

Report on BUSTER refinement run in directory 00_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:
2052 bond lengths. Worst is 27.3σ 1.61 Å A|501:C17=C16 (468)
18 bond angles. Worst is 17.3σ 99.37° A|501:C2=C3=N11 (468)
2 planes. Worst is 13.8σ 0.28 Å A|501:C8=C7=N11=C3 (468)
5 idealD contacts. Worst 15.7σ 1.17 Å A|864:O=O (HOH) symm: 1555=11656

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:
2052 bond lengths. Worst is 27.3σ 1.61 Å A|501:C17=C16 (468)
18 bond angles. Worst is 17.3σ 99.37° A|501:C2=C3=N11 (468)
2 planes. Worst is 13.8σ 0.28 Å A|501:C8=C7=N11=C3 (468)
5 idealD contacts. Worst 15.7σ 1.17 Å A|864:O=O (HOH) symm: 1555=11656

See [logs/screen_final.txt](#) for more detail

1.2 Run conditions

refine command	<pre>/mnt/scratch_fs1/osmart/autobuster/Server/- autoBUSTER/bin/linux64/refine -p 2h7p.hydro- genate.pdb -m 2h7p/2h7p.mtz -l 468.grade_PDB_- ligand.cif -M MapOnly -d 00_MapOnly -report ?, Mon Jun 16 17:49:22 BST 2014, osmart /home/osmart/2014/06/erice_workshop/- introtutorial/buster</pre>
BUSTER version, run at, by user in directory	<pre>6, hypatia, Ubuntu precise (12.04.4 LTS) /home/osmart/autobuster/Server/scripts/- buster-report -d 00_MapOnly -dr 00_- MapOnly.report -f</pre>
nthreads, hostname, OS buster-report command	<pre>1.1.4 <July 25 2015>, Sat Jul 25 19:23:04 2015, osmart</pre>
buster-report version, run at, by user	<pre>/home/osmart/2014/06/erice_workshop/- introtutorial/buster/00_MapOnly</pre>
buster-report run on refine directory	<pre>/home/osmart/2014/06/erice_workshop/- introtutorial/buster/00_MapOnly.report</pre>
buster-report output directory	<pre>00_MapOnly.report.pdb</pre>
final pdb coordinates	<pre>00_MapOnly.report.mtz</pre>
final mtzfile	

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

1.3 Refinement vital statistics

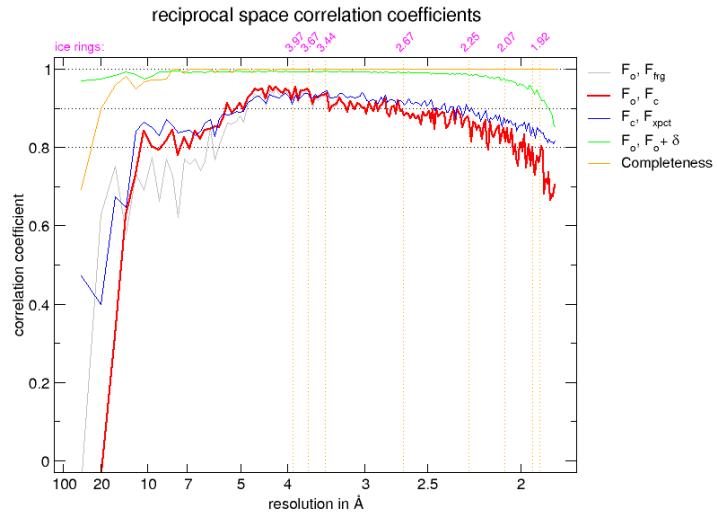
	start	final
N_{cycles} big	0	2
N_{cycles} small	0	0
X-ray weight	n/a	n/a
R_{work}	0.1822	0.1822
R_{free}	0.1837	0.1837
100 (R_{free} – R_{work})	0.2%	0.2%
LLG_{work} (cumulative Log-Likelihood Gain, working set)	0	0.0000
LLG_{free} (cumulative Log-Likelihood Gain, free set)	0	0.0000
High resolution limit in Å	n/a	n/a
Low resolution limit in Å	n/a	n/a
Number of waters	368	368

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

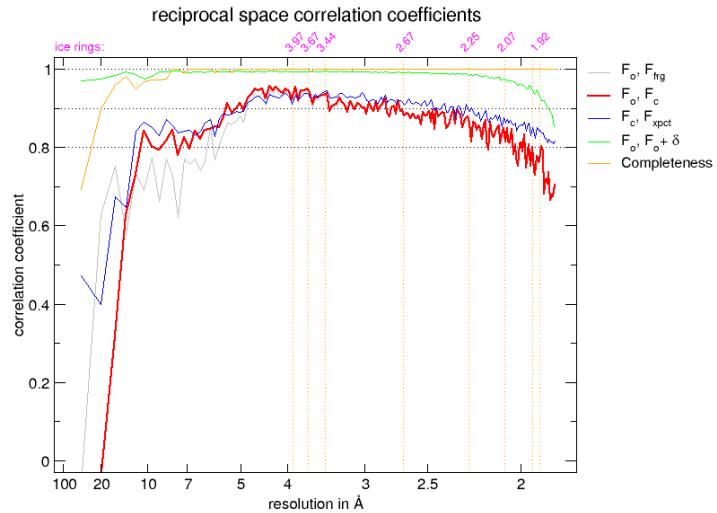
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

