# Report on BUSTER refinement run in directory ./1pmq_08_rebuild3

## Contents

# 1 Run overview

## 1.1 Run conditions

| | |
|---|---|
| refine command | /mnt/public/xtal/Server-nightly-beta-consortium-linux64/autoBUSTER/bin/-linux64/refine -p 1pmq_07_rebuild2-coot-4_edit.pdb -m dataAnsisotropy-Server.mtz -l 880_cation.grade.cif -Gelly 03_occupancy_refine.Gelly -M TLSbasic -nbig 3 -d /scratch/osmart/2014/11/./1pmq_08_rebuild3 |
| BUSTER version, run at, by user | 2.11.6, Mon Nov 10 10:21:33 GMT 2014, osmart |
| in directory | /home/osmart/2014/11/1pmq_rerefine |
| nthreads, hostname, OS | 6, hypatia, Ubuntu precise (12.04.4 LTS) |
| buster-report command | /public/xtal/Server-nightly-beta-consortium-linux64/scripts/buster-report -d ./-1pmq_08_rebuild3 -f |
| buster-report version, run at, by user | 1.1.3 <July 23 2014>, Mon Nov 10 10:26:17 2014, osmart |
| buster-report run on refine directory | /home/osmart/2014/11/1pmq_rerefine/-1pmq_08_rebuild3 |
| buster-report output directory | /home/osmart/2014/11/1pmq_rerefine/-1pmq_08_rebuild3-report |
| final pdb coordinates | 1pmq_08_rebuild3.pdb |
| final mtzfile | 1pmq_08_rebuild3.mtz |

For help on "Run conditions table" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRrunConditions

## 1.2 Refinement vital statistics

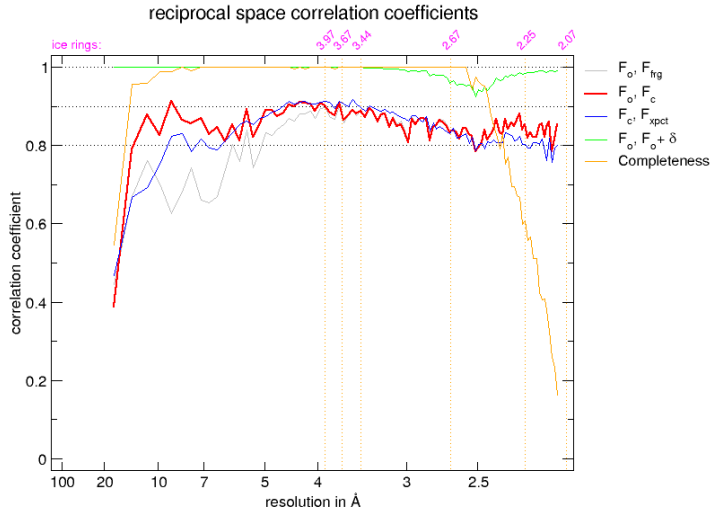
| | start | final |
|---|---|---|
| **$N_{cycles}$ big** | 0 | 3 |
| **$N_{cycles}$ small** | 0 | 126 |
| **X-ray weight** | 5.82 | 5.88 |
| **$R_{work}$** | 0.2185 | 0.1997 |
| **$R_{free}$** | 0.2359 | 0.2256 |
| **100** ($R_{free} - R_{work}$) | 1.7% | 2.6% |
| **$LLG_{work}$** *(cumulative Log-Likelihood Gain, working set)* | 0 | 0.1206 |
| **$LLG_{free}$** *(cumulative Log-Likelihood Gain, free set)* | 0 | -0.0324 |
| **RMS bond in Å** | 0.0100 | 0.0099 |
| **RMS angle in degrees** | 1.02 | 1.00 |
| **High resolution limit in Å** | 2.10 | 2.10 |
| **Low resolution limit in Å** | 16.94 | 16.94 |
| **Number of waters** | 69 | 69 |

For help on "Refinement vital statistics" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRTblVitalStats

