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

Structure Factor Check

4HEI

Title: 2A X−RAY STRUCTURE OF HPF FROM VIBRIO CHOLERAE
Date: 03−OCT−12
PDB code: 4HEI

Crystal

Cell parameters:

a: 46.35 A b: 46.35 A c: 174.49 A
α: 90.00 β: 90.00 γ: 90.00

Space group: P 41 21 2

Model

1675 atoms (138 water molecules)

Number of chains:	21
Volume not occupied by model:	20.4 %
<B> (for atomic model):	31.2 A^2
σ(B):	11.82 A^2
Matthews coefficient:	2.00
Corresponding solvent % :	37.97

Refinement

Program:	CNS 1.1
Nominal resolution range:	43.6 − 1.60 A
Reported R−factor:	0.262
Number of reflections used:	19305
Reported Rfree:	0.28
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		43.6 − 1.60 A
Reflections in file:		19305
Unique reflections	above 0:	19305
	above 1σ:	18763
	above 3σ:	15384

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Nominal resolution range: 43.6 − 1.60 A
\05max. from input data, min. from author\05

Used reflections:	19305
Completeness:	73.7 %
R_stand(F) = <σ(F)>/<F> :	0.034

Anisotropic distribution of Structure Factors
ratio of eigen values: 1.0000 1.0000 0.7278

B_overall (by Patterson):	28.A^2
Optical resolution:	1.44 A
Expected opt. resol. for complete data set:	1.44 A
Estimated minimal error:	0.010 A

Model vs. Structure Factors

R−factor for all reflections:	0.262
Correlation factor:	0.923
R−factor:	0.263

for F > 2.0 σ
nom. resolution range: 43.62 − 1.60A
reflections used: 18807

Rfree:	0.283
Nfree:	1035
R−factor without free−refl.:	0.261
Non free−reflections:	17772
<u> (error in coords by Luzzati plot):	0.272 A
Estimated maximal error:	0.073 A
DPI:	0.147 A

Scaling

Scale:	1.292
Bdiff:	−1.81

Anisothermal Scaling (Beta):
2.0460 2.0460 −0.0994 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.821 180.546