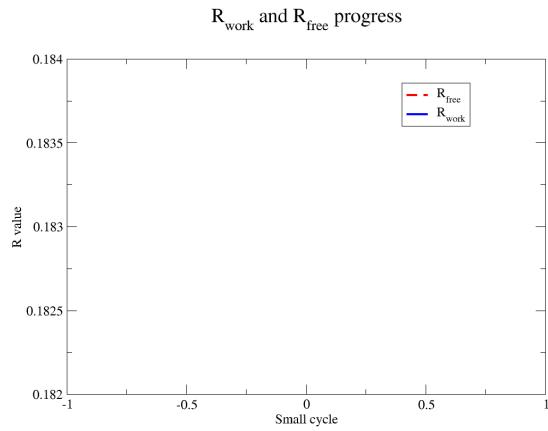
2.1.1 Initial RSCC plot



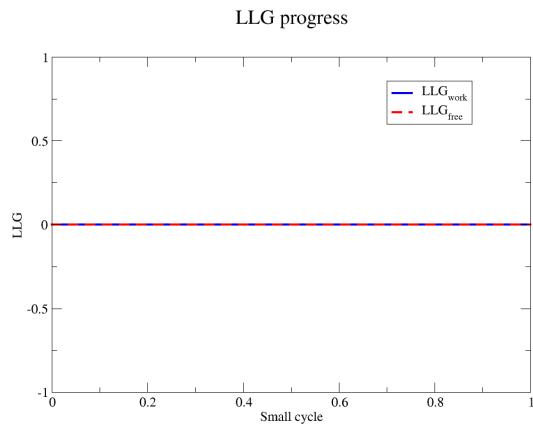
2.1.2 Final RSCC plot



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:	6.55	93 rd percentile* N=777, 1.86Å± 0.25Å
Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	5	2.45% Goal: <1%
	Ramachandran outliers	1	0.38% Goal: <0.05%
	Ramachandran favored	255	95.86% Goal: >98%
	Cβ deviations >0.25Å	0	0.00% Goal: 0
	MolProbity score [†]	1.94	72 nd percentile* N=11957, 1.86Å± 0.25Å
	Bad backbone bonds:	0 / 1071	0.00% Goal: 0%
	Bad backbone angles:	1 / 1337	0.07% Goal: <0.1%

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

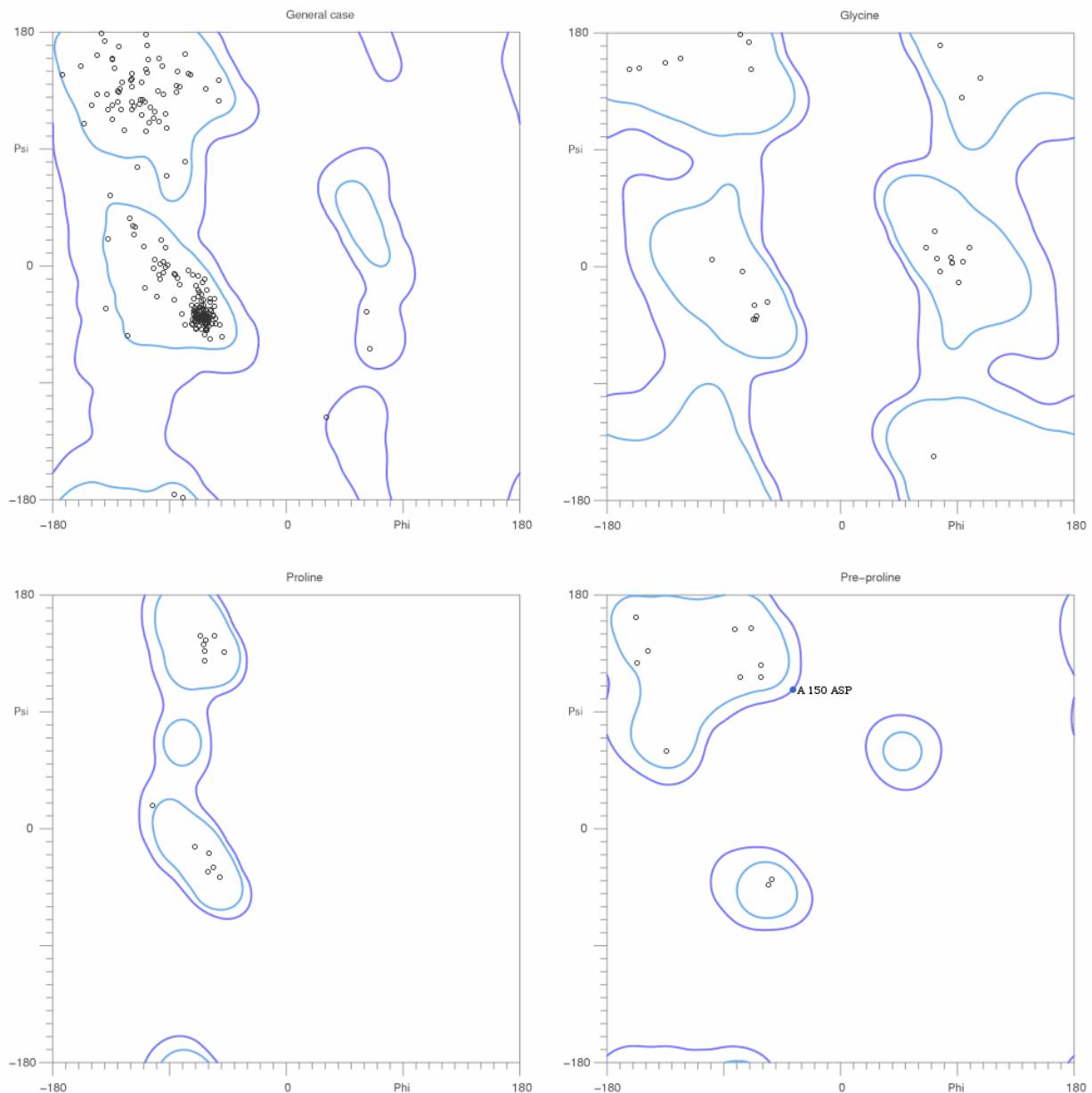
* 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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. D* **66**: 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



266 residues were evaluated in total for general, glycine, proline, and pre-pro.

