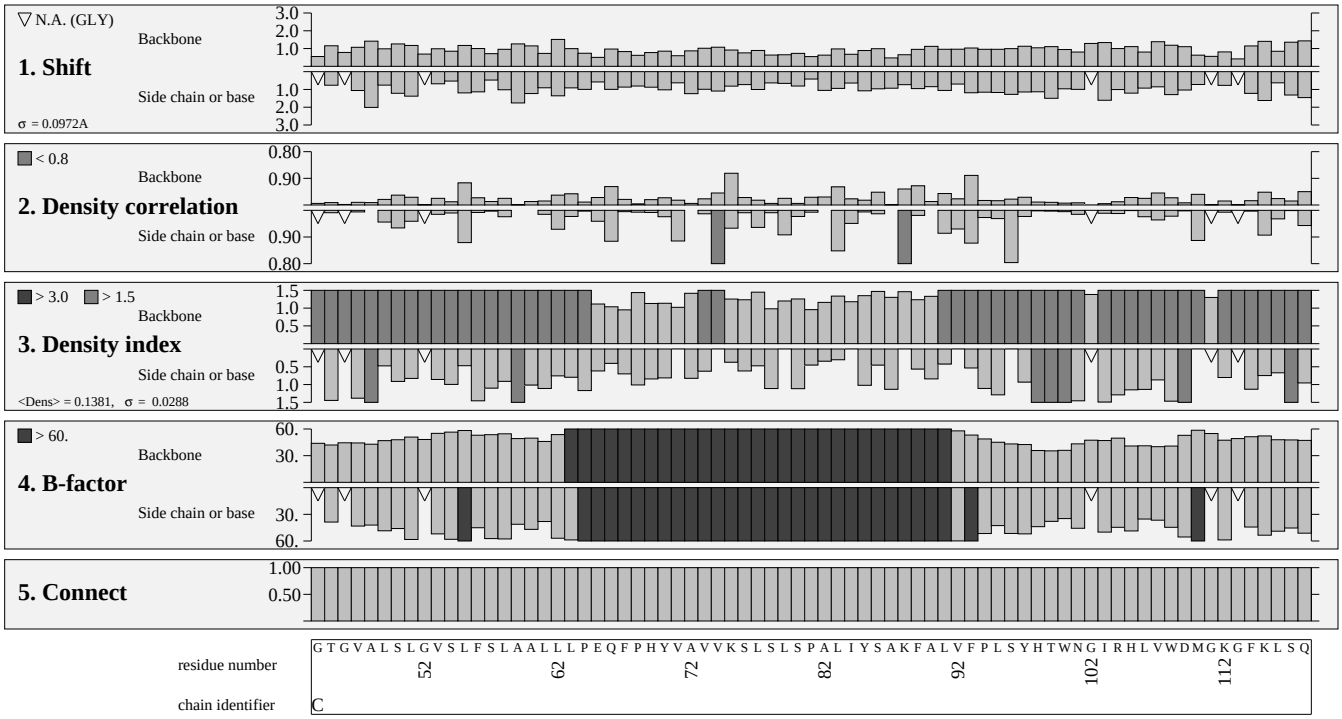
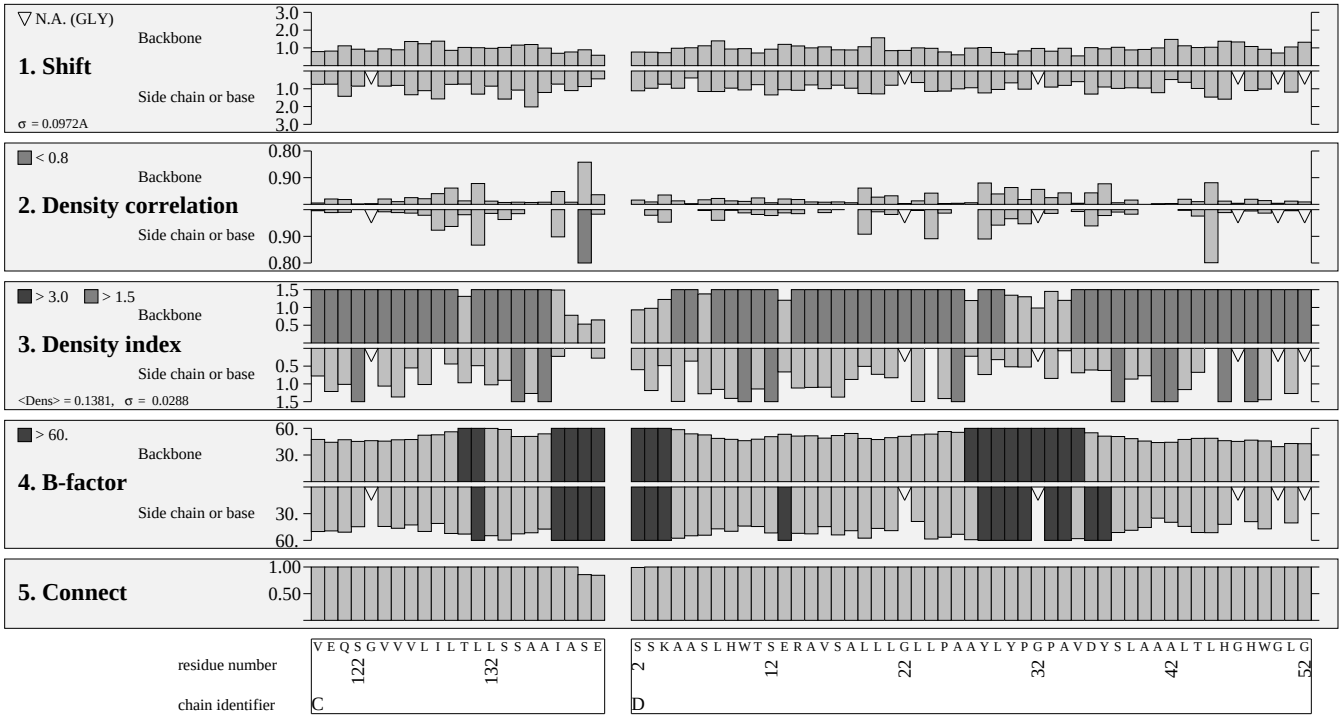
Local estimation (7)





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Structure Factor Check

