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 σ. Number of outliers for each term:
49 bond lengths. Worst is 15.5 σ 0.86 Å `A|501:N19=H19 (880)`
13 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 σ. Number of outliers for each term:
1 bond angles. Worst is 5.7 σ 140.80° `A|501:C50=N54=C55 (880)`

See logs/screen_final.txt for more detail

1.2 Run conditions

refine command	/mnt/scratch_fs1/osmart/autobuster/Server/-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	2.13.0, Mon Jun 16 15:24:15 BST 2014, osmart
in directory	/home/osmart/2014/06/erice_workshop/1pmq_tutorial
nthreads, hostname, OS	6, hypatia, Ubuntu precise (12.04.4 LTS)
buster-report command	/home/osmart/autobuster/Server/scripts/-buster-report -d 1pmq_02_refine -dr 1pmq_-02_refine-report
buster-report version, run at, by user	1.1.4 <July 25 2015>, Sat Jul 25 18:53:01 2015, osmart
buster-report run on refine directory	/home/osmart/2014/06/erice_workshop/1pmq_-tutorial/1pmq_02_refine
buster-report output directory	/home/osmart/2014/06/erice_workshop/1pmq_-tutorial/1pmq_02_refine-report
final pdb coordinates	1pmq_02_refine-report.pdb
final mtzfile	1pmq_02_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

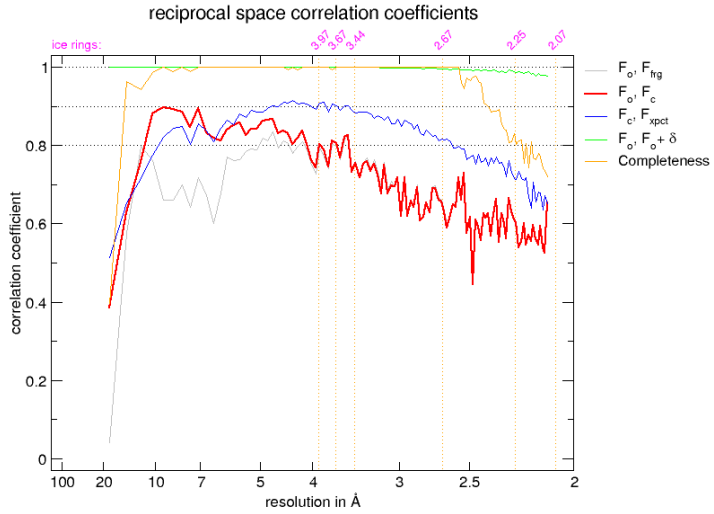
	start	final
N_{cycles} big	0	5
N_{cycles} small	0	296
X-ray weight	4.00	4.44
R_{work}	0.2253	0.2062
R_{free}	0.2636	0.2361
100 $(R_{free} - R_{work})$	3.8%	3.0%
LLG_{work} *(cumulative Log-Likelihood Gain, working set)*	0	0.1121
LLG_{free} *(cumulative Log-Likelihood Gain, free set)*	0	0.0817
RMS bond in Å	0.0175	0.0089
RMS angle in degrees	1.47	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

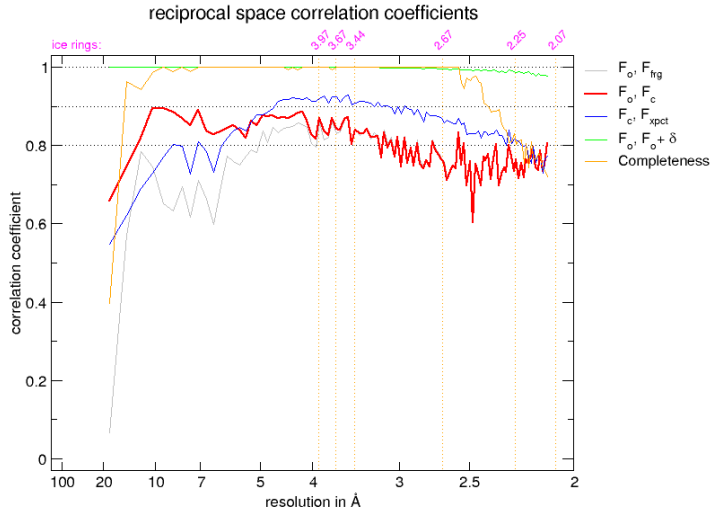
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

