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

Structure Factor Check

3L71

Title:	CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH AZOXYSTROBIN BOUND
Date:	27−DEC−09
PDB code:	3L71

Crystal

Cell parameters:

a: 170.15 A b: 181.31 A c: 240.50 A

α: 90.00 β: 90.00 γ: 90.00

Space group: P 21 21 21

Model

32655 atoms (19 water molecules)

Number of chains:	51
Volume not occupied by model:	62.0 %
<B> (for atomic model):	73.6 A^2
σ(B):	18.83 A^2
Matthews coefficient:	4.06
Corresponding solvent % :	69.45

Refinement

Program:	CNS 1.1
Nominal resolution range:	24.9 − 2.84 A
Reported R−factor:	0.247
Number of reflections used:	165215
Reported Rfree:	0.28
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		144.8 − 2.80 A
Reflections in file:		170949
Unique reflections	above 0:	170949
	above 1σ:	167603
	above 3σ:	112140

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Nominal resolution range:	144.8 − 2.84 A
\05max. from input data, min. from author\05	
Used reflections:	165523
Reflections out of resolution:	5426
Completeness:	94.5 %
R_stand(F) = <σ(F)>/<F> :	0.062
Anisotropic distribution of Structure Factors	
ratio of eigen values:	1.0000 0.4725 0.4425
B_overall (by Patterson):	49.A^2
Optical resolution:	2.13 A
Expected opt. resol. for complete data set:	2.13 A
Estimated minimal error:	0.067 A

Model vs. Structure Factors

R−factor for all reflections:	0.298
Correlation factor:	0.865
R−factor:	0.302
for F > 2.0 σ	
nom. resolution range:	24.94 − 2.84A
reflections used:	162125
Rfree:	0.331
Nfree:	3168
R−factor without free−refl.:	0.301
Non free−reflections:	158957
<u> (error in coords by Luzzati plot):	0.459 A
Estimated maximal error:	0.353 A
DPI:	0.350 A

Scaling

Scale:	0.476
Bdiff:	−9.70

Anisothermal Scaling (Beta):

10.9330 −1.7389 −2.6990 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.750 250.127

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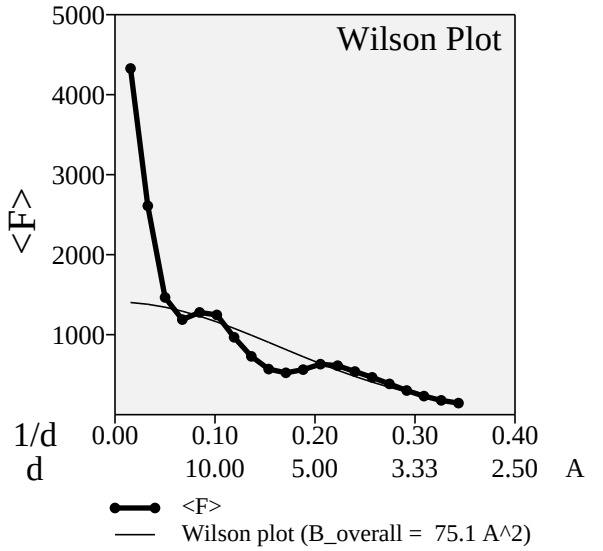
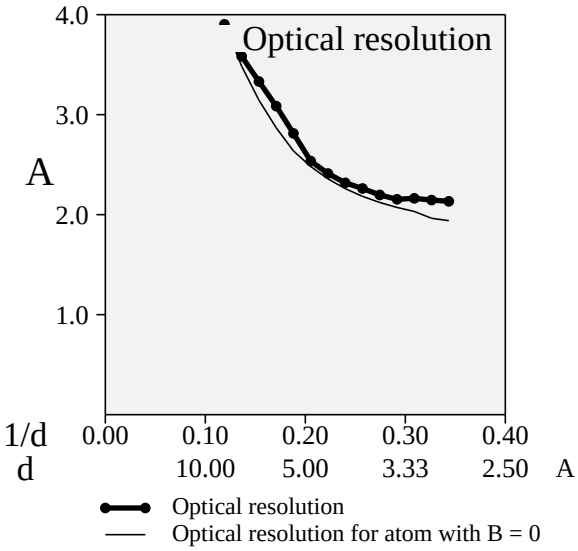
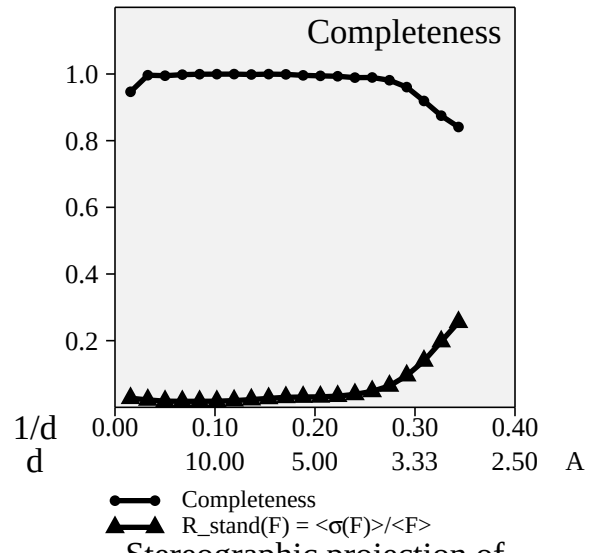


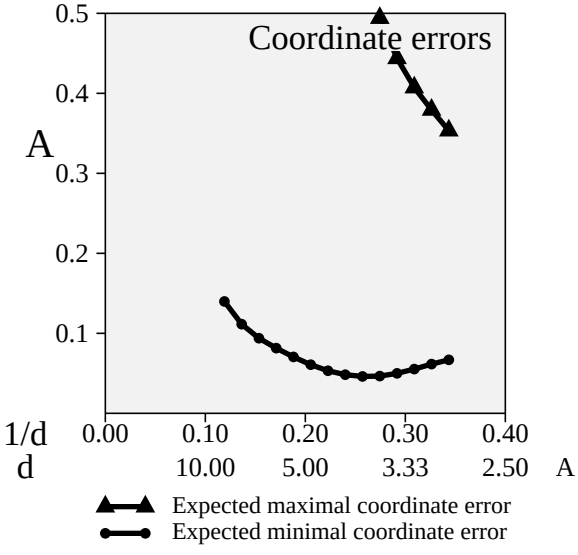
<F>
Wilson plot (B_overall = 75.1 A^2)



Optical resolution
Optical resolution for atom with B = 0

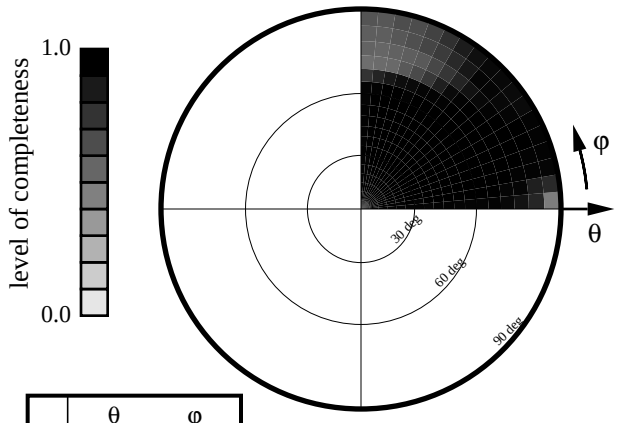


Completeness
R_stand(F) = <σ(F)>/<F>



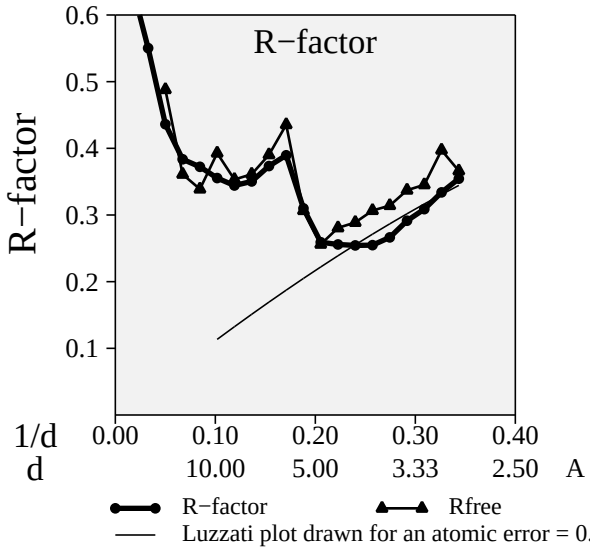
Expected maximal coordinate error
Expected minimal coordinate error

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 = 0.459

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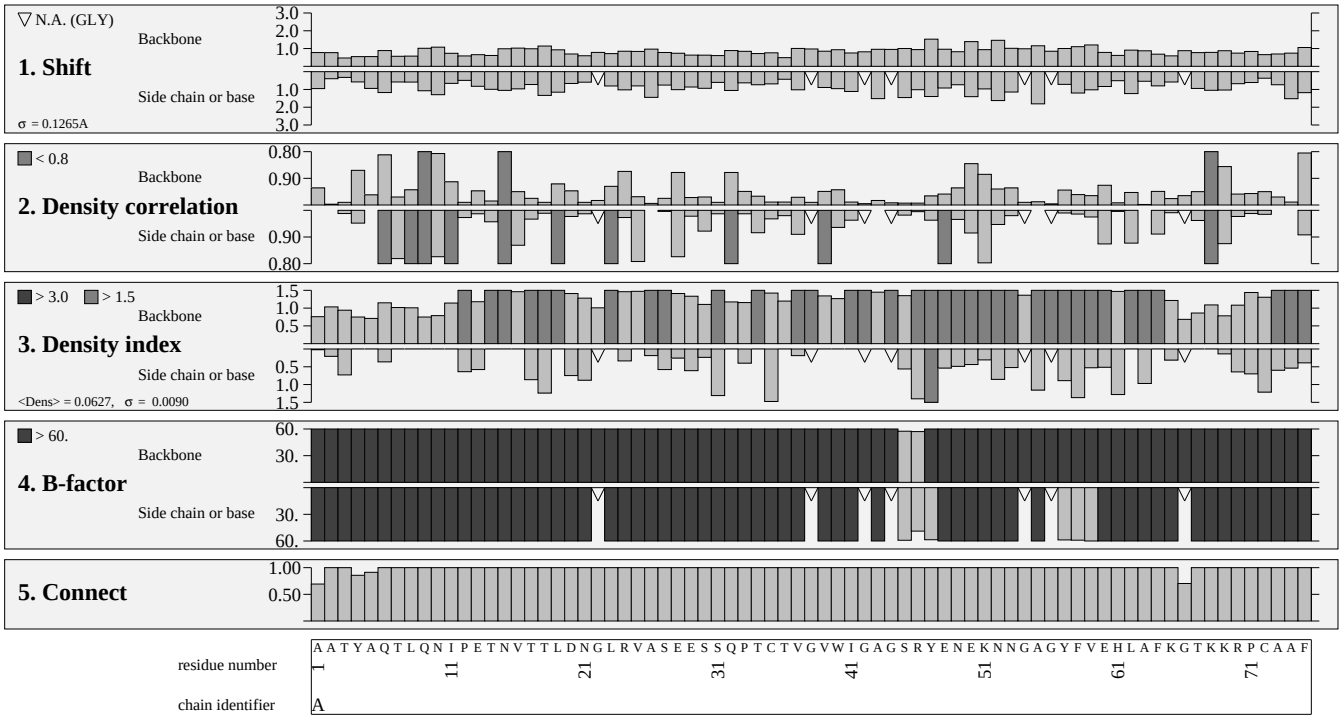
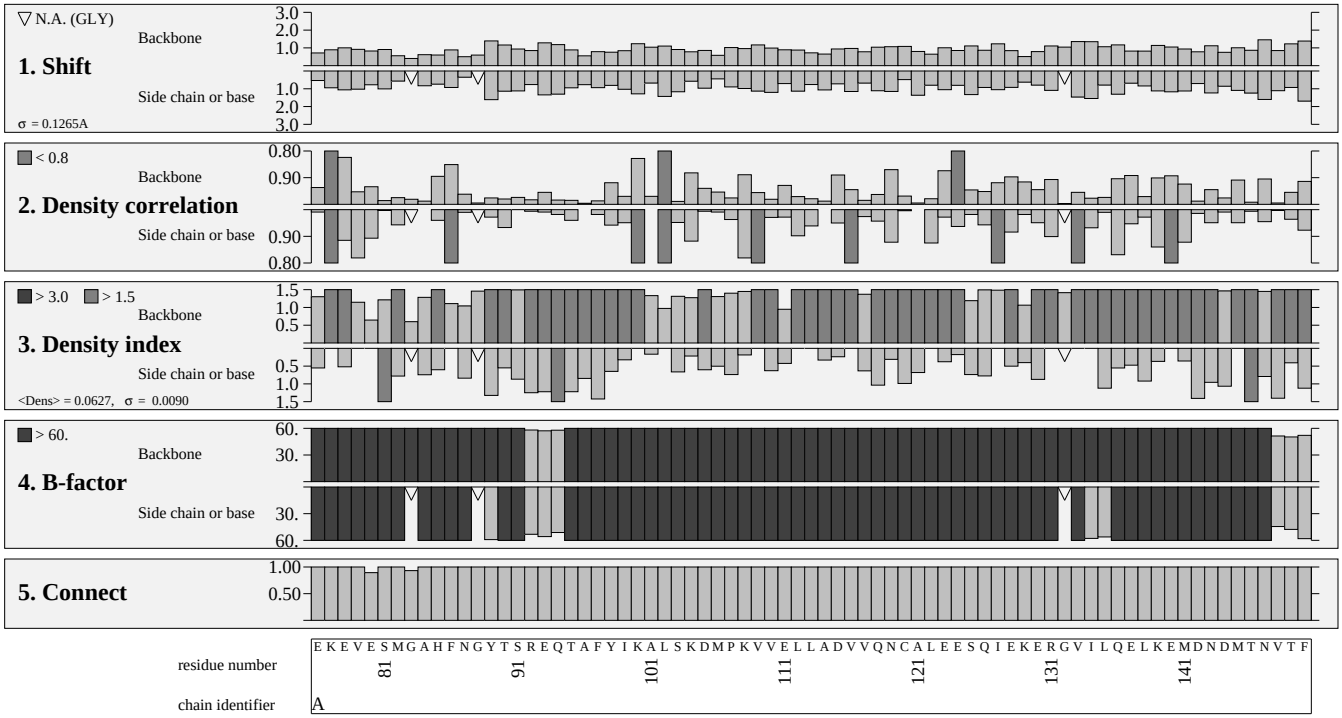
Local estimation





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Structure Factor Check

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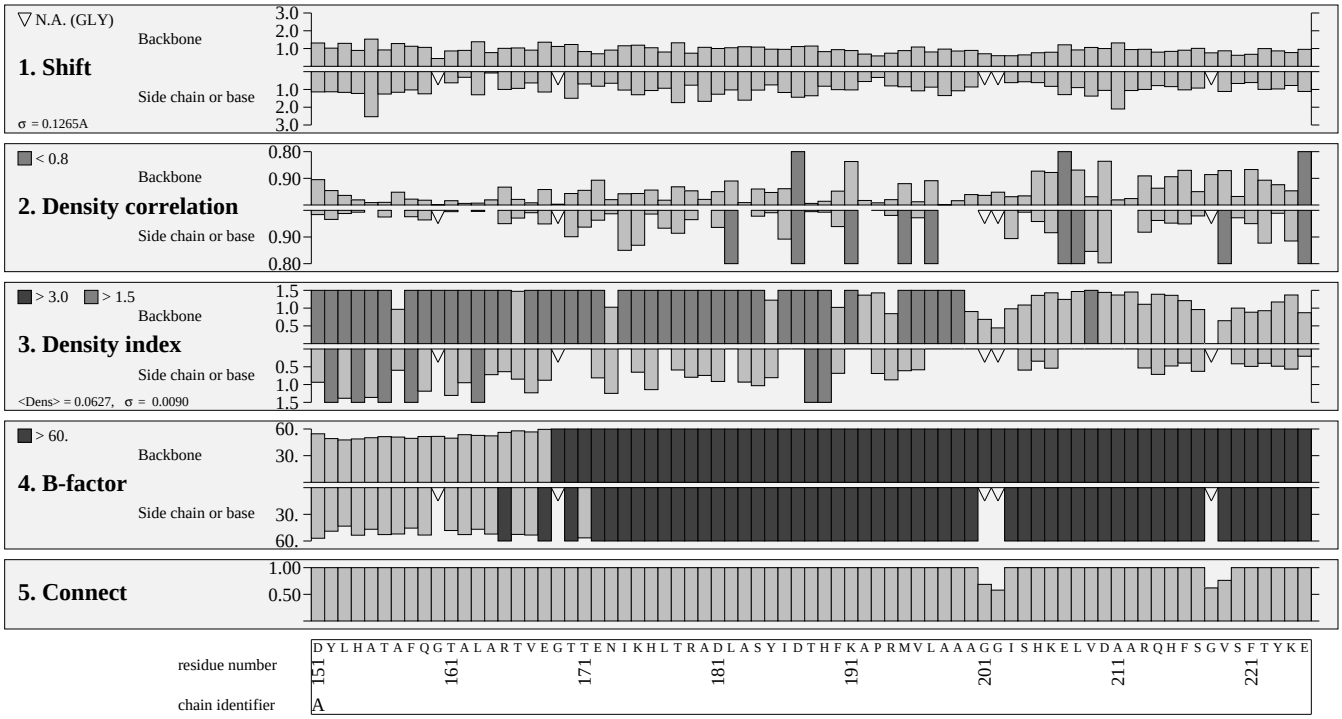
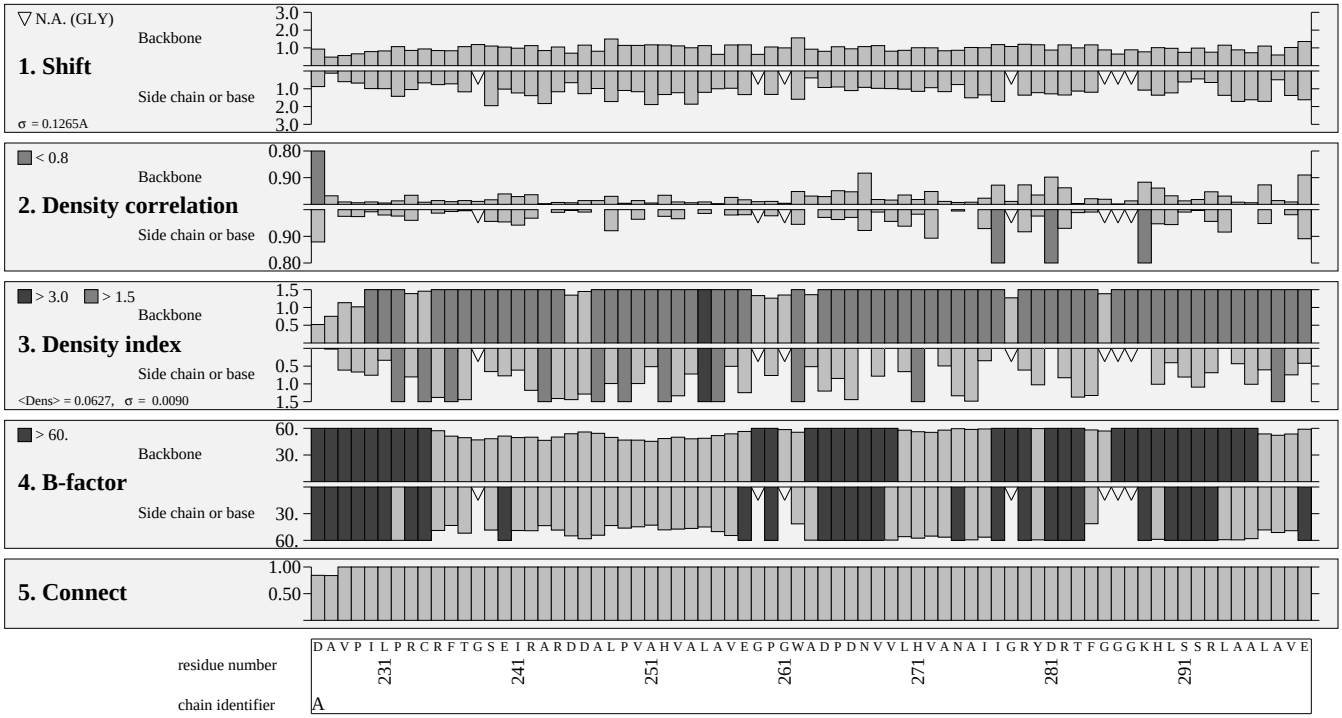
Local estimation (2)