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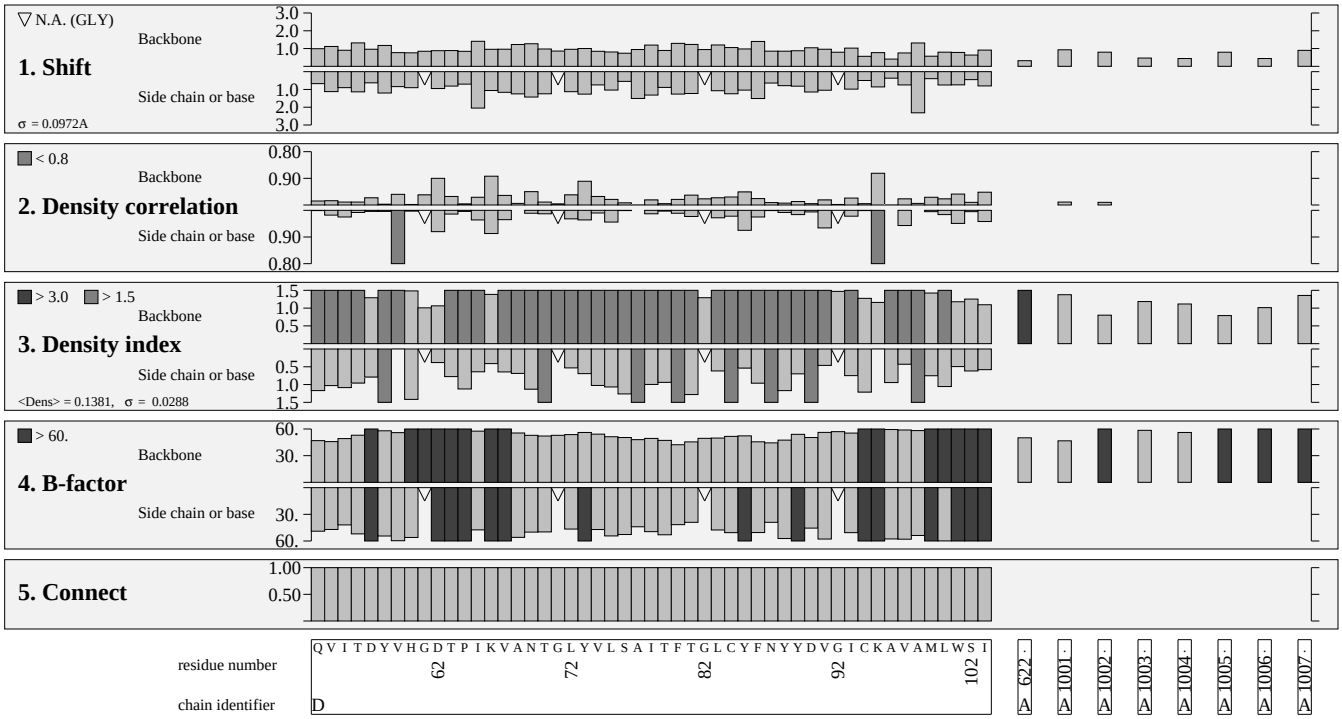
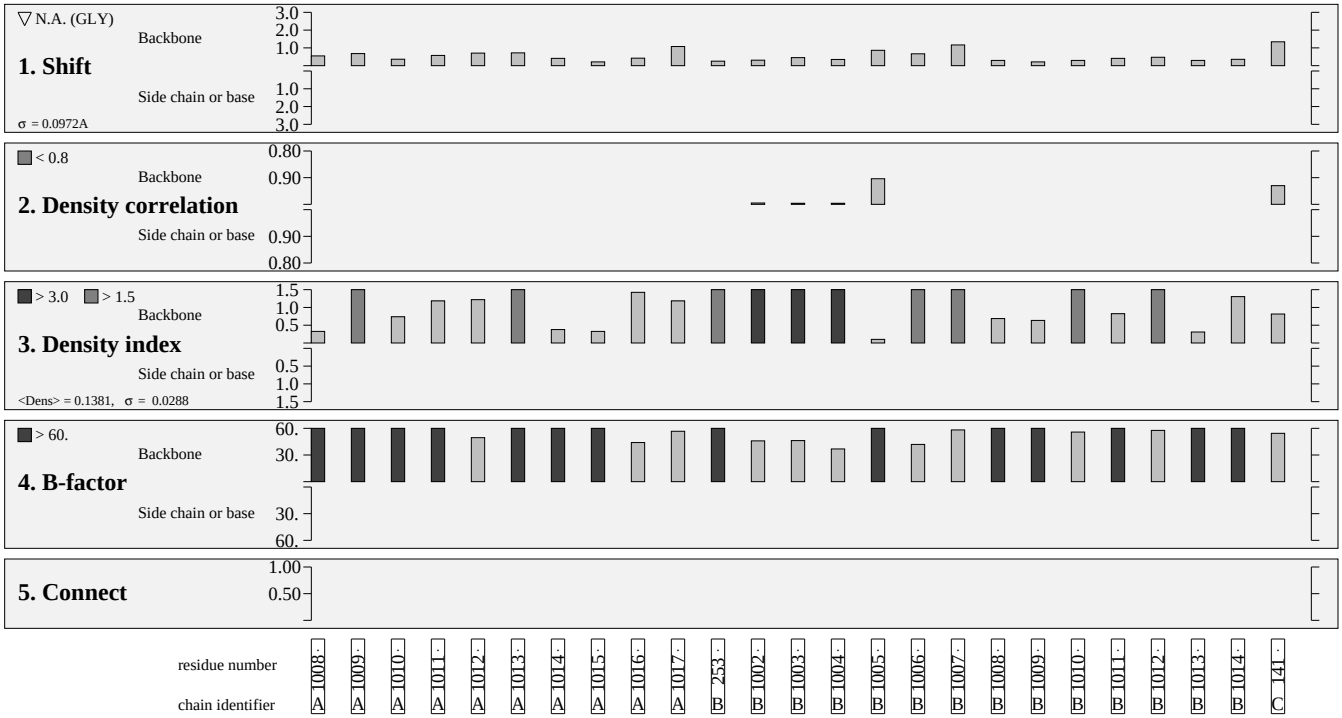
Local estimation (8)





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Structure