Report on BUSTER refinement run in directory 1pmq_01_MapOnly

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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:
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_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_01_MapOnly -l 880.grade_PDB_ligand.cif -M MapOnly -report
BUSTER version, run at, by user	?, Thu May 29 07:24:21 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_01_MapOnly -dreport 1pmq_01_MapOnly.report
buster-report version, run at, by user	1.1.2 <May 05 2014>, Thu May 29 07:25:16 2014, osmart
buster-report run on refine directory	/home/osmart/erice_workshop/1pmq_tutorial/-1pmq_01_MapOnly
buster-report output directory	/home/osmart/erice_workshop/1pmq_tutorial/-1pmq_01_MapOnly.report
final pdb coordinates	1pmq_01_MapOnly.report.pdb
final mtzfile	1pmq_01_MapOnly.report.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

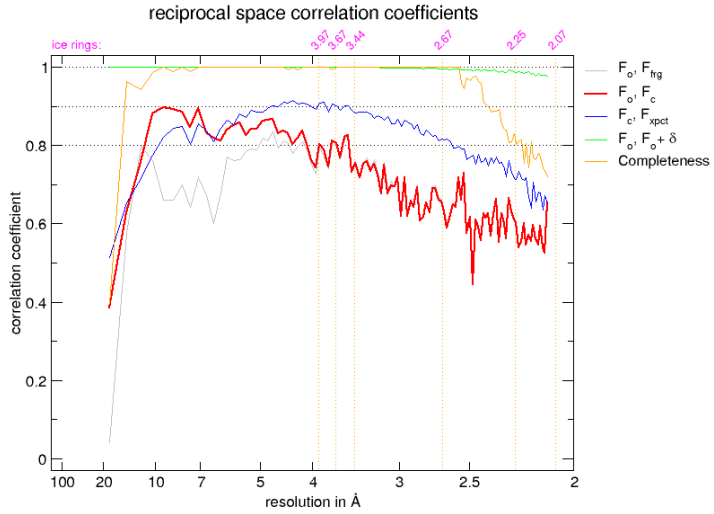
	start	final
N_{cycles} big	0	2
N_{cycles} small	0	0
X-ray weight	n/a	n/a
R_{work}	0.2253	0.2231
R_{free}	0.2636	0.2619
100 $(R_{free} - R_{work})$	3.8%	3.9%
LLG_{work} *(cumulative Log-Likelihood Gain, working set)*	0	0.0000
LLG_{free} *(cumulative Log-Likelihood Gain, free set)*	0	0.0000
High resolution limit in Å	n/a	n/a
Low resolution limit in Å	n/a	n/a
Number of waters	54	54

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

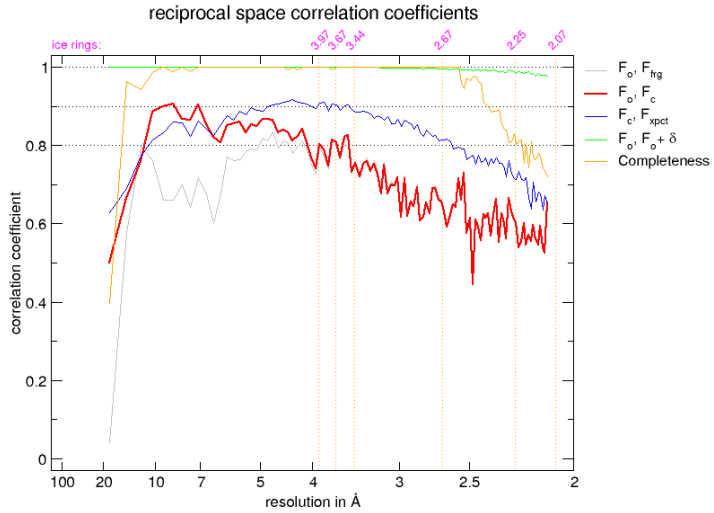
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

