Report on BUSTER refinement run in directory MapOnly.01

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:
2 bond lengths. Worst is 9.3 σ 1.47 Å `A|401:C24=O25 (OEW)`
10 bond angles. Worst is 14.9 σ 134.19° `A|401:C24=O25=C27 (OEW)`
8 planes. Worst is 9.3 σ 0.19 Å `A|401:C19=N23=C24=O25 (OEW)`
2 idealD contacts. Worst 7.2 σ 2.48 Å `A|401:C1=C4 (OEW)`
14 Bcorrel. Worst is 17.4 σ -43.48 Å^2 `A|402:S=O (DMS)`

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:
2 bond lengths. Worst is 9.3 σ 1.47 Å `A|401:C24=O25 (OEW)`
10 bond angles. Worst is 14.9 σ 134.19° `A|401:C24=O25=C27 (OEW)`
8 planes. Worst is 9.3 σ 0.19 Å `A|401:C19=N23=C24=O25 (OEW)`
2 idealD contacts. Worst 7.2 σ 2.48 Å `A|401:C1=C4 (OEW)`
14 Bcorrel. Worst is 17.4 σ -43.48 Å^2 `A|402:S=O (DMS)`

See logs/screen_final.txt for more detail

1.2 Run conditions

refine command	/home/software/xtal/GPhL/20200316/-autoBUSTER/bin/linux64/refine PdbChk_-ChecksNotToDo=PdbChk_WeirdCellParameters UseCcp4MonomerLibrary=yes -nthreads 1 -M MapOnly -p 6y7m.pdb -m 6y7m.mtz -l /home/-vonrhein/PDB/OEW.grade_PDB_ligand.cif -d MapOnly.01
BUSTER version, run at, by user	?, Wed Mar 25 10:28:30 CET 2020, vonrhein
in directory	/home/vonrhein/PDB/6Y7M
nthreads, hostname, OS	1, staraniso, CentOS Linux 7 (Core)
buster-report command	/public/xtal/Server-nightly-alpha-bdg-linux64/scripts/buster-report -d MapOnly.01 -dreport MapOnly.01.report
buster-report version, run at, by user	1.1.11 <January 13 2020>, Wed Mar 25 14:01:52 2020, vonrhein
buster-report run on refine directory	/scratch_babinet1/vonrhein/Projects/Covid-19/6Y7M/server10/MapOnly.01
buster-report output directory	/scratch_babinet1/vonrhein/Projects/Covid-19/6Y7M/server10/MapOnly.01.report
final pdb coordinates	MapOnly.01.report.pdb
final mtzfile	MapOnly.01.report.mtz
final model mmCIF	none
final refln mmCIF	none

For help on "Run conditions table" see BUSTER wiki page

http://www.globalphasing.com/buster/wiki/index.cgi?BRrunConditions

1.3 Refinement vital statistics

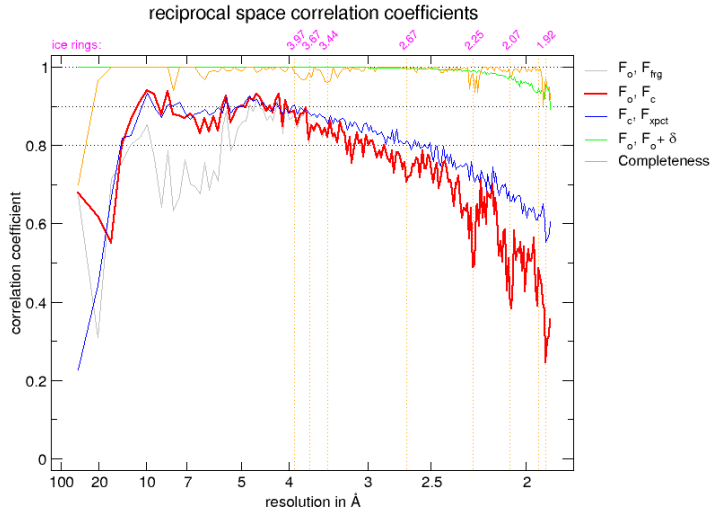
	start	final
N_{cycles} big	0	2
N_{cycles} small	0	0
X-ray weight	4	4
R_{work}	0.2171	0.2160
R_{free}	0.2608	0.2583
100 ($R_{free} - R_{work}$)	4.4%	4.2%
LLG_{work} *(cumulative Log-Likelihood Gain, working set)*	0	0.0000
LLG_{free} *(cumulative Log-Likelihood Gain, free set)*	0	0.0000
RMS bond in Å	0.0161	0.0161
RMS angle in degrees	1.81	1.81
High resolution limit in Å	1.89995	1.89995
Low resolution limit in Å	42.40000	42.40000
Number of waters	197	197

