Report on BUSTER refinement run in directory 1pmq_01_MapOnly

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:
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 $> 5.0\ \sigma$. 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_final.txt` for more detail

1.2 Run conditions

refine command	`/mnt/scratch_fs1/osmart/autobuster/Server/-autoBUSTER/bin/linux64/refine -p 1pmq_hydro-genate_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 in directory	`?, Mon Jun 16 15:21:43 BST 2014, osmart` `/home/osmart/2014/06/erice_workshop/1pmq_tuto-rial`
nthreads, hostname, OS	`6, hypatia, Ubuntu precise (12.04.4 LTS)`
buster-report command	`/home/osmart/autobuster/Server/scripts/-buster-report -d 1pmq_01_MapOnly -dr 1pmq_-01_MapOnly.report -f`
buster-report version, run at, by user	`1.1.4 <July 25 2015>, Sat Jul 25 18:42:14 2015, osmart`
buster-report run on refine directory	`/home/osmart/2014/06/erice_workshop/1pmq_-tutorial/1pmq_01_MapOnly`
buster-report output directory	`/home/osmart/2014/06/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
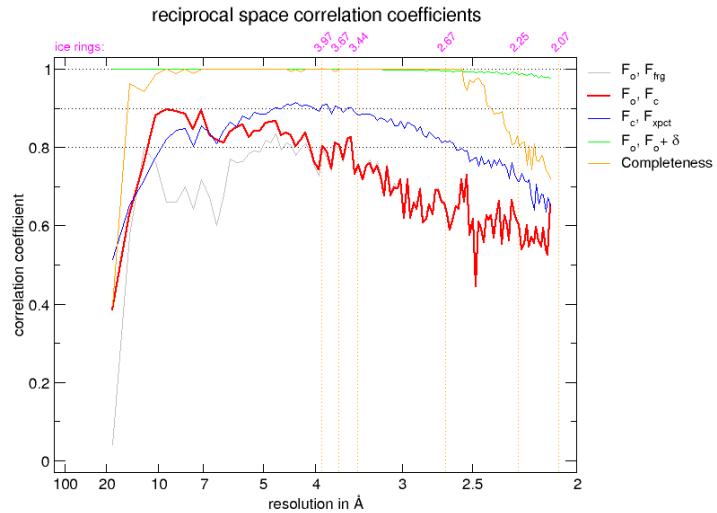
2.1.2 Final RSCC plot
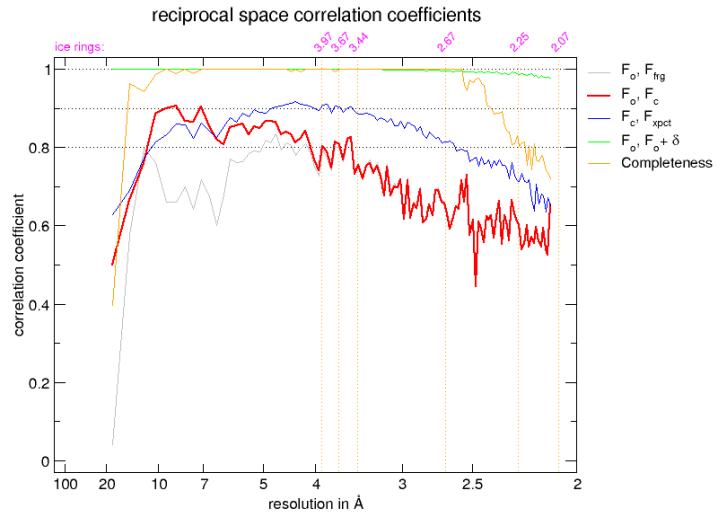
2.2 R-factor behaviour during refinement

R_{work} and R_{free} progress
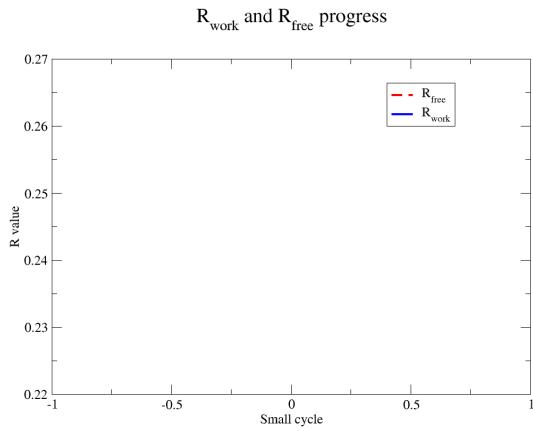
2.3 LLG behaviour during refinement

