# Report on BUSTER refinement run in directory aB_refine.01/03

## Contents

# 1 Run overview

## 1.1 Run conditions

| | |
|---|---|
| refine command | /home/software/xtal/GPhL/20200316/-autoBUSTER/bin/linux64/refine -p aB_-refine.01/02/refine.pdb -m 6y7m.mtz -autoncs -M TLSalternate -TLS -M WaterUpdateP-kmaps -nthreads 8 -l /home/vonrhein/PDB/-OEW.grade_PDB_ligand.cif -CS aB_refine.01/02/-refine.scales UseMtzchk=no -d aB_refine.01/03 |
| BUSTER version, run at, by user | 2.13.0 (16-MAR-2020), Tue Mar 24 19:15:39 CET 2020, vonrhein |
| in directory | /home/vonrhein/PDB/6Y7M |
| nthreads, hostname, OS | 8, staraniso, CentOS Linux 7 (Core) |
| buster-report command | /public/xtal/Server-nightly-alpha-bdg-linux64/scripts/buster-report -d aB_-refine.01/03 -dreport aB_refine.01/03.report |
| buster-report version, run at, by user | 1.1.11 <January 13 2020>, Wed Mar 25 15:37:59 2020, vonrhein |
| buster-report run on refine directory | /scratch_babinet1/vonrhein/Projects/Covid-19/6Y7M/server10/aB_refine.01/03 |
| buster-report output directory | /scratch_babinet1/vonrhein/Projects/Covid-19/6Y7M/server10/aB_refine.01/03.report |
| final pdb coordinates | 03.report.pdb |
| final mtzfile | 03.report.mtz |
| final model mmCIF | BUSTER_model.cif |
| final refln mmCIF | BUSTER_refln.cif |

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

## 1.2 Refinement vital statistics

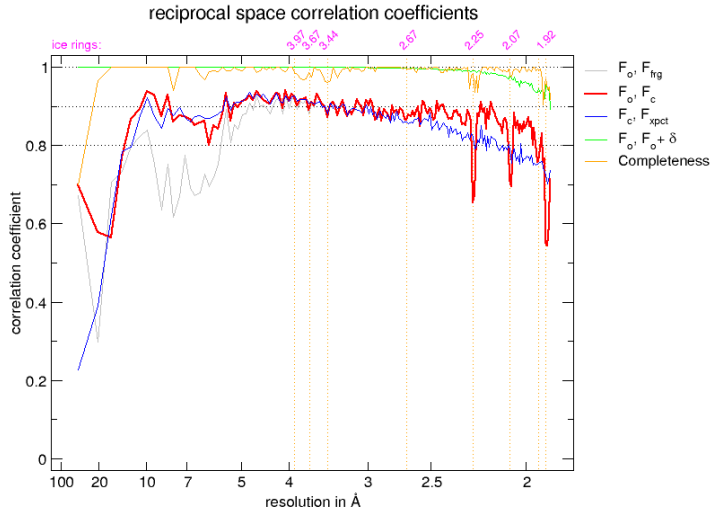
| | start | final |
|---|---|---|
| **$N_{cycles}$ big** | 0 | 5 |
| **$N_{cycles}$ small** | 0 | 205 |
| **X-ray weight** | 4.73 | 4.45 |
| **$R_{work}$** | 0.2038 | 0.1985 |
| **$R_{free}$** | 0.2345 | 0.2226 |
| **100** ($R_{free} - R_{work}$) | 3.1% | 2.4% |
| **$LLG_{work}$** *(cumulative Log-Likelihood Gain, working set)* | 0 | 0.0308 |
| **$LLG_{free}$** *(cumulative Log-Likelihood Gain, free set)* | 0 | 0.0171 |
| **RMS bond in Å** | 0.0082 | 0.0081 |
| **RMS angle in degrees** | 0.98 | 0.97 |
| **High resolution limit in Å** | 1.89995 | 1.89995 |
| **Low resolution limit in Å** | 42.40000 | 42.40000 |
| **Number of waters** | 197 | 222 |

