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

Structure Factor Check

3L73

Title:	CYTOCHROME BC1 COMPLEX FROM CHICKEN WITH TRIAZOLONE INHIBITOR
Date:	27−DEC−09
PDB code:	3L73

Crystal

Cell parameters:

a: 171.50 A b: 182.93 A c: 241.03 A

α: 90.00 β: 90.00 γ: 90.00

Space group: P 21 21 21

Model

32645 atoms (19 water molecules)

Number of chains:	51
Volume not occupied by model:	62.4 %
<B> (for atomic model):	79.6 A^2
σ(B):	18.27 A^2
Matthews coefficient:	4.14
Corresponding solvent % :	70.03

Refinement

Program:	CNS 1.1
Nominal resolution range:	25.0 − 3.04 A
Reported nominal resolution:	3.00 A
Reported R−factor:	0.259
Number of reflections used:	145117
Reported Rfree:	0.29
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		25.0 − 2.90 A
Reflections in file:		166720
Unique reflections	above 0:	166720
	above 1σ:	161882
	above 3σ:	96414

SFCHECK

Nominal resolution range:	25.0 − 3.04 A
\05max. from input data, min. from author\05	
Used reflections:	145117
Reflections out of resolution:	21603
Completeness:	99.7 %
R_stand(F) = <σ(F)>/<F> :	0.073
Anisotropic distribution of Structure Factors	
ratio of eigen values:	1.0000 0.4474 0.4507
B_overall (by Patterson):	53.A^2
Optical resolution:	2.25 A
Expected opt. resol. for complete data set:	2.25 A
Estimated minimal error:	0.093 A

Model vs. Structure Factors

R−factor for all reflections:	0.306
Correlation factor:	0.851
R−factor:	0.307
for F > 2.0σ	
nom. resolution range:	24.97 − 3.04A
reflections used:	141488
Rfree:	0.335
Nfree:	2775
R−factor without free−refl.:	0.307
Non free−reflections:	138713
<u> (error in coords by Luzzati plot):	0.604 A
Estimated maximal error:	0.414 A
DPI:	0.376 A

Scaling

Scale:	0.483
Bdiff:	−9.31

Anisothermal Scaling (Beta):

12.5073 −4.4573 −3.7911 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.416 250.040

Structure Factor Check

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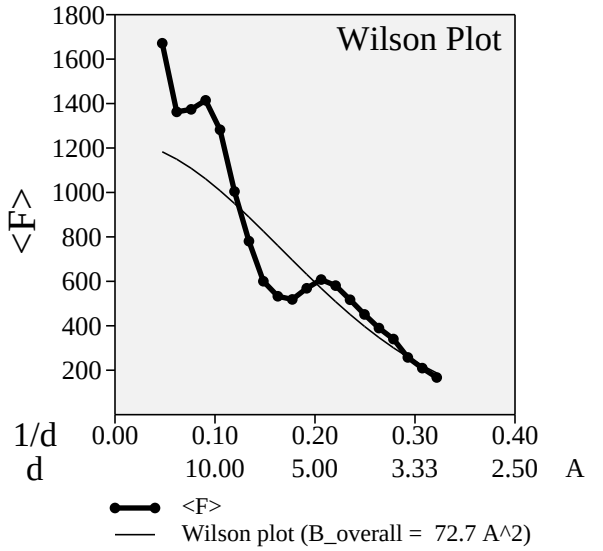
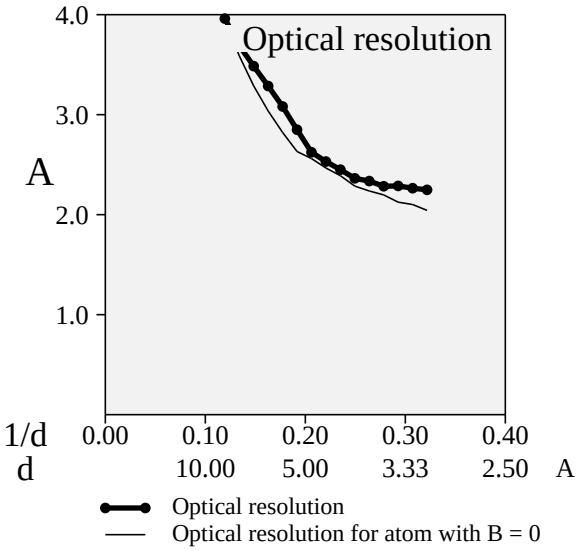
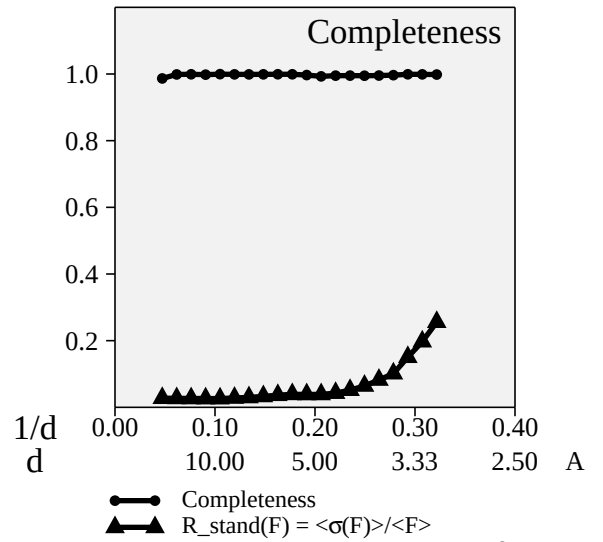
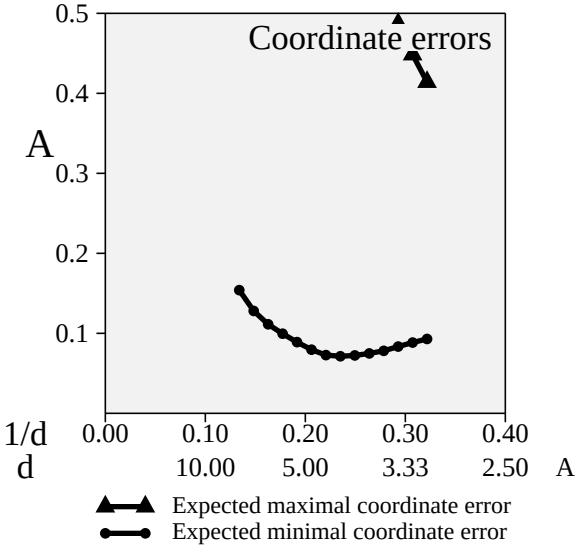
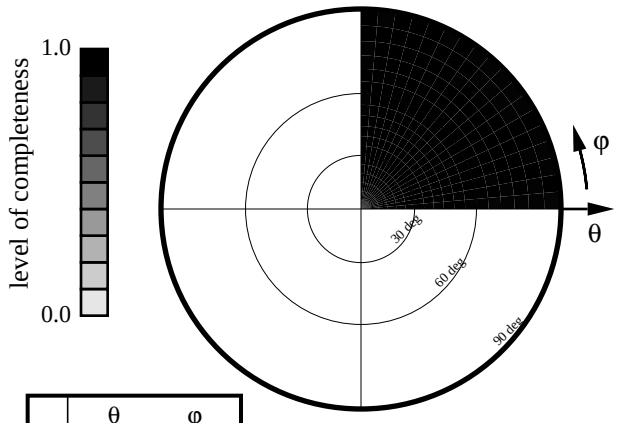






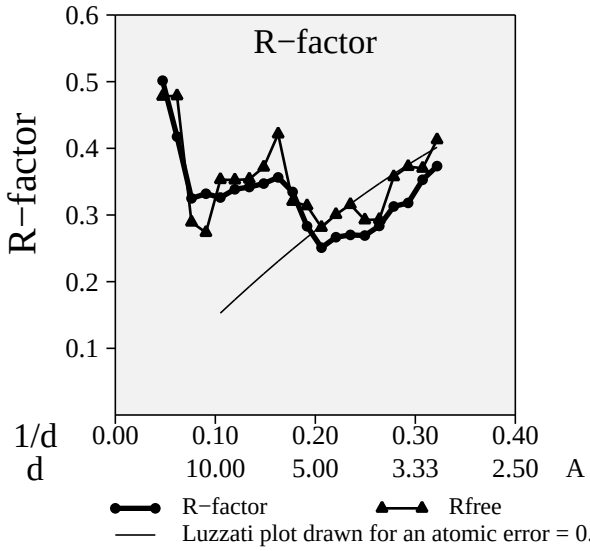


Stereographic projection of
the averaged radial completeness



	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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Structure Factor Check

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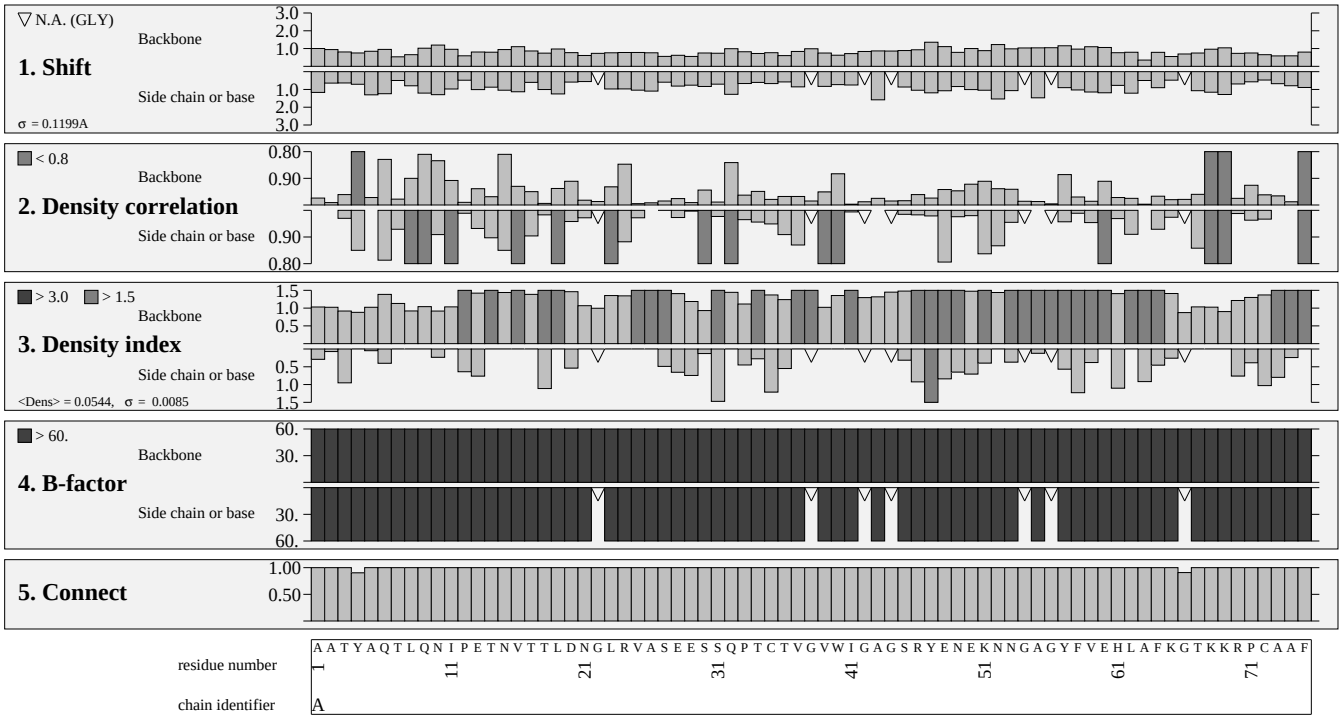
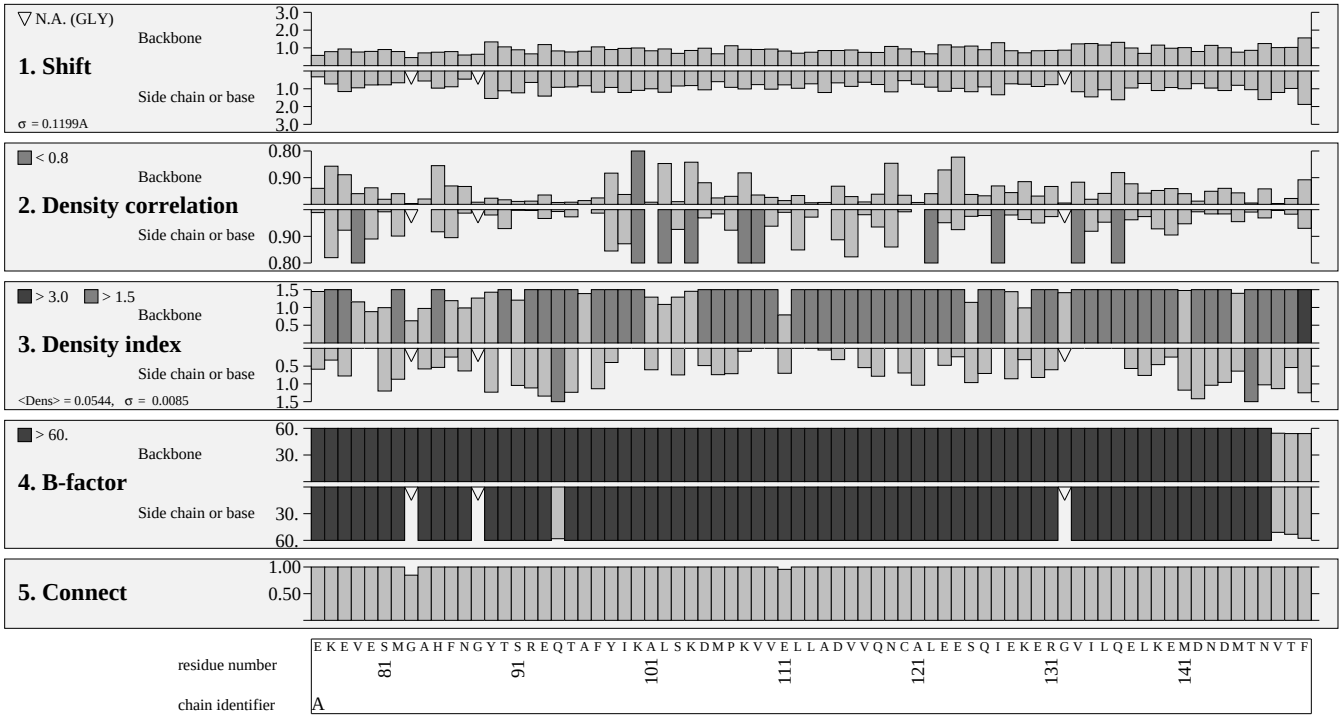
Local estimation





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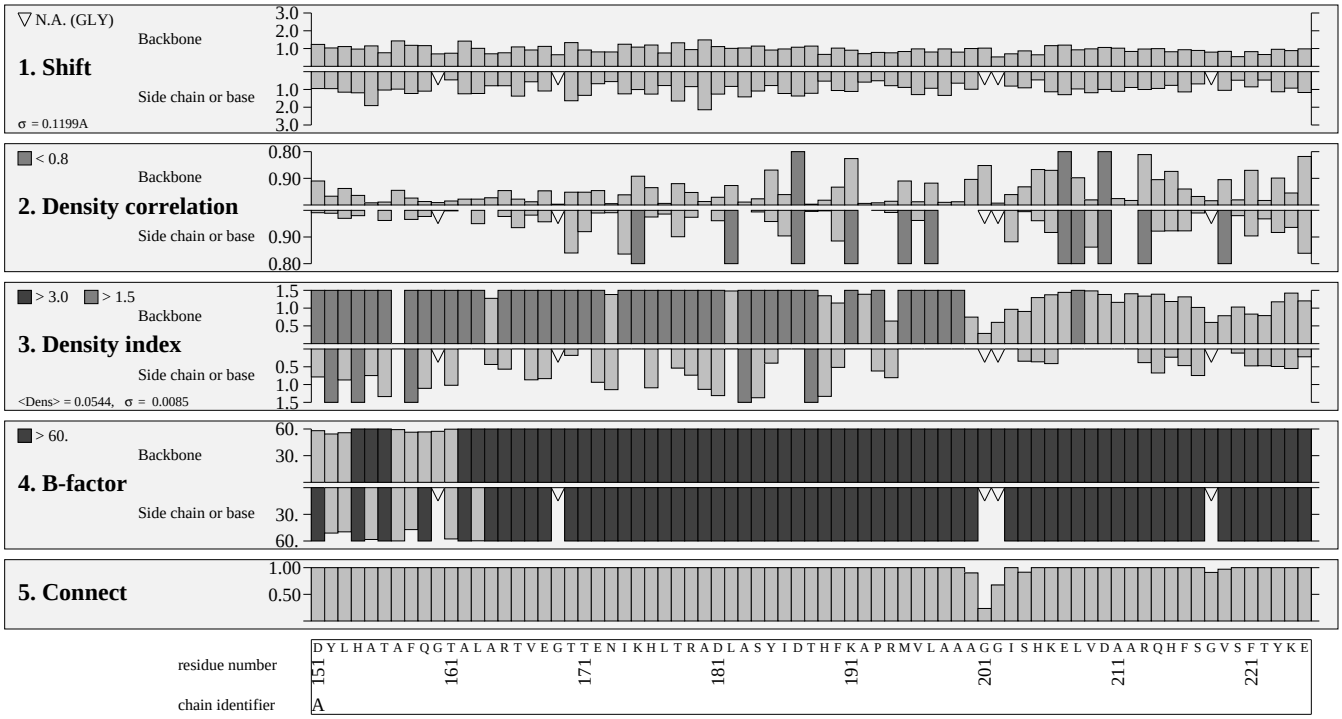
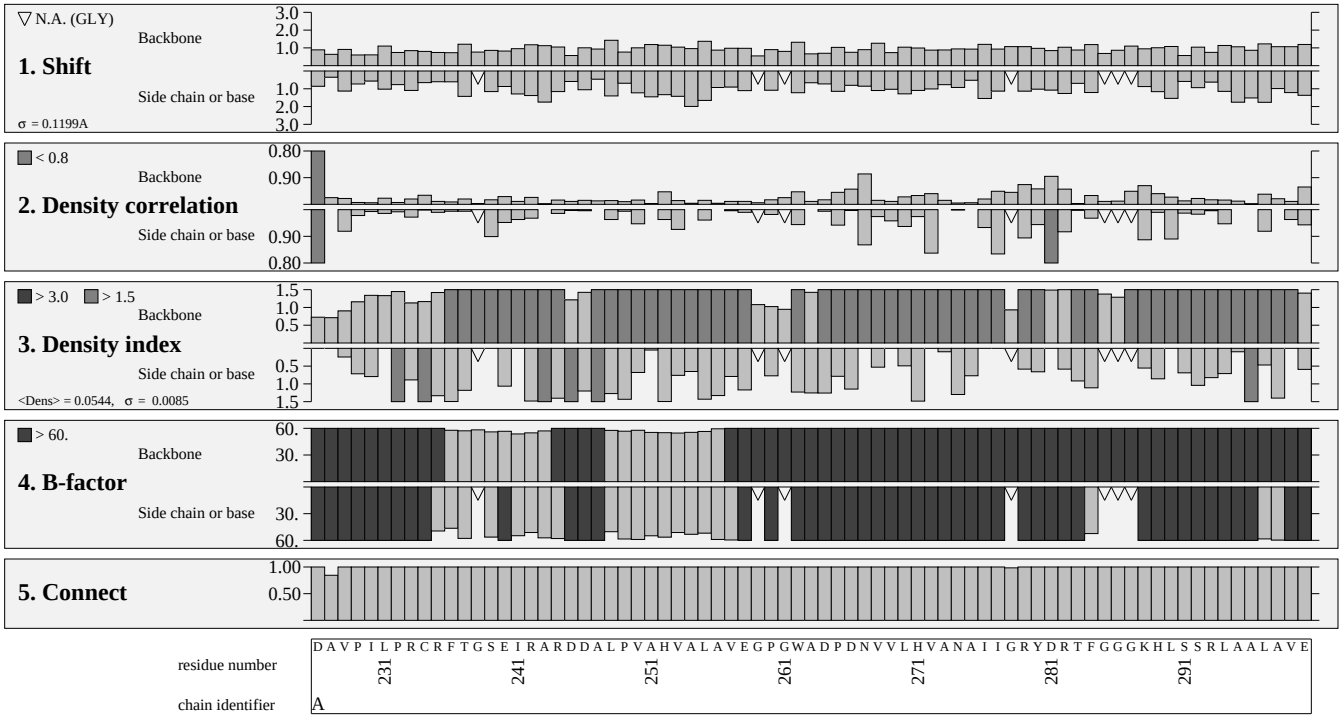
Structure Factor Check

3L73

Local estimation (2)