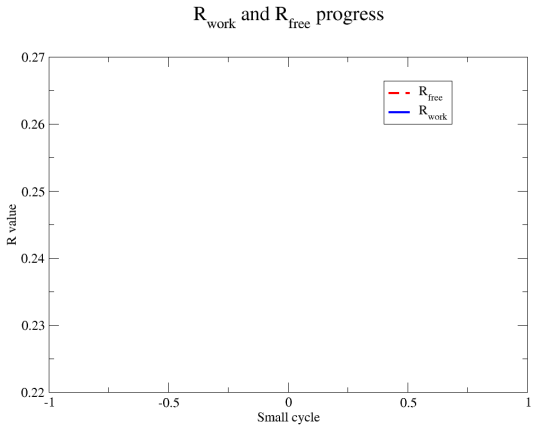
2.1.1 Initial RSCC plot



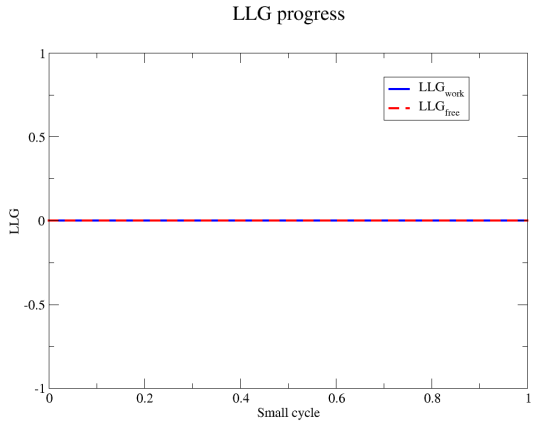
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement



2.3 LLG behaviour during refinement



2.4 Geometry behaviour during optimisation

3 MolProbity analysis

3.1 Summary statistics

All–Atom Contacts	Clashscore, all atoms:	7.39		97th 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	11	3.56%	Goal: <1%
	Ramachandran outliers	3	0.88%	Goal: <0.05%
	Ramachandran favored	321	93.86%	Goal: >98%
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	MolProbity score†	2.23		71st 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.

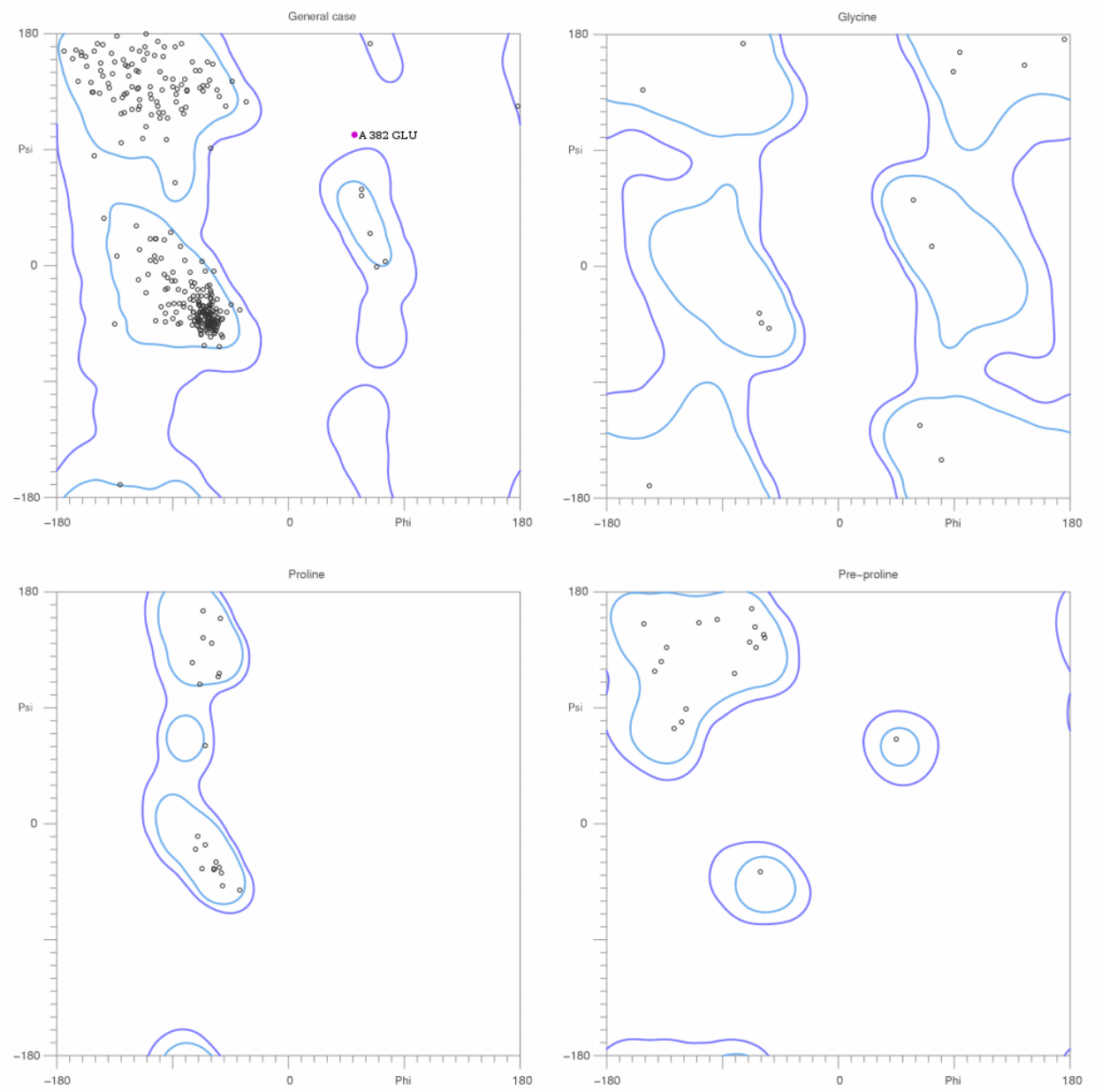
∗ 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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:

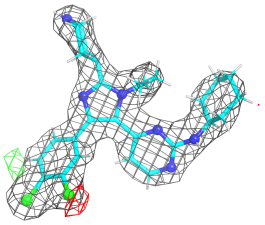
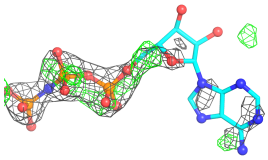
- MolProbity homepage: http://molprobity.biochem.duke.edu/
- MolProbity paper: Chen et al. (2010) "MolProbity: all-atom structure validation for macromolecular crystallography." *Acta Cryst.* **D66**: 12-21. http://dx.doi.org/10.1107/S0907444909042073
- MolProbity Ramachandran plot paper: Lovell et al. (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.
95.61% of all residues were in favored (98%) regions. (327 residues)
99.71% of all residues were in allowed (>99.8%) regions. (341 residues)
There were 1 outliers:
    A 382 GLU: (phi,psi) = (52.05, 100.76)

4 Ligand analysis

Ligand	Picture	Residue in model	$F_o - F_c$ correlation	RMS z_{bond}	RMS z_{angle}
880		A 501	0.950	4.207	3.063
ANP		A 502	0.769	4.747	4.412

4.1 Individual outliers

Ligand	Residue	Term type	Atoms	Observed value	Ideal value	Z
880	A 501	BOND	C17-C18	1.585	1.512	5.2
880	A 501	BOND	C5-C4	1.493	1.377	8.4
880	A 501	BOND	C57-C56	1.559	1.524	3.0
880	A 501	BOND	C17-C16	1.575	1.531	2.9
880	A 501	BOND	C37-C35	1.420	1.391	3.2
880	A 501	BOND	C59-C60	1.571	1.524	4.0
880	A 501	BOND	C5-N1	1.520	1.389	8.8
880	A 501	BOND	C36-N51	1.367	1.341	3.8
880	A 501	BOND	C41-C40	1.466	1.383	9.1
880	A 501	BOND	C47-C36	1.428	1.388	4.0
880	A 501	BOND	C41-C35	1.441	1.391	4.0
880	A 501	BOND	C38-CL45	1.672	1.734	5.1
880	A 501	BOND	C36-C5	1.555	1.478	10.5
880	A 501	BOND	C47-C48	1.418	1.381	3.0
880	A 501	BOND	C2-N3	1.366	1.316	3.4
880	A 501	BOND	C40-C39	1.459	1.384	5.7
880	A 501	BOND	C4-N3	1.443	1.384	4.6
880	A 501	BOND	C21-C16	1.590	1.531	3.9
880	A 501	BOND	C60-C55	1.587	1.518	4.6
880	A 501	BOND	C21-C20	1.595	1.512	6.0
880	A 501	ANGLE	C41-C40-C39	118.1	120.2	2.8
880	A 501	ANGLE	C56-C55-N54	122.7	110.4	7.8
