Report on BUSTER refinement run in directory 01_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 σ. Number of outliers for each term:
2052 bond lengths. Worst is 27.3 σ 1.61 Å `A|501:C17=C16 (468)`
18 bond angles. Worst is 17.3 σ 99.37° `A|501:C2=C3=N11 (468)`
2 planes. Worst is 13.8 σ 0.28 Å `A|501:C8=C7=N11=C3 (468)`
5 idealD contacts. Worst 15.7 σ 1.17 Å `A|864:O=O (HOH) symm: 1555=11656`

See logs/screen_initial.txt for more detail

1.2 Run conditions

refine command	/mnt/scratch_fs1/osmart/autobuster/Server/-autoBUSTER/bin/linux64/refine -p 2h7p_hydrogenate.pdb -m 2h7p/2h7p.mtz -l 468.grade_PDB_-ligand.cif -M TLSbasic -d 01_refine -report
BUSTER version, run at, by user	2.13.0, Mon Jun 16 17:53:36 BST 2014, osmart
in directory	/home/osmart/2014/06/erice_workshop/-introtutorial/buster
nthreads, hostname, OS	6, hypatia, Ubuntu precise (12.04.4 LTS)
buster-report command	/home/osmart/autobuster/Server/scripts/-buster-report -d 01_refine -dr 01_refine.report -f
buster-report version, run at, by user	1.1.4 <July 25 2015>, Sat Jul 25 19:27:21 2015, osmart
buster-report run on refine directory	/home/osmart/2014/06/erice_workshop/-introtutorial/buster/01_refine
buster-report output directory	/home/osmart/2014/06/erice_workshop/-introtutorial/buster/01_refine.report
final pdb coordinates	01_refine.report.pdb
final mtzfile	01_refine.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

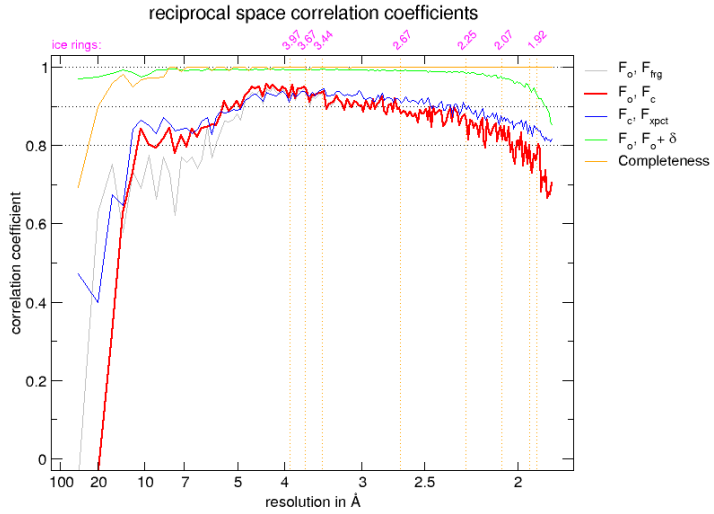
	start	final
N_{cycles} big	0	5
N_{cycles} small	0	307
X-ray weight	4.00	3.24
R_{work}	0.1822	0.1518
R_{free}	0.1837	0.1778
100 ($R_{free} - R_{work}$)	0.2%	2.6%
LLG_{work} *(cumulative Log-Likelihood Gain, working set)*	0	0.2141
LLG_{free} *(cumulative Log-Likelihood Gain, free set)*	0	0.0122
RMS bond in Å	0.0231	0.0094
RMS angle in degrees	1.66	1.04
High resolution limit in Å	1.86	1.86
Low resolution limit in Å	46.20	17.34
Number of waters	368	368

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

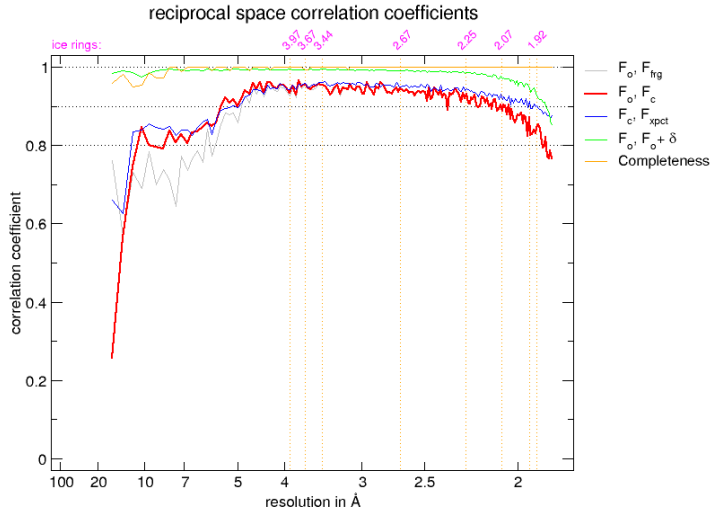
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