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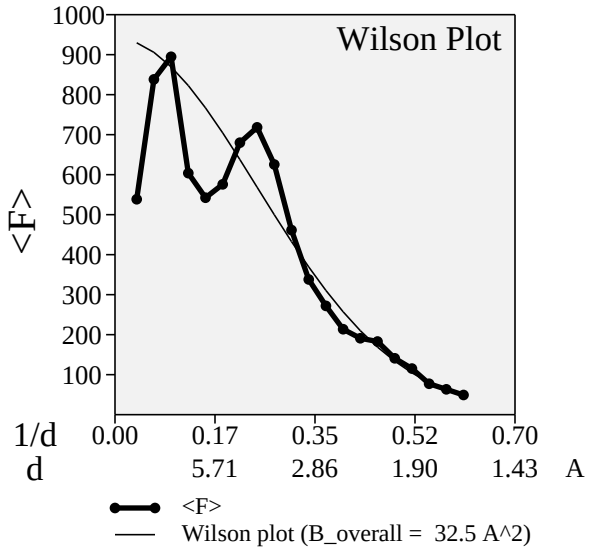
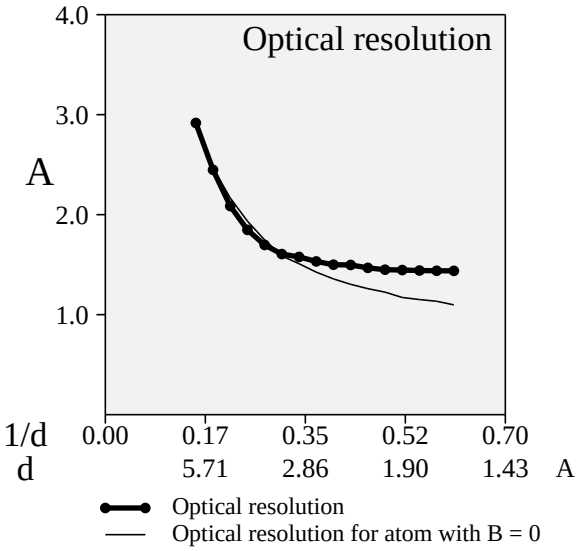
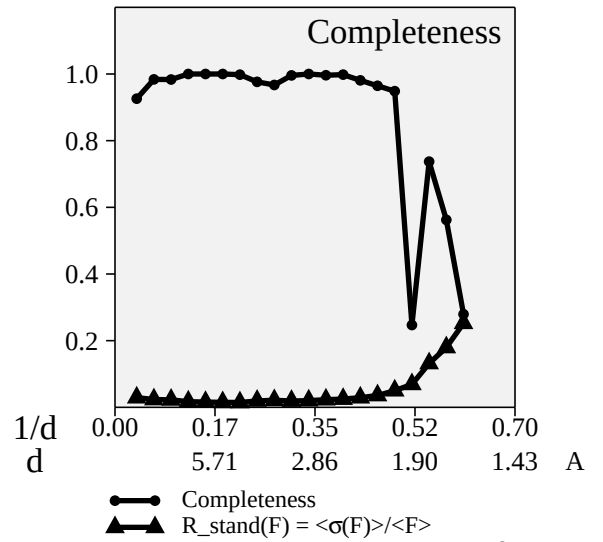
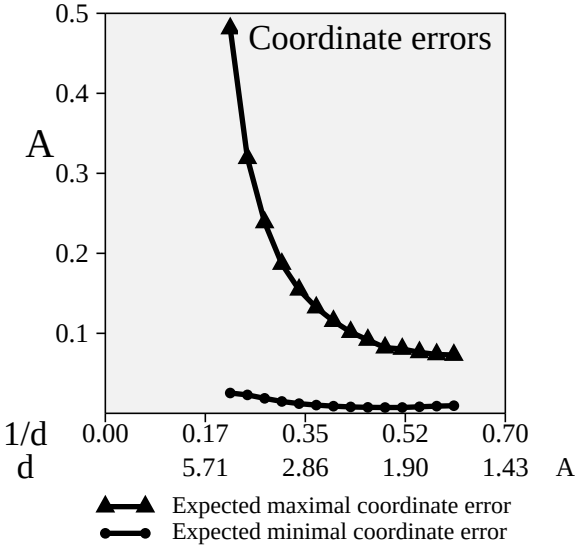
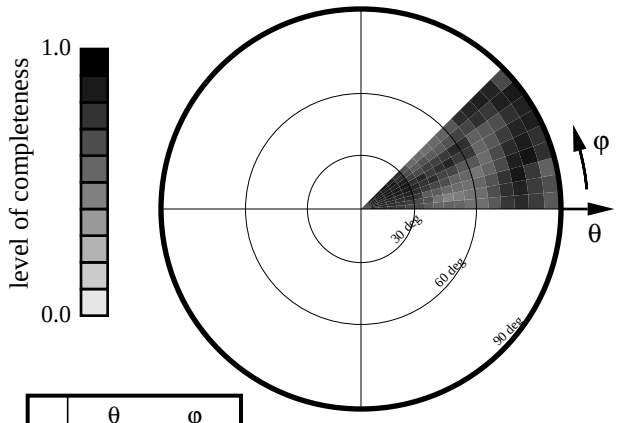






