Report on BUSTER refinement run in directory ./1pmq_06_rebuild1

Contents

1 Run overview

1.1 Geometry WARNING messages

1.1.1 At start of refinement

N.B. initial structure has some really bad geometry restraint violations
Have $|\delta/\sigma|$ deviations > 5.0 σ. Number of outliers for each term:
1 bond lengths. Worst is 19.2 σ 0.90 Å `A|47:C(GLN)=A|48:N(PHE)`
2 bond angles. Worst is 12.2 σ 103.25° `A|47:O(GLN)=A|47:C(GLN)=A|48:N(PHE)`
1 idealD contacts. Worst 5.4 σ 2.13 Å `A|47:O(GLN)=A|48:CA(PHE)`

See logs/screen_initial.txt for more detail

1.2 Run conditions

refine command	/mnt/public/xtal/Server-nightly-beta-consortium-linux64/autoBUSTER/bin/linux64/-refine -p 1pmq_05_dataAnsisotropyServer-edit111-coot-0-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_06_rebuild1
BUSTER version, run at, by user	2.11.6, Sun Nov 9 16:38:19 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_06_rebuild1 -f
buster-report version, run at, by user	1.1.3 <July 23 2014>, Sun Nov 9 16:43:33 2014, osmart
buster-report run on refine directory	/home/osmart/2014/11/1pmq_rerefine/-1pmq_06_rebuild1
buster-report output directory	/home/osmart/2014/11/1pmq_rerefine/-1pmq_06_rebuild1-report
final pdb coordinates	1pmq_06_rebuild1.pdb
final mtzfile	1pmq_06_rebuild1.mtz

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

1.3 Refinement vital statistics

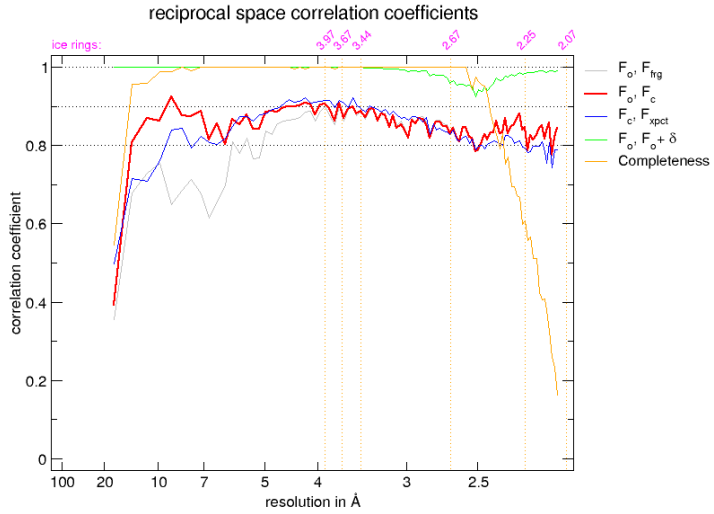
	start	final
N_{cycles} big	0	3
N_{cycles} small	0	137
X-ray weight	5.80	5.31
R_{work}	0.2175	0.2003
R_{free}	0.2307	0.2270
100 $(R_{free} - R_{work})$	1.3%	2.7%
LLG_{work} *(cumulative Log-Likelihood Gain, working set)*	0	0.1007
LLG_{free} *(cumulative Log-Likelihood Gain, free set)*	0	-0.0275
RMS bond in Å	0.0120	0.0091
RMS angle in degrees	1.08	0.99
High resolution limit in Å	2.10	2.10
Low resolution limit in Å	16.94	16.94
Number of waters	60	60

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

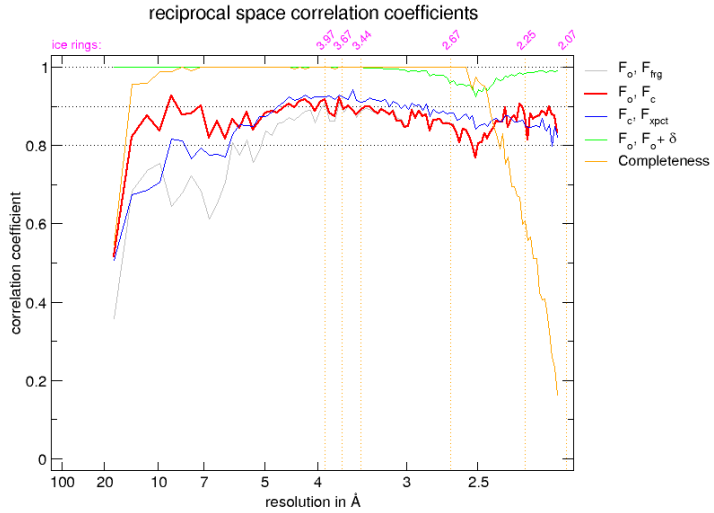
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