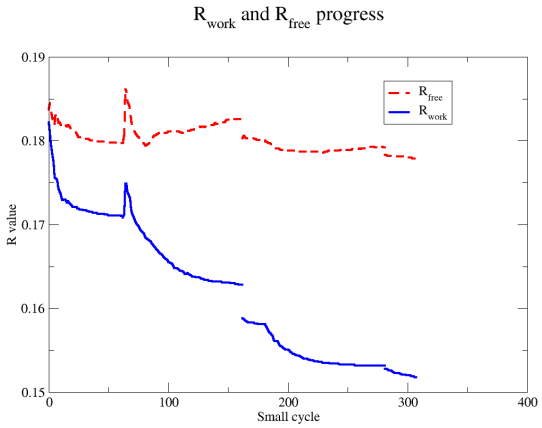
2.1.1 Initial RSCC plot



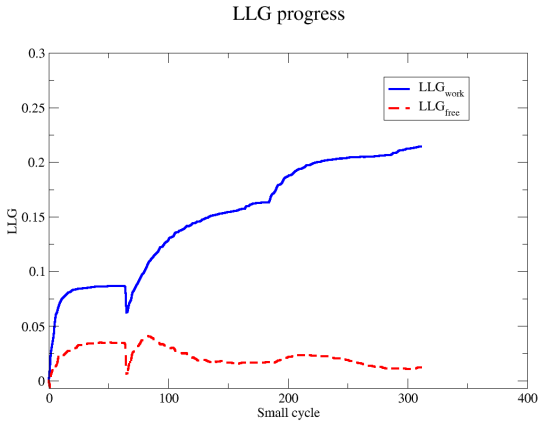
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement

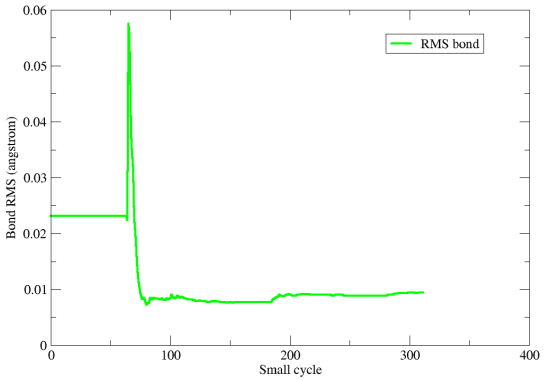


2.3 LLG behaviour during refinement

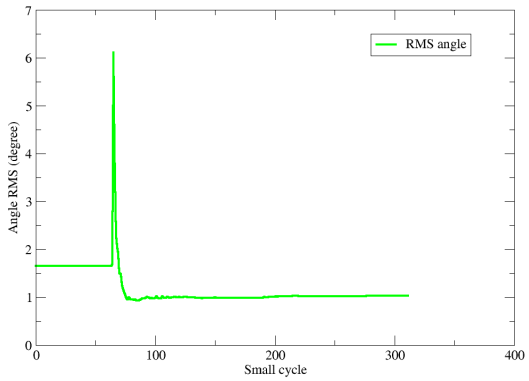


2.4 Geometry behaviour during optimisation

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:	0.24		100th 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	4	1.96%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	257	96.62%	Goal: >98%
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	MolProbity score†	1.03		100th percentile* N=11957, 1.86Å± 0.25Å
	Bad backbone bonds:	0 / 1071	0.00%	Goal: 0%
	Bad backbone angles:	0 / 1337	0.00%	Goal: <0.1%

