

Structure Factor Check

4YTP

Title: CRYSTAL STRUCTURE OF PORCINE HEART MITOCHONDRIAL COMPLEX II
 N-[\054-TERT-BUTYLPHENYL\05METHYL]-2-\05TRIFLUOROMETHYL\05BENZAMIDE
 Date: 18-MAR-15
 PDB code: 4YTP

Crystal

Cell parameters:

a: 71.43 A b: 84.01 A c: 294.82 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Model

8641 atoms (22 water molecules)

Number of chains: 14
 Volume not occupied by model: 58.3 %
 $\langle B \rangle$ (for atomic model): 69.7 A²
 $\sigma(B)$: 15.77 A²
 Matthews coefficient: 3.66
 Corresponding solvent % : 66.09

Refinement

Program: REFMAC 5.7.0029
 Nominal resolution range: 20.0 – 3.10 A
 Reported R-factor: 0.206
 Number of reflections used: 25461
 Reported Rfree: 0.27
 Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 20.0 – 3.10 A
 Reflections in file: 33004
 Unique reflections above 0: 26706
 above 1 σ : 26238
 above 3 σ : 18993
 Reflections > 0: 6298

SFCHECK

Nominal resolution range: 20.0 – 3.10 A
 \05max. from input data, min. from author\05
 Used reflections: 26705
 Reflections out of resolution: 1
 Completeness: 80.9 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.073
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.8495 0.9458 1.0000
 B_{overall} (by Patterson): 50.A²
 Optical resolution: 2.23 A
 Expected opt. resol. for complete data set: 2.23 A
 Estimated minimal error: 0.112 A

Model vs. Structure Factors

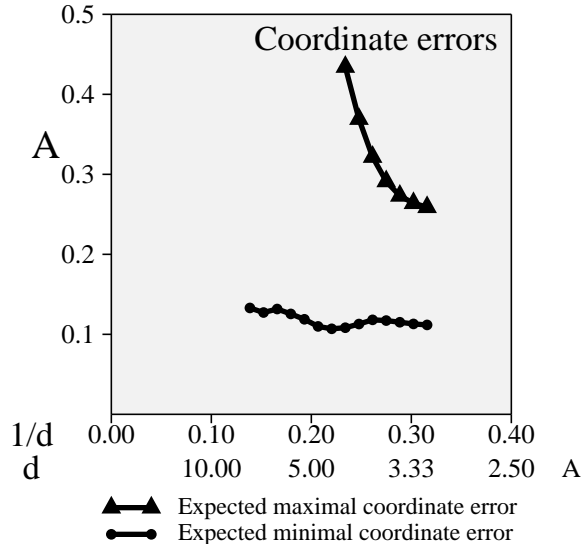
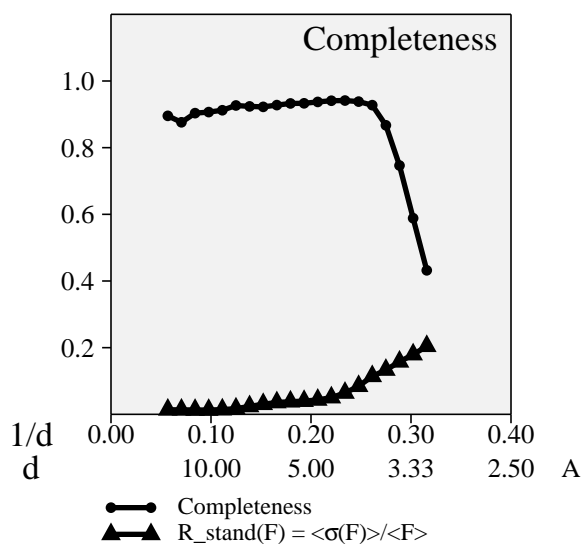
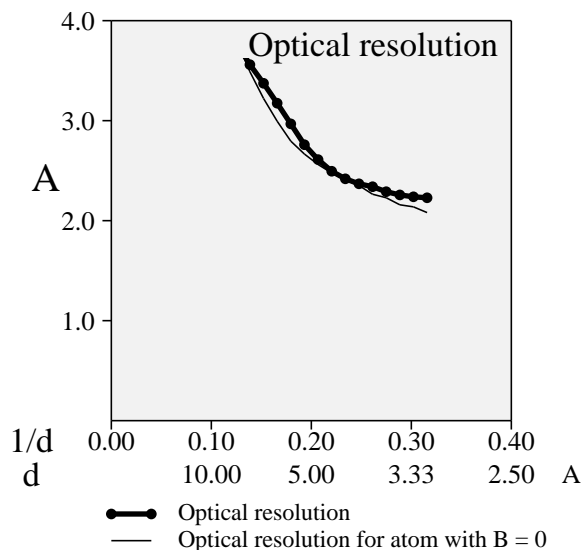
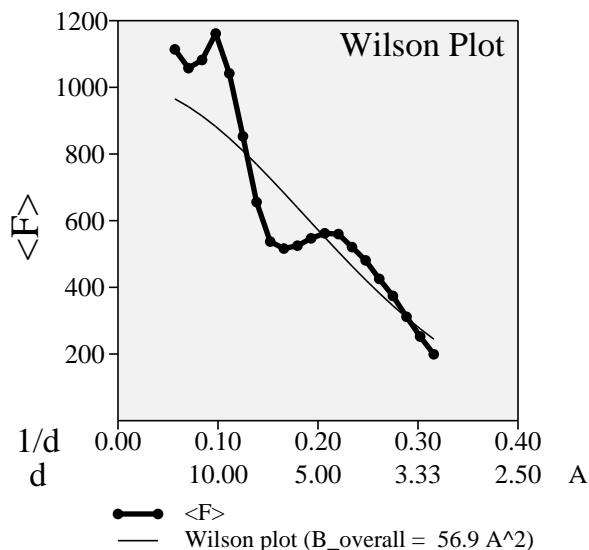
R-factor for all reflections: 0.265
 Correlation factor: 0.818
 R-factor: 0.271
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 – 3.10A
 reflections used: 26237
 Rfree: 0.326
 Nfree: 1330
 R-factor without free-refl.: 0.268
 Non free-reflections: 24907
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.533 A
 Estimated maximal error: 0.259 A
 DPI: 0.509 A