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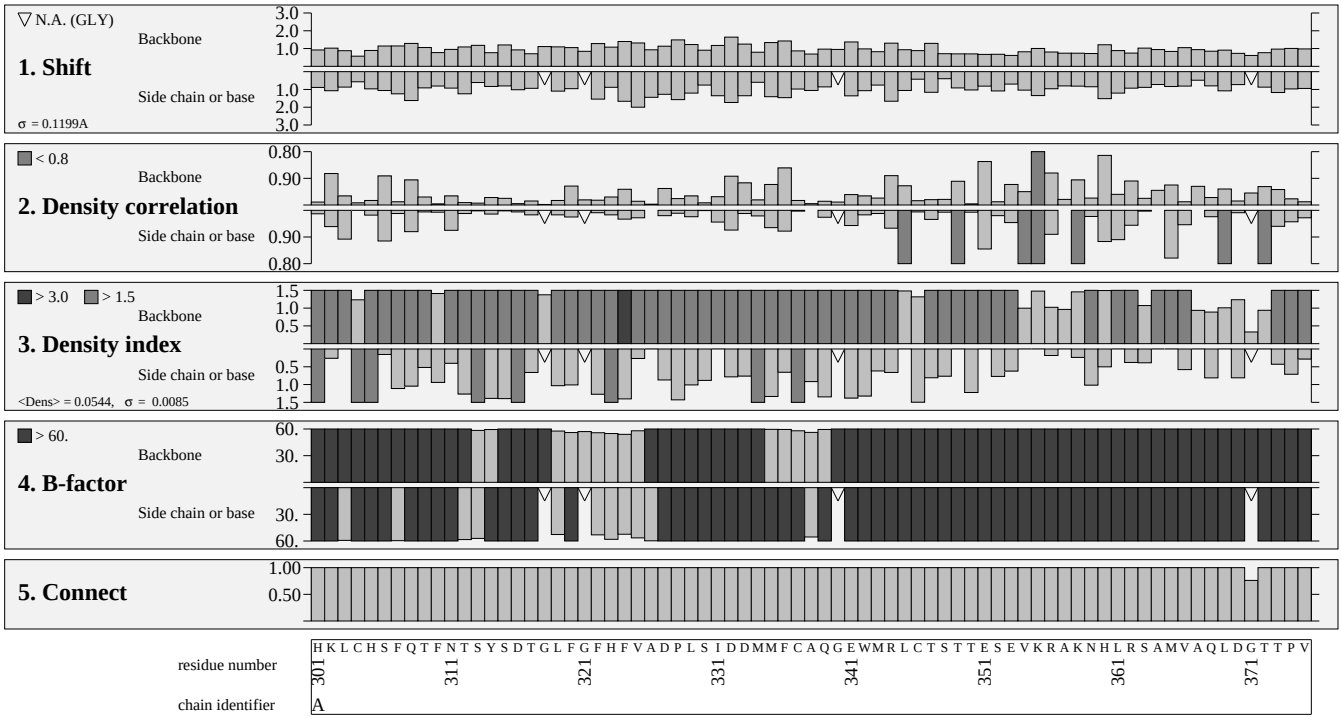
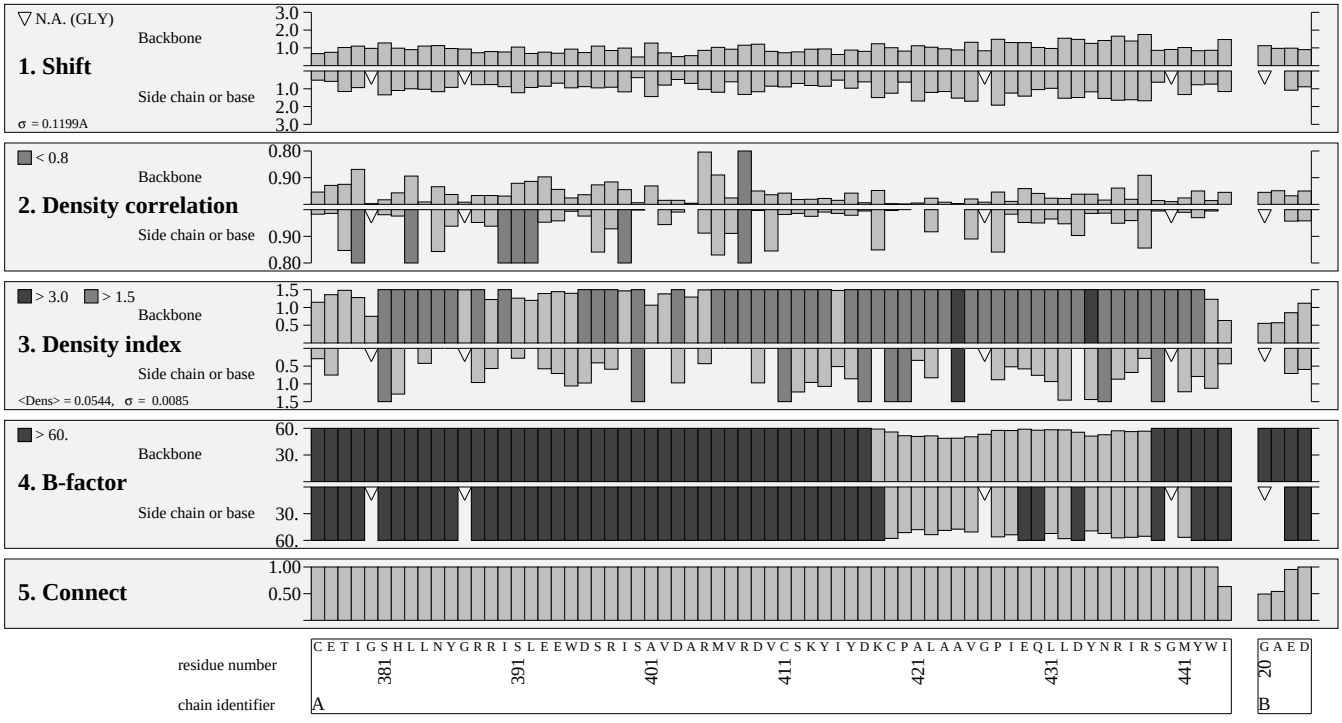
Structure Factor Check

3L73

Local estimation (3)





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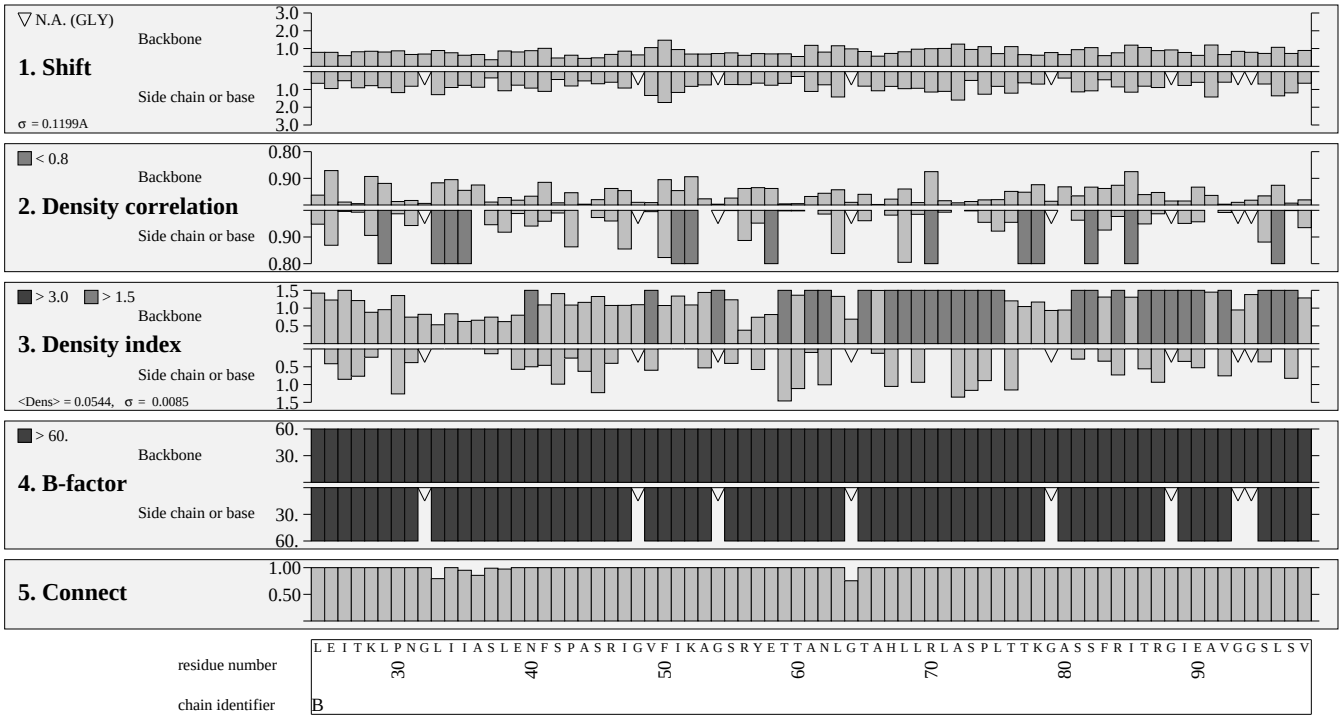
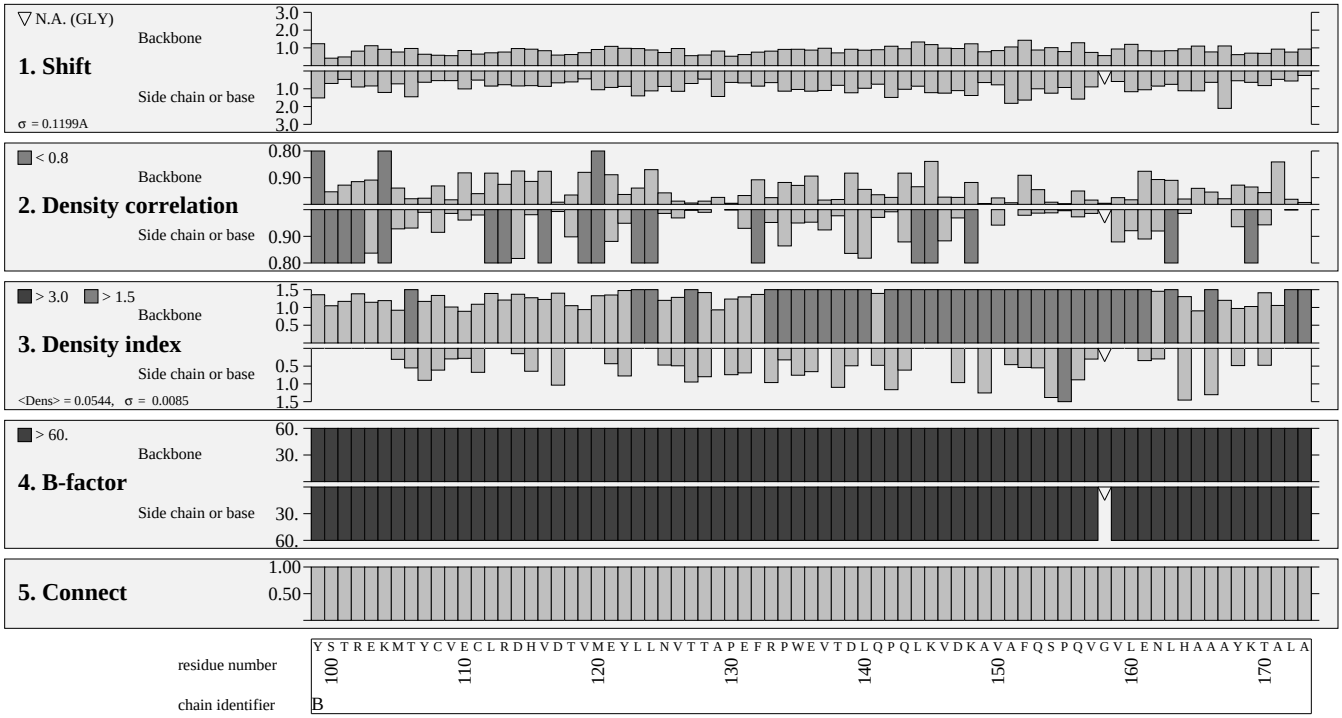
Structure Factor Check

3L73

Local estimation (4)

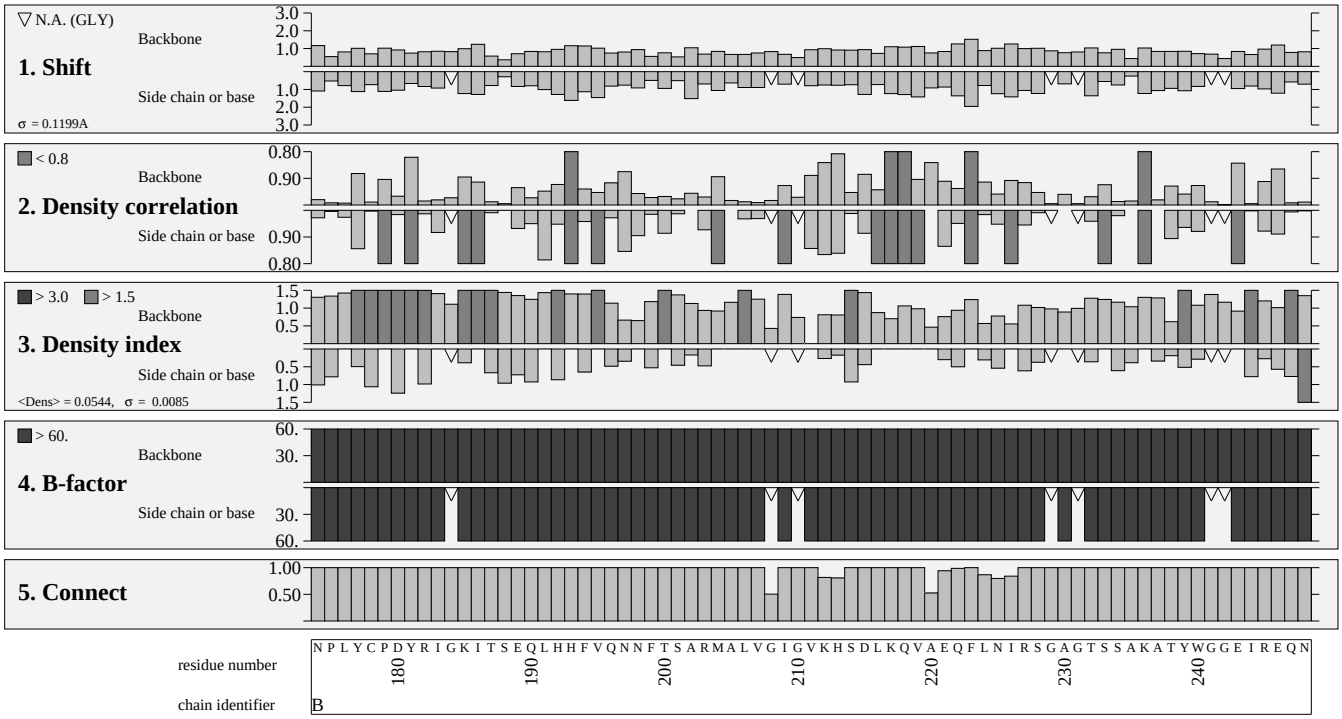


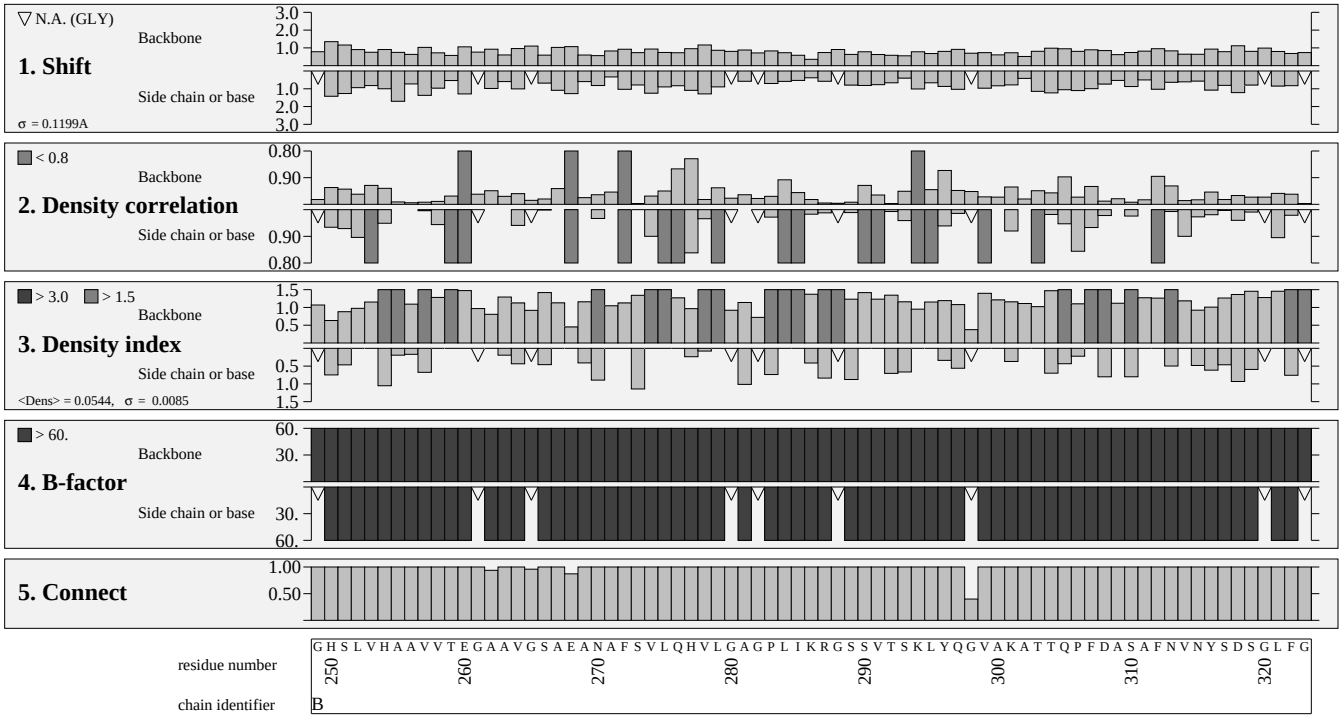


Structure Factor Check

3L73

Local estimation (5)



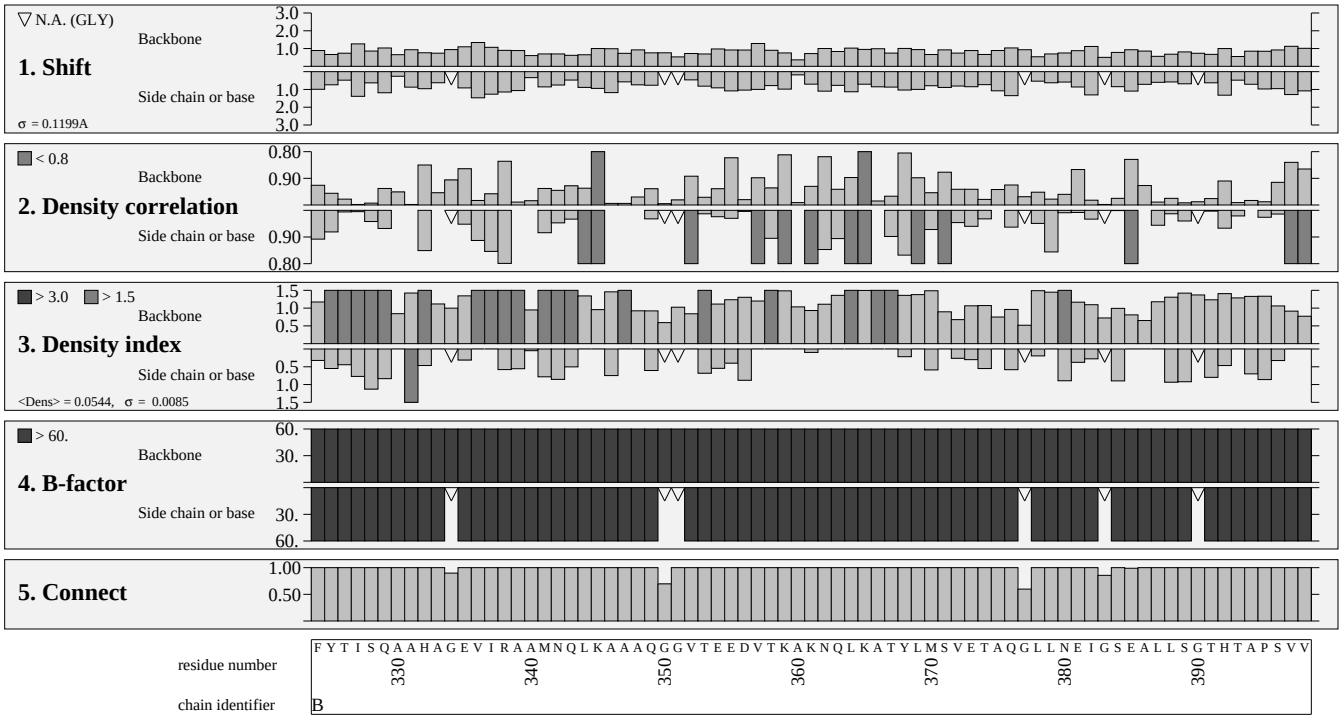


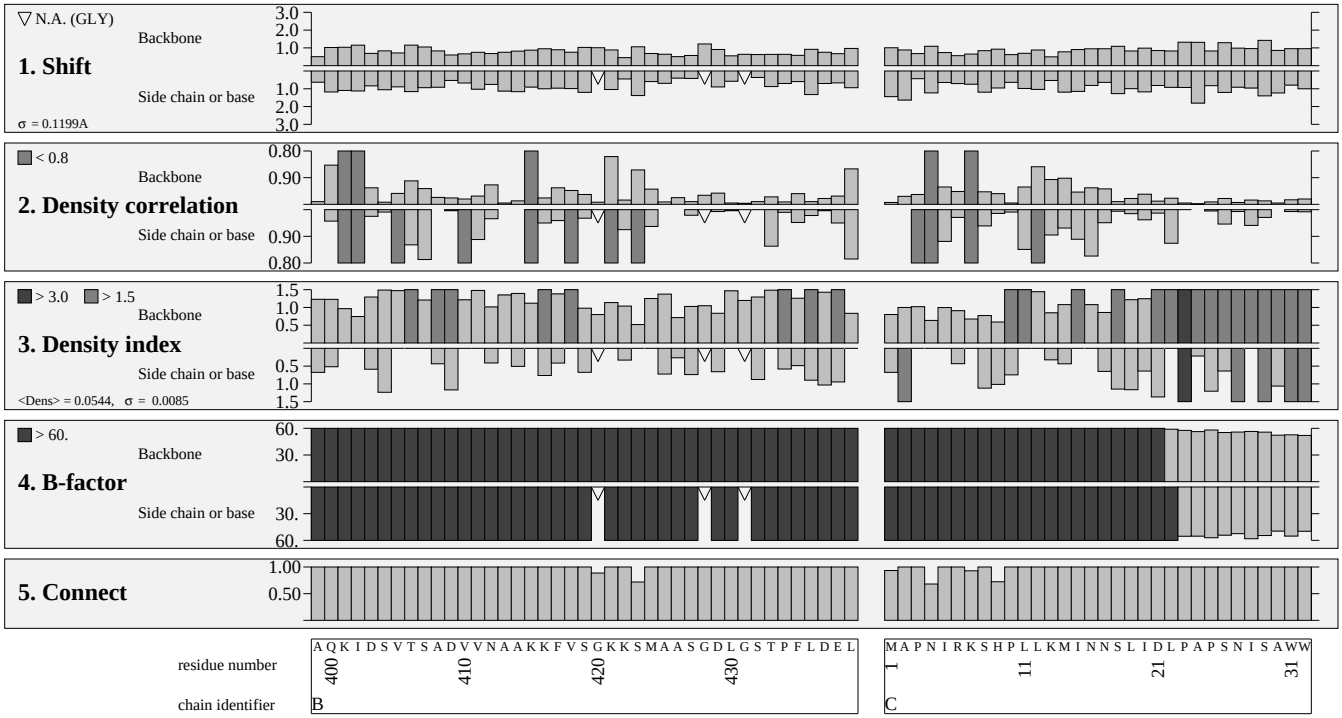
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (6)