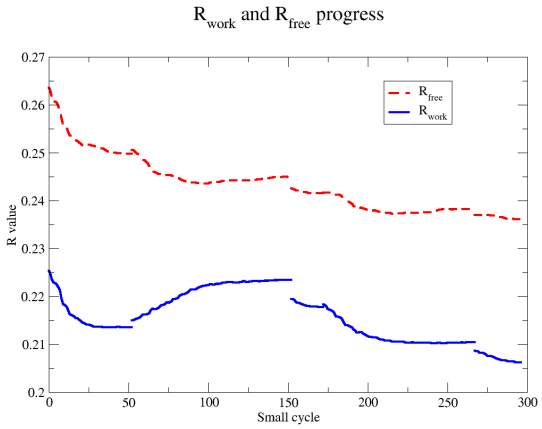
2.1.1 Initial RSCC plot



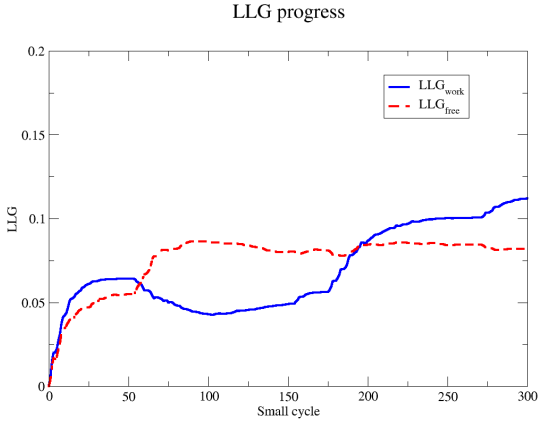
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement

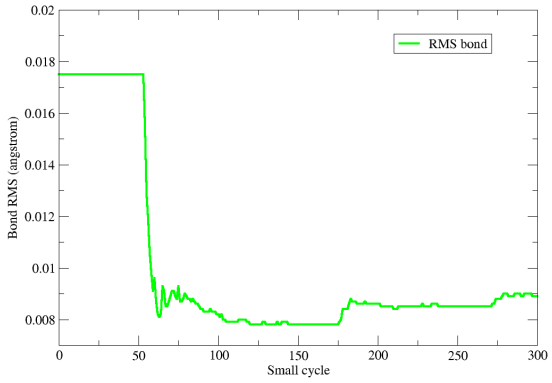


2.3 LLG behaviour during refinement

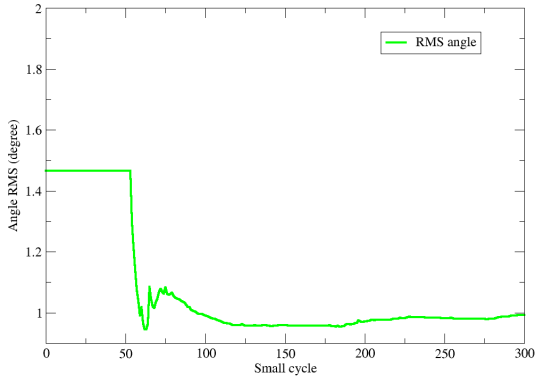


2.4 Geometry behaviour during optimisation

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:	1.94		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†	1.56		98th 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.

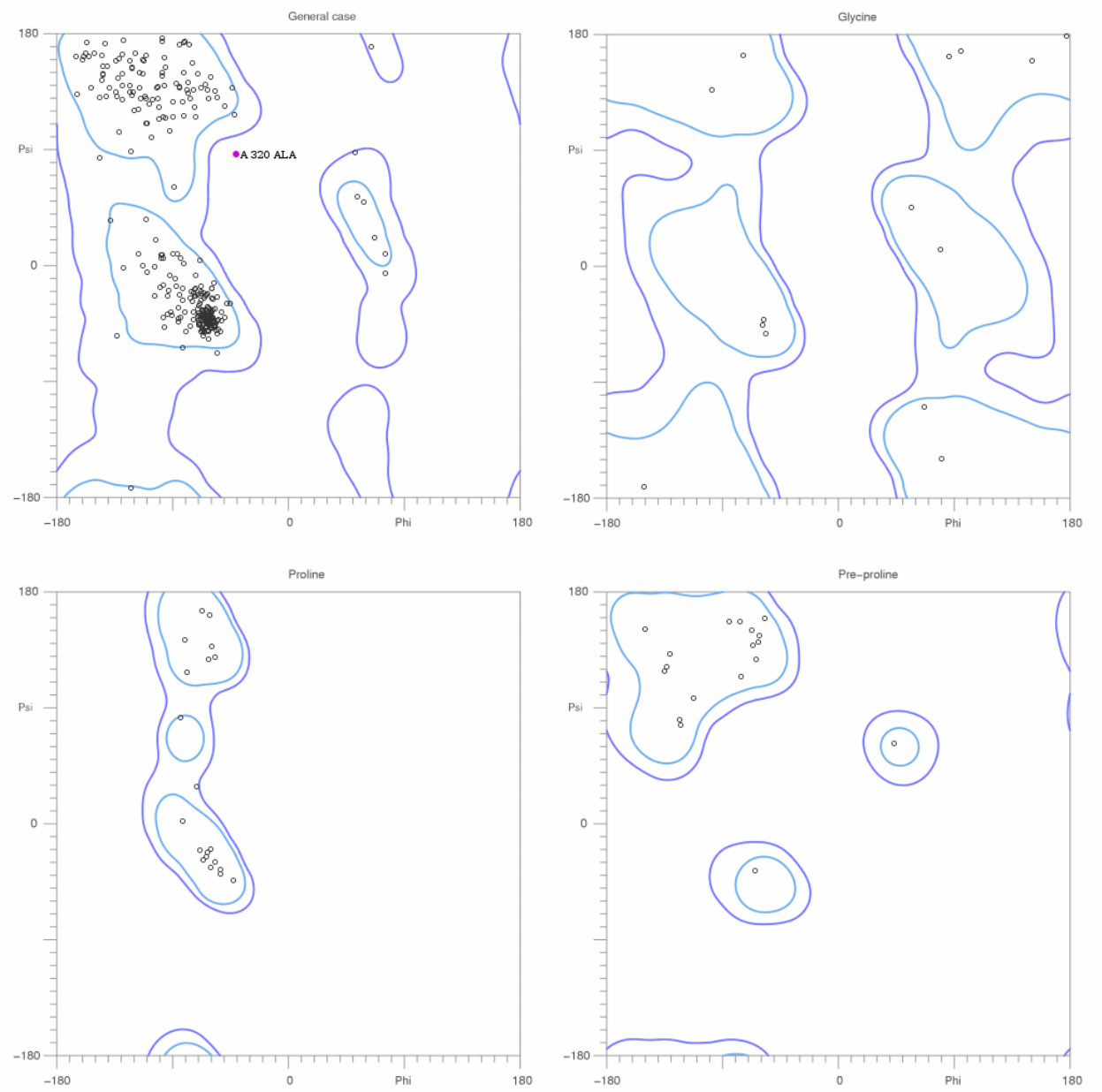
∗ 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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.
97.08% of all residues were in favored (98%) regions. (332 residues)
99.71% of all residues were in allowed (>99.8%) regions. (341 residues)
There were 1 outliers:
    A 320 ALA: (phi,psi) = (-39.57, 85.59)