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

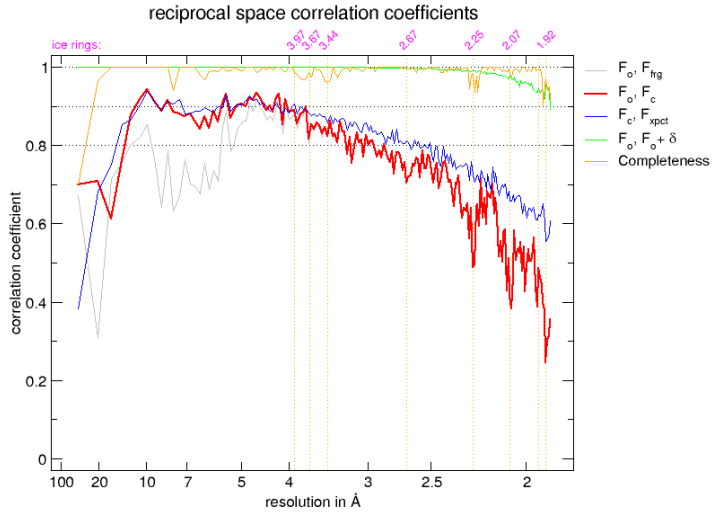
2 RSCC, R-factor, LLG and geometry evolution over the refine