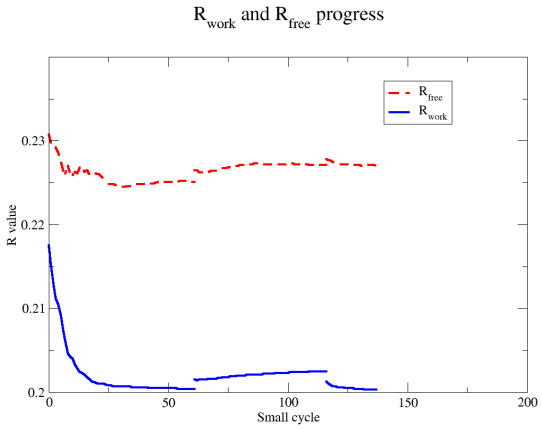
2.1.1 Initial RSCC plot



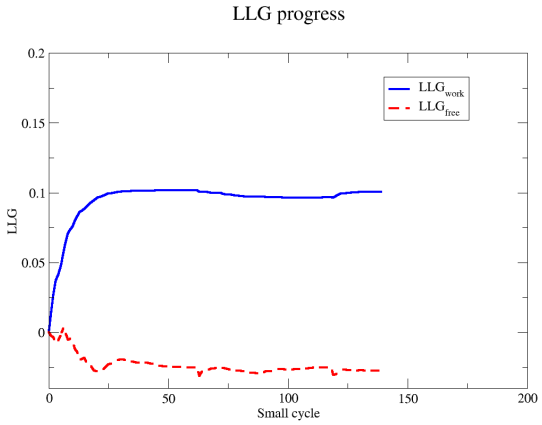
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement

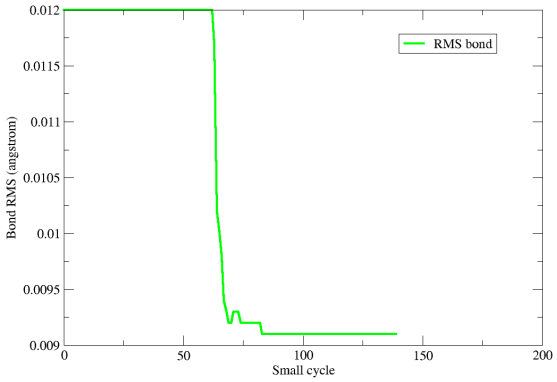


2.3 LLG behaviour during refinement

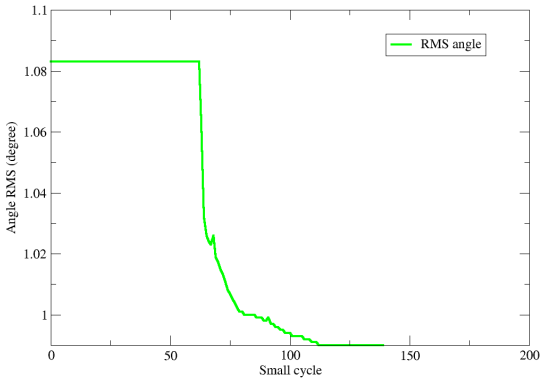


2.4 Geometry behaviour during optimisation

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:	0.88		100th 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	9	2.91%	Goal: <1%
	Ramachandran outliers	2	0.58%	Goal: <0.05%
	Ramachandran favored	327	95.61%	Goal: >98%
	Cβ deviations >0.25Å	1	0.30%	Goal: 0
	MolProbity score†	1.43		99th percentile* N=11758, 2.10Å± 0.25Å
	Bad backbone bonds:	0 / 1389	0.00%	Goal: 0%
	Bad backbone angles:	1 / 1731	0.06%	Goal: <0.1%