96.99% of all residues were in favored (98%) regions. (258 residues)

99.62% of all residues were in allowed (>99.8%) regions. (265 residues)

There were 1 outliers:

A 150 ASP: $(\phi, \psi) = (-36.39, 106.99)$

4 Ligand analysis

4.1 468 A 501

4.1.1 Statistics for ligand

Database ID	468 (PDB)
3-letter code	468
CC($2mF_o$ -DF _c)	0.9043
min(B-factor)‡	30.3
avg(B-factor)‡	32.4
max(B-factor)‡	36.2
min(occupancy)‡	1.00
max(occupancy)‡	1.00
‡hydrogen atoms excluded	

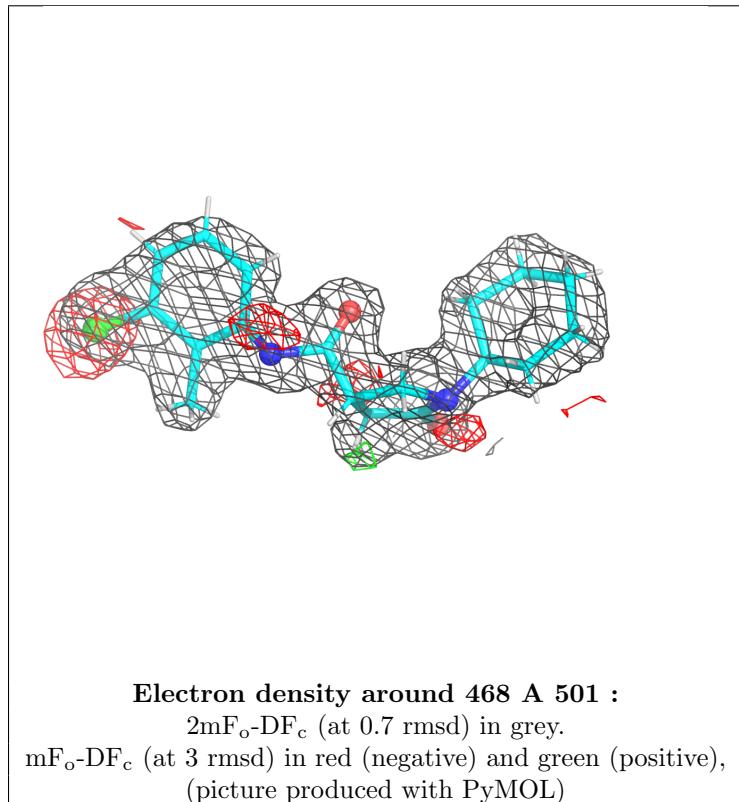
Restraints used

restraints for 468 (-3S-N-3-CHLORO-2-METHYLPHENYL-1-CYCLOHEXYL-5-OXOPYRROLIDINE-3-CARBOXAMIDE) from cif dictionary 468.grade_PDB_ligand.cif; generated by GRADE_PDB_LIGAND 1.2.9pre (June 16 2014) using MOGUL 1.6.1(DEV7), CSD as535be, with quantum mechanics RM1

For help on “Ligand Statistics Table” see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#statistics>

4.1.2 Picture of ligand in electron density



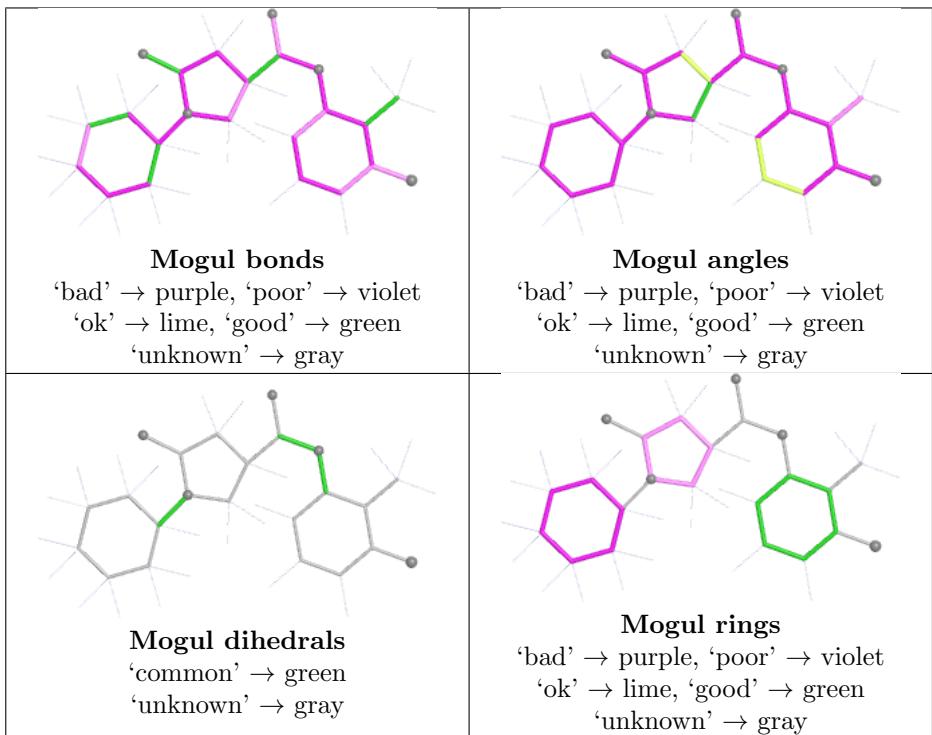
For help on “Ligand Electron Density Picture” see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#density>