Scaling

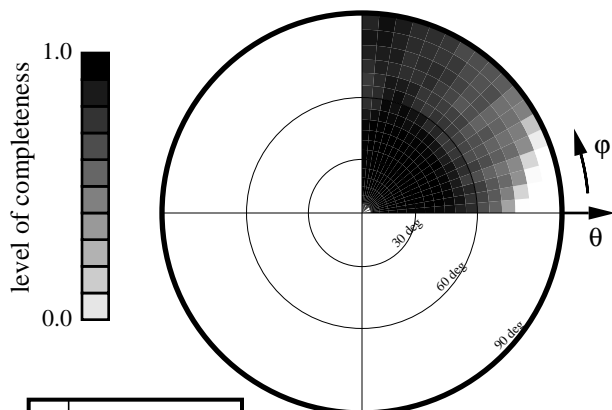
Scale: 0.862
 Bdiff: -6.97
 Anisothermal Scaling (Beta):
 -3.2537 -2.8956 -2.9859 0.0000 -0.0000 -0.0000
 Solvent correction – Ks,Bs: 0.318 249.827

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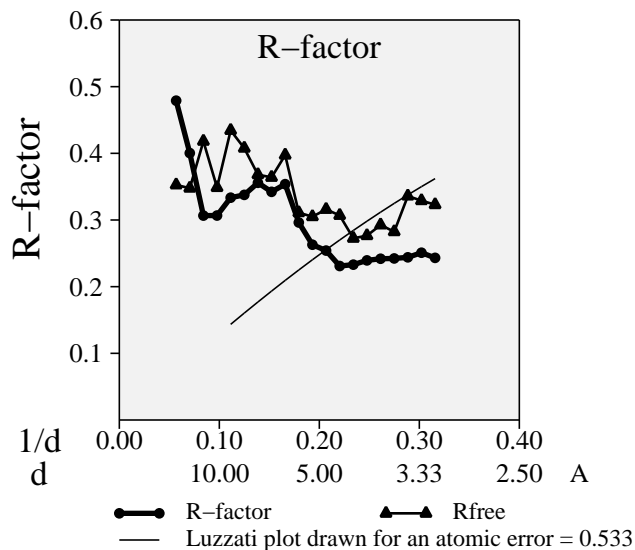