2.1 Reciprocal space correlation coefficient plots

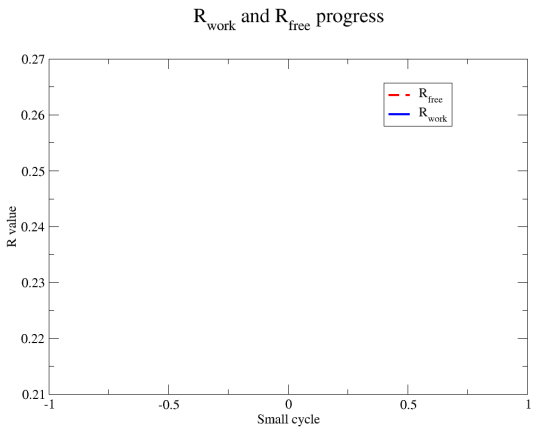
2.1.1 Initial RSCC plot



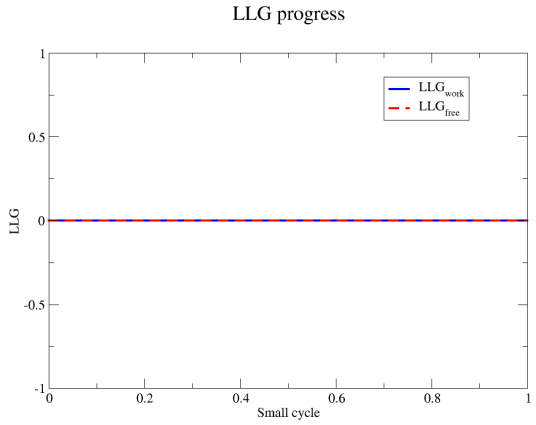
2.1.2 Final RSCC plot



2.2 R-factor behaviour during refinement

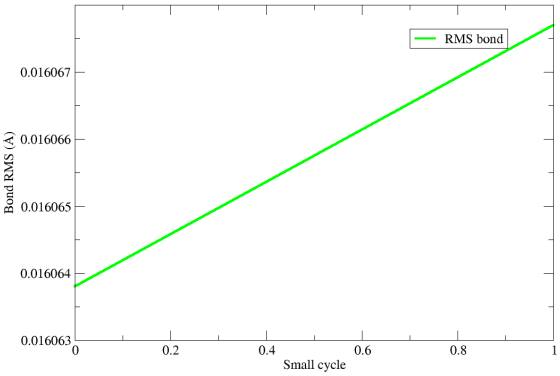


2.3 LLG behaviour during refinement

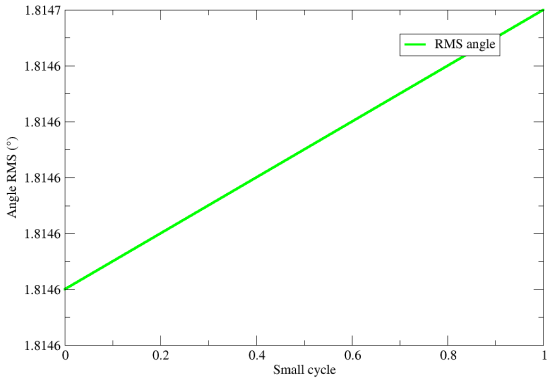


2.4 Geometry behaviour during optimisation

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:	3.36		98th percentile* N=773, 1.90Å± 0.25Å
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	7	2.66%	Goal: <1%
	Ramachandran outliers	1	0.33%	Goal: <0.05%
	Ramachandran favored	294	96.71%	Goal: >98%
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	MolProbity score†	1.66		89th percentile* N=12147, 1.90Å± 0.25Å
	Bad backbone bonds:	0 / 1223	0.00%	Goal: 0%
	Bad backbone angles:	0 / 1527	0.00%	Goal: <0.1%

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

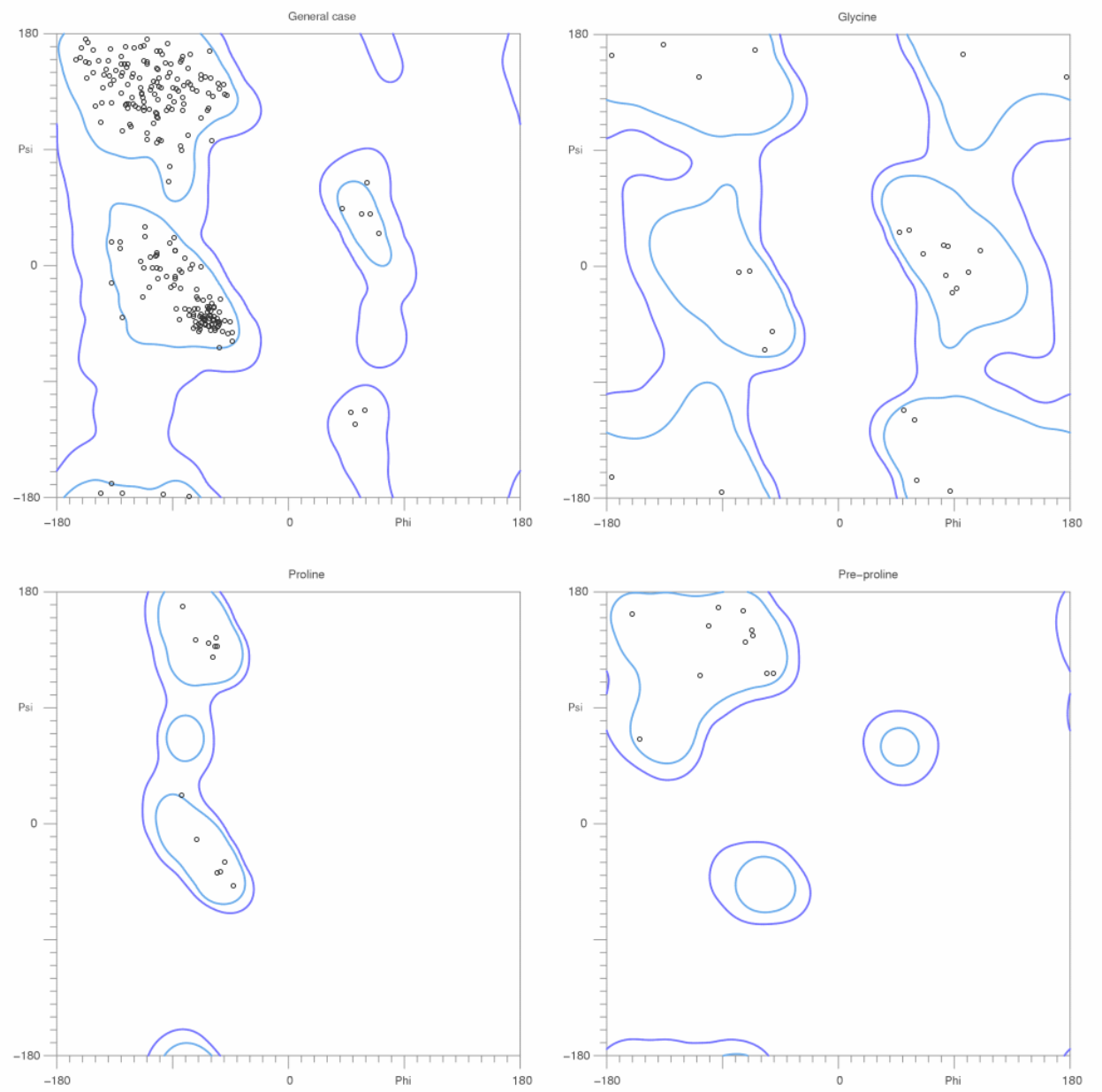
∗ 100th percentile is the best among structures of comparable resolution; 0th is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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