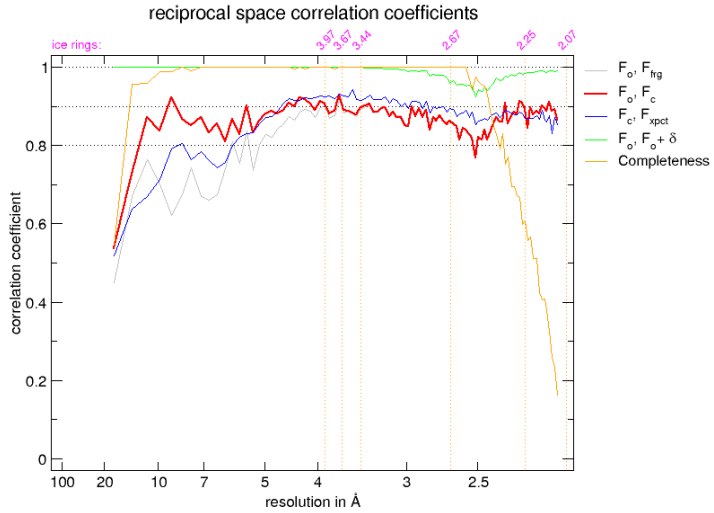
# 2 RSCC, R-factor, LLG and geometry evolution over the refine