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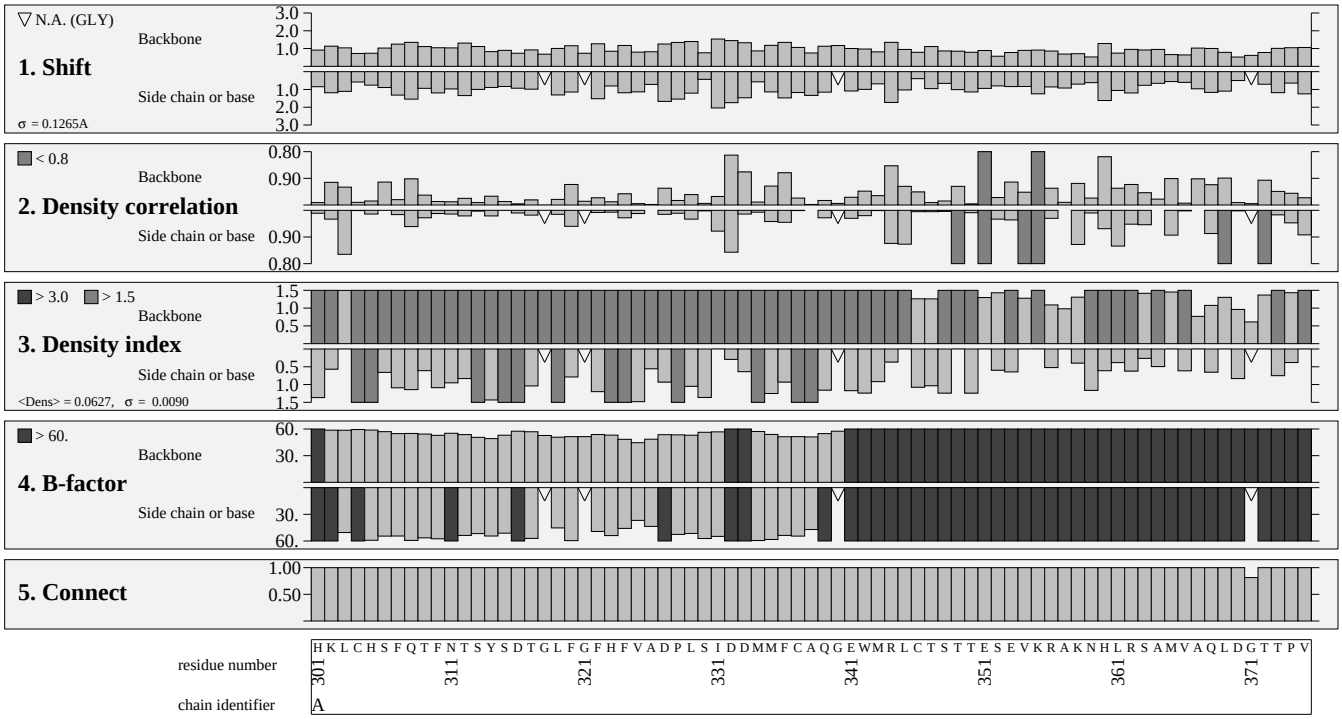
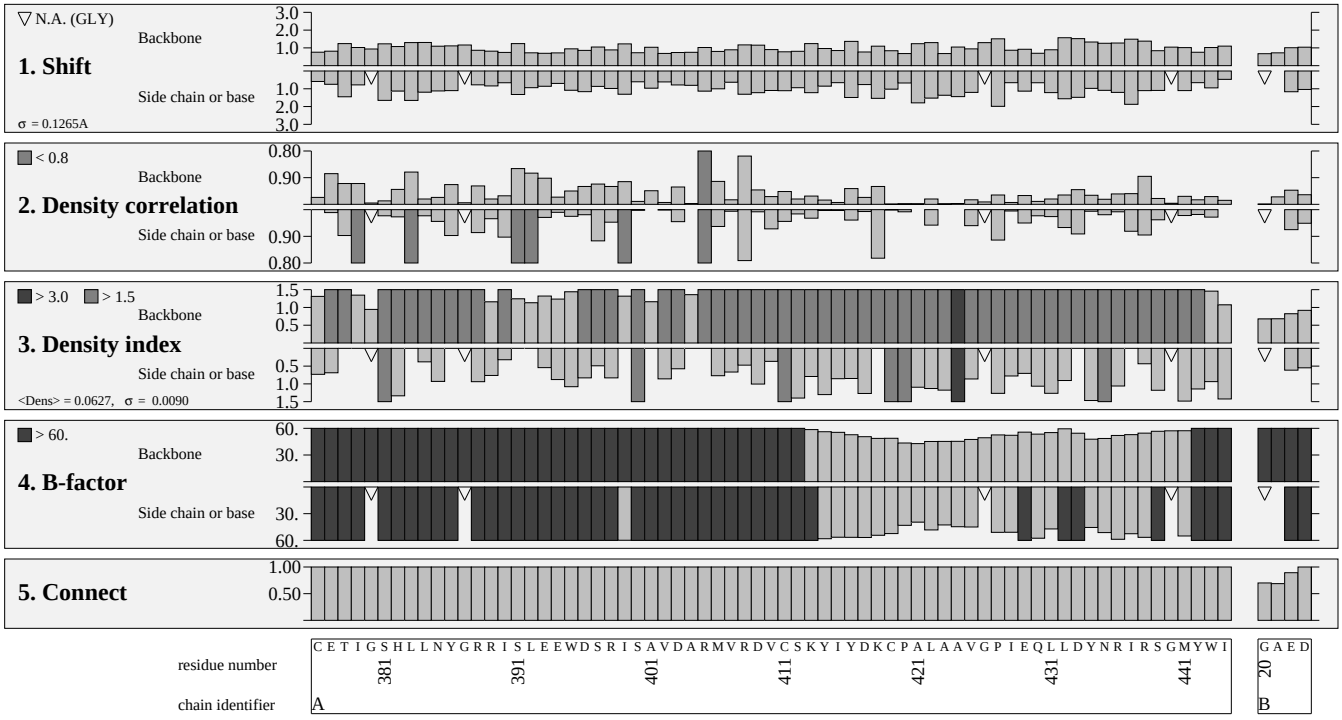
Structure Factor Check

3L71

Local estimation (3)





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Structure Factor Check

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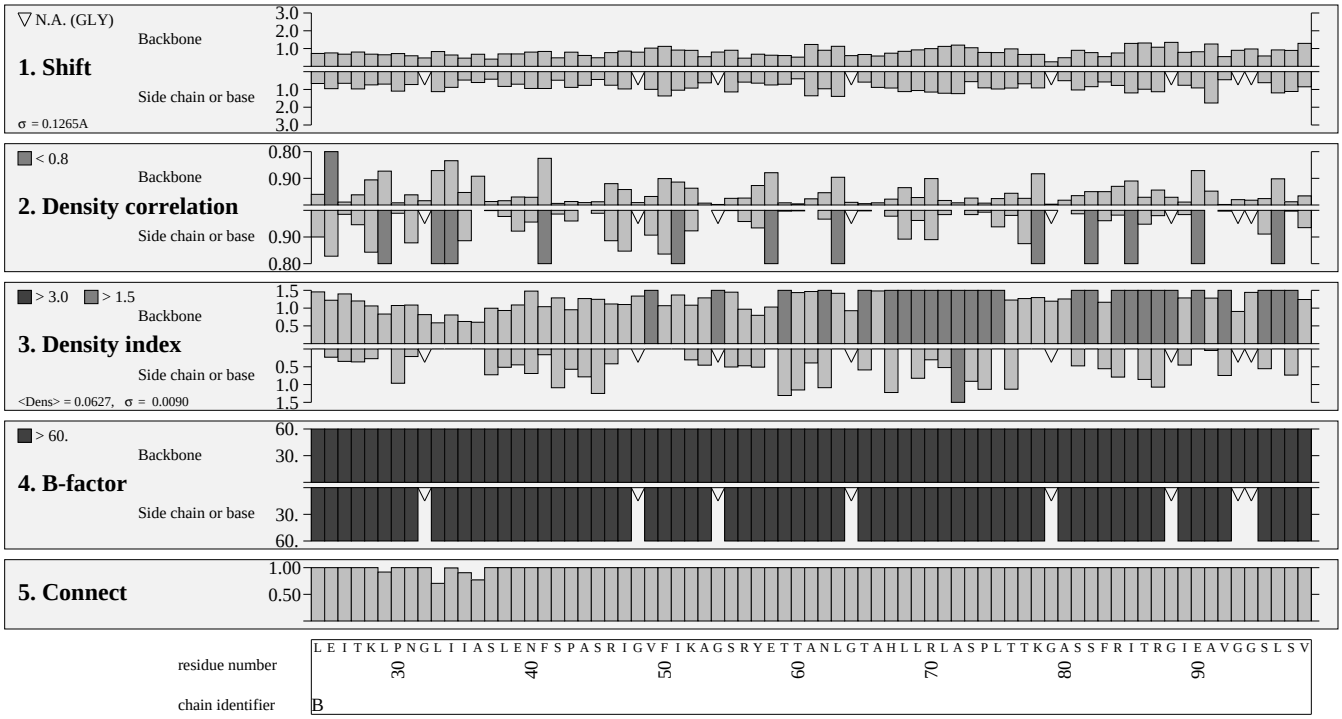
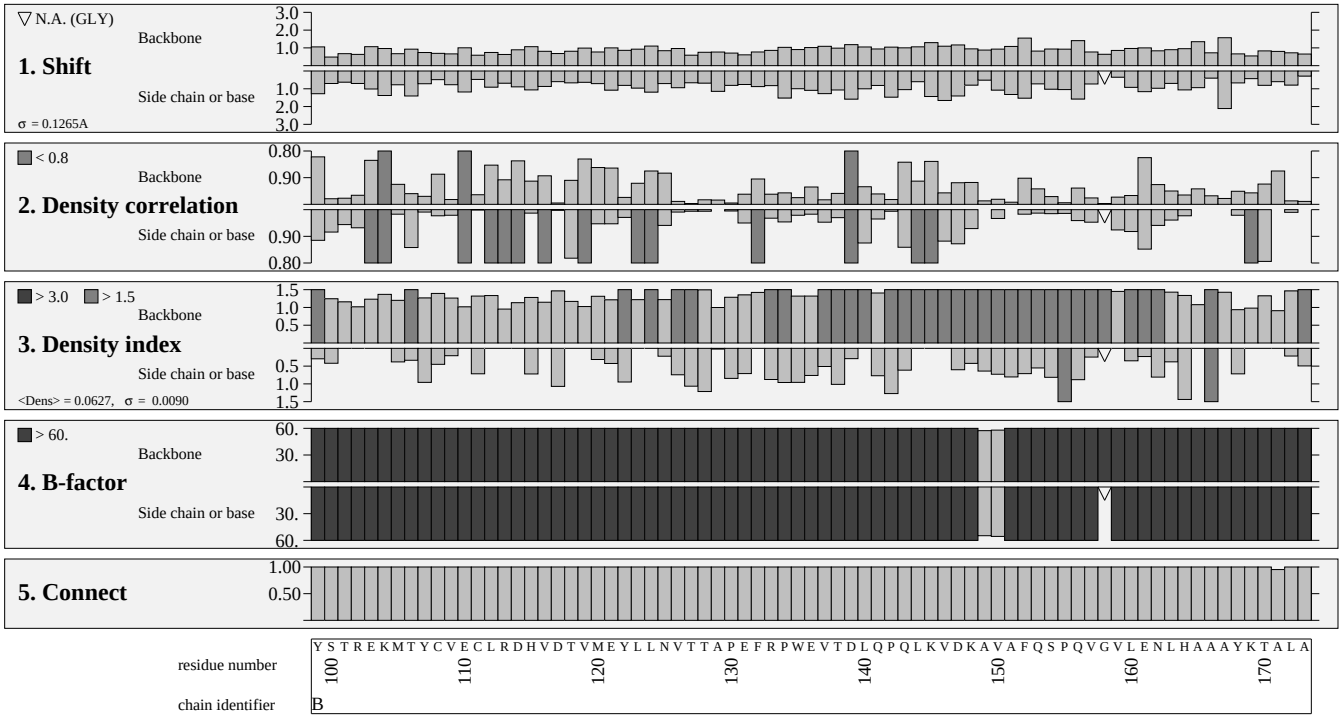
Local estimation (4)





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Structure Factor Check

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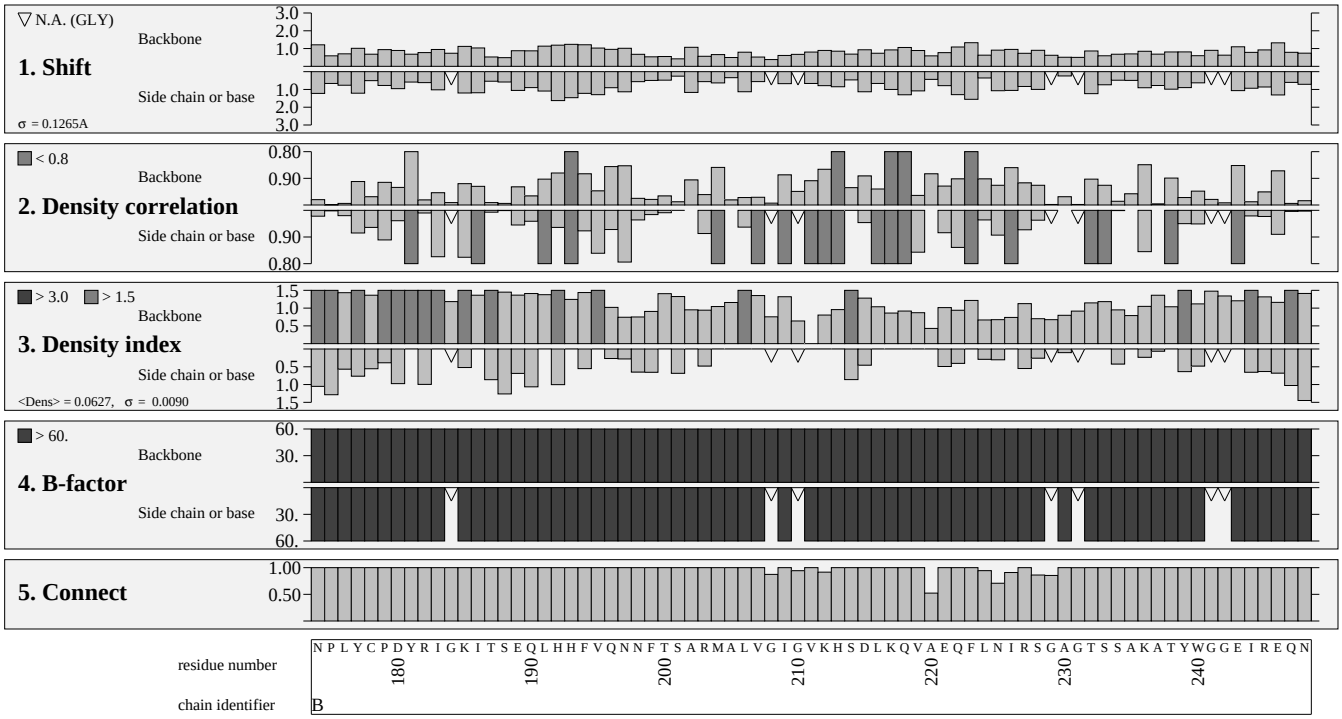
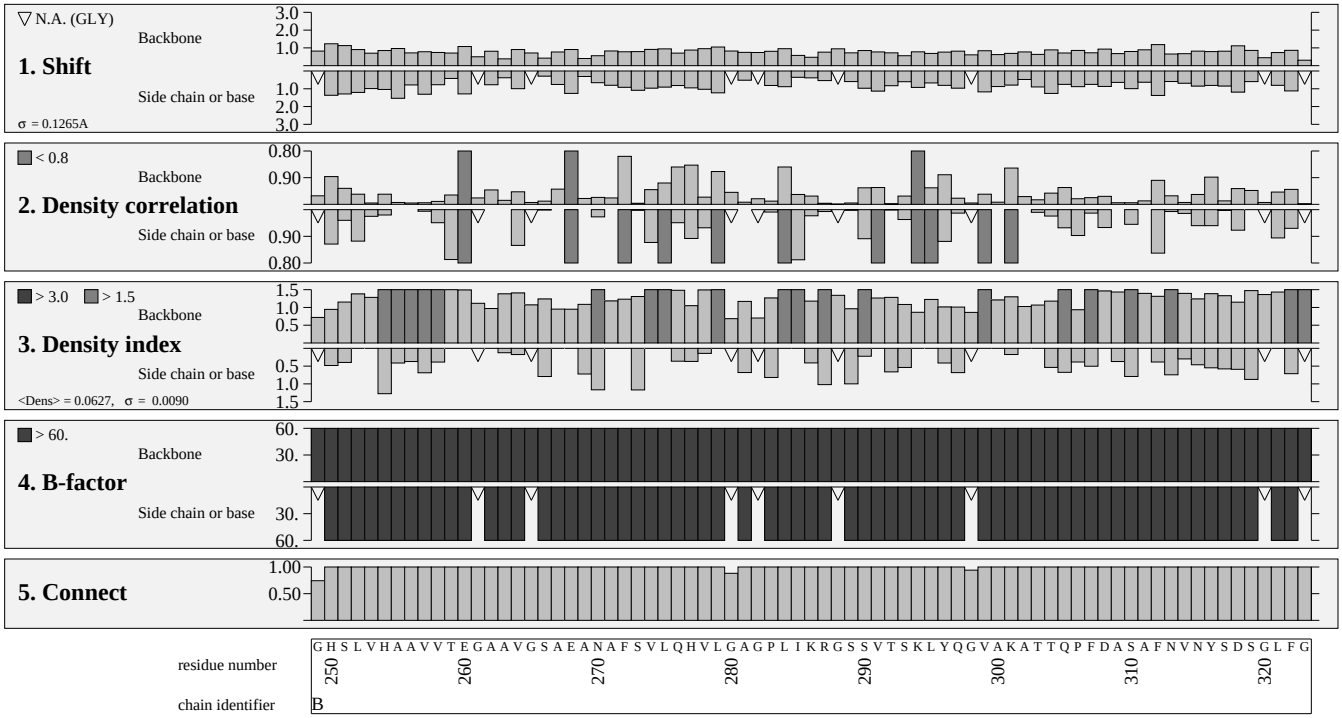
Local estimation (5)





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Structure Factor Check

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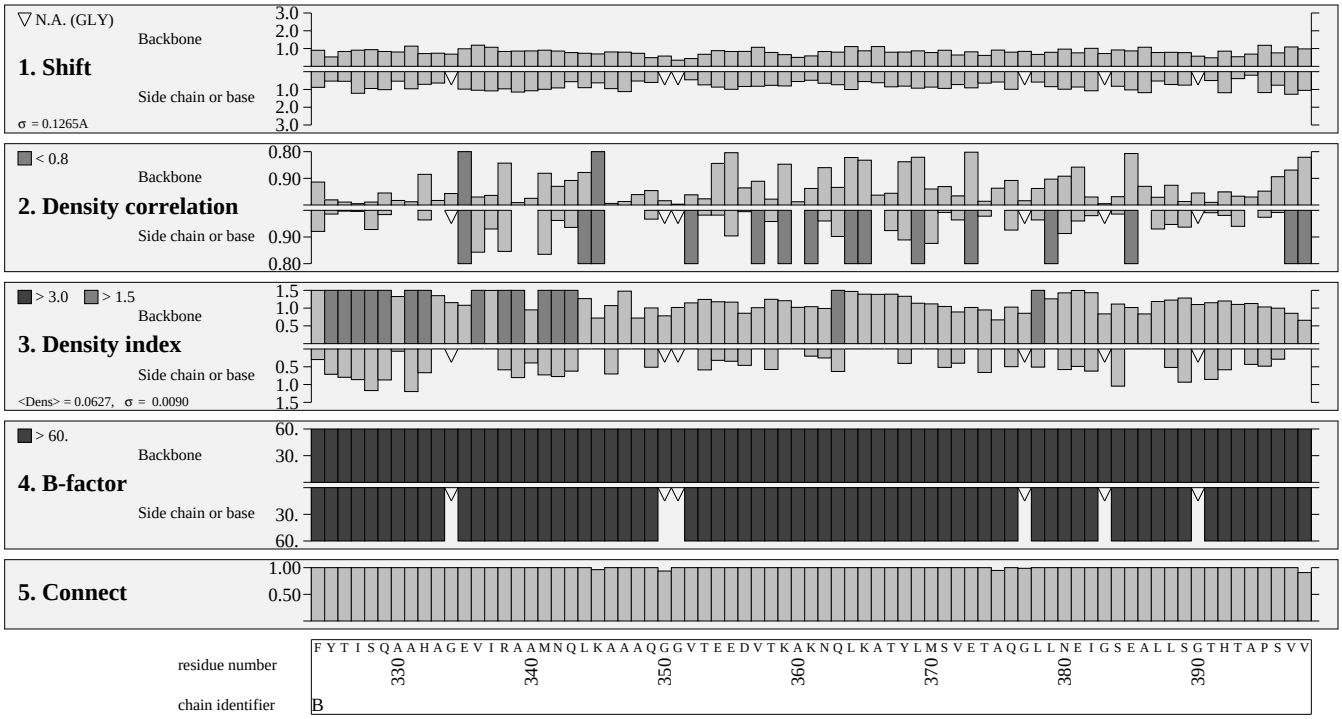
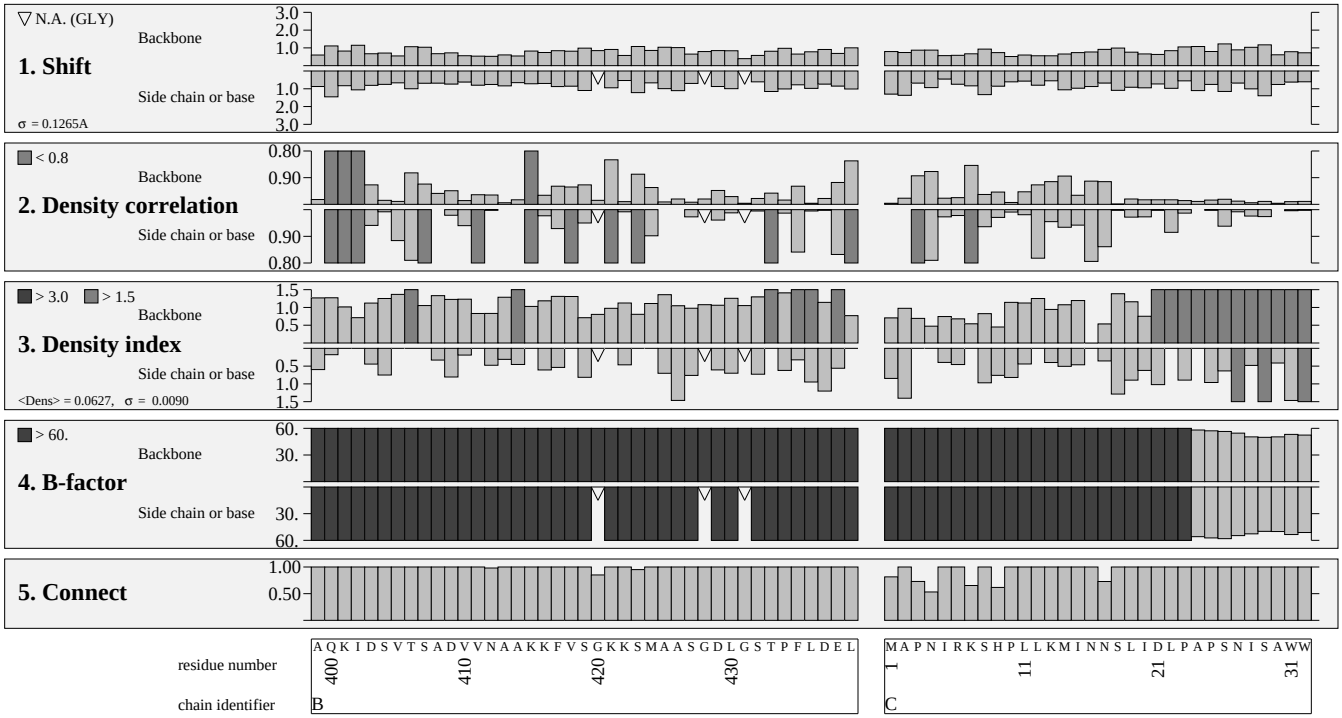
Local estimation (6)