304 residues were evaluated in total for general, glycine, proline, and pre-pro.
97.04% of all residues were in favored (98%) regions. (295 residues)
100.00% of all residues were in allowed (>99.8%) regions. (304 residues)
There were no outliers.

4 Ligand analysis

4.1 OEW A 401

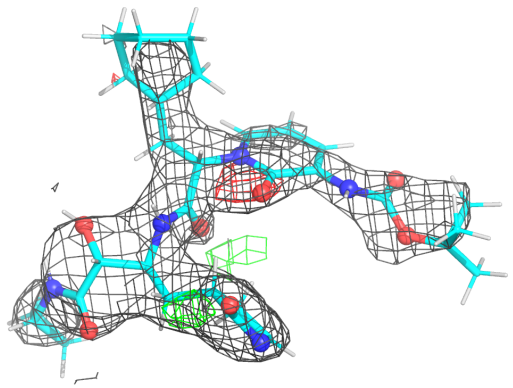
4.1.1 Statistics for ligand

Database ID	OEW (PDB)
3-letter code	OEW
CC(2mF$_o$-DF$_c$)	0.8570
min(B-factor)‡	43.4
avg(B-factor)‡	68.4
max(B-factor)‡	99.3
min(occupancy)‡	0.80
max(occupancy)‡	0.80
‡hydrogen atoms excluded	

Restraints used
restraints for OEW (__tert_-butyl __N_-_1-__2__S__-3-cyclohexyl-1-___2__S_,3__R__-4-_cyclopropylamino_-3-oxidanyl-4-oxidanylidene-1-__3__R__-2-oxidanylidene-3,4-dihydropyrrol-3-yl_butan-2-yl_amino_-1-oxidanylidene-propan-2-yl_-2-oxidanylidene-pyridin-3-yl_carbamate) from cif dictionary OEW.grade_PDB_ligand.cif; generated by GRADE_PDB_LIGAND 1.2.19 (Nov 11 2019) using GRADE 1.2.19 (Nov 11 2019) using MOGUL 1.8.5(274361), CSD as541be, 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



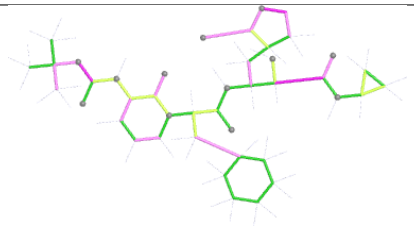
Electron density around OEW A 401 :
2mF$_o$-DF$_c$ (at 0.7 rmsd) in grey.
mF$_o$-DF$_c$ (at 3 rmsd) in red (negative) and green (positive),
(picture produced with PyMOL)

