

Report on BUSTER refinement run in directory 1pmq_10_improvedANP_final2

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1 Run overview

1.1 Run conditions

refine command	/mnt/public/xtal/Server-nightly-beta-consortium-linux64/autoBUSTER/bin/linux64/-refine -p 1pmq_09_final1-report/1pmq_09_final1.pdb -m dataAnisotropyServer.mtz -l 880.cation.grade.cif -Gelly 03_occupancy_refine.Gelly -M TLSbasic -nbig 3 -d /scratch/osmart/2015/11/./1pmq_10_improvedANP_final2
BUSTER version, run at, by user in directory	2.11.6, Mon Mar 9 12:17:07 GMT 2015, osmart/home/osmart/2014/11/1pmq_rerefine
nthreads, hostname, OS buster-report command	6, hypatia, Ubuntu precise (12.04.5 LTS) /home/osmart/autobuster/Server/scripts/-buster-report -d 1pmq_10_improvedANP_final2
buster-report version, run at, by user	-dr 1pmq_10_improvedANP_final2-report 1.1.4 <July 25 2015>, Sat Jul 25 19:41:10 2015, osmart
buster-report run on refine directory	/home/osmart/2014/11/1pmq_rerefine/1pmq_10_improvedANP_final2
buster-report output directory	/home/osmart/2014/11/1pmq_rerefine/1pmq_10_improvedANP_final2-report
final pdb coordinates	1pmq_10_improvedANP_final2-report.pdb
final mtzfile	1pmq_10_improvedANP_final2-report.mtz

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

1.2 Refinement vital statistics

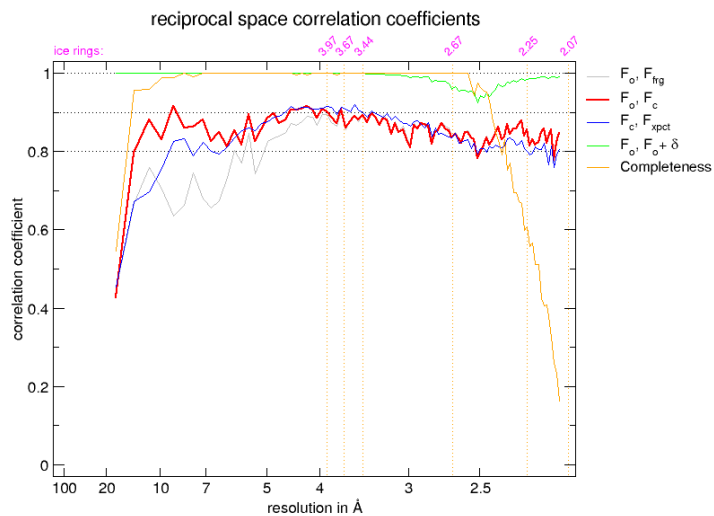
	start	final
N_{cycles} big	0	3
N_{cycles} small	0	88
X-ray weight	5.43	5.78
R_{work}	0.2172	0.1997
R_{free}	0.2341	0.2258
100 (R_{free} - R_{work})	1.7%	2.6%
LLG_{work} (cumulative Log-Likelihood Gain, working set)	0	0.1135
LLG_{free} (cumulative Log-Likelihood Gain, free set)	0	-0.0274
RMS bond in Å	0.0096	0.0098
RMS angle in degrees	1.01	0.99
High resolution limit in Å	2.10	2.10
Low resolution limit in Å	16.94	16.94
Number of waters	67	67

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

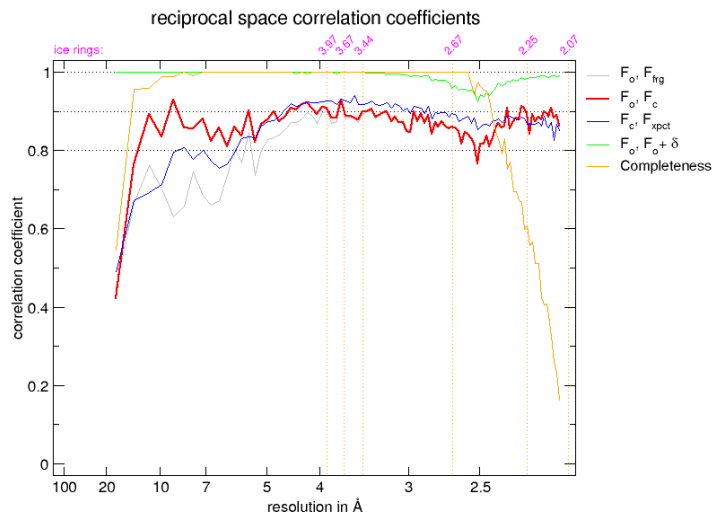
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

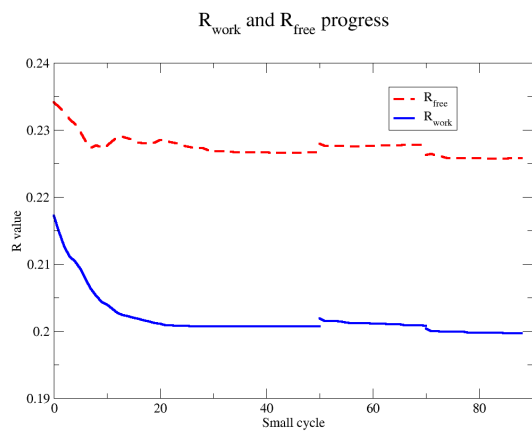
2.1.1 Initial RSCC plot



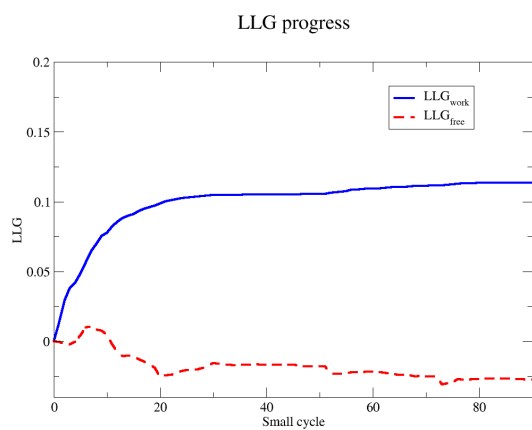
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement