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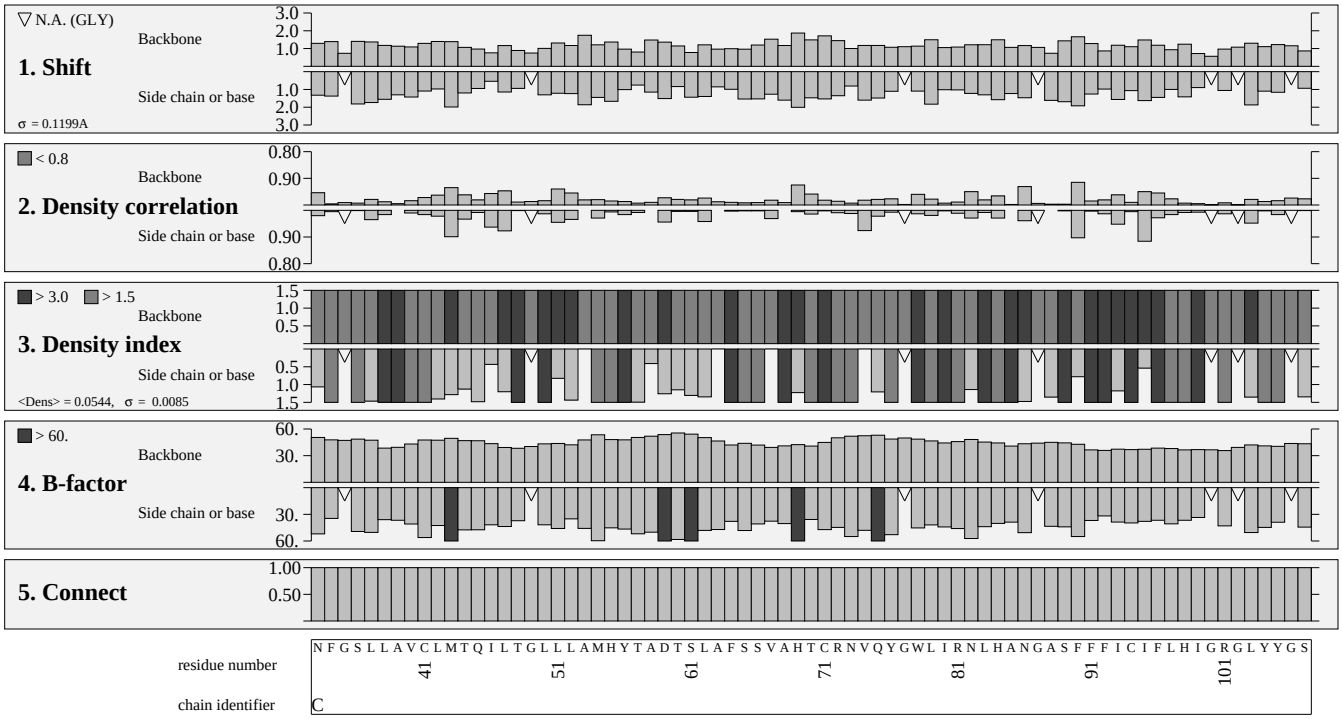
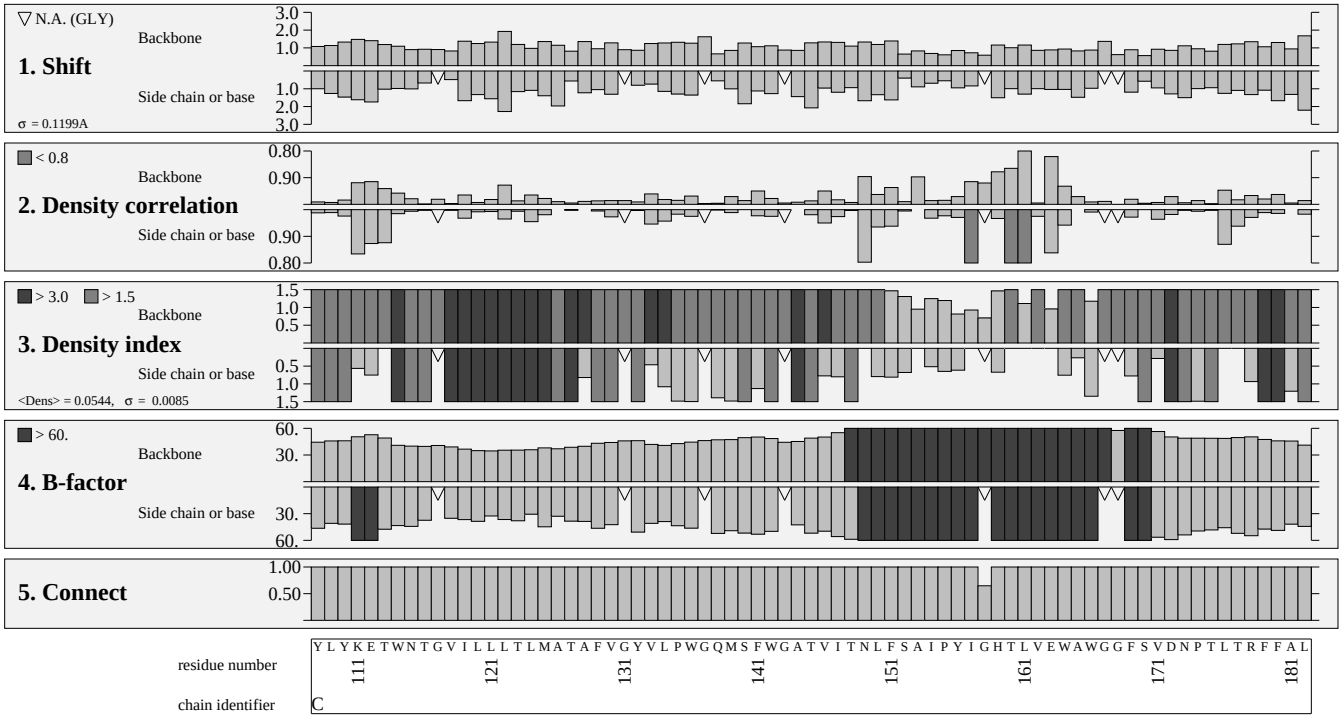
Structure Factor Check

3L73

Local estimation (7)





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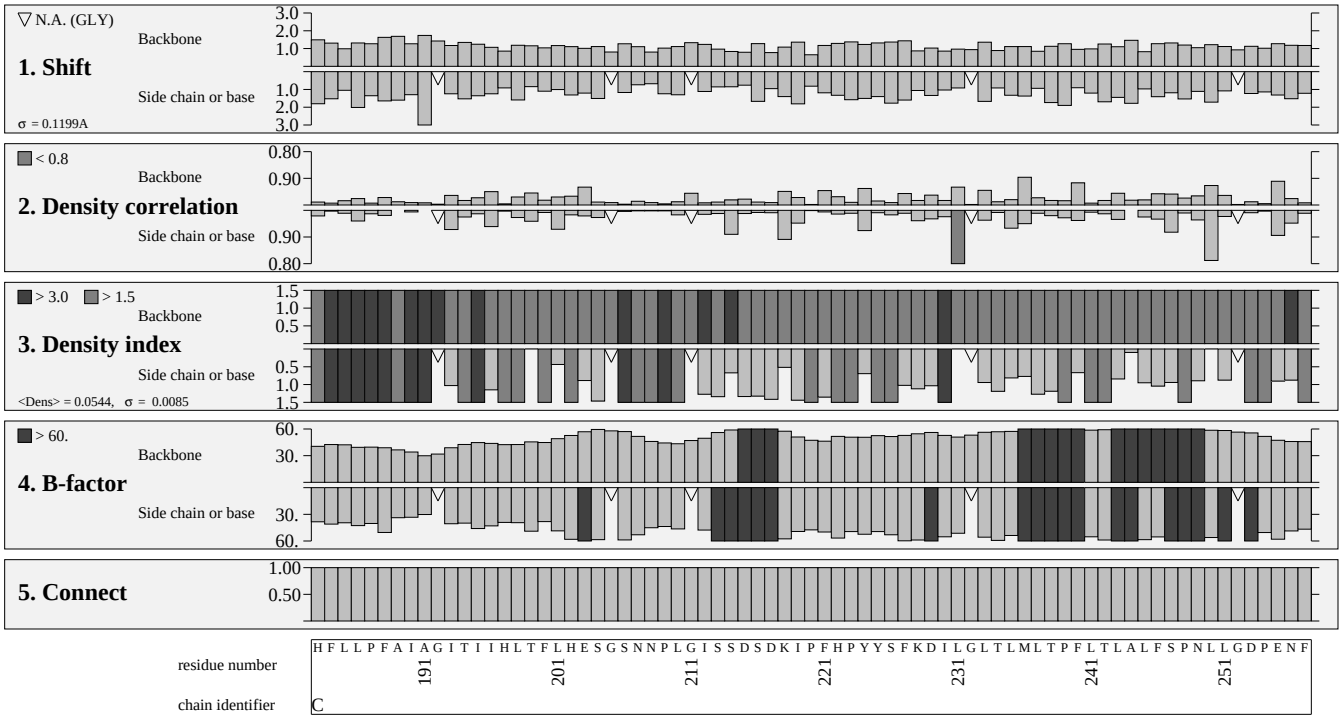
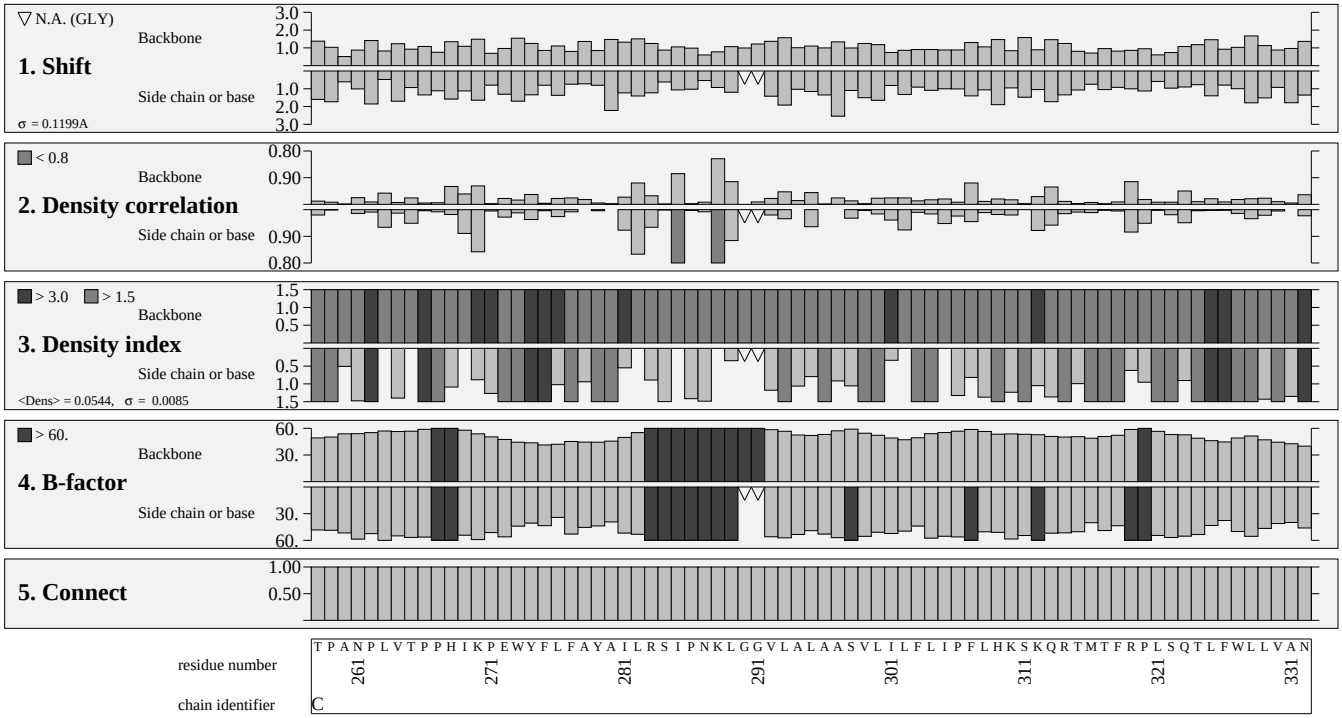
Structure Factor Check

3L73

Local estimation (8)





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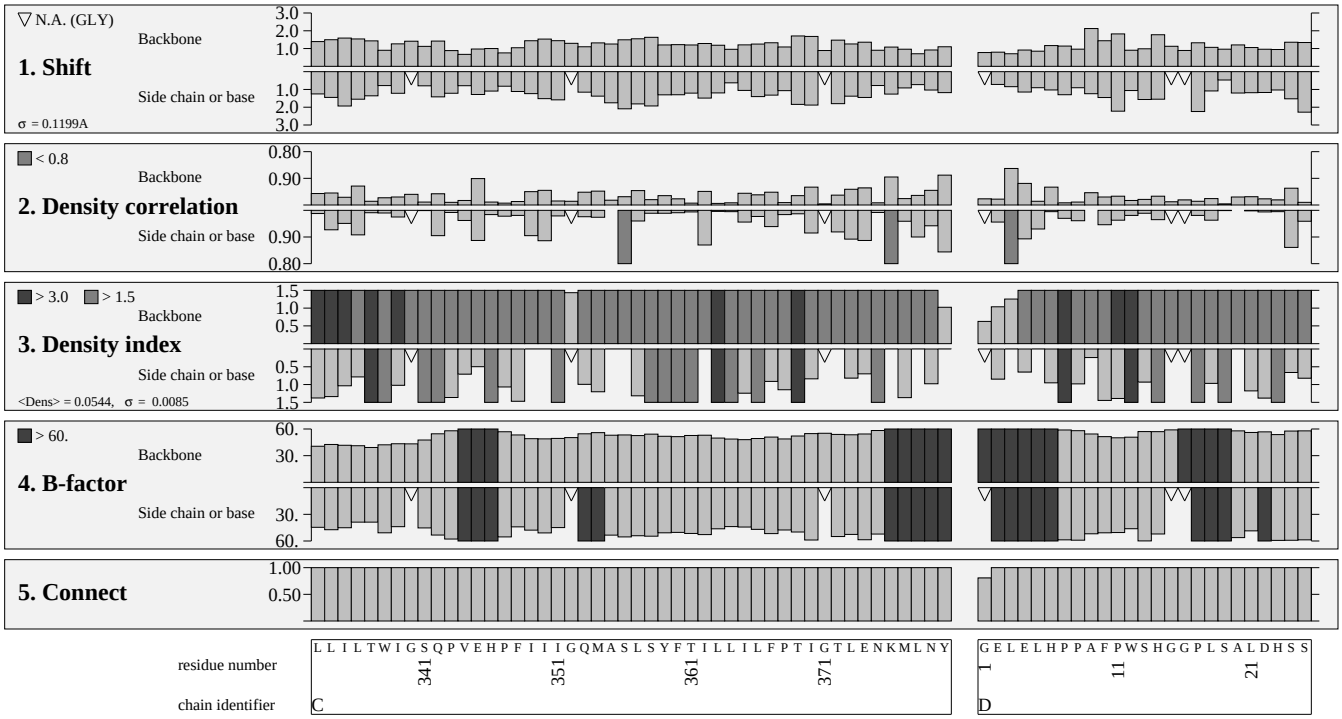
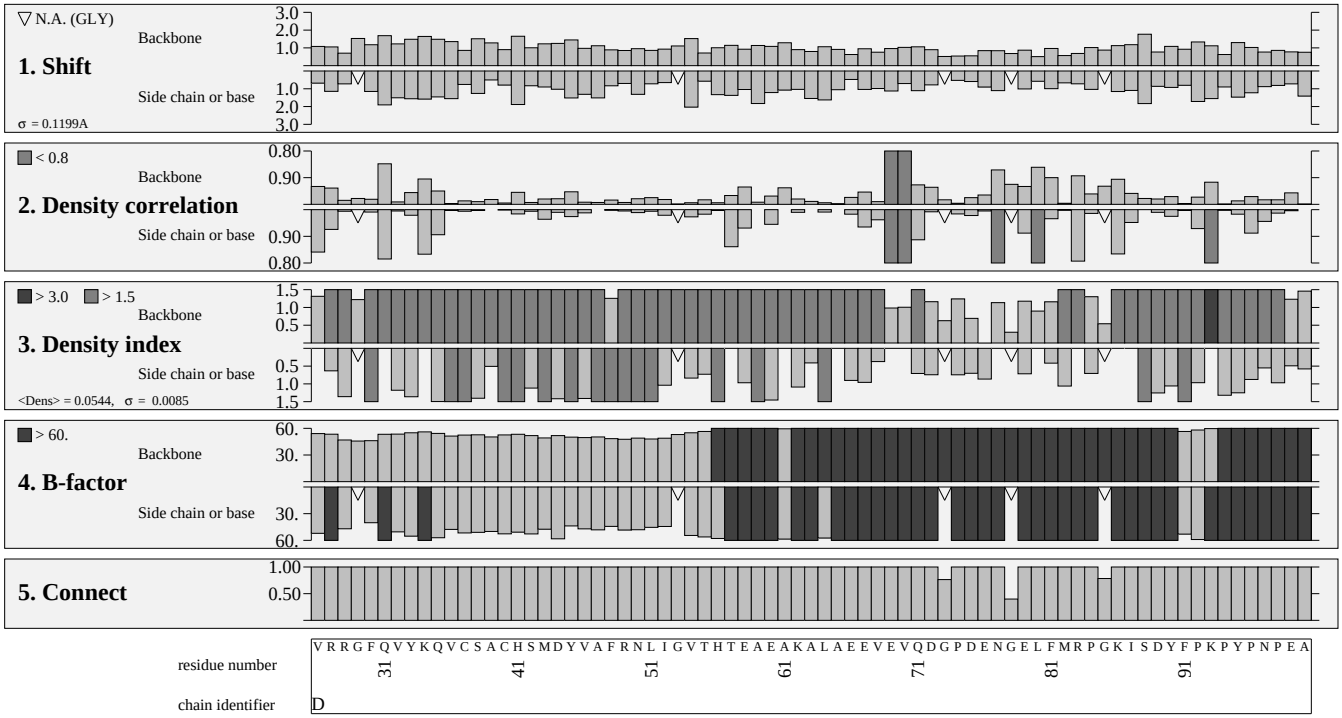
Structure Factor Check

3L73

Local estimation (9)

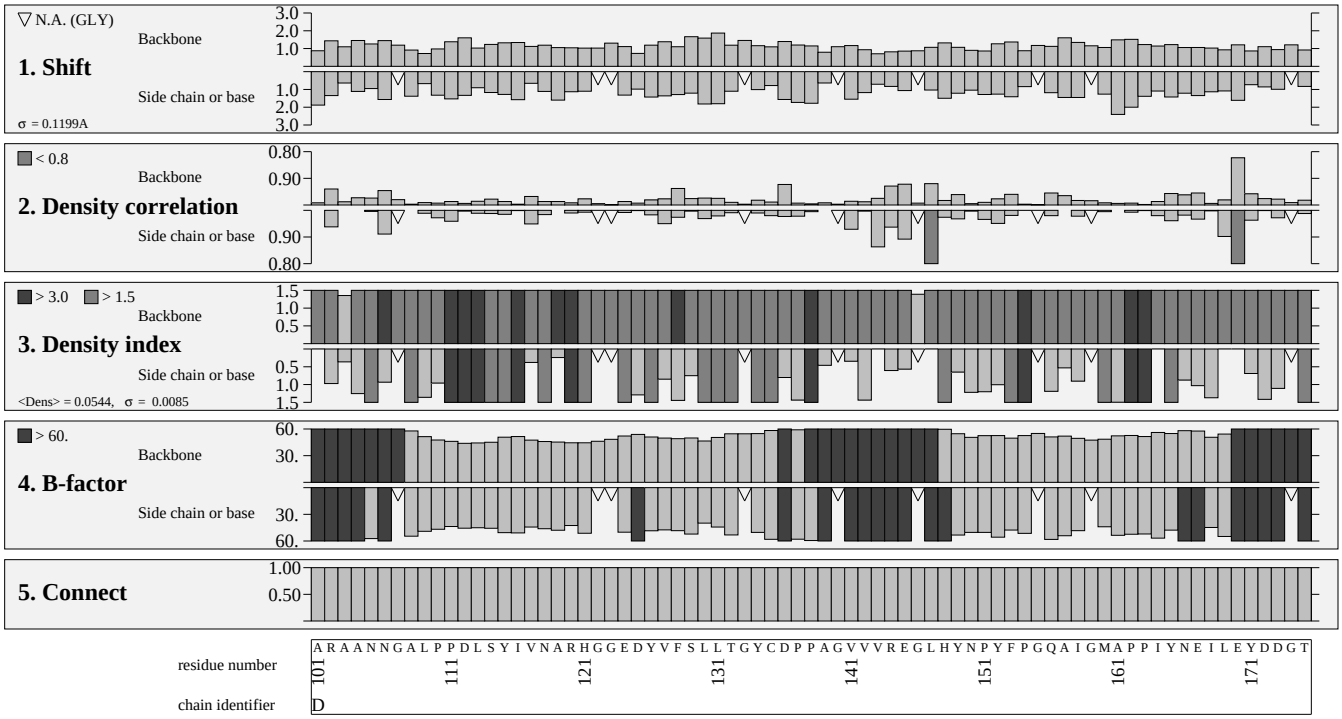


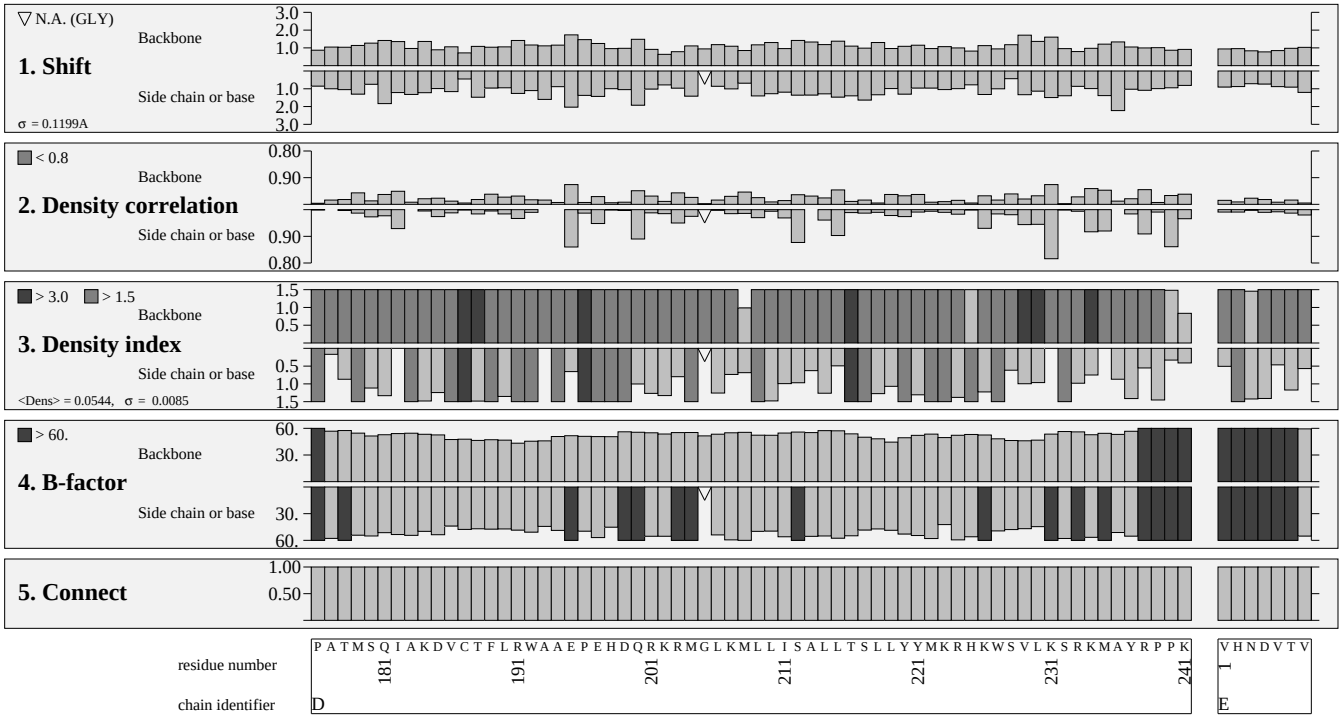


Structure Factor Check

3L73

Local estimation (10)