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

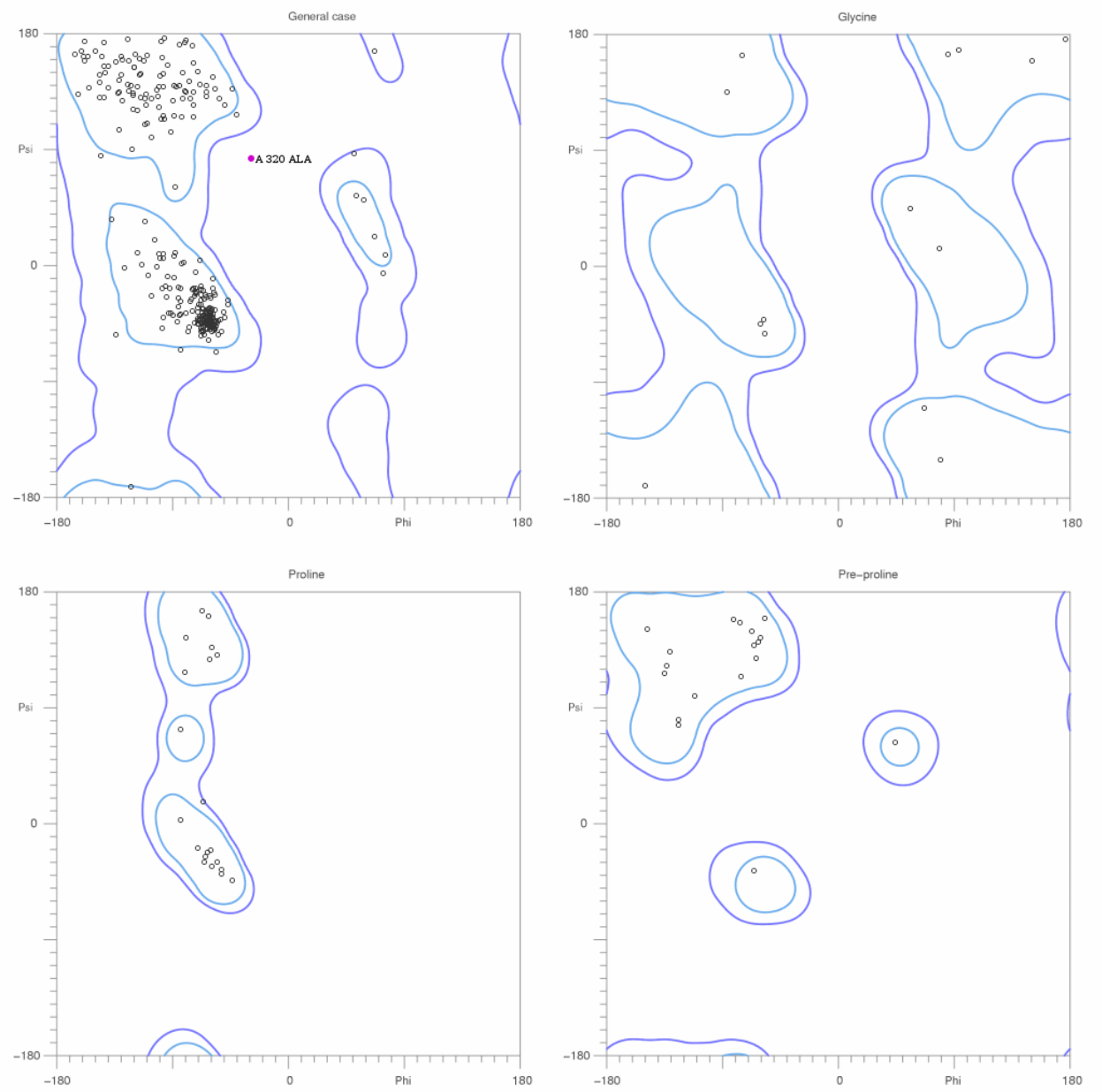
∗ 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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:

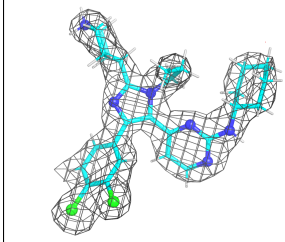
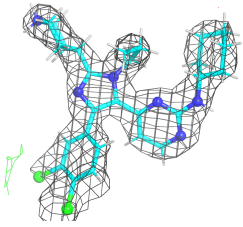
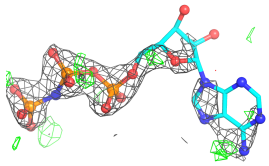
- MolProbity homepage: http://molprobity.biochem.duke.edu/
- MolProbity paper: Chen et al. (2010) "MolProbity: all-atom structure validation for macromolecular crystallography." *Acta Cryst.* **D66**: 12-21. http://dx.doi.org/10.1107/S0907444909042073
- MolProbity Ramachandran plot paper: Lovell et al.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