4.1.3 Mogul analysis for 468 A 501

Summary

‘bad’ bonds	14/25
‘bad’ bond angles	16/31
‘unusual’ dihedrals	0/3
‘bad’ rings	1/3
bonds rms Z	9.335
angles rms Z	5.532



For help on “Ligand Mogul Analysis” see BUSTER wiki page
<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#Mogul>

Mogul bond results for 468 A 501

Mogul bonds schematic						
atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
C17-C16	1.610	1.391	0.219	0.008	28	26.28
C15-N13	1.098	1.415	-0.317	0.014	1552	22.23
C10-N11	1.654	1.465	0.188	0.013	181	14.69
C19-C20	1.524	1.384	0.139	0.010	2659	13.39
C8-C7	1.402	1.505	-0.103	0.010	228	10.42
C12-N13	1.492	1.350	0.142	0.014	362	9.82
C3-N11	1.577	1.470	0.107	0.013	21	8.20
C15-C16	1.502	1.399	0.103	0.013	49	7.79
C19-C18	1.455	1.384	0.071	0.010	2659	6.81
C6-C5	1.622	1.516	0.106	0.018	1743	5.99
C5-C4	1.600	1.525	0.074	0.013	1827	5.61
C2-C3	1.596	1.522	0.074	0.014	1191	5.24
C8-C9	1.424	1.531	-0.107	0.021	57	5.06
C7-N11	1.410	1.346	0.064	0.013	191	4.82
C20-C15	1.436	1.392	0.044	0.012	3256	3.76
C6-C1	1.582	1.516	0.066	0.018	1743	3.75
C10-C9	1.595	1.530	0.064	0.019	36	3.40
C18-C17	1.429	1.384	0.045	0.013	2673	3.38
O14-C12	1.188	1.228	-0.040	0.012	3021	3.38
C17-CL1	1.771	1.734	0.037	0.012	3693	3.12

(table limited to 20 rows)

For help on “Ligand Mogul Analysis: Bonds” see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulBonds>

Mogul angle results for 468 A 501

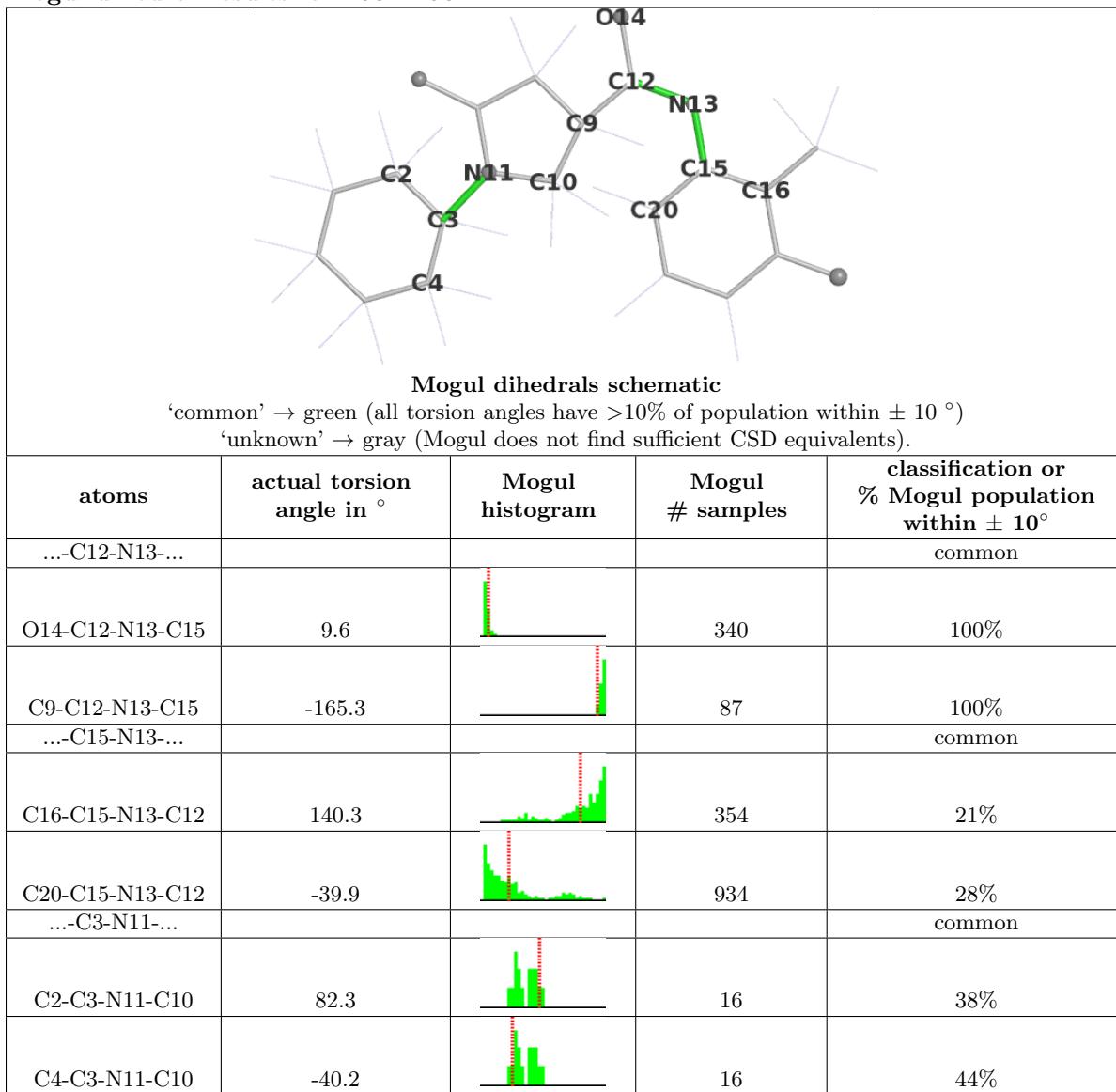
atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C2-C3-N11	99.4	111.7	-12.3	0.9	18	14.33
C4-C3-N11	121.0	111.7	9.3	0.9	18	10.84
C10-N11-C7	105.2	113.8	-8.6	1.0	14	8.84
C9-C12-N13	110.1	114.8	-4.8	0.6	11	8.23
C18-C17-C16	119.2	123.0	-3.9	0.5	22	8.13
O15-C7-C8	118.5	127.3	-8.8	1.1	174	7.84
C16-C17-CL1	123.7	119.6	4.1	0.6	26	7.02
C3-N11-C7	107.9	122.7	-14.8	2.1	16	6.92
C16-C15-N13	110.5	119.3	-8.9	1.6	18	5.62
C1-C2-C3	118.7	110.9	7.8	1.4	901	5.41
C8-C7-N11	113.3	108.2	5.1	1.0	22	5.12
C5-C6-C1	115.9	110.9	5.1	1.0	1269	4.88
C6-C1-C2	115.9	111.3	4.6	1.0	1421	4.74
C6-C5-C4	115.8	111.3	4.6	1.0	1421	4.71
O14-C12-N13	129.2	124.2	5.0	1.2	305	4.30
C20-C15-N13	130.9	121.9	9.0	2.2	1192	4.11
C5-C4-C3	105.7	110.9	-5.1	1.4	901	3.55
C20-C15-C16	118.7	121.3	-2.6	0.8	35	3.36
C23-C16-C17	119.1	122.2	-3.0	0.9	26	3.17
O15-C7-N11	128.2	124.8	3.4	1.1	162	3.04