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

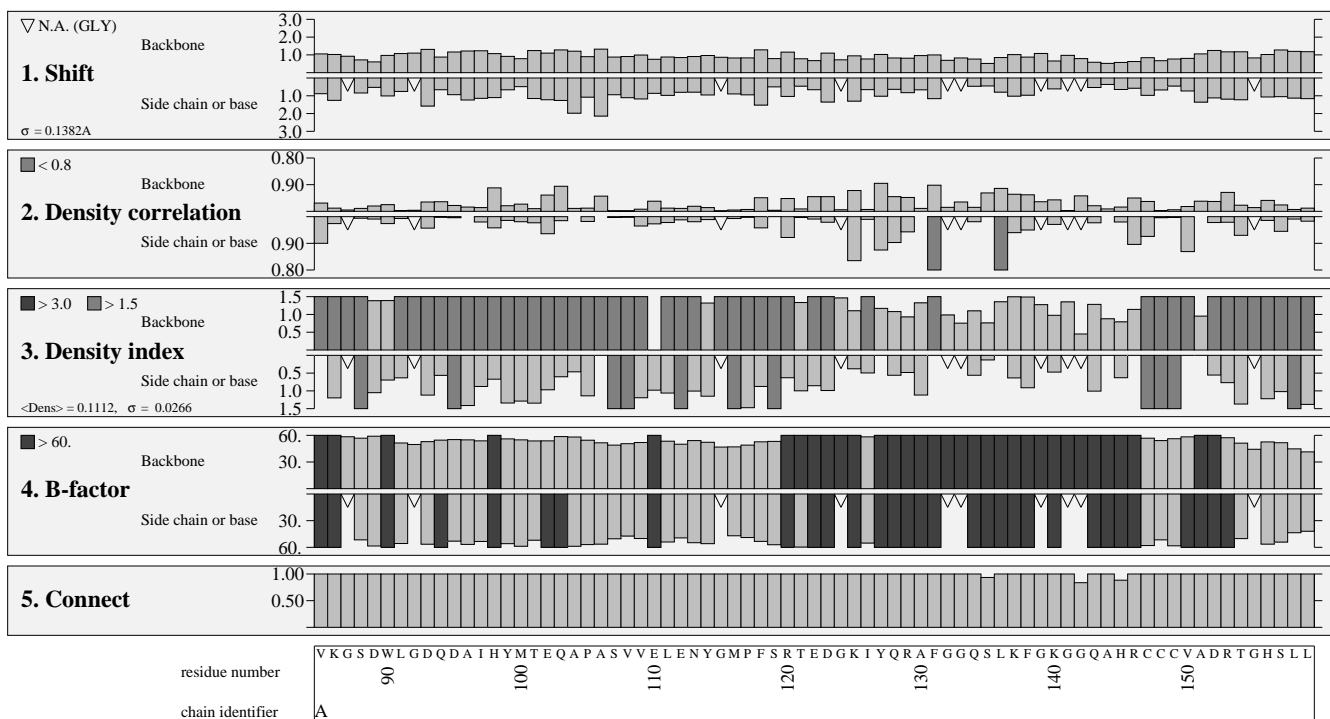
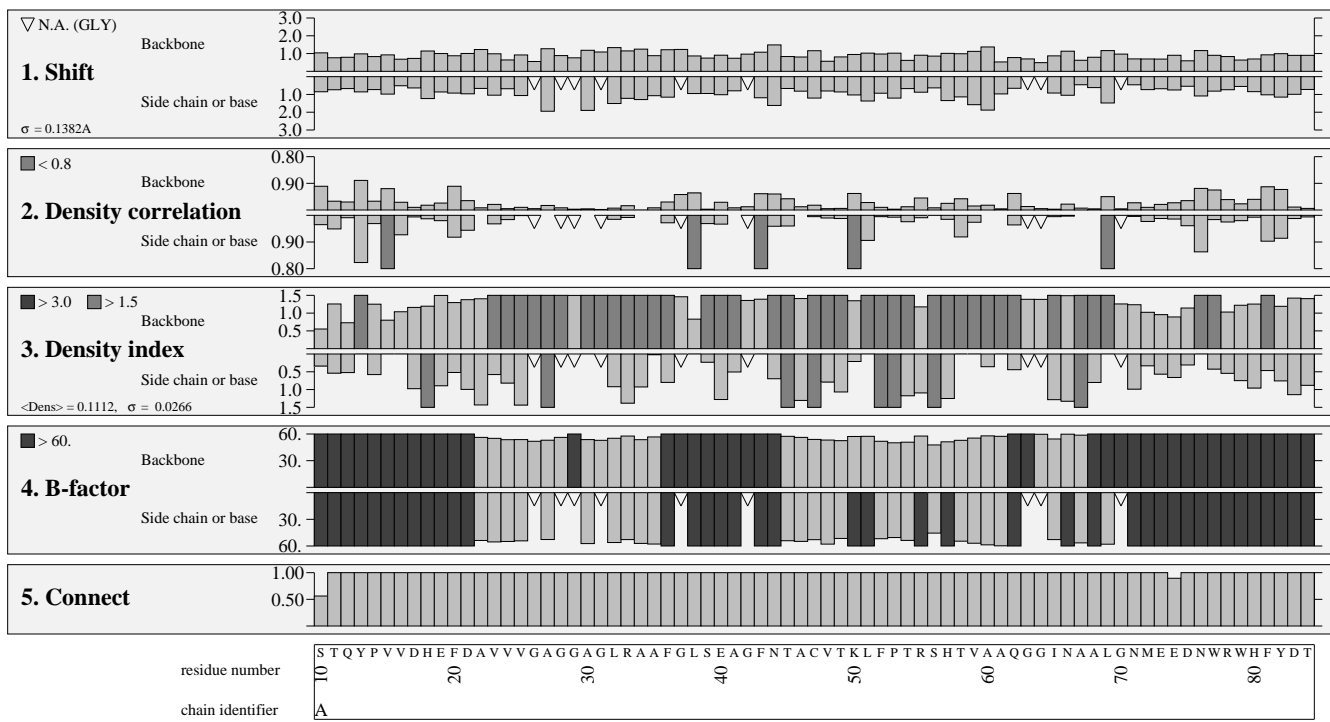
polar coordinates of the crystallographical axes