4 Ligand analysis

4.1 880 A 501

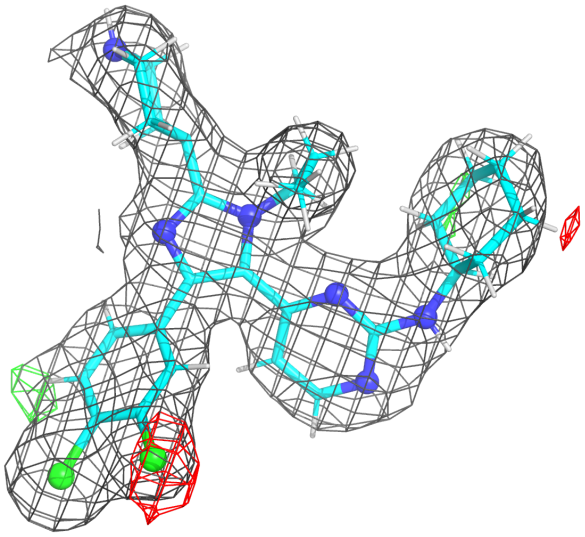
4.1.1 Statistics for ligand

Database ID	880 (PDB)
3-letter code	880
CC(2mF$_o$-DF$_c$)	0.9557
min(B-factor)‡	28.7
avg(B-factor)‡	36.1
max(B-factor)‡	44.2
min(occupancy)‡	1.00
max(occupancy)‡	1.00
‡hydrogen atoms excluded	

Restraints used
restraints for 880 (CYCLOHEXYL-_4-_5-_3,4-DICHLOROPHENYL_-2-PIPERIDIN-4-YL-3-PROPYL-3H-IMIDAZOL-4-YL_-PYRIMIDIN-2-YL_AMINE) from cif dictionary 880.grade_PDB_ligand.cif; generated by GRADE_PDB_LIGAND 1.2.9 (pre-release) (June 15 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



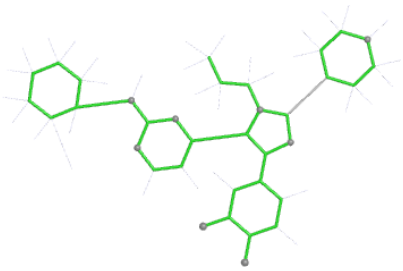
Electron density around 880 A 501 :
2mF$_o$-DF$_c$ (at 0.7 rmsd) in grey.
mF$_o$-DF$_c$ (at 3 rmsd) in red (negative) and green (positive),
(picture produced with PyMOL)

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

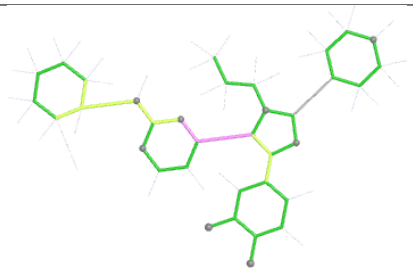
4.1.3 Mogul analysis for 880 A 501

Summary

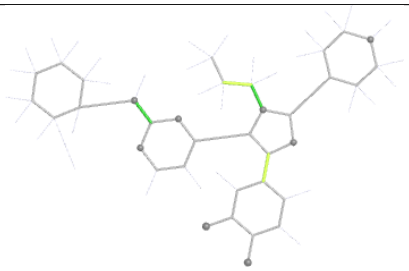
'bad' bonds	0/38
'bad' bond angles	0/43
'unusual' dihedrals	0/4
'bad' rings	0/4
bonds rms Z	0.554
angles rms Z	1.028