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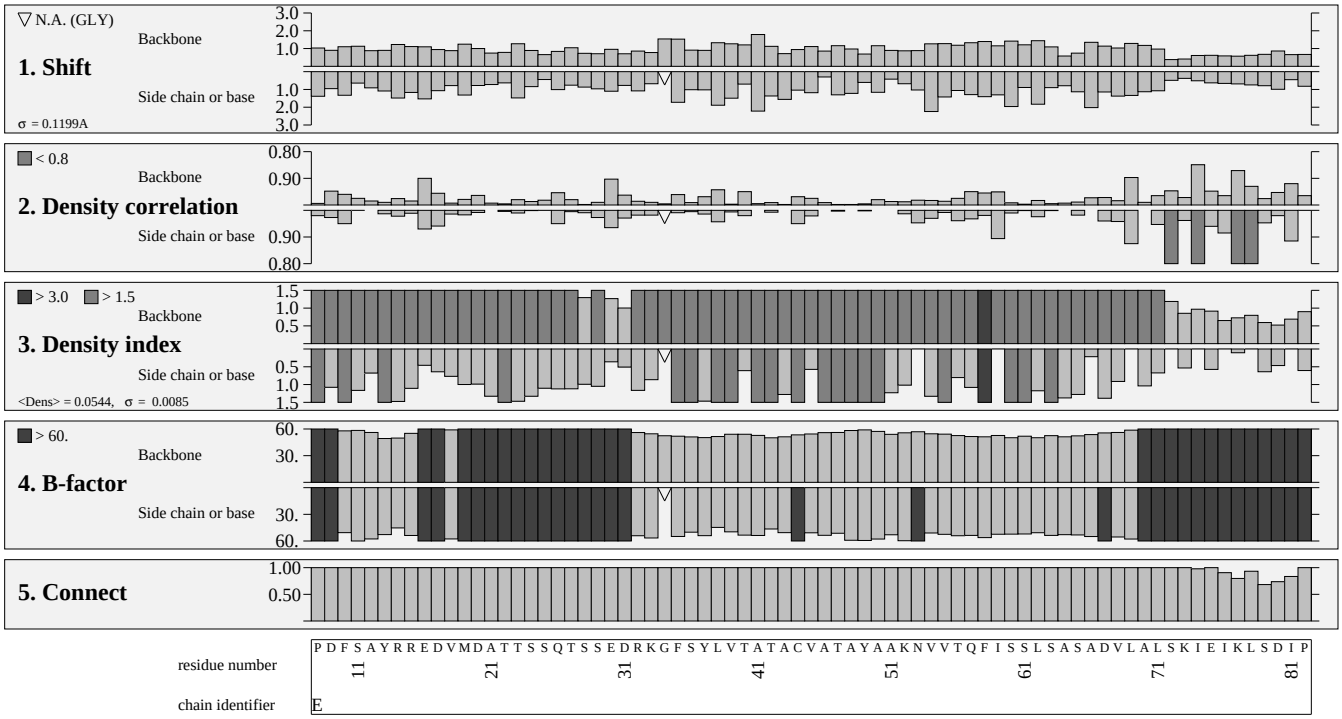
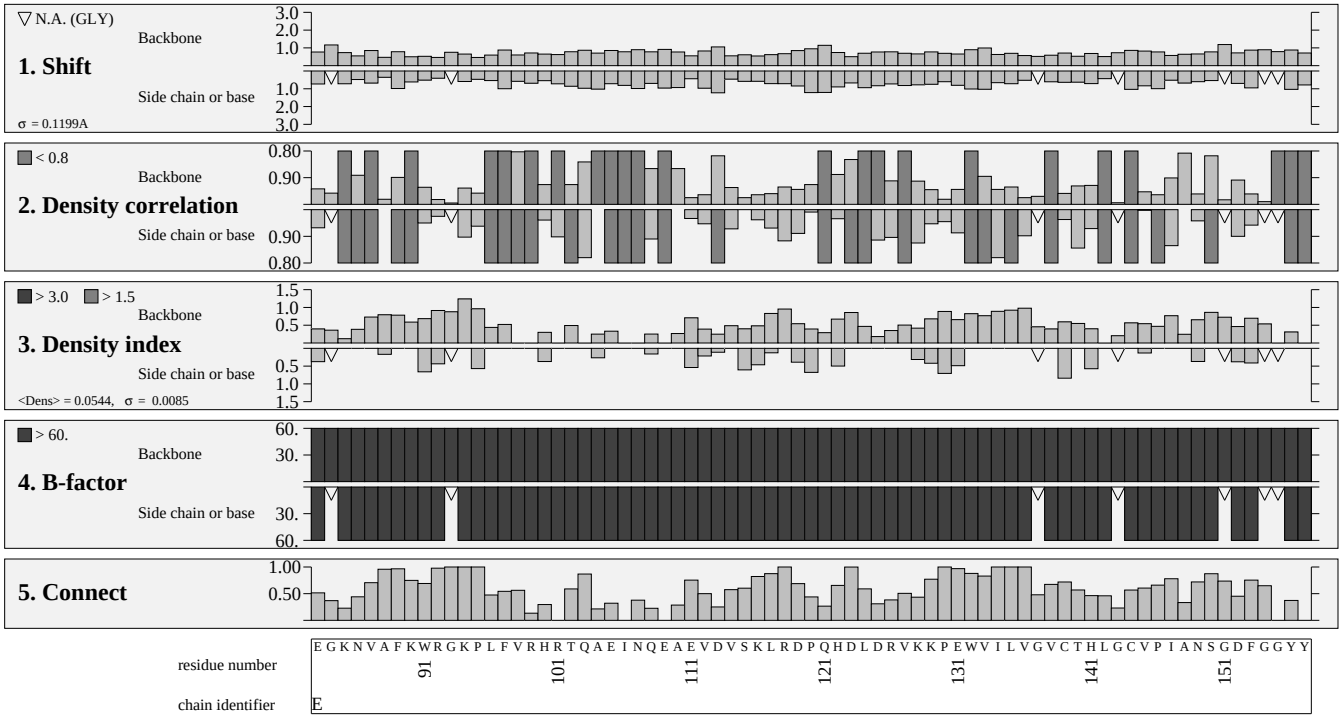
Structure Factor Check

3L73

Local estimation (11)



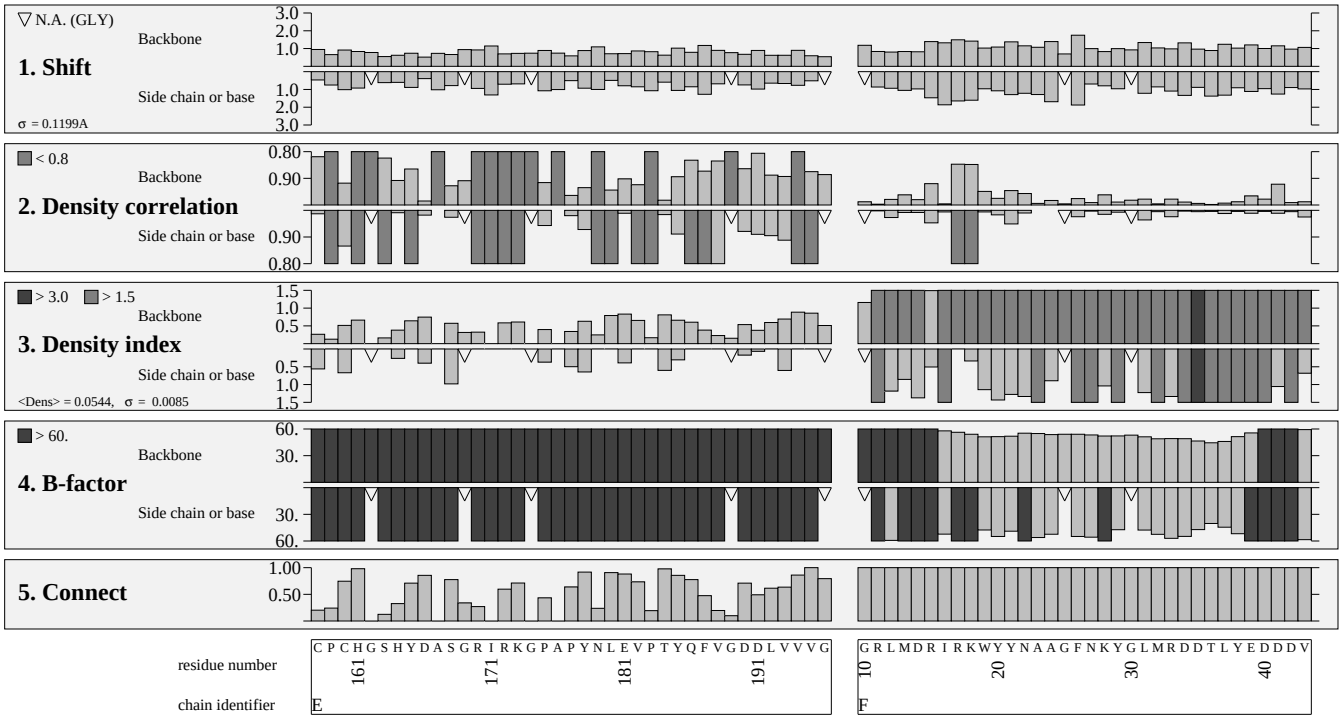


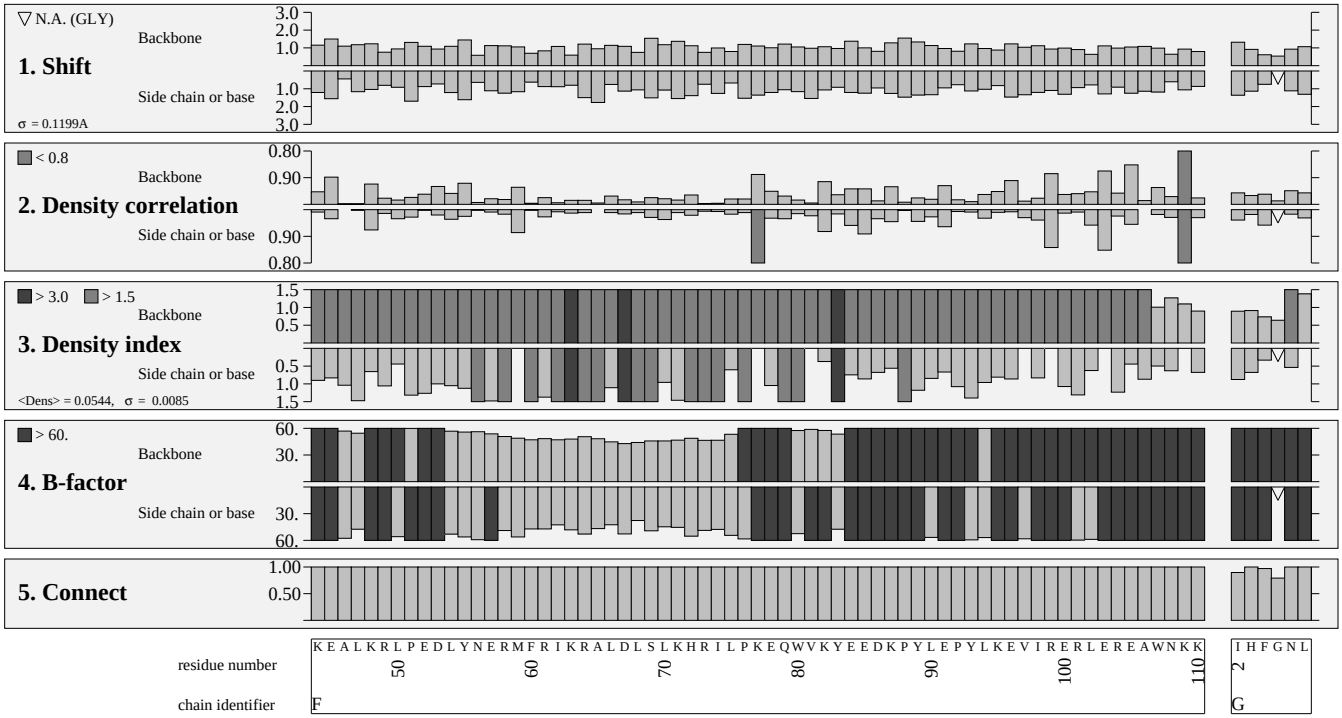
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (12)



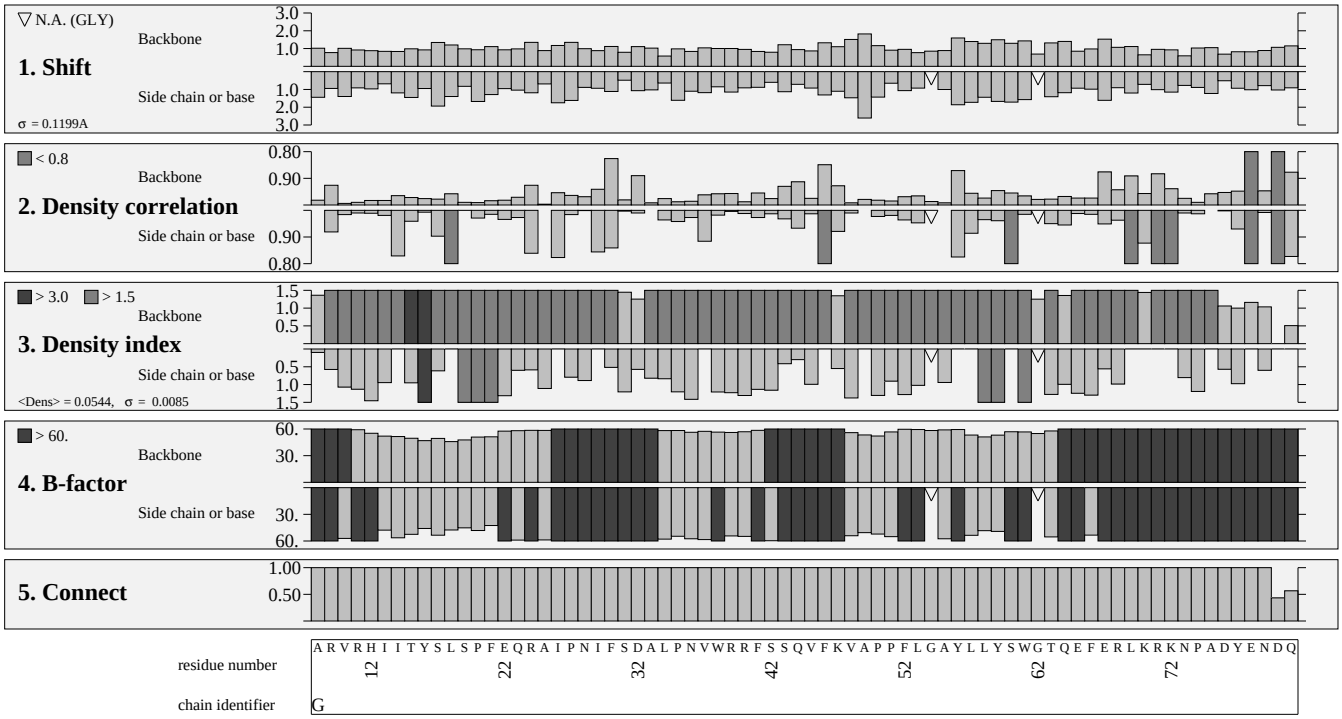


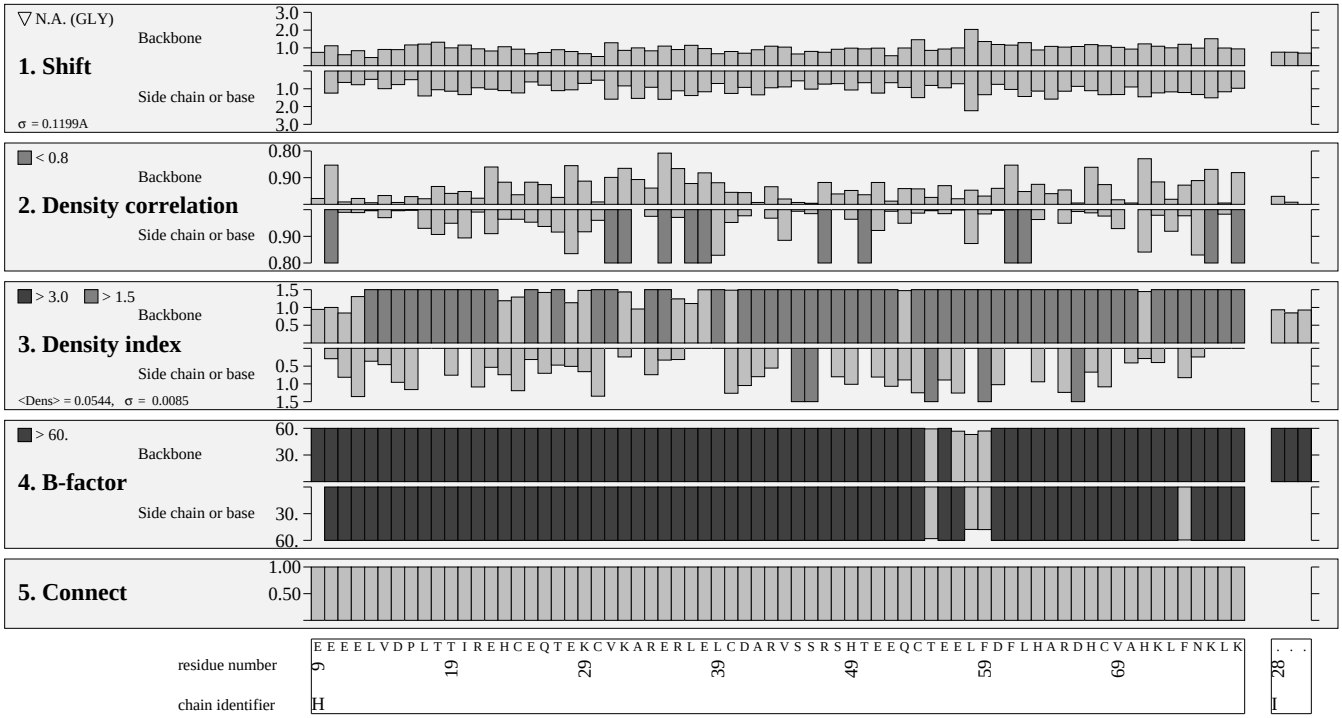
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (13)



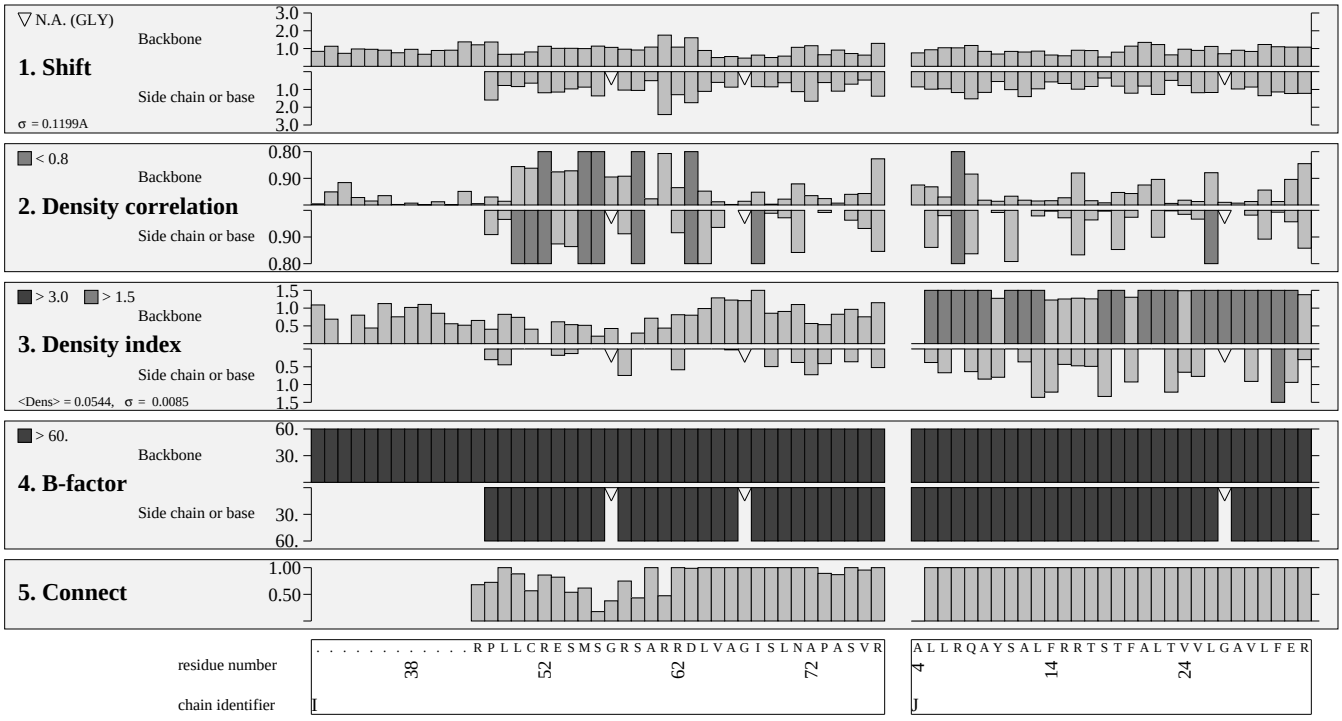


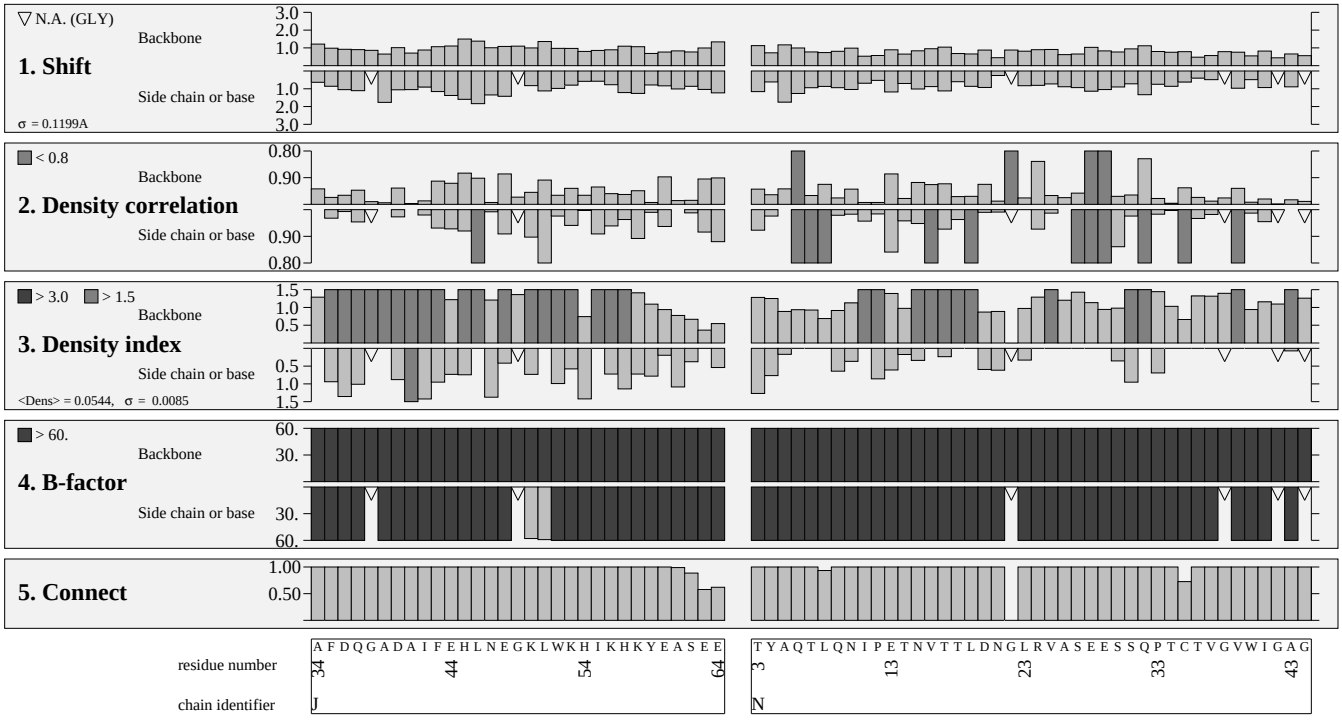
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (14)