Factor Check

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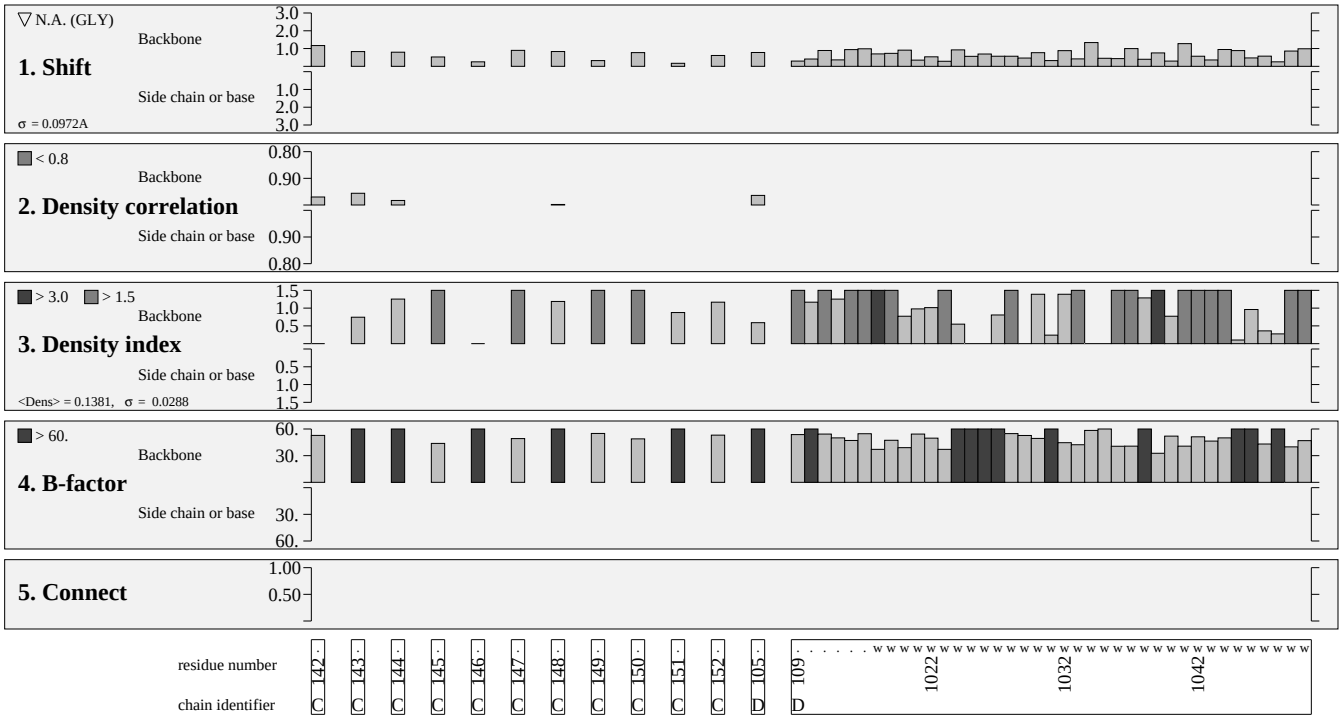
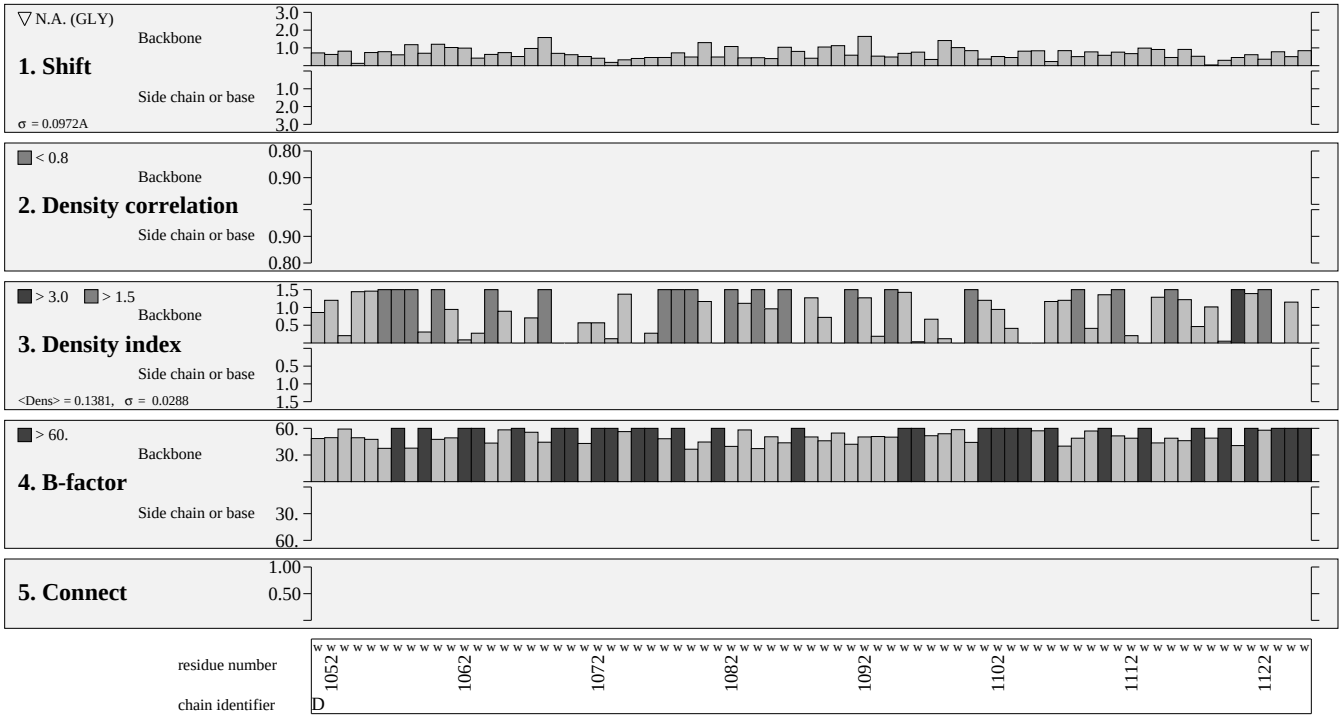
Local estimation (9)