## 2.1 Reciprocal space correlation coefficient plots

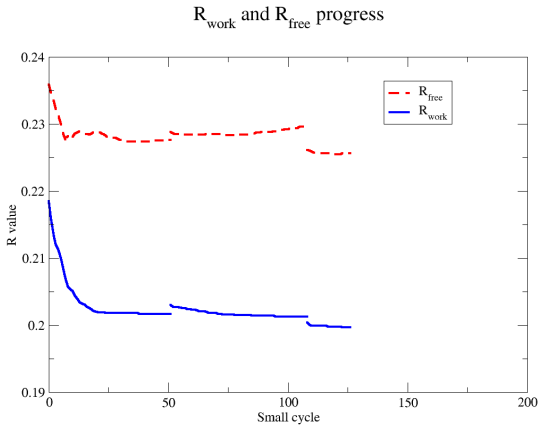
### 2.1.1 Initial RSCC plot



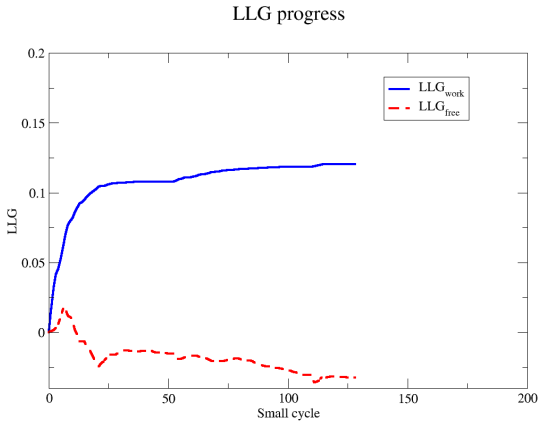

### 2.1.2 Final RSCC plot



## 2.2 R-factor behaviour during refinement

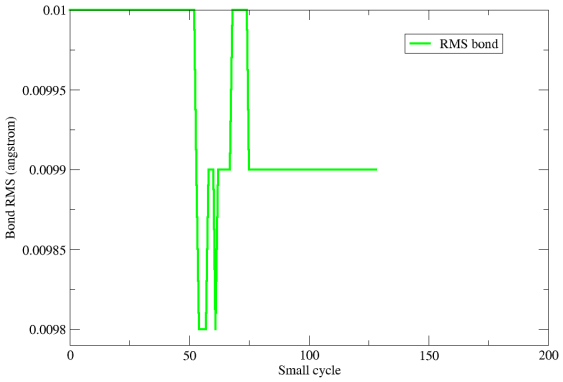



## 2.3 LLG behaviour during refinement

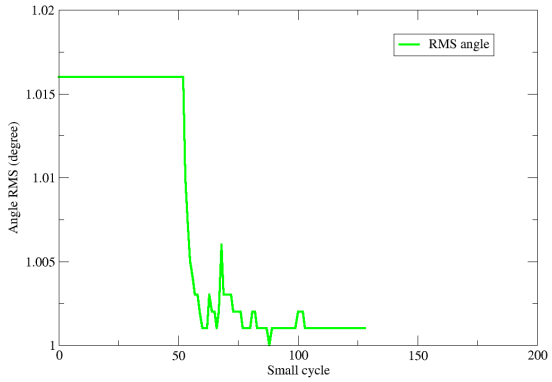


## 2.4 Geometry behaviour during optimisation

### 2.4.1 Graph of RMS(bond) against cycle of refinement




### 2.4.2 Graph of RMS(angle) against cycle of refinement



# 3 MolProbity analysis

## 3.1 Summary statistics

| | | | | |
|---|---|---|---|---|
| All–Atom Contacts | Clashscore, all atoms: | 0.94 | | 100$^{th}$ percentile* N=576, 2.10Å± 0.25Å |
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 2 | 0.71% | Goal: <1% |
| | Ramachandran outliers | 0 | 0.00% | Goal: <0.05% |
| | Ramachandran favored | 312 | 96.59% | Goal: >98% |
| | C$\beta$ deviations >0.25Å | 1 | 0.31% | Goal: 0 |
| | MolProbity score† | 1.00 | | 100$^{th}$ percentile* N=11758, 2.10Å± 0.25Å |
| | Bad backbone bonds: | 0 / 1327 | 0.00% | Goal: 0% |
| | Bad backbone angles: | 0 / 1650 | 0.00% | Goal: <0.1% |

In the two column results, the left column gives the raw count, right column gives the percentage.

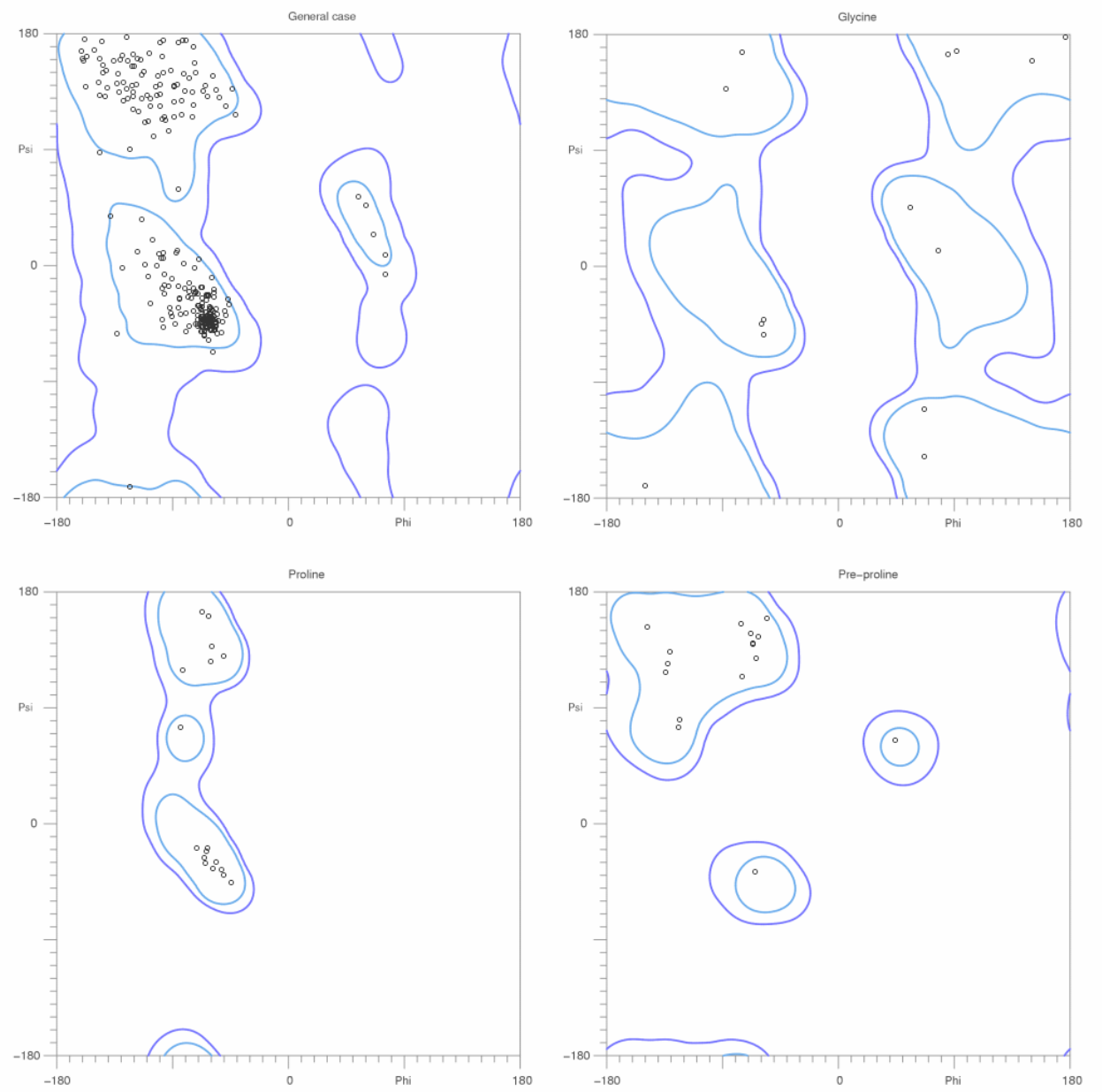
∗ 100$^{th}$ percentile is the best among structures of comparable resolution; 0$^{th}$ is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