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

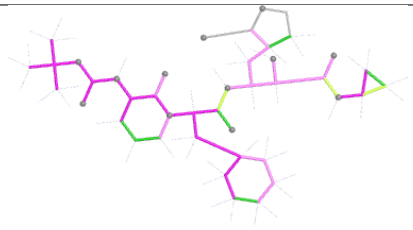
4.1.3 Mogul analysis for OEW A 401

Summary

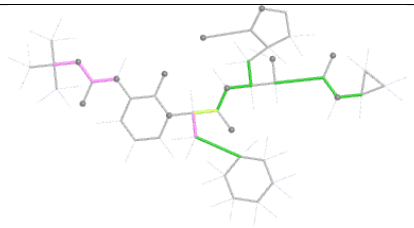
'bad' bonds	3/45
'bad' bond angles	13/56
'unusual' dihedrals	4/12
'bad' rings	1/3
bonds rms Z	2.708
angles rms Z	4.921



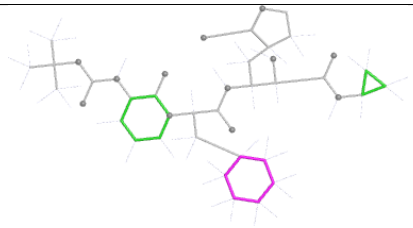
Mogul bonds
'bad' → purple, 'poor' → violet
'ok' → lime, 'good' → green
'unknown' → gray



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



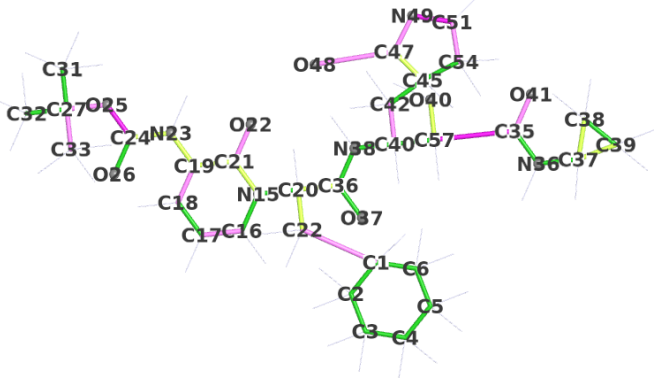
Mogul dihedrals
'unusual' → violet
'rare' → lime, 'common' → green
'unknown' → gray



Mogul rings
'bad' → purple, 'poor' → violet
'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 OEW A 401

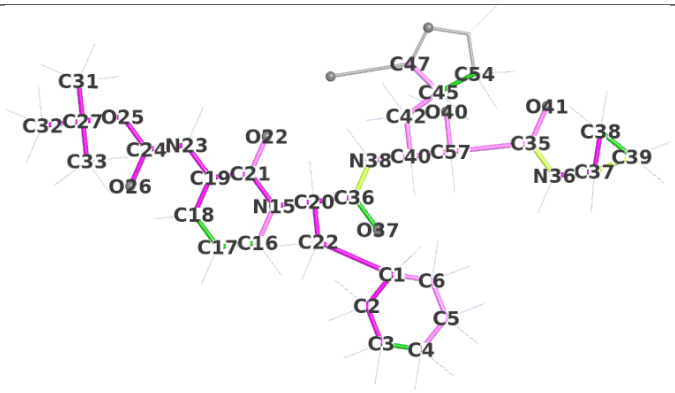


Mogul bonds schematic
'bad' → purple (Z >4)
'poor' → violet (2.5 <Z <4)
'ok' → lime (1.5 <Z <2.5)
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in Å	Mogul mean in Å	difference in Å	Mogul σ in Å	Mogul # samples	Zscore
O25-C24	1.465	1.344	0.122	0.013	1568	9.37
C51-N49	1.442	1.285	0.157	0.029	15	5.41
C57-C35	1.474	1.523	-0.049	0.010	77	5.07
C42-C40	1.561	1.529	0.032	0.008	39	3.99
C18-C19	1.411	1.369	0.042	0.011	48	3.73
C16-C17	1.390	1.349	0.041	0.011	786	3.68
C22-C1	1.497	1.527	-0.030	0.008	93	3.60
O25-C27	1.439	1.481	-0.042	0.012	4459	3.57
C33-C27	1.561	1.512	0.048	0.014	2893	3.49
O41-C35	1.184	1.228	-0.044	0.013	3078	3.33
C54-C51	1.526	1.483	0.043	0.014	22	3.08
O48-C47	1.193	1.226	-0.033	0.011	40	2.87
O22-C21	1.267	1.225	0.043	0.015	3852	2.77
C47-N49	1.321	1.363	-0.042	0.016	20	2.56
C22-C20	1.505	1.531	-0.026	0.010	128	2.48
O40-C57	1.446	1.416	0.029	0.013	1937	2.32
C45-C47	1.490	1.512	-0.022	0.009	2401	2.30
C20-C36	1.501	1.527	-0.026	0.012	563	2.25
C19-N23	1.370	1.409	-0.038	0.018	203	2.16
C19-C21	1.515	1.469	0.046	0.021	35	2.16
(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 OEW A 401