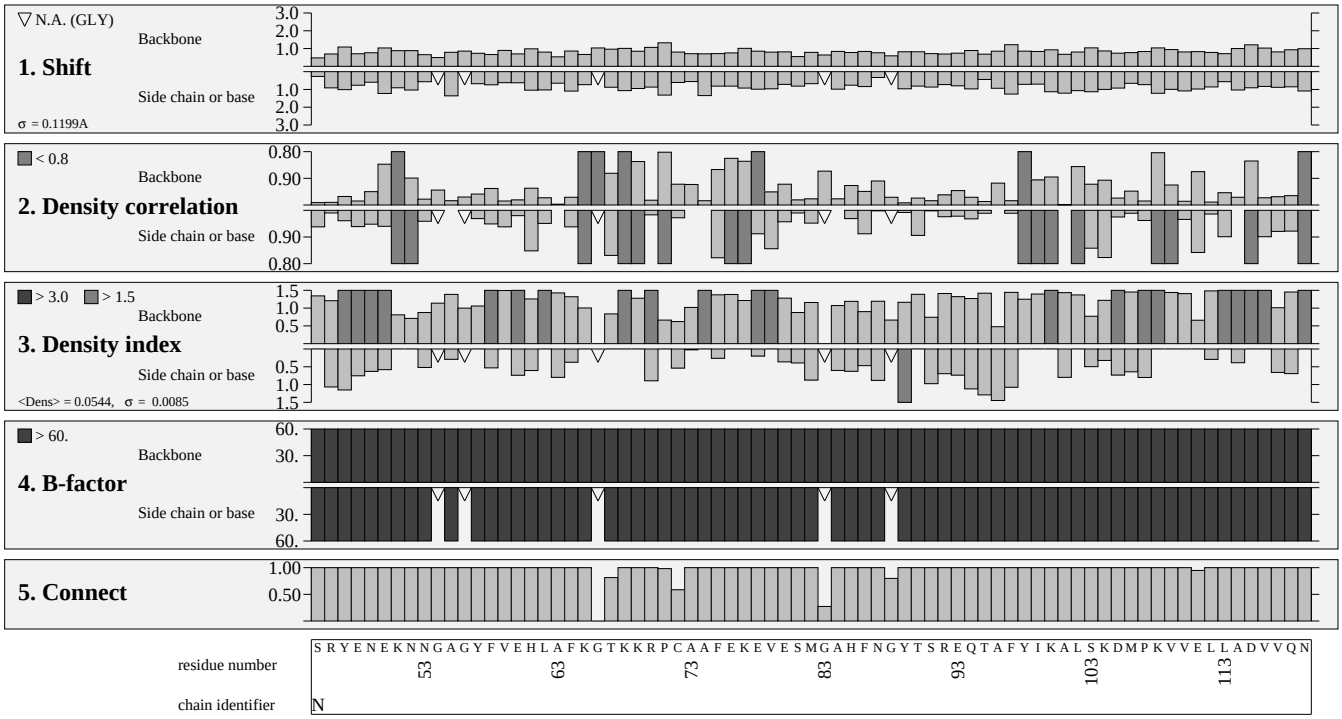


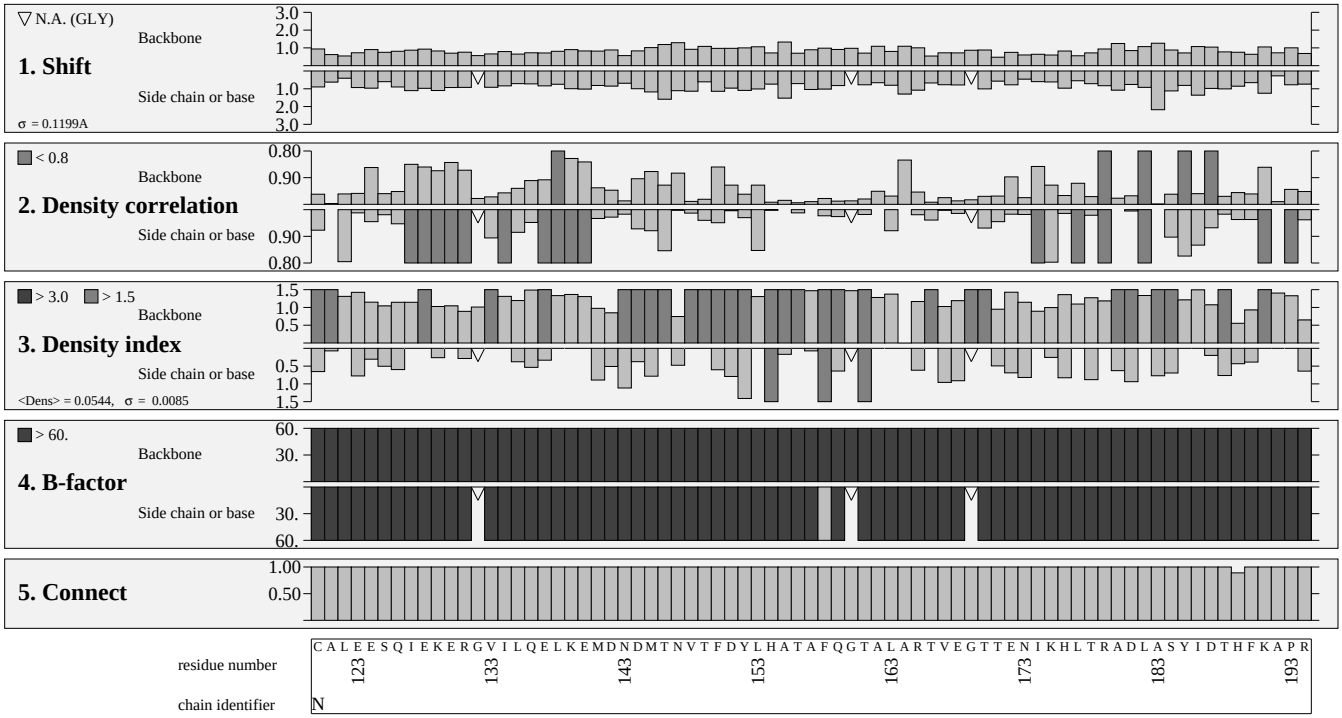
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (15)





SFCHECK 7.1.01

Structure Factor Check

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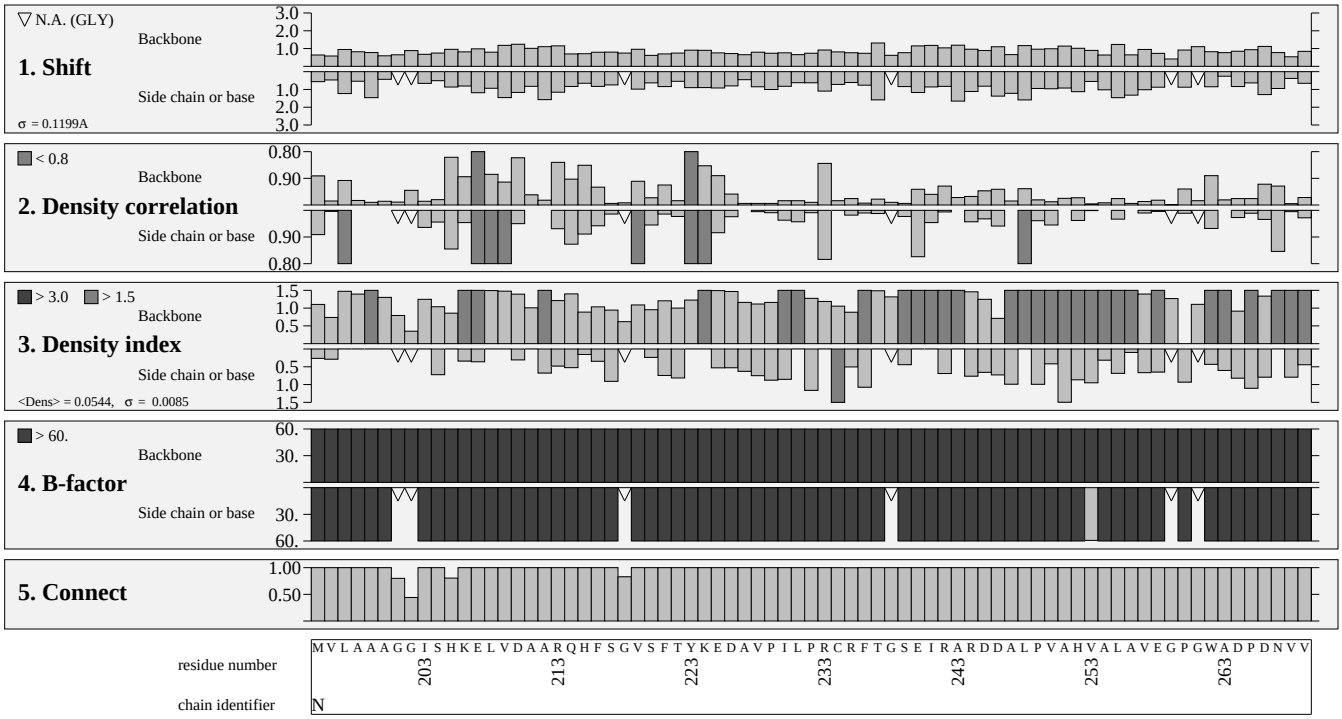
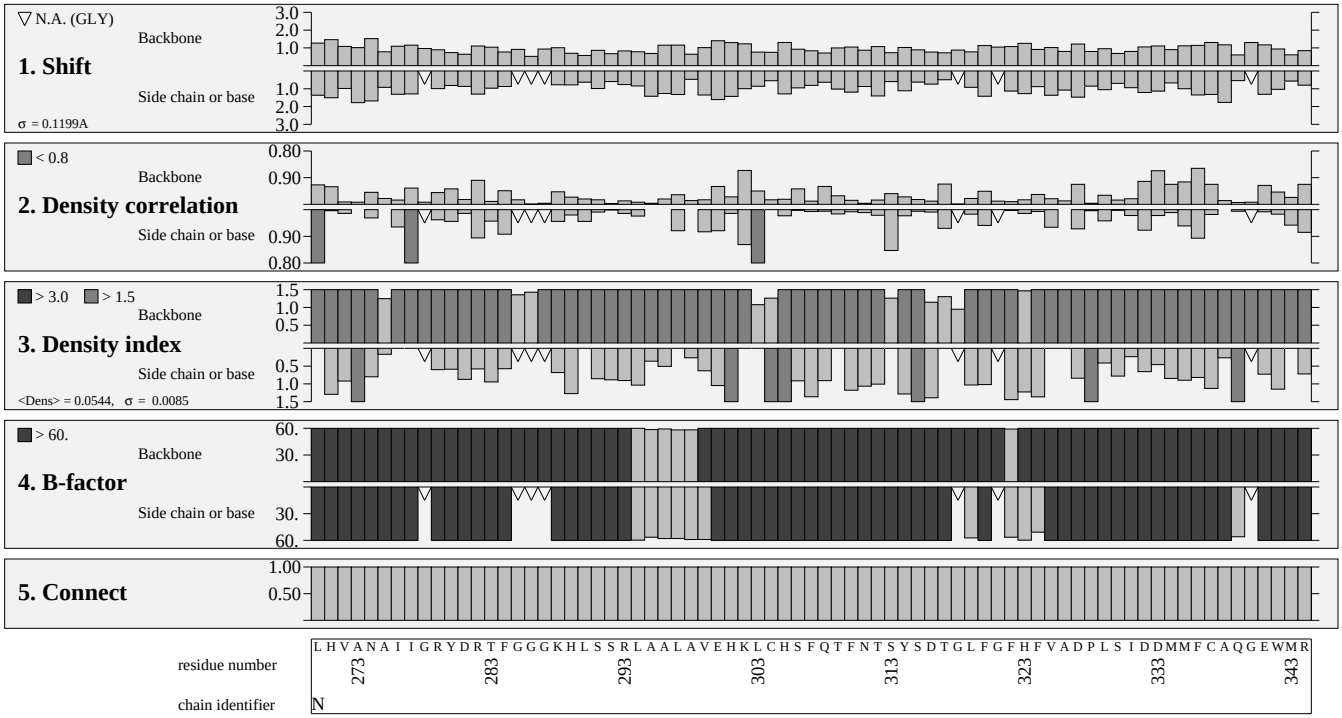
Local estimation (16)





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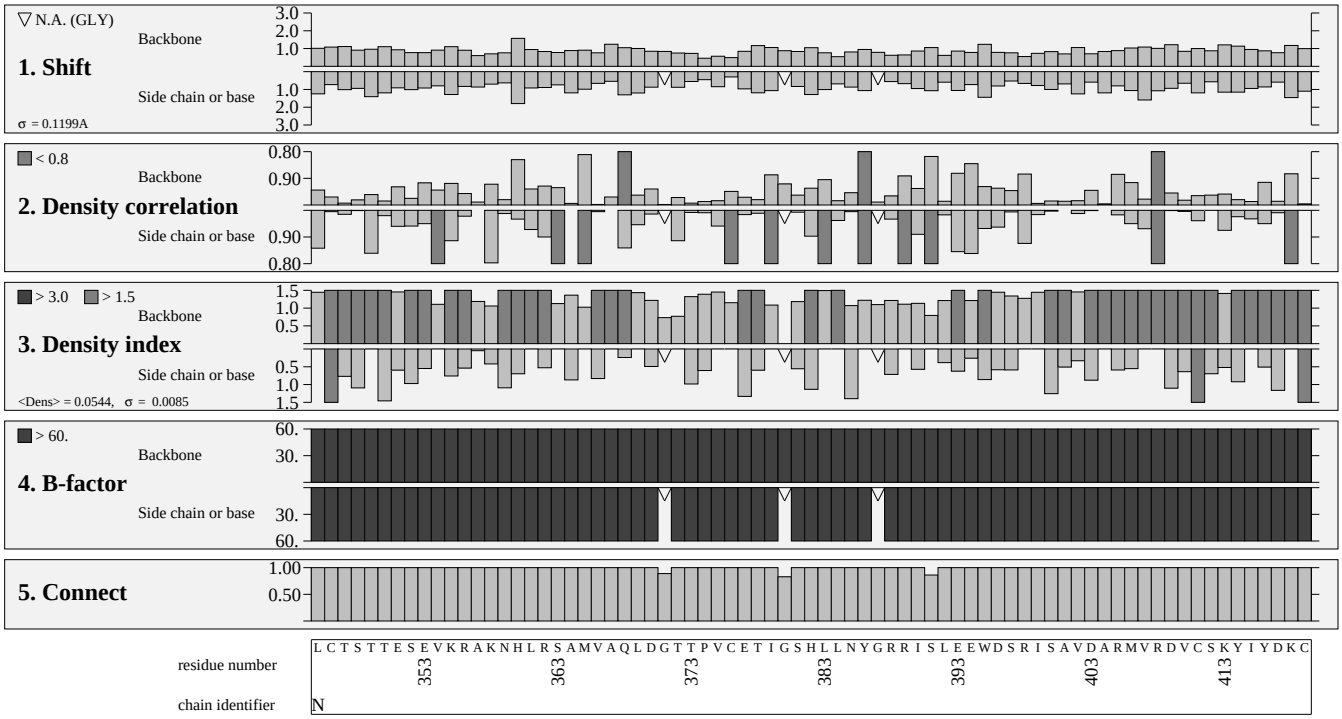
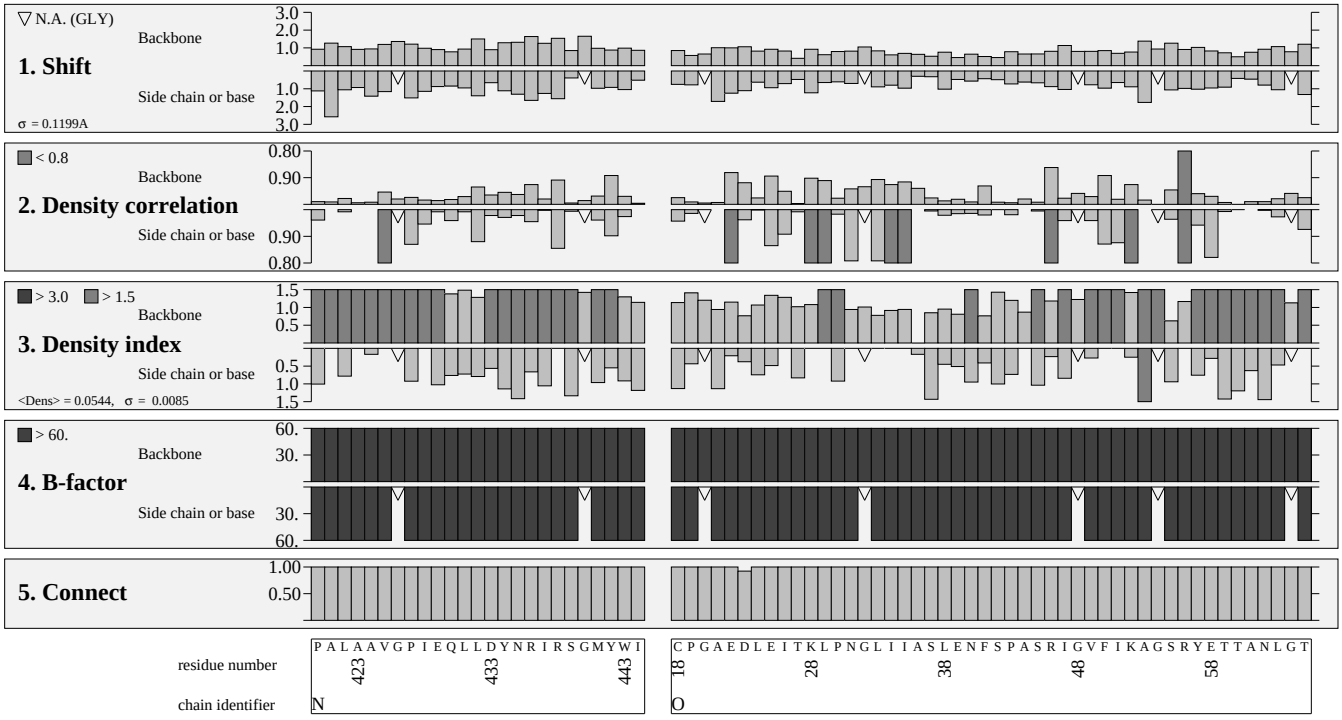
Structure Factor Check

3L73

Local estimation (17)