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

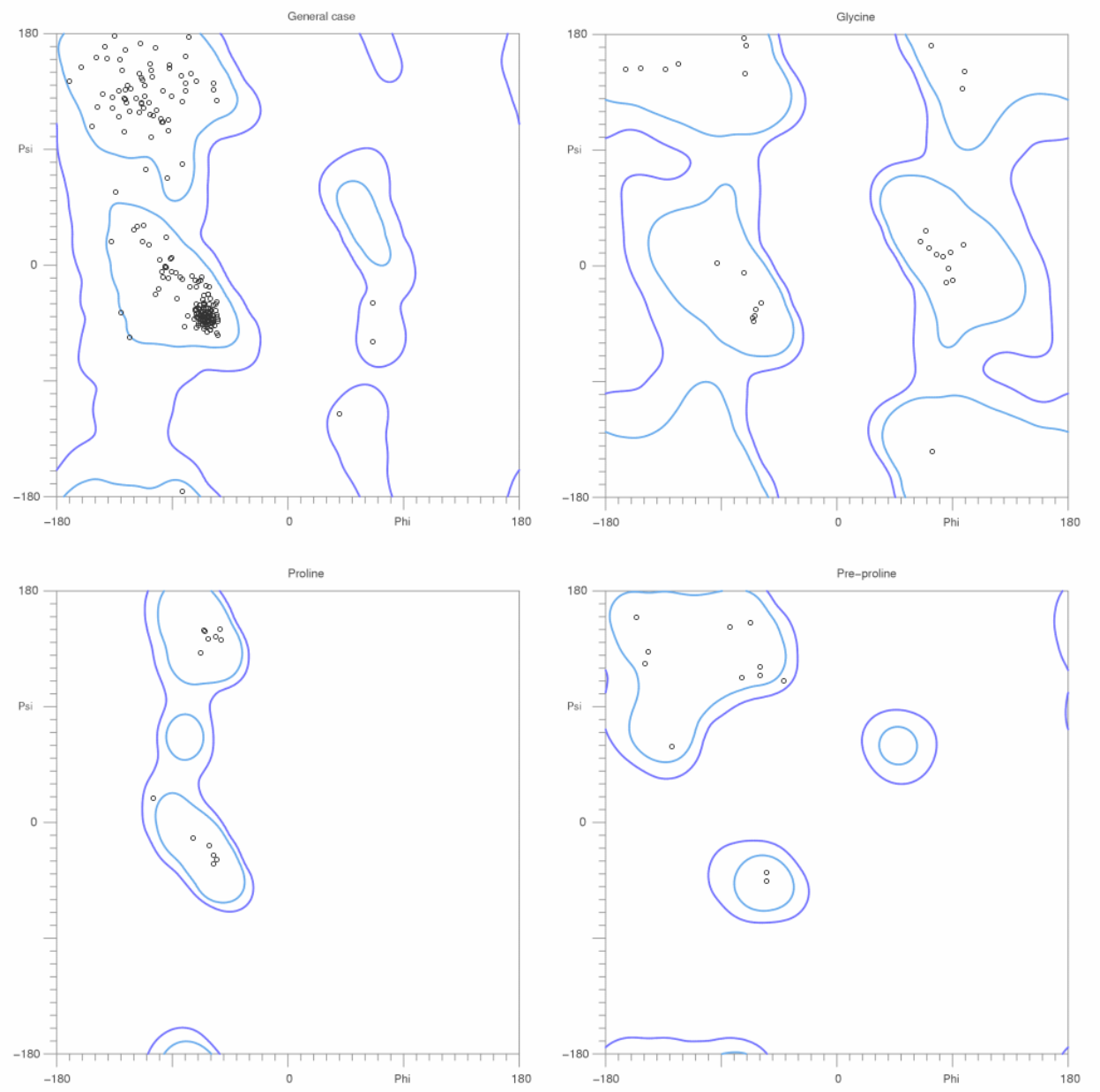
∗ 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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



266 residues were evaluated in total for general, glycine, proline, and pre-pro.
96.62% of all residues were in favored (98%) regions. (257 residues)
100.00% of all residues were in allowed (>99.8%) regions. (266 residues)
There were no outliers.

4 Ligand analysis

4.1 468 A 501

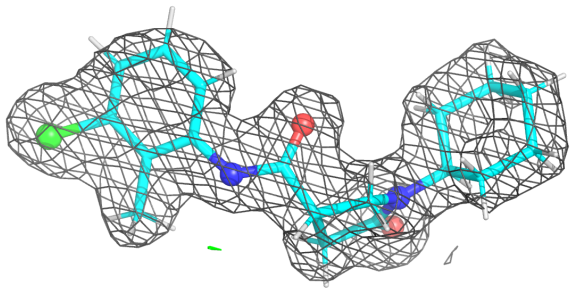
4.1.1 Statistics for ligand

Database ID	468 (PDB)
3-letter code	468
CC(2mF$_o$-DF$_c$)	0.9643
min(B-factor)‡	26.3
avg(B-factor)‡	32.7
max(B-factor)‡	54.8
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



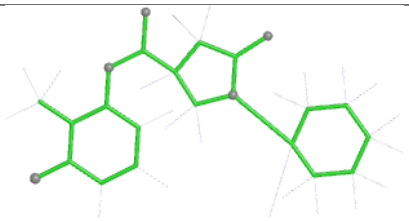
Electron density around 468 A 501 :
2mF$_o$-DF$_c$ (at 0.7 rmsd) in grey.
mF$_o$-DF$_c$ (at 3 rmsd) in red (negative) and green (positive),
(picture produced with PyMOL)

For help on "Ligand Electron Density Picture" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#density

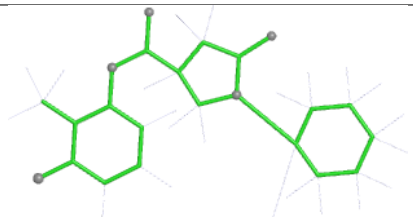
4.1.3 Mogul analysis for 468 A 501

Summary

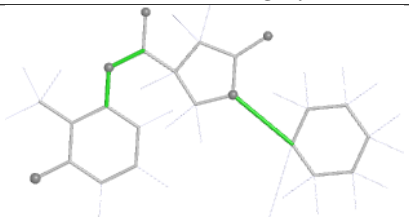
'bad' bonds	0/25
'bad' bond angles	0/31
'unusual' dihedrals	0/3
'bad' rings	0/3
bonds rms Z	0.282
angles rms Z	0.486