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Structure Factor Check

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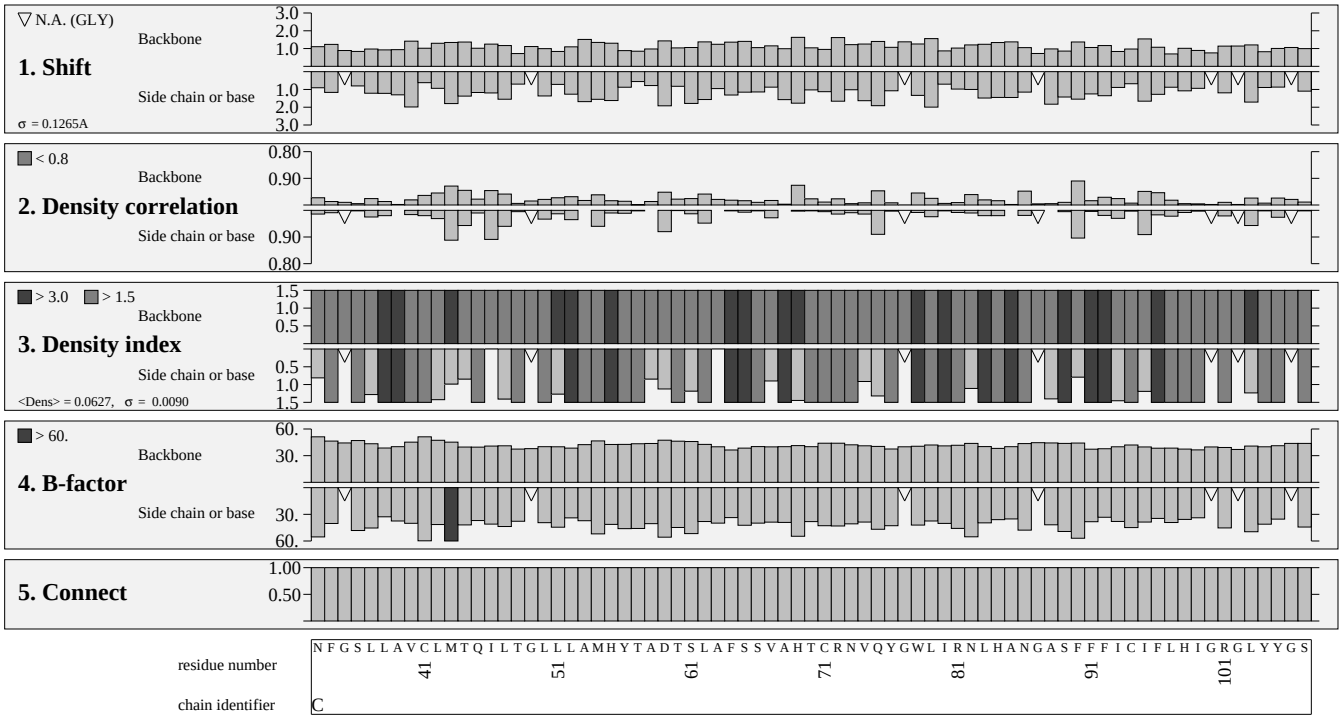
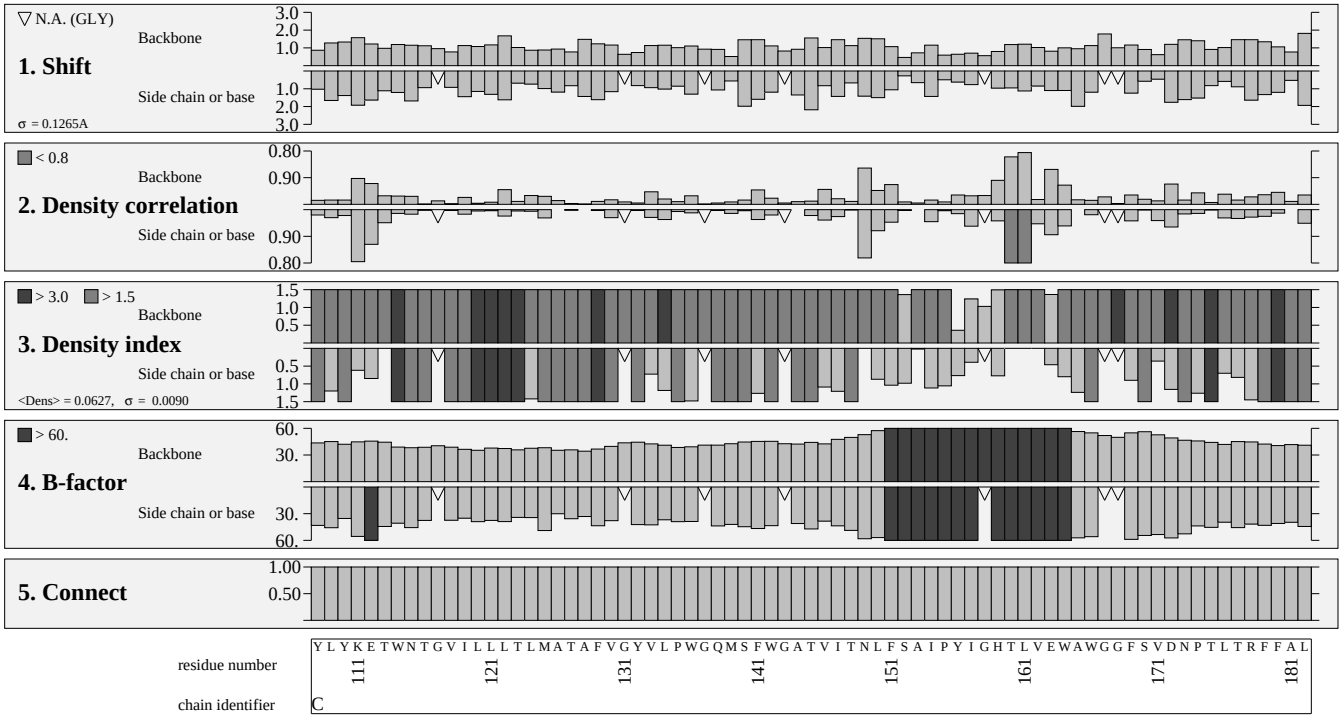
Local estimation (7)





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Structure Factor Check

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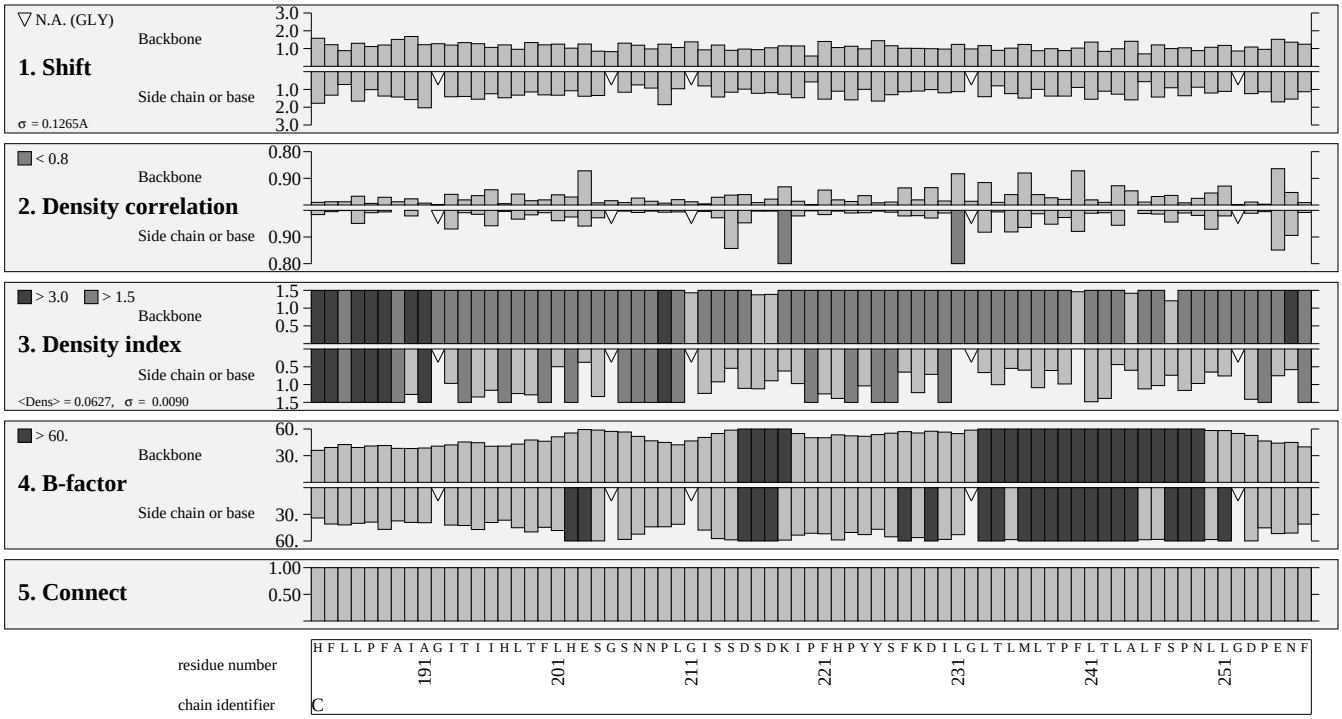
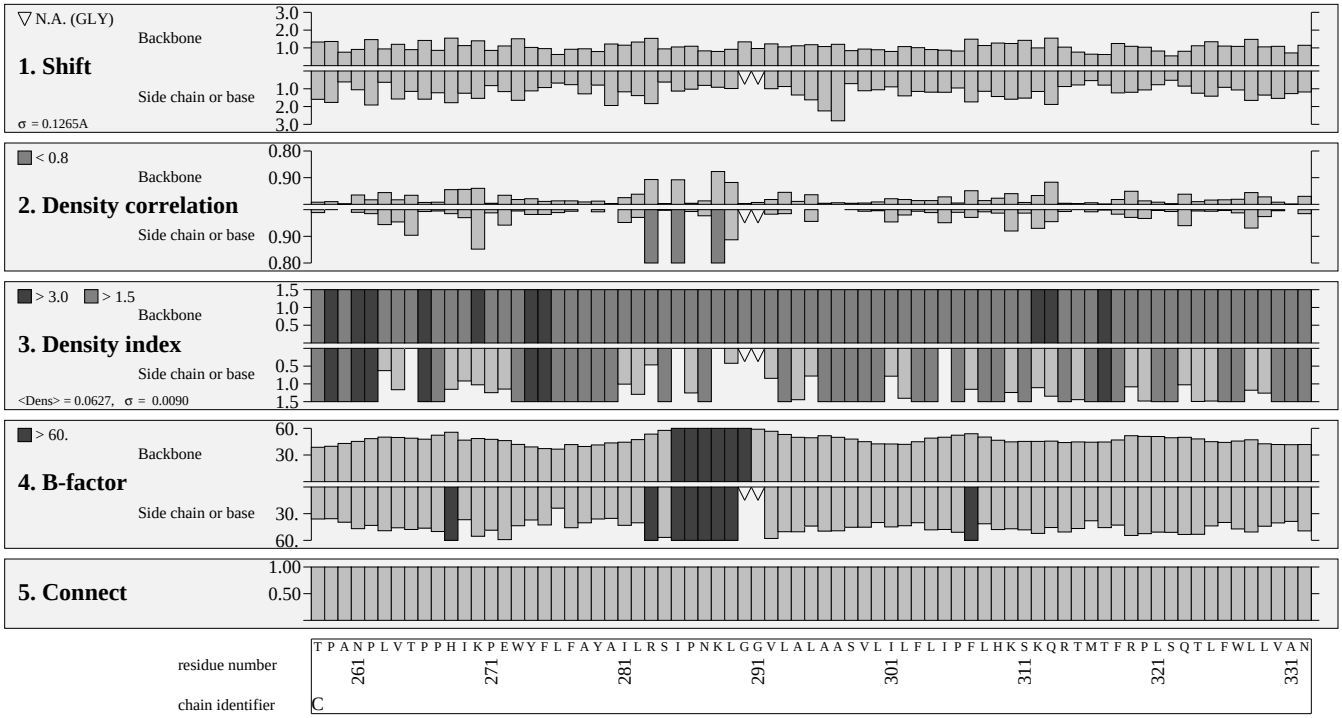
Local estimation (8)





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Structure Factor Check

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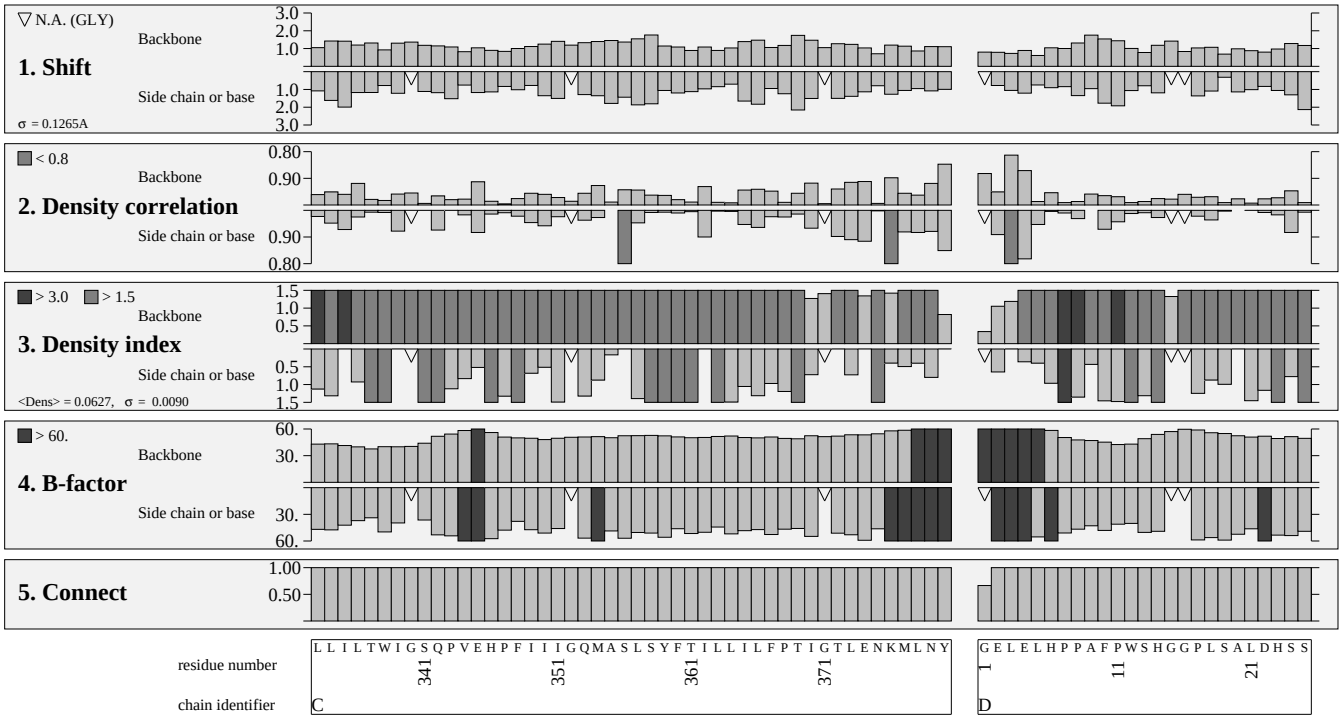
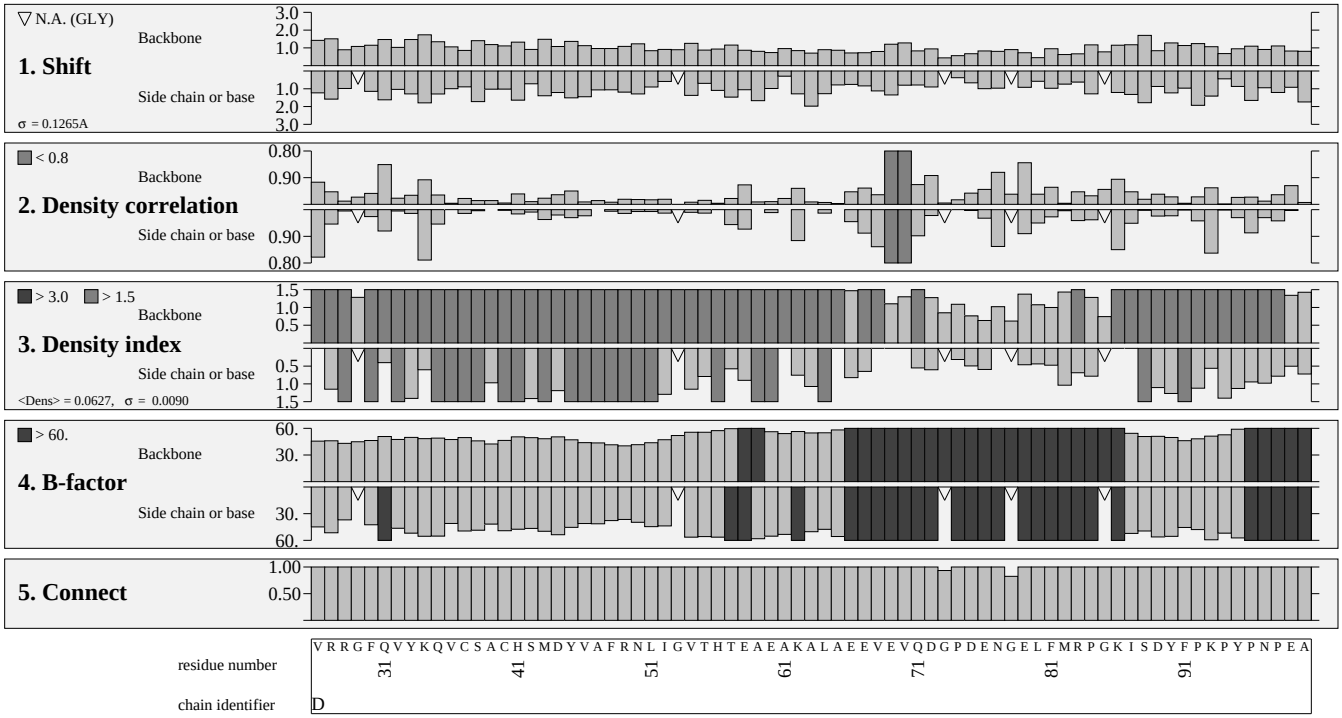
Local estimation (9)





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Structure Factor Check

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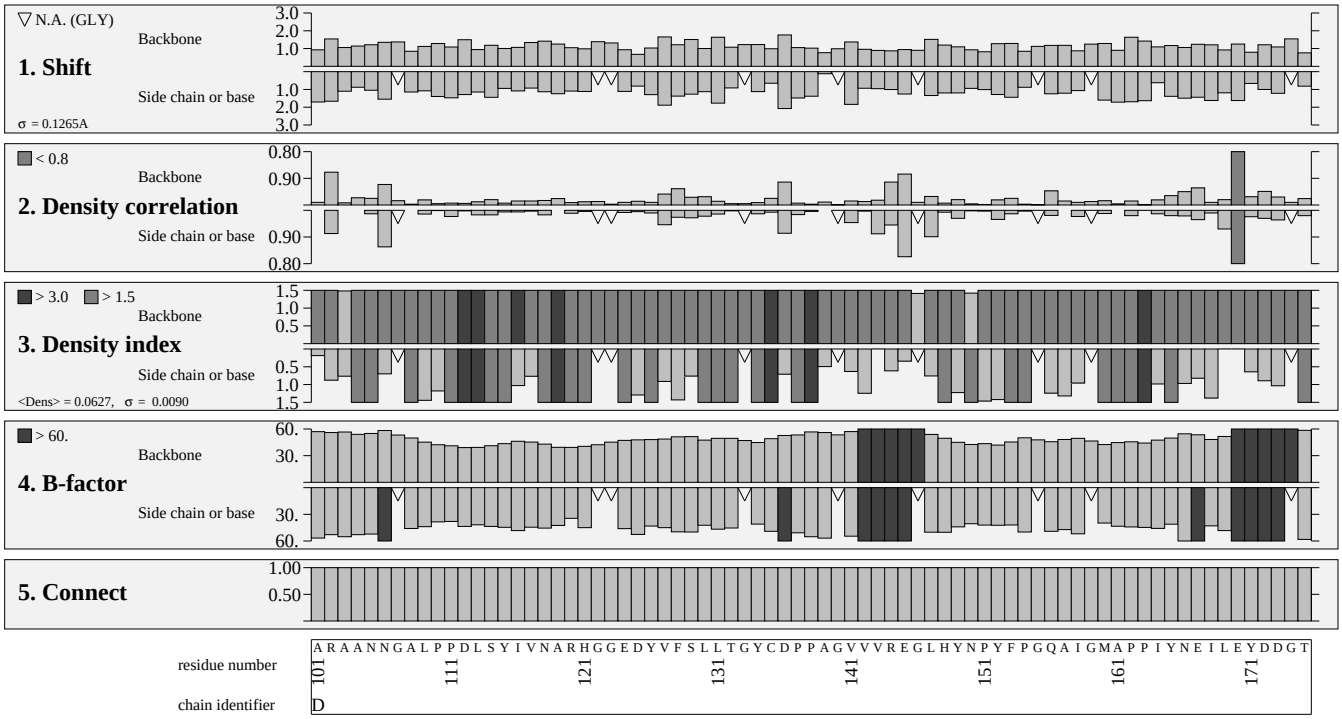
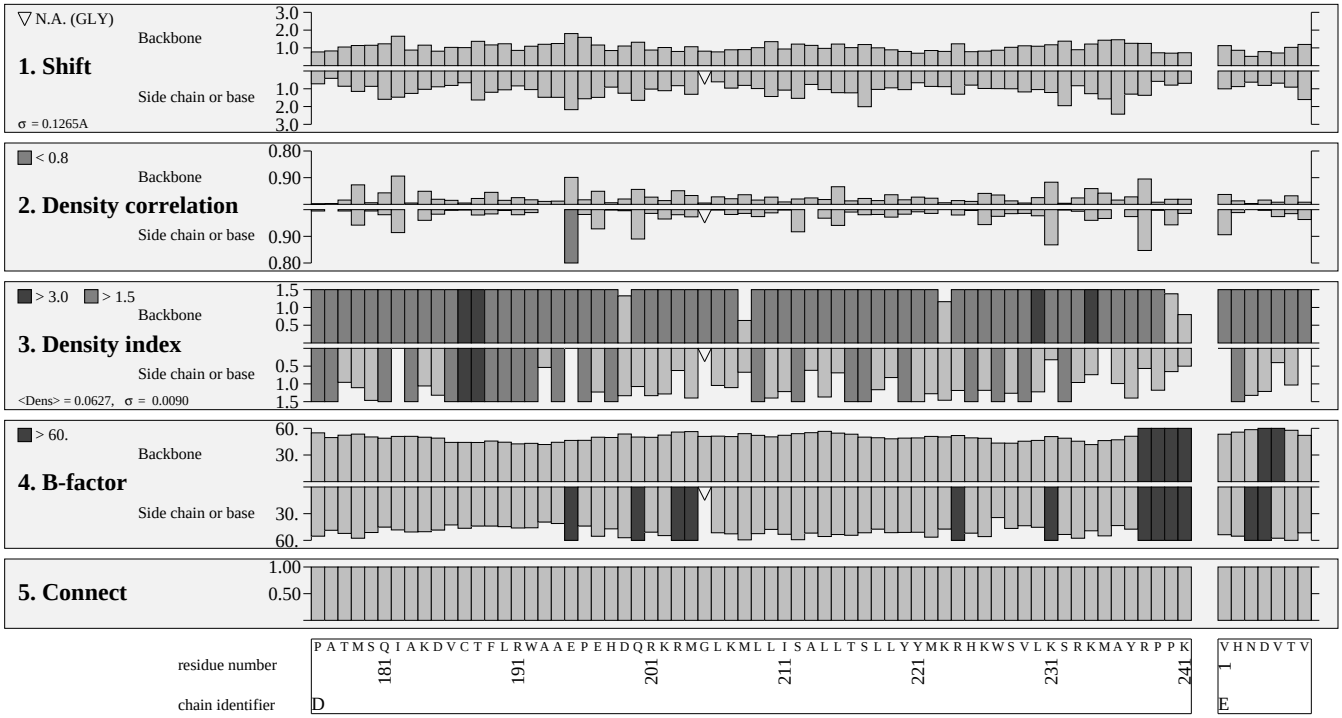
Local estimation (10)





