Report on BUSTER refinement run in directory 1pmq_02_refine

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 $> 5.0\ \sigma$. Number of outliers for each term:
47 bond lengths. Worst is 15.5 σ 0.86 Å `A|501:N19=H19 (880)`
12 bond angles. Worst is 12.1 σ 108.55° `A|502:C8=N7=C5 (ANP)`
1 planes. Worst is 11.9 σ 0.24 Å `A|501:N49=C50=N54=C55 (880)`
1 idealD contacts. Worst 5.1 σ 2.67 Å `A|283:SG(CYS)=A|346:NZ(LYS)`

See logs/screen_initial.txt for more detail

1.1.2 At end of refinement (problem with model or restraints?)

N.B. final structure has some really bad geometry restraint violations This is serious - check the final map with `visualise_geometry_coot`
Have $|\delta/\sigma|$ deviations $> 5.0\ \sigma$. Number of outliers for each term:
1 bond angles. Worst is 5.7 σ 140.85° `A|501:C50=N54=C55 (880)`

See logs/screen_final.txt for more detail

1.2 Run conditions

refine command	/software/GPhL/BUSTER_stable_production_20140512/-autoBUSTER/bin/linux64/refine -p 1pmq_hydrogenate_880.pdb -m 1pmq/1pmq.mtz -d 1pmq_02_refine -l 880.grade_PDB_ligand.cif -M TLSbasic
BUSTER version, run at, by user	2.10.1, Thu May 29 07:26:35 BST 2014, osmart
in directory	/home/osmart/erice_workshop/1pmq_tutorial
nthreads, hostname, OS	2, fuji01vm, Ubuntu precise (12.04.4 LTS)
buster-report command	/home/software/GPhL/-BUSTER_stable_production_20140512/scripts/-buster-report -d 1pmq_02_refine
buster-report version, run at, by user	1.1.2 <May 05 2014>, Thu May 29 08:37:45 2014, osmart
buster-report run on refine directory	/home/osmart/erice_workshop/1pmq_tutorial/-1pmq_02_refine
buster-report output directory	/home/osmart/erice_workshop/1pmq_tutorial/-1pmq_02_refine-report
final pdb coordinates	1pmq_02_refine.pdb
final mtzfile	1pmq_02_refine.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

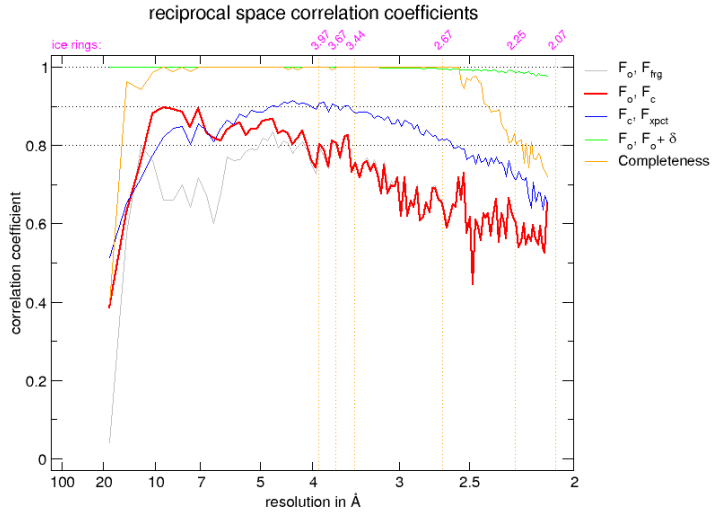
	start	final
N_{cycles} big	0	5
N_{cycles} small	0	285
X-ray weight	4.00	4.49
R_{work}	0.2253	0.2062
R_{free}	0.2636	0.2362
100 ($R_{free} - R_{work}$)	3.8%	3.0%
LLG_{work} *(cumulative Log-Likelihood Gain, working set)*	0	0.1125
LLG_{free} *(cumulative Log-Likelihood Gain, free set)*	0	0.0802
RMS bond in Å	0.0166	0.0090
RMS angle in degrees	1.46	0.99
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

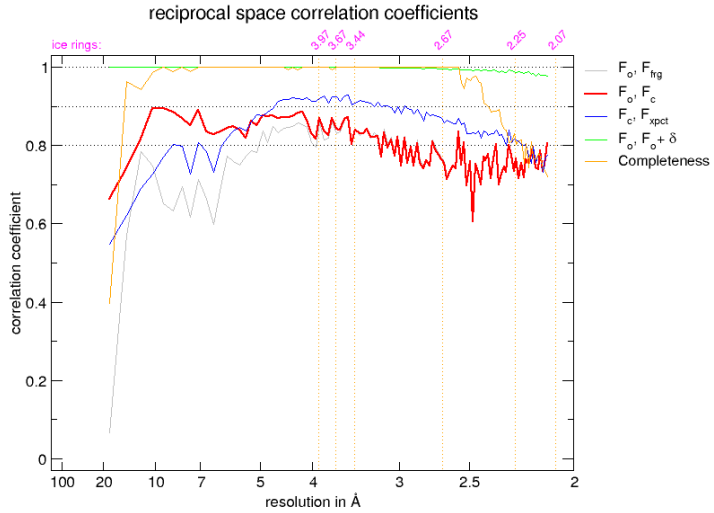
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