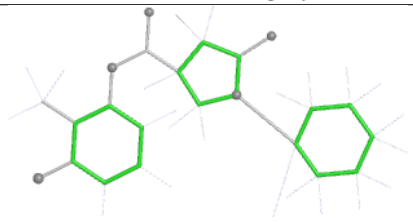
Mogul bonds
'good' → green
'unknown' → gray



Mogul angles
'good' → green
'unknown' → gray



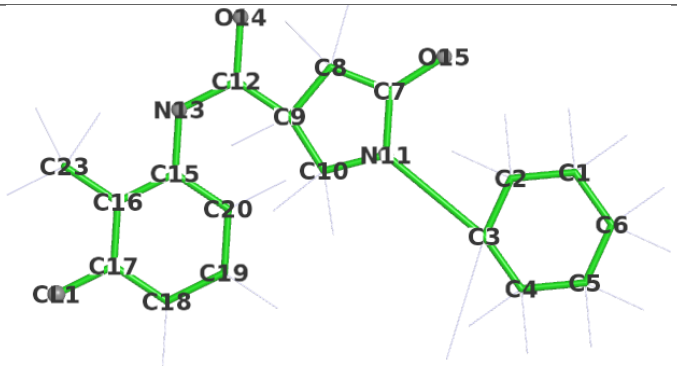
Mogul dihedrals
'common' → green
'unknown' → gray



Mogul rings
'good' → green
'unknown' → gray

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

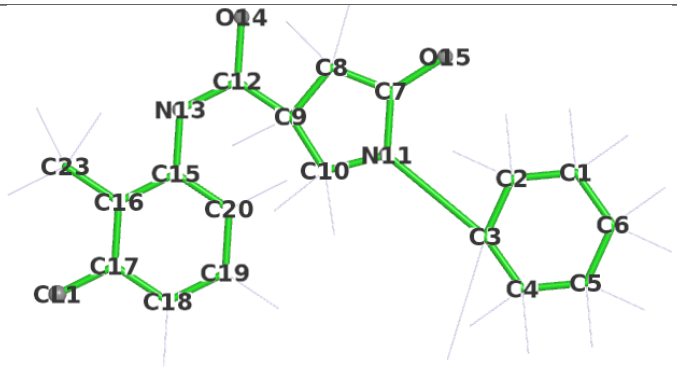


Mogul bonds schematic
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
C20-C15	1.400	1.392	0.008	0.012	3256	0.73
C3-N11	1.477	1.470	0.007	0.013	21	0.51
C6-C5	1.525	1.516	0.009	0.018	1743	0.51
C10-C9	1.539	1.530	0.009	0.019	36	0.45
C15-C16	1.405	1.399	0.006	0.013	49	0.44
C2-C3	1.527	1.522	0.006	0.014	1191	0.39
C18-C17	1.379	1.384	-0.005	0.013	2673	0.34
C6-C1	1.521	1.516	0.005	0.018	1743	0.30
C17-C16	1.393	1.391	0.002	0.008	28	0.26
C8-C9	1.527	1.531	-0.004	0.021	57	0.20
C19-C18	1.383	1.384	-0.002	0.010	2659	0.16
C17-CL1	1.732	1.734	-0.002	0.012	3693	0.15
C5-C4	1.526	1.525	0.001	0.013	1827	0.08
C9-C12	1.511	1.509	0.002	0.019	46	0.08
C23-C16	1.508	1.509	-0.001	0.011	1974	0.07
C1-C2	1.526	1.525	0.001	0.013	1827	0.06
C12-N13	1.351	1.350	0.001	0.014	362	0.05
O15-C7	1.220	1.220	-0.000	0.014	2954	0.04
C19-C20	1.384	1.384	-0.000	0.010	2659	0.04
C7-N11	1.345	1.346	-0.001	0.013	191	0.04
(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