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Structure Factor Check

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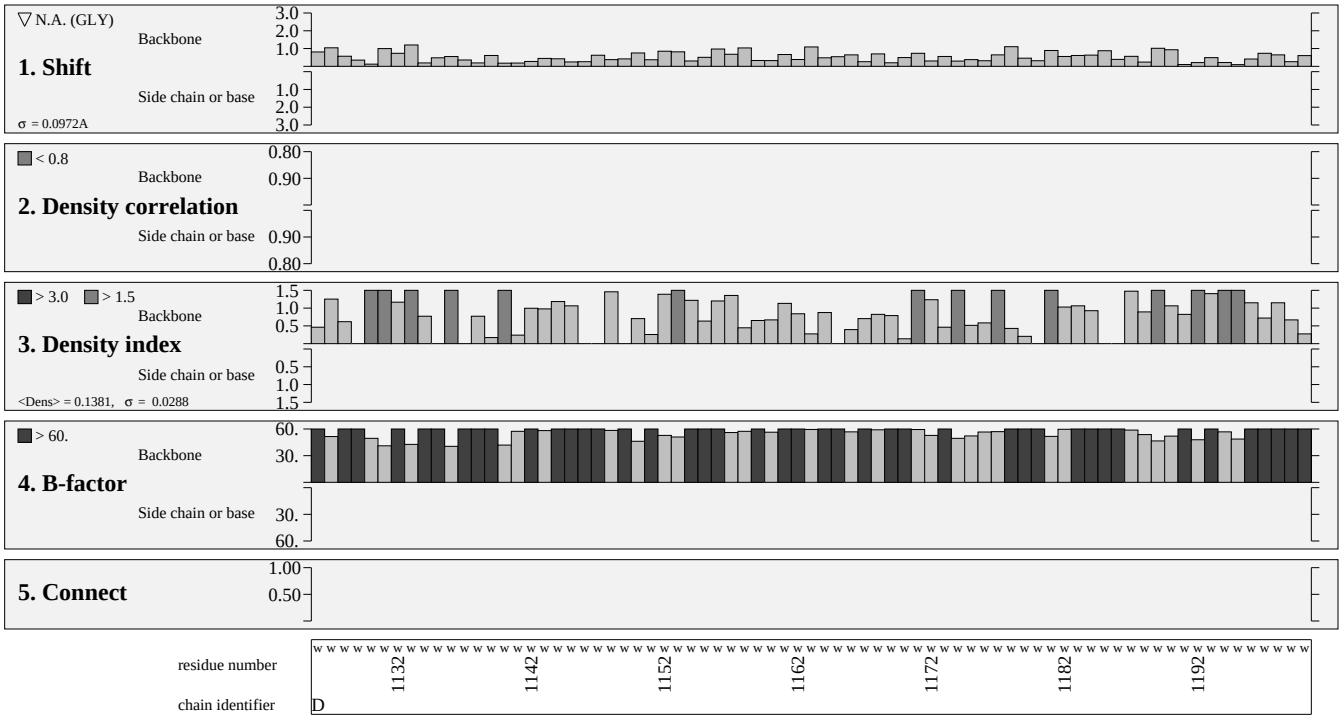
