Report on BUSTER refinement run in directory ./1pmq_09_final1

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:
15 bond lengths. Worst is 15.5 σ 0.86 Å `A|502:N3B=HNB1 (ANP)`
2 bond angles. Worst is 6.1 σ 141.16° `A|371:C(PRO)=A|372:N(PRO)=A|372:CD(PRO)`
4 idealD contacts. Worst 9.6 σ 1.52 Å `A|117:O(CYS)=A|373:CB(PRO)`

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_08_rebuild3-coot-1_edit_hydrogenate_ANP_edit.pdb -m dataAnsisotropyServer.mtz -l 880_cation.grade.cif -Gelly 03_occupancy_refine.Gelly -M TLSbasic -nbig 3 -d /scratch/osmart/2014/11/./-1pmq_09_final1
BUSTER version, run at, by user	2.11.6, Mon Nov 10 13:05:34 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_09_final1 -f
buster-report version, run at, by user	1.1.3 <July 23 2014>, Mon Nov 10 13:10:37 2014, osmart
buster-report run on refine directory	/home/osmart/2014/11/1pmq_rerefine/-1pmq_09_final1
buster-report output directory	/home/osmart/2014/11/1pmq_rerefine/-1pmq_09_final1-report
final pdb coordinates	1pmq_09_final1.pdb
final mtzfile	1pmq_09_final1.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

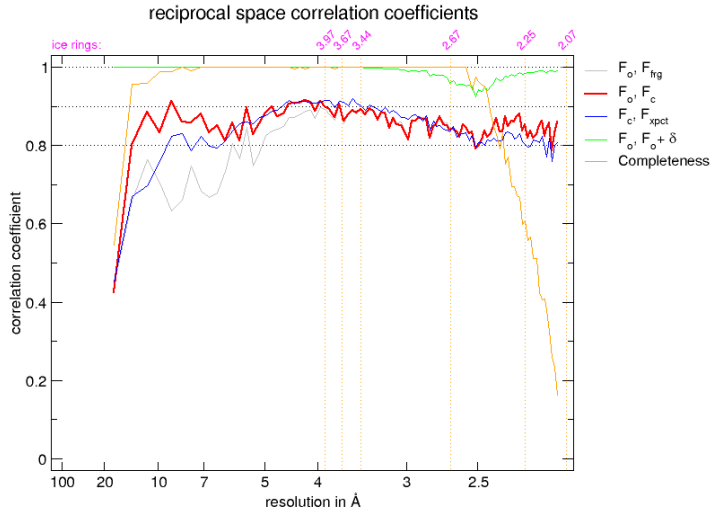
	start	final
N_{cycles} big	0	3
N_{cycles} small	0	136
X-ray weight	5.88	5.43
R_{work}	0.2162	0.2005
R_{free}	0.2357	0.2249
100 ($R_{free} - R_{work}$)	1.9%	2.4%
LLG_{work} *(cumulative Log-Likelihood Gain, working set)*	0	0.1049
LLG_{free} *(cumulative Log-Likelihood Gain, free set)*	0	-0.0222
RMS bond in Å	0.0114	0.0095
RMS angle in degrees	1.07	0.99
High resolution limit in Å	2.10	2.10
Low resolution limit in Å	16.94	16.94
Number of waters	67	67

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

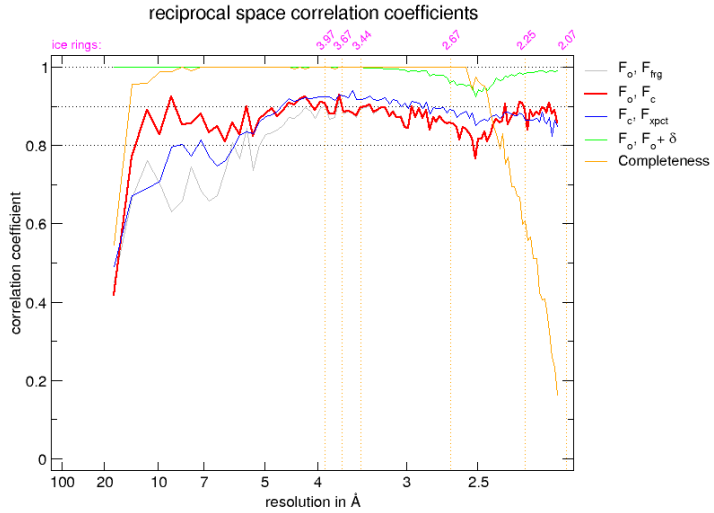
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