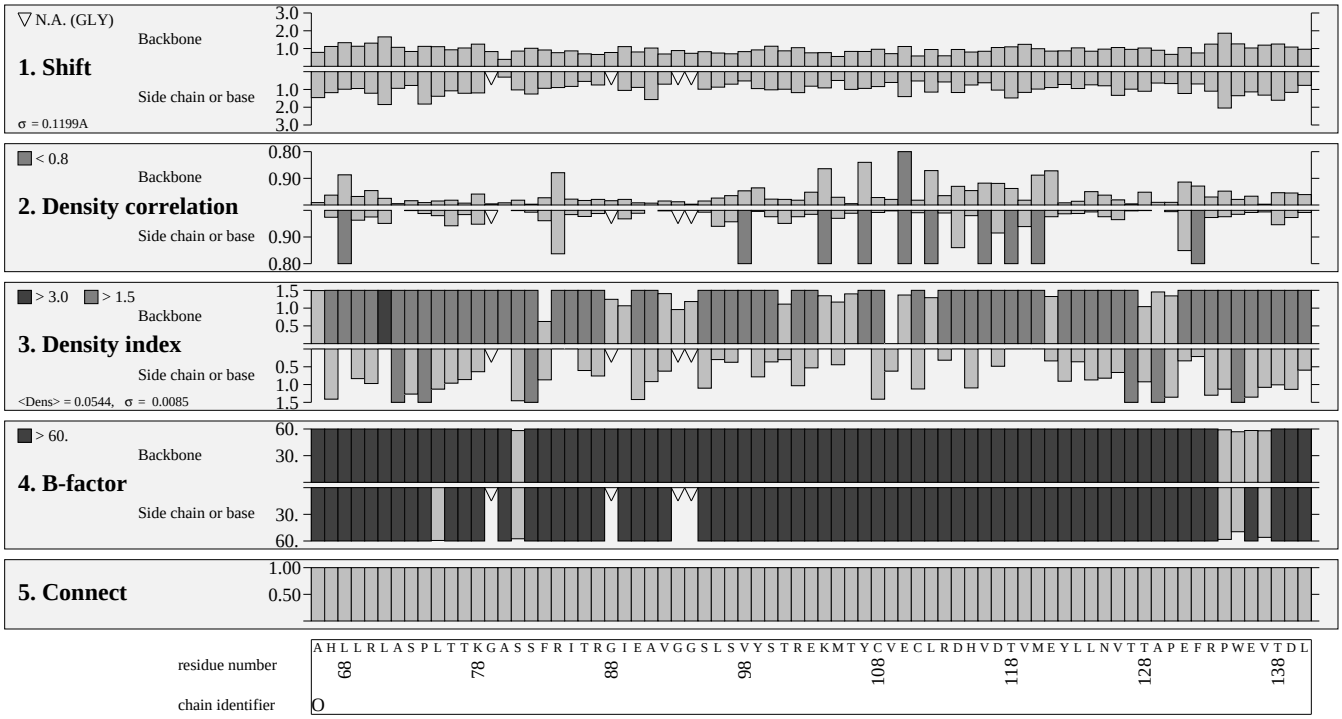


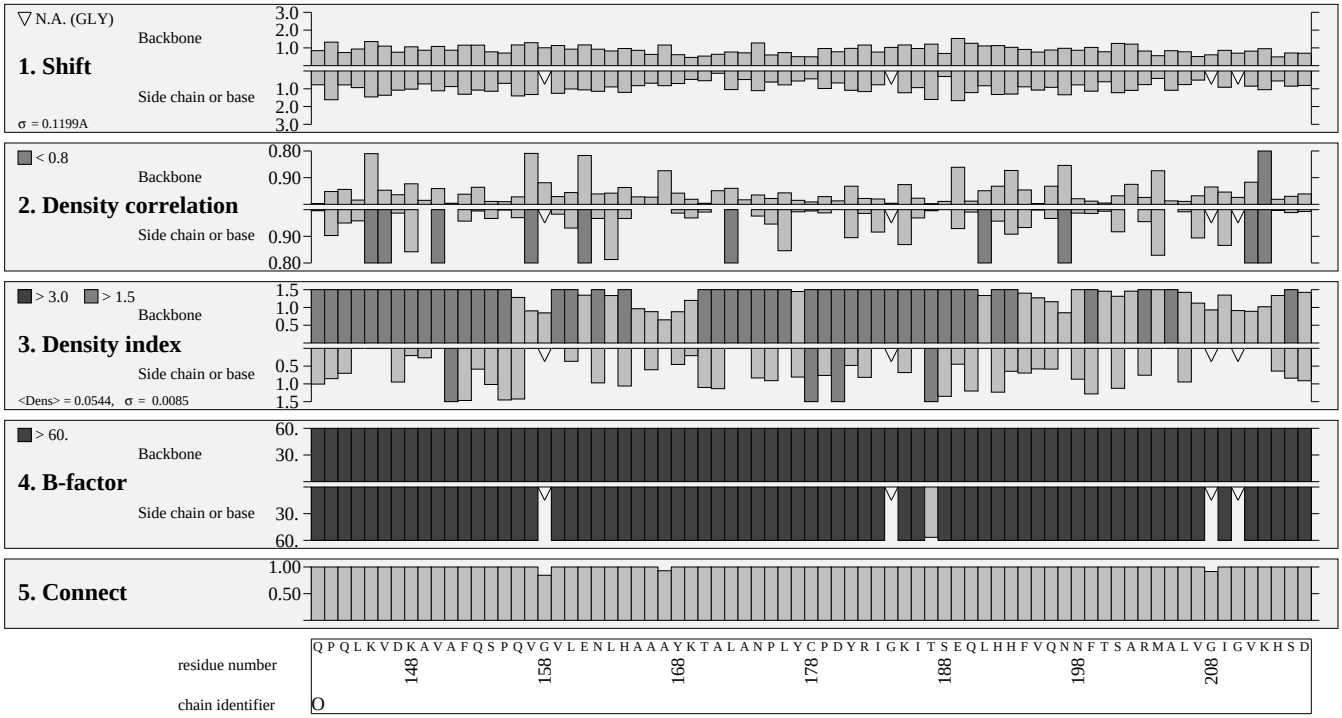


Structure Factor Check

3L73

Local estimation (18)





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Structure Factor Check

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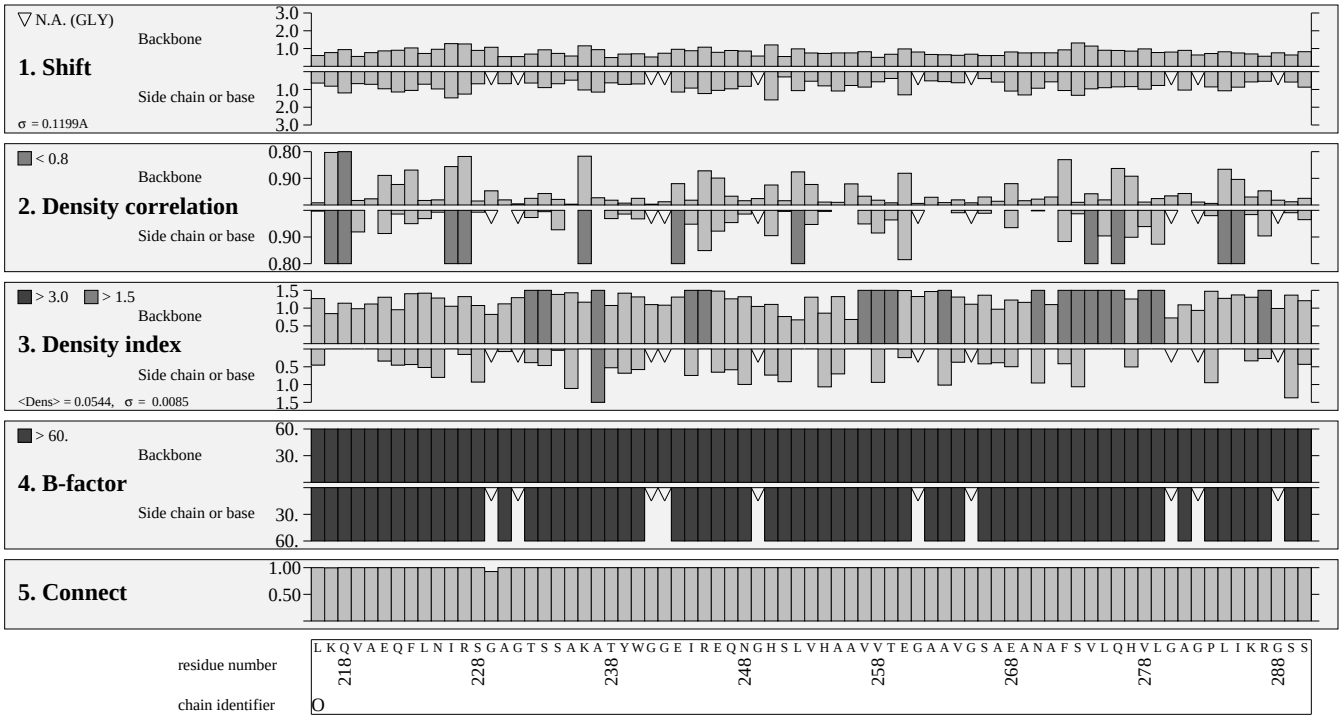
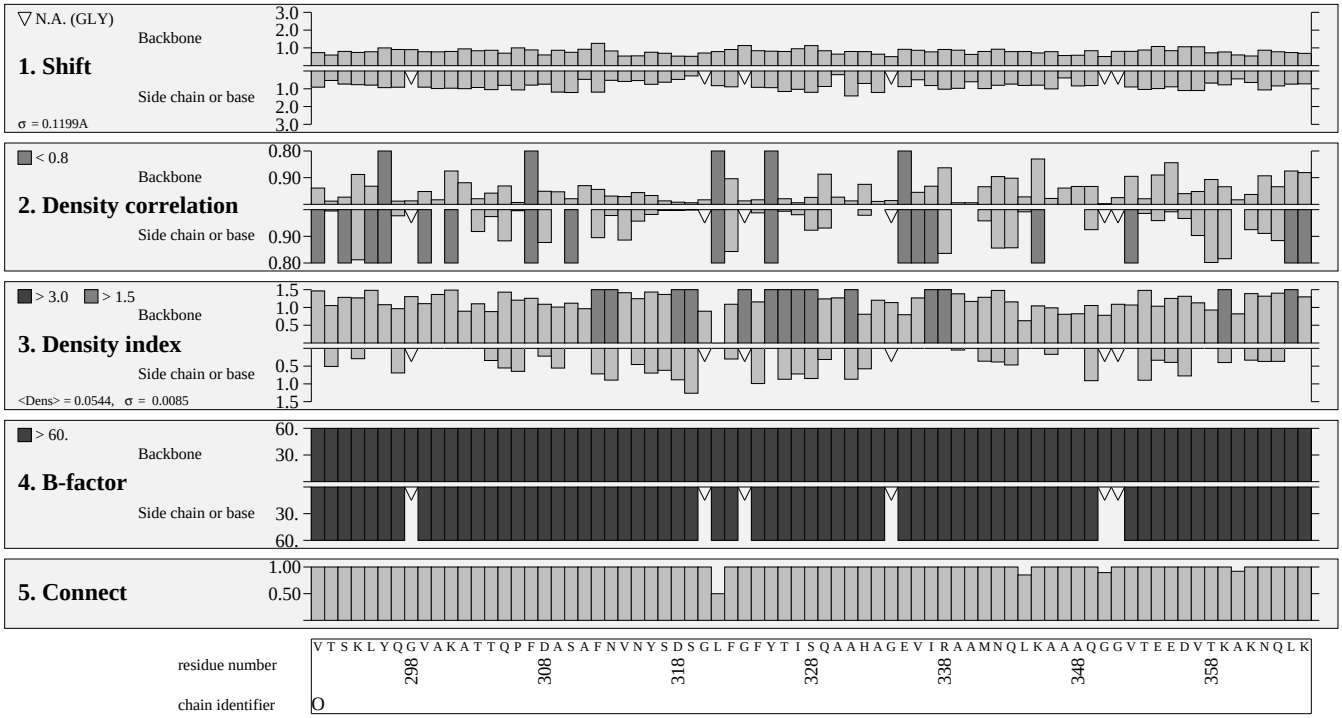
Local estimation (19)



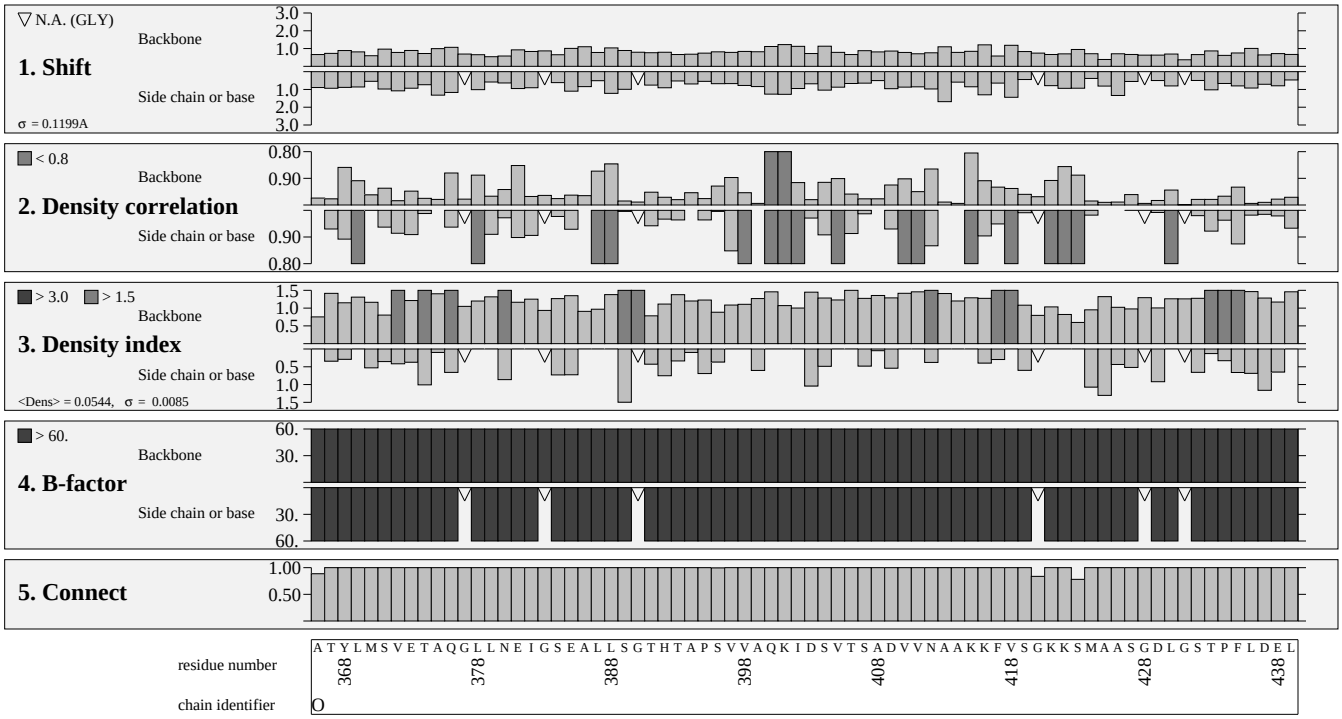


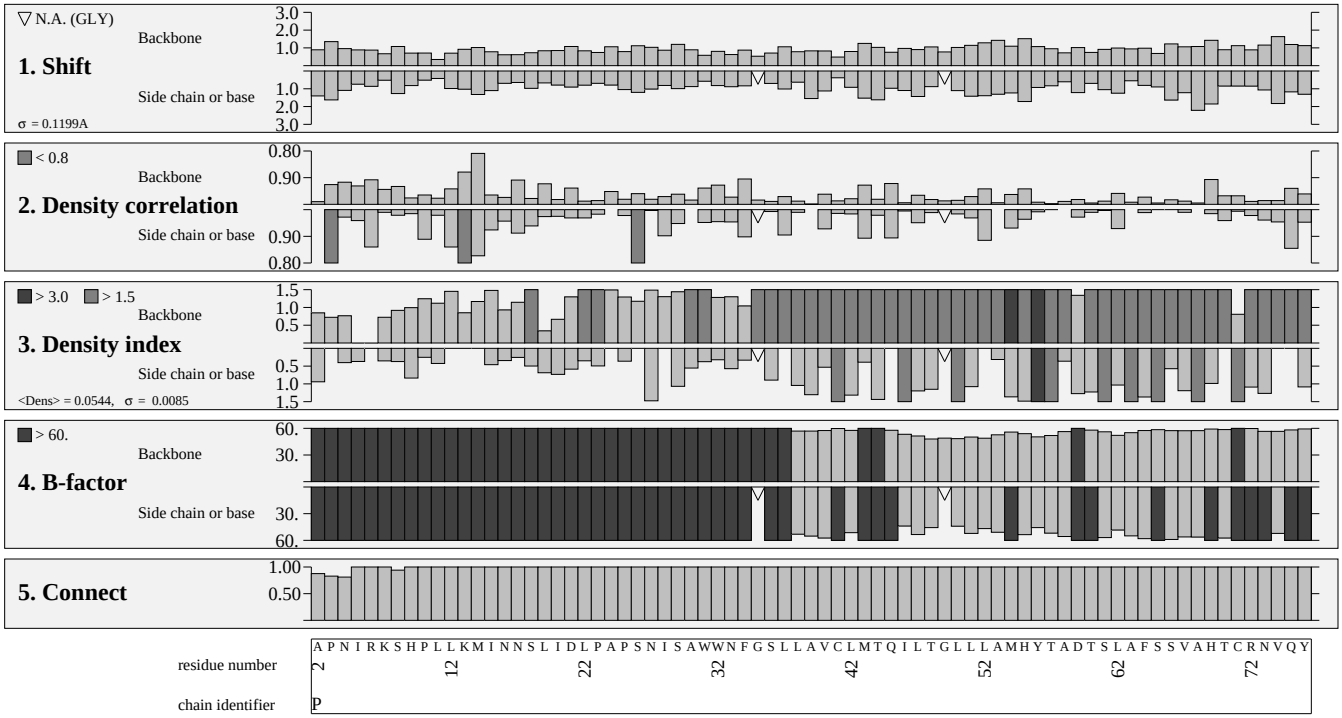
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (20)



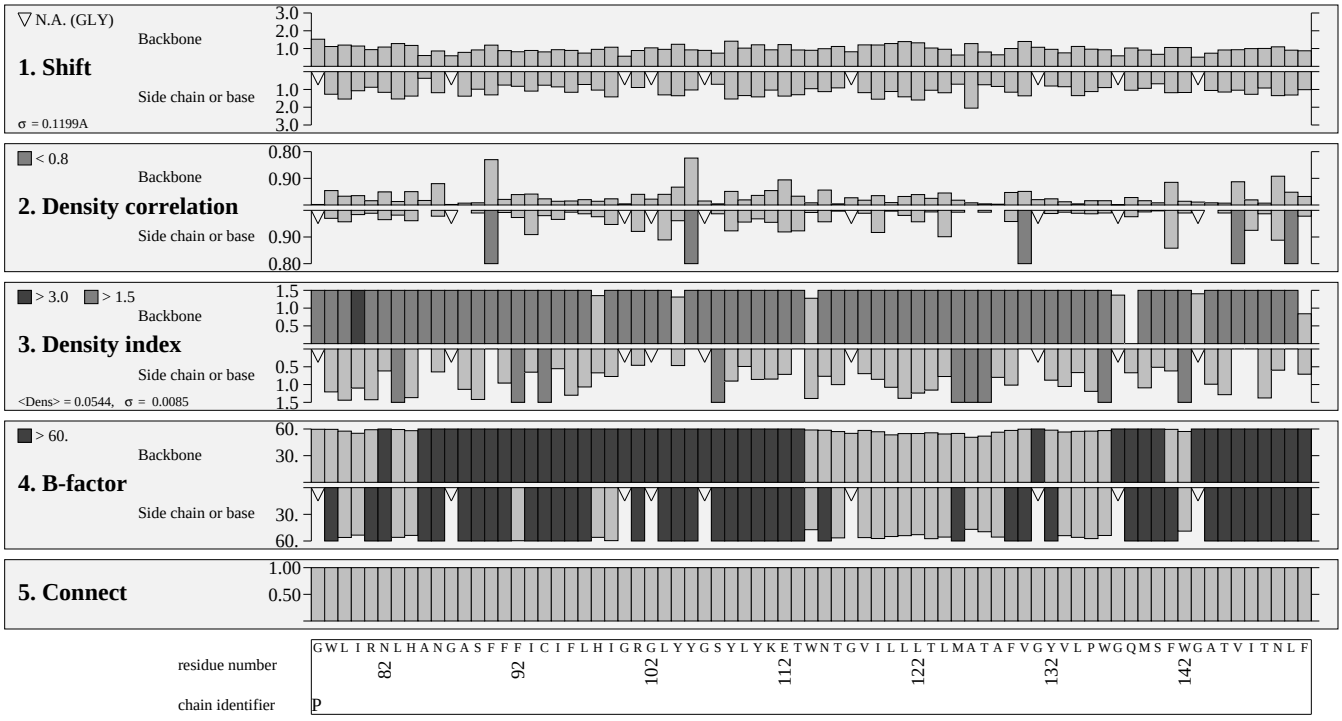


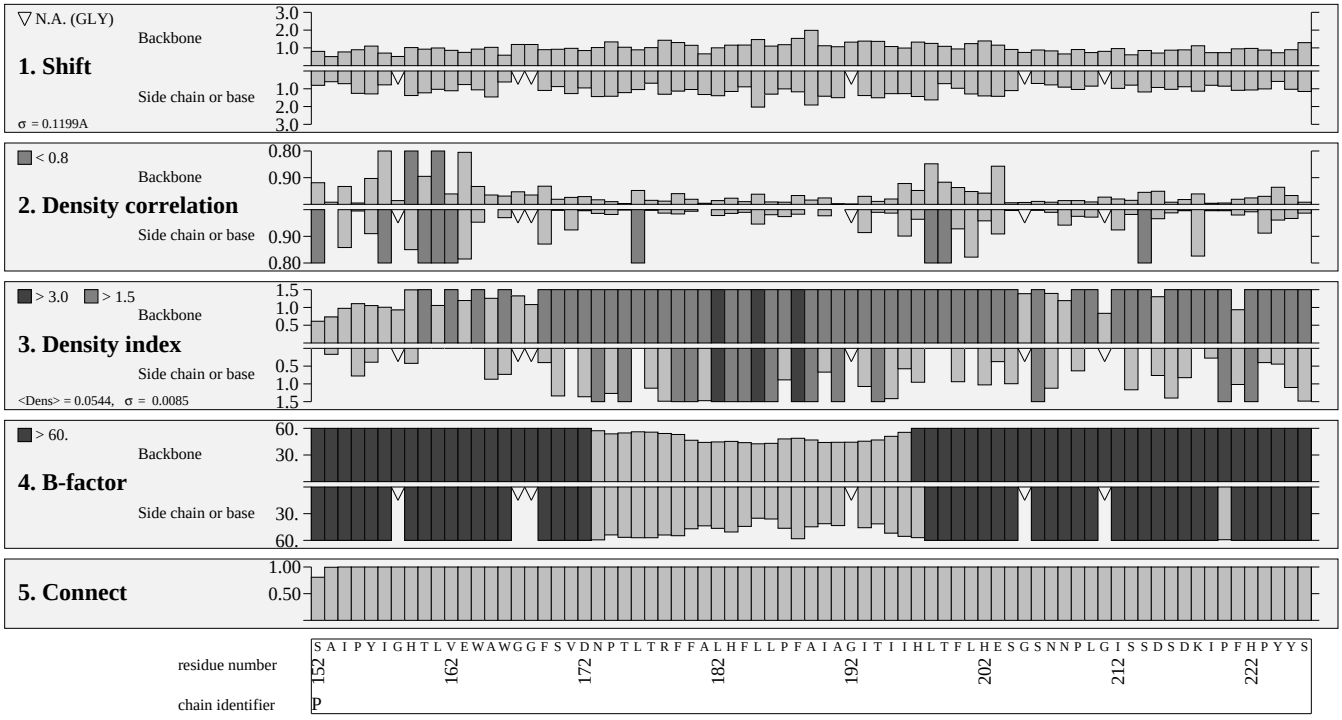
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (21)