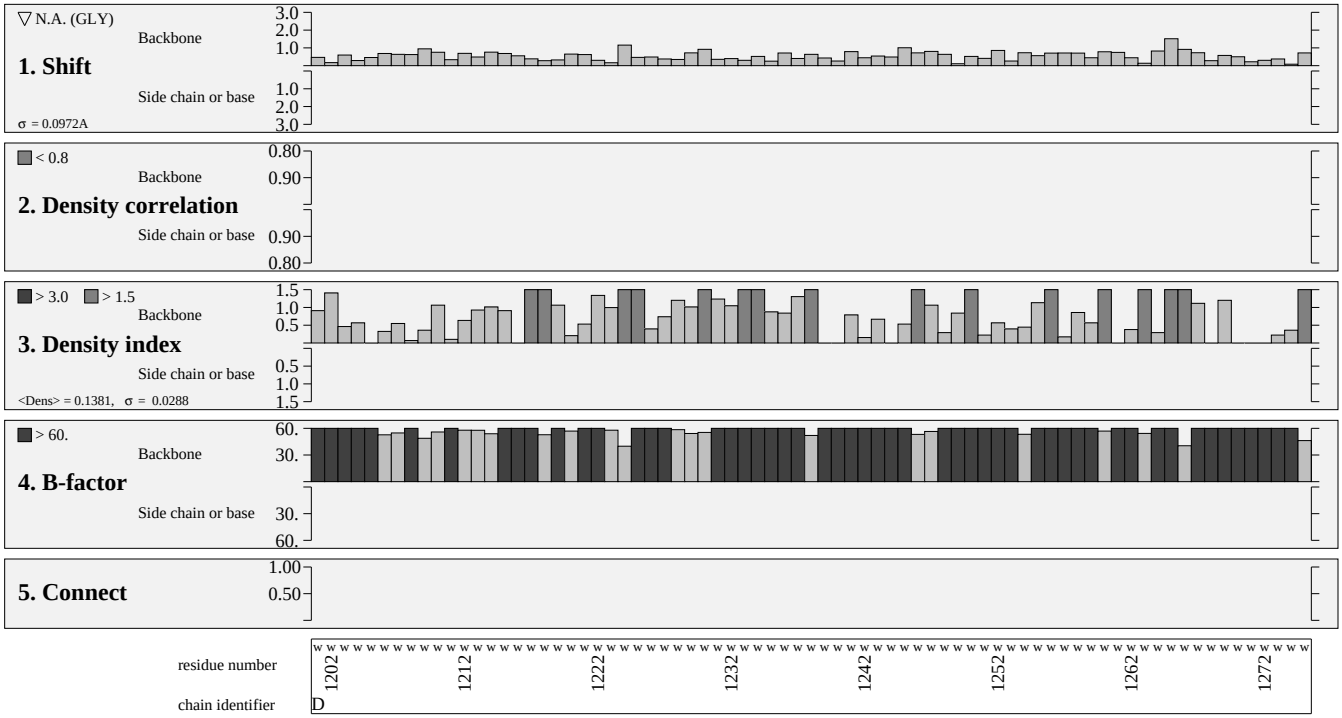
Local estimation (10)





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Structure Factor Check

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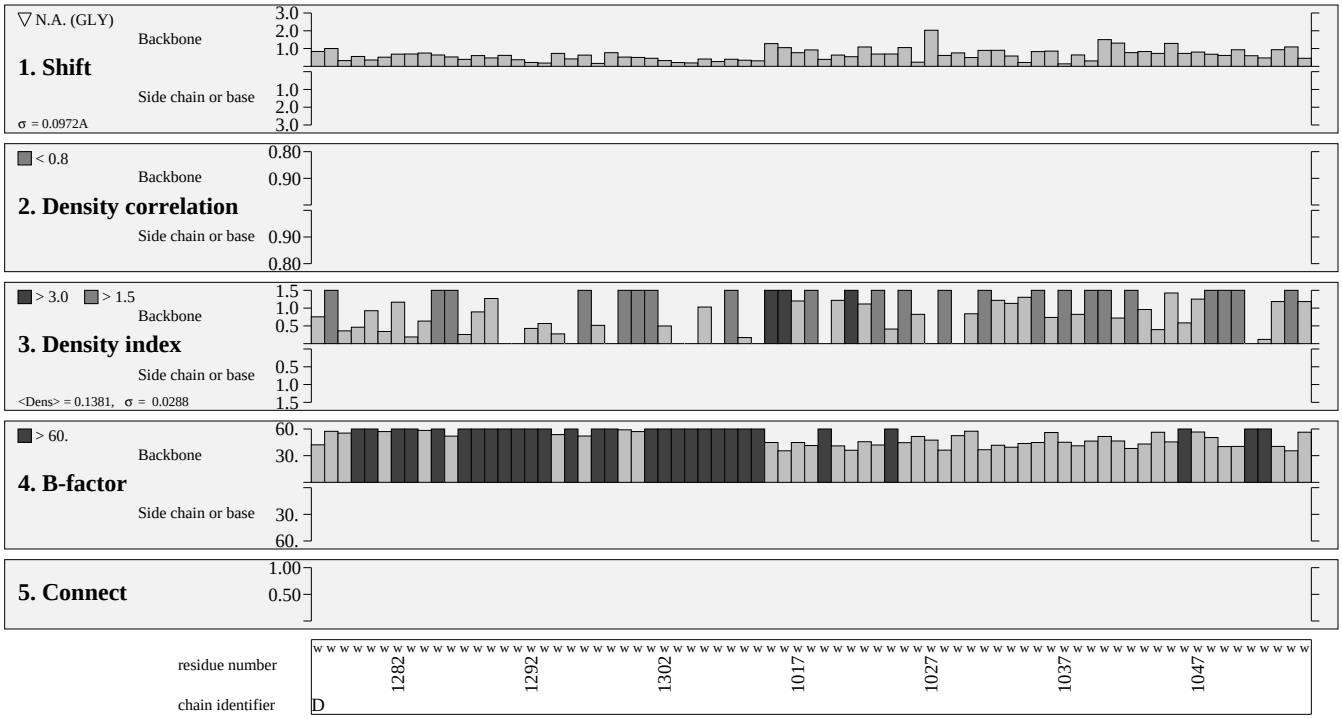