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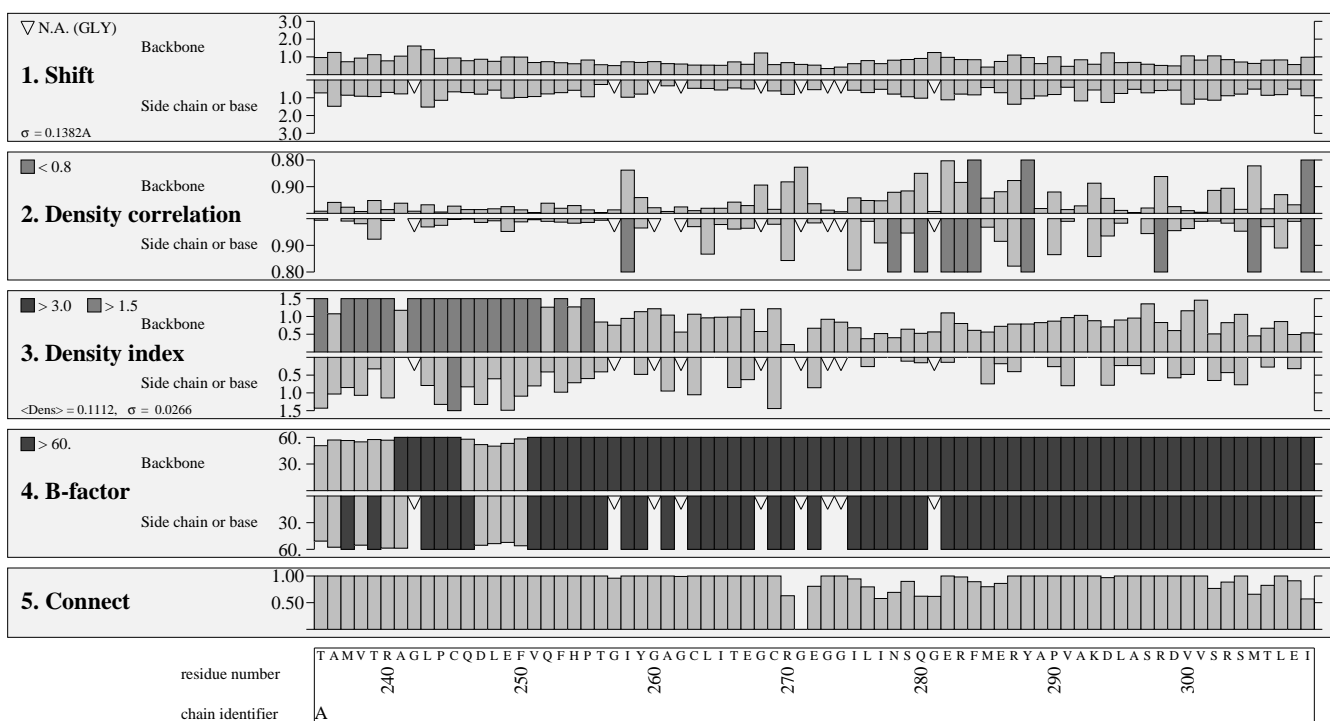
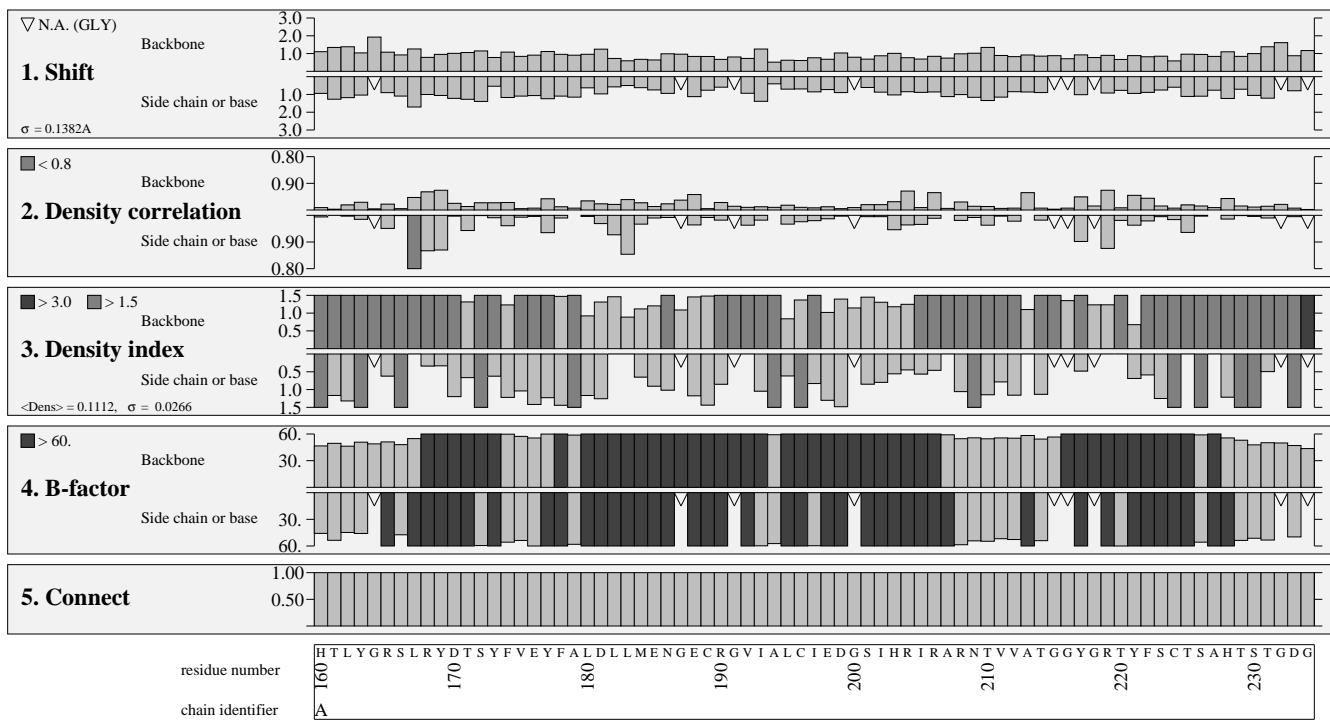
Local estimation