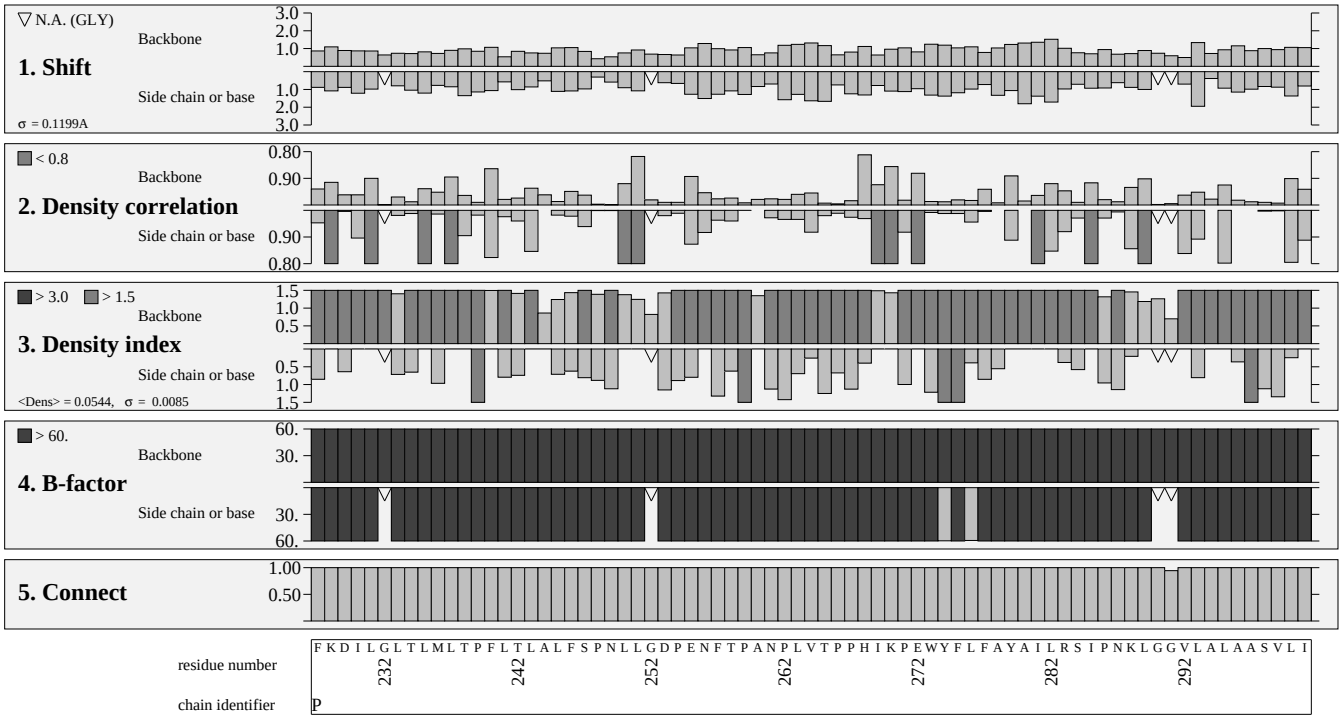


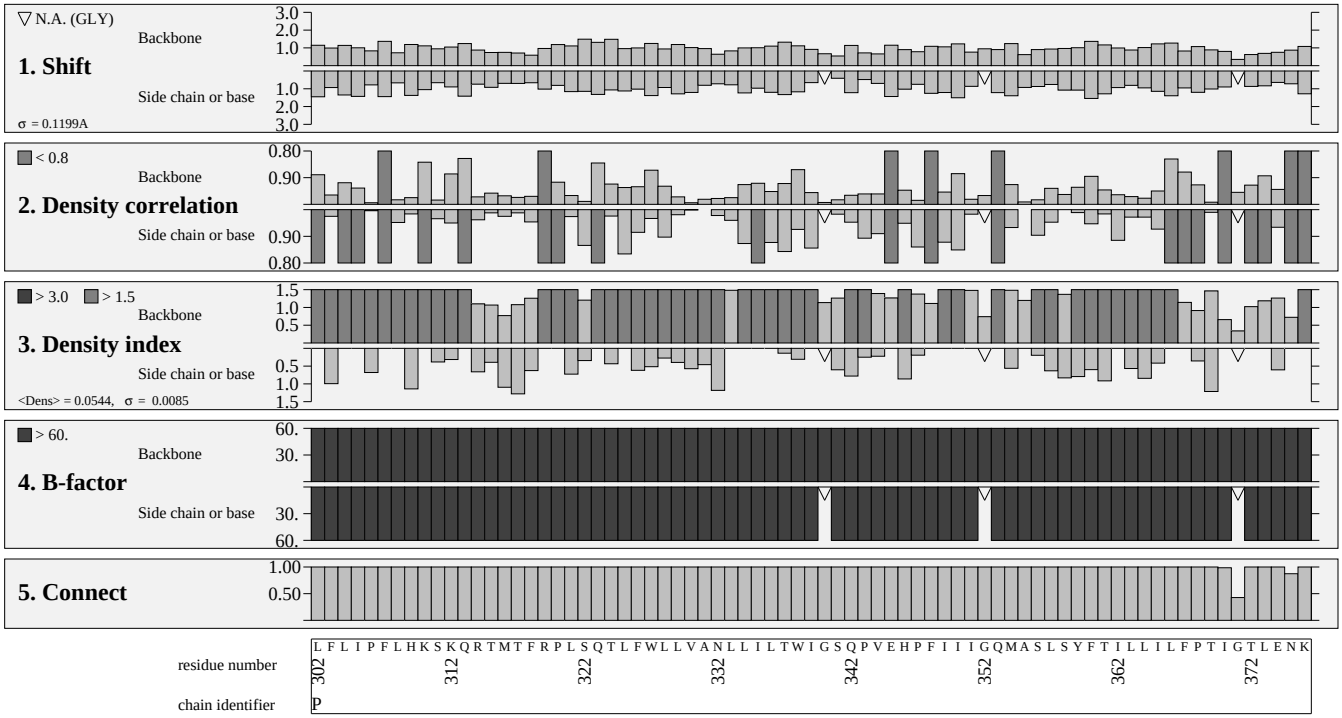
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (22)



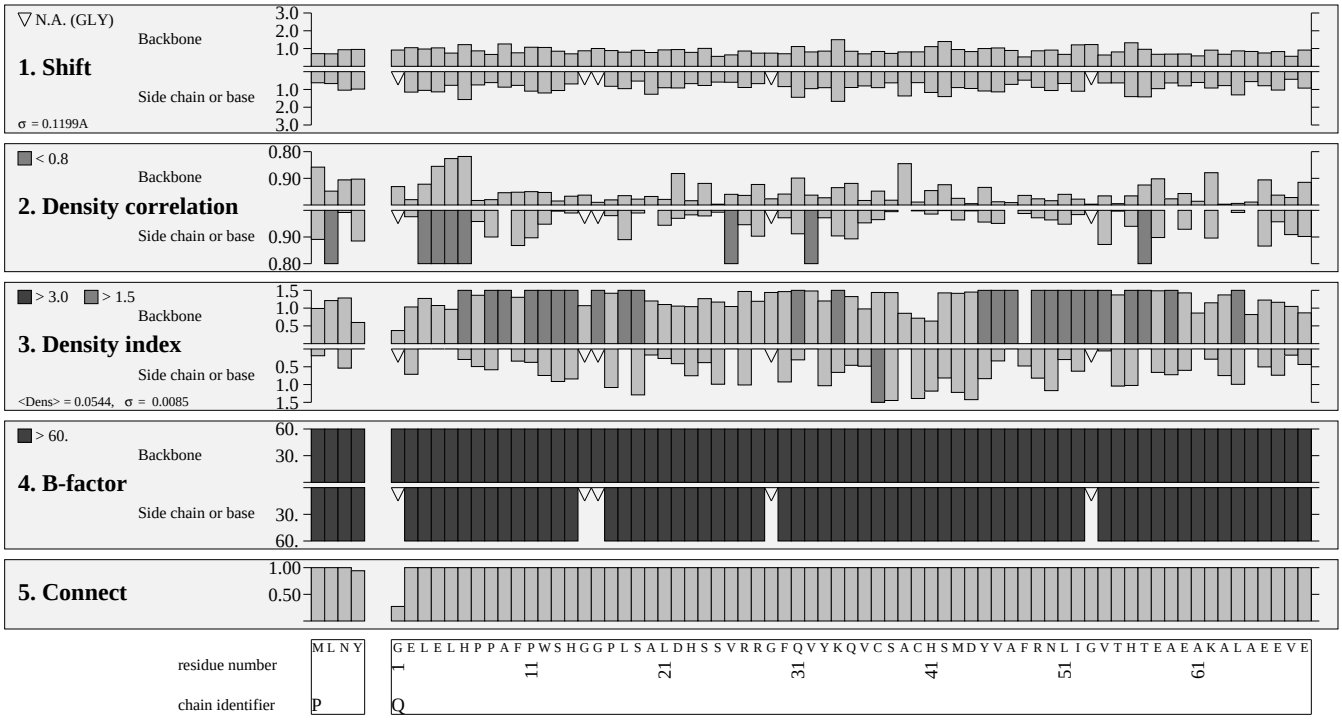


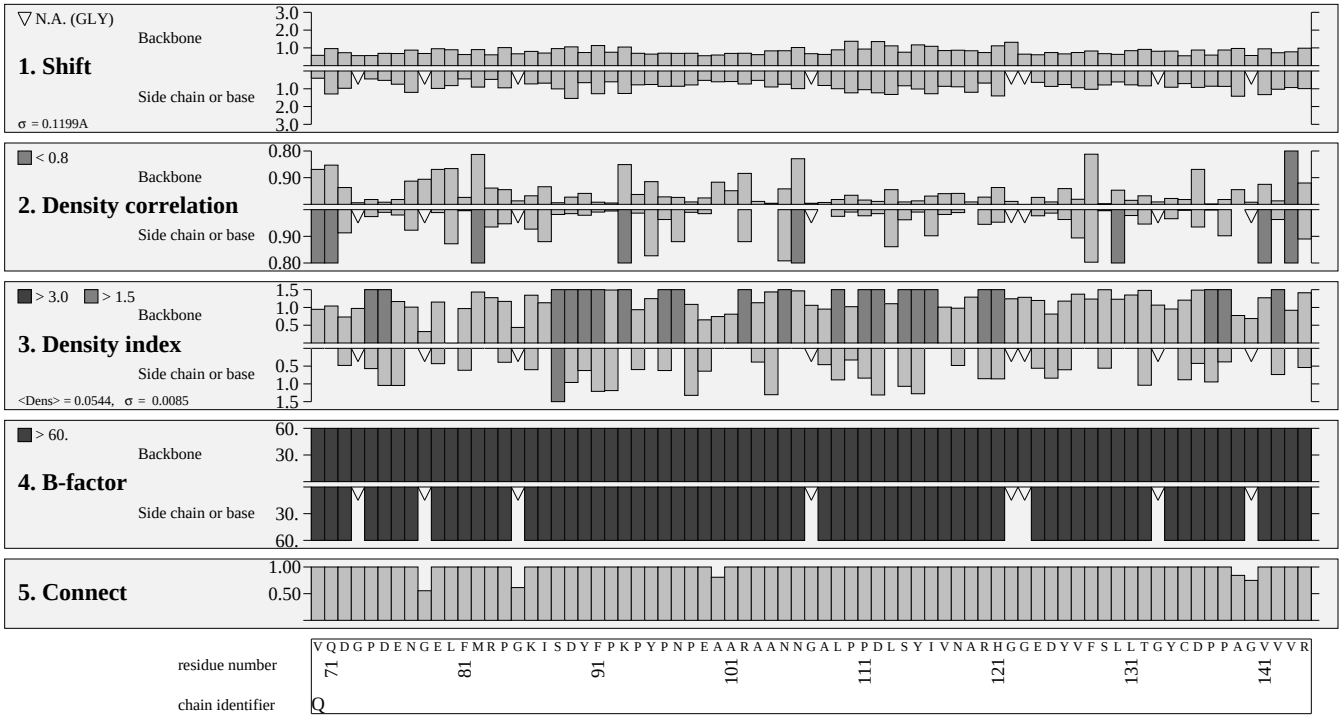
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (23)

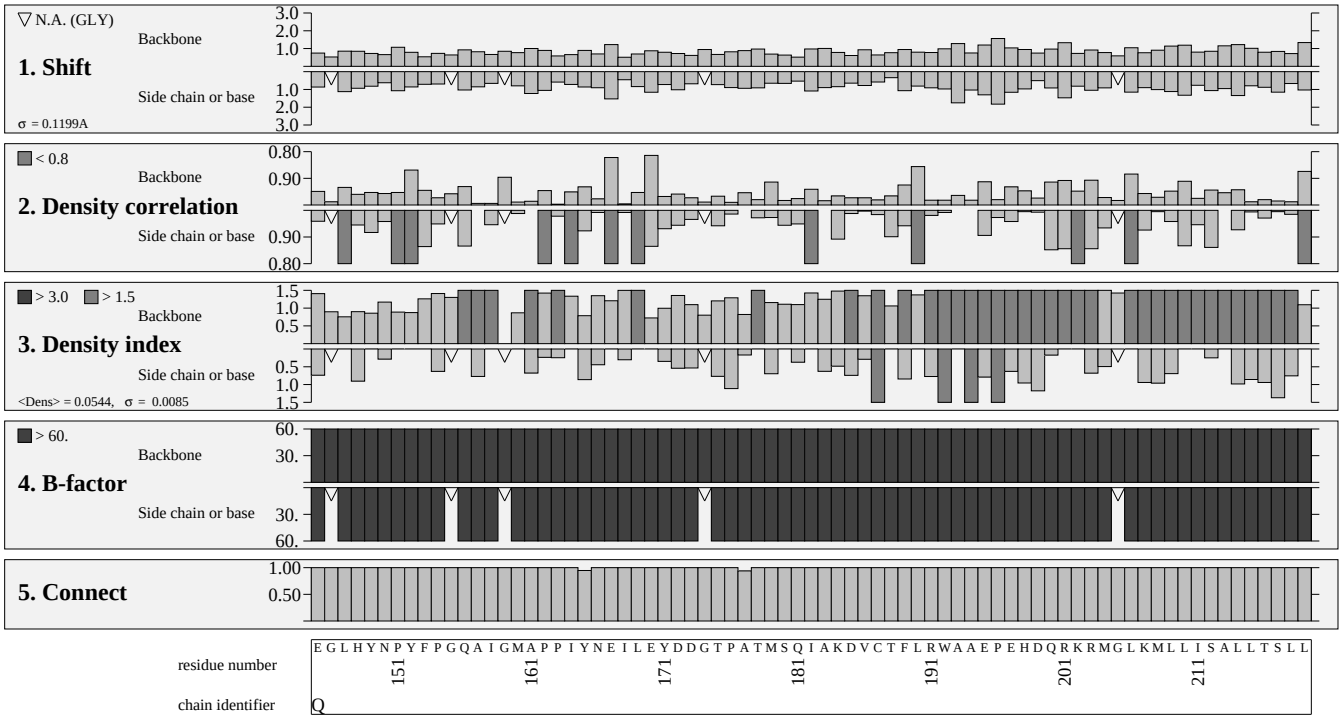


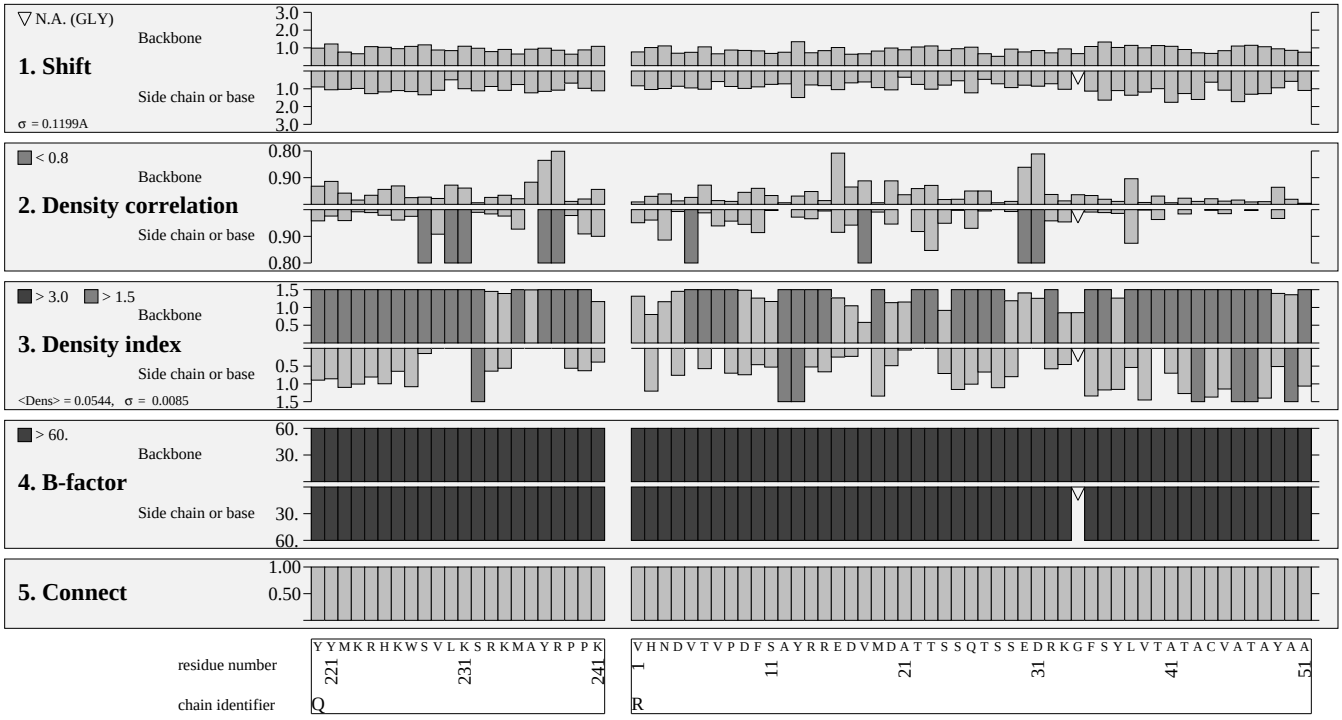


Structure Factor Check

3L73

Local estimation (24)



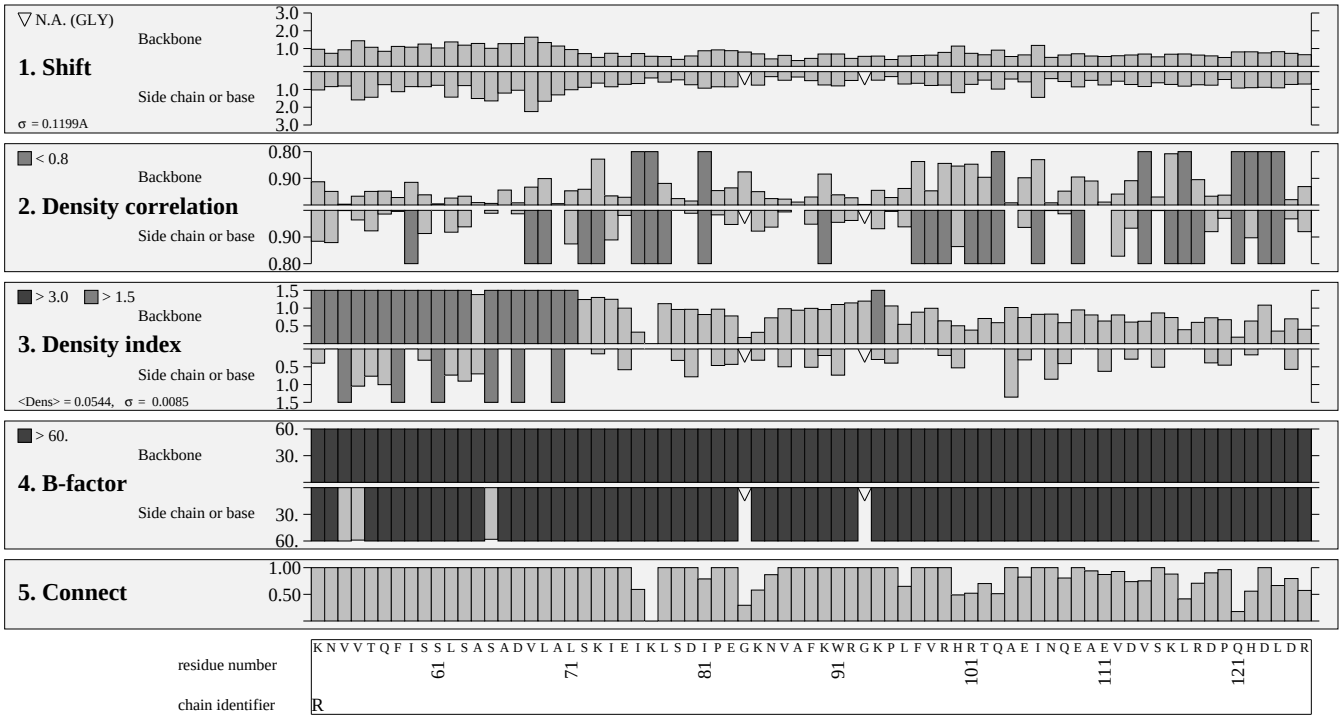


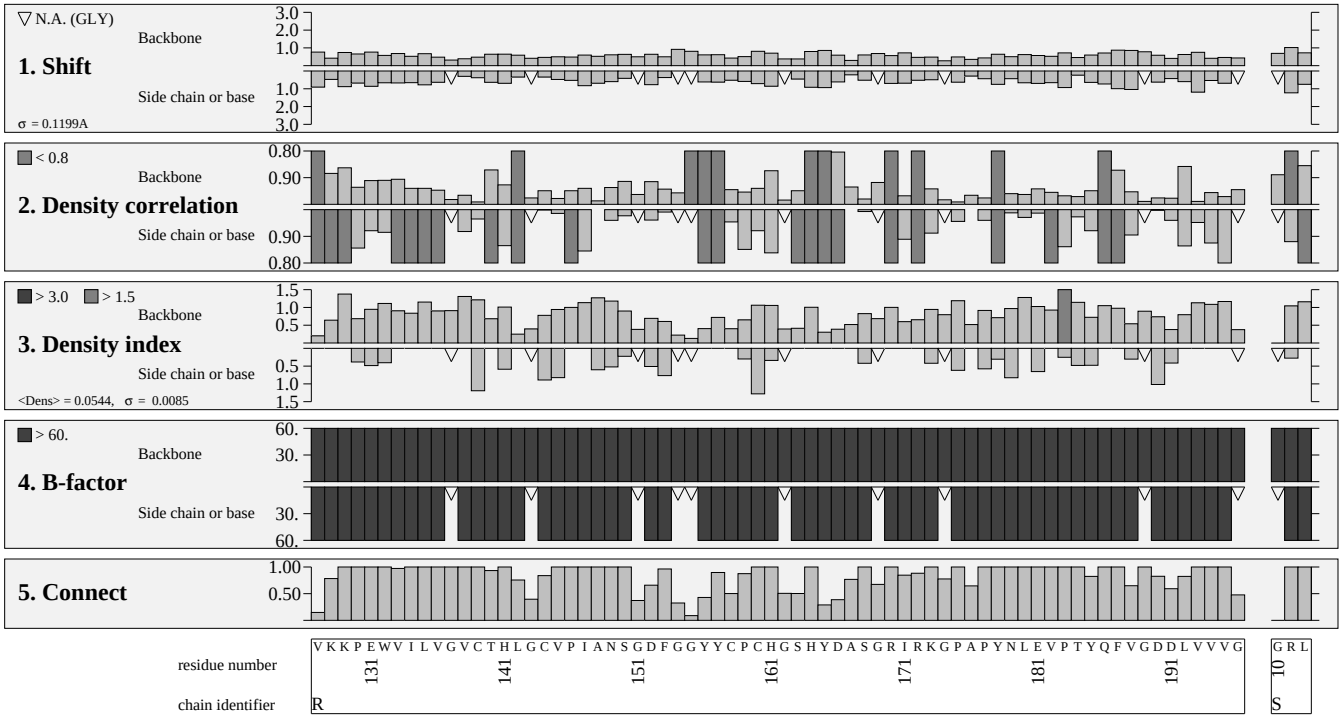
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (25)



