

Report on BUSTER refinement run in directory ./1pmq_04_ab_cation_two_alts

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1 Run overview

1.1 Run conditions

refine command	<code>/mnt/public/xtal/Server-nightly-beta-consortium-linux64/autoBUSTER/bin/linux64/-refine -p 1pmq_03_cation880-twoalts_init.pdb -m 1pmq/1pmq.mtz -l 880_cation.grade.cif -Gelly 03_occupancy_refine.Gelly -M TLSbasic -nbig 3 -d /scratch/osmart/2014/11/./-1pmq_04_ab_cation_two_alts</code>
BUSTER version, run at, by user in directory	2.11.6, Fri Nov 7 18:24:51 GMT 2014, osmart /home/osmart/2014/11/1pmq_rerefine
nthreads, hostname, OS	6, hypatia, Ubuntu precise (12.04.4 LTS)
buster-report command	<code>/public/xtal/Server-nightly-beta-consortium-linux64/scripts/buster-report -d ./-1pmq_04_ab_cation_two_alts -f</code>
buster-report version, run at, by user	1.1.3 <July 23 2014>, Fri Nov 7 18:31:09 2014, osmart
buster-report run on refine directory	/home/osmart/2014/11/1pmq_rerefine/-1pmq_04_ab_cation_two_alts
buster-report output directory	/home/osmart/2014/11/1pmq_rerefine/-1pmq_04_ab_cation_two_alts-report
final pdb coordinates	1pmq_04_ab_cation_two_alts.pdb
final mtzfile	1pmq_04_ab_cation_two_alts.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

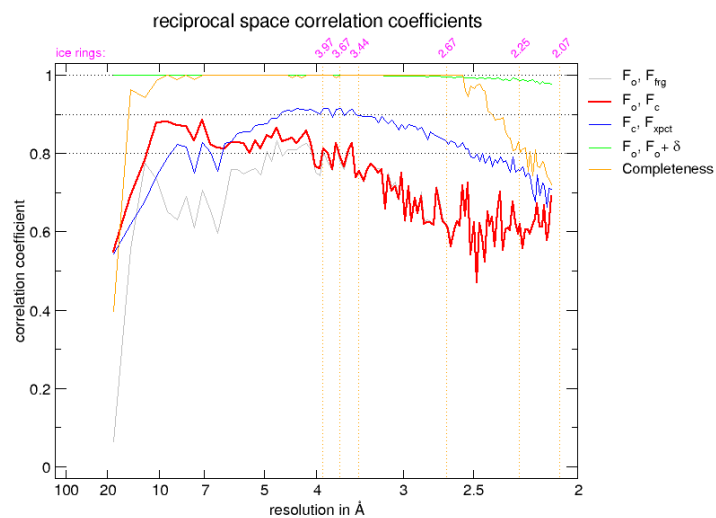
	start	final
N_{cycles} big	0	3
N_{cycles} small	0	144
X-ray weight	4.00	4.90
R_{work}	0.2192	0.2044
R_{free}	0.2459	0.2337
100 (R_{free} - R_{work})	2.7%	2.9%
LLG_{work} (cumulative Log-Likelihood Gain, working set)	0	0.0846
LLG_{free} (cumulative Log-Likelihood Gain, free set)	0	0.0176
RMS bond in Å	0.0094	0.0088
RMS angle in degrees	0.99	0.97
High resolution limit in Å	2.10	2.10
Low resolution limit in Å	16.94	16.94
Number of waters	54	54

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

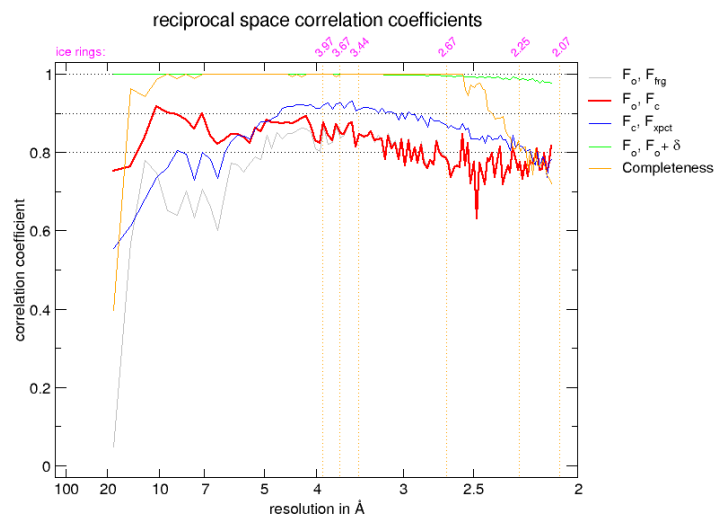
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