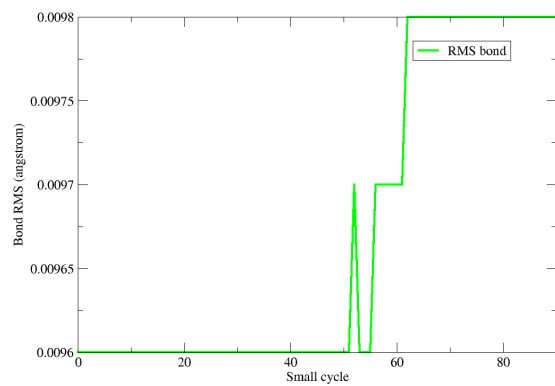


2.3 LLG behaviour during refinement

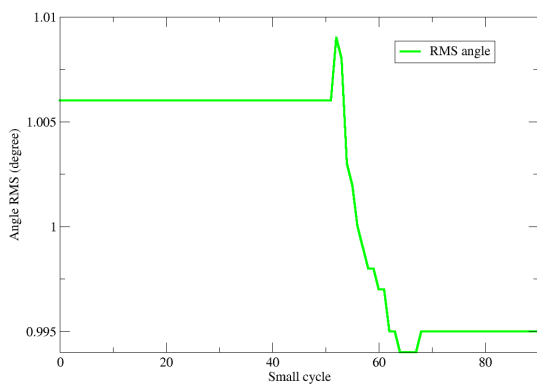


2.4 Geometry behaviour during optimisation

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:	1.89		100 th percentile* N=576, 2.10Å ± 0.25Å
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	0.71%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	311	96.28%	Goal: >98%
	Cβ deviations >0.25Å	1	0.31%	Goal: 0
	MolProbity score [†]	1.20		100 th percentile* N=11758, 2.10Å ± 0.25Å
	Bad backbone bonds:	0 / 1327	0.00%	Goal: 0%
Bad backbone angles:	0 / 1650	0.00%	Goal: <0.1%	

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

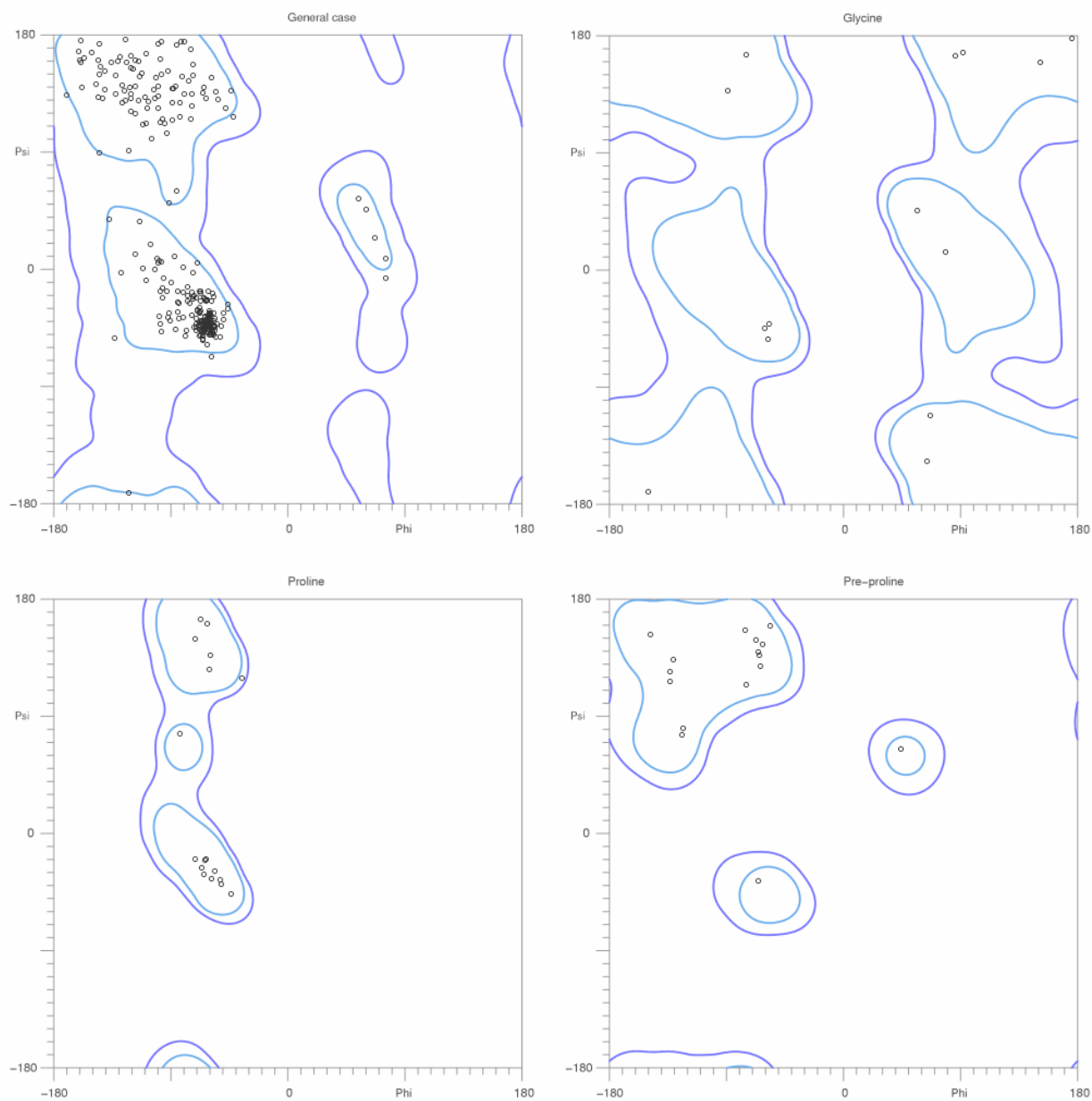
* 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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



323 residues were evaluated in total for general, glycine, proline, and pre-pro.
97.52% of all residues were in favored (98%) regions. (315 residues)
100.00% of all residues were in allowed (>99.8%) regions. (323 residues)
There were no outliers.

4 Ligand analysis

4.1 880 A 501 A

4.1.1 Statistics for ligand

Database ID	880 (PDB)
3-letter code	880
CC(2mF _o -DF _c)	-
min(B-factor)‡	5.7
avg(B-factor)‡	13.5
max(B-factor)‡	23.6
min(occupancy)‡	0.71
max(occupancy)‡	1.00
‡hydrogen atoms excluded	

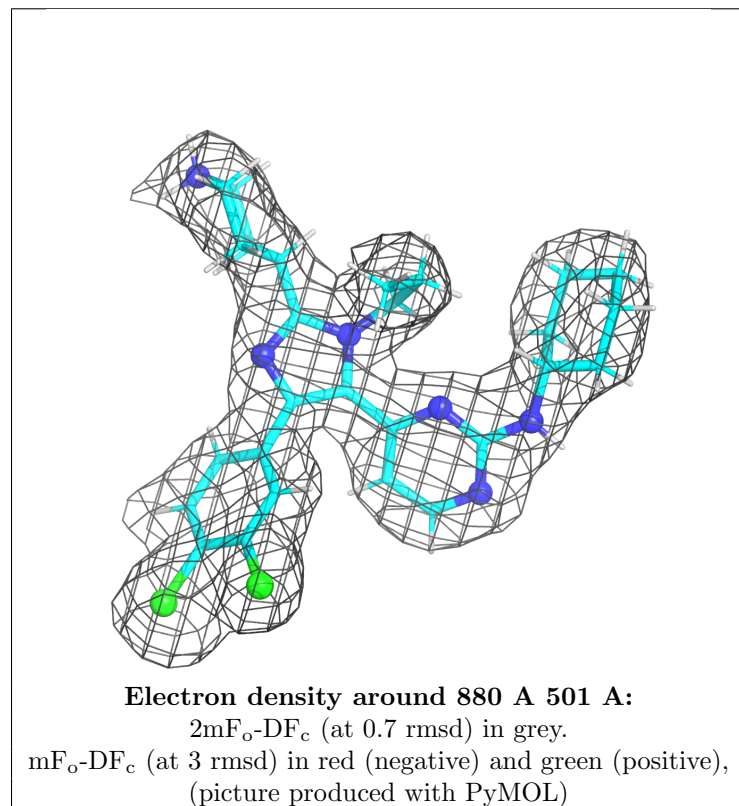
Restraints used

restraints for 880 (VUSAVSDZIWIWIDPM-UHFFFAOYSA-N) from cif dictionary 880_cation.grade.cif; generated by GRADE 1.2.9 (July 24 2014) from mol2 file using MOGUL 1.6(RC5), 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