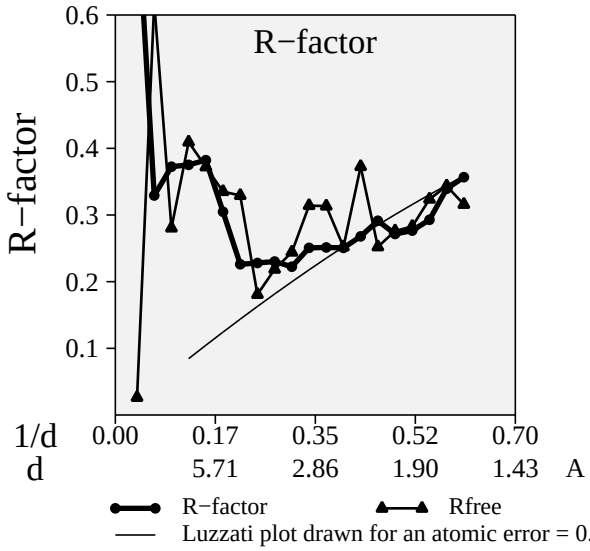


Stereographic projection of
the averaged radial completeness



	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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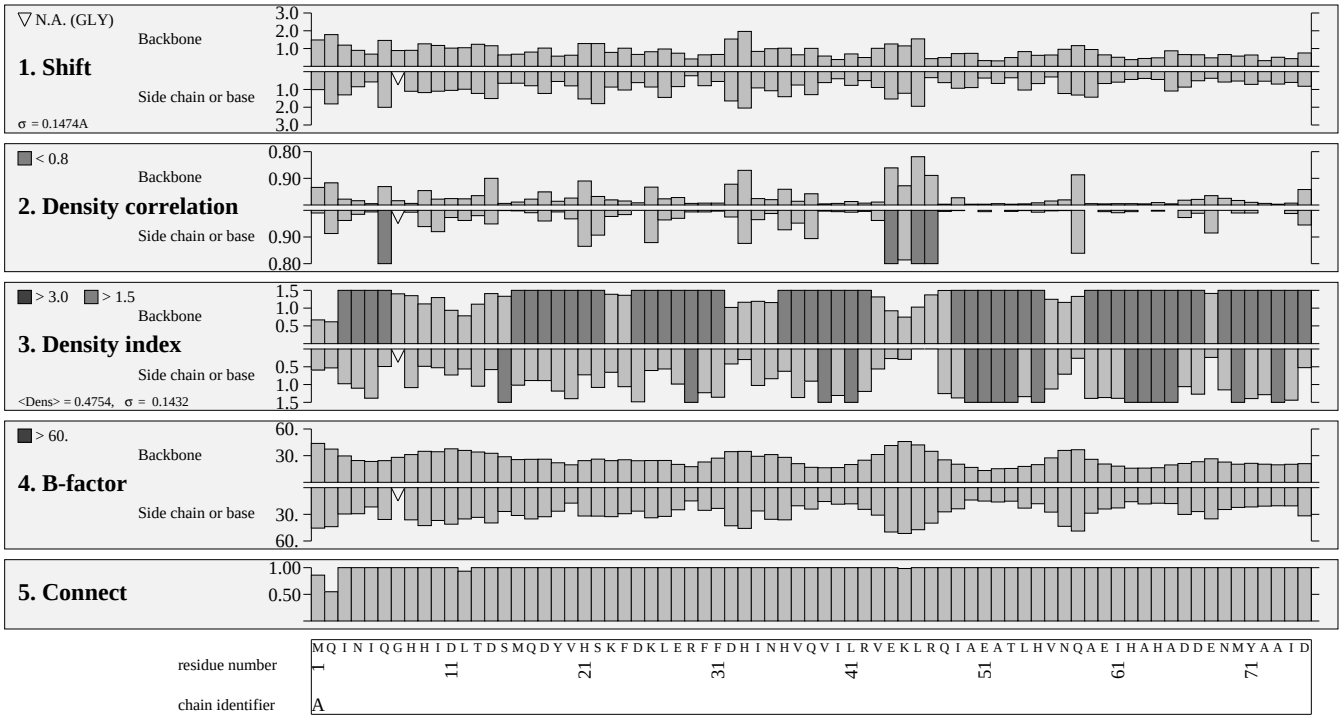
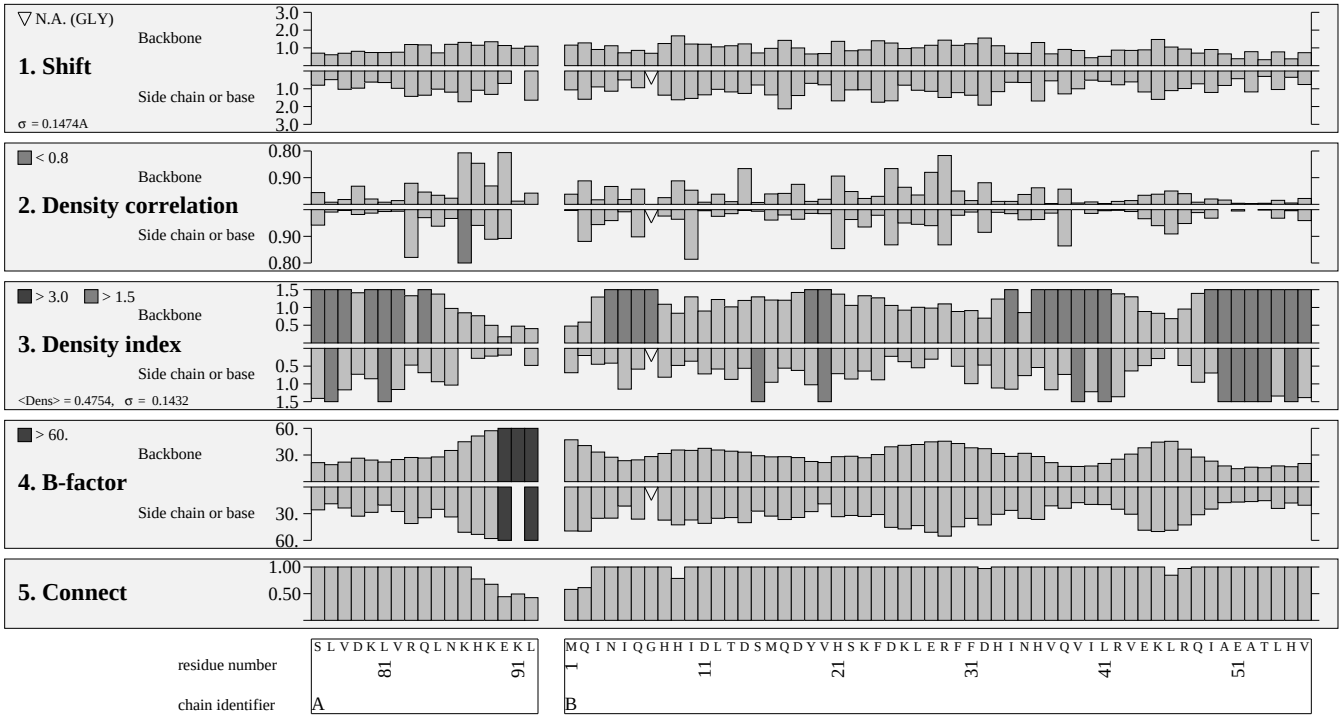
Local estimation