880	A 501	ANGLE	C4-N3-C2	110.4	105.2	3.3
880	A 501	ANGLE	C60-C55-C56	114.9	110.7	5.2
880	A 501	ANGLE	C47-C36-N51	119.7	123.0	3.9

880	A 501	ANGLE	C20-N19-C18	114.6	110.5	3.0
880	A 501	ANGLE	C59-C58-C57	114.7	110.9	3.4
880	A 501	ANGLE	C5-C36-N51	123.6	115.8	7.6
880	A 501	ANGLE	C58-C57-C56	116.0	111.3	4.5
880	A 501	ANGLE	C47-C36-C5	116.2	121.1	4.4
880	A 501	ANGLE	C57-C56-C55	114.0	111.2	3.4
880	A 501	ANGLE	C6-N1-C5	130.4	126.8	2.7
880	A 501	ANGLE	C5-C4-N3	105.2	110.3	4.1
880	A 501	ANGLE	C7-C6-N1	117.5	112.3	2.5
880	A 501	ANGLE	C60-C55-N54	97.7	110.4	8.0
880	A 501	ANGLE	C36-N51-C50	119.0	116.6	2.7
ANP	A 502	BOND	O2'-C2'	1.458	1.423	2.6
ANP	A 502	BOND	PG-N3B	1.572	1.637	8.0
ANP	A 502	BOND	C5-C4	1.476	1.387	7.8
ANP	A 502	BOND	C6-N6	1.384	1.336	3.5
ANP	A 502	BOND	O5'-C5'	1.626	1.443	11.8
ANP	A 502	BOND	C4-N9	1.395	1.374	2.6
ANP	A 502	BOND	PG-O2G	1.546	1.454	9.7
ANP	A 502	BOND	PB-N3B	1.562	1.637	9.1
ANP	A 502	BOND	C5'-C4'	1.539	1.508	2.5
ANP	A 502	BOND	PB-O1B	1.532	1.454	8.2
ANP	A 502	BOND	C8-N7	1.350	1.311	5.1
ANP	A 502	BOND	C4-N3	1.424	1.339	6.8
ANP	A 502	ANGLE	N3-C2-N1	123.3	128.8	6.4
ANP	A 502	ANGLE	C5-N7-C8	108.5	103.7	10.9
ANP	A 502	ANGLE	C5-C4-N9	102.5	105.8	7.3
ANP	A 502	ANGLE	N9-C8-N7	109.0	114.1	7.4
ANP	A 502	ANGLE	O4'-C1'-N9	111.8	108.4	2.6
ANP	A 502	ANGLE	N3-C4-N9	133.5	127.1	5.5
ANP	A 502	ANGLE	O5'-C5'-C4'	102.3	108.7	2.7
ANP	A 502	ANGLE	C6-C5-C4	113.3	117.0	5.6
ANP	A 502	ANGLE	C4-C5-N7	108.7	110.7	3.8
ANP	A 502	ANGLE	C2-N1-C6	123.4	118.6	5.2
ANP	A 502	ANGLE	C5-C4-N3	124.1	126.8	3.8
ANP	A 502	ANGLE	C4-N9-C8	111.3	105.7	12.1
ANP	A 502	ANGLE	O4'-C1'-C2'	110.4	106.5	3.4
ANP	A 502	ANGLE	C6-C5-N7	138.0	132.1	5.5
ANP	A 502	ANGLE	C5-C6-N6	120.6	123.6	2.9
ANP	A 502	ANGLE	C5-C6-N1	120.6	117.6	4.1
ANP	A 502	ANGLE	C5'-C4'-C3'	110.3	115.3	2.8