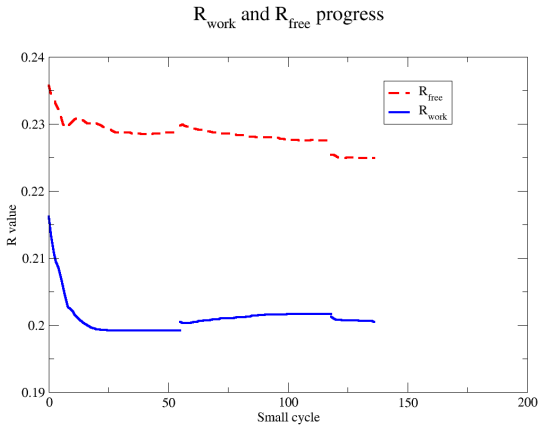
2.1.1 Initial RSCC plot



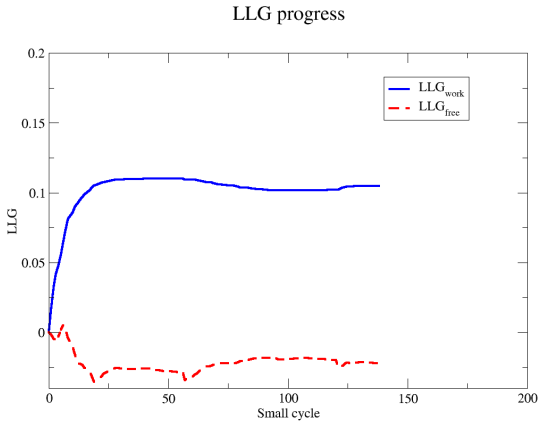
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement

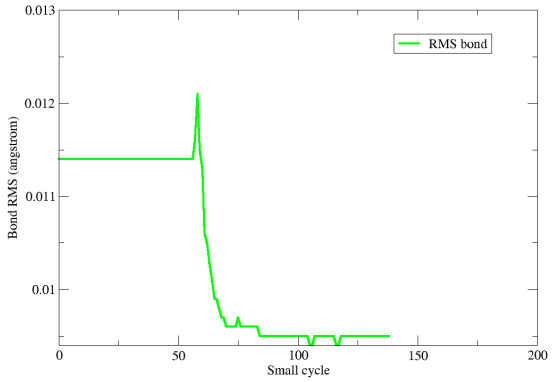


2.3 LLG behaviour during refinement

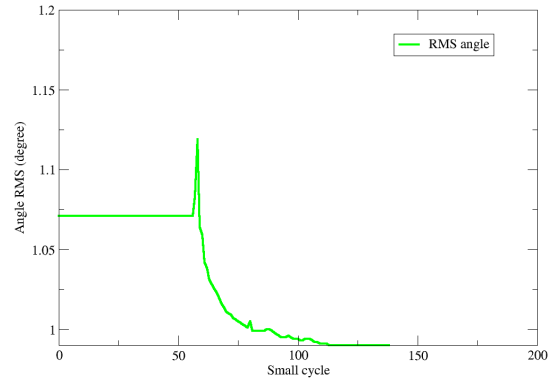


2.4 Geometry behaviour during optimisation

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:	1.13		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	2	0.71%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	312	96.59%	Goal: >98%
	Cβ deviations >0.25Å	1	0.31%	Goal: 0
	MolProbity score†	1.04		100th 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.