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Structure Factor Check

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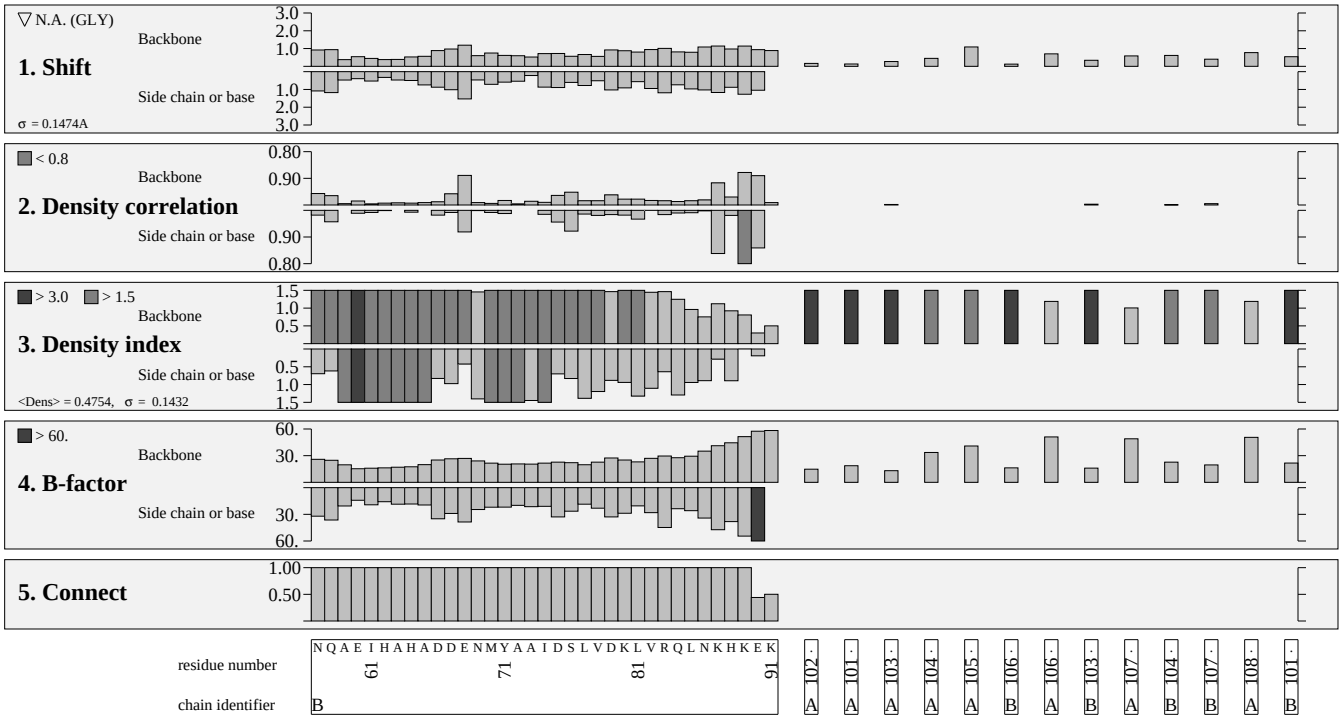
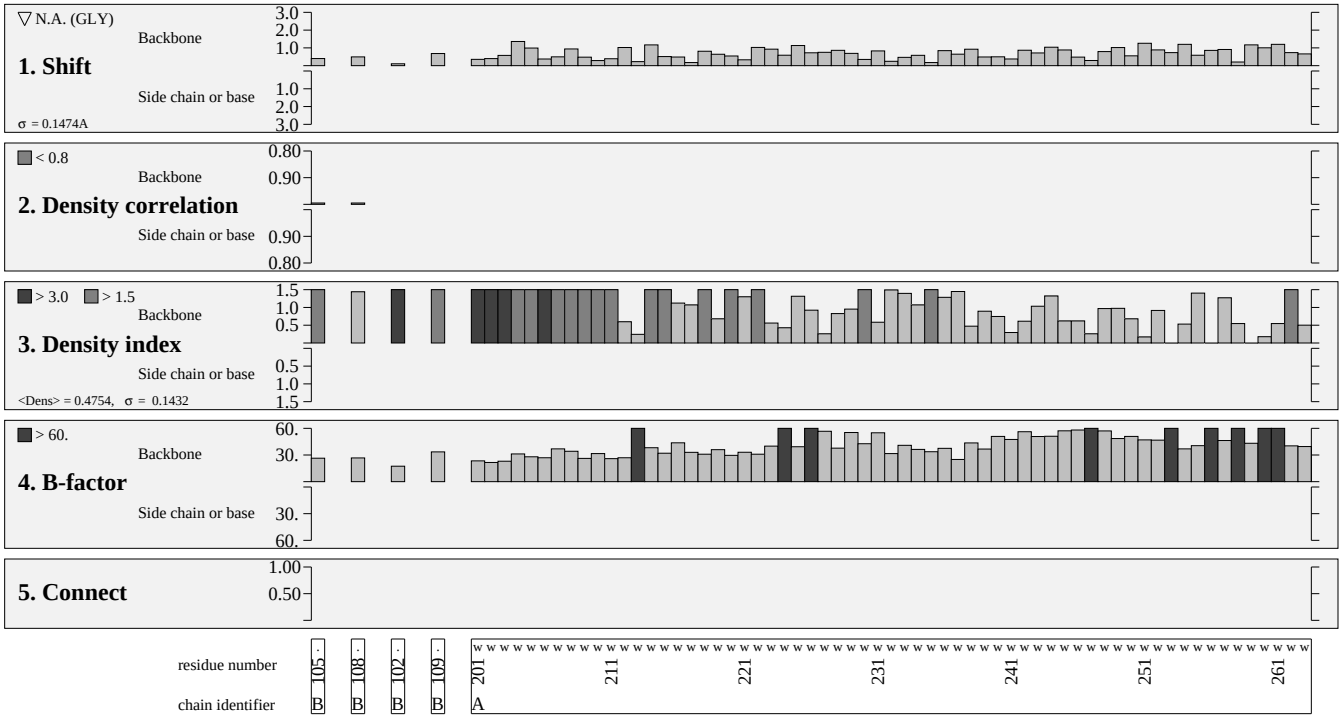
Local estimation (2)





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Local estimation (3)