LLG progress
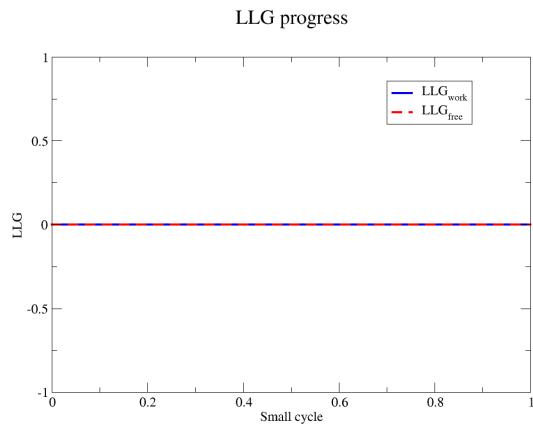
2.4 Geometry behaviour during optimisation

3 MolProbity analysis

3.1 Summary statistics

| All–Atom Contacts	Clashscore, all atoms:	10.39		88th 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†	2.36		62nd 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
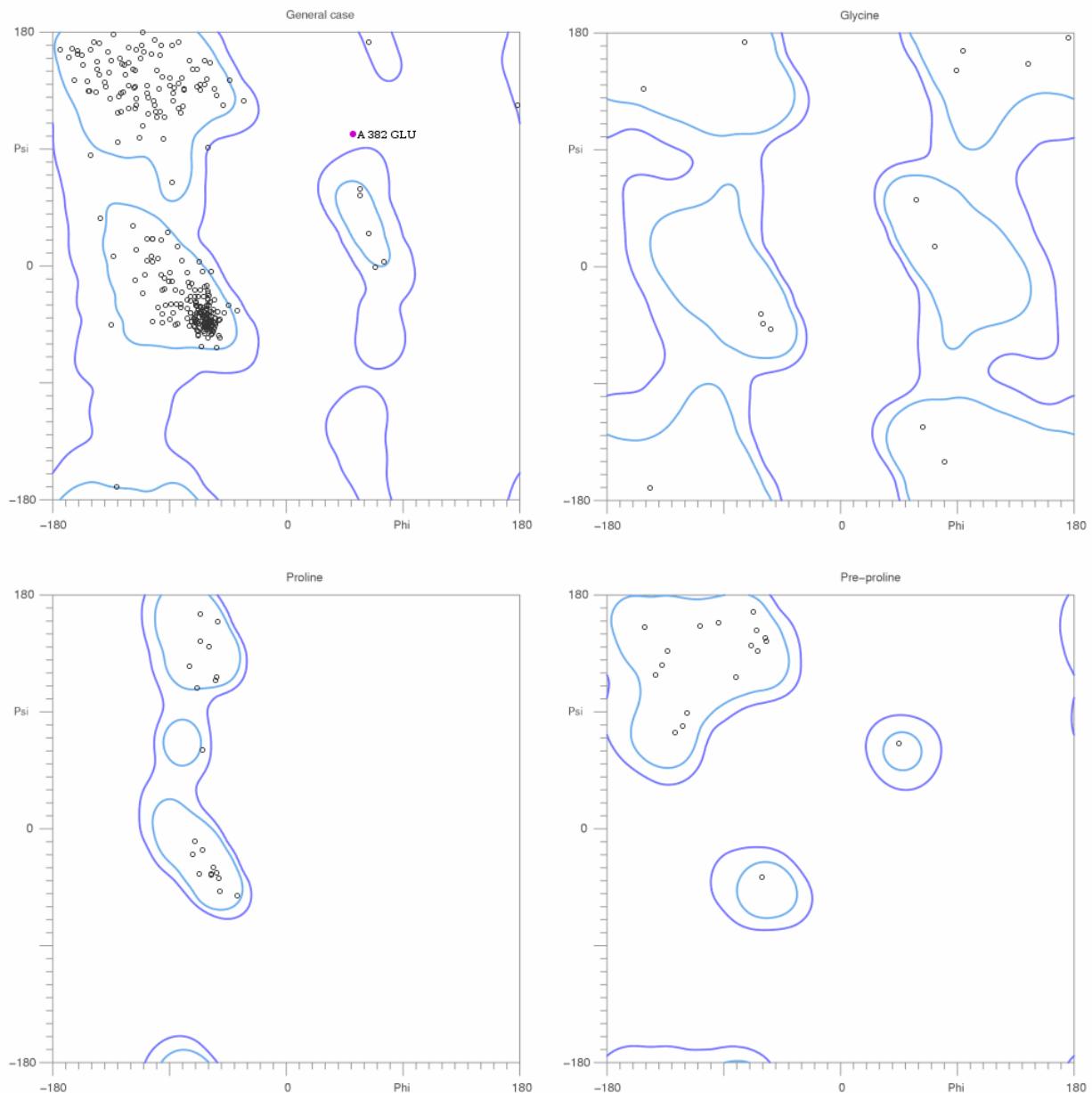
342 residues were evaluated in total for general, glycine, proline, and pre-pro.
95.61% of all residues were in favored (98%) regions. (327 residues)
99.71% of all residues were in allowed (>99.8%) regions. (341 residues)
There were 1 outliers:
    A 382 GLU: (phi,psi) = (52.05, 100.76)