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

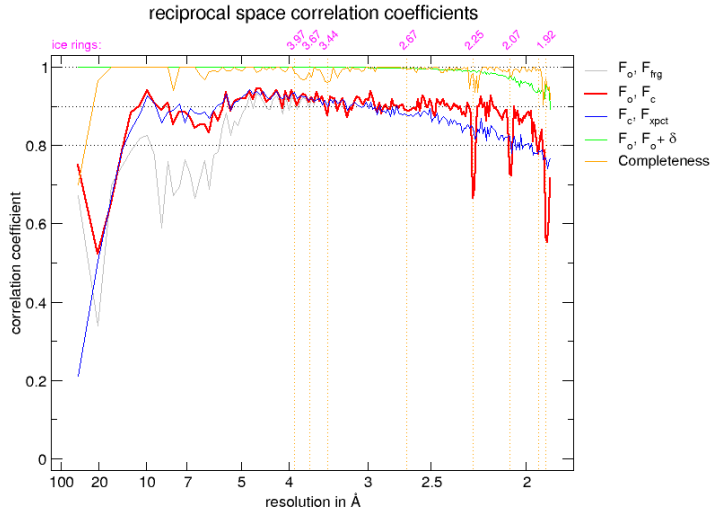
# 2 RSCC, R-factor, LLG and geometry evolution over the refine

## 2.1 Reciprocal space correlation coefficient plots

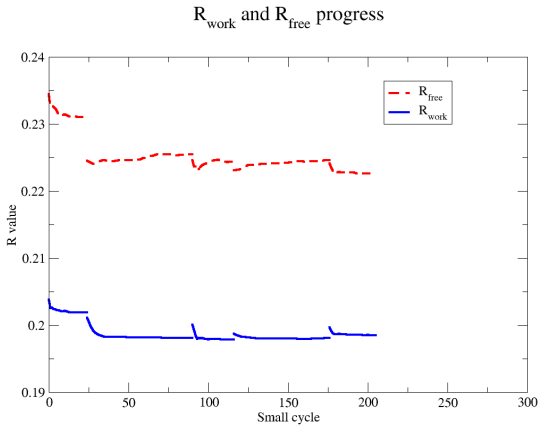
### 2.1.1 Initial RSCC plot



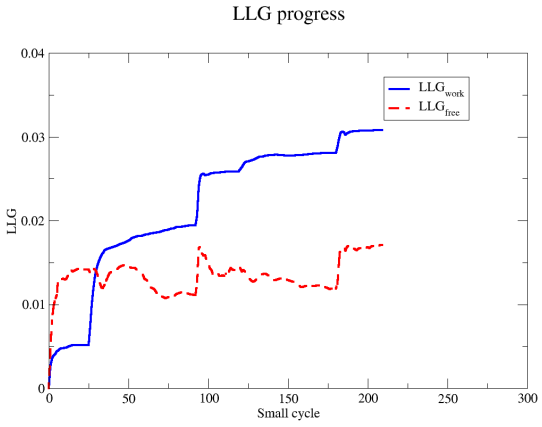

### 2.1.2 Final RSCC plot



## 2.2 R-factor behaviour during refinement

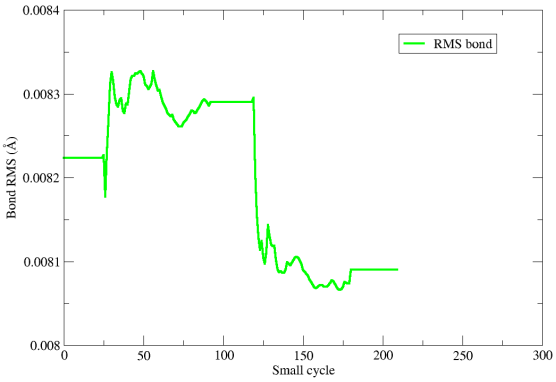



## 2.3 LLG behaviour during refinement

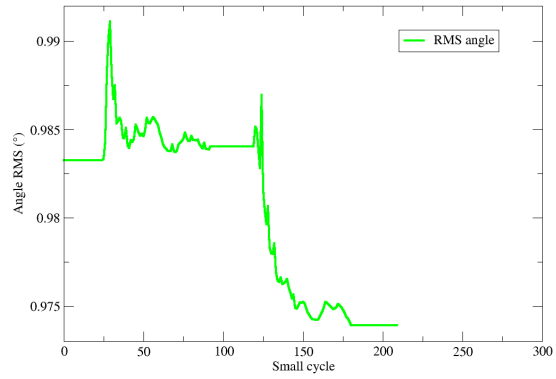


## 2.4 Geometry behaviour during optimisation

### 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: | 1.68 | | 100$^{th}$ 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 | 6 | 2.28% | Goal: <1% |
| | Ramachandran outliers | 0 | 0.00% | Goal: <0.05% |
| | Ramachandran favored | 298 | 98.03% | Goal: >98% |
| | C$\beta$ deviations >0.25Å | 1 | 0.36% | Goal: 0 |
| | MolProbity score† | 1.19 | | 99$^{th}$ 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.