(table limited to 20 rows)

For help on "Ligand Mogul Analysis: Angles" see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulAngles>

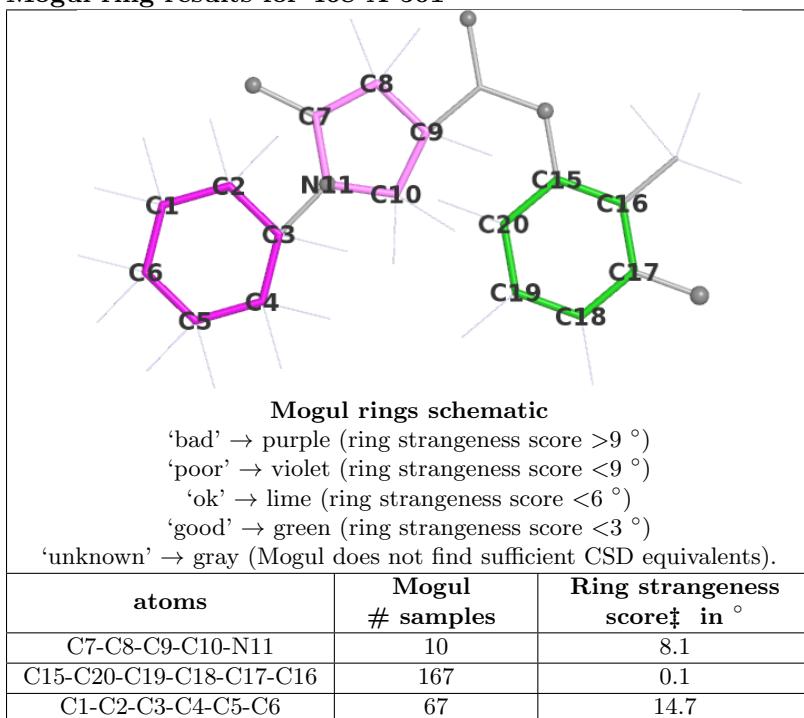
Mogul dihedral results for 468 A 501



For help on “Ligand Mogul Analysis: Dihedrals” see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulDihedrals>

Mogul ring results for 468 A 501



‡‘ring strangeness score’ is the RMS difference in torsion angles between the instance of the ring in the ligand in the model, and the nearest instance that mogul finds in the CSD.

For help on “Ligand Mogul Analysis: Rings” see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulRings>

4.2 NAD A 500

4.2.1 Statistics for ligand

Database ID	NAD (PDB)
3-letter code	NAD
CC($2mF_o - DF_c$)	0.9633
min(B-factor)‡	18.4
avg(B-factor)‡	21.9
max(B-factor)‡	25.7
min(occupancy)‡	1.00
max(occupancy)‡	1.00
‡hydrogen atoms excluded	