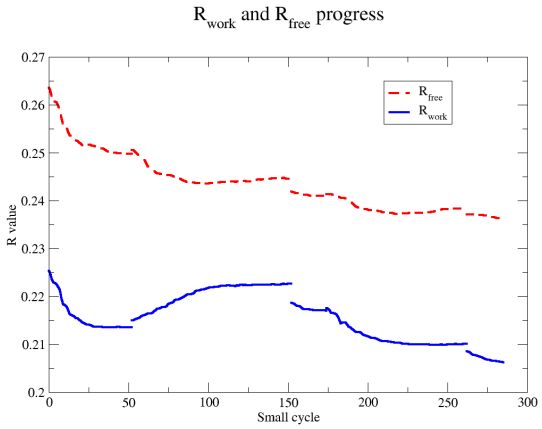
2.1.1 Initial RSCC plot



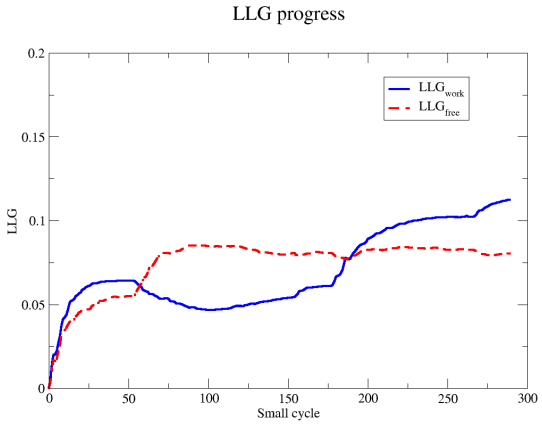
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement

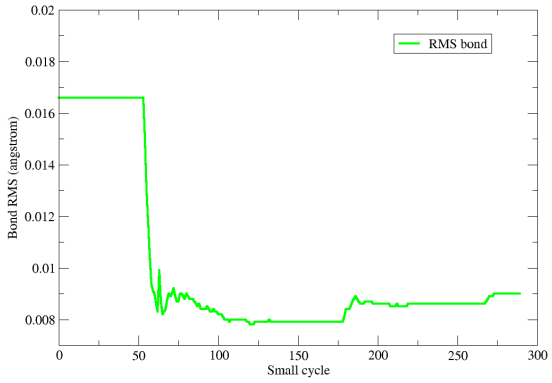


2.3 LLG behaviour during refinement

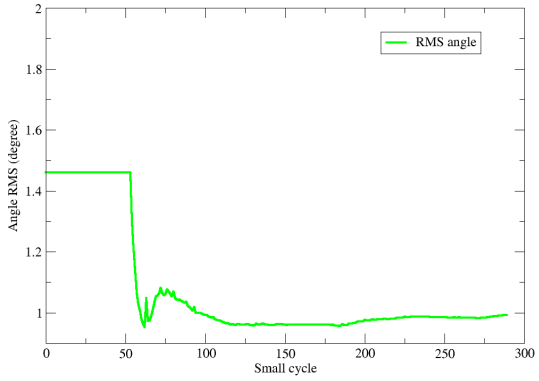


2.4 Geometry behaviour during optimisation

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:	0.35		100th percentile* N=456, 2.20Å± 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	328	95.91%	Goal: >98%
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	MolProbity score†	1.22		100th percentile* N=10167, 2.20Å± 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.