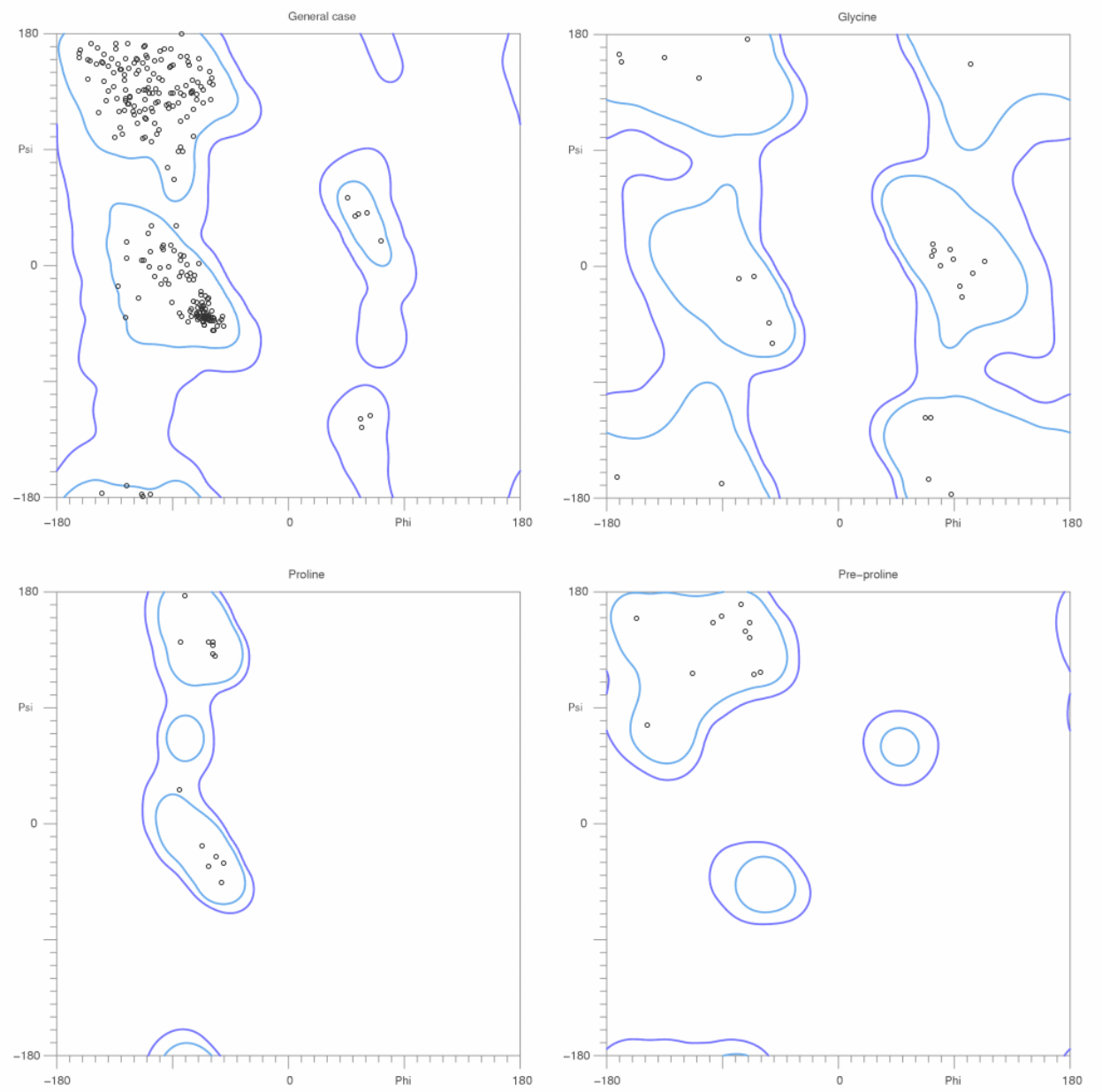
∗ 100$^{th}$ percentile is the best among structures of comparable resolution; 0$^{th}$ is the worst " For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