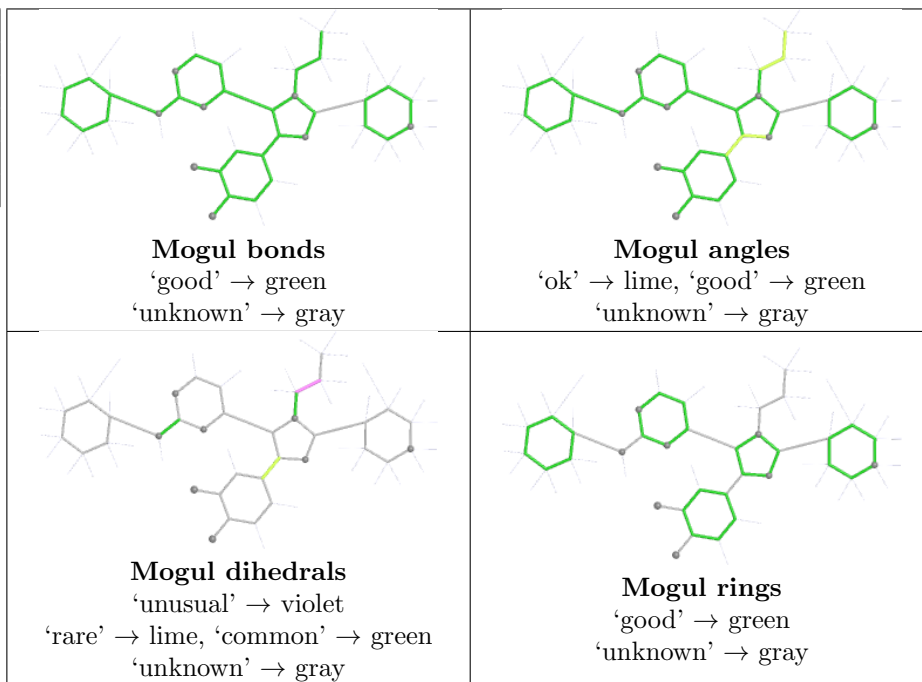
For help on “Ligand Electron Density Picture” see BUSTER wiki page

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

4.1.3 Mogul analysis for 880 A 501 A

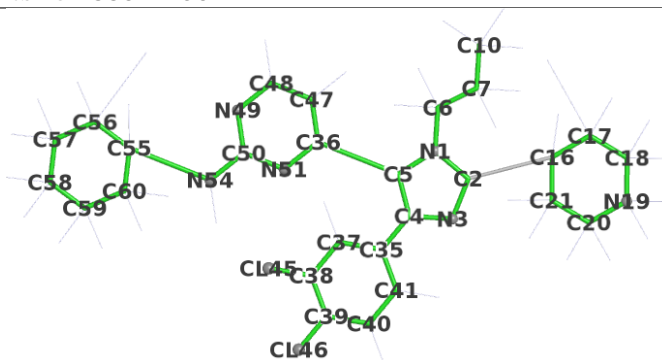
Summary

'bad' bonds	0/38
'bad' bond angles	0/45
'unusual' dihedrals	1/4
'bad' rings	0/5
bonds rms Z	0.392
angles rms Z	0.692



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 A



Mogul bonds schematic

'good' → green (Z < 1.5)

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

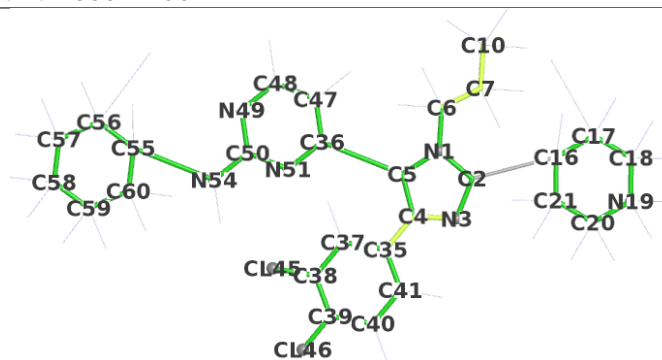
atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
C50-N51	1.353	1.341	0.012	0.013	434	0.91
C5-C4	1.387	1.377	0.010	0.013	125	0.79
C59-C58	1.529	1.516	0.014	0.018	1743	0.77
C36-C5	1.483	1.478	0.005	0.007	10	0.74
C2-N3	1.305	1.316	-0.011	0.015	17	0.72
C5-N1	1.398	1.389	0.009	0.014	79	0.62
C58-C57	1.525	1.516	0.009	0.018	1743	0.53
C38-CL45	1.728	1.734	-0.006	0.012	3693	0.52
C7-C6	1.525	1.514	0.012	0.023	243	0.49
C56-C55	1.525	1.518	0.007	0.015	793	0.46
C36-N51	1.344	1.341	0.003	0.007	892	0.43
C20-N19	1.491	1.488	0.004	0.008	1052	0.43
C60-C55	1.523	1.518	0.006	0.015	793	0.37
C4-N3	1.380	1.385	-0.005	0.013	288	0.36
C55-N54	1.462	1.458	0.004	0.013	47	0.32
C50-N54	1.346	1.342	0.004	0.013	12	0.31
C50-N49	1.344	1.340	0.003	0.011	146	0.30
C10-C7	1.498	1.509	-0.011	0.040	1023	0.27
C41-C35	1.394	1.391	0.003	0.013	4266	0.22
C20-C21	1.517	1.515	0.001	0.007	139	0.21

(table limited to 20 rows)

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

http://www.globalphasing.com/buster/wiki/index.cgi?BR_LigandReportAfter201507#MogulBonds

Mogul angle results for 880 A 501 A



Mogul angles schematic

'ok' → lime (1.5 < Z < 2.5)

'good' → green (Z < 1.5)