Structure Factor Check

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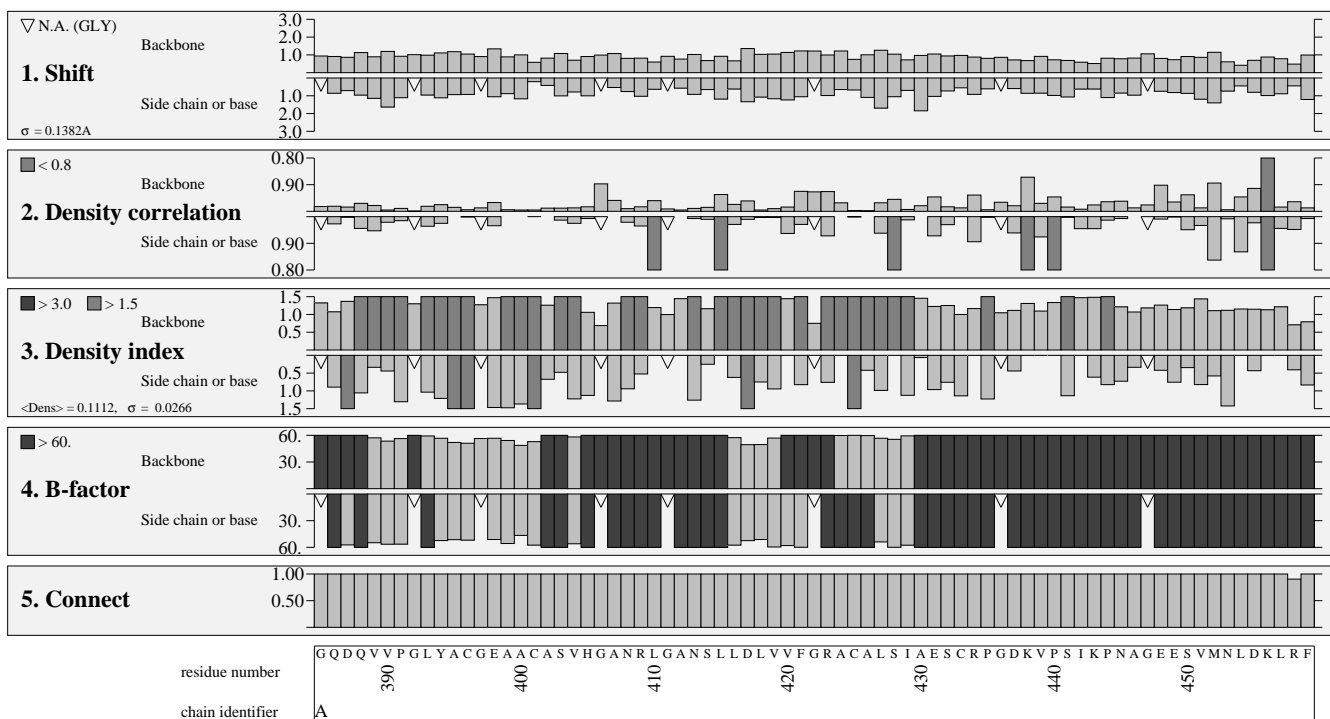
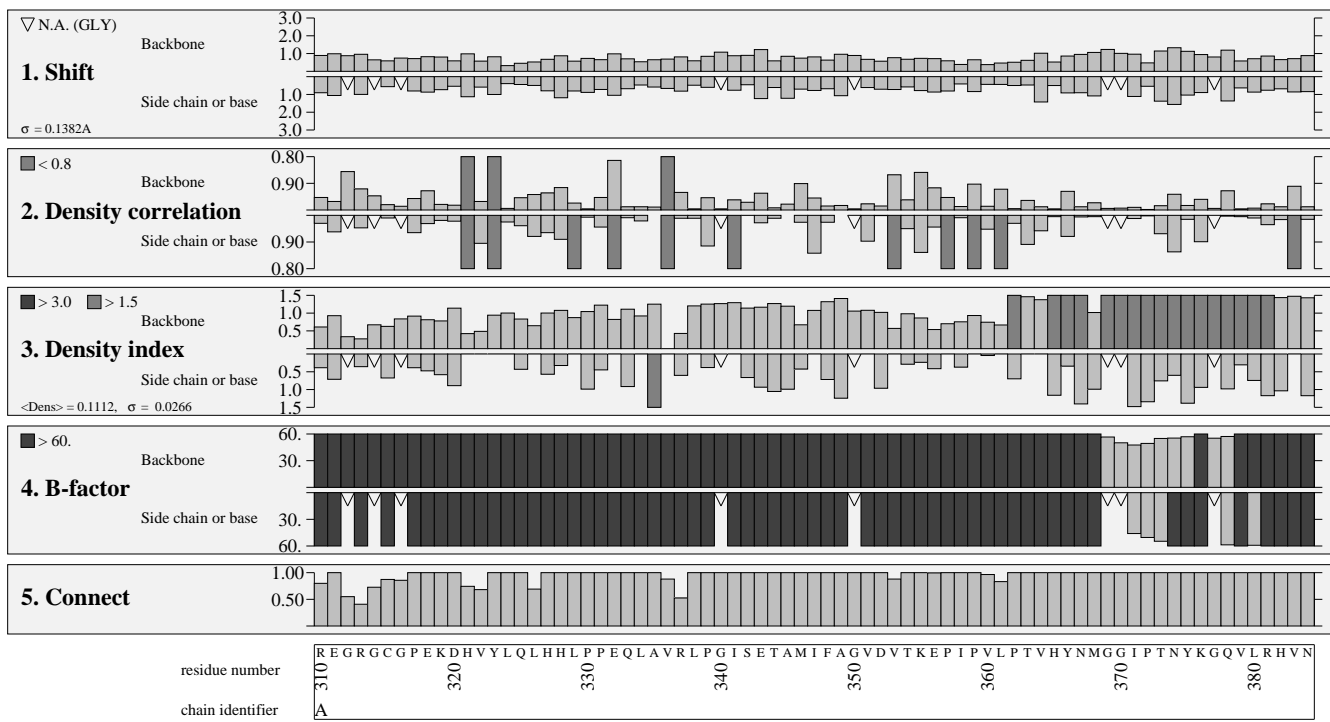
Local estimation (2)