3.2 Ramachandran plot



342 residues were evaluated in total for general, glycine, proline, and pre-pro.
97.08% of all residues were in favored (98%) regions. (332 residues)
99.71% of all residues were in allowed (>99.8%) regions. (341 residues)
There were 1 outliers:
    A 320 ALA: (phi,psi) = (-27.81, 82.11)

4 Ligand analysis

Ligand	Picture	Residue in model	$F_o - F_c$ correlation	RMS z_{bond}	RMS z_{angle}
880		A 501 A	-	0.378	0.646
		A 501 B	-	0.365	0.571
ANP		A 502	0.852	1.019	0.526

4.1 Individual outliers

Ligand	Residue	Term type	Atoms	Observed value	Ideal value	Z
ANP	A 502	BOND	PG-N3B	1.666	1.637	3.5
ANP	A 502	BOND	PG-O1G	1.480	1.454	2.8

5 X-ray statistics

5.1 Scaling parameters in last cycle

Refined parameters		Unrefined parameters	
K_OVER	0.77769974	K_MISS	1.00000000
B_IMPF_FRAG	1.17596500	B_MISS	0.00000000
K_SOLV	0.75018270	K_IMPF_MISS	1.00000000
B_SOLV	20.83726411	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	41.55582599	K_IMPF_SOLV	1.00000000
B_11	7.61814969	B_OVER	0.00000000
B_22	-2.86393341	B_12	0.00000000
B_33	-4.75421628	B_13	0.00000000
		B_23	0.00000000

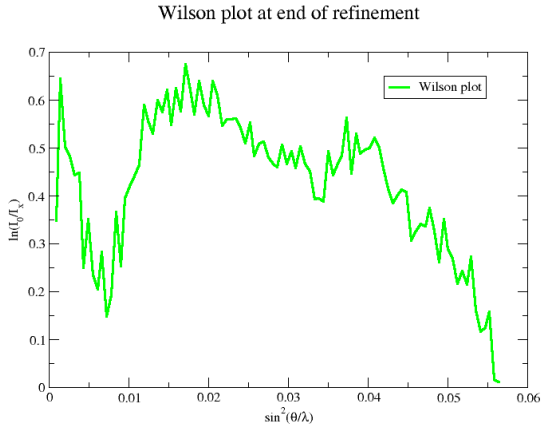
Anisotropic ratio	0.39

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

5.2 Wilson plots

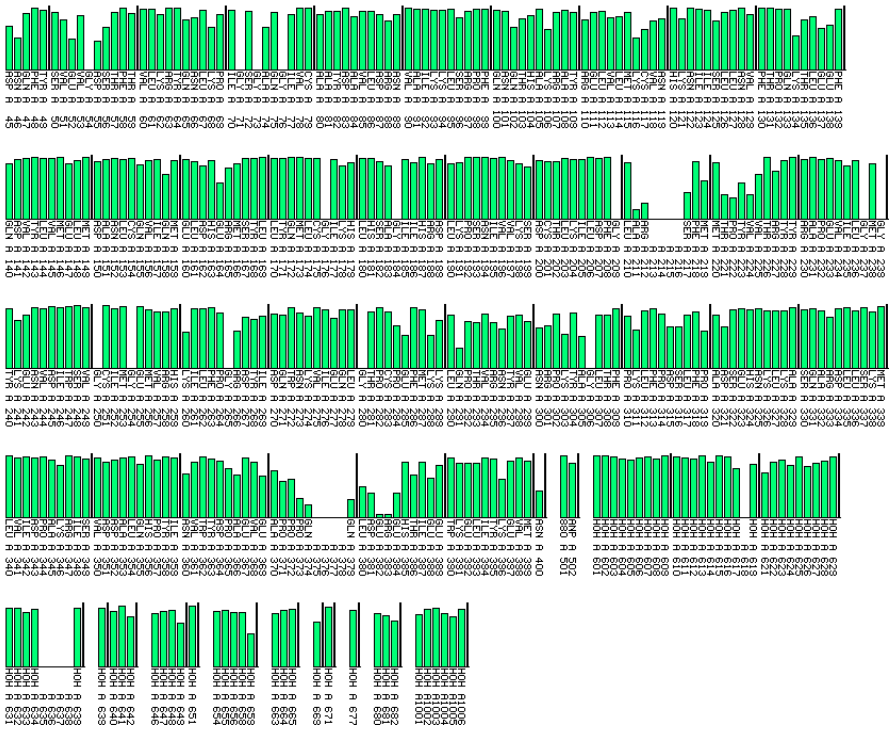
5.2.1 Wilson plot at start of refinement

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