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

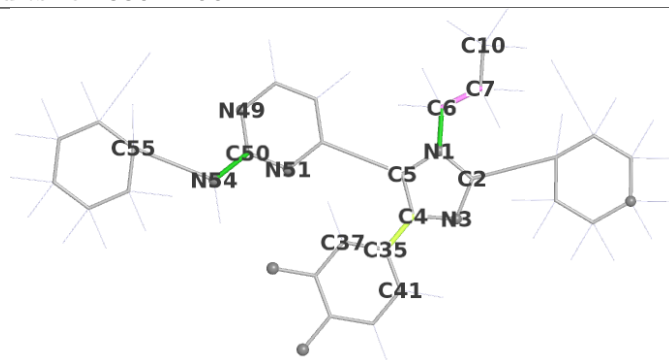
atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C10-C7-C6	115.9	111.8	4.1	2.5	217	1.62
C35-C4-N3	117.0	119.3	-2.3	1.4	227	1.62
C47-C36-N51	121.8	123.0	-1.2	0.8	691	1.49
C35-C4-C5	132.0	130.0	1.9	1.3	92	1.47
C6-N1-C2	125.1	127.1	-2.1	1.6	26	1.32
C4-C5-N1	104.4	105.4	-1.1	0.9	25	1.19
C47-C36-C5	122.2	121.1	1.0	1.1	10	0.90
C21-C16-C17	108.4	109.5	-1.1	1.2	259	0.90
N54-C50-N51	117.7	116.5	1.2	1.4	22	0.87
C6-N1-C5	127.9	126.6	1.2	1.4	14	0.86
C47-C48-N49	123.4	124.1	-0.7	0.9	427	0.78
C20-N19-C18	112.2	111.6	0.6	0.9	452	0.68
C37-C35-C4	120.9	119.9	1.0	1.4	31	0.68
C40-C39-CL46	119.2	118.4	0.8	1.3	2376	0.64
C48-C47-C36	116.7	117.1	-0.4	0.7	16	0.63
C7-C6-N1	113.6	112.5	1.2	1.9	33	0.62
C18-C17-C16	110.9	111.2	-0.4	0.6	72	0.61
C41-C35-C4	119.7	120.7	-1.0	1.7	1605	0.58
C60-C55-N54	109.7	110.6	-0.9	1.7	34	0.53
C4-N3-C2	106.0	105.2	0.8	1.6	12	0.50

(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 A



Mogul dihedrals schematic

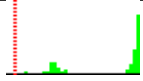
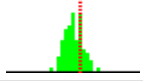
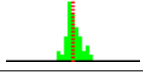
'unusual' → violet (some torsion angles have <0.5% of population within $\pm 10^\circ$)

'rare' → lime (all torsion angles have >0.5% of population within $\pm 10^\circ$)

'common' → green (all torsion angles have >10% of population within $\pm 10^\circ$)

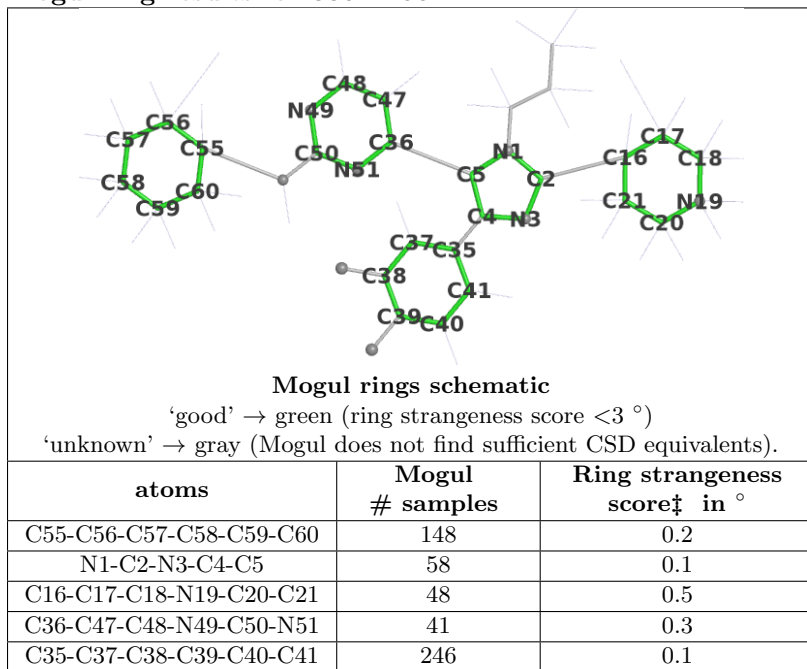
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual torsion angle in $^\circ$	Mogul histogram	Mogul # samples	classification or % Mogul population within $\pm 10^\circ$
...-C35-C4-...				rare
C41-C35-C4-C5	-126.8		452	6%
C37-C35-C4-N3	-131.9		528	19%
C41-C35-C4-N3	45.1		528	16%
C37-C35-C4-C5	56.2		452	4%
...-C50-N54-...				common
N51-C50-N54-C55	0.6		22	45%
N49-C50-N54-C55	176.9		22	55%
...-C6-C7-...				unusual

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within $\pm 10^\circ$
N1-C6-C7-C10 ...-C6-N1-...	-9.6		196	0% common
C7-C6-N1-C5	-95.6		97	56%
C7-C6-N1-C2	87.4		49	82%

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 A



‡‘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>

4.2 880 A 501 B

4.2.1 Statistics for ligand

Database ID	880 (PDB)
3-letter code	880
CC($2mF_o-DF_c$)	-
min(B-factor) \ddagger	4.4
avg(B-factor) \ddagger	12.3
max(B-factor) \ddagger	23.6
min(occupancy) \ddagger	0.29
max(occupancy) \ddagger	1.00
\ddagger hydrogen atoms excluded	

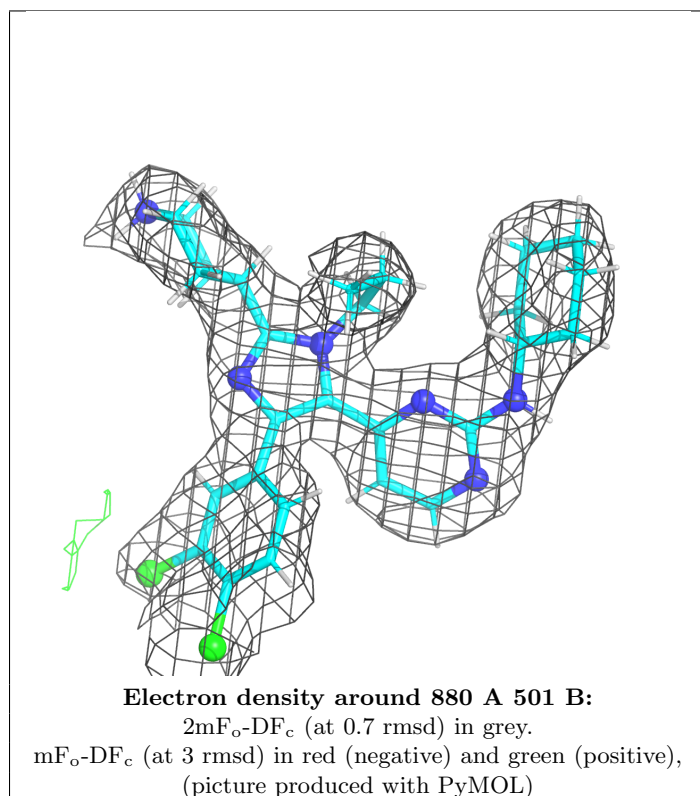
Restraints used

restraints for 880 (VUSAVSDZIWIWIDPM-UHFFFAOYSA-N) from cif dictionary 880_cation.grade.cif; generated by GRADE 1.2.9 (July 24 2014) from mol2 file using MOGUL 1.6(RC5), 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