For more information see:

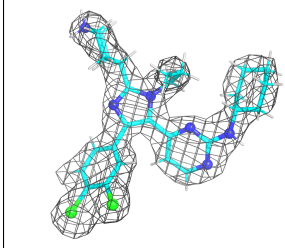
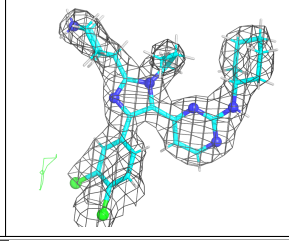
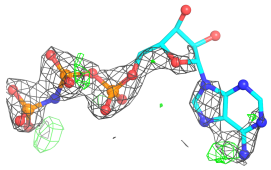
- MolProbity homepage: http://molprobity.biochem.duke.edu/
- MolProbity paper: Chen et al. (2010) "MolProbity: all-atom structure validation for macromolecular crystallography." *Acta Cryst.* **D66**: 12-21. http://dx.doi.org/10.1107/S0907444909042073
- MolProbity Ramachandran plot paper: Lovell et al. (2003) "Structure Validation by C$\alpha$ Geometry: $\phi$, $\psi$ and C$\beta$ Deviation." *Proteins: Struc Func Genet* **50**: 437-450. http://dx.doi.org/10.1002/prot.10286

## 3.2 Ramachandran plot




323 residues were evaluated in total for general, glycine, proline, and pre-pro.
98.14% of all residues were in favored (98%) regions. (317 residues)
100.00% of all residues were in allowed (>99.8%) regions. (323 residues)
There were no outliers.

# 4 Ligand analysis

| Ligand | Picture | Residue in model | $F_o - F_c$ correlation | RMS $z_{bond}$ | RMS $z_{angle}$ |
|---|---|---|---|---|---|
| **880** |  | A 501 A | - | 0.402 | 0.664 |
| |  | A 501 B | - | 0.398 | 0.576 |
| **ANP** |  | A 502 | 0.854 | 1.371 | 0.538 |

## 4.1 Individual outliers

| Ligand | Residue | Term type | Atoms | Observed value | Ideal value | Z |
|---|---|---|---|---|---|---|
| **ANP** | A 502 | BOND | PG-N3B | 1.678 | 1.637 | 5.0 |
| **ANP** | A 502 | BOND | PB-O1B | 1.478 | 1.454 | 2.5 |
| **ANP** | A 502 | BOND | PG-O1G | 1.488 | 1.454 | 3.6 |