4 Ligand analysis

4.1 880 A 501

4.1.1 Statistics for ligand

Database ID	880 (PDB)
3-letter code	880
CC(2mF$_o$-DF$_c$)	0.9495
min(B-factor)‡	30.2
avg(B-factor)‡	35.5
max(B-factor)‡	45.5
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

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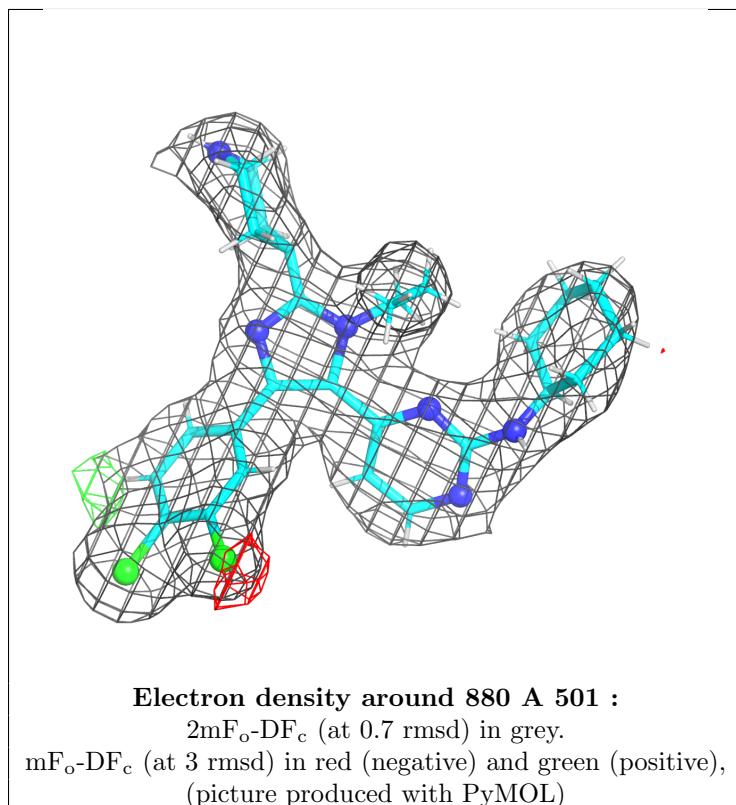
4.1.3 Mogul analysis for 880 A 501

Summary

'bad' bonds	11/38
'bad' bond angles	7/43
'unusual' dihedrals	2/4
'bad' rings	0/4
bonds rms Z	4.186
angles rms Z	3.033

Mogul bonds
'bad' → purple, 'poor' → violet
'ok' → lime, 'good' → green
'unknown' → gray