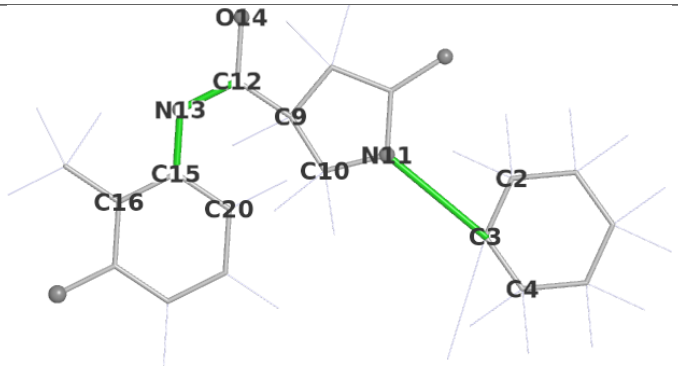


Mogul angles schematic
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C8-C9-C12	109.4	112.1	-2.7	1.8	16	1.47
C18-C17-CL1	117.0	118.4	-1.4	1.3	2376	1.02
C10-N11-C3	122.0	124.2	-2.2	2.4	11	0.90
C3-N11-C7	124.5	122.7	1.8	2.1	16	0.85
C20-C15-N13	120.3	121.9	-1.6	2.2	1192	0.76
C16-C15-N13	118.4	119.3	-0.9	1.6	18	0.58
C4-C3-C2	110.1	111.0	-0.9	1.7	435	0.51
O14-C12-C9	121.6	122.1	-0.5	1.0	39	0.49
C1-C2-C3	110.2	110.9	-0.7	1.4	901	0.46
O14-C12-N13	123.7	124.2	-0.5	1.2	305	0.44
C19-C20-C15	119.6	119.0	0.6	1.7	2995	0.36
C9-C12-N13	114.7	114.8	-0.2	0.6	11	0.30
C10-N11-C7	113.5	113.8	-0.3	1.0	14	0.29
C5-C4-C3	110.5	110.9	-0.4	1.4	901	0.28
C18-C19-C20	120.2	120.4	-0.3	1.0	1853	0.27
C4-C3-N11	111.5	111.7	-0.2	0.9	18	0.22
C23-C16-C17	122.4	122.2	0.2	0.9	26	0.22
C5-C6-C1	111.1	110.9	0.2	1.0	1269	0.20
C18-C17-C16	122.9	123.0	-0.1	0.5	22	0.20
C6-C1-C2	111.4	111.3	0.2	1.0	1421	0.19
(table limited to 20 rows)						

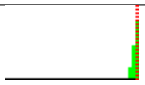
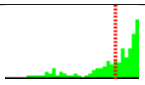
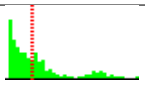
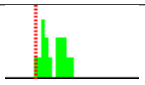
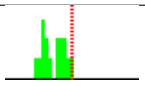
For help on "Ligand Mogul Analysis: Angles" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulAngles

Mogul dihedral results for 468 A 501



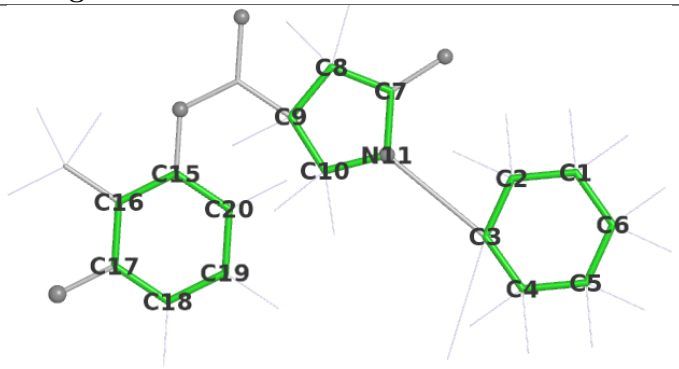
Mogul dihedrals schematic

'common' → green (all torsion angles have >10% of population within ± 10 °)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
...-C12-N13-...				common
O14-C12-N13-C15	3.7		340	99%
C9-C12-N13-C15	-175.2		87	100%
...-C15-N13-...				common
C16-C15-N13-C12	146.5		354	27%
C20-C15-N13-C12	-32.1		934	30%
...-C3-N11-...				common
C2-C3-N11-C10	36.5		16	31%
C4-C3-N11-C10	-87.3		16	25%

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



Mogul rings schematic
'good' → green (ring strangeness score <3 °)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	Mogul # samples	Ring strangeness score‡ in °
C7-C8-C9-C10-N11	10	1.1
C15-C20-C19-C18-C17-C16	167	1.1
C1-C2-C3-C4-C5-C6	67	0.5

‡'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

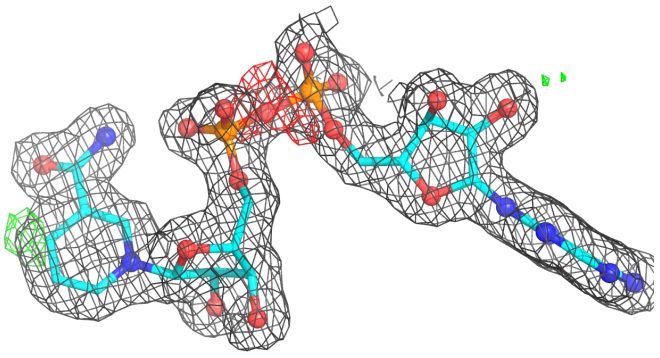
4.2.1 Statistics for ligand

Database ID	NAD (PDB)
3-letter code	NAD
CC(2mF$_o$-DF$_c$)	0.9812
min(B-factor)‡	17.7
avg(B-factor)‡	22.0
max(B-factor)‡	25.5
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