Structure Factor Check

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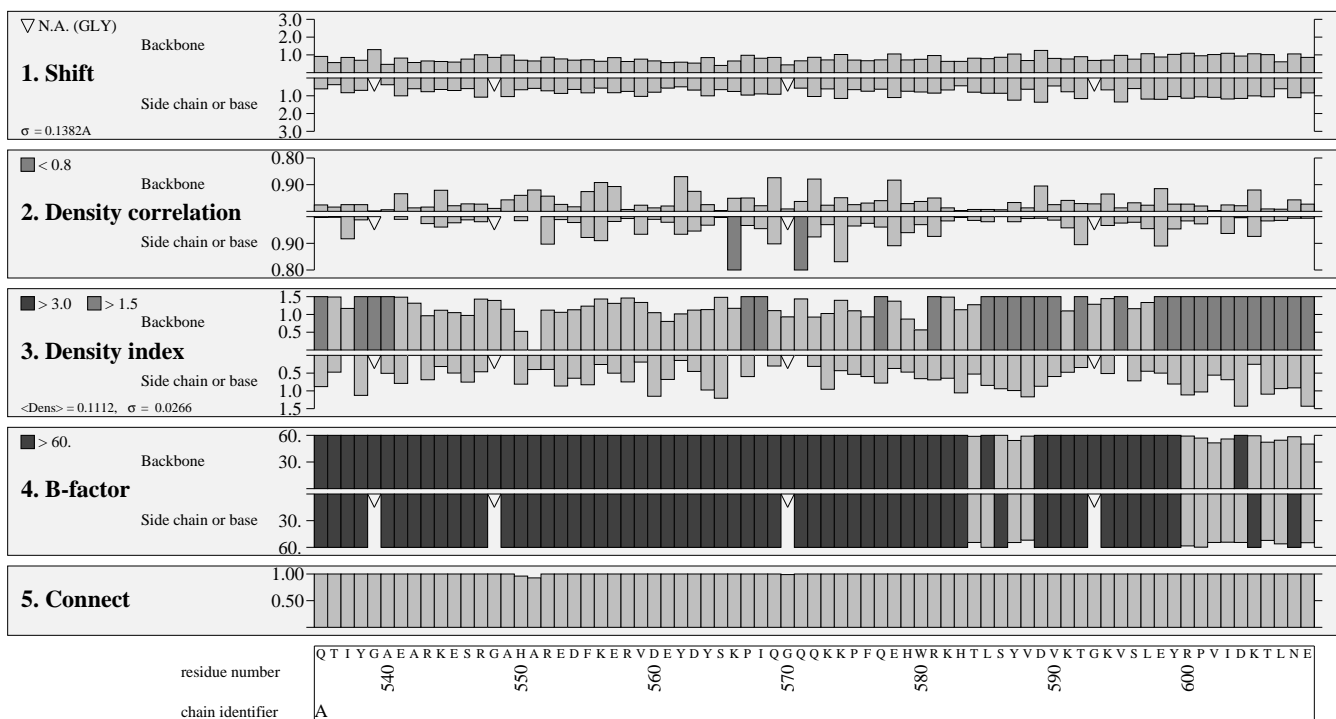
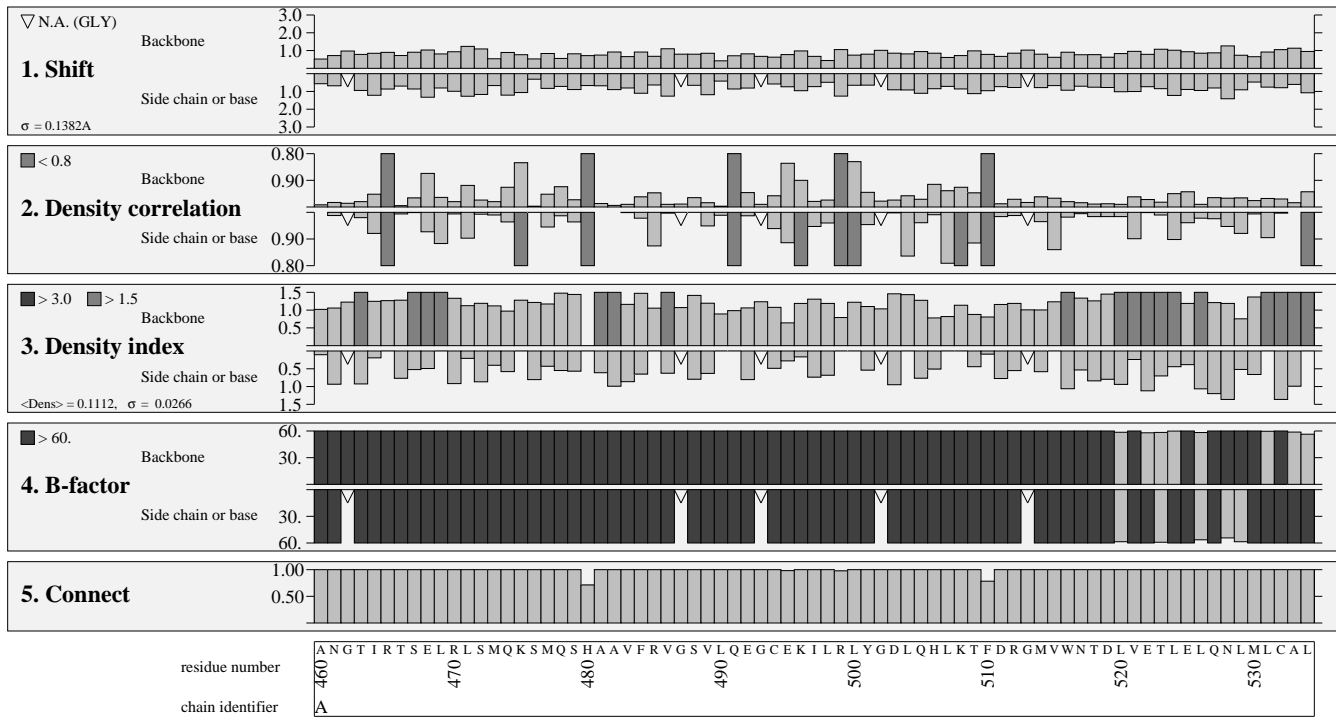
Local estimation (3)