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

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

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

For help on "Ligand Mogul Analysis" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#Mogul
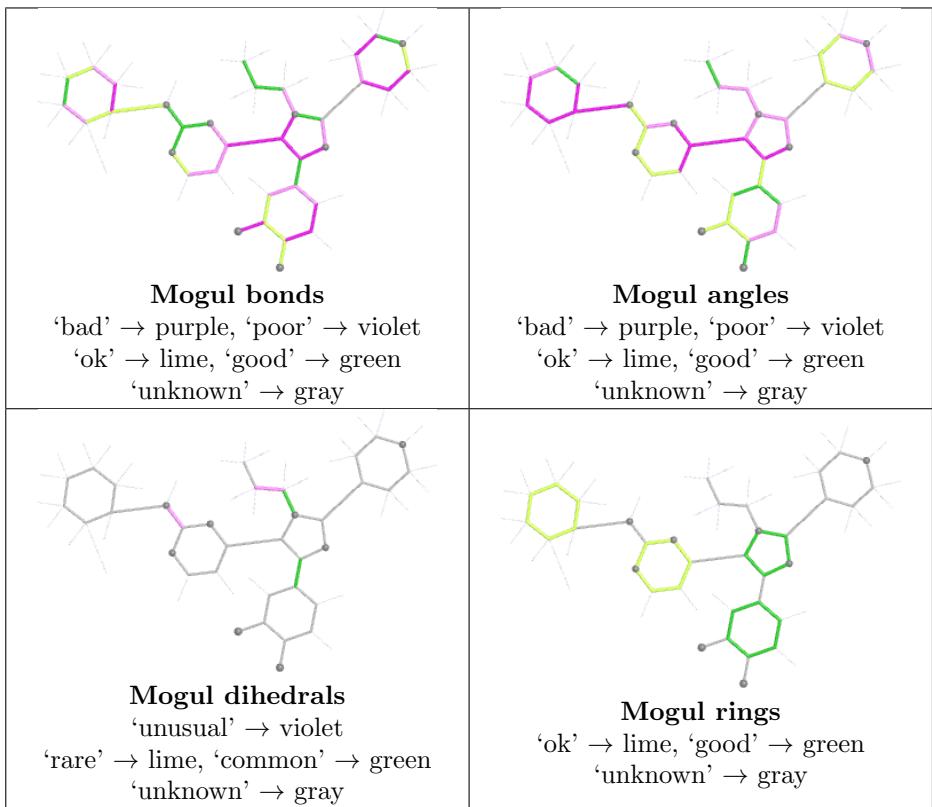
Mogul bond results for 880 A 501

Mogul bonds schematic
'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
C36-C5	1.555	1.478	0.078	0.007	10	10.49
C5-N1	1.520	1.389	0.131	0.014	79	9.07
C5-C4	1.493	1.377	0.116	0.013	125	8.72
C41-C40	1.466	1.382	0.083	0.010	4486	8.42
C21-C20	1.595	1.512	0.083	0.014	29	5.98
C40-C39	1.459	1.384	0.075	0.013	2673	5.62
C17-C18	1.585	1.512	0.072	0.014	29	5.23
C38-CL45	1.672	1.734	-0.061	0.012	3693	5.22
C60-C55	1.587	1.518	0.069	0.015	793	4.56
C4-N3	1.443	1.385	0.059	0.013	288	4.47
C21-C16	1.590	1.531	0.059	0.014	1072	4.06
C41-C35	1.441	1.391	0.050	0.013	4266	3.95
C47-C36	1.428	1.389	0.039	0.010	1673	3.93
C36-N51	1.367	1.341	0.026	0.007	892	3.79
C59-C60	1.571	1.525	0.046	0.013	1827	3.48
C2-N3	1.366	1.316	0.050	0.015	17	3.39
C47-C48	1.418	1.381	0.037	0.011	2637	3.27
C37-C35	1.420	1.391	0.029	0.009	1816	3.18
C17-C16	1.575	1.531	0.043	0.014	1072	3.00
C57-C56	1.559	1.525	0.034	0.013	1827	2.57
(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
'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 °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C5-C36-N51	123.6	115.8	7.8	1.0	10	7.61
C60-C55-N54	97.7	110.6	-12.8	1.7	34	7.49
C56-C55-N54	122.7	110.6	12.1	1.7	34	7.08
C60-C55-C56	114.9	110.7	4.3	0.8	315	5.15
C58-C57-C56	116.0	111.3	4.8	1.0	1421	4.92
C47-C36-C5	116.2	121.1	-5.0	1.1	10	4.38
C5-C4-N3	105.2	110.3	-5.1	1.2	77	4.25
C47-C36-N51	119.7	123.0	-3.2	0.8	691	3.93
C59-C58-C57	114.7	110.9	3.9	1.0	1269	3.74
C57-C56-C55	114.0	111.2	2.8	0.8	586	3.47
C4-N3-C2	110.4	105.2	5.1	1.6	12	3.26
C20-N19-C18	114.6	110.5	4.1	1.3	60	3.10
C41-C40-C39	118.1	120.2	-2.1	0.7	492	2.80
C7-C6-N1	117.5	112.5	5.0	1.9	33	2.67
C6-N1-C5	130.4	126.6	3.7	1.4	14	2.65
C36-N51-C50	119.0	116.7	2.3	0.9	14	2.65
C6-N1-C2	123.1	127.1	-4.0	1.6	26	2.55
C35-C4-N3	122.9	119.3	3.6	1.4	227	2.48
C37-C38-CL45	115.9	118.4	-2.5	1.2	1948	1.99
C18-C17-C16	112.7	109.8	2.9	1.5	90	1.91
(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