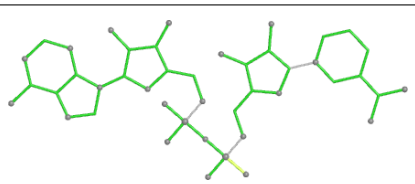
Electron density around NAD A 500 :
2mF$_o$-DF$_c$ (at 0.7 rmsd) in grey.
mF$_o$-DF$_c$ (at 3 rmsd) in red (negative) and green (positive),
(picture produced with PyMOL)

For help on "Ligand Electron Density Picture" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#density

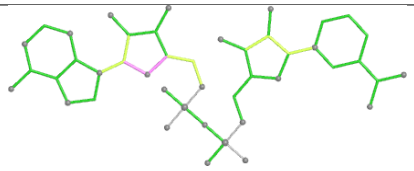
4.2.3 Mogul analysis for NAD A 500

Summary

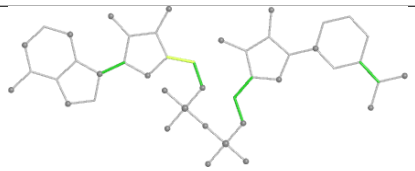
'bad' bonds	0/45
'bad' bond angles	0/60
'unusual' dihedrals	0/6
'bad' rings	0/4
bonds rms Z	0.553
angles rms Z	0.907



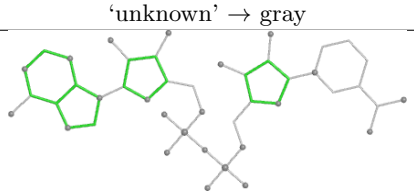
Mogul bonds
'ok' → lime, 'good' → green
'unknown' → gray



Mogul angles
'poor' → violet
'ok' → lime, 'good' → green
'unknown' → gray



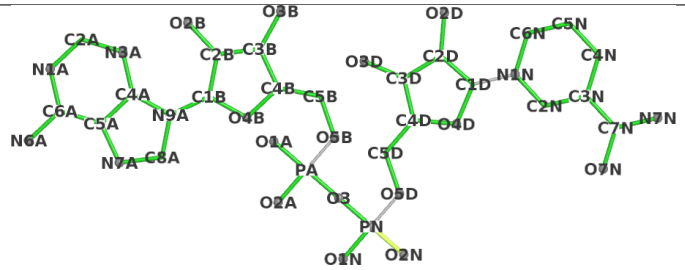
Mogul dihedrals
'rare' → lime, 'common' → green
'unknown' → gray



Mogul rings
'good' → green
'unknown' → gray

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

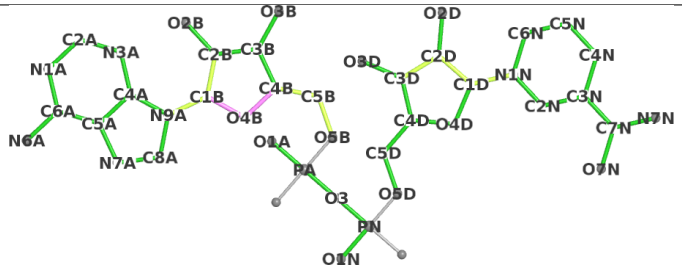


Mogul bonds schematic
'ok' → lime (1.5 <Z <2.5)
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
PN-O2N	1.481	1.527	-0.046	0.030	30	1.54
C3B-C4B	1.543	1.526	0.018	0.014	577	1.28
PA-O2A	1.489	1.527	-0.038	0.030	30	1.28
O4D-C4D	1.455	1.444	0.011	0.011	1633	1.01
C2B-C1B	1.518	1.530	-0.013	0.014	341	0.90
C4N-C3N	1.401	1.391	0.011	0.013	4266	0.84
O3D-C3D	1.434	1.423	0.010	0.013	3264	0.79
C7N-N7N	1.344	1.327	0.016	0.021	568	0.79
C6N-N1N	1.352	1.347	0.006	0.008	44	0.76
C3D-C4D	1.535	1.526	0.010	0.014	577	0.72
C6A-N1A	1.355	1.350	0.005	0.010	239	0.51
C6A-N6A	1.343	1.336	0.007	0.014	531	0.50
O4B-C1B	1.410	1.415	-0.006	0.011	592	0.49
O2B-C2B	1.418	1.423	-0.006	0.013	3264	0.43
O4B-C4B	1.448	1.444	0.005	0.011	1633	0.42
C2A-N1A	1.339	1.335	0.005	0.011	829	0.41
C4A-N3A	1.344	1.339	0.005	0.012	542	0.40
C8A-N7A	1.314	1.311	0.003	0.008	447	0.38
PN-O3	1.598	1.594	0.004	0.011	21	0.38
C2D-C3D	1.526	1.530	-0.005	0.013	510	0.36
(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