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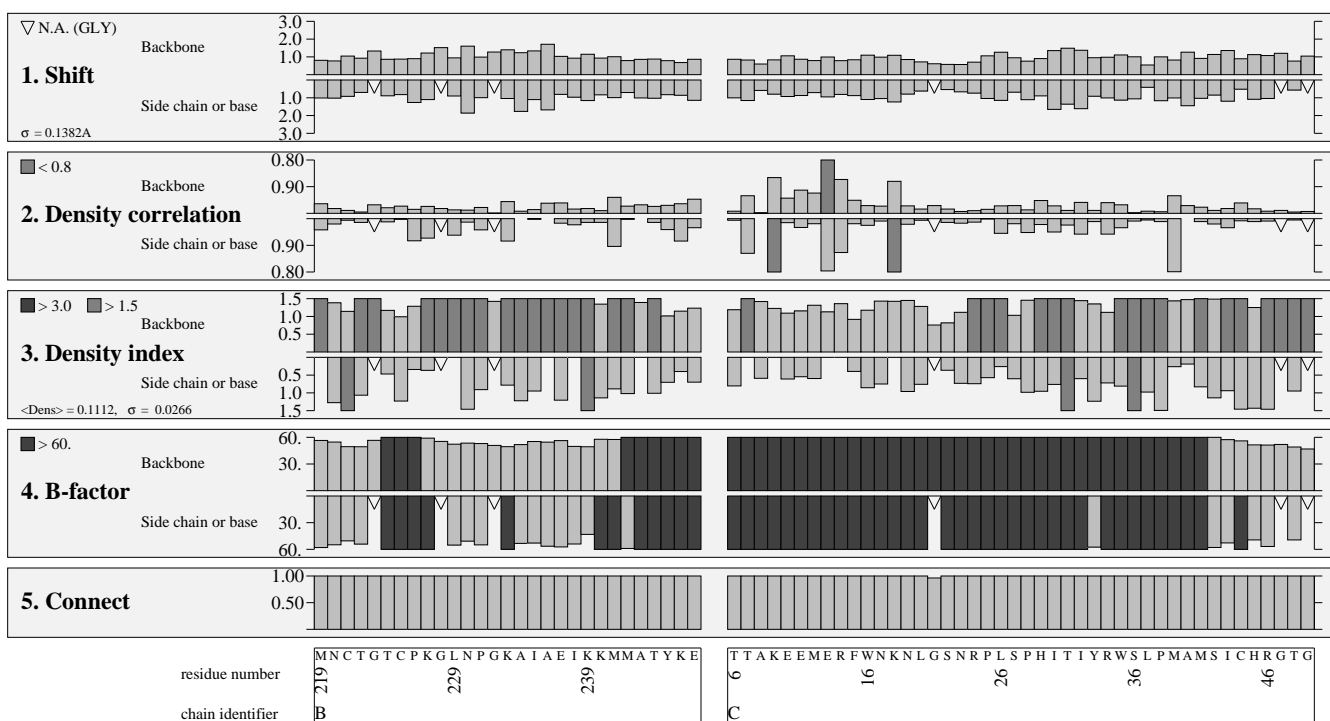
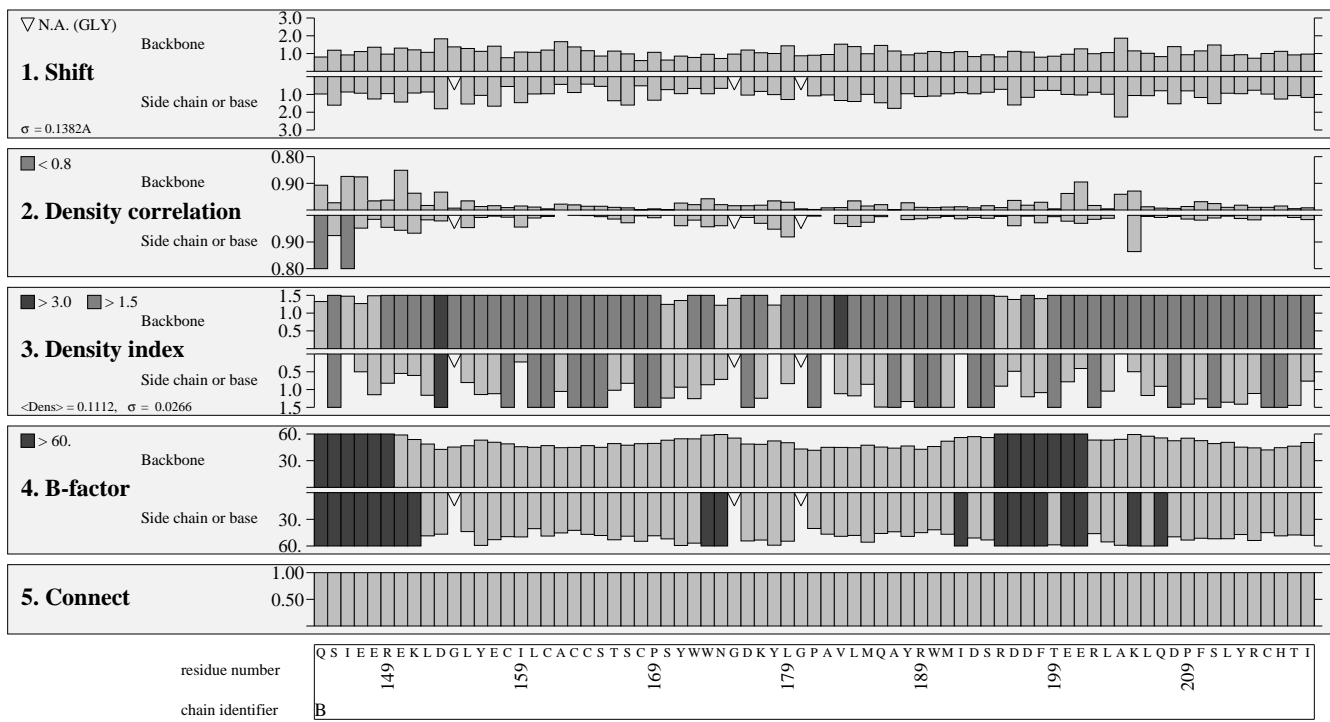
Local estimation (4)