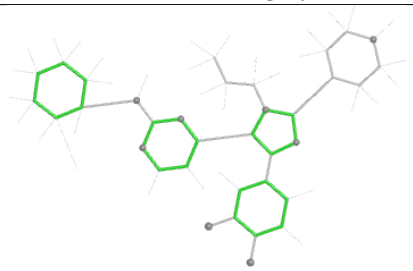
Mogul bonds
'good' → green
'unknown' → gray



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



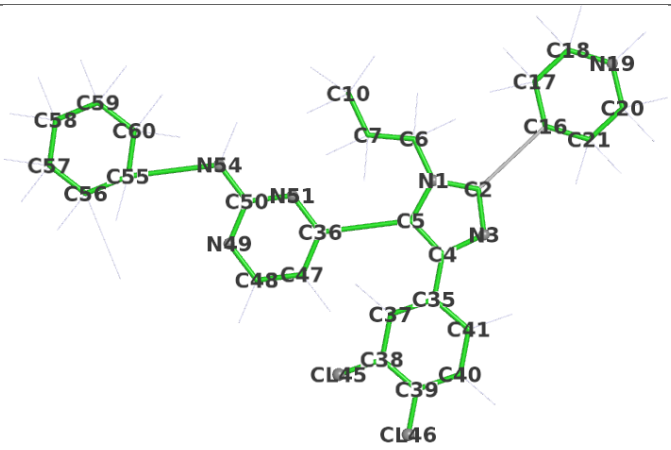
Mogul dihedrals
'rare' → lime, 'common' → green
'unknown' → gray



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 880 A 501



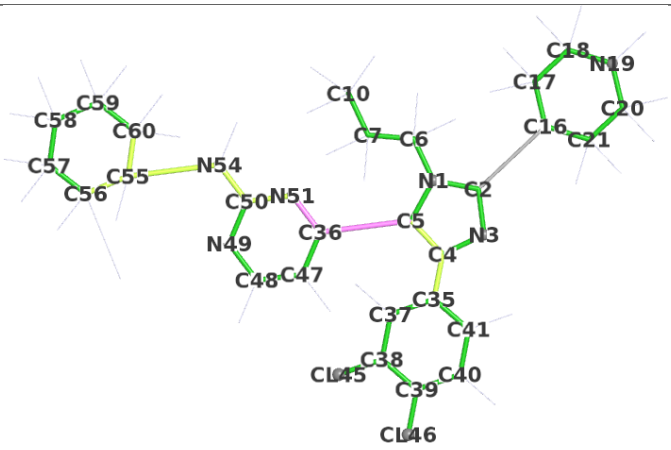
Mogul bonds schematic
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
C38-CL45	1.718	1.734	-0.016	0.012	3693	1.34
C5-C4	1.392	1.377	0.015	0.013	125	1.09
C39-C38	1.375	1.388	-0.013	0.013	403	0.98
C2-N3	1.302	1.316	-0.014	0.015	17	0.95
C50-N51	1.354	1.341	0.012	0.013	434	0.95
C36-C5	1.484	1.478	0.006	0.007	10	0.88
C7-C6	1.532	1.514	0.018	0.023	243	0.78
C58-C57	1.528	1.516	0.012	0.018	1743	0.71
C50-N54	1.350	1.342	0.008	0.013	12	0.67
C59-C58	1.527	1.516	0.011	0.018	1743	0.62
C5-N1	1.398	1.389	0.008	0.014	79	0.59
C55-N54	1.466	1.458	0.008	0.013	47	0.59
C4-N3	1.377	1.385	-0.008	0.013	288	0.58
C56-C55	1.509	1.518	-0.008	0.015	793	0.55
C21-C20	1.520	1.512	0.008	0.014	29	0.55
C6-N1	1.472	1.467	0.005	0.012	575	0.42
C10-C7	1.492	1.509	-0.017	0.040	1023	0.42
C20-N19	1.474	1.467	0.007	0.018	139	0.42
C50-N49	1.345	1.340	0.004	0.011	146	0.39
C41-C35	1.396	1.391	0.005	0.013	4266	0.39