† 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 C$\alpha$ Geometry: $\phi$, $\psi$ and C$\beta$ 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.
98.03% of all residues were in favored (98%) regions. (298 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

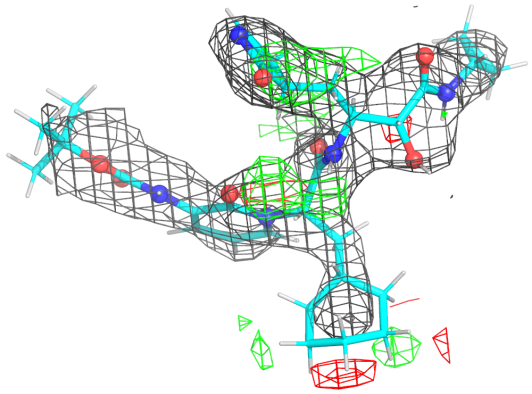
### 4.1.1 Statistics for ligand

| Database ID | OEW (PDB) |
|---|---|
| **3-letter code** | OEW |
| **CC(2mF$_o$-DF$_c$)** | 0.8203 |
| **min(B-factor)‡** | 47.5 |
| **avg(B-factor)‡** | 59.2 |
| **max(B-factor)‡** | 68.4 |
| **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



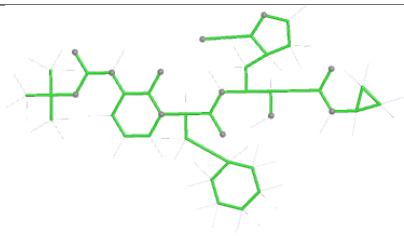
**Electron density around OEW A 401 :**
2mF$_o$-DF$_c$ (at 0.7 rmsd) in grey.
mF$_o$-DF$_c$ (at 3 rmsd) in red (negative) and green (positive),
(picture produced with PyMOL)

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

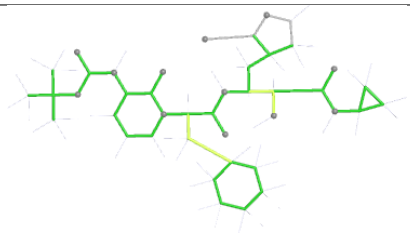
### 4.1.3 Mogul analysis for OEW A 401

**Summary**

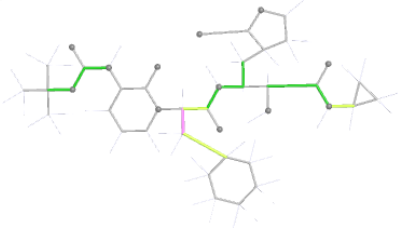
| | |
|---|---|
| **'bad' bonds** | 0/45 |
| **'bad' bond angles** | 0/56 |
| **'unusual' dihedrals** | 1/12 |
| **'bad' rings** | 1/3 |
| **bonds rms Z** | 0.357 |
| **angles rms Z** | 0.586 |



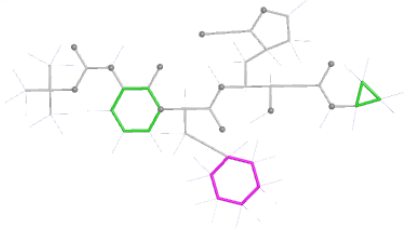
**Mogul bonds**
'good' → green
'unknown' → gray



**Mogul angles**
'ok' → lime, 'good' → green
'unknown' → gray



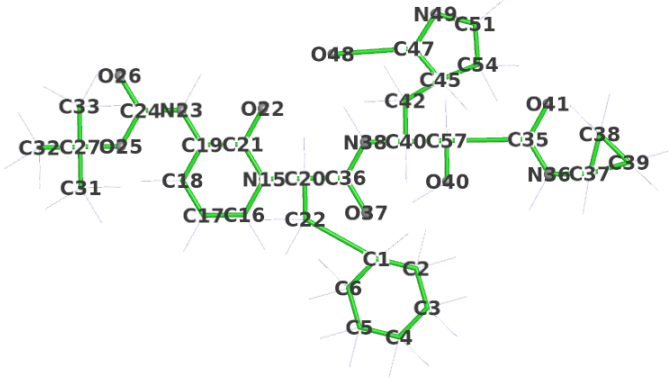
**Mogul dihedrals**
'unusual' → violet
'rare' → lime, 'common' → green
'unknown' → gray