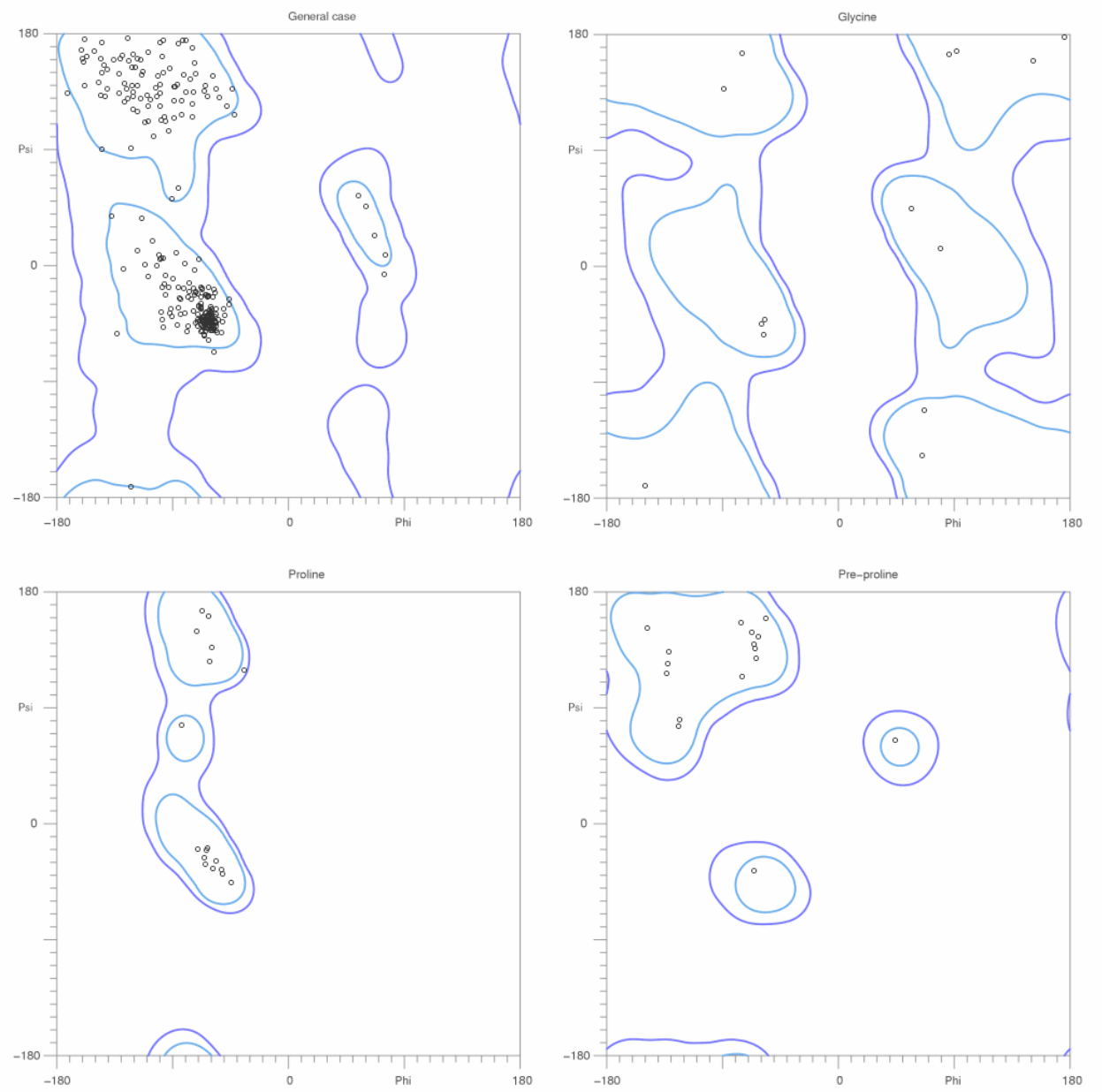
∗ 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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:

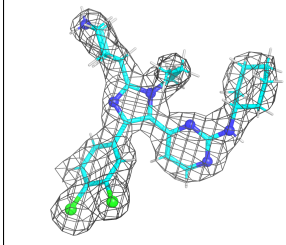
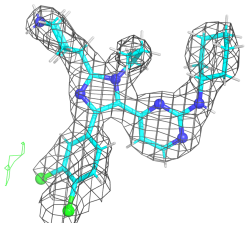
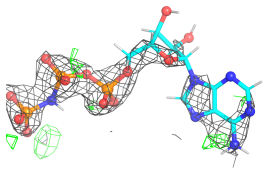
- MolProbity homepage: http://molprobity.biochem.duke.edu/
- MolProbity paper: Chen et al. (2010) "MolProbity: all-atom structure validation for macromolecular crystallography." *Acta Cryst.* **D66**: 12-21. http://dx.doi.org/10.1107/S0907444909042073
- MolProbity Ramachandran plot paper: Lovell et al. (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