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Mogul dihedral results for 880 A 501
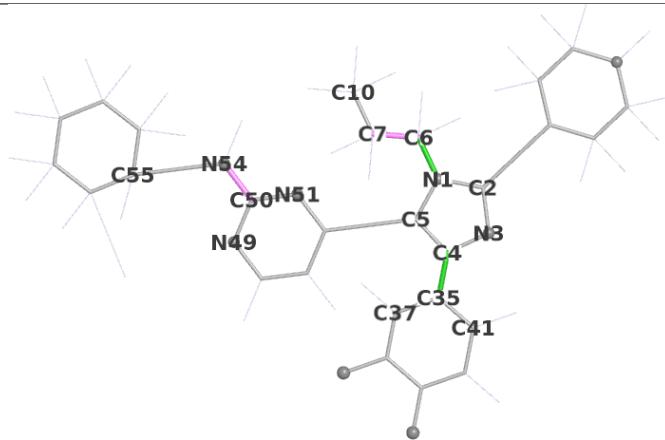

Mogul dihedrals schematic
'unusual' → violet (some torsion angles have <0.5% of population within ± 10 °)
'rare' → lime (all torsion angles have >0.5% of population within ± 10 °)
'common' → green (all torsion angles have >10% of population within ± 10 °)
'unknown' → gray (Mogul does not find sufficient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

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
...-C35-C4-...				common
C41-C35-C4-C5	-133.4		452	12%
C37-C35-C4-N3	-131.7		528	19%
C41-C35-C4-N3	48.8		528	16%
C37-C35-C4-C5	46.1		452	15%
...-C50-N54-...				unusual
N51-C50-N54-C55	-61.8		22	0%
N49-C50-N54-C55	119.9		22	0%
...-C6-C7-...				unusual

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
N1-C6-C7-C10	0.3		196	0%
...-C6-N1-...				common
C7-C6-N1-C5	-90.3		97	64%
C7-C6-N1-C2	91.3		49	76%
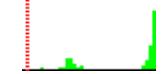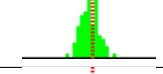
For help on "Ligand Mogul Analysis: Dihedrals" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulDihedrals

Mogul ring results for 880 A 501

Mogul rings schematic
'ok' → lime (ring strangeness score <6 °)
'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	5.8
N1-C2-N3-C4-C5	58	0.2
C36-C47-C48-N49-C50-N51	41	4.2
C35-C37-C38-C39-C40-C41	246	0.2

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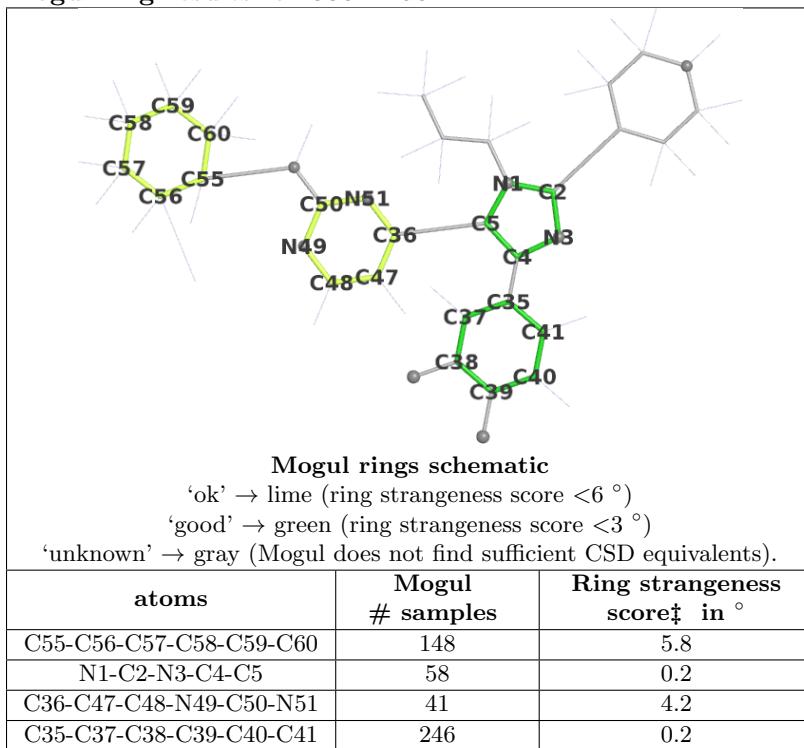
For help on "Ligand Mogul Analysis: Rings" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulRings