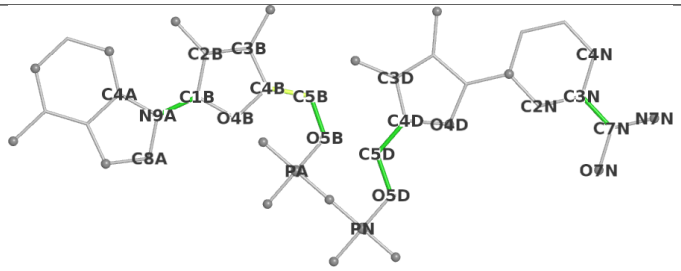


Mogul angles schematic
'poor' → violet (2.5 <Z <4)
'ok' → lime (1.5 <Z <2.5)
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C4B-O4B-C1B	105.7	109.5	-3.8	1.4	434	2.61
C2D-C1D-N1N	117.8	113.6	4.2	1.8	20	2.30
O4B-C1B-N9A	111.3	108.4	2.9	1.3	66	2.25
O5B-C5B-C4B	104.6	109.1	-4.5	2.3	84	1.93
C3D-C2D-C1D	99.4	101.5	-2.1	1.2	285	1.82
O4B-C1B-C2B	104.4	106.5	-2.1	1.2	307	1.82
C4N-C3N-C7N	117.2	120.7	-3.5	2.4	598	1.45
C3B-C2B-C1B	99.8	101.5	-1.7	1.2	273	1.45
O3D-C3D-C2D	108.6	111.9	-3.3	2.6	938	1.26
C4A-N9A-C1B	125.0	127.0	-1.9	1.8	67	1.10
O4D-C1D-C2D	105.9	107.0	-1.1	1.1	17	1.07
O3-PA-O1A	111.2	108.7	2.5	2.4	19	1.02
O4B-C4B-C3B	106.6	105.3	1.3	1.3	448	1.02
O7N-C7N-C3N	118.7	119.5	-0.8	0.8	373	1.00
C1B-N9A-C8A	128.6	126.8	1.8	1.9	65	0.96
O2D-C2D-C1D	113.2	110.6	2.6	2.8	336	0.93
C2B-C1B-N9A	115.5	114.1	1.4	1.5	59	0.92
C6N-C5N-C4N	119.2	119.9	-0.7	0.7	149	0.92
C6N-N1N-C2N	121.8	122.2	-0.3	0.4	10	0.88
C3N-C7N-N7N	118.7	117.9	0.8	1.0	373	0.84
(table limited to 20 rows)						

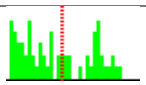
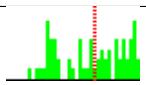
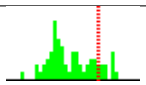
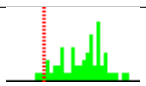
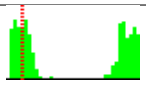
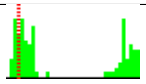
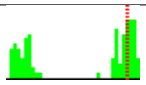
For help on "Ligand Mogul Analysis: Angles" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulAngles

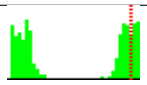
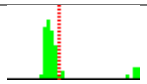
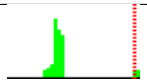
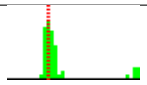
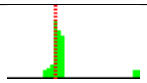
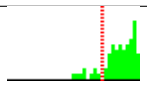
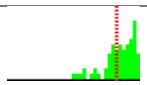
Mogul dihedral results for NAD A 500



Mogul dihedrals schematic

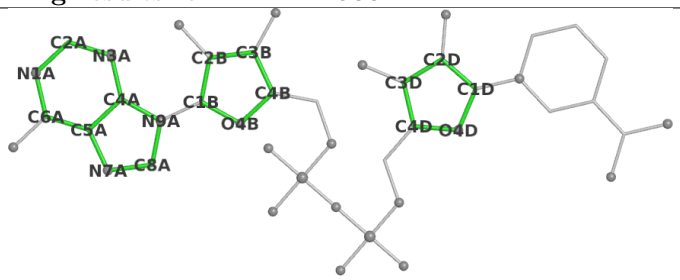
'rare' → lime (all torsion angles have >0.5% of population within ± 10 °)
'common' → green (all torsion angles have >10% of population within ± 10 °)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
...-C1B-N9A-...				common
O4B-C1B-N9A-C8A	71.1		64	12%
O4B-C1B-N9A-C4A	-119.9		68	16%
C2B-C1B-N9A-C4A	121.4		66	18%
C2B-C1B-N9A-C8A	-47.7		63	11%
...-C3N-C7N-...				common
C4N-C3N-C7N-O7N	-19.1		707	39%
C2N-C3N-C7N-N7N	-12.0		111	42%
C2N-C3N-C7N-O7N	160.6		111	43%