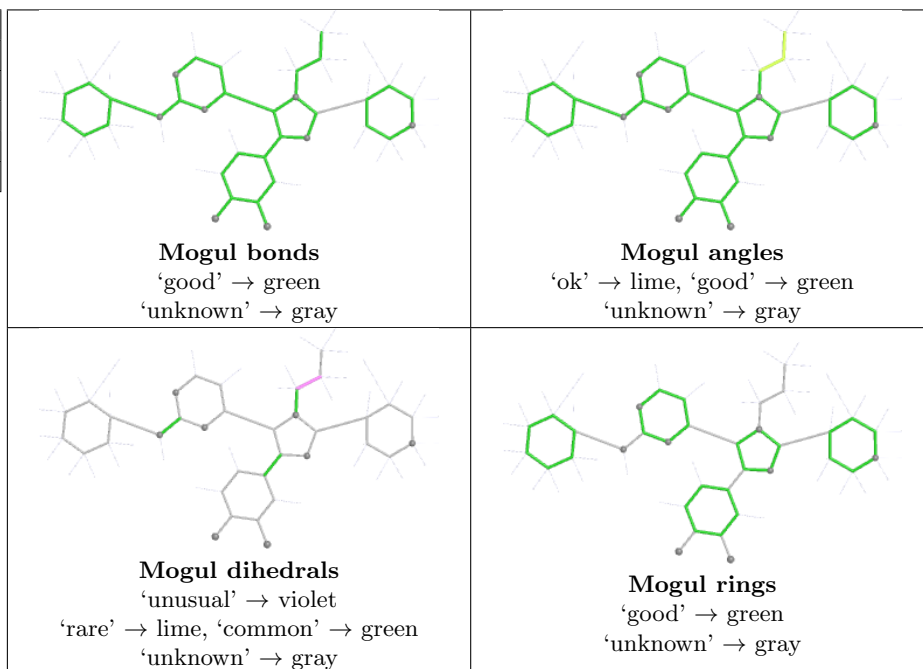
For help on “Ligand Electron Density Picture” see BUSTER wiki page

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

4.2.3 Mogul analysis for 880 A 501 B

Summary

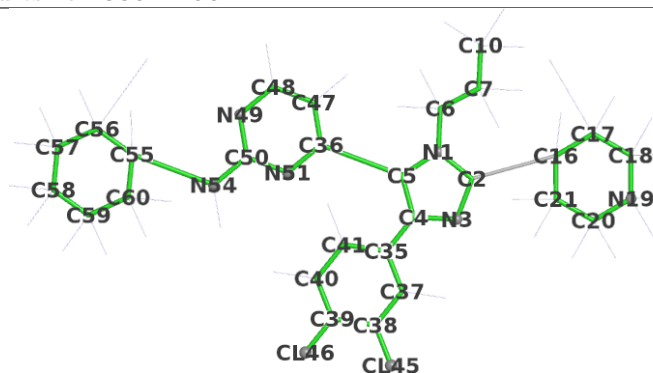
'bad' bonds	0/38
'bad' bond angles	0/45
'unusual' dihedrals	1/4
'bad' rings	0/5
bonds rms Z	0.392
angles rms Z	0.595



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 B



Mogul bonds schematic

'good' → green (Z < 1.5)

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

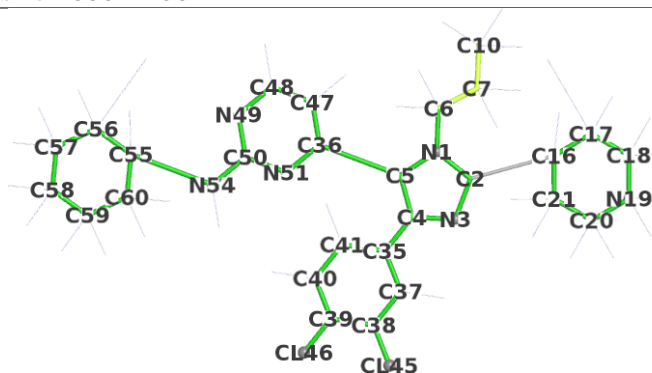
atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
C50-N51	1.353	1.341	0.012	0.013	434	0.91
C5-C4	1.387	1.377	0.010	0.013	125	0.79
C59-C58	1.529	1.516	0.014	0.018	1743	0.77
C36-C5	1.483	1.478	0.005	0.007	10	0.74
C2-N3	1.305	1.316	-0.011	0.015	17	0.72
C5-N1	1.398	1.389	0.009	0.014	79	0.62
C58-C57	1.525	1.516	0.009	0.018	1743	0.53
C7-C6	1.525	1.514	0.012	0.023	243	0.49
C56-C55	1.525	1.518	0.007	0.015	793	0.46
C36-N51	1.344	1.341	0.003	0.007	892	0.43
C20-N19	1.491	1.488	0.004	0.008	1052	0.43
C60-C55	1.523	1.518	0.006	0.015	793	0.37
C41-C35	1.395	1.391	0.005	0.013	4266	0.36
C4-N3	1.380	1.385	-0.005	0.013	288	0.36
C39-C38	1.393	1.388	0.004	0.013	403	0.33
C55-N54	1.462	1.458	0.004	0.013	47	0.32
C50-N54	1.346	1.342	0.004	0.013	12	0.31
C50-N49	1.344	1.340	0.003	0.011	146	0.30
C10-C7	1.498	1.509	-0.011	0.040	1023	0.27
C37-C38	1.384	1.381	0.002	0.009	2188	0.26

(table limited to 20 rows)

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

<http://www.globalphasing.com/buster/wiki/index.cgi?BR LigandReportAfter201507#MogulBonds>

Mogul angle results for 880 A 501 B



Mogul angles schematic

'ok' → lime (1.5 < Z < 2.5)

'good' → green (Z < 1.5)