5 X-ray statistics

5.1 Scaling parameters in last cycle

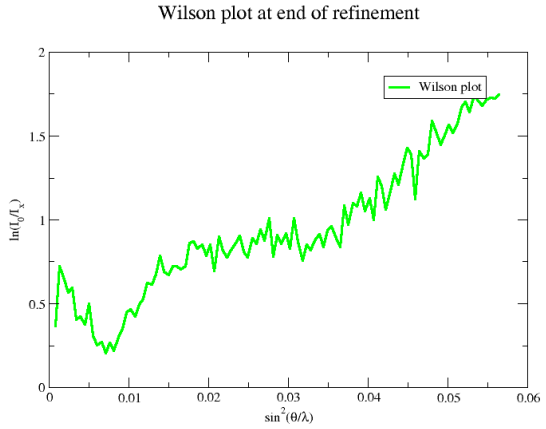
Refined parameters		Unrefined parameters	
K_OVER	0.78579614	K_MISS	1.00000000
B_IMPF_FRAG	2.30750020	B_MISS	0.00000000
K_SOLV	0.66124584	K_IMPF_MISS	1.00000000
B_SOLV	70.43197712	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	19.60604606	K_IMPF_SOLV	1.00000000
B_11	-34.04047314	B_OVER	0.00000000
B_22	13.97100678	B_12	0.00000000
B_33	20.06946636	B_13	0.00000000
		B_23	0.00000000

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

5.2 Wilson plots

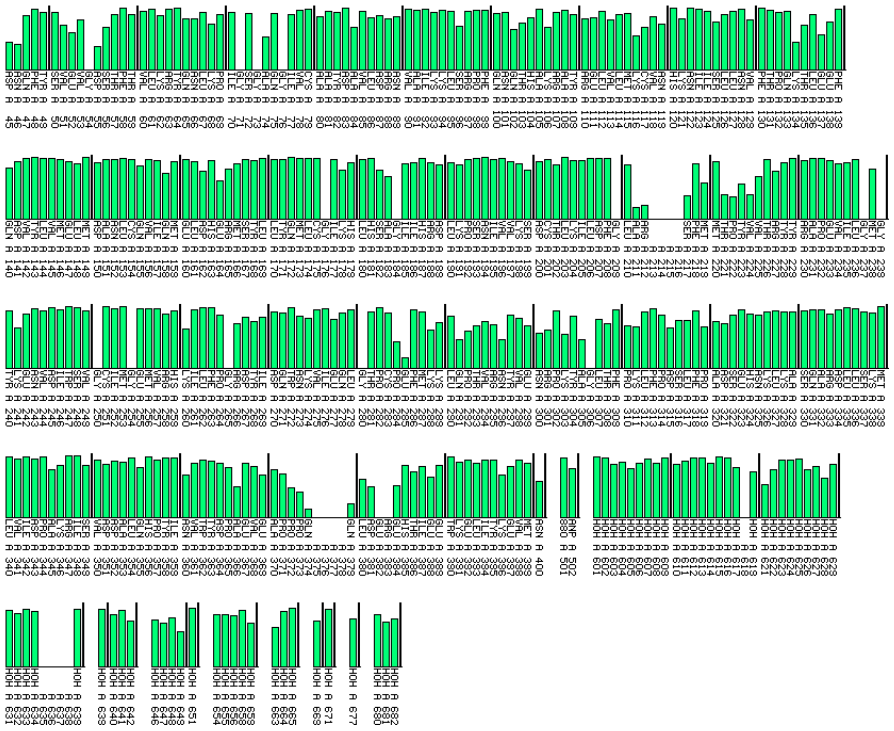
5.2.1 Wilson plot at start of refinement

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