(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 880 A 501

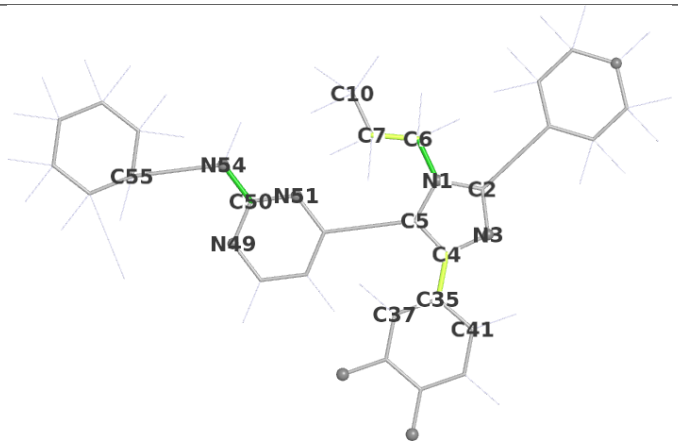


Mogul angles schematic
'poor' → violet (2.5 <Z <4)
'ok' → lime (1.5 <Z <2.5)
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C5-C36-N51	118.5	115.8	2.7	1.0	10	2.62
C56-C55-N54	114.8	110.6	4.3	1.7	34	2.49
C60-C55-N54	114.4	110.6	3.8	1.7	34	2.24
N54-C50-N51	119.2	116.5	2.7	1.4	22	1.95
C35-C4-C5	132.1	130.0	2.0	1.3	92	1.54
C47-C36-C5	119.5	121.1	-1.6	1.1	10	1.45
C40-C39-CL46	120.2	118.4	1.9	1.3	2376	1.42
C35-C4-N3	117.3	119.3	-2.0	1.4	227	1.39
N54-C50-N49	114.6	116.5	-1.9	1.4	22	1.38
C47-C36-N51	122.0	123.0	-1.0	0.8	691	1.22
C39-C38-CL45	119.9	120.9	-1.0	0.8	728	1.16
C38-C39-CL46	120.0	120.9	-0.9	0.8	728	1.02
C4-C5-N1	104.5	105.4	-0.9	0.9	25	1.02
C6-N1-C2	125.6	127.1	-1.6	1.6	26	1.00
C59-C58-C57	111.8	110.9	0.9	1.0	1269	0.87
C6-N1-C5	127.8	126.6	1.2	1.4	14	0.86
C48-C47-C36	116.5	117.1	-0.6	0.7	16	0.86
C47-C48-N49	123.4	124.1	-0.7	0.9	427	0.81
C37-C38-C39	120.9	120.2	0.7	1.0	476	0.73
C20-N19-C18	111.4	110.5	0.9	1.3	60	0.67
(table limited to 20 rows)						

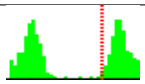
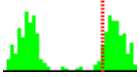
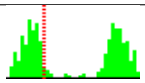
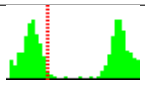
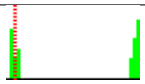
For help on "Ligand Mogul Analysis: Angles" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulAngles

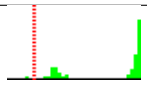
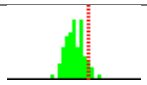
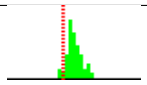
Mogul dihedral results for 880 A 501



Mogul dihedrals schematic

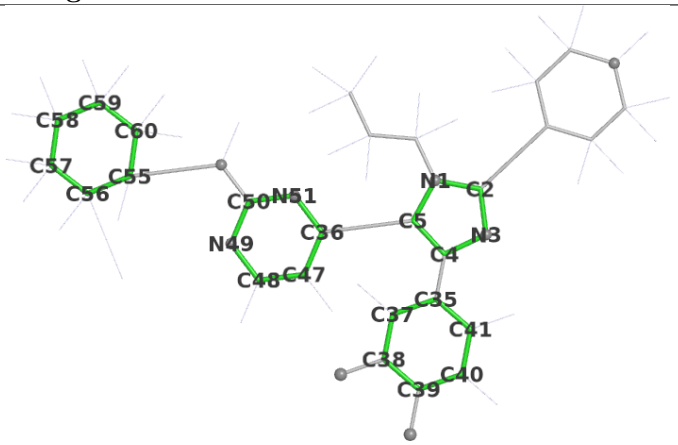
'rare' → lime (all torsion angles have >0.5% of population within ± 10 °)
'common' → green (all torsion angles have >10% of population within ± 10 °)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
...-C35-C4-...				rare
C41-C35-C4-C5	-129.6		452	6%
C37-C35-C4-N3	-130.9		528	19%
C41-C35-C4-N3	46.6		528	16%
C37-C35-C4-C5	52.9		452	9%
...-C50-N54-...				common
N51-C50-N54-C55	-7.8		22	45%
N49-C50-N54-C55	167.4		22	55%
...-C6-C7-...				rare

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
N1-C6-C7-C10	32.4		196	1%
...-C6-N1-...				common
C7-C6-N1-C5	-108.2		97	32%
C7-C6-N1-C2	71.6		49	43%

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 880 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 °
C55-C56-C57-C58-C59-C60	148	0.5
N1-C2-N3-C4-C5	58	0.1
C36-C47-C48-N49-C50-N51	41	0.7
C35-C37-C38-C39-C40-C41	246	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