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

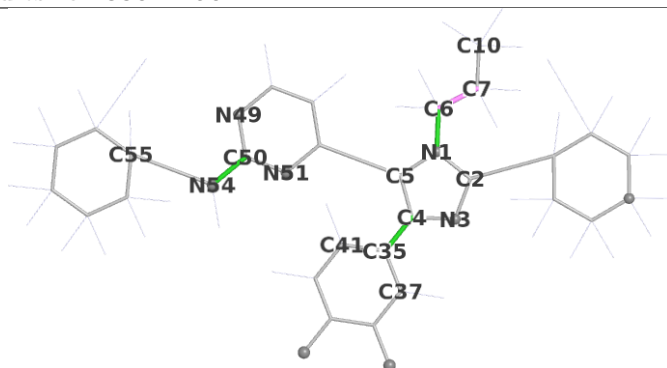
atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C10-C7-C6	115.9	111.8	4.1	2.5	217	1.62
C47-C36-N51	121.8	123.0	-1.2	0.8	691	1.49
C6-N1-C2	125.1	127.1	-2.1	1.6	26	1.32
C4-C5-N1	104.4	105.4	-1.1	0.9	25	1.19
C47-C36-C5	122.2	121.1	1.0	1.1	10	0.90
C21-C16-C17	108.4	109.5	-1.1	1.2	259	0.90
N54-C50-N51	117.7	116.5	1.2	1.4	22	0.87
C6-N1-C5	127.9	126.6	1.2	1.4	14	0.86
C47-C48-N49	123.4	124.1	-0.7	0.9	427	0.78
C20-N19-C18	112.2	111.6	0.6	0.9	452	0.68
C48-C47-C36	116.7	117.1	-0.4	0.7	16	0.63
C7-C6-N1	113.6	112.5	1.2	1.9	33	0.62
C18-C17-C16	110.9	111.2	-0.4	0.6	72	0.61
C60-C55-N54	109.7	110.6	-0.9	1.7	34	0.53
C4-N3-C2	106.0	105.2	0.8	1.6	12	0.50
C40-C39-CL46	119.0	118.4	0.7	1.3	2376	0.49
C38-C39-CL46	121.2	120.9	0.4	0.8	728	0.44
N49-C50-N51	126.2	126.6	-0.4	1.0	20	0.43
C48-N49-C50	115.3	115.6	-0.3	0.7	106	0.42
C20-C21-C16	111.0	111.2	-0.2	0.6	72	0.39

(table limited to 20 rows)

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

<http://www.globalphasing.com/buster/wiki/index.cgi?BRLLigandReportAfter201507#MogulAngles>

Mogul dihedral results for 880 A 501 B



Mogul dihedrals schematic

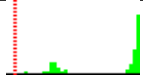
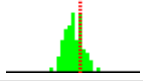
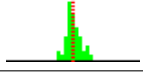
'unusual' → violet (some torsion angles have <0.5% of population within $\pm 10^\circ$)

'rare' → lime (all torsion angles have >0.5% of population within $\pm 10^\circ$)

'common' → green (all torsion angles have >10% of population within $\pm 10^\circ$)

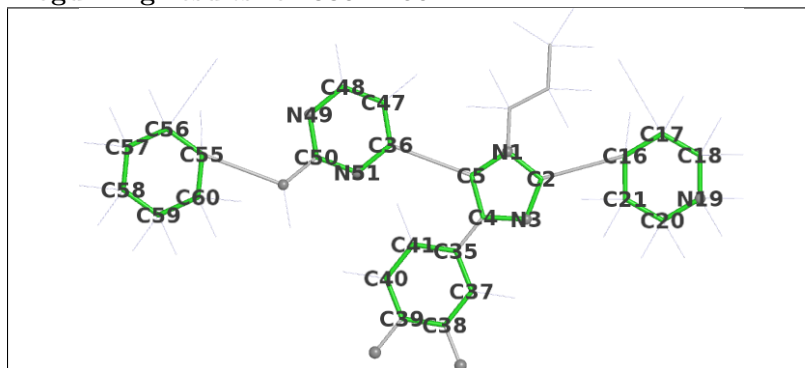
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual torsion angle in $^\circ$	Mogul histogram	Mogul # samples	classification or % Mogul population within $\pm 10^\circ$
...-C35-C4-...				common
C41-C35-C4-C5	40.9		452	23%
C37-C35-C4-N3	49.6		528	16%
C41-C35-C4-N3	-135.0		528	19%
C37-C35-C4-C5	-134.6		452	12%
...-C50-N54-...				common
N51-C50-N54-C55	0.6		22	45%
N49-C50-N54-C55	176.9		22	55%
...-C6-C7-...				unusual

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within $\pm 10^\circ$
N1-C6-C7-C10 ...-C6-N1-...	-9.6		196	0% common
C7-C6-N1-C5	-95.6		97	56%
C7-C6-N1-C2	87.4		49	82%

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 B



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	0.2
N1-C2-N3-C4-C5	58	0.1
C16-C17-C18-N19-C20-C21	48	0.5
C36-C47-C48-N49-C50-N51	41	0.3
C35-C37-C38-C39-C40-C41	246	0.0

‡'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>

4.3 ANP A 502

4.3.1 Statistics for ligand

Database ID	ANP (PDB)
3-letter code	ANP
CC(2mF _o -DF _c)	0.8619
min(B-factor)‡	22.9
avg(B-factor)‡	33.6
max(B-factor)‡	43.4
min(occupancy)‡	0.66
max(occupancy)‡	0.66
‡hydrogen atoms excluded	

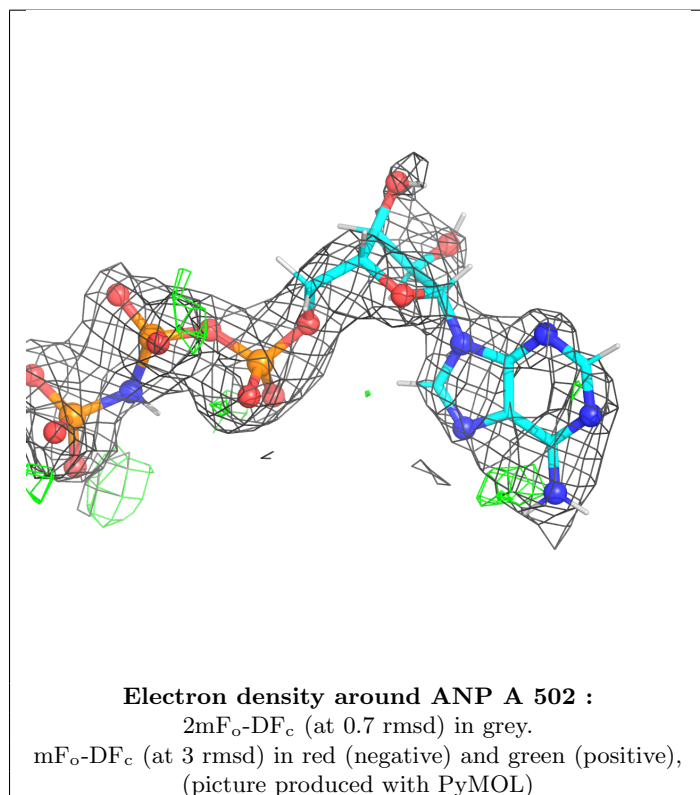
Restraints used

restraints for ANP (PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER) from cif dictionary ANP.cif; buster common-compounds v 3.1 (07 Mar 2014); Generated by GRADE_PDB.LIGAND 1.2.9 (July 24 2014) using MOGUL 1.7(RC5), CSD as536be, with quantum mechanics RM1