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Structure Factor Check

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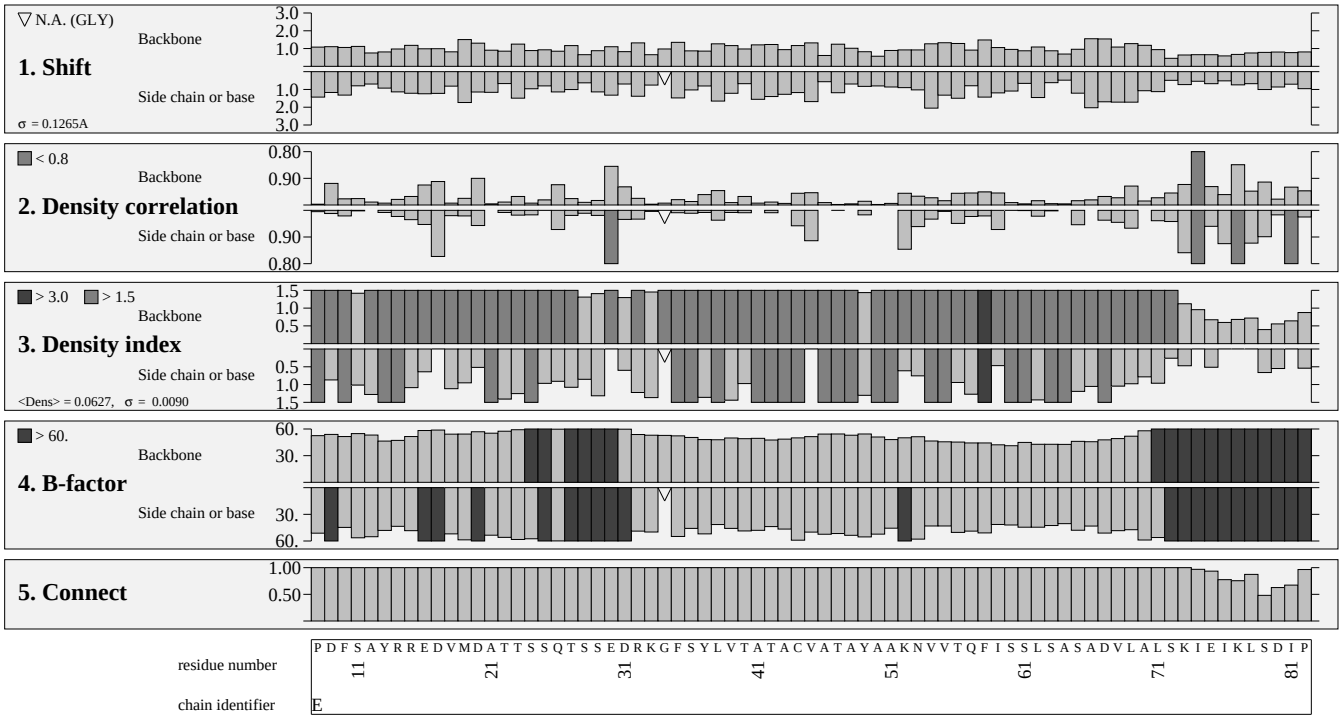
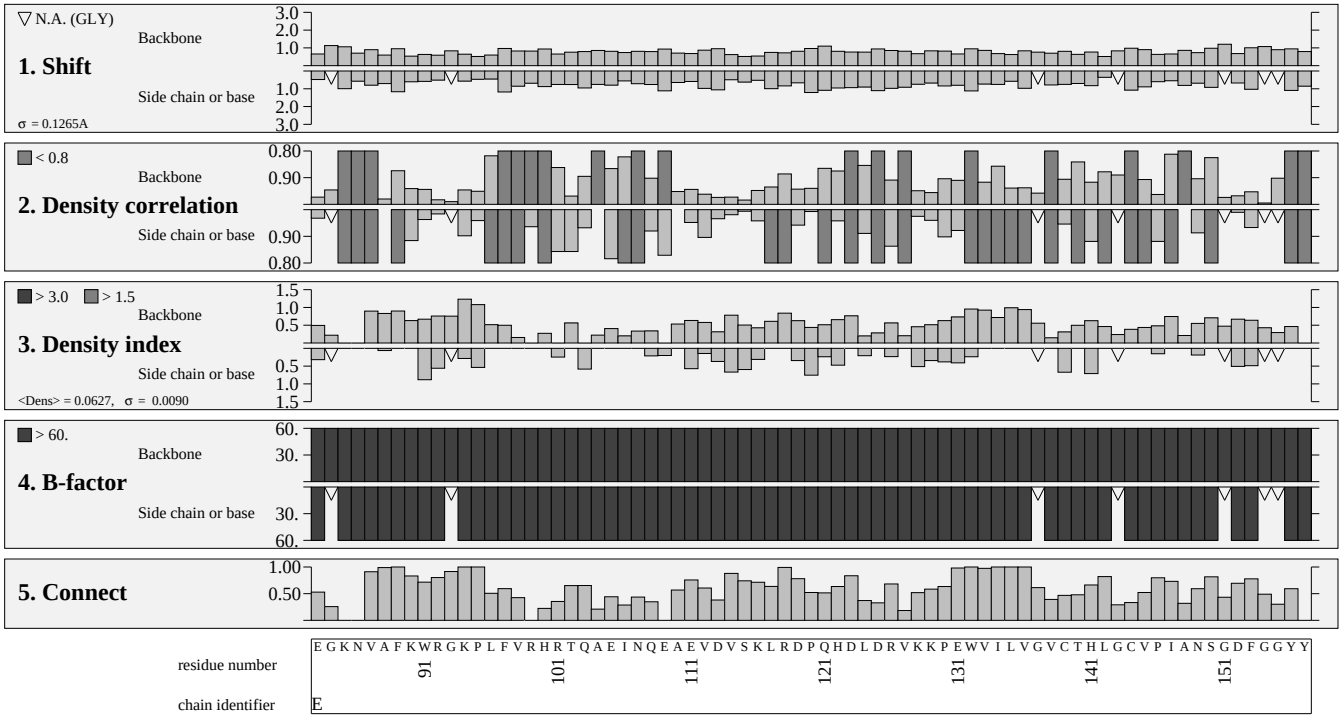
Local estimation (11)





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Structure Factor Check

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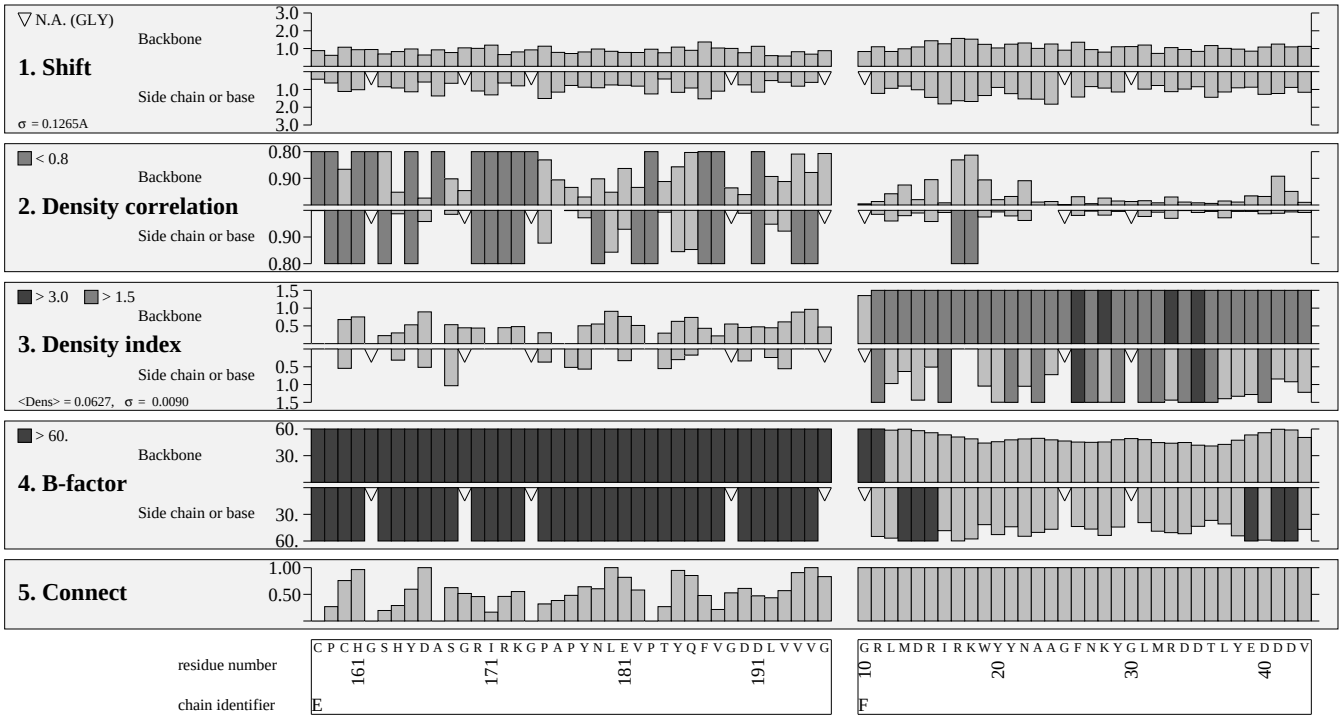
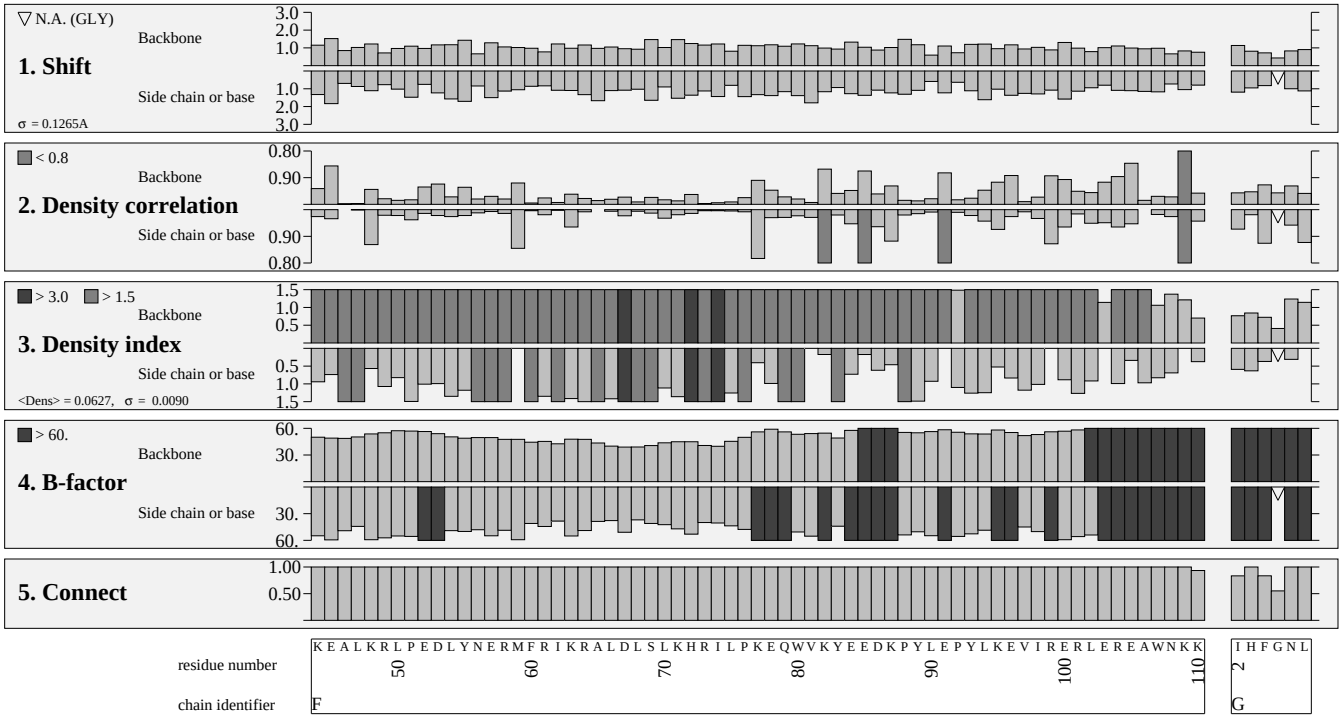
Local estimation (12)





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Structure Factor Check

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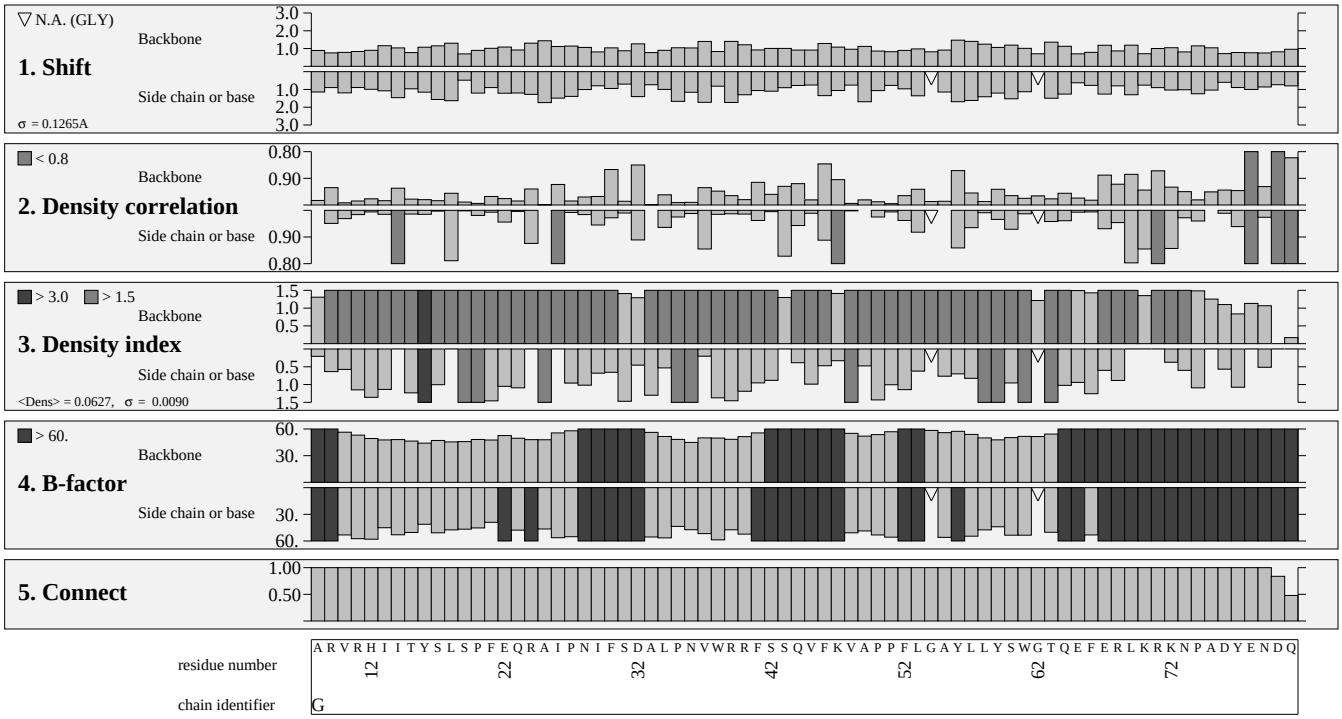
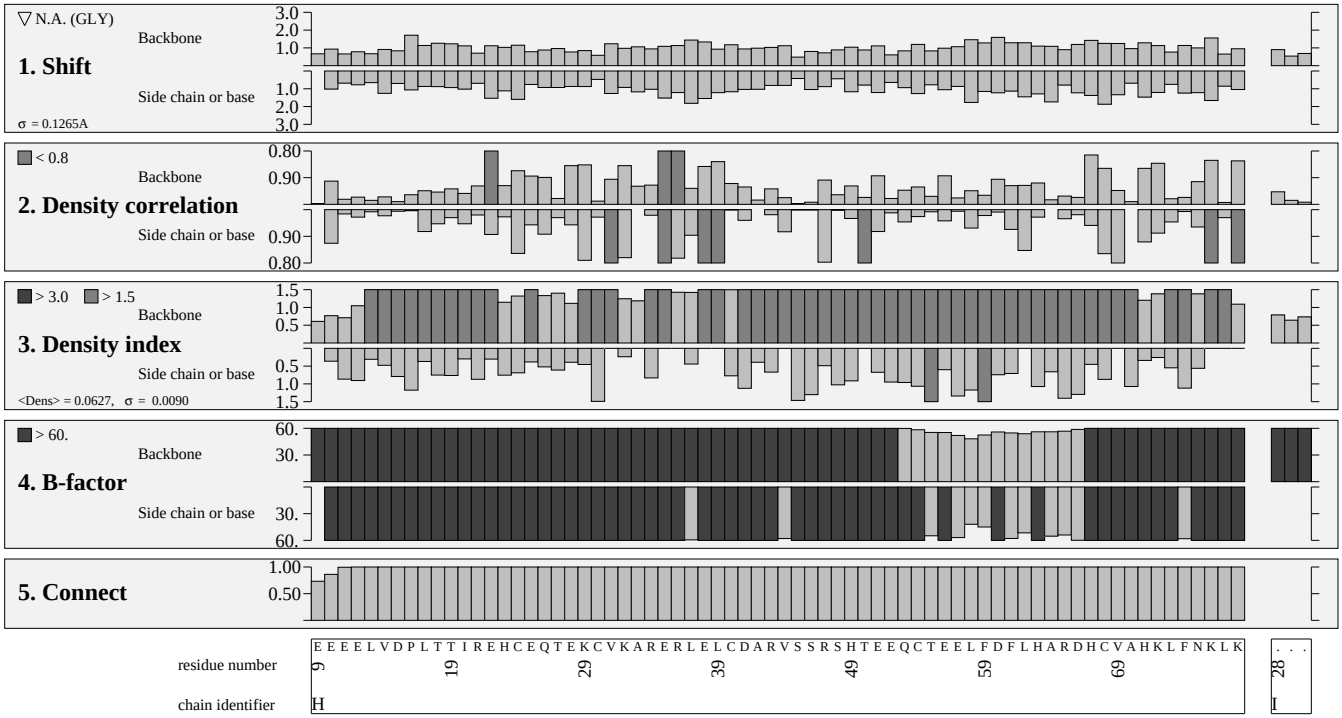
Local estimation (13)





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Structure Factor Check

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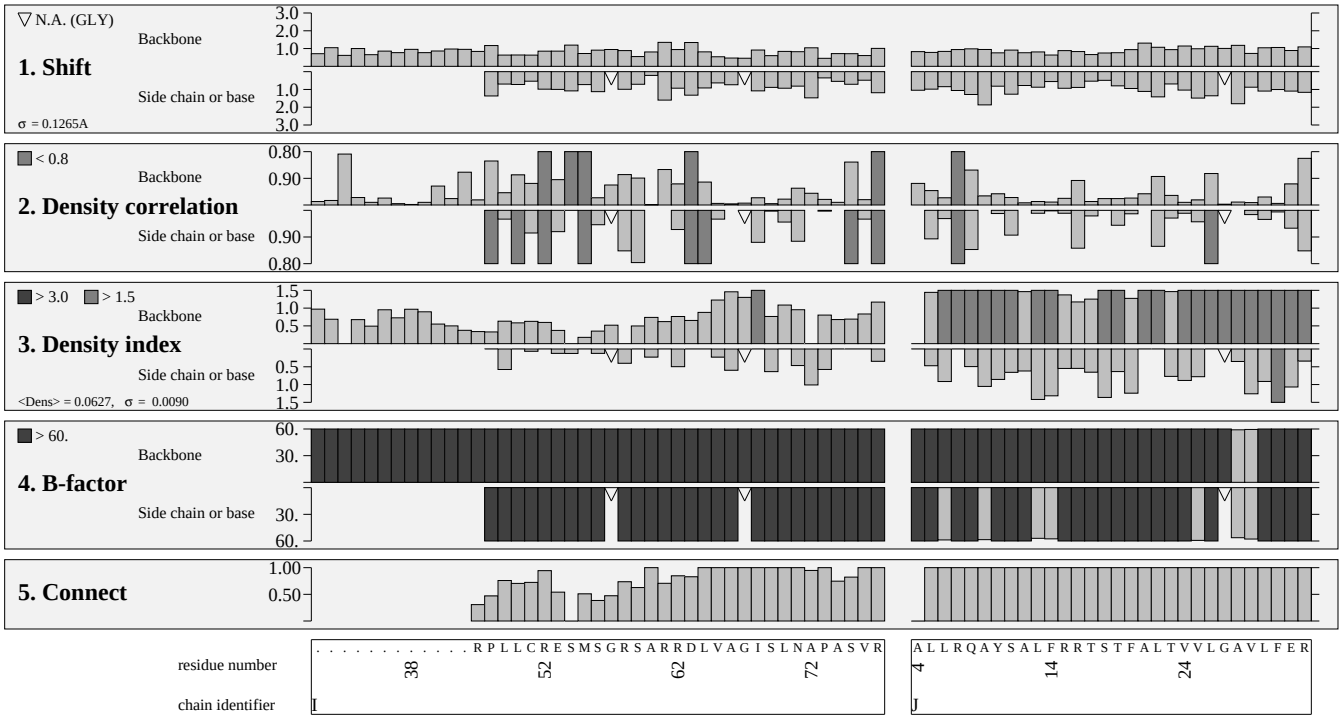
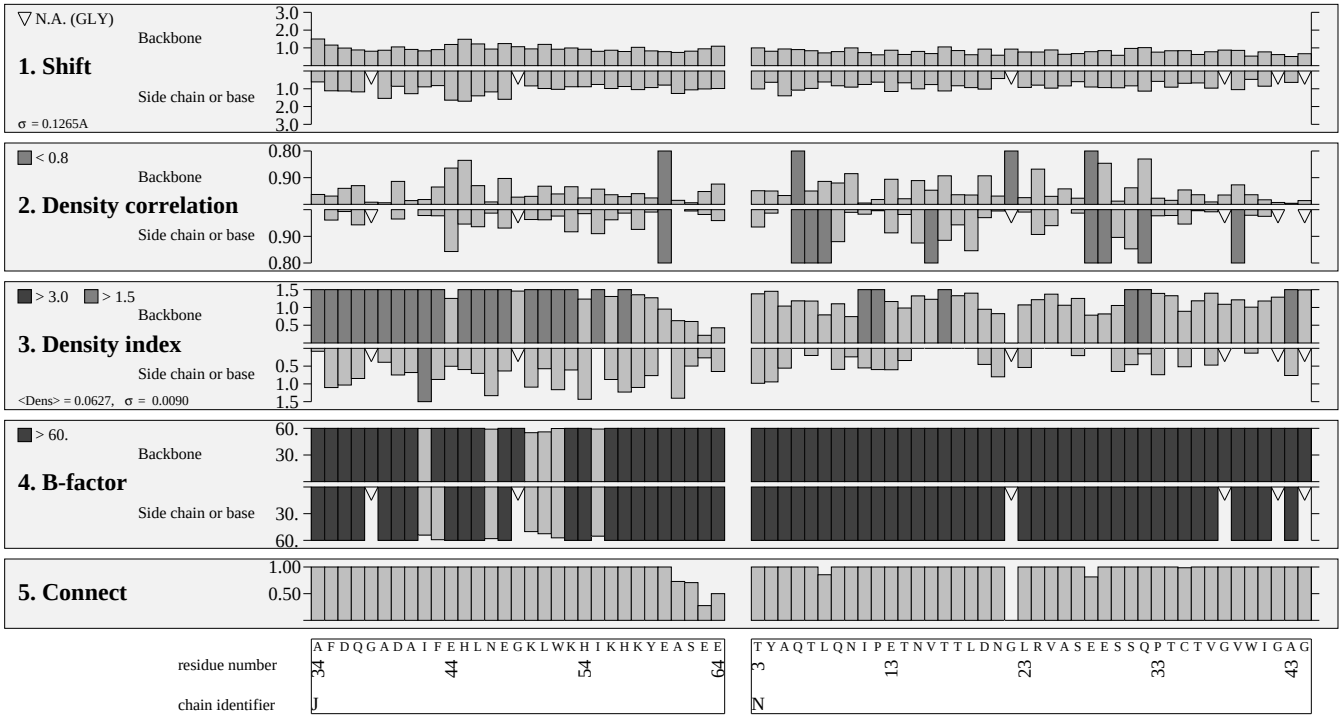
Local estimation (14)