4.2 ANP A 502

4.2.1 Statistics for ligand

| Database ID	ANP (PDB)
3-letter code	ANP
$CC(2mF_o\text{-}DF_c)$	0.7687
min(B-factor)‡	43.6
avg(B-factor)‡	48.9
max(B-factor)‡	54.1
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 :
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in grey.
$mF_o\text{-}DF_c$ (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
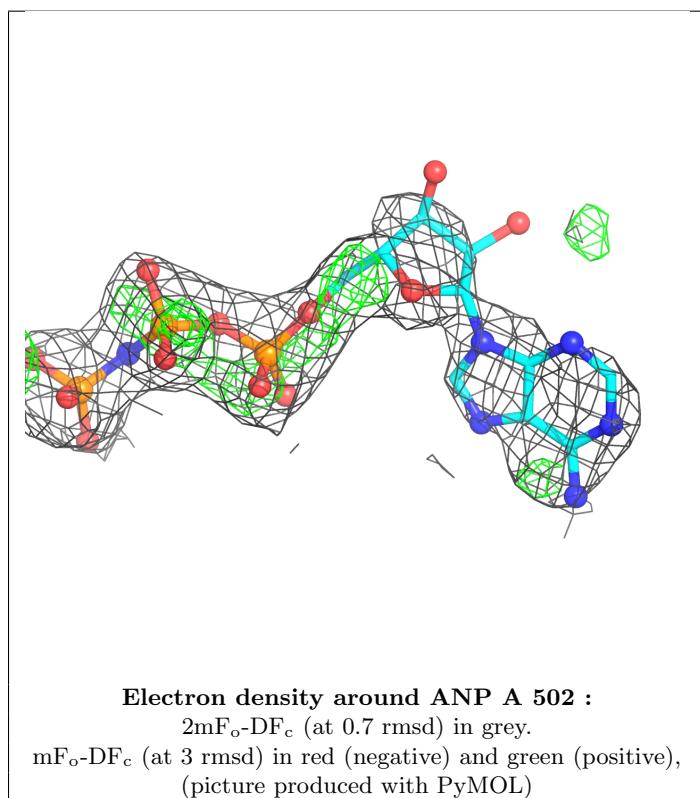
4.2.3 Mogul analysis for ANP A 502

Summary

'bad' bonds	6/28
'bad' bond angles	9/33
'unusual' dihedrals	0/3
'bad' rings	0/3
bonds rms Z	4.275
angles rms Z	4.310

Mogul bonds
'bad' → purple, 'poor' → violet
'ok' → lime, 'good' → green
'unknown' → gray

Mogul angles
'bad' → purple, '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
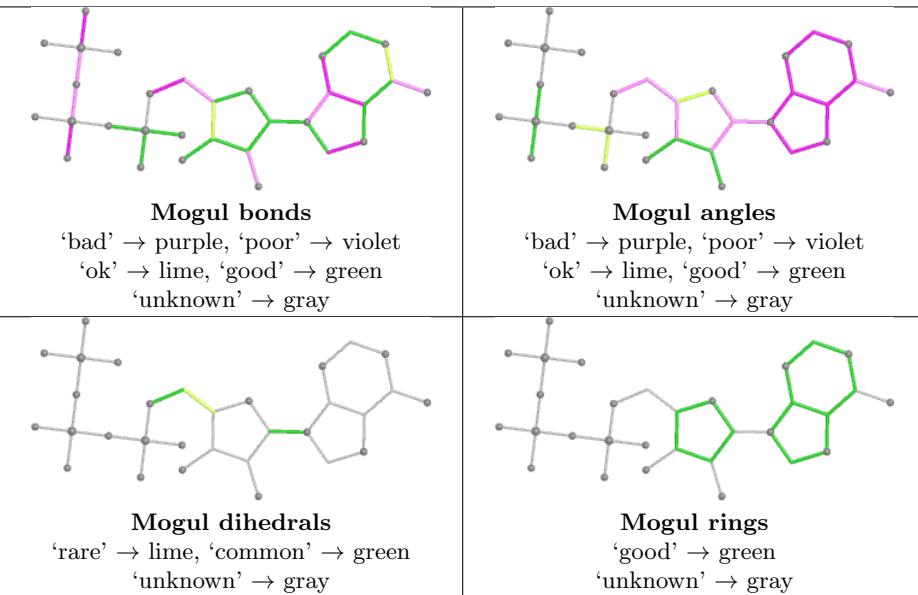
Mogul bond results for ANP A 502