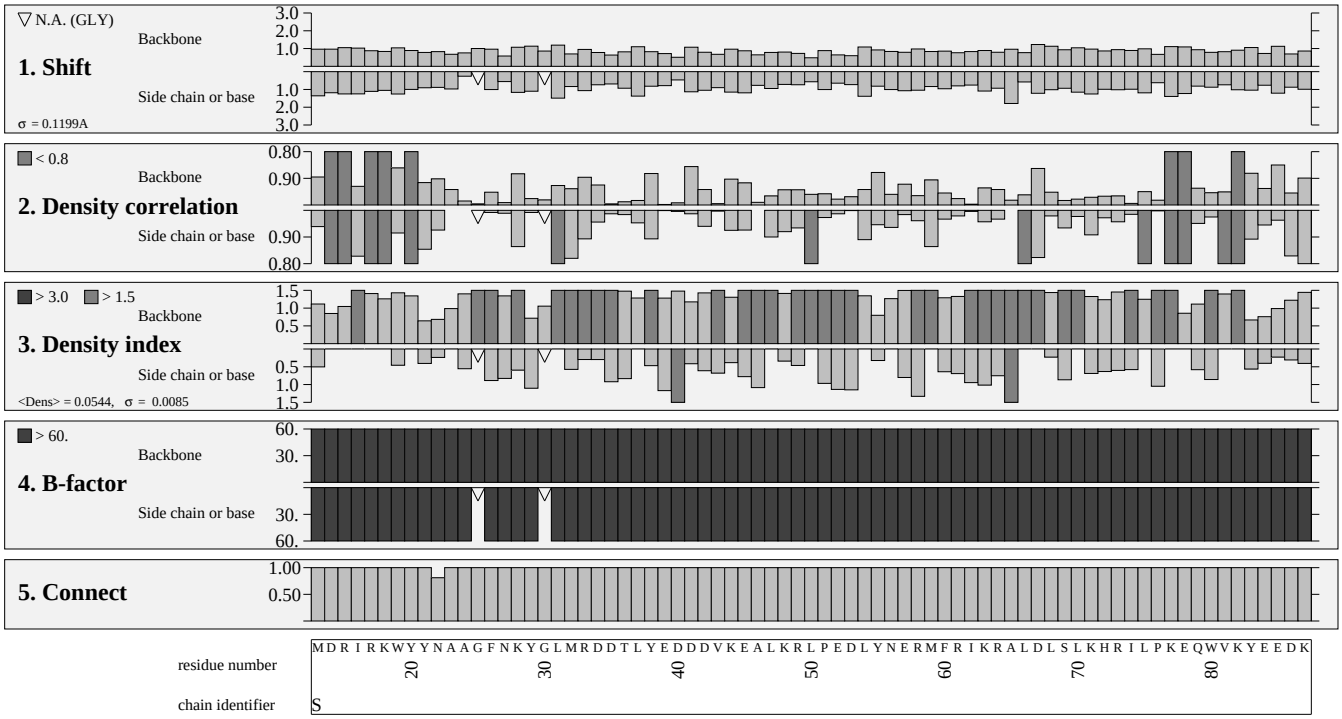


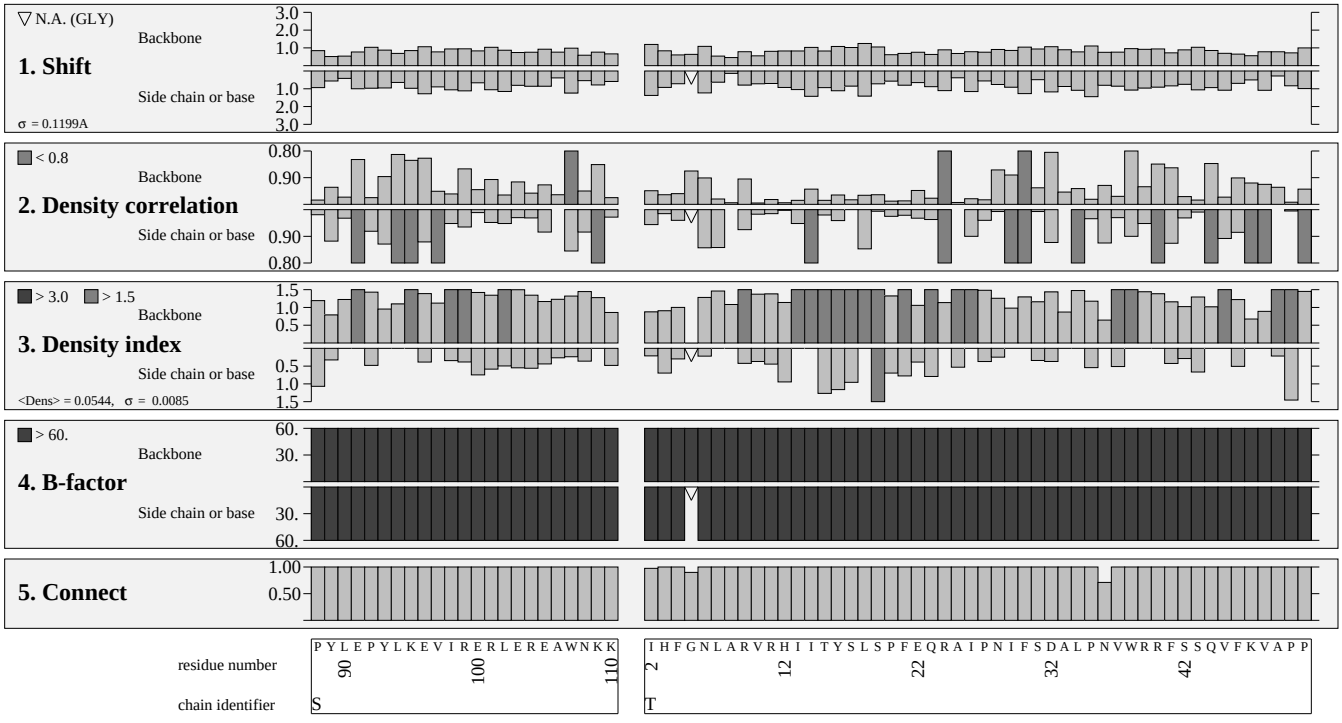
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (26)



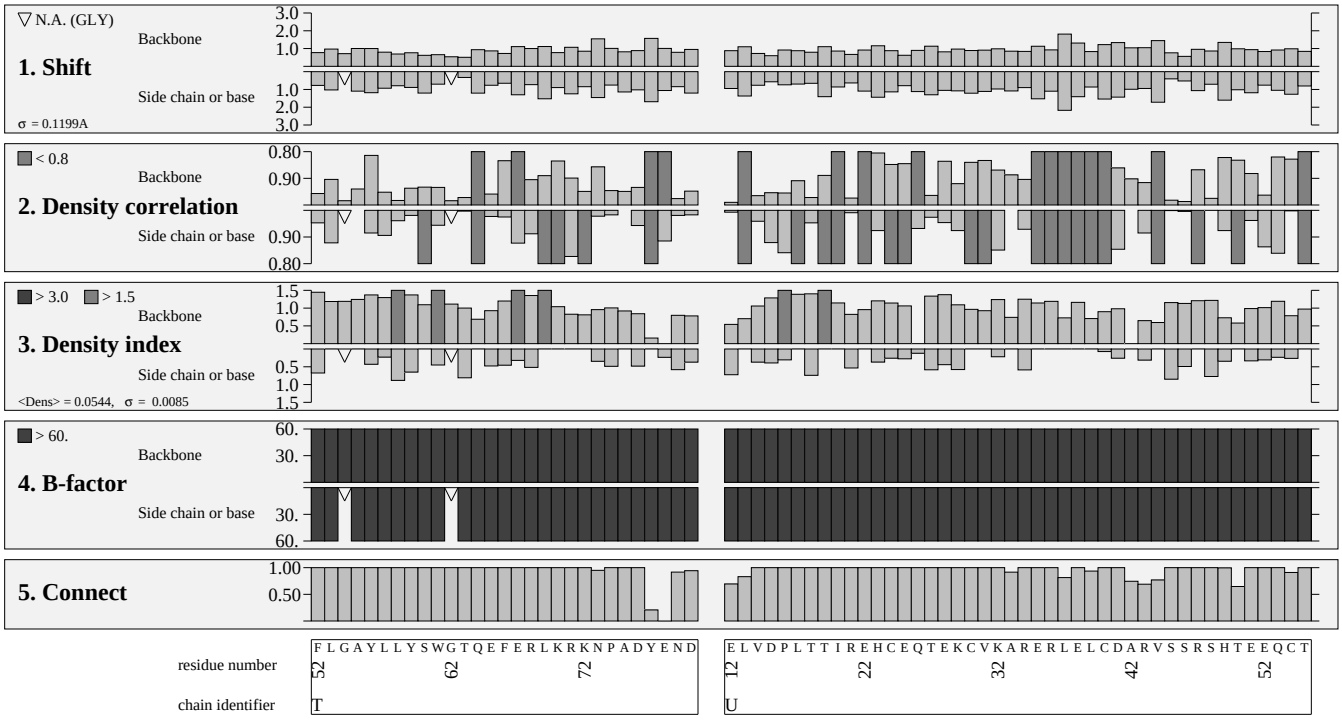


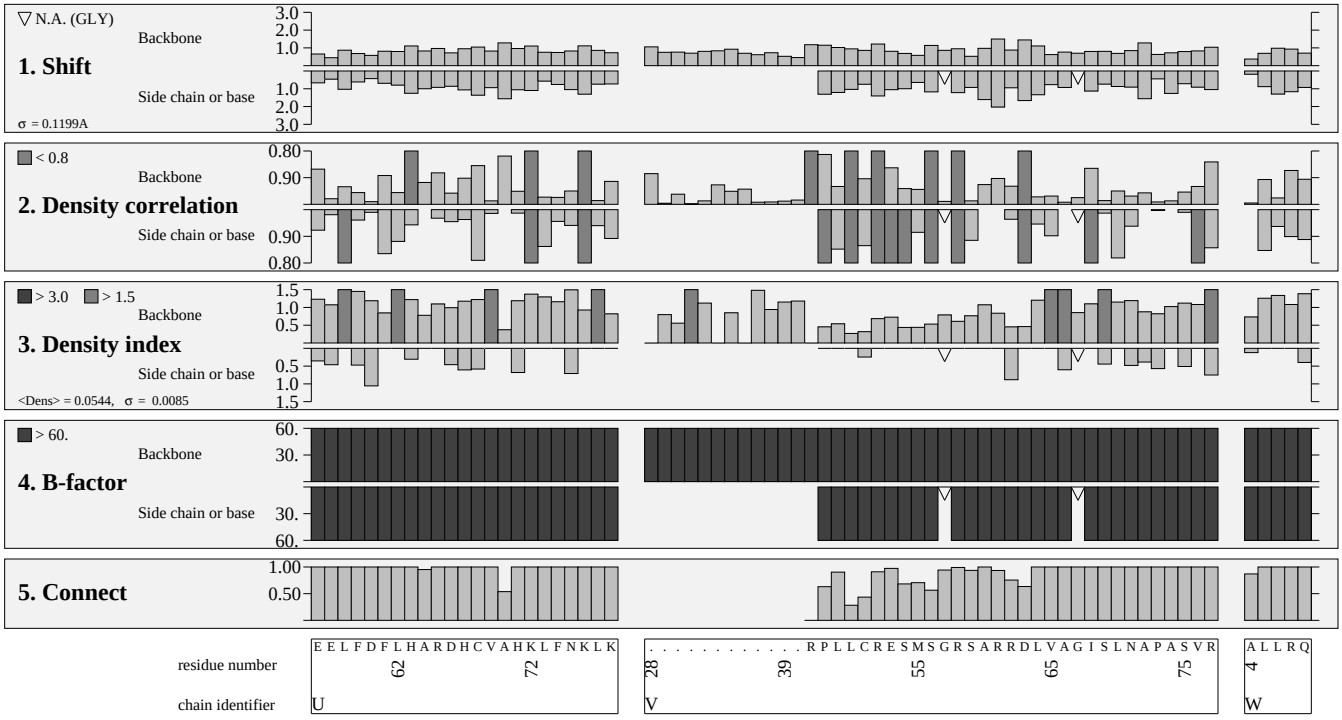
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (27)



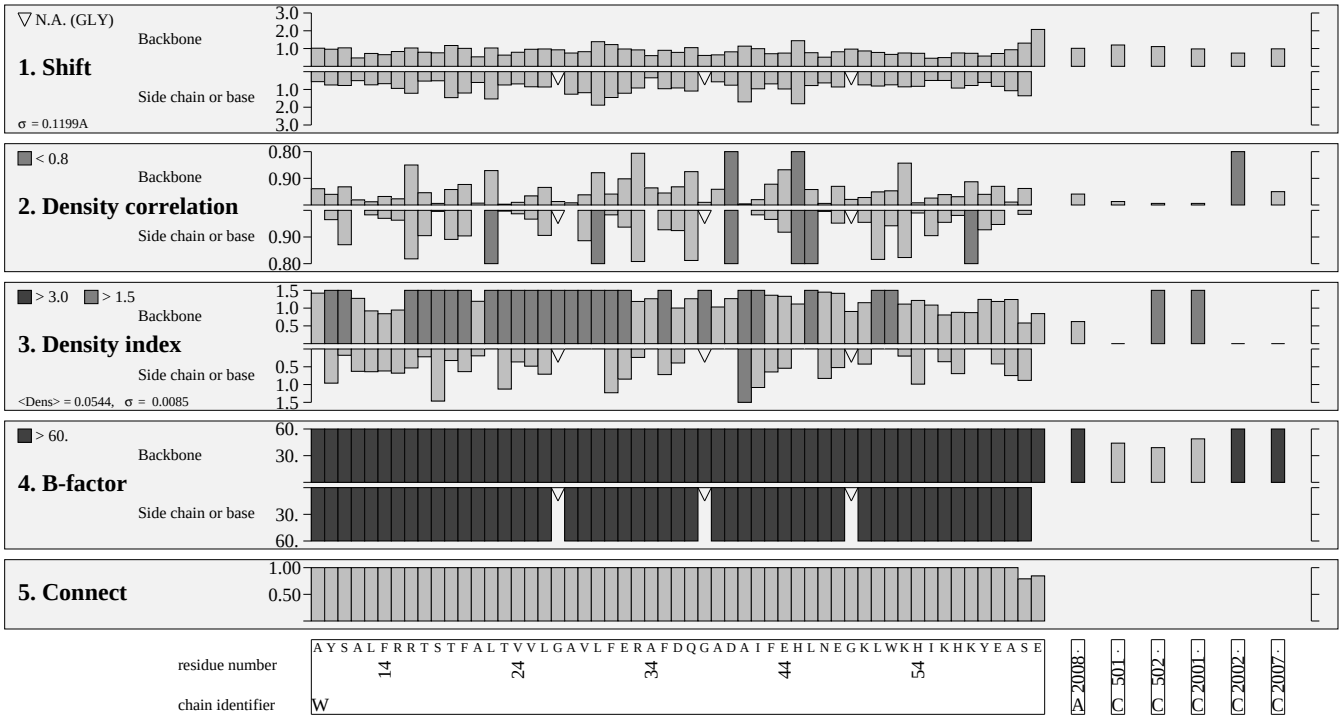


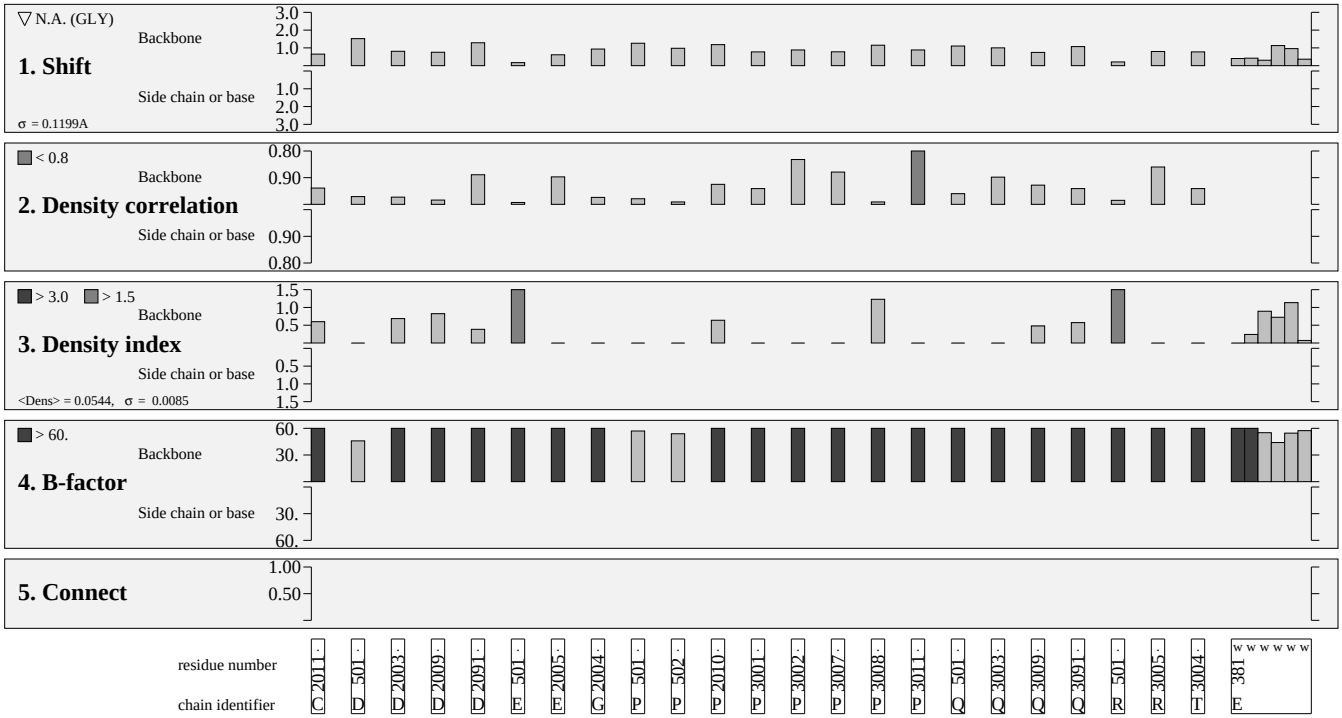
SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (28)



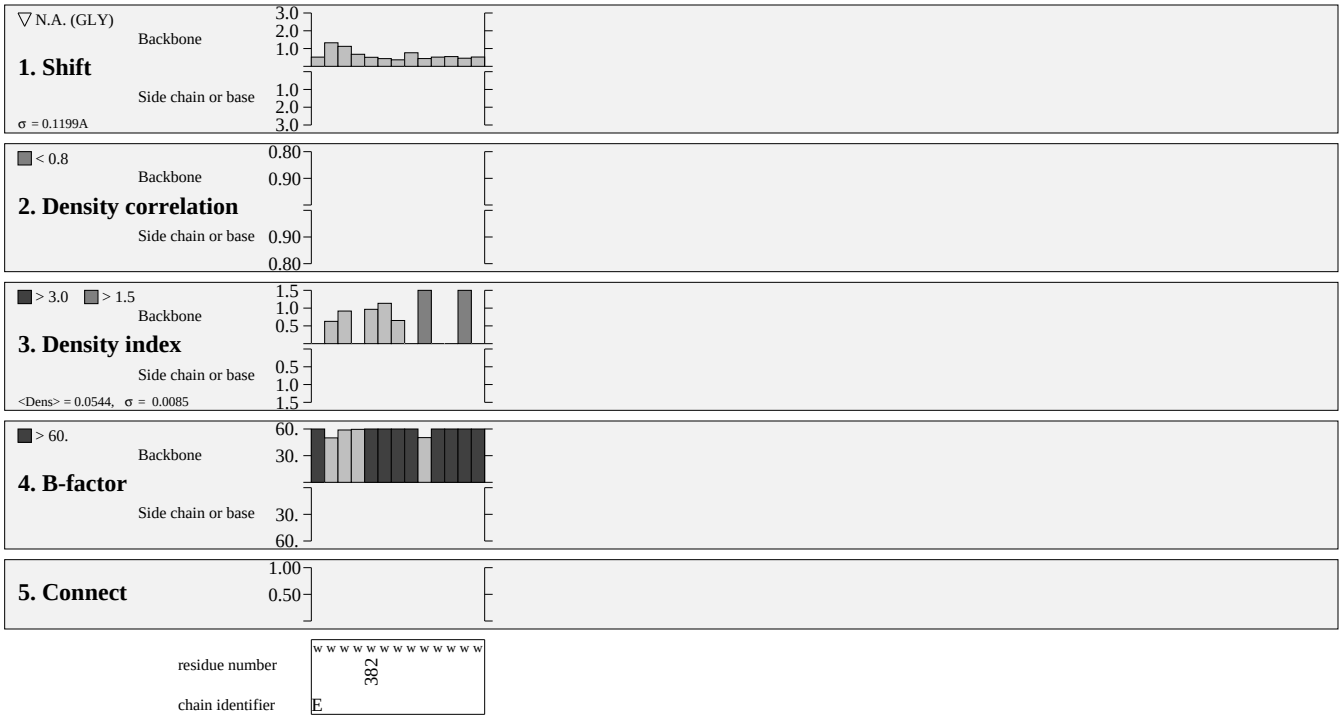


SFCHECK 7.1.01

Structure Factor Check

3L73

Local estimation (29)



SFCHECK 7.1.01