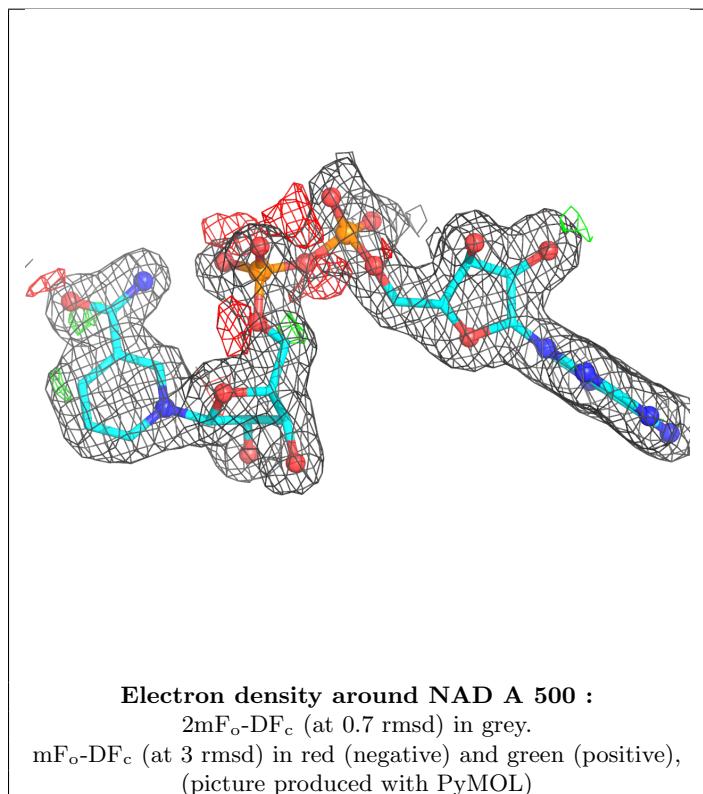
Restraints used

restraints for NAD (NICOTINAMIDE-ADENINE-DINUCLEOTIDE) from cif dictionary NAD.cif; buster common-compounds v 3.0, Generated by GRADE_PDB_LIGAND 1.2.9pre (June 16 2014) using MOGUL 1.6.1(DEV7), CSD as535be, with quantum mechanics RM1

For help on “Ligand Statistics Table” see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#statistics>

4.2.2 Picture of ligand in electron density



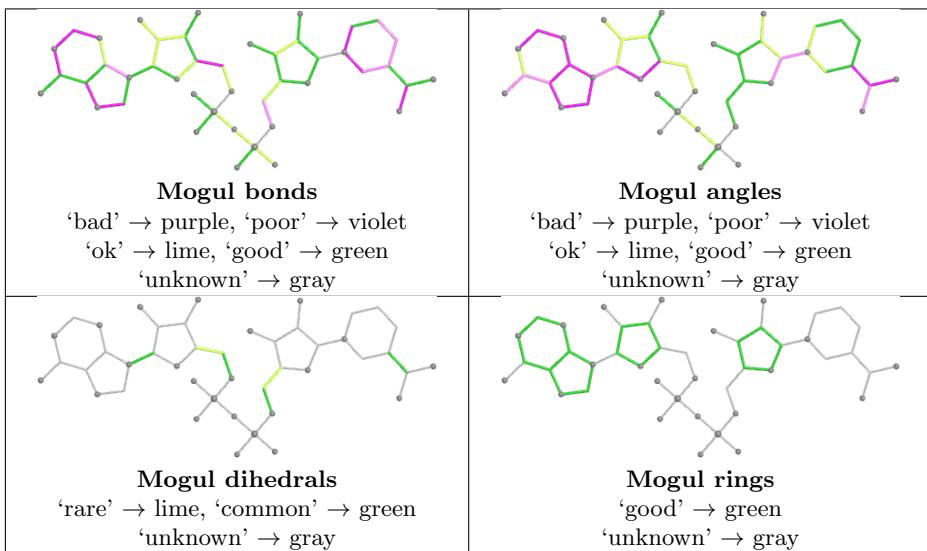
For help on “Ligand Electron Density Picture” see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#density>

4.2.3 Mogul analysis for NAD A 500

Summary

'bad' bonds	9/45
'bad' bond angles	8/60
'unusual' dihedrals	0/6
'bad' rings	0/4
bonds rms Z	3.044
angles rms Z	3.054



For help on "Ligand Mogul Analysis" see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#Mogul>

Mogul bond results for NAD A 500

<p>Mogul bonds schematic</p> <ul style="list-style-type: none"> ‘bad’ → purple ($Z > 4$) ‘poor’ → violet ($2.5 < Z < 4$) ‘ok’ → lime ($1.5 < Z < 2.5$) ‘good’ → green ($Z < 1.5$) ‘unknown’ → gray (Mogul does not find sufficient CSD equivalents). 						
atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
C2N-N1N	1.397	1.344	0.053	0.006	10	9.44
C5B-C4B	1.593	1.508	0.085	0.012	1182	7.03
C5A-N7A	1.349	1.387	-0.037	0.007	359	5.56
C6N-N1N	1.389	1.347	0.043	0.008	44	5.54
C2A-N1A	1.393	1.335	0.058	0.011	829	5.35
O7N-C7N	1.362	1.239	0.123	0.025	568	4.96
C8A-N7A	1.348	1.311	0.037	0.008	447	4.95
C6A-N1A	1.397	1.350	0.047	0.010	239	4.86
C2A-N3A	1.381	1.335	0.046	0.011	829	4.27
C2N-C3N	1.407	1.381	0.026	0.007	79	3.44
O5D-C5D	1.394	1.443	-0.048	0.015	124	3.14
C5N-C4N	1.412	1.384	0.028	0.010	2659	2.69
C4N-C3N	1.424	1.391	0.033	0.013	4266	2.61
C4A-N9A	1.354	1.374	-0.020	0.008	181	2.55
C4A-N3A	1.367	1.339	0.028	0.012	542	2.35
O5B-C5B	1.407	1.443	-0.035	0.015	124	2.29
C2D-C3D	1.501	1.530	-0.029	0.013	510	2.25
C2B-C3B	1.502	1.530	-0.029	0.013	510	2.21
C2B-C1B	1.501	1.530	-0.030	0.014	341	2.13
PA-O3	1.616	1.594	0.022	0.011	21	2.08

(table limited to 20 rows)

For help on “Ligand Mogul Analysis: Bonds” see BUSTER wiki page
<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulBonds>