Mogul bonds schematic
'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
O5'-C5'	1.626	1.443	0.183	0.015	124	11.89
PG-O2G	1.546	1.454	0.092	0.009	68	9.72
PB-O1B	1.532	1.454	0.078	0.009	68	8.25
C5-C4	1.476	1.388	0.088	0.011	332	7.92
C4-N3	1.424	1.339	0.085	0.012	542	7.10
C8-N7	1.350	1.311	0.039	0.008	447	5.17
C6-N6	1.384	1.336	0.048	0.014	531	3.35
PB-N3B	1.562	1.631	-0.068	0.022	23	3.06
O2'-C2'	1.458	1.423	0.035	0.013	3264	2.67
PG-N3B	1.572	1.631	-0.059	0.022	23	2.65
C5'-C4'	1.539	1.508	0.031	0.012	1182	2.55
C4-N9	1.395	1.374	0.020	0.008	181	2.52
C6-N1	1.370	1.350	0.020	0.010	239	2.03
C3'-C4'	1.551	1.526	0.026	0.014	577	1.87
C8-N9	1.381	1.370	0.011	0.008	190	1.47
O3'-C3'	1.442	1.423	0.019	0.013	3264	1.45
C2'-C1'	1.549	1.530	0.019	0.014	341	1.39
O4'-C4'	1.458	1.444	0.015	0.011	1633	1.31
PA-O1A	1.492	1.527	-0.035	0.030	30	1.17
O4'-C1'	1.427	1.415	0.012	0.011	592	1.06
(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
'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 °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C4-N9-C8	111.3	105.7	5.5	0.5	150	11.81
C5-N7-C8	108.5	103.7	4.9	0.5	265	10.64
N9-C8-N7	109.0	114.1	-5.1	0.7	173	7.20
C5-C4-N9	102.5	105.7	-3.3	0.5	148	7.10
N3-C2-N1	123.3	128.8	-5.5	0.9	329	6.26
C6-C5-C4	113.3	117.0	-3.7	0.7	127	5.67
N3-C4-N9	133.5	127.1	6.4	1.2	126	5.53
C2-N1-C6	123.4	118.5	4.8	1.0	154	5.05
C6-C5-N7	138.0	132.1	5.9	1.2	118	5.02
C5-C4-N3	124.1	126.8	-2.8	0.7	212	3.88
C4-C5-N7	108.7	110.7	-2.0	0.5	241	3.77
C5-C6-N1	120.6	117.6	3.0	0.9	133	3.48
O4'-C1'-C2'	110.4	106.5	3.9	1.2	307	3.37
C5-C6-N6	120.6	123.7	-3.0	1.0	144	2.95
O5'-C5'-C4'	102.3	109.1	-6.8	2.3	84	2.93
C5'-C4'-C3'	110.3	115.3	-5.0	1.8	70	2.81
O4'-C1'-N9	111.8	108.4	3.4	1.3	66	2.63
C2-N3-C4	115.4	111.5	3.9	2.0	224	1.98
C1'-N9-C8	123.3	126.8	-3.5	1.9	65	1.83
O4'-C4'-C5'	112.2	109.6	2.7	1.5	204	1.79
(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
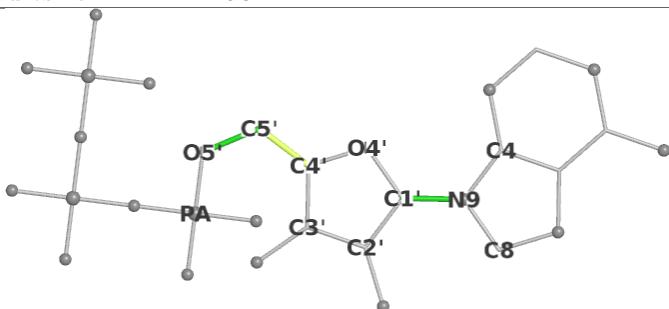
Mogul dihedrals schematic