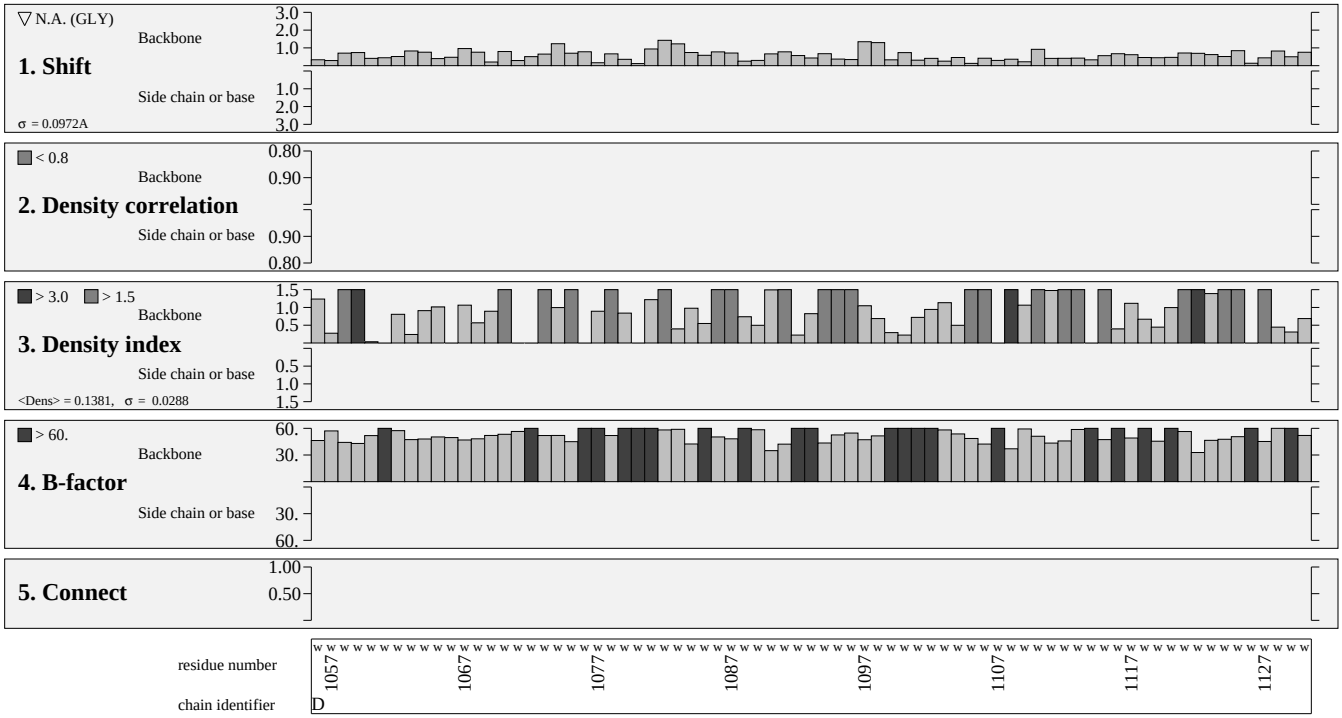
Local estimation (11)





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Structure Factor Check