4.2 ANP A 502

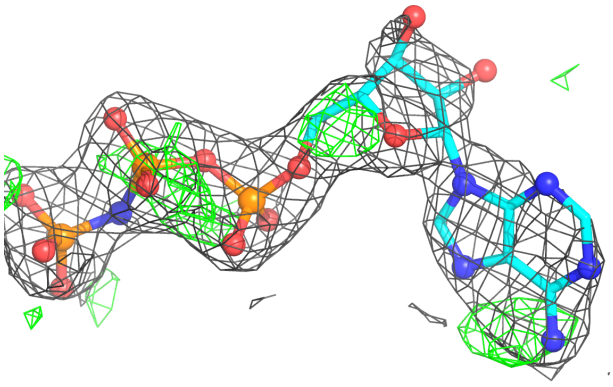
4.2.1 Statistics for ligand

Database ID	ANP (PDB)
3-letter code	ANP
CC(2mF$_o$-DF$_c$)	0.7959
min(B-factor)‡	35.8
avg(B-factor)‡	46.5
max(B-factor)‡	56.1
min(occupancy)‡	0.50
max(occupancy)‡	0.50
‡hydrogen atoms excluded	

Restraints used
restraints for ANP (PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER) from cif dictionary ANP.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



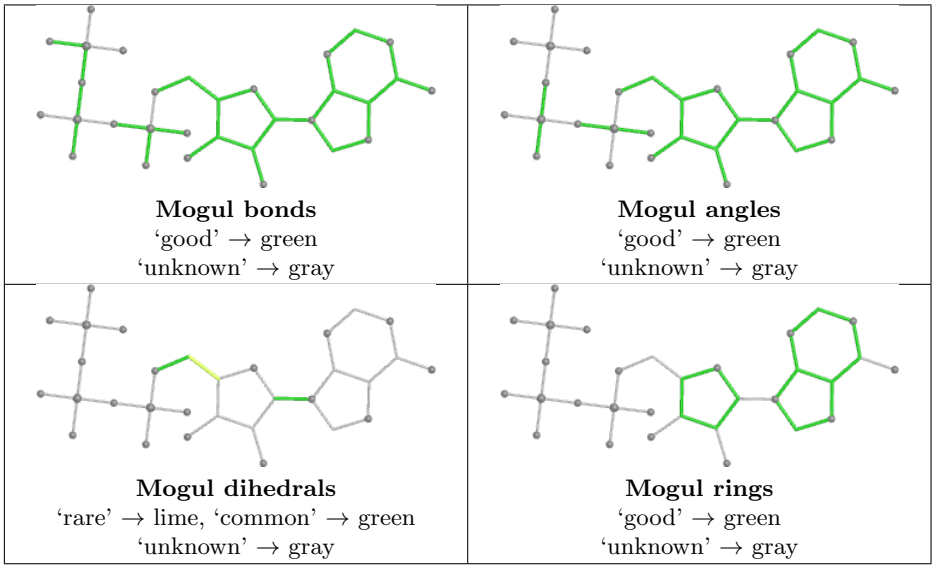
Electron density around ANP A 502 :
2mF$_o$-DF$_c$ (at 0.7 rmsd) in grey.
mF$_o$-DF$_c$ (at 3 rmsd) in red (negative) and green (positive),
(picture produced with PyMOL)

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 ANP A 502

Summary

'bad' bonds	0/28
'bad' bond angles	0/33
'unusual' dihedrals	0/3
'bad' rings	0/3
bonds rms Z	0.249
angles rms Z	0.326



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

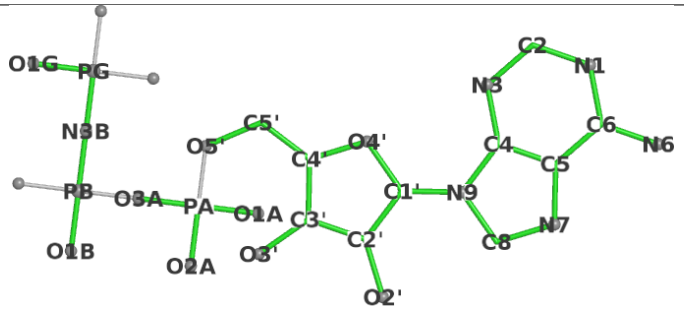
Mogul angles
'good' → green
'unknown' → gray