'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	102.5		66	18%
O4'-C1'-N9-C8	47.0		64	17%
O4'-C1'-N9-C4	-131.2		68	15%
C2'-C1'-N9-C8	-79.3		63	22%
...-C4'-C5'-...				rare
O4'-C4'-C5'-O5'	59.6		63	71%
C3'-C4'-C5'-O5'	179.1		63	10%
...-C5'-O5'-...				common

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
C4'-C5'-O5'-PA	-171.5		74	43%
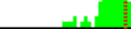
For help on "Ligand Mogul Analysis: Dihedrals" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulDihedrals

Mogul ring results for 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	0.2
C4'-O4'-C1'-C2'-C3'	191	1.1

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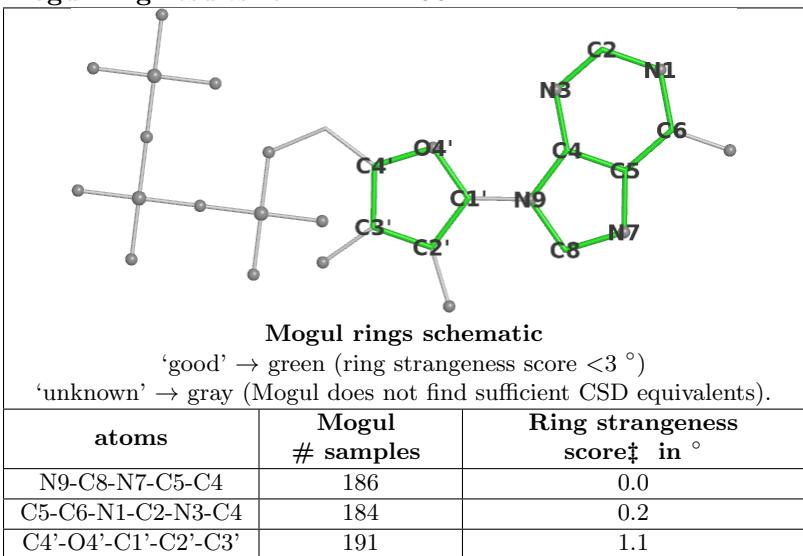
For help on "Ligand Mogul Analysis: Rings" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulRings

5 X-ray statistics

5.1 Scaling parameters in last cycle

Refined parameters		Unrefined parameters	
K_OVER	0.78579614	K_MISS	1.00000000
B_IMPF_FRAG	2.30750044	B_MISS	0.00000000
K_SOLV	0.66124588	K_IMPF_MISS	1.00000000
B_SOLV	70.43196690	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	19.60605014	K_IMPF_SOLV	1.00000000
B_11	-34.04047358	B_OVER	0.00000000
B_22	13.97100696	B_12	0.00000000
B_33	20.06946661	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
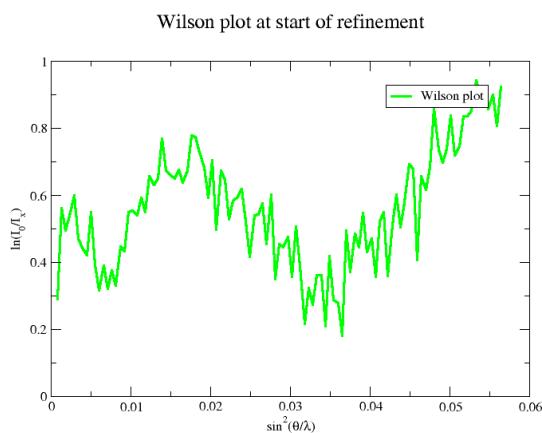
5.2.2 Wilson plot at end of refinement
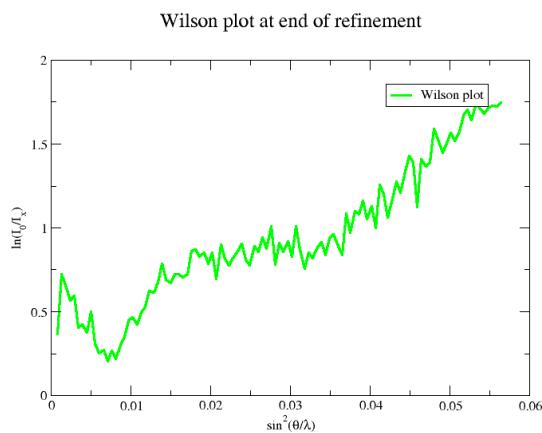
6 Real-space correlations

6.1 Side chains of chain A

6.2 Mainchain of chain A