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

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

4.3.2 Picture of ligand in electron density



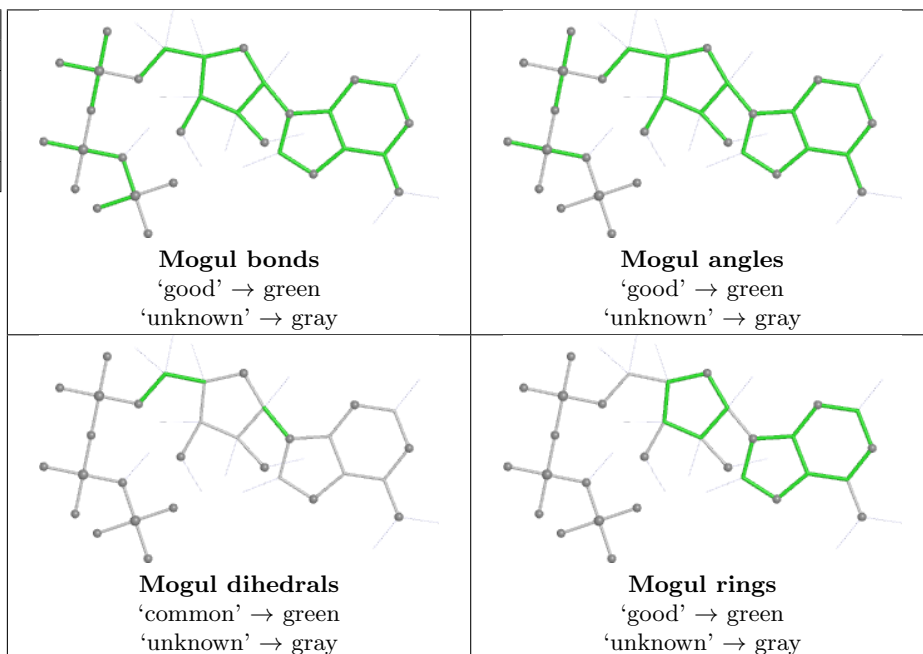
For help on “Ligand Electron Density Picture” see BUSTER wiki page

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

4.3.3 Mogul analysis for ANP A 502

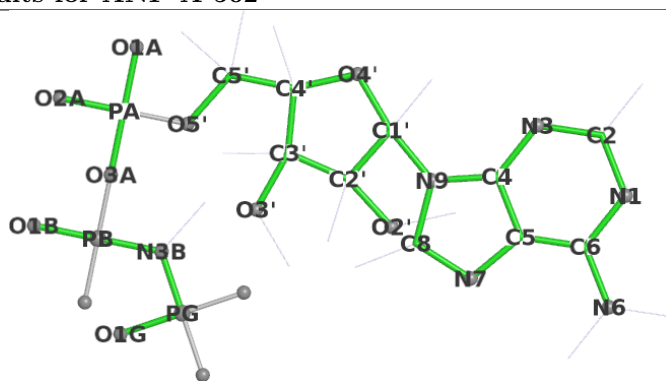
Summary

'bad' bonds	0/28
'bad' bond angles	0/33
'unusual' dihedrals	0/3
'bad' rings	0/3
bonds rms Z	0.283
angles rms Z	0.298



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).

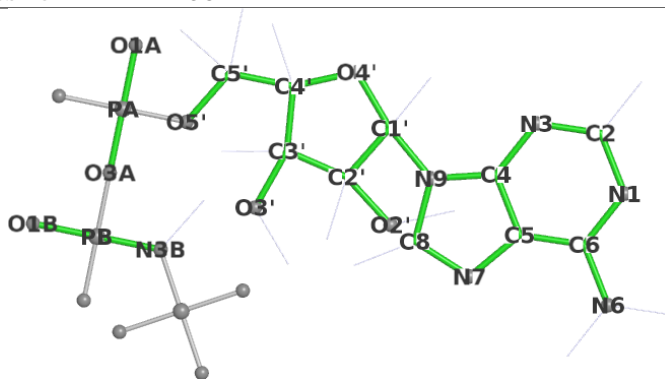
atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
C3'-C4'	1.536	1.526	0.010	0.014	577	0.75
PG-N3B	1.646	1.631	0.015	0.022	23	0.67
C2-N3	1.339	1.335	0.005	0.011	829	0.46
C6-N1	1.354	1.350	0.004	0.010	239	0.39
C2'-C3'	1.535	1.530	0.005	0.013	510	0.36
C2-N1	1.338	1.335	0.004	0.011	829	0.34
C6-N6	1.331	1.336	-0.005	0.014	531	0.33
PA-O3A	1.597	1.594	0.003	0.011	21	0.27
PA-O2A	1.520	1.527	-0.008	0.030	30	0.26
C1'-N9	1.462	1.459	0.003	0.012	78	0.25
O3'-C3'	1.426	1.423	0.003	0.013	3264	0.24
O4'-C4'	1.446	1.444	0.003	0.011	1633	0.23
C2'-C1'	1.527	1.530	-0.003	0.014	341	0.20
C4-N9	1.373	1.374	-0.002	0.008	181	0.19
C4-N3	1.341	1.339	0.002	0.012	542	0.19
PA-O1A	1.478	1.482	-0.003	0.018	31	0.18
C5-N7	1.386	1.387	-0.001	0.007	359	0.16
O2'-C2'	1.425	1.423	0.001	0.013	3264	0.09
C5-C4	1.387	1.388	-0.001	0.011	332	0.06
O4'-C1'	1.415	1.415	-0.001	0.011	592	0.06

(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

'good' → green (Z < 1.5)

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

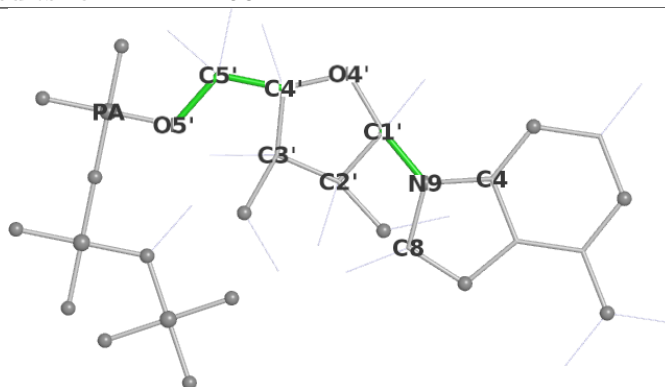
atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
O4'-C4'-C3'	106.5	105.3	1.3	1.3	448	0.99
C2'-C3'-C4'	103.0	102.5	0.6	1.0	376	0.57
N3-C4-N9	127.7	127.1	0.6	1.2	126	0.55
O2'-C2'-C3'	113.3	111.9	1.3	2.6	938	0.50
C2'-C1'-N9	114.9	114.1	0.8	1.5	59	0.50
C5'-C4'-C3'	115.9	115.3	0.6	1.8	70	0.36
C5-C4-N3	126.6	126.8	-0.2	0.7	212	0.34
O1B-PB-N3B	111.6	112.1	-0.5	1.7	15	0.31
O4'-C1'-C2'	106.2	106.5	-0.3	1.2	307	0.27
C4'-O4'-C1'	109.9	109.5	0.4	1.4	434	0.26
O3A-PA-O1A	108.1	108.7	-0.6	2.4	19	0.25
C2-N3-C4	111.0	111.5	-0.4	2.0	224	0.23
O3'-C3'-C4'	111.6	111.0	0.6	2.6	541	0.22
O3'-C3'-C2'	112.4	111.9	0.4	2.6	938	0.16
C5-C6-N1	117.7	117.6	0.1	0.9	133	0.15
C2-N1-C6	118.7	118.5	0.1	1.0	154	0.14
C3'-C2'-C1'	101.3	101.5	-0.2	1.2	273	0.14
C6-C5-N7	132.3	132.1	0.2	1.2	118	0.14
C5-C4-N9	105.7	105.7	-0.1	0.5	148	0.12
N6-C6-N1	118.3	118.2	0.1	1.2	214	0.11