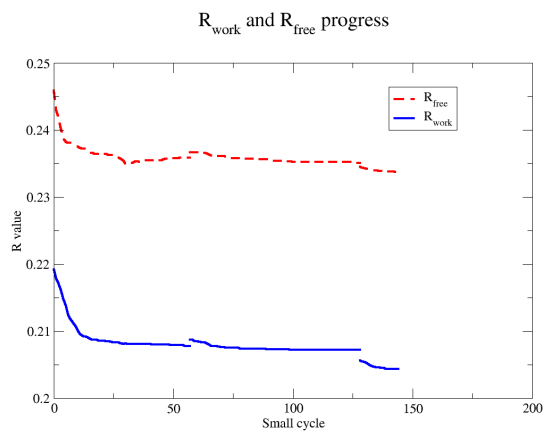
2.1.1 Initial RSCC plot



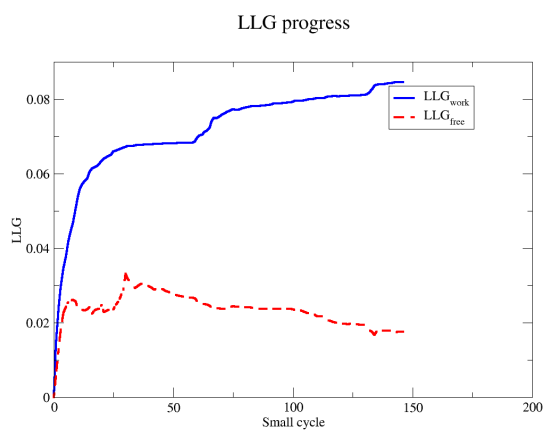
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement

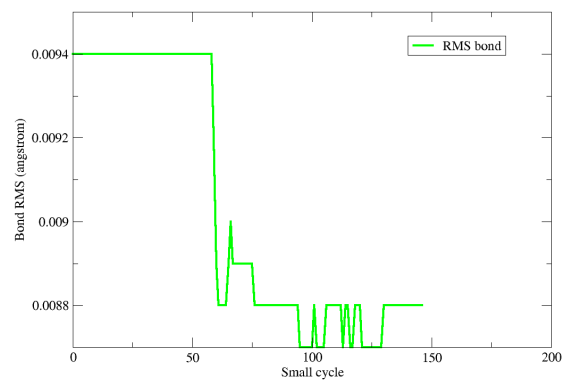


2.3 LLG behaviour during refinement

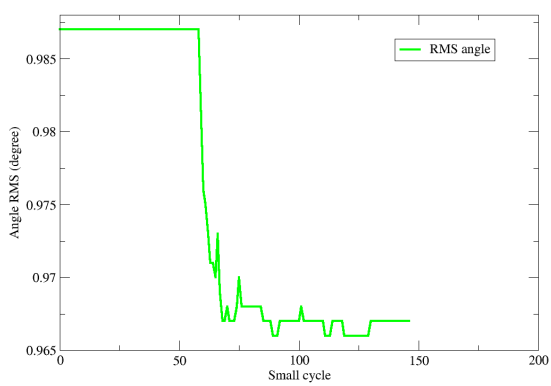


2.4 Geometry behaviour during optimisation

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:	0.7		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	8	2.59%	Goal: <1%
	Ramachandran outliers	2	0.58%	Goal: <0.05%
	Ramachandran favored	329	96.20%	Goal: >98%
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	MolProbity score [†]	1.30		99 th percentile* N=11758, 2.10Å ± 0.25Å
	Bad backbone bonds:	0 / 1389	0.00%	Goal: 0%
Bad backbone angles:	0 / 1731	0.00%	Goal: <0.1%	