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 ANP A 502

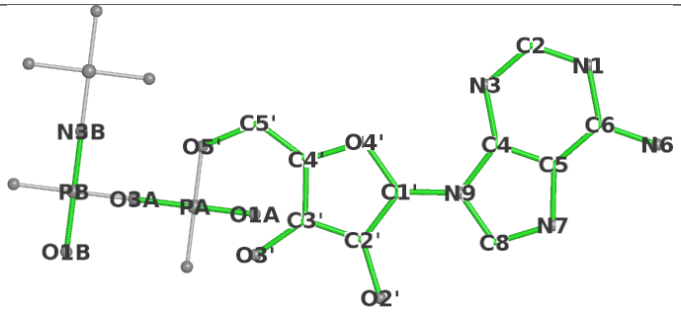


Mogul bonds schematic
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
PA-O2A	1.511	1.527	-0.016	0.030	30	0.55
O4'-C4'	1.448	1.444	0.004	0.011	1633	0.40
C6-N1	1.354	1.350	0.004	0.010	239	0.39
C1'-N9	1.463	1.459	0.004	0.012	78	0.34
C2-N3	1.338	1.335	0.004	0.011	829	0.33
C4-N3	1.343	1.339	0.004	0.012	542	0.33
C2-N1	1.338	1.335	0.003	0.011	829	0.30
C8-N9	1.372	1.370	0.002	0.008	190	0.29
PG-N3B	1.637	1.631	0.006	0.022	23	0.28
C4-N9	1.372	1.374	-0.002	0.008	181	0.28
PA-O1A	1.477	1.482	-0.005	0.018	31	0.26
C5'-C4'	1.511	1.508	0.003	0.012	1182	0.25
C3'-C4'	1.529	1.526	0.003	0.014	577	0.22
C5-N7	1.385	1.387	-0.001	0.007	359	0.22
C6-N6	1.333	1.336	-0.003	0.014	531	0.20
PB-N3B	1.635	1.631	0.004	0.022	23	0.20
O3'-C3'	1.426	1.423	0.003	0.013	3264	0.19
O4'-C1'	1.417	1.415	0.002	0.011	592	0.14
PA-O3A	1.595	1.594	0.001	0.011	21	0.13
C5-C4	1.386	1.388	-0.001	0.011	332	0.13
(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 ANP A 502



Mogul angles schematic

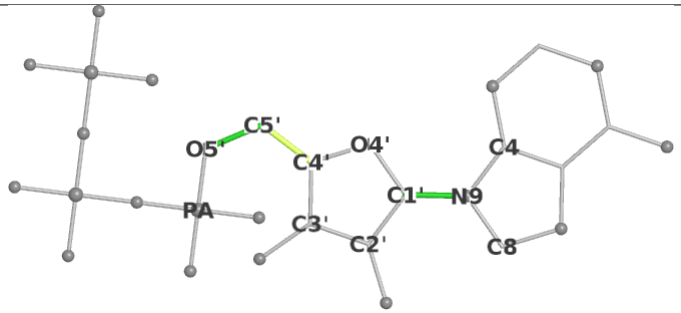
'good' → green (Z <1.5)

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

atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
O5'-C5'-C4'	111.1	109.1	2.0	2.3	84	0.87
O3'-C3'-C2'	113.7	111.9	1.7	2.6	938	0.66
O2'-C2'-C3'	113.6	111.9	1.7	2.6	938	0.65
C2'-C1'-N9	114.9	114.1	0.8	1.5	59	0.51
O4'-C4'-C5'	110.3	109.6	0.7	1.5	204	0.48
C4'-O4'-C1'	110.2	109.5	0.7	1.4	434	0.47
N3-C4-N9	127.5	127.1	0.5	1.2	126	0.41
O4'-C4'-C3'	105.8	105.3	0.5	1.3	448	0.39
C5'-C4'-C3'	114.7	115.3	-0.6	1.8	70	0.34
C5-C4-N3	126.6	126.8	-0.2	0.7	212	0.33
N6-C6-N1	118.6	118.2	0.4	1.2	214	0.30
C2-N1-C6	118.8	118.5	0.3	1.0	154	0.29
C3'-C2'-C1'	101.2	101.5	-0.3	1.2	273	0.29
O2'-C2'-C1'	111.4	110.6	0.8	2.8	323	0.28
O1B-PB-N3B	111.7	112.1	-0.4	1.7	15	0.24
C5-C4-N9	105.9	105.7	0.1	0.5	148	0.23
C1'-N9-C8	127.1	126.8	0.4	1.9	65	0.21
C2-N3-C4	111.1	111.5	-0.4	2.0	224	0.20
O4'-C1'-N9	108.6	108.4	0.2	1.3	66	0.18
C6-C5-N7	132.3	132.1	0.2	1.2	118	0.17
(table limited to 20 rows)						

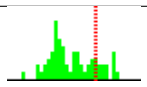
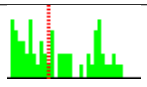
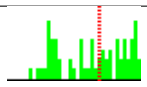
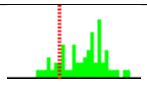
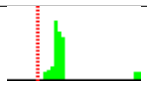
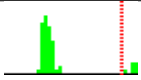
For help on "Ligand Mogul Analysis: Angles" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulAngles

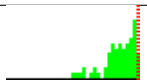
Mogul dihedral results for ANP A 502



Mogul dihedrals schematic

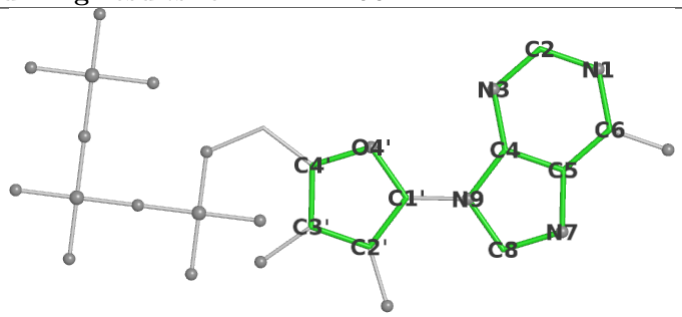
'rare' → lime (all torsion angles have >0.5% of population within ± 10 °)
'common' → green (all torsion angles have >10% of population within ± 10 °)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
...-C1'-N9-...				common
C2'-C1'-N9-C4	119.7		66	18%
O4'-C1'-N9-C8	54.0		64	16%
O4'-C1'-N9-C4	-121.0		68	18%
C2'-C1'-N9-C8	-65.3		63	17%
...-C4'-C5'-...				rare
O4'-C4'-C5'-O5'	36.3		63	3%
C3'-C4'-C5'-O5'	155.5		63	2%
...-C5'-O5'-...				common

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
C4'-C5'-O5'-PA	-179.2		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 ANP A 502



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 °
N9-C8-N7-C5-C4	186	0.0
C5-C6-N1-C2-N3-C4	184	0.1
C4'-O4'-C1'-C2'-C3'	191	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

5 X-ray statistics

5.1 Scaling parameters in last cycle

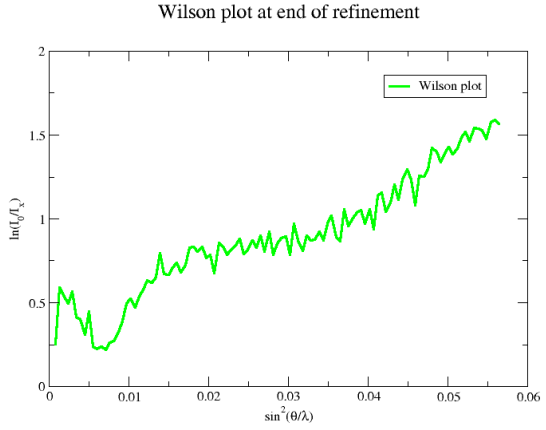
Refined parameters		Unrefined parameters	
K_OVER	0.77997902	K_MISS	1.00000000
B_IMPF_FRAG	1.31938221	B_MISS	0.00000000
K_SOLV	0.74732490	K_IMPF_MISS	1.00000000
B_SOLV	42.69776549	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	41.06995858	K_IMPF_SOLV	1.00000000
B_11	-28.61001361	B_OVER	0.00000000
B_22	11.87356543	B_12	0.00000000
B_33	16.73644818	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

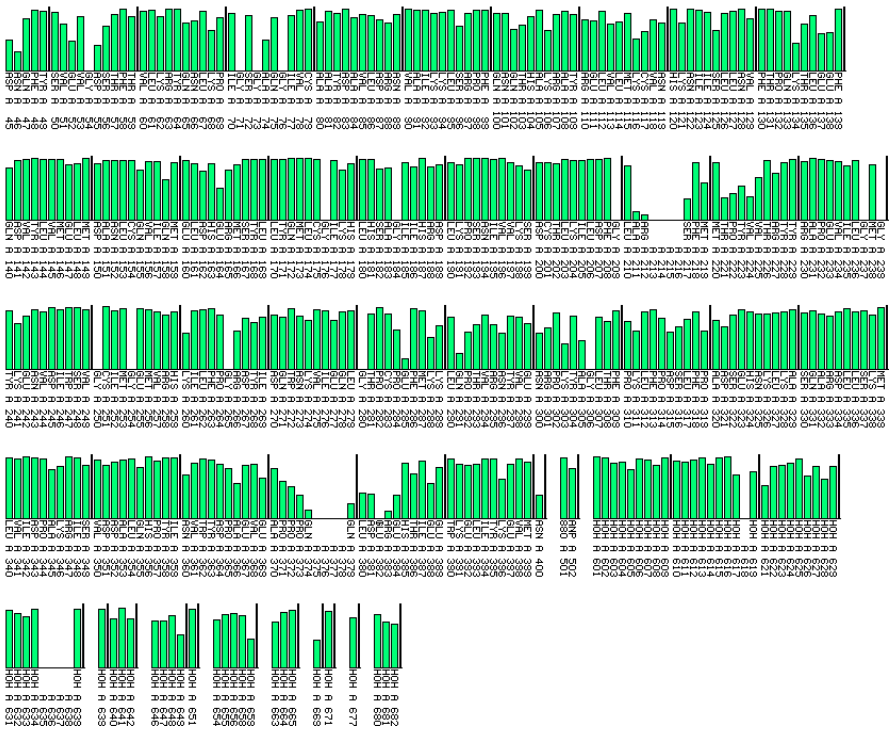
5.2.1 Wilson plot at start of refinement

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