# 5 X-ray statistics

## 5.1 Scaling parameters in last cycle

| Refined parameters | | Unrefined parameters | |
|---|---|---|---|
| K_OVER | 0.77384540 | K_MISS | 1.00000000 |
| B_IMPF_FRAG | 0.88584184 | B_MISS | 0.00000000 |
| K_SOLV | 0.73621504 | K_IMPF_MISS | 1.00000000 |
| B_SOLV | 15.16289184 | B_IMPF_MISS | 0.00000000 |
| B_IMPF_SOLV | 51.56237539 | K_IMPF_SOLV | 1.00000000 |
| B_11 | 7.80894464 | B_OVER | 0.00000000 |
| B_22 | -2.94399096 | B_12 | 0.00000000 |
| B_33 | -4.86495367 | B_13 | 0.00000000 |
| | | B_23 | 0.00000000 |

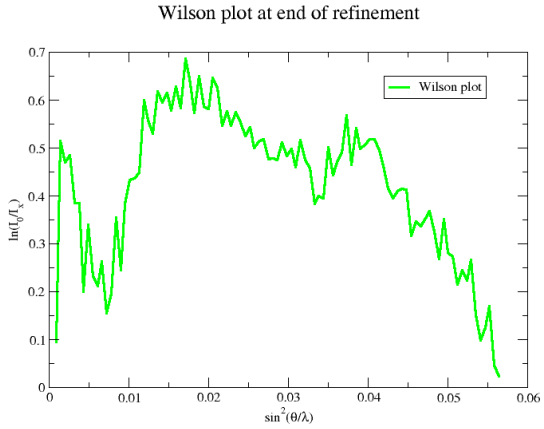
| | |
|---|---|
| Anisotropic ratio | 0.43 |

For help on "X-ray scaling parameters" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRScalingInfo

## 5.2 Wilson plots

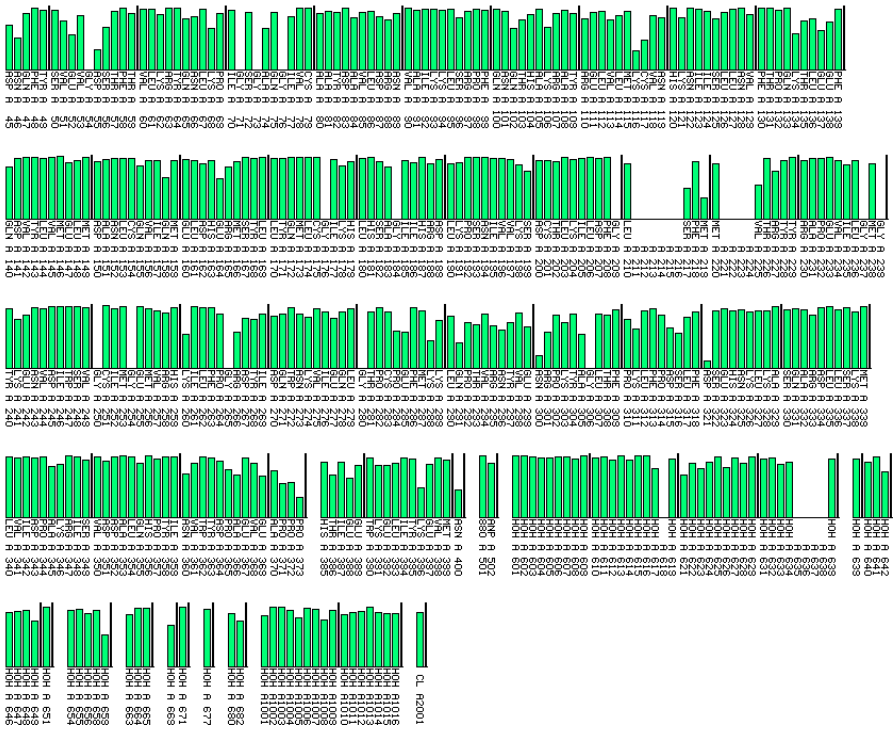
### 5.2.1 Wilson plot at start of refinement


### 5.2.2 Wilson plot at end of refinement



# 6 Real-space correlations

## 6.1 Side chains of chain A



## 6.2 Mainchain of chain A