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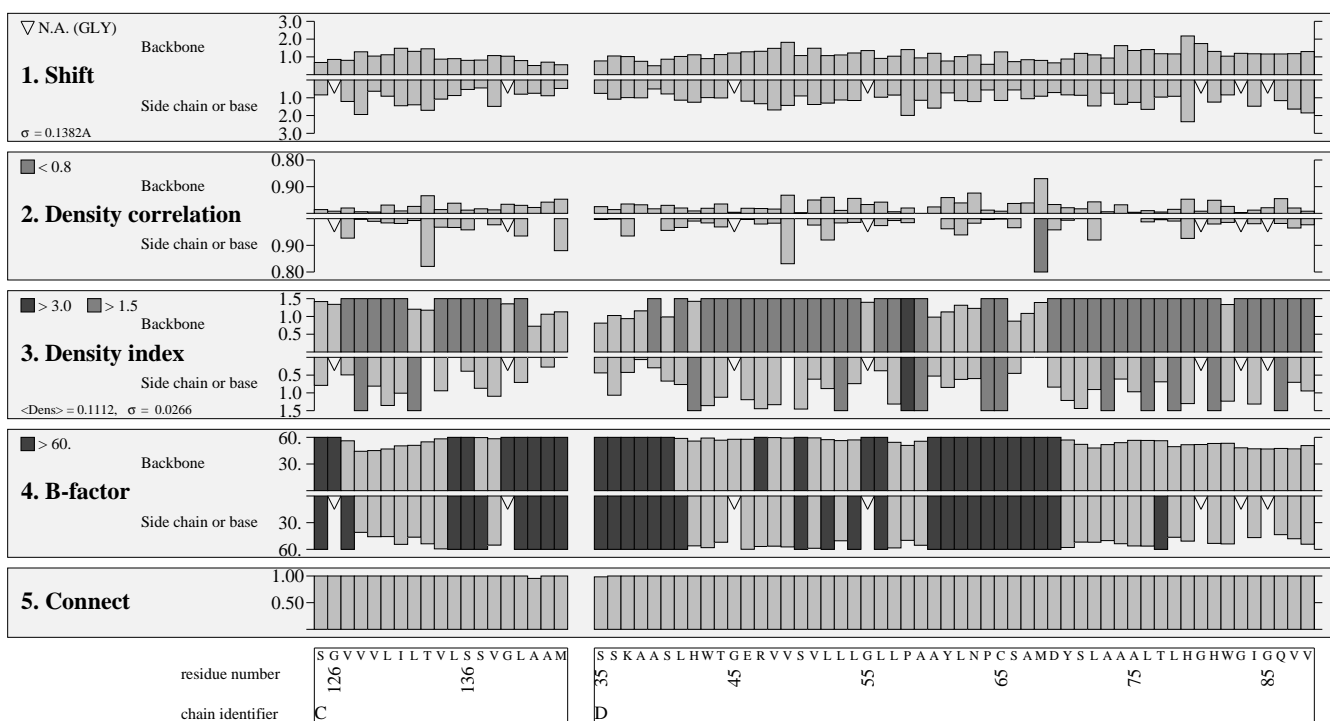
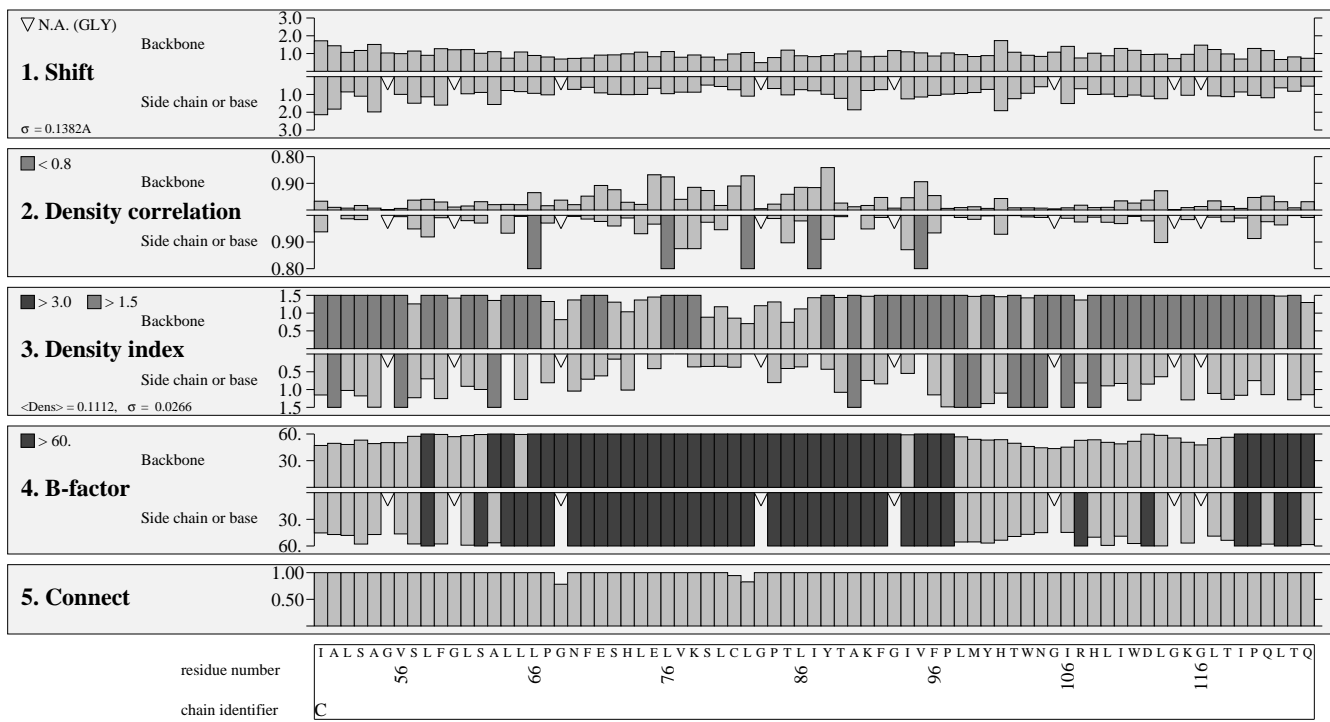
Local estimation (6)



Structure Factor Check

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Local estimation (7)



Structure Factor Check

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Local estimation (8)