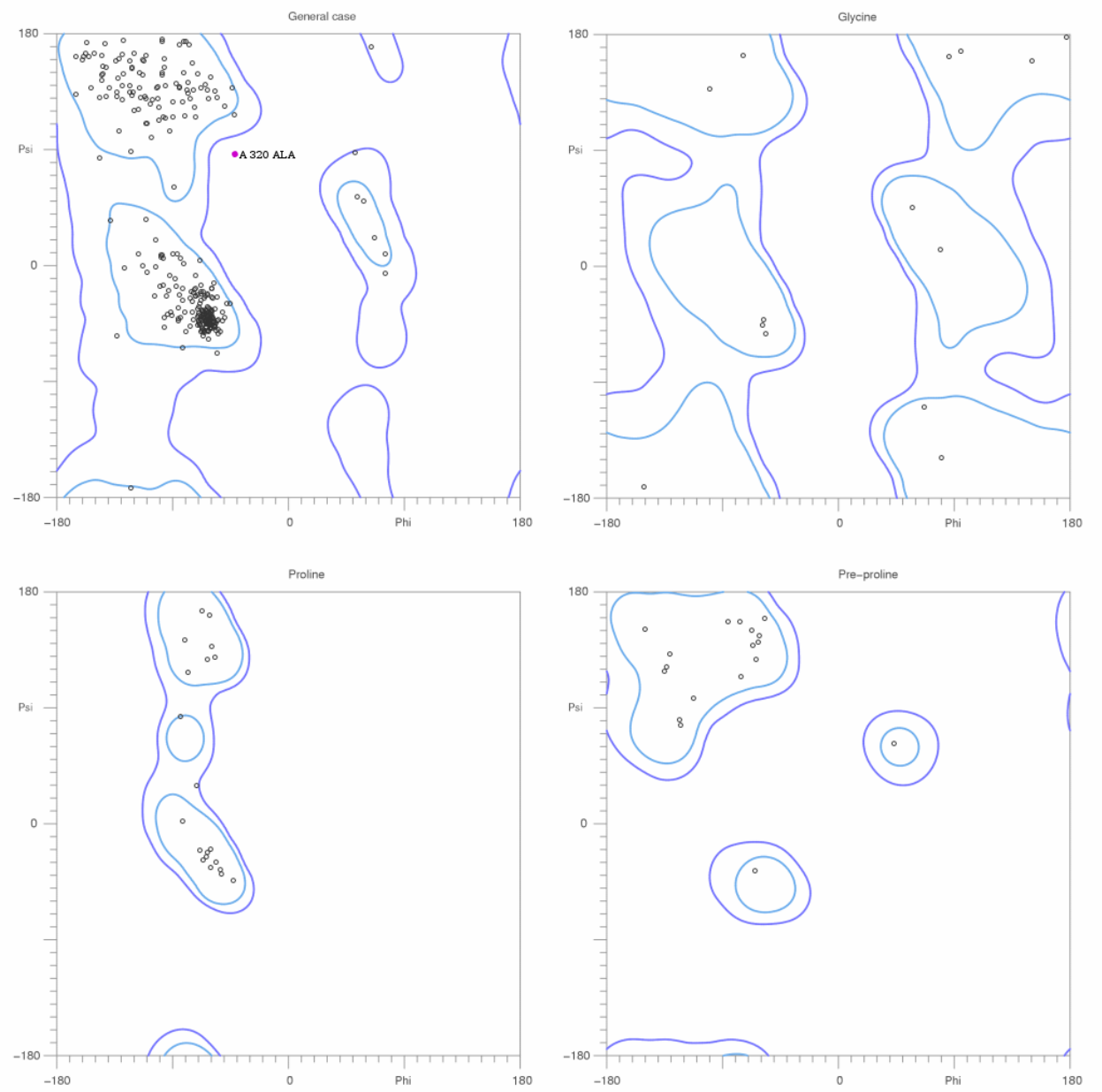
∗ 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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:

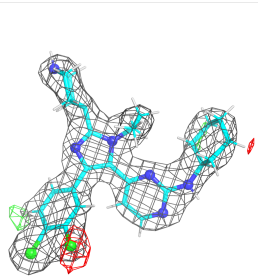
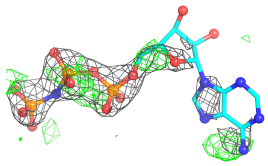
- MolProbity homepage: http://molprobity.biochem.duke.edu/
- MolProbity paper: Chen et al. (2010) "MolProbity: all-atom structure validation for macromolecular crystallography." *Acta Cryst.* **D66**: 12-21. http://dx.doi.org/10.1107/S0907444909042073
- MolProbity Ramachandran plot paper: Lovell et al. (2003) "Structure Validation by Cα Geometry: ϕ, ψ and Cβ Deviation." *Proteins: 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.
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) = (-40.48, 85.71)

4 Ligand analysis

Ligand	Picture	Residue in model	$F_o - F_c$ correlation	RMS z_{bond}	RMS z_{angle}
880		A 501	0.956	0.539	1.043
ANP		A 502	0.790	0.821	0.524

4.1 Individual outliers

Ligand	Residue	Term type	Atoms	Observed value	Ideal value	Z
880	A 501	ANGLE	C56-C55-N54	114.8	110.4	2.8
880	A 501	ANGLE	C5-C36-N51	118.5	115.8	2.6
880	A 501	ANGLE	C60-C55-N54	114.4	110.4	2.6
ANP	A 502	BOND	PG-N3B	1.659	1.637	2.7