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

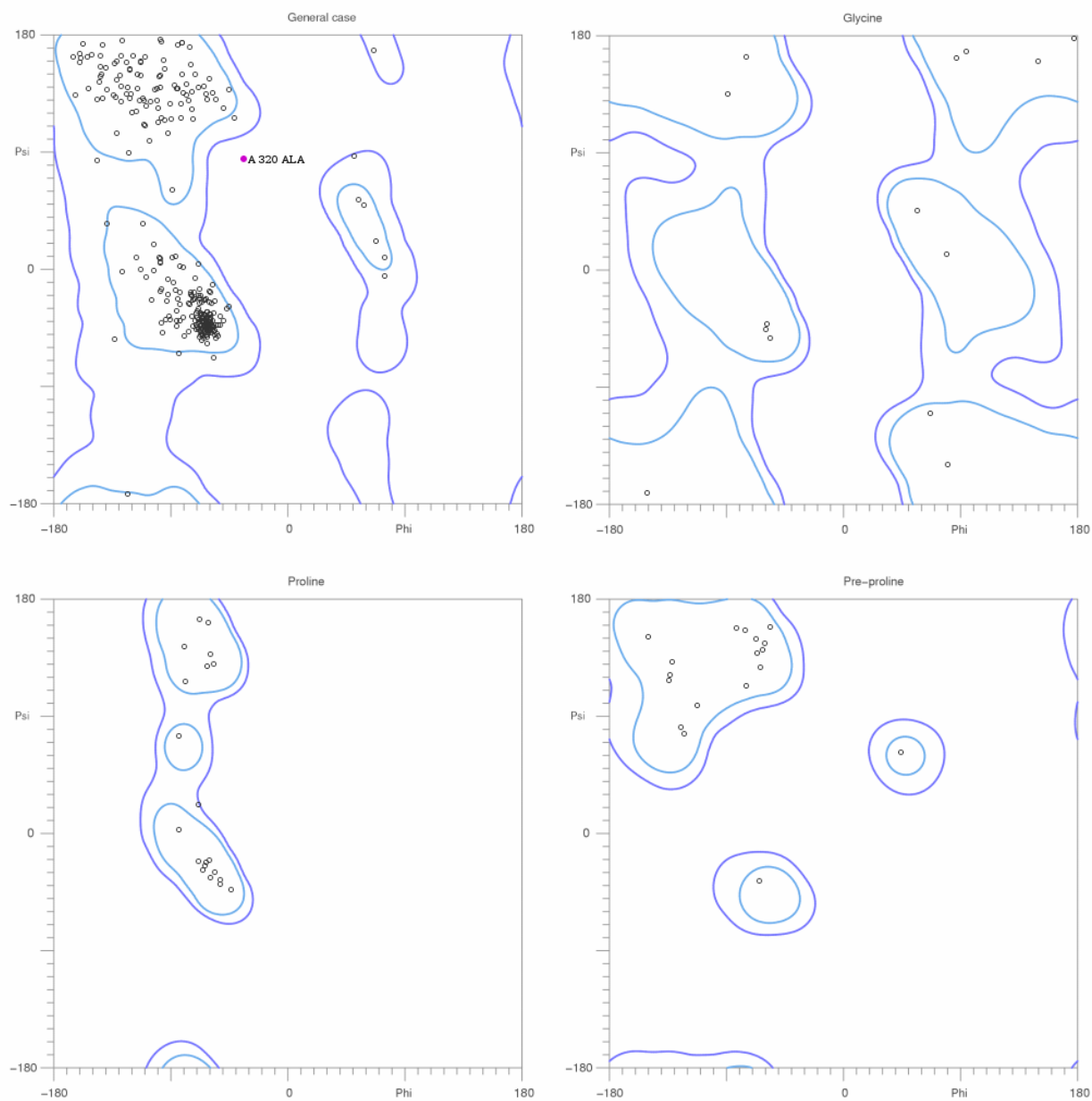
* 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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: Struct 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.