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Structure Factor Check

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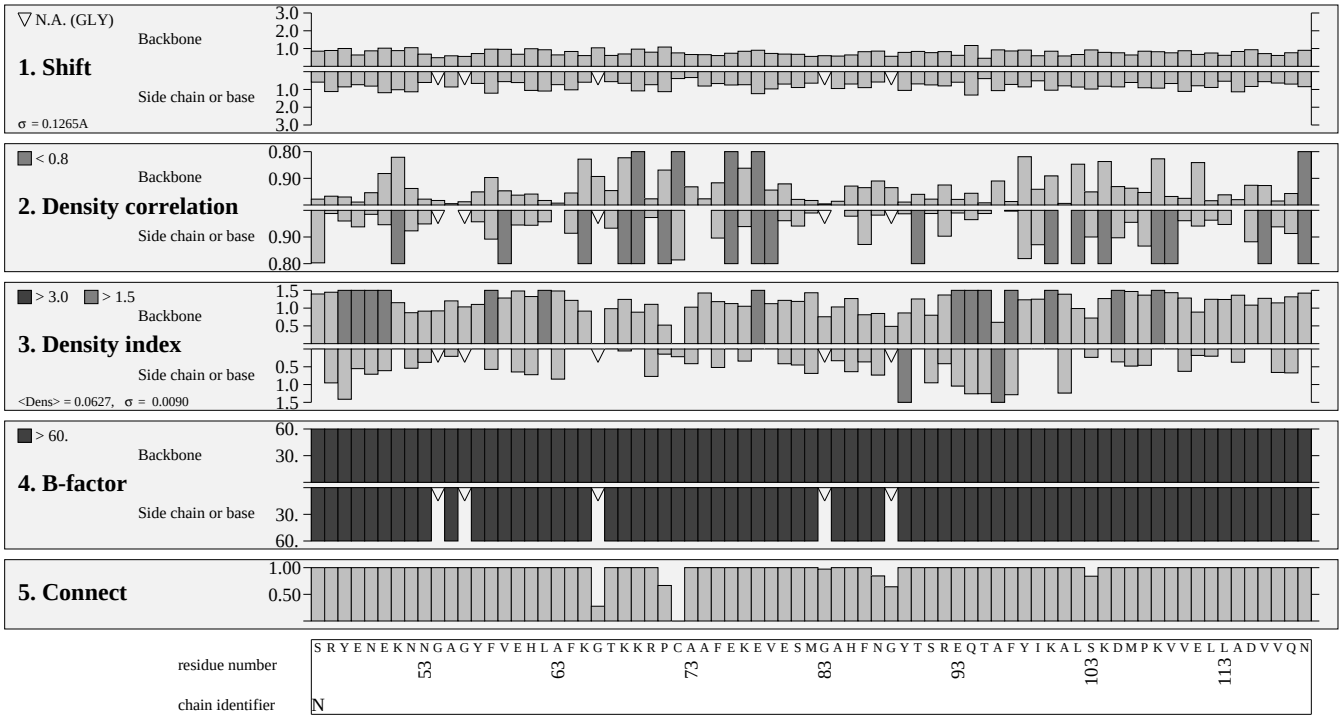
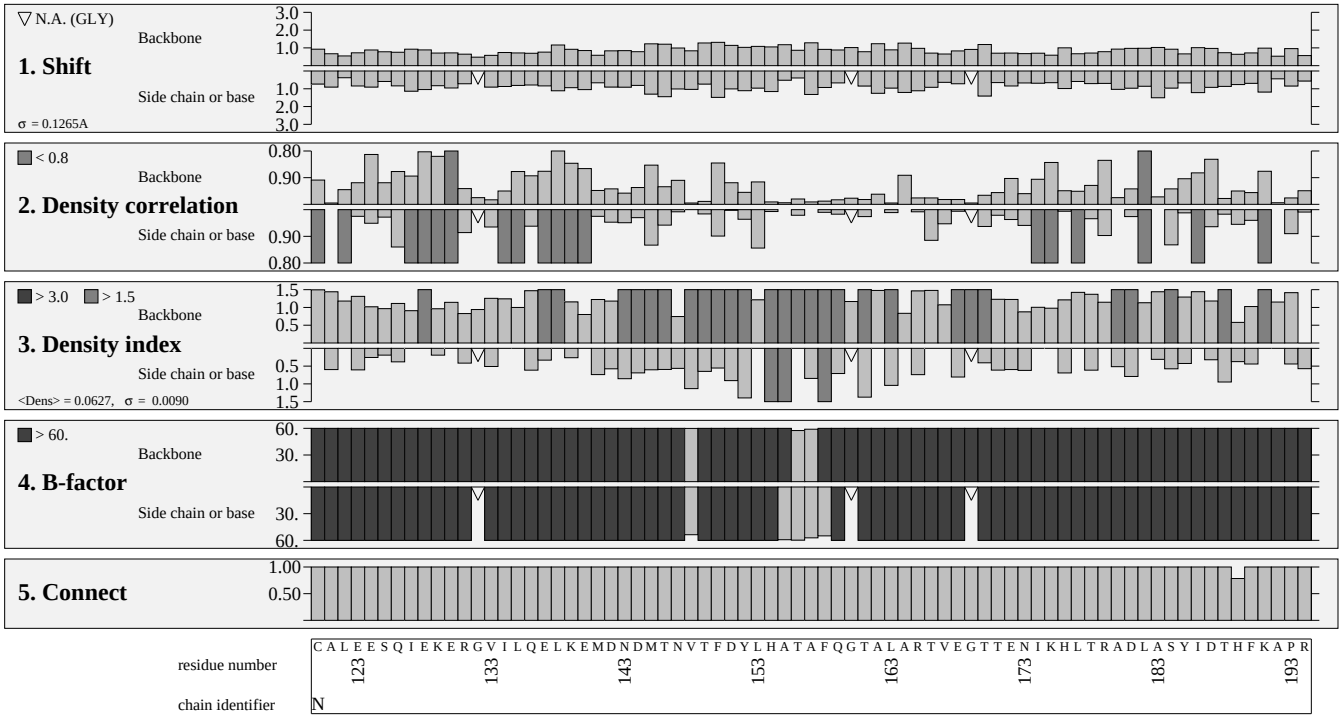
Local estimation (15)





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Structure Factor Check

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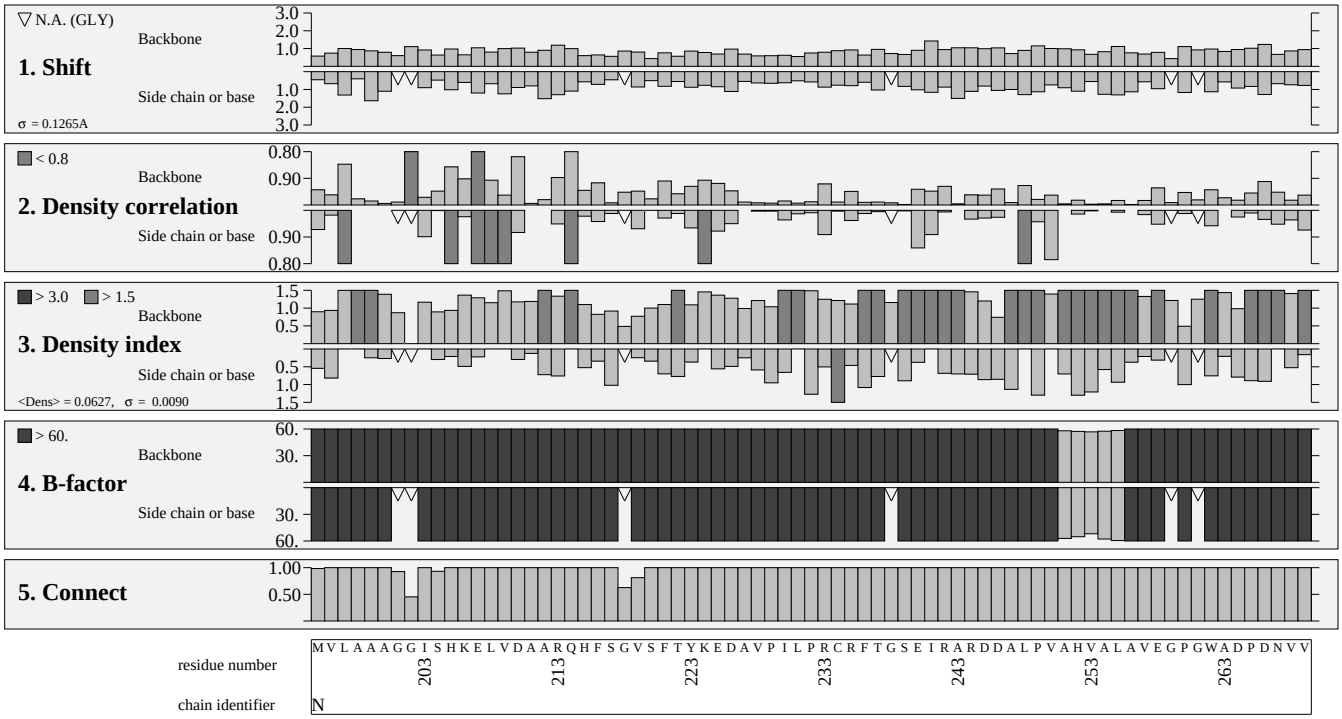
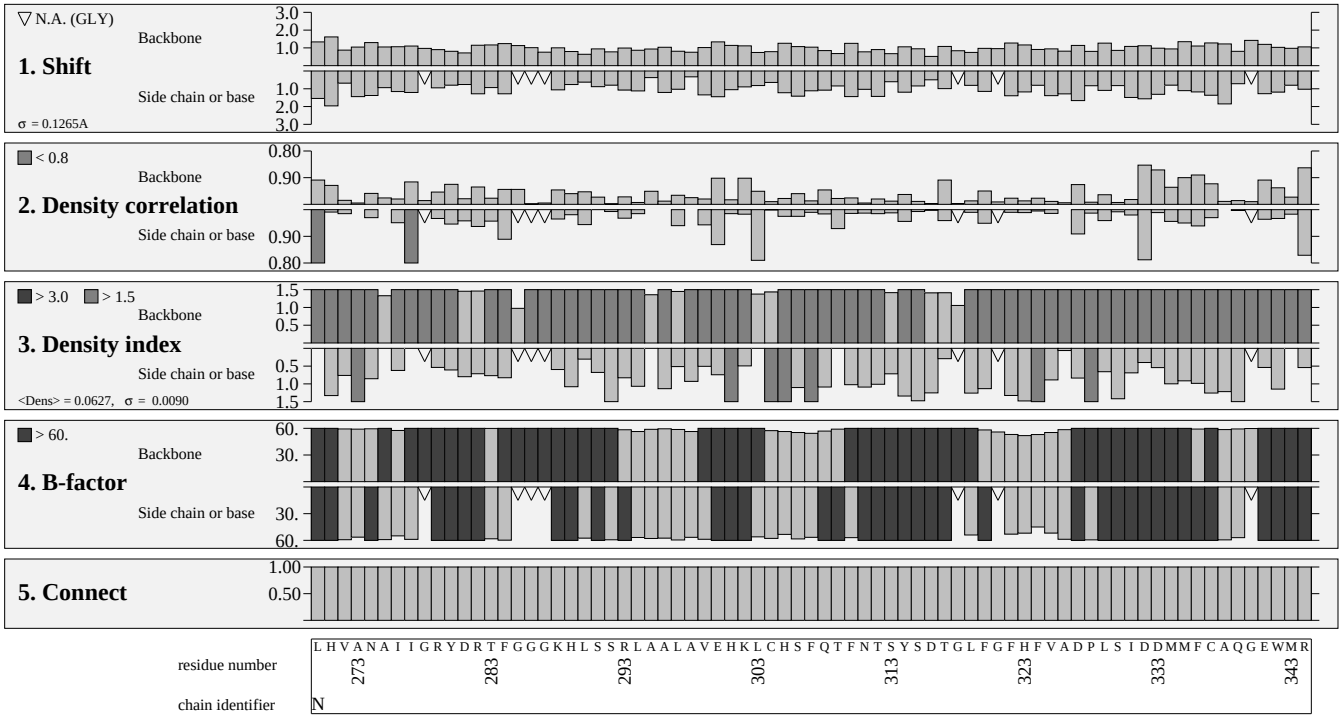
Local estimation (16)





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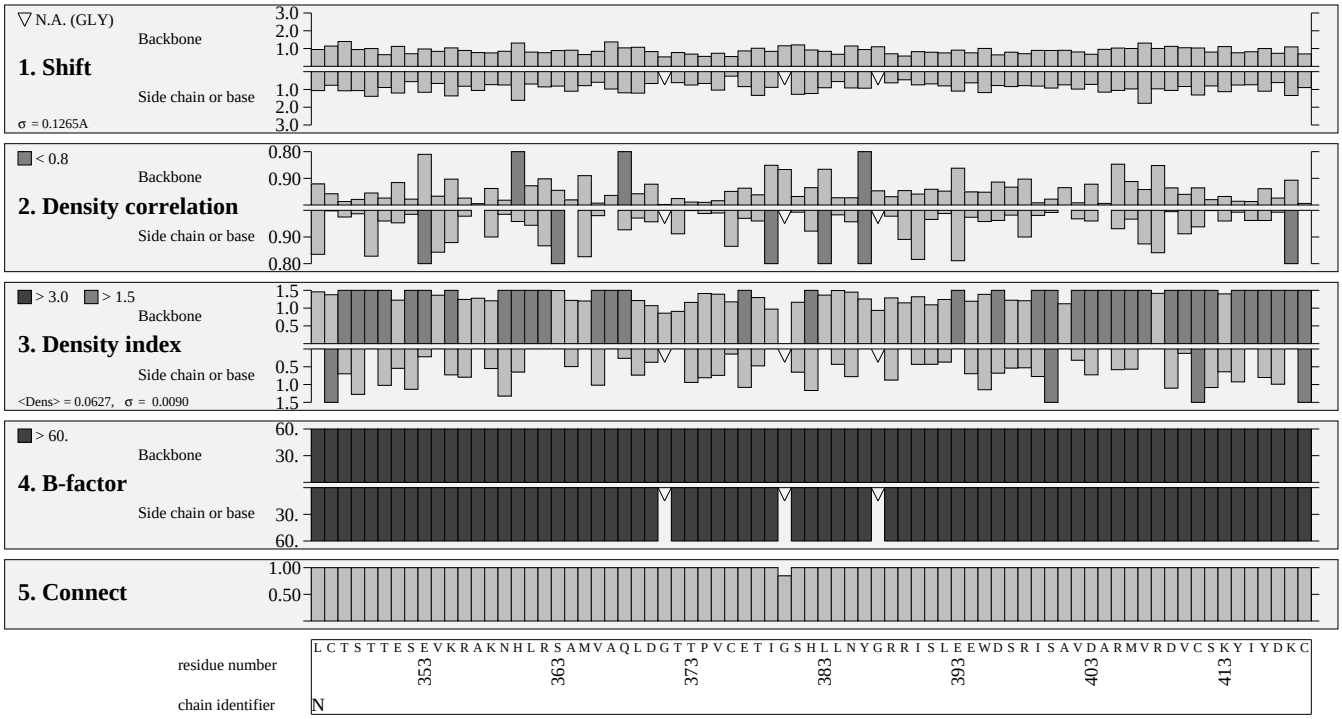
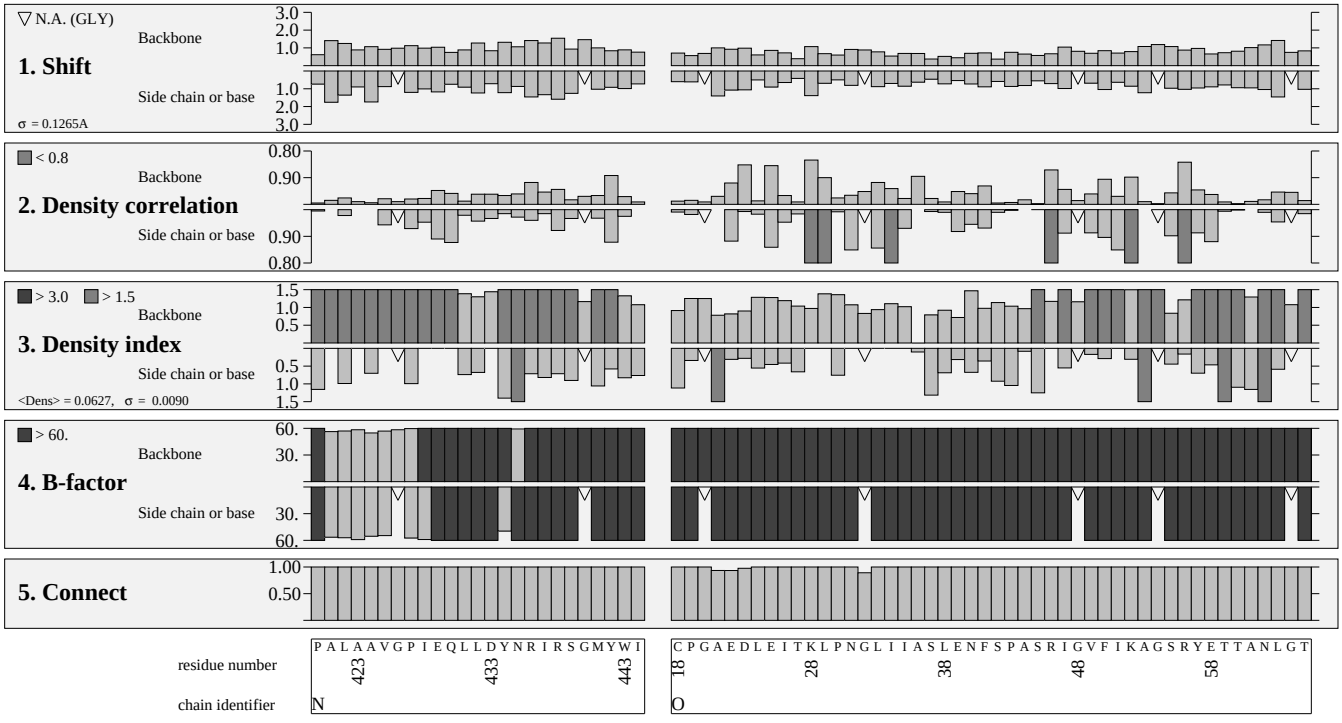
Local estimation (17)