(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>

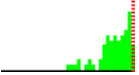
Mogul dihedral results for ANP A 502



Mogul dihedrals schematic

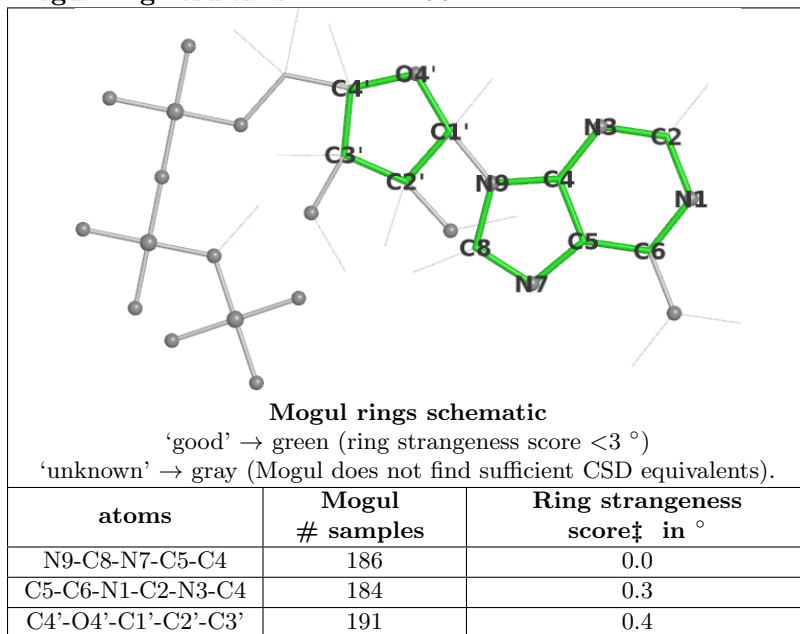
'common' → green (all torsion angles have >10% of population within $\pm 10^\circ$)
 'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual torsion angle in $^\circ$	Mogul histogram	Mogul # samples	classification or % Mogul population within $\pm 10^\circ$
...-C1'-N9-...				common
C2'-C1'-N9-C4	139.5		66	14%
O4'-C1'-N9-C8	70.2		64	12%
O4'-C1'-N9-C4	-102.1		68	15%
C2'-C1'-N9-C8	-48.3		63	11%
...-C4'-C5'-...				common
O4'-C4'-C5'-O5'	-63.7		63	90%
C3'-C4'-C5'-O5'	56.8		63	84%
...-C5'-O5'-...				common

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within $\pm 10^\circ$
C4'-C5'-O5'-PA	175.6		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



‡'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	0.77241712	K_MISS	1.00000000
B_IMPF_FRAG	0.92226895	B_MISS	0.00000000
K_SOLV	0.74618836	K_IMPF_MISS	1.00000000
B_SOLV	15.72499038	B_IMPF_MISS	0.00000000
B_IMPF_SOLV	49.90967985	K_IMPF_SOLV	1.00000000
B_11	7.80691621	B_OVER	0.00000000
B_22	-3.02914084	B_12	0.00000000
B_33	-4.7777537	B_13	0.00000000
		B_23	0.00000000
Anisotropic ratio		0.43	

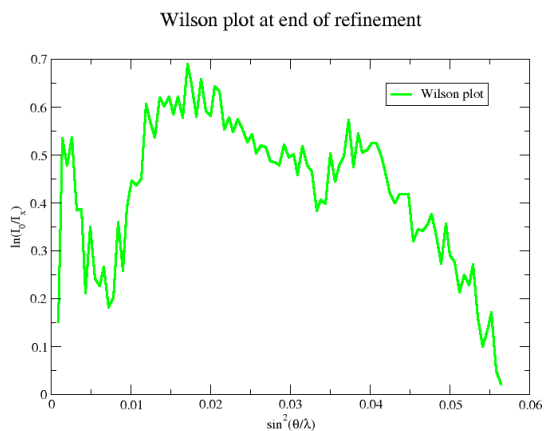
For help on “X-ray scaling parameters” see BUSTER wiki page
<http://www.globalphasing.com/buster/wiki/index.cgi?BRScalingInfo>

5.2 Wilson plots

5.2.1 Wilson plot at start of refinement

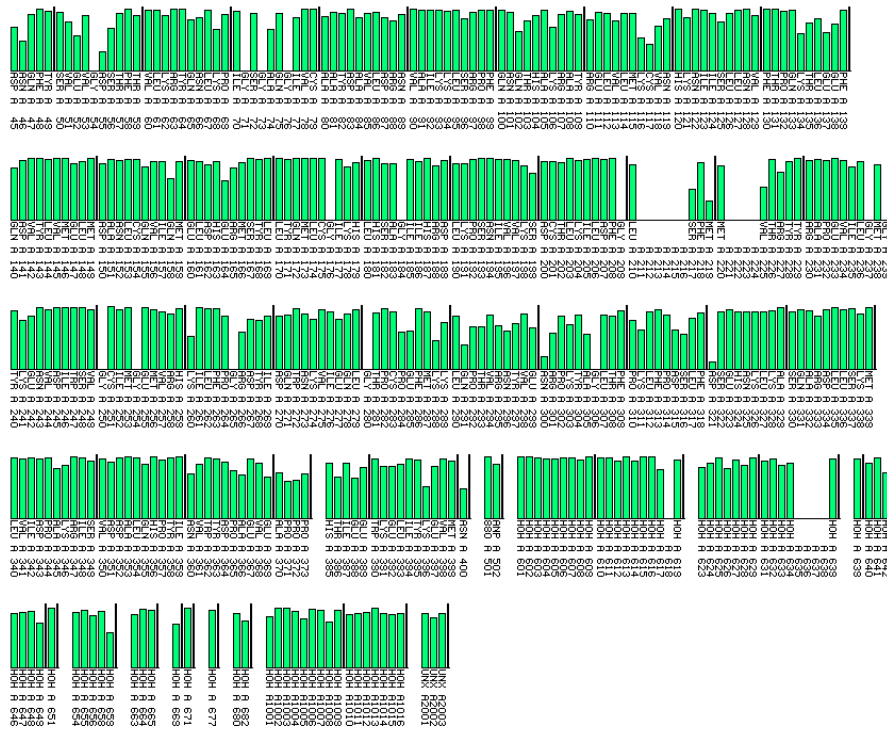


5.2.2 Wilson plot at end of refinement



6 Real-space correlations

6.1 Side chains of chain A



6.2 Mainchain of chain A