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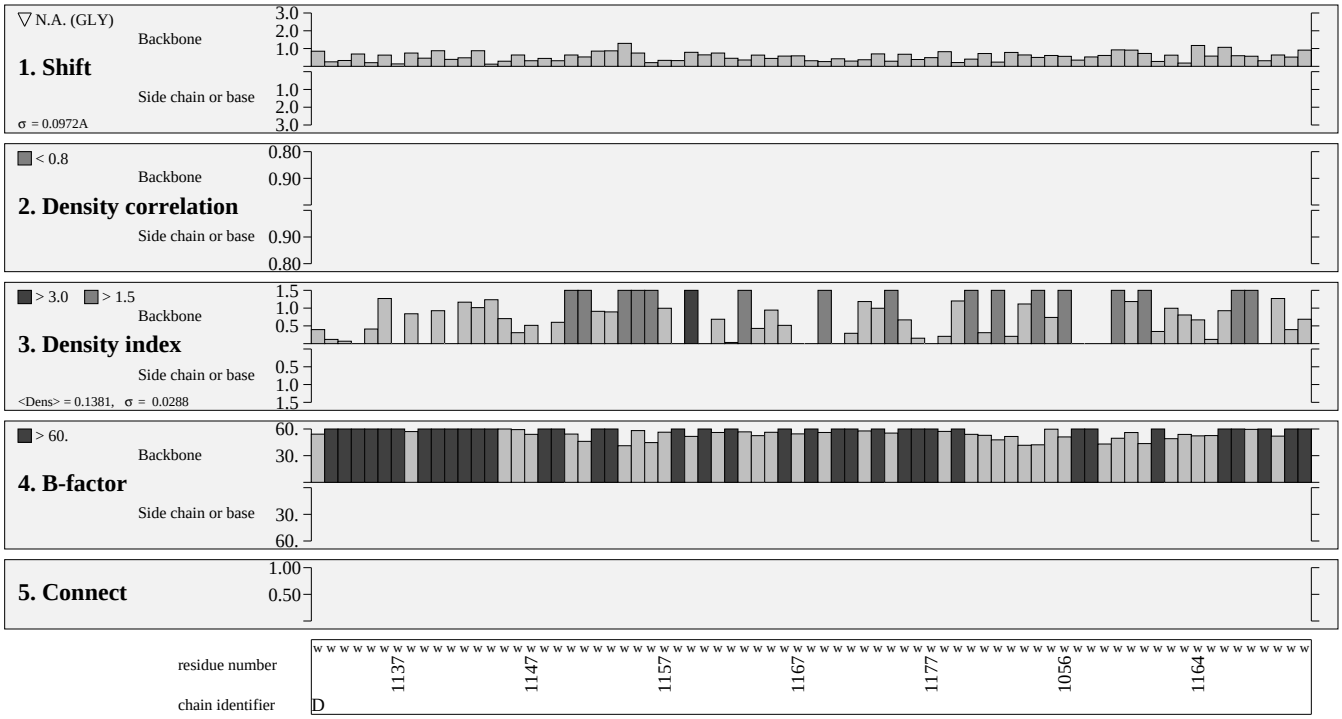
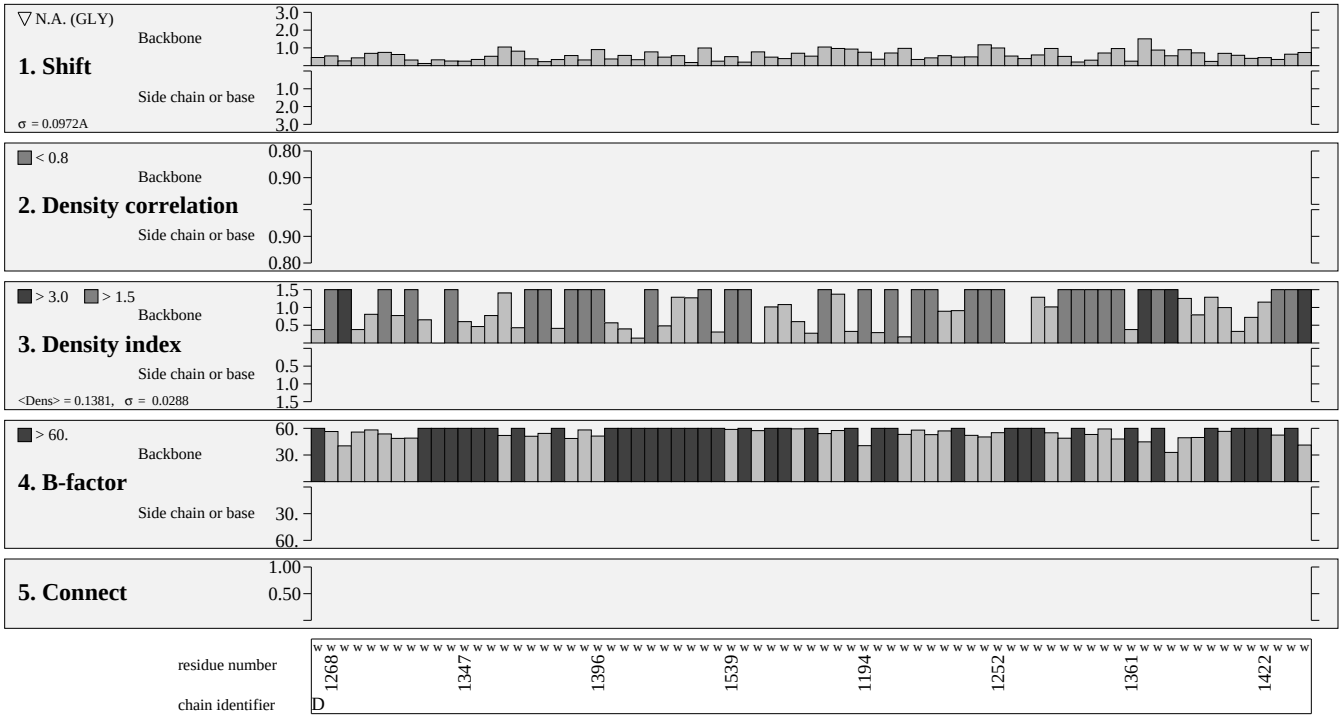
Local estimation (12)





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Structure Factor Check