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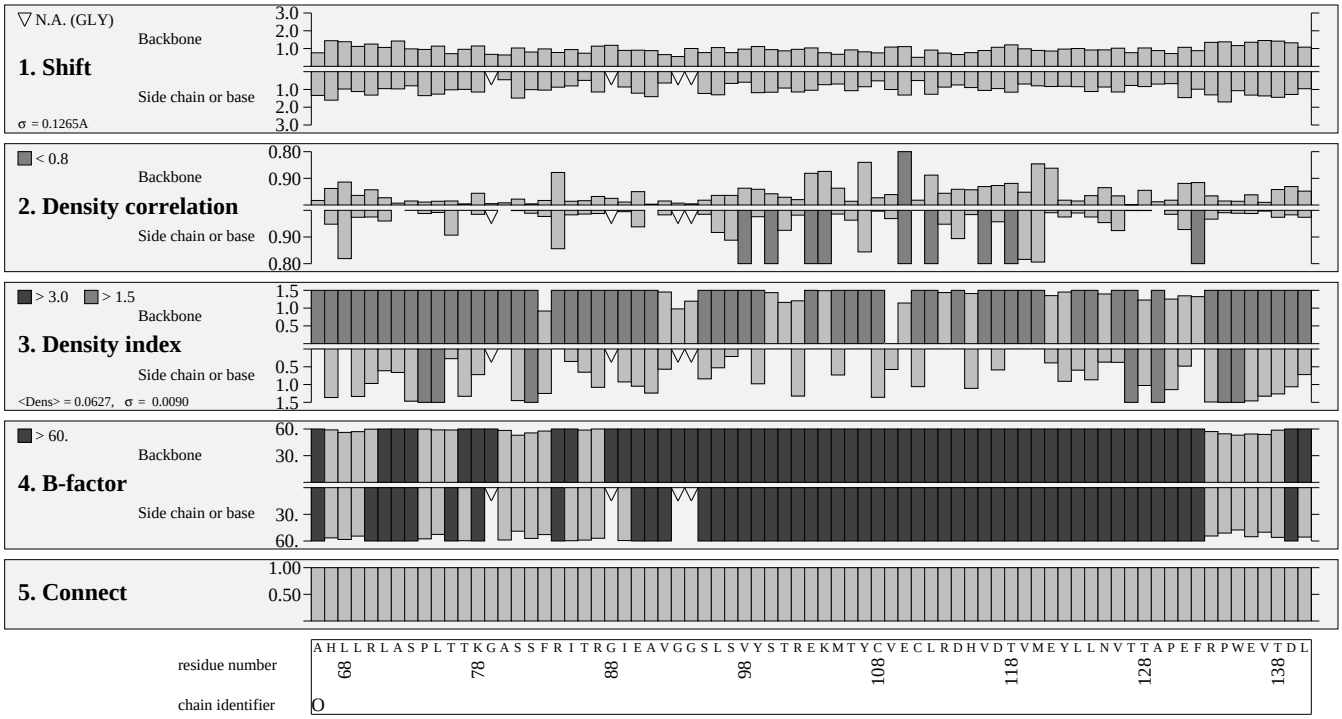
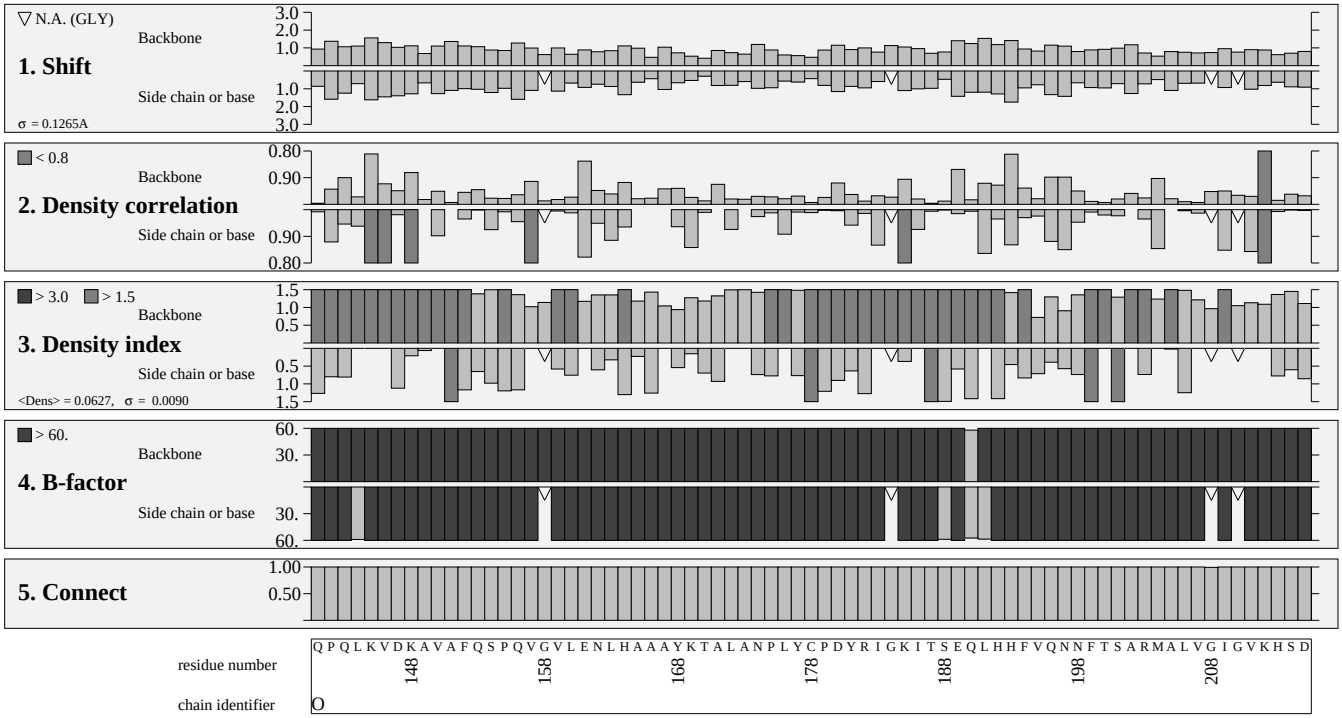
Local estimation (18)





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Structure Factor Check

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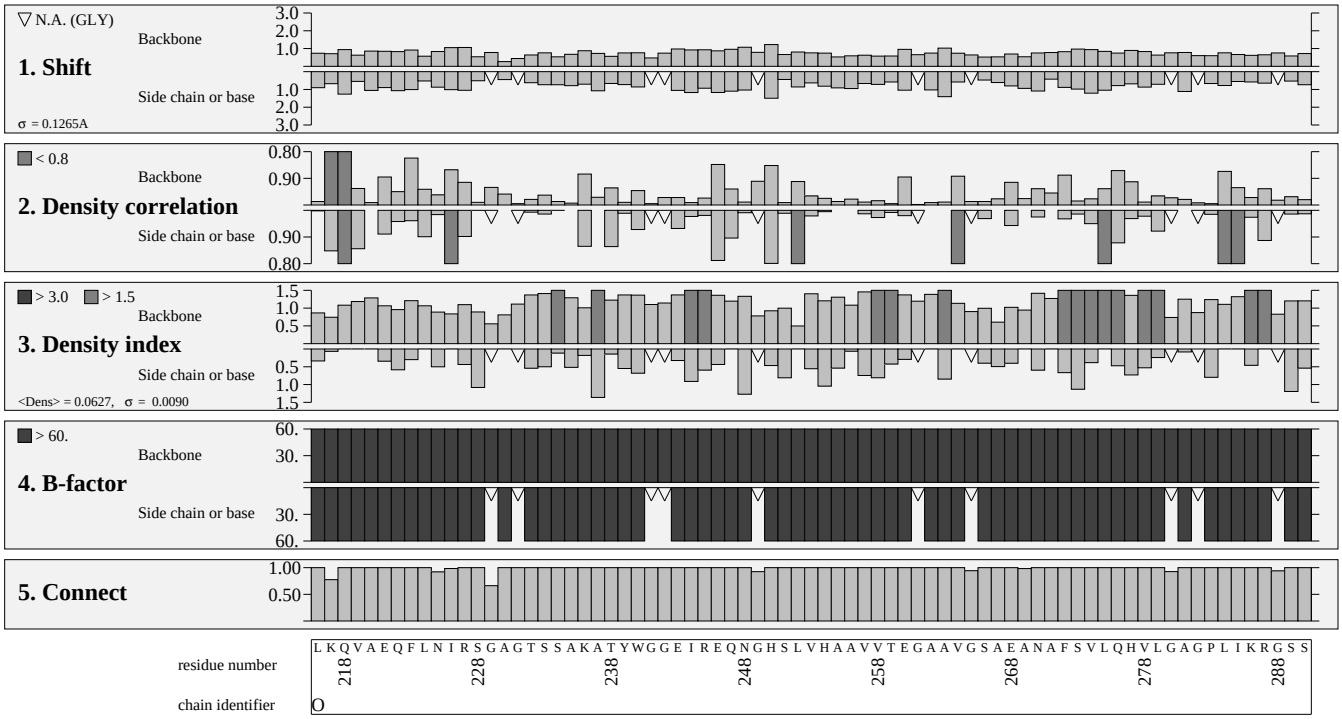
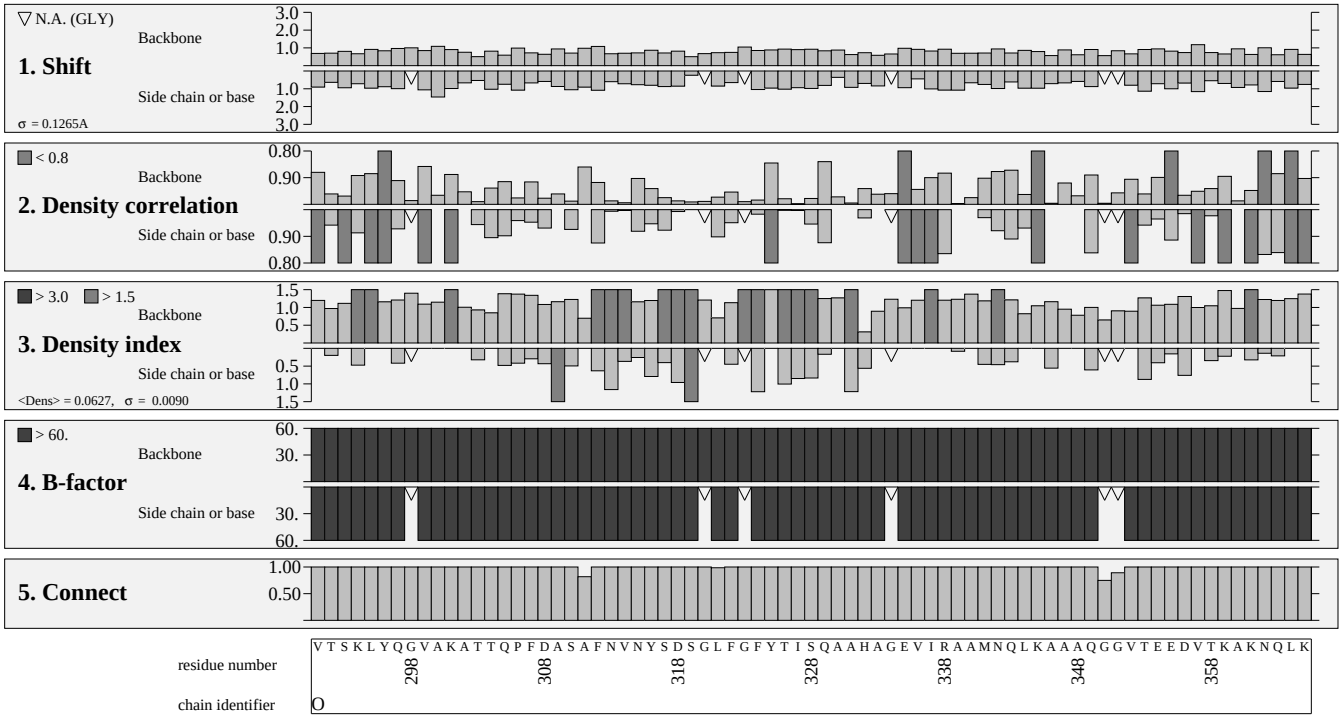
Local estimation (19)





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Structure Factor Check

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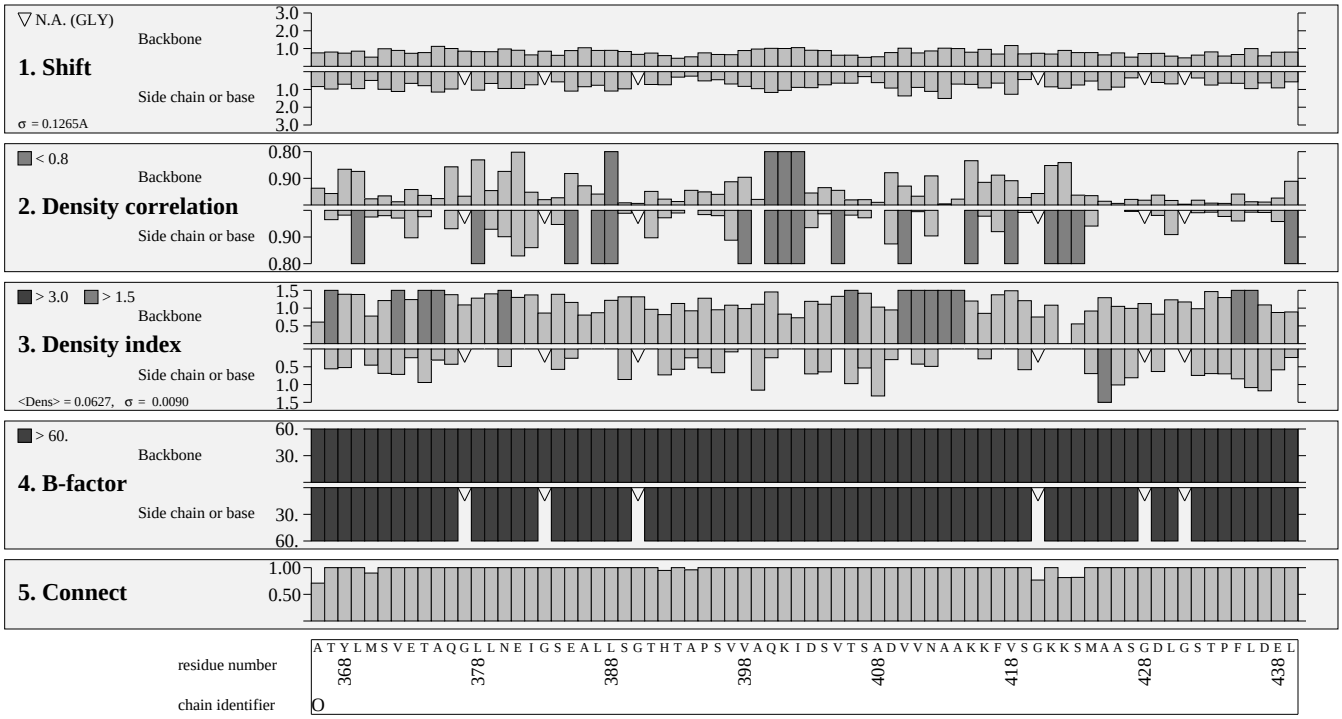
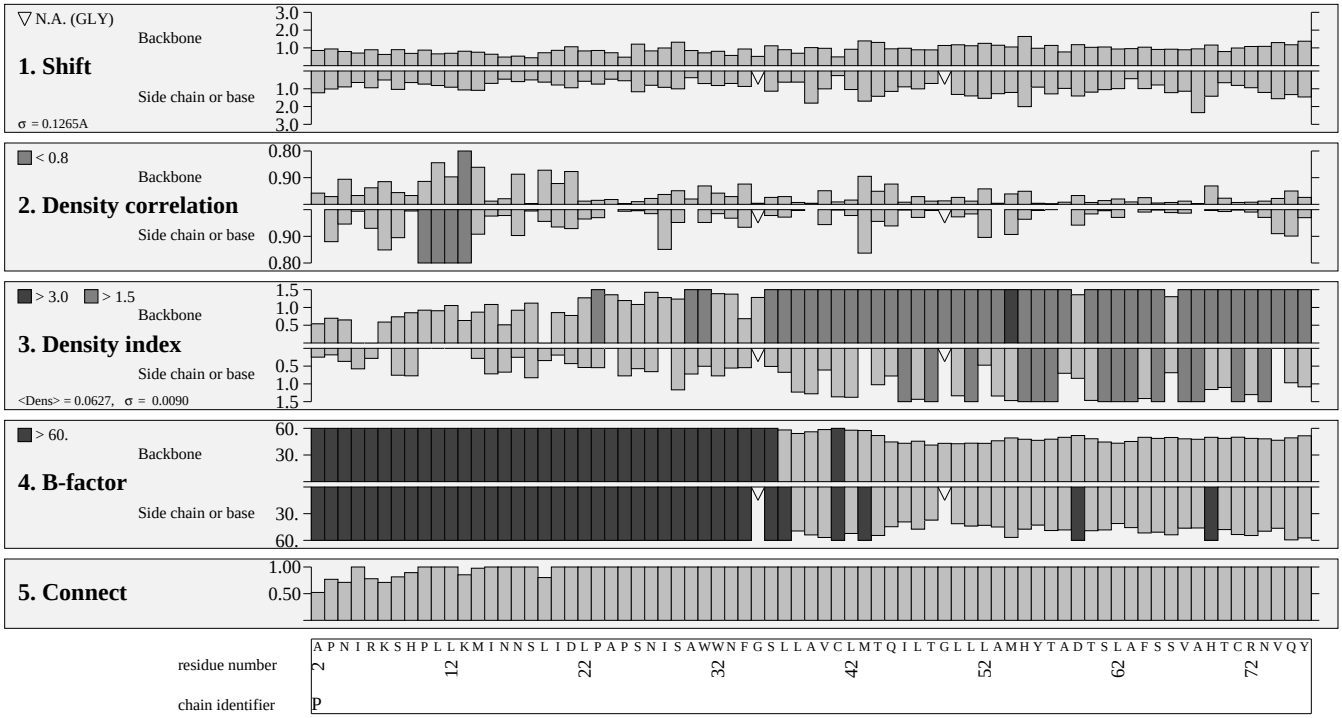
Local estimation (20)





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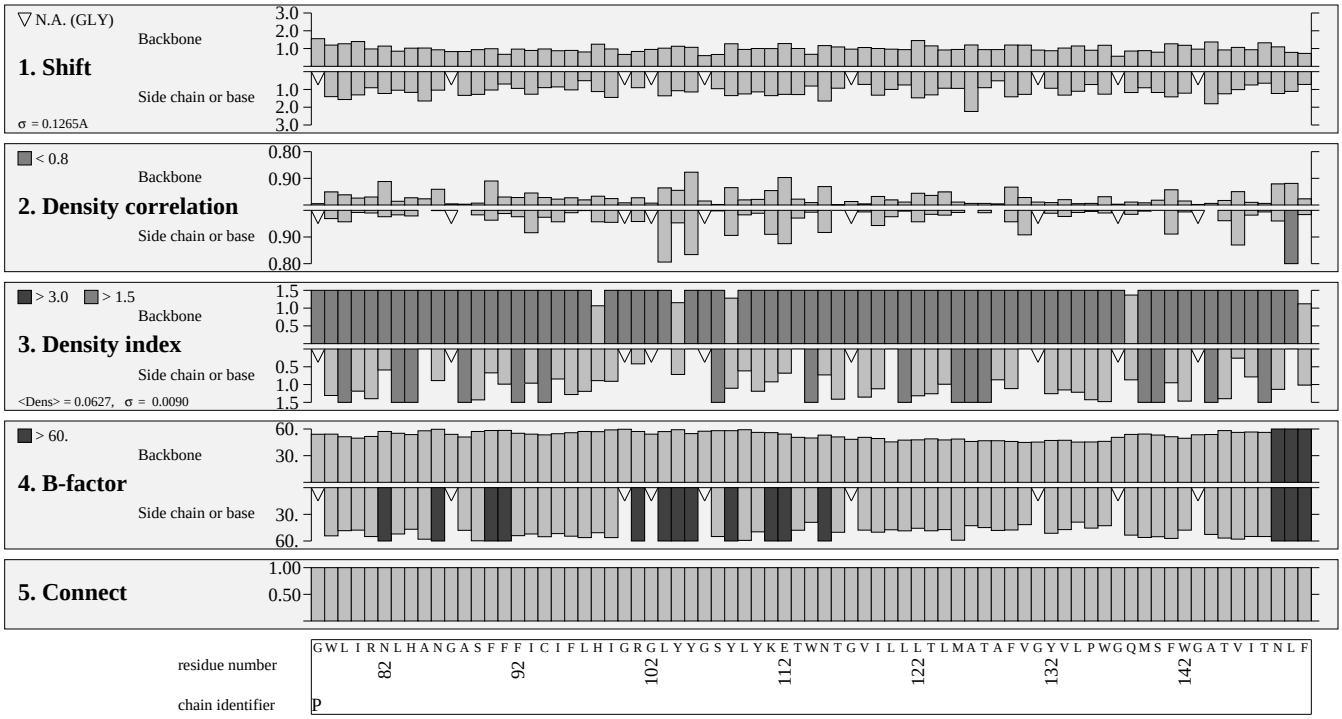
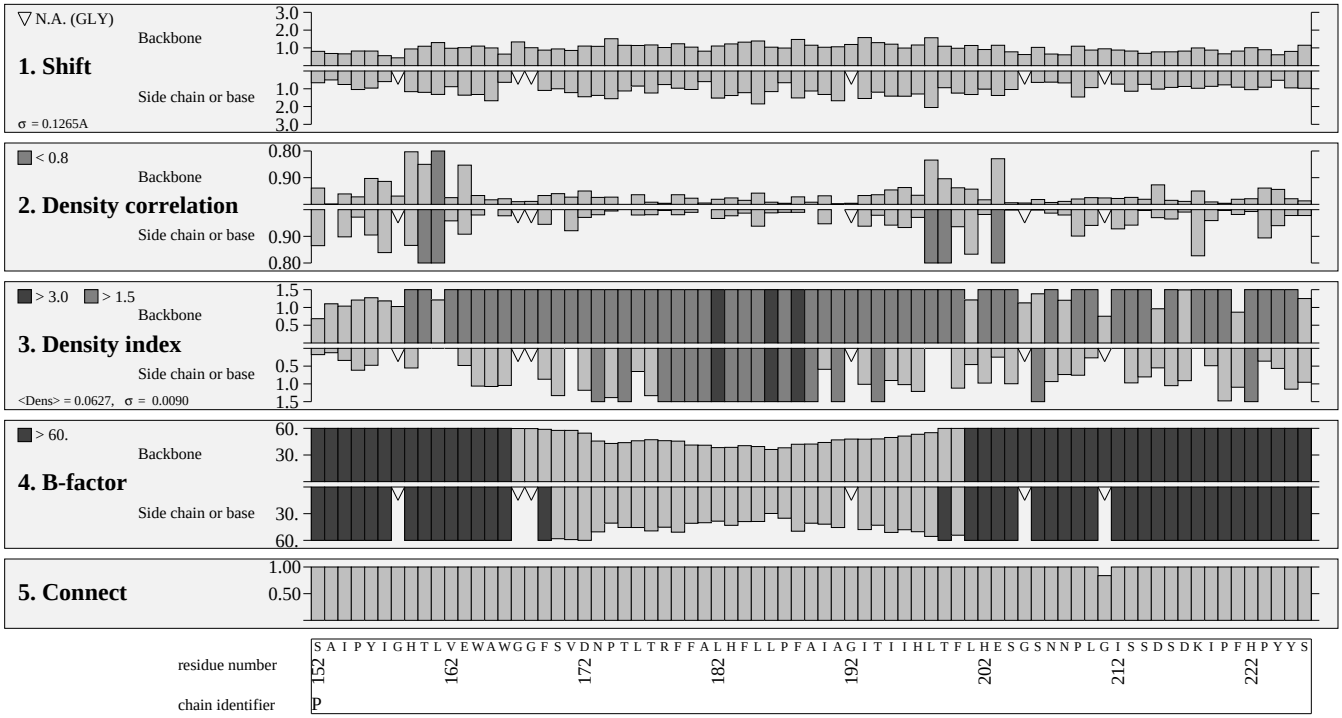
Structure Factor Check

3L71

Local estimation (21)