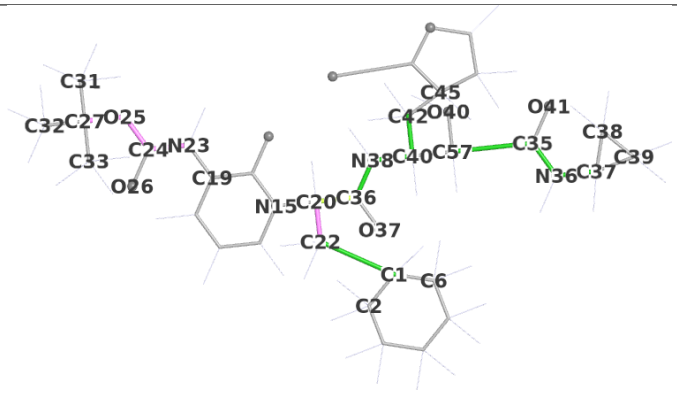


Mogul angles schematic
'bad' → purple (Z >4)
'poor' → violet (2.5 <Z <4)
'ok' → lime (1.5 <Z <2.5)
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

atoms	actual in °	Mogul mean in °	difference in °	Mogul σ in °	Mogul # samples	Zscore
C27-O25-C24	134.2	120.8	13.4	0.9	1559	14.55
C32-C27-C33	91.0	111.5	-20.5	1.4	2900	14.54
C31-C27-C33	91.2	111.5	-20.3	1.4	2900	14.37
C21-C19-N23	120.8	112.4	8.4	0.8	10	10.72
O25-C24-O26	116.1	125.8	-9.7	1.0	1568	9.89
O25-C24-N23	119.8	108.6	11.2	1.3	67	8.62
C1-C22-C20	106.0	114.3	-8.3	1.1	16	7.56
C31-C27-C32	121.1	111.5	9.6	1.4	2900	6.80
C18-C19-C21	116.3	120.2	-3.8	0.6	16	6.70
C3-C2-C1	106.7	112.2	-5.4	1.2	289	4.45
C20-N15-C21	114.1	118.7	-4.6	1.0	16	4.41
C22-C20-C36	104.1	111.8	-7.7	1.9	17	4.13
C38-C37-N36	113.9	118.5	-4.6	1.1	26	4.08
C42-C40-N38	115.0	110.1	4.9	1.2	19	3.92
C4-C5-C6	107.6	111.3	-3.7	1.0	1280	3.76
C20-N15-C16	125.3	119.8	5.6	1.6	11	3.53
O25-C27-C31	120.5	107.2	13.3	3.8	4436	3.49
C42-C40-C57	116.8	111.7	5.0	1.5	19	3.40
O22-C21-N15	114.8	121.6	-6.8	2.1	14	3.31
C57-C40-N38	103.9	109.6	-5.7	1.7	36	3.28
(table limited to 20 rows)						

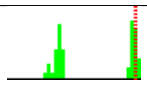
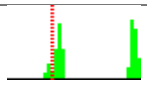
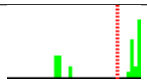
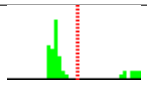
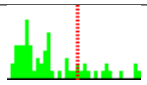
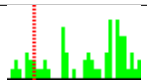
For help on "Ligand Mogul Analysis: Angles" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulAngles

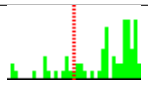
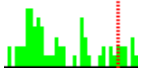
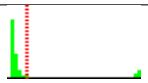
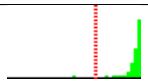
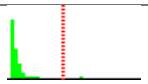
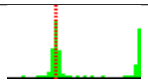
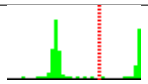
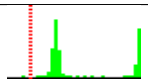
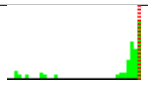
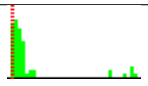
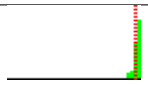
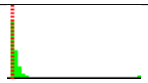
Mogul dihedral results for OEW A 401

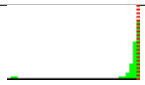
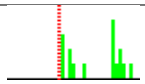
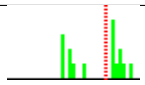
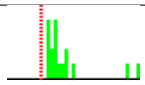
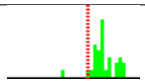
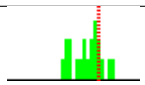


Mogul dihedrals schematic

'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).

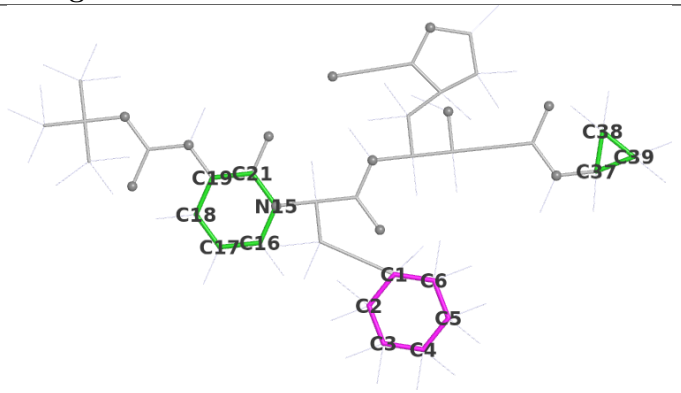
atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
...-C1-C22-...				common
C6-C1-C22-C20	174.1		56	50%
C2-C1-C22-C20	55.6		56	39%
...-C20-C22-...				unusual
C36-C20-C22-C1	147.2		31	0%
N15-C20-C22-C1	-93.5		51	0%
...-C20-C36-...				rare
C22-C20-C36-O37	90.7		70	10%
N15-C20-C36-O37	-31.1		69	13%

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
C22-C20-C36-N38	-87.2		70	13%
N15-C20-C36-N38	150.9		69	13%
...-C24-N23-...				unusual
O25-C24-N23-C19	-144.2		59	0%
O26-C24-N23-C19	24.6		59	10%
...-C24-O25-...				unusual
N23-C24-O25-C27	-119.1		1491	0%
O26-C24-O25-C27	71.3		1568	0%
...-C27-O25-...				unusual
C32-C27-O25-C24	64.7		4576	65%
C31-C27-O25-C24	-123.5		4576	0%
C33-C27-O25-C24	-29.1		4576	0%
...-C35-C57-...				common
O41-C35-C57-O40	178.0		77	71%
N36-C35-C57-O40	0.5		72	68%
...-C35-N36-...				common
O41-C35-N36-C37	-4.9		1546	97%
C57-C35-N36-C37	172.3		90	100%
...-C36-N38-...				common
O37-C36-N38-C40	-2.8		1546	97%

atoms	actual torsion angle in °	Mogul histogram	Mogul # samples	classification or % Mogul population within ± 10°
C20-C36-N38-C40	175.1		1158	94%
...-C37-N36-...				common
C38-C37-N36-C35	-66.3		16	19%
C39-C37-N36-C35	-133.0		16	25%
...-C40-C42-...				common
N38-C40-C42-C45	-43.4		17	24%
...-C40-N38-...				common
C42-C40-N38-C36	106.6		32	22%
C57-C40-N38-C36	-124.5		20	40%

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 OEW A 401



Mogul rings schematic
'bad' → purple (ring strangeness score >9 °)
'poor' → violet (ring strangeness score <9 °)
'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 °
N15-C21-C19-C18-C17-C16	18	0.7
C1-C6-C5-C4-C3-C2	113	69.7
C37-C39-C38	190	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