5 X-ray statistics

5.1 Scaling parameters in last cycle

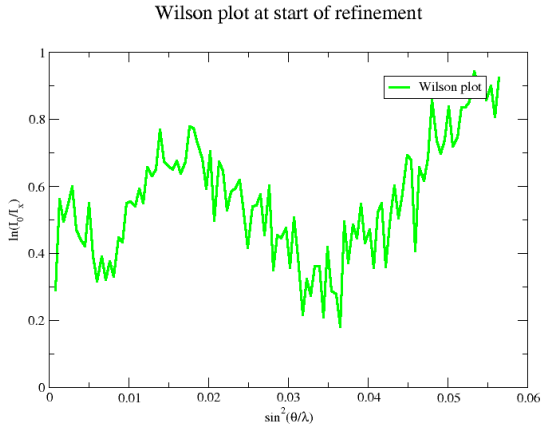
Refined parameters		**Unrefined parameters**	
K_OVER	0.77880594	K_MISS	1.00000000
B_IMPF_FRAG	1.30611781	B_MISS	0.00000000
K_SOLV	0.74735006	K_IMPF_MISS	1.00000000
B_SOLV	42.44850275	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	41.26283878	K_IMPF_SOLV	1.00000000
B_11	-28.58283827	B_OVER	0.00000000
B_22	11.87236777	B_12	0.00000000
B_33	16.71047050	B_13	0.00000000
		B_23	0.00000000

Anisotropic ratio	0.87

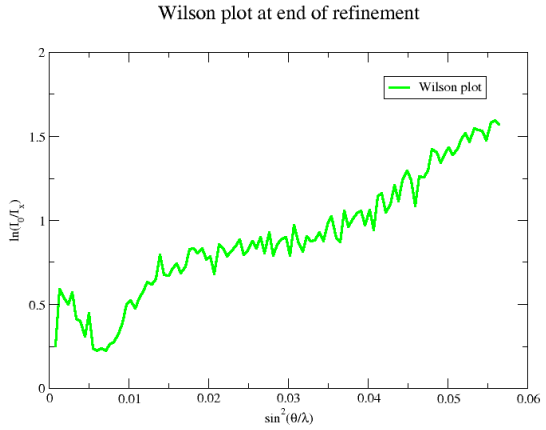
For help on "X-ray scaling parameters" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRScalingInfo

5.2 Wilson plots

5.2.1 Wilson plot at start of refinement

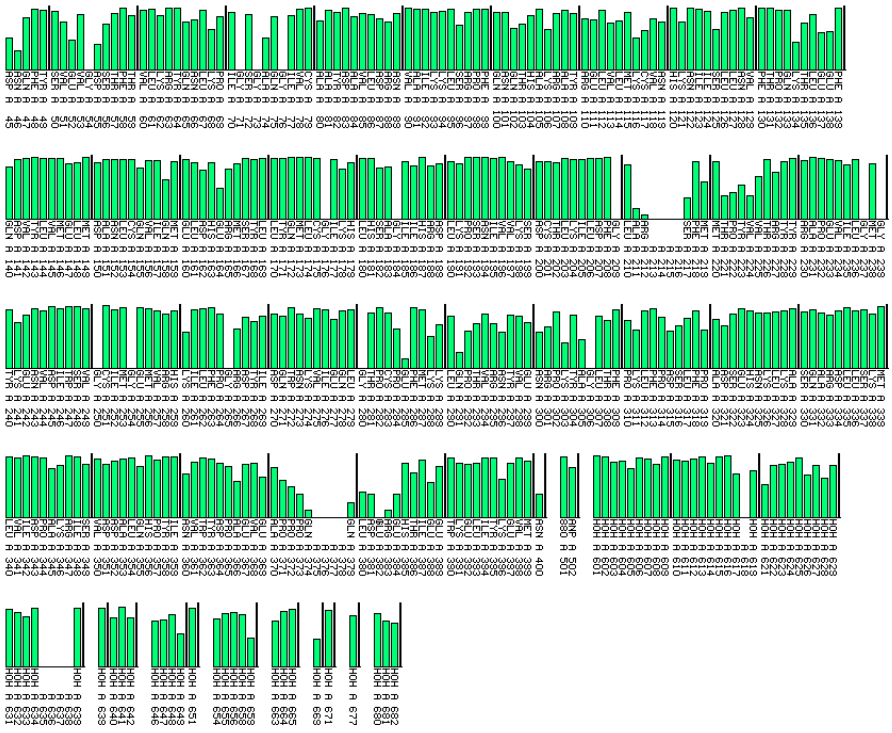


5.2.2 Wilson plot at end of refinement



6 Real-space correlations

6.1 Side chains of chain A



6.2 Mainchain of chain A