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Structure Factor Check

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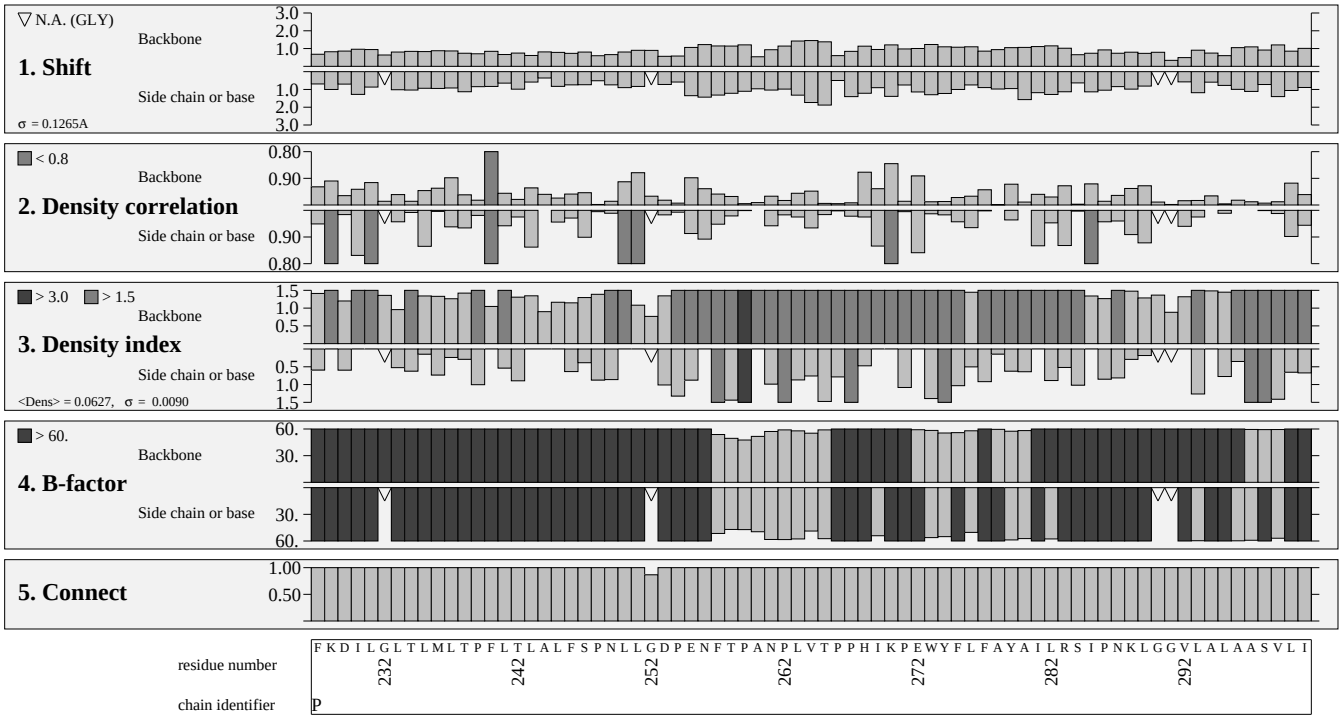
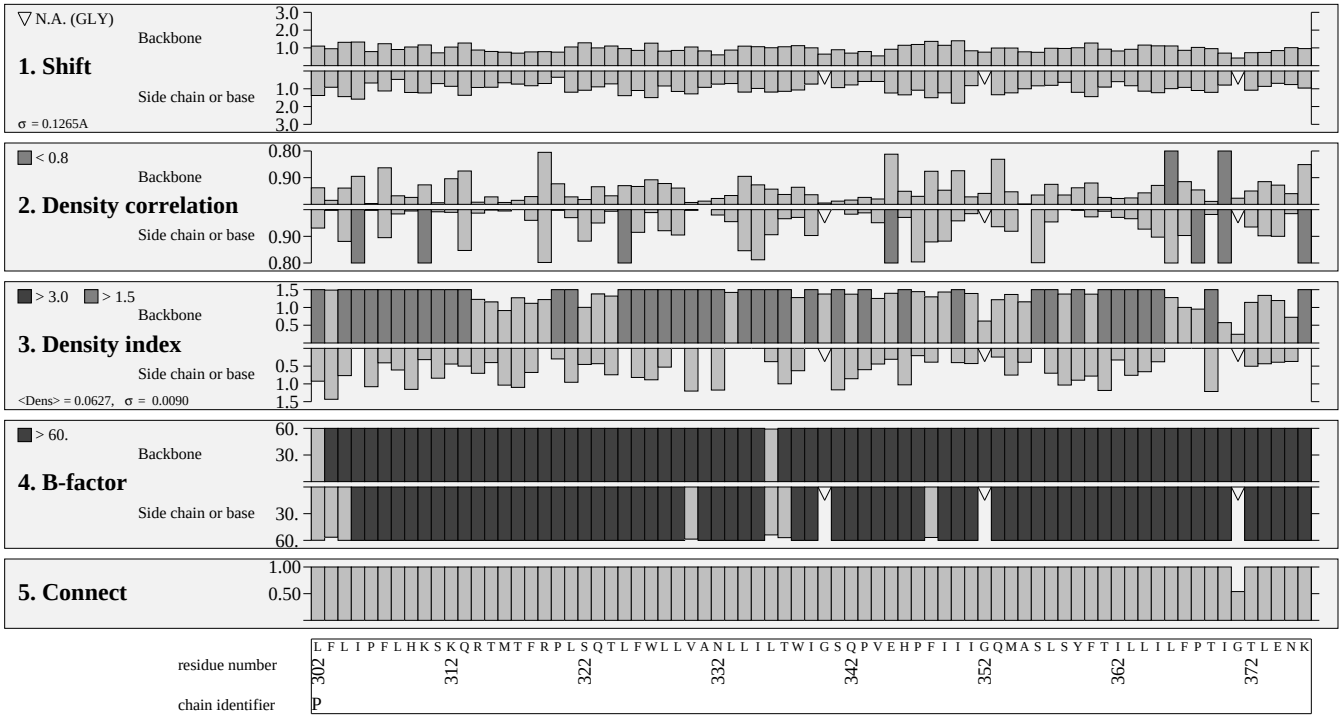
Local estimation (22)





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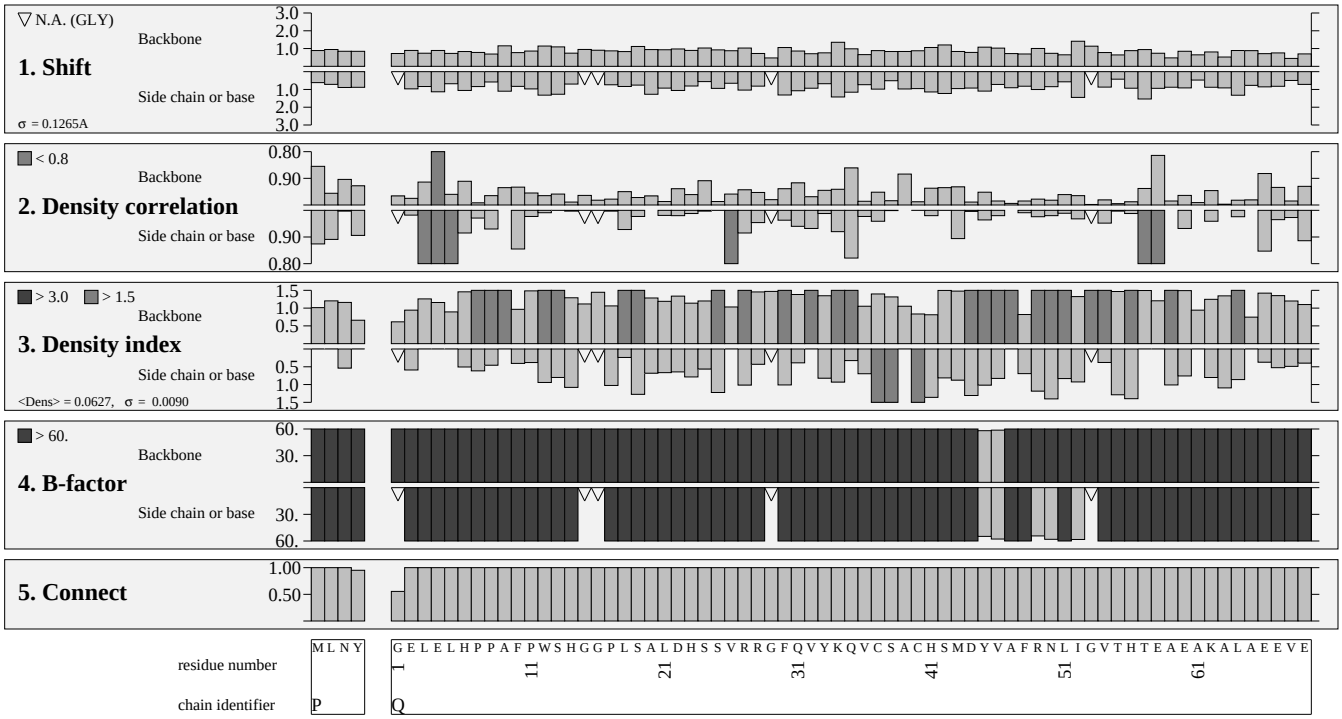
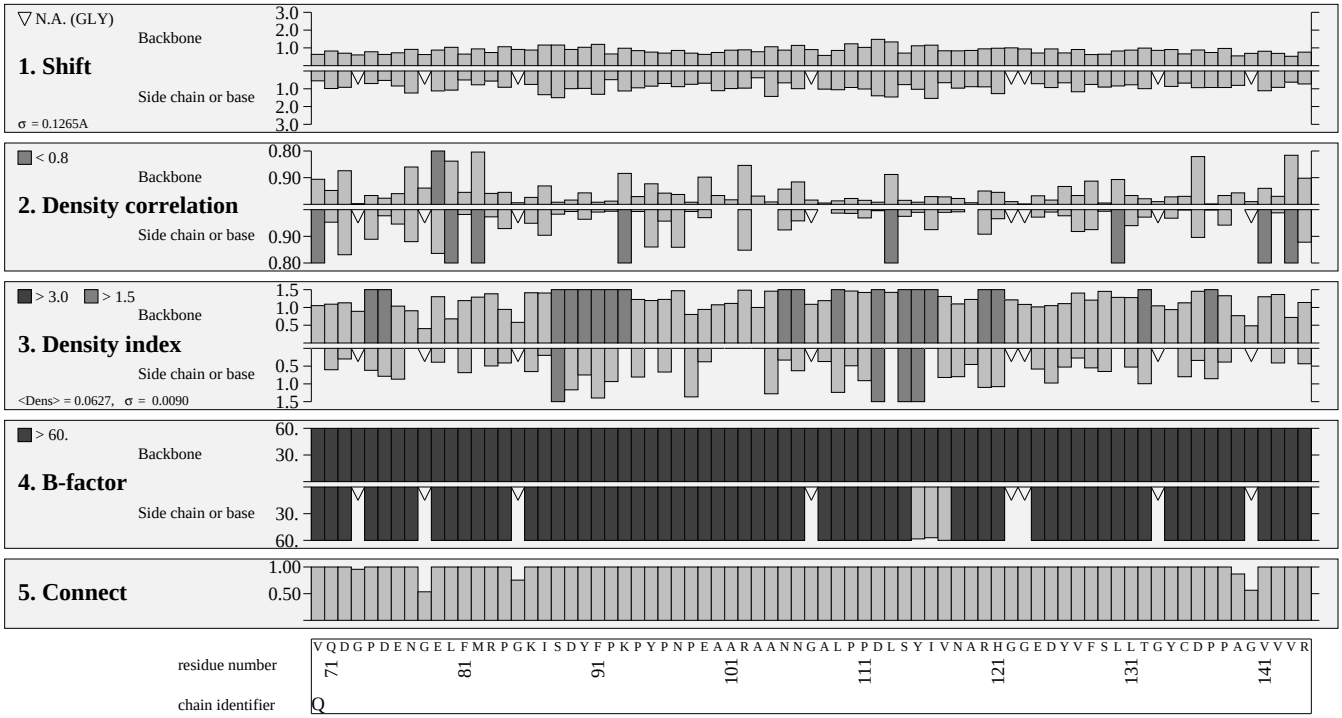
Structure Factor Check

3L71

Local estimation (23)



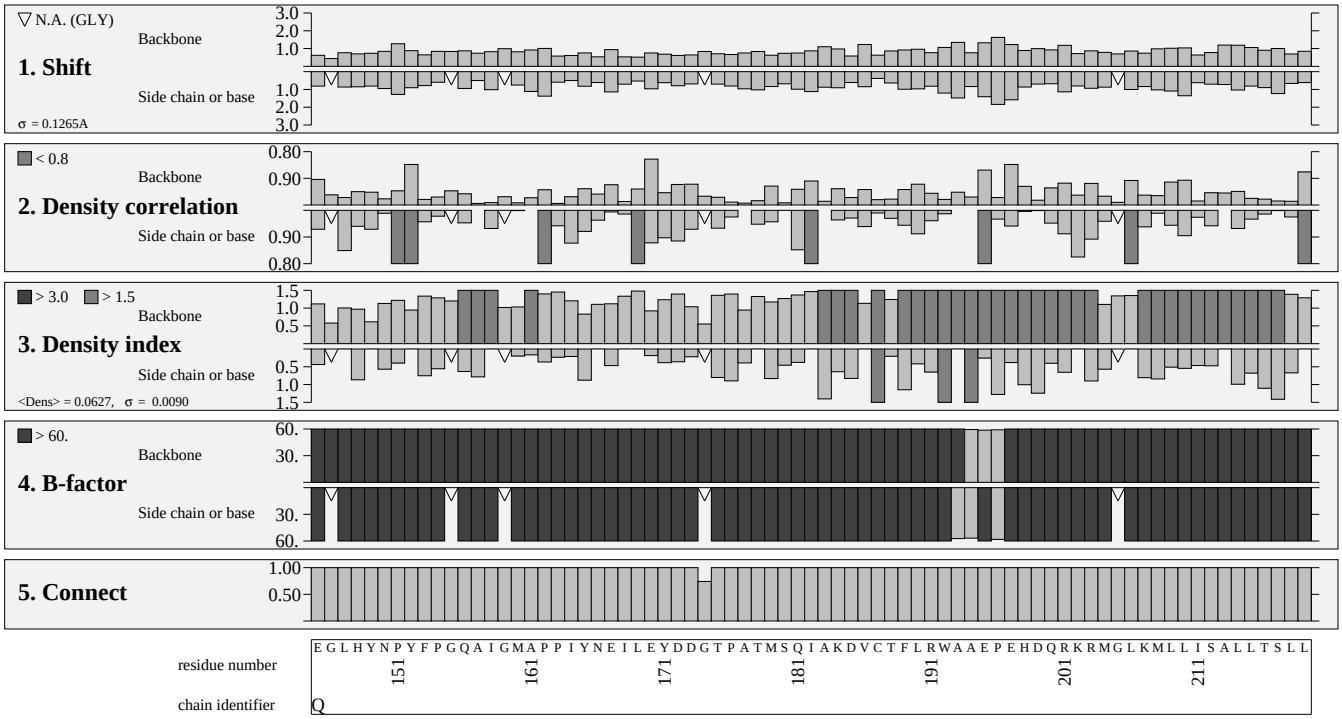


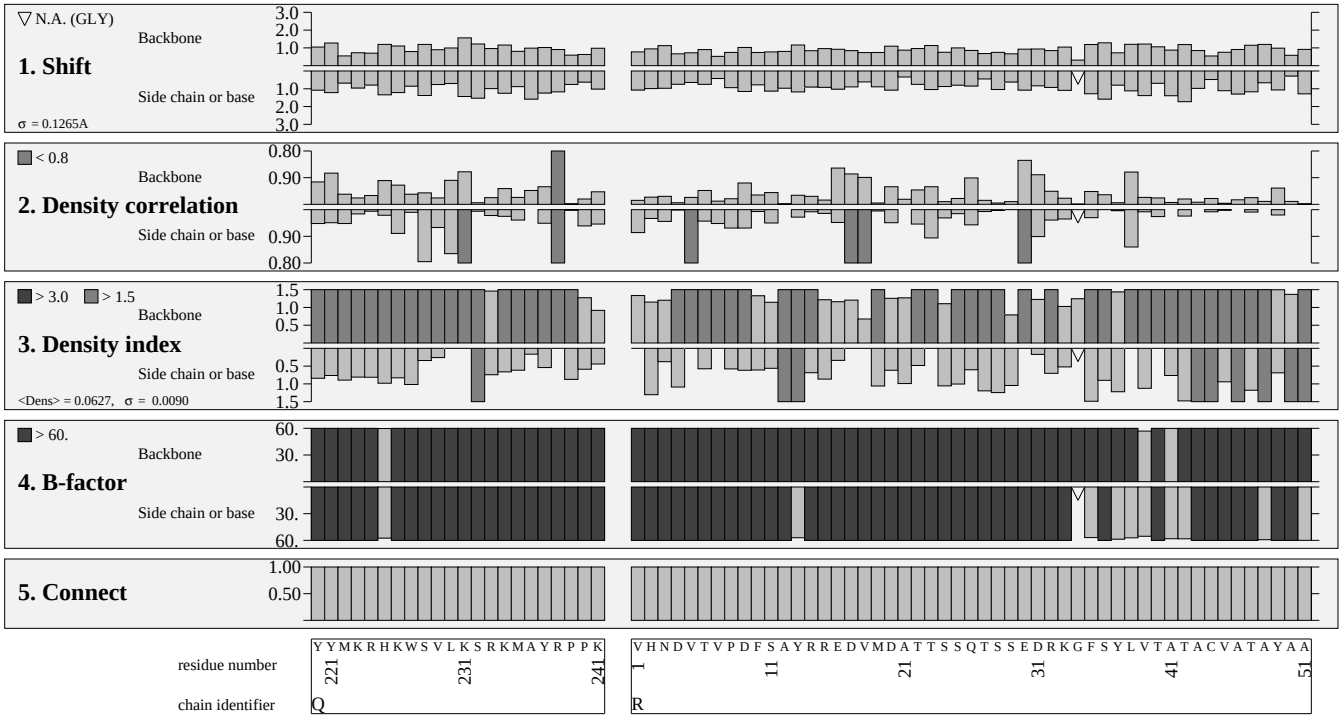
SFCHECK 7.03.16

Structure Factor Check

3L71

Local estimation (24)



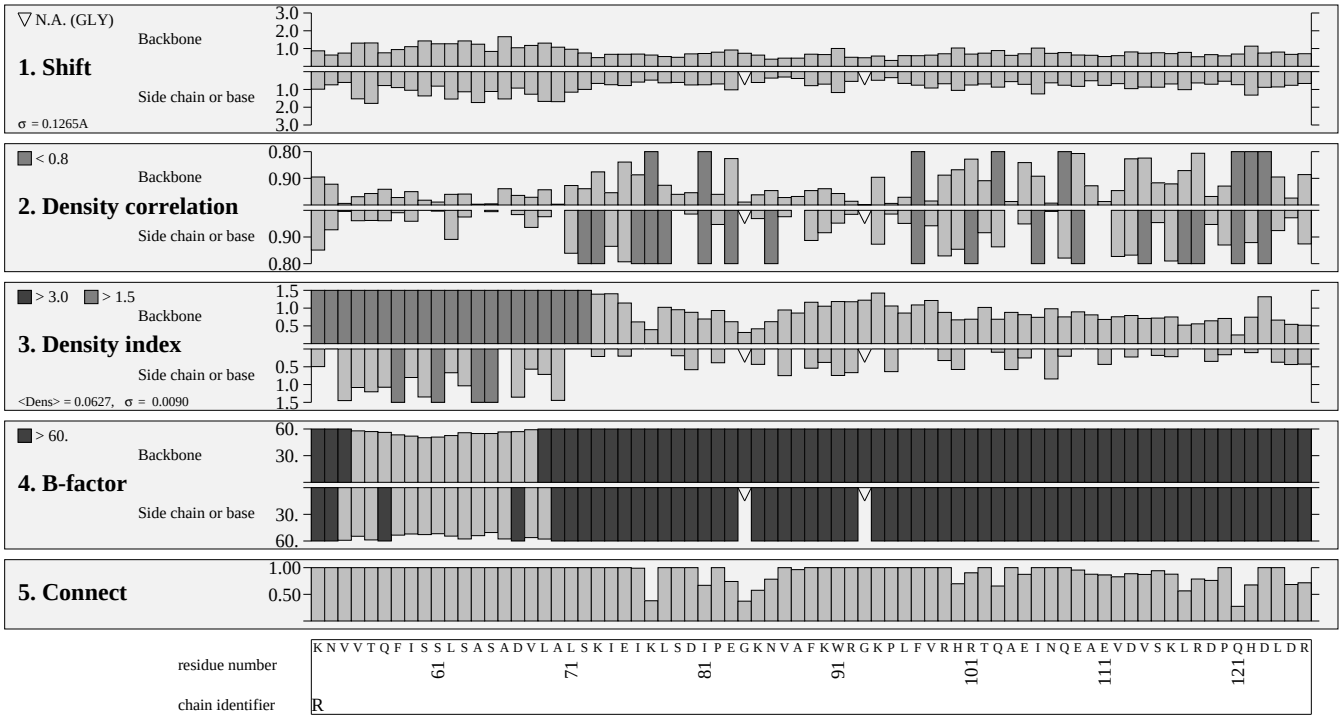


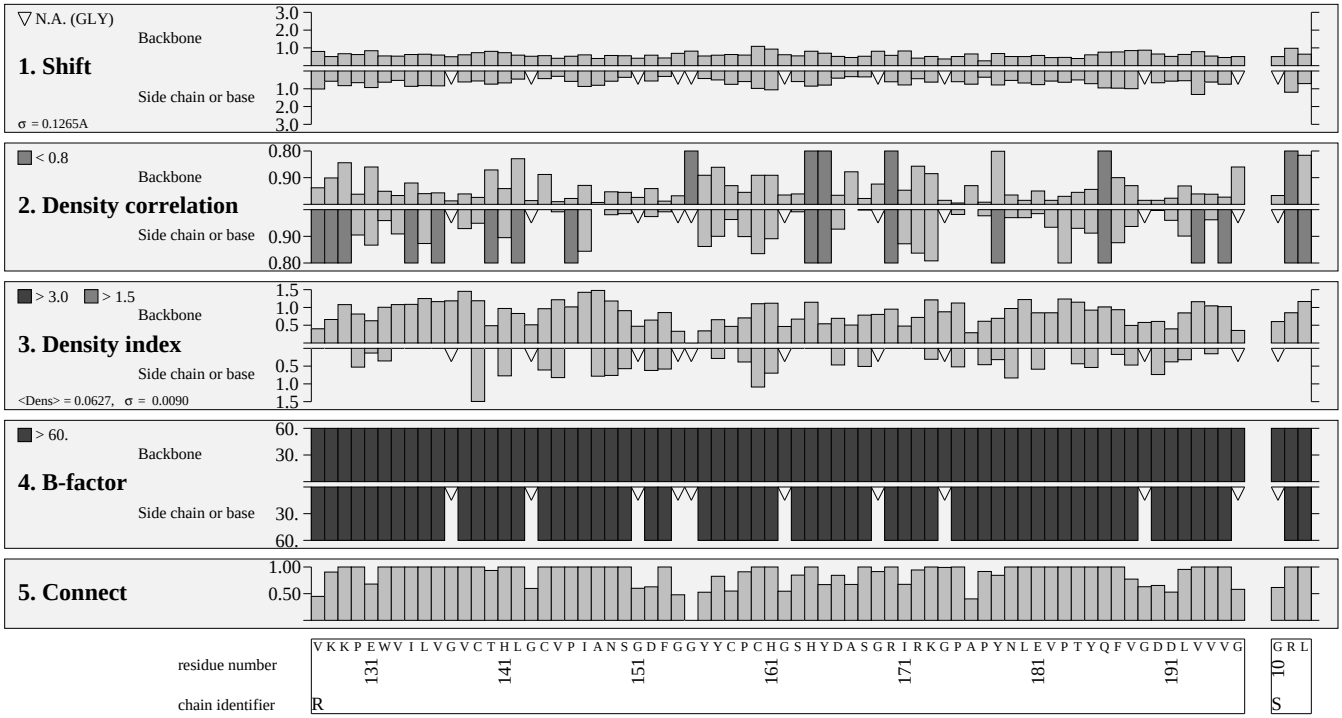
SFCHECK 7.03.16

Structure Factor Check

3L71

Local estimation (25)