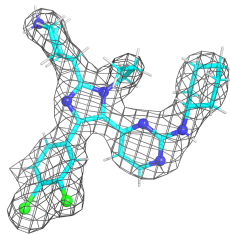
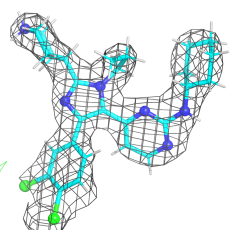
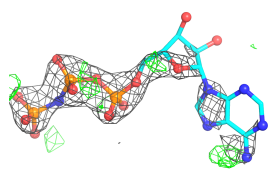
96.78% of all residues were in favored (98%) regions. (331 residues)

99.71% of all residues were in allowed (>99.8%) regions. (341 residues)

There were 1 outliers:

A 320 ALA: (phi,psi) = (-33.10, 84.41)

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	0.662
		A 501 B	-	0.399	0.593
ANP		A 502	0.827	0.902	0.523

4.1 Individual outliers

Ligand	Residue	Term type	Atoms	Observed value	Ideal value	Z
ANP	A 502	BOND	PG-N3B	1.660	1.637	2.7
ANP	A 502	BOND	PG-O1G	1.481	1.454	2.9

5 X-ray statistics

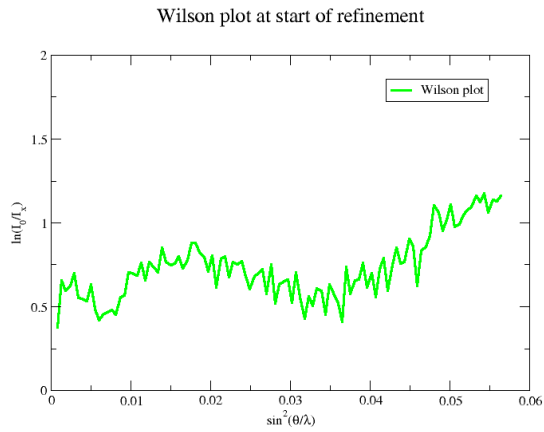
5.1 Scaling parameters in last cycle

Refined parameters		Unrefined parameters	
K_OVER	0.78103234	K_MISS	1.00000000
B_IMPF_FRAG	1.28293565	B_MISS	0.00000000
K_SOLV	0.74726989	K_IMPF_MISS	1.00000000
B_SOLV	41.99591832	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	41.19417746	K_IMPF_SOLV	1.00000000
B_11	-27.53761632	B_OVER	0.00000000
B_22	11.12326672	B_12	0.00000000
B_33	16.41434959	B_13	0.00000000
		B_23	0.00000000
Anisotropic ratio		0.85	

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

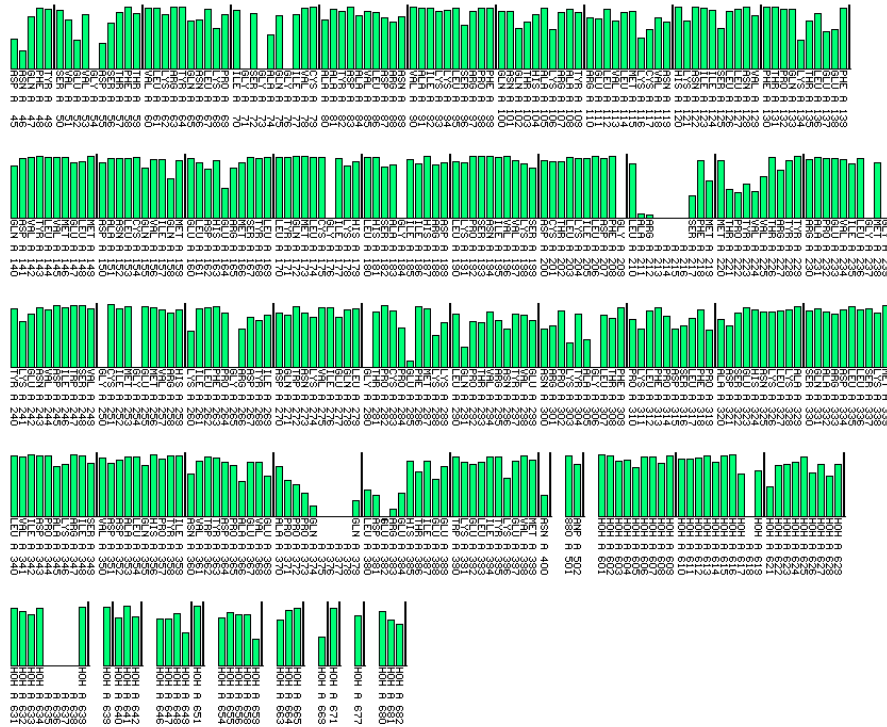


5.2.2 Wilson plot at end of refinement



6 Real-space correlations

6.1 Side chains of chain A



6.2 Mainchain of chain A