Mogul angle results for NAD A 500

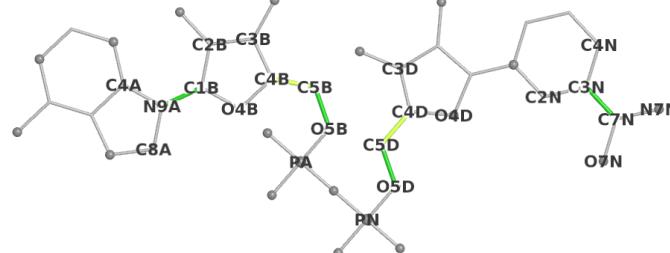
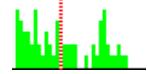
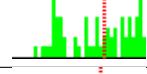
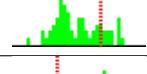
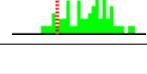
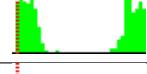
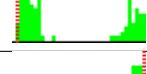
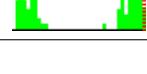
Mogul angles schematic						
atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C5A-N7A-C8A	108.3	103.7	4.7	0.5	265	10.21
N3A-C2A-N1A	120.0	128.8	-8.9	0.9	329	10.06
N9A-C8A-N7A	109.0	114.1	-5.0	0.7	173	7.09
C3N-C7N-N7N	124.2	117.9	6.4	1.0	373	6.70
C4A-C5A-N7A	107.7	110.7	-3.0	0.5	241	5.82
C5A-C4A-N3A	122.8	126.8	-4.0	0.7	212	5.63
C4B-O4B-C1B	102.3	109.5	-7.2	1.4	434	5.02
C4A-N9A-C8A	107.7	105.7	2.0	0.5	150	4.17
C2A-N3A-C4A	119.1	111.5	7.6	2.0	224	3.87
O4B-C1B-N9A	113.1	108.4	4.7	1.3	66	3.62
C5A-C4A-N9A	107.3	105.7	1.5	0.5	148	3.31
O7N-C7N-N7N	118.7	122.8	-4.0	1.3	516	3.16
O7N-C7N-C3N	117.0	119.5	-2.5	0.8	373	3.11
O4D-C1D-N1N	110.5	108.4	2.1	0.7	16	2.90
C5A-C6A-N6A	120.9	123.7	-2.7	1.0	144	2.66
N3A-C4A-N9A	129.9	127.1	2.9	1.2	126	2.48
C2A-N1A-C6A	120.8	118.5	2.3	1.0	154	2.40
C4A-N9A-C1B	122.8	127.0	-4.2	1.8	67	2.36
C5A-C6A-N1A	119.5	117.6	1.9	0.9	133	2.16
O2D-C2D-C1D	116.7	110.6	6.1	2.8	336	2.15

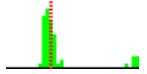
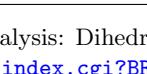
(table limited to 20 rows)

For help on “Ligand Mogul Analysis: Angles” see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulAngles>

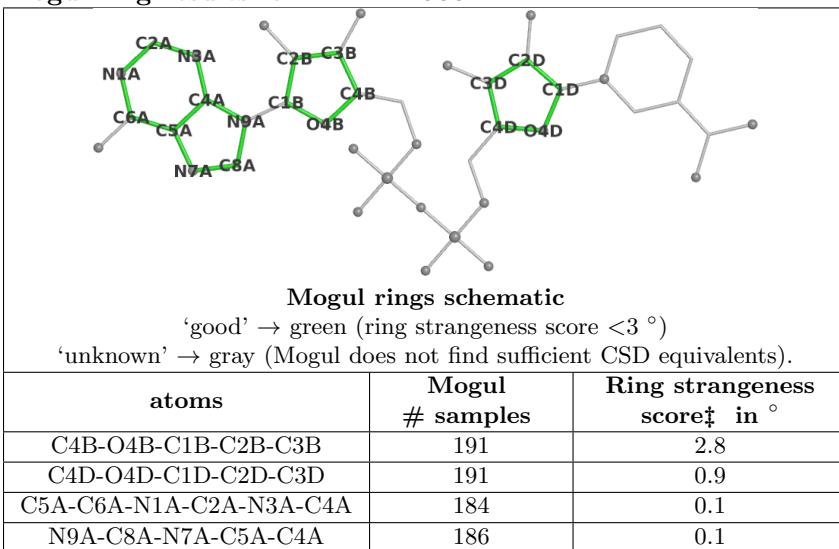
Mogul dihedral results for NAD A 500

 <p>Mogul dihedsals schematic</p> <p>'rare' → lime (all torsion angles have >0.5% of population within $\pm 10^\circ$) 'common' → green (all torsion angles have >10% of population within $\pm 10^\circ$) 'unknown' → gray (Mogul does not find sufficient CSD equivalents).</p>				
atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within $\pm 10^\circ$
...-C1B-N9A-...				common
O4B-C1B-N9A-C8A	61.0		64	14%
O4B-C1B-N9A-C4A	-120.6		68	18%
C2B-C1B-N9A-C4A	119.7		66	18%
C2B-C1B-N9A-C8A	-58.7		63	14%
...-C3N-C7N-...				common
C4N-C3N-C7N-O7N	-1.0		707	24%
C2N-C3N-C7N-N7N	-1.0		111	23%
C2N-C3N-C7N-O7N	178.6		111	25%

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within $\pm 10^\circ$
C4N-C3N-C7N-N7N ...-C4B-C5B-...	179.4		707	24% rare
C3B-C4B-C5B-O5B	-56.0		63	84%
O4B-C4B-C5B-O5B ...-C4D-C5D-...	-174.9		63	6% rare
C3D-C4D-C5D-O5D	79.2		63	5%
O4D-C4D-C5D-O5D ...-C5B-O5B-...	-38.9		63	3% common
C4B-C5B-O5B-PA ...-C5D-O5D-...	140.6		74	36% common
C4D-C5D-O5D-PN	176.2		74	34%

For help on “Ligand Mogul Analysis: Dihedrals” see BUSTER wiki page
<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulDihedrals>

Mogul ring results for NAD A 500



‡'ring strangeness score' is the RMS difference in torsion angles between the instance of the ring in the ligand in the model, and the nearest instance that mogul finds in the CSD.