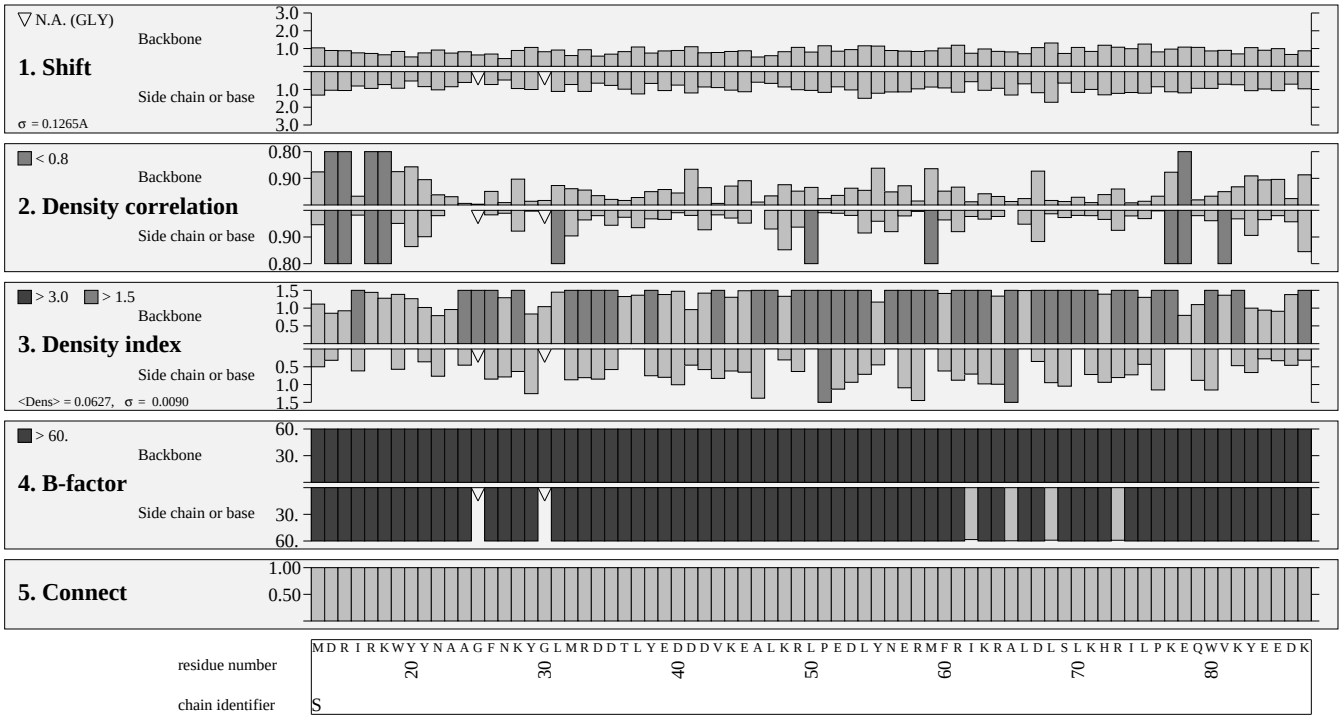


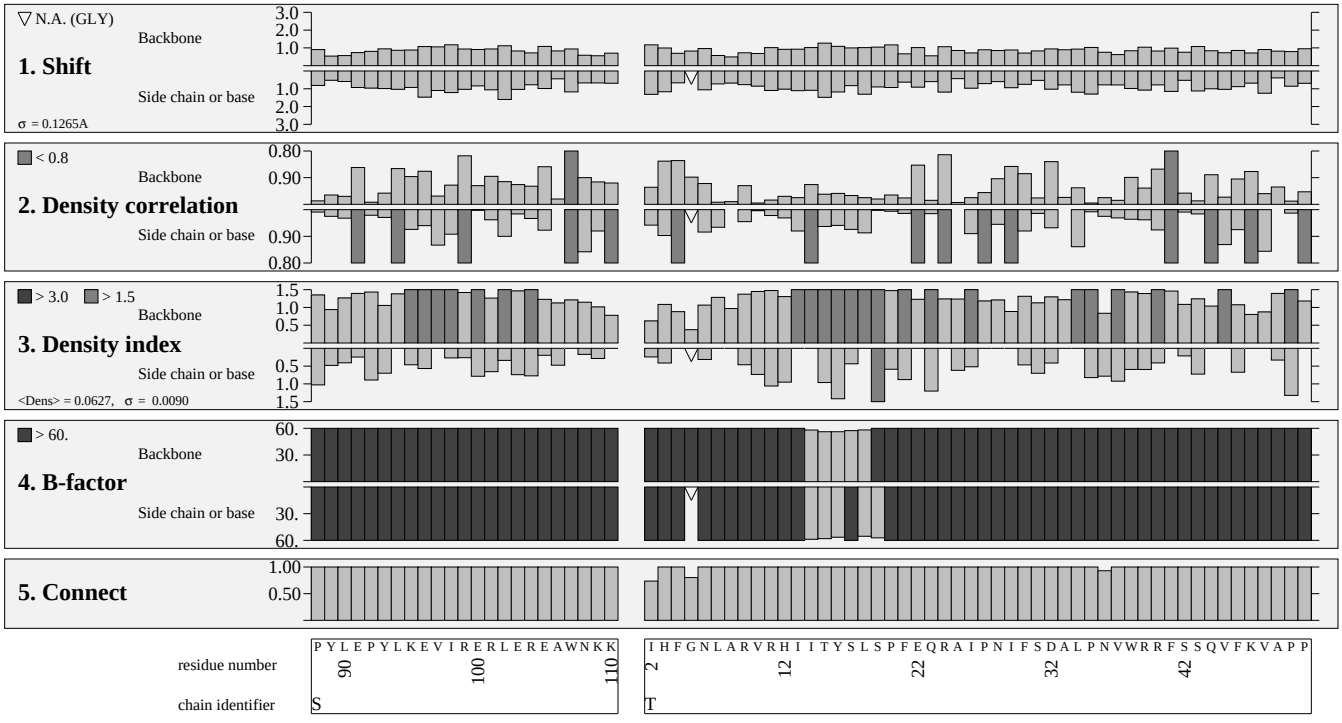
SFCHECK 7.03.16

Structure Factor Check

3L71

Local estimation (26)



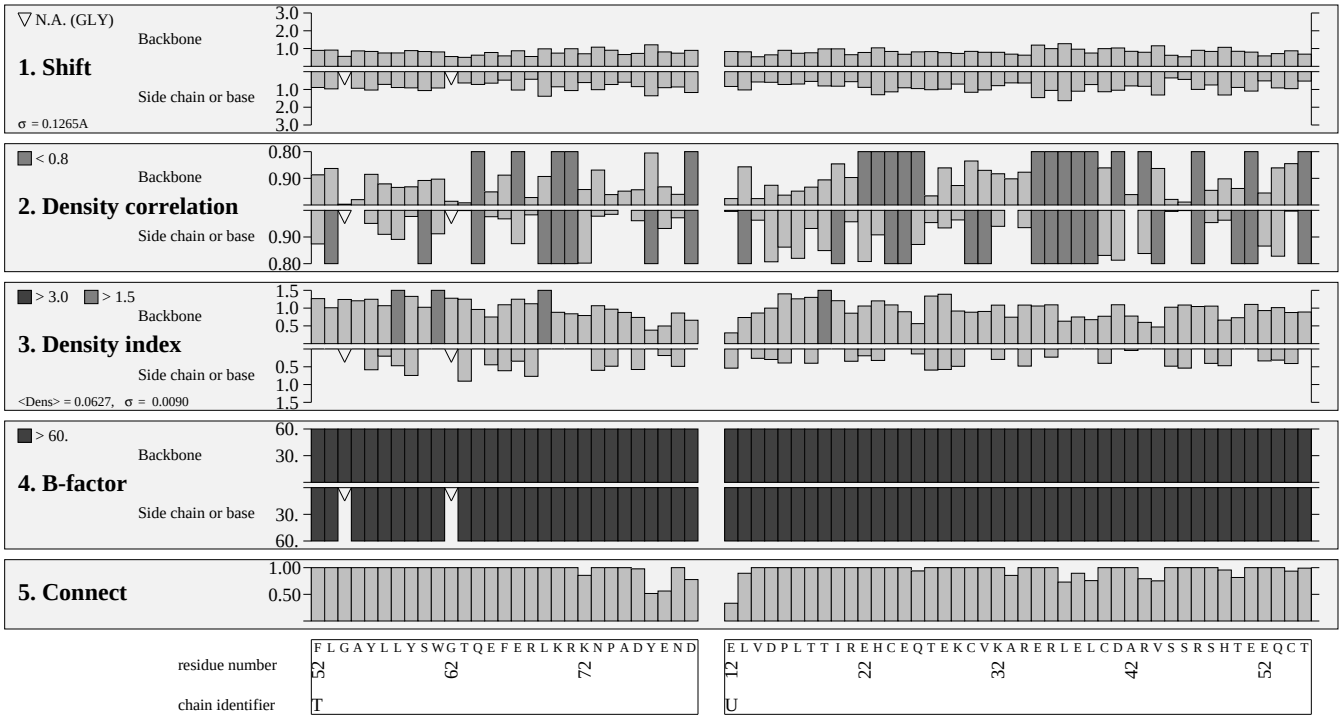


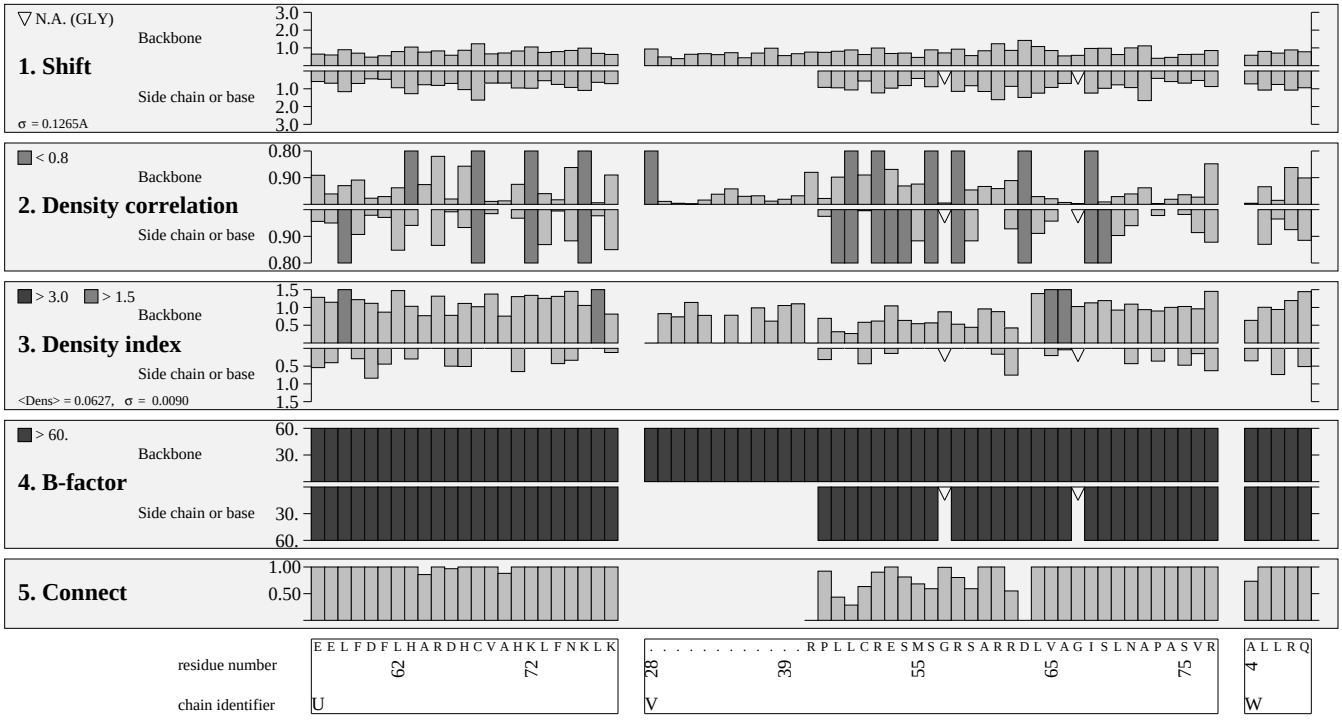
SFCHECK 7.03.16

Structure Factor Check

3L71

Local estimation (27)



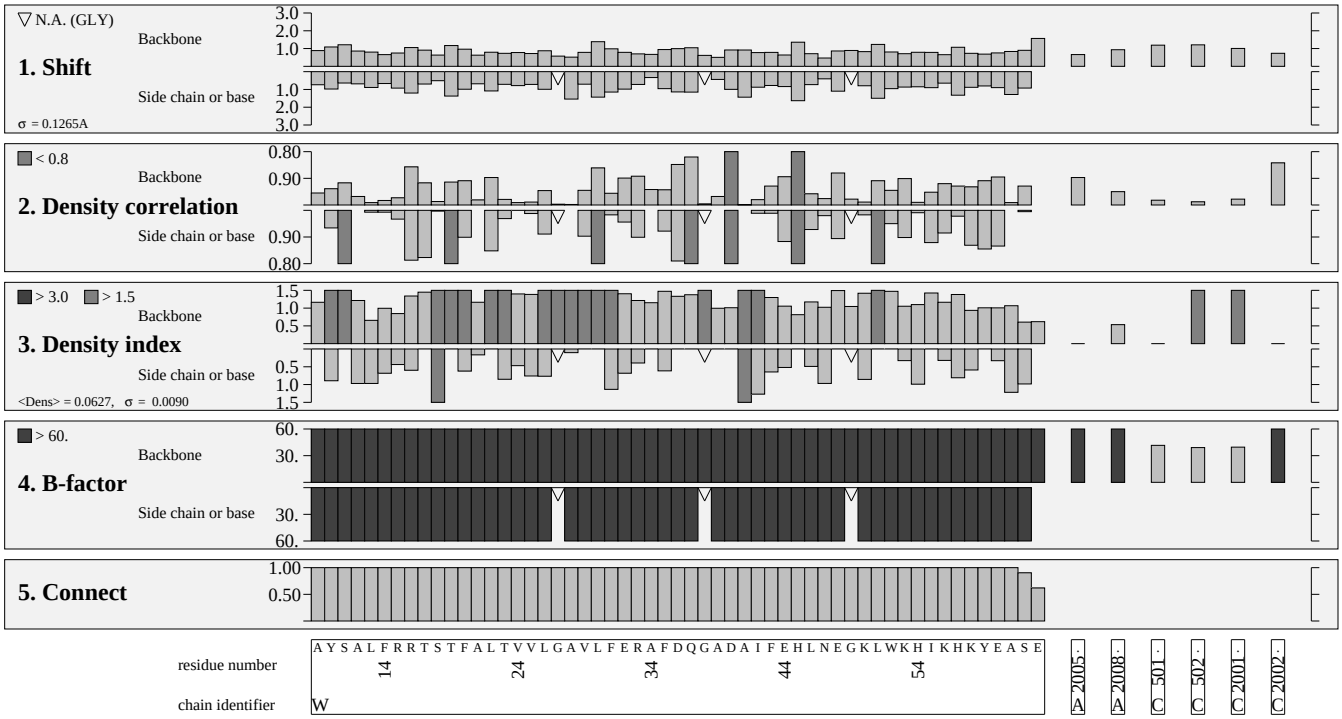


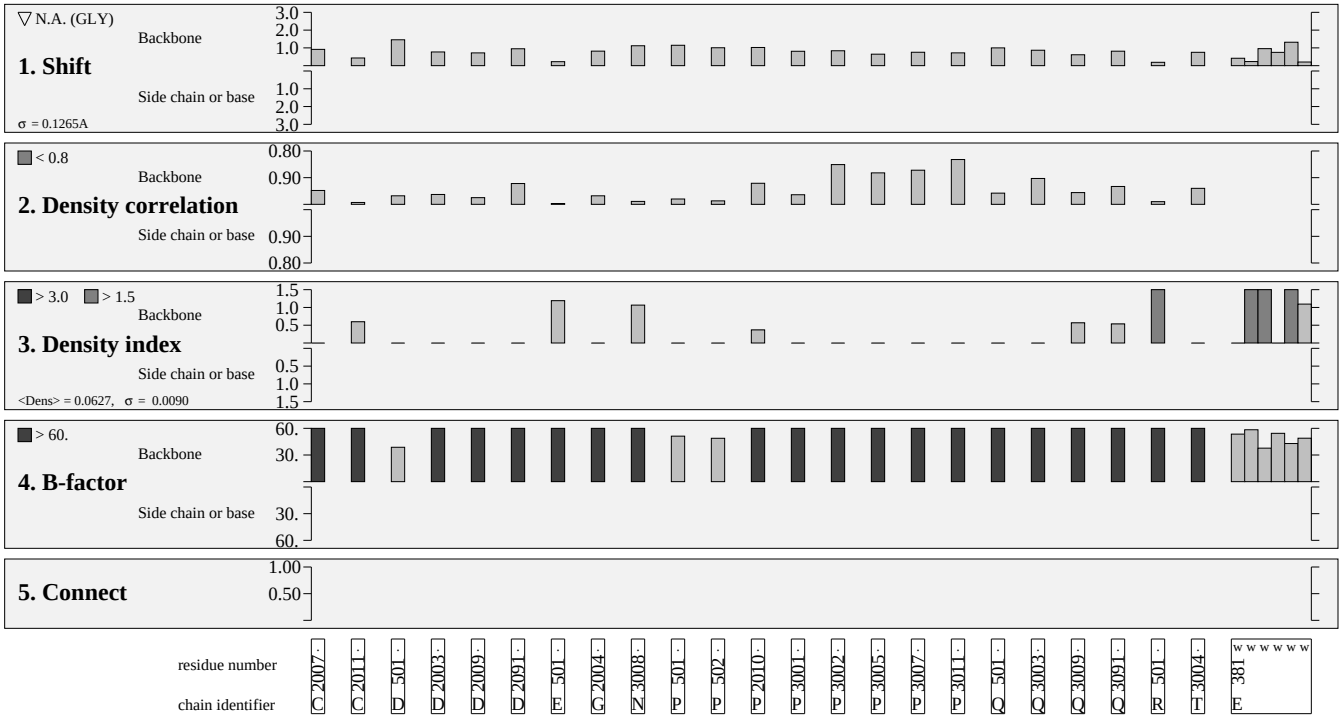
SFCHECK 7.03.16

Structure Factor Check

3L71

Local estimation (28)



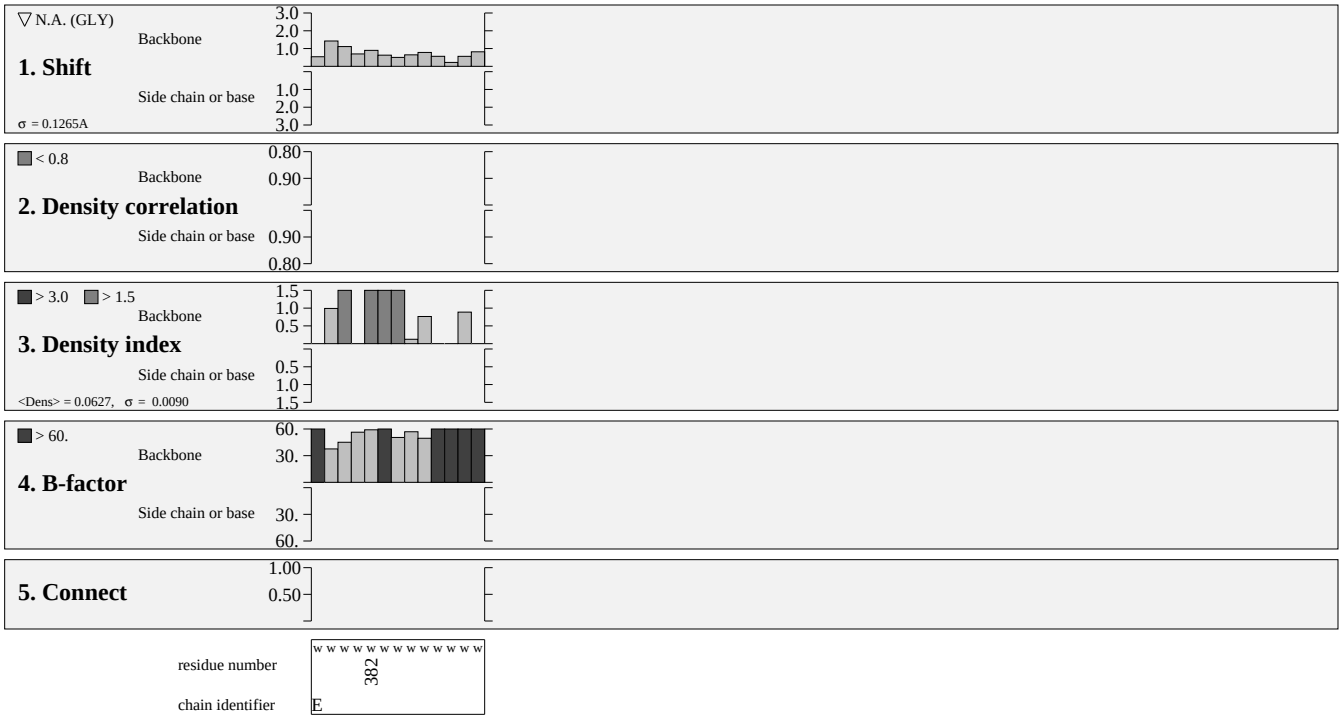


SFCHECK 7.03.16

Structure Factor Check

3L71

Local estimation (29)



SFCHECK 7.03.16