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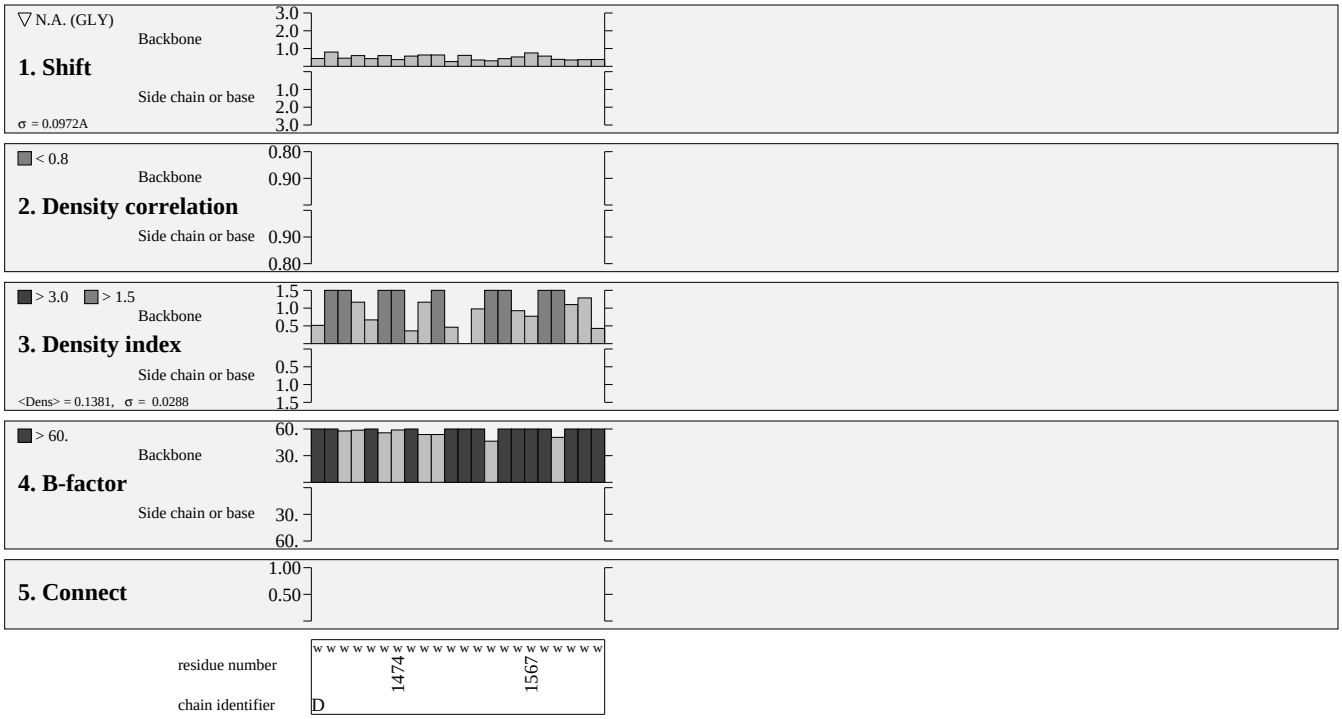
Local estimation (13)



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