For help on "Ligand Mogul Analysis: Rings" see BUSTER wiki page

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulRings>

5 X-ray statistics

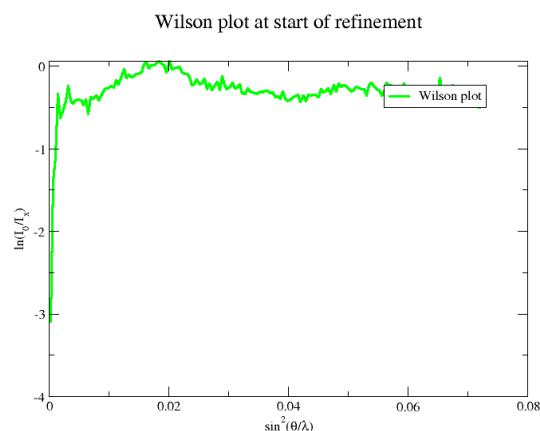
5.1 Scaling parameters in last cycle

Refined parameters		Unrefined parameters	
K_OVER	1.11331176	K_MISS	1.00000000
B_IMPF_FRAG	0.85410099	B_MISS	0.00000000
K_SOLV	0.74384128	K_IMPF_MISS	1.00000000
B_SOLV	30.41999119	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	56.01302087	K_IMPF_SOLV	1.00000000
B_11	-2.61272803	B_OVER	0.00000000
B_22	-2.61272803	B_12	0.00000000
B_33	5.22545607	B_13	0.00000000
		B_23	0.00000000

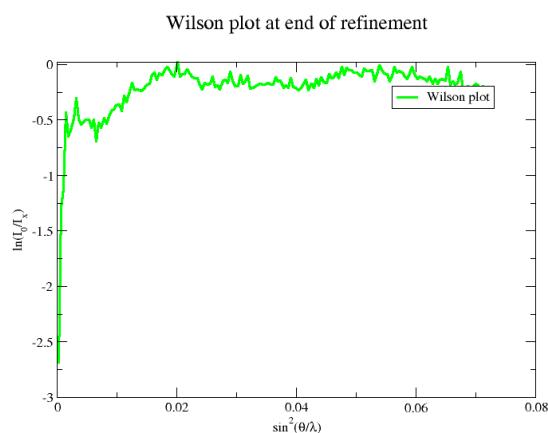
For help on “X-ray scaling parameters” see BUSTER wiki page
<http://www.globalphasing.com/buster/wiki/index.cgi?BRScalingInfo>

5.2 Wilson plots

5.2.1 Wilson plot at start of refinement

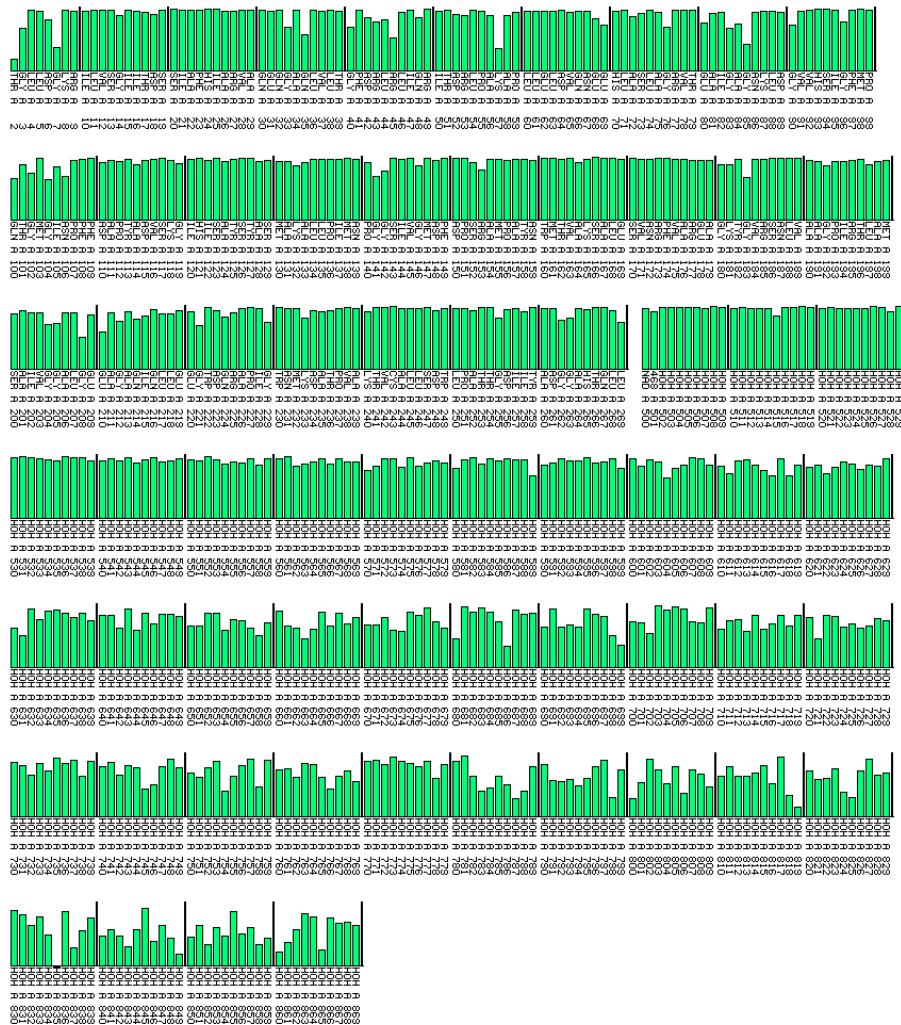


5.2.2 Wilson plot at end of refinement



6 Real-space correlations

6.1 Side chains of chain A



6.2 Mainchain of chain A