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
C4N-C3N-C7N-N7N	168.4		707	40%
...-C4B-C5B-...				rare
C3B-C4B-C5B-O5B	-67.1		63	40%
O4B-C4B-C5B-O5B	172.8		63	6%
...-C4D-C5D-...				common
C3D-C4D-C5D-O5D	54.8		63	84%
O4D-C4D-C5D-O5D	-65.0		63	90%
...-C5B-O5B-...				common
C4B-C5B-O5B-PA	128.4		74	14%
...-C5D-O5D-...				common
C4D-C5D-O5D-PN	147.5		74	42%

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



Mogul rings schematic

'good' → green (ring strangeness score <3 °)

'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	Mogul # samples	Ring strangeness score‡ in °
C4B-O4B-C1B-C2B-C3B	191	1.4
C4D-O4D-C1D-C2D-C3D	191	0.5
C5A-C6A-N1A-C2A-N3A-C4A	184	0.2
N9A-C8A-N7A-C5A-C4A	186	0.1

‡'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	1.06710468	K_MISS	1.00000000
B_IMPF_FRAG	0.38117391	B_MISS	0.00000000
K_SOLV	0.71777213	K_IMPF_MISS	1.00000000
B_SOLV	35.79420156	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	56.24216365	K_IMPF_SOLV	1.00000000
B_11	-1.98137423	B_OVER	0.00000000
B_22	-1.98137423	B_12	0.00000000
B_33	3.96274847	B_13	0.00000000
		B_23	0.00000000
Anisotropic ratio	0.20		

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

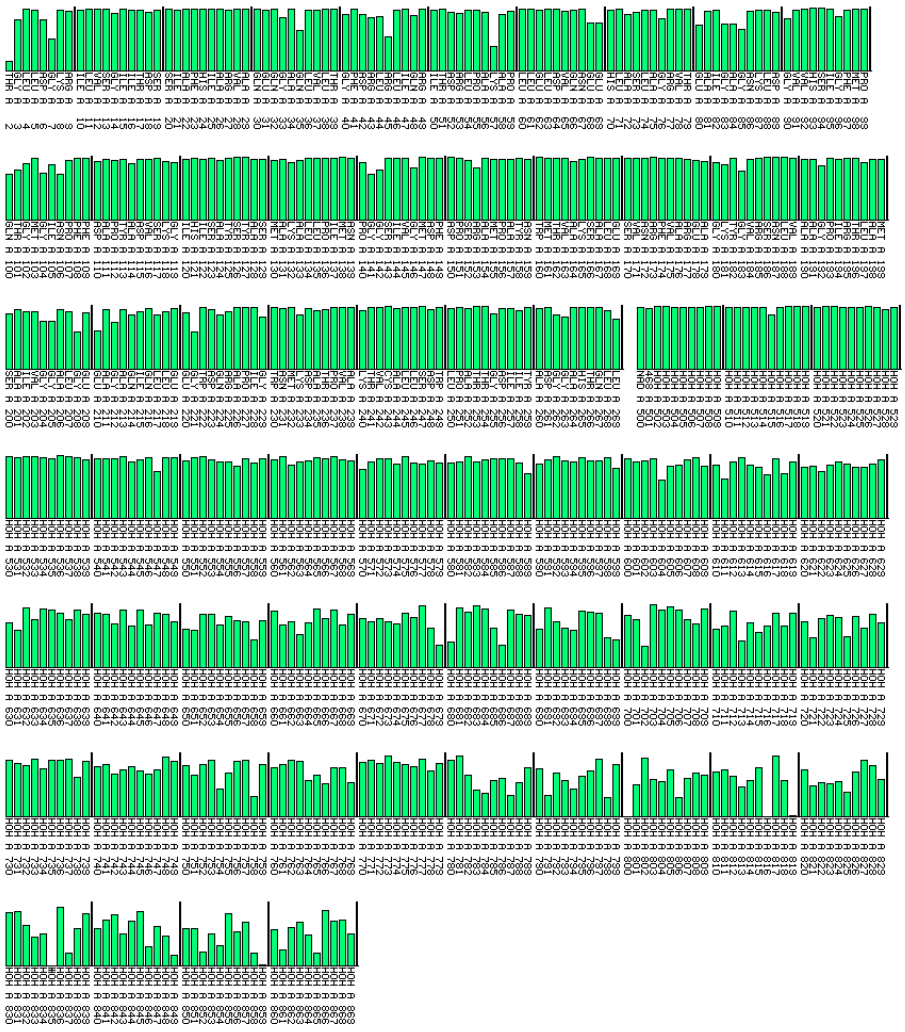
5.2 Wilson plots

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