5 X-ray statistics

5.1 Scaling parameters in last cycle

Refined parameters	
K_OVER	0.3355
B_IMPF_FRAG	2.7630
K_SOLV	0.7817
B_SOLV	86.8642
B_IMPF_SOLV	19.7430
B_OVER	5.9963
B_11	11.3906
B_22	-7.9944
B_13	-5.6459
B_33	-3.3961

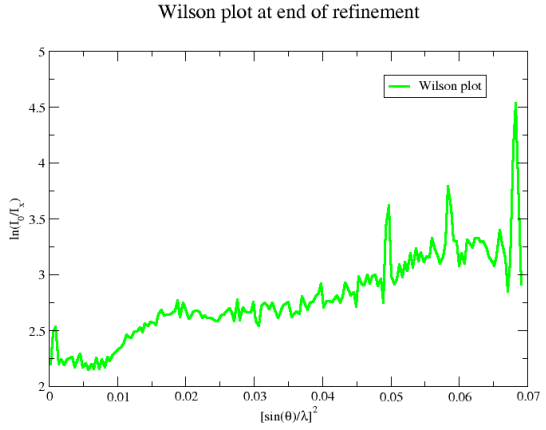
Unrefined parameters	
K_MISS	1.0000
B_MISS	0.0000
K_IMPF_MISS	1.0000
B_IMPF_MISS	0.0000
K_IMPF_SOLV	1.0000
B_12	0.0000
B_23	0.0000

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

5.2 Wilson plots

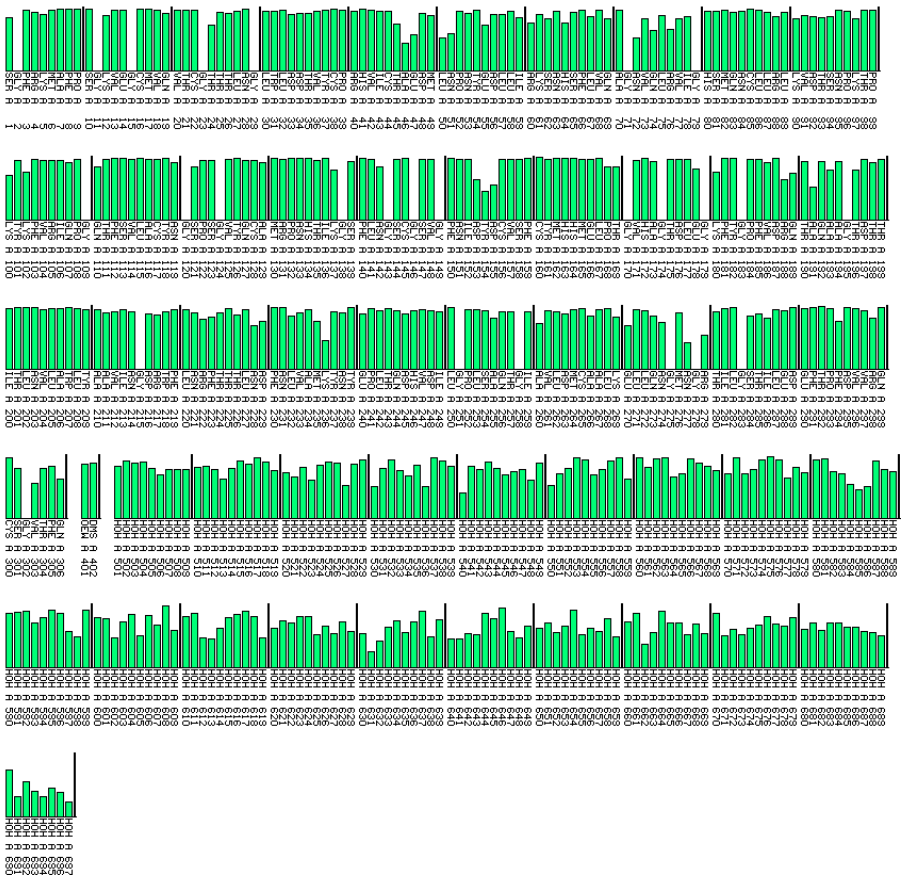
5.2.1 Wilson plot at start of refinement

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