323 residues were evaluated in total for general, glycine, proline, and pre-pro.
97.52% of all residues were in favored (98%) regions. (315 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	-	0.390	0.659
		A 501 B	-	0.380	0.577
ANP		A 502	0.861	1.081	0.569

4.1 Individual outliers

Ligand	Residue	Term type	Atoms	Observed value	Ideal value	Z
ANP	A 502	BOND	PG-N3B	1.669	1.637	3.9
ANP	A 502	BOND	PG-O1G	1.483	1.454	3.1

5 X-ray statistics

5.1 Scaling parameters in last cycle

Refined parameters		**Unrefined parameters**	
K_OVER	0.77324101	K_MISS	1.00000000
B_IMPF_FRAG	0.94103661	B_MISS	0.00000000
K_SOLV	0.74779332	K_IMPF_MISS	1.00000000
B_SOLV	15.68984174	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	49.97886645	K_IMPF_SOLV	1.00000000
B_11	7.78026578	B_OVER	0.00000000
B_22	-3.03733855	B_12	0.00000000
B_33	-4.74292723	B_13	0.00000000
		B_23	0.00000000

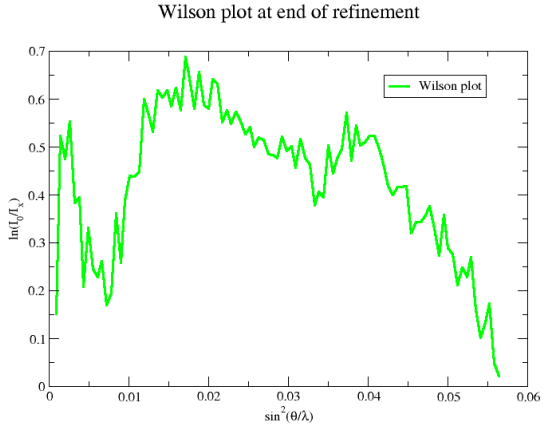
Anisotropic ratio	0.43

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

5.2 Wilson plots

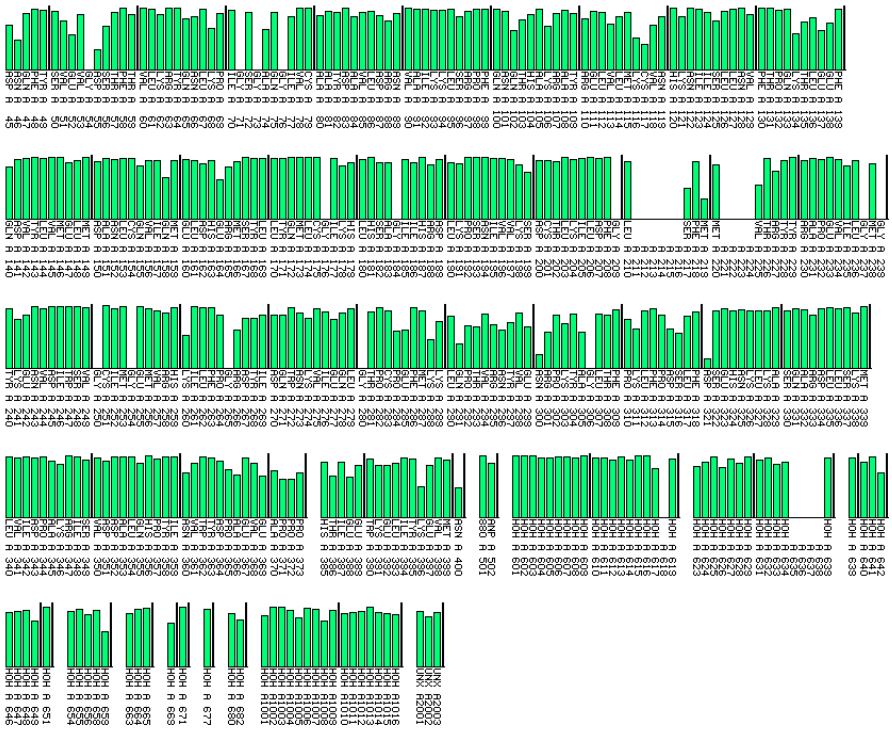
5.2.1 Wilson plot at start of refinement

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