**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**

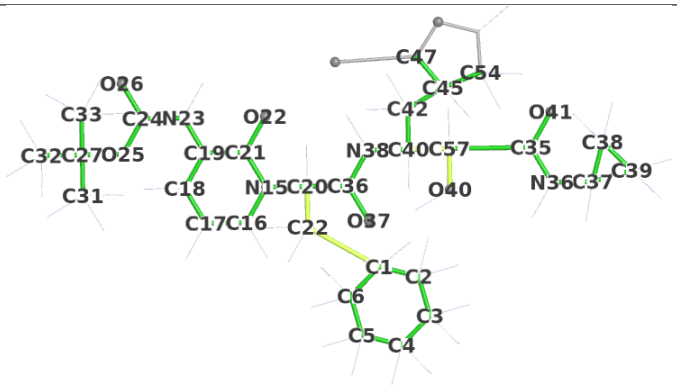



**Mogul bonds schematic**
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

| atoms | actual in Å | Mogul mean in Å | difference in Å | Mogul $\sigma$ in Å | Mogul # samples | Zscore |
|---|---|---|---|---|---|---|
| O41-C35 | 1.217 | 1.228 | -0.010 | 0.013 | 3078 | 0.79 |
| C3-C4 | 1.529 | 1.517 | 0.012 | 0.016 | 1489 | 0.75 |
| O40-C57 | 1.425 | 1.416 | 0.009 | 0.013 | 1937 | 0.72 |
| C57-C40 | 1.546 | 1.538 | 0.008 | 0.012 | 223 | 0.70 |
| O48-C47 | 1.218 | 1.226 | -0.008 | 0.011 | 40 | 0.68 |
| C22-C1 | 1.522 | 1.527 | -0.005 | 0.008 | 93 | 0.66 |
| O25-C24 | 1.351 | 1.344 | 0.007 | 0.013 | 1568 | 0.55 |
| C42-C40 | 1.534 | 1.529 | 0.004 | 0.008 | 39 | 0.53 |
| C4-C5 | 1.525 | 1.517 | 0.008 | 0.016 | 1489 | 0.47 |
| C19-N23 | 1.417 | 1.409 | 0.008 | 0.018 | 203 | 0.46 |
| C5-C6 | 1.530 | 1.525 | 0.005 | 0.012 | 1525 | 0.43 |
| C22-C20 | 1.527 | 1.531 | -0.004 | 0.010 | 128 | 0.41 |
| O25-C27 | 1.486 | 1.481 | 0.005 | 0.012 | 4459 | 0.40 |
| C24-N23 | 1.378 | 1.373 | 0.005 | 0.014 | 222 | 0.36 |
| C20-N15 | 1.475 | 1.471 | 0.004 | 0.012 | 14 | 0.35 |
| C16-N15 | 1.380 | 1.375 | 0.005 | 0.016 | 465 | 0.33 |
| C3-C2 | 1.529 | 1.525 | 0.004 | 0.012 | 1525 | 0.32 |
| C45-C47 | 1.509 | 1.512 | -0.003 | 0.009 | 2401 | 0.31 |
| C42-C45 | 1.541 | 1.537 | 0.004 | 0.014 | 68 | 0.28 |
| C20-C36 | 1.524 | 1.527 | -0.003 | 0.012 | 563 | 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?BRLigandReportAfter201507#MogulBonds

**Mogul angle results for OEW A 401**

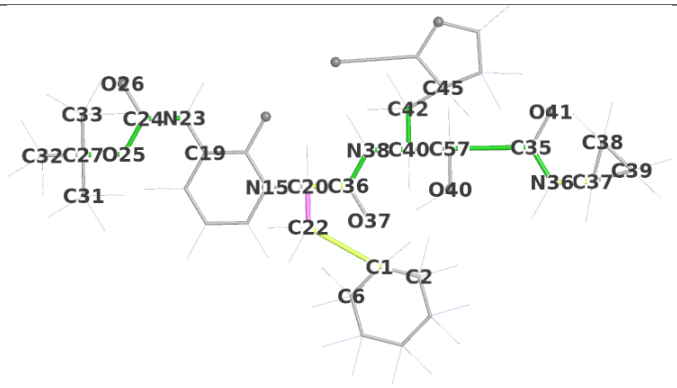



**Mogul angles schematic**
'ok' → lime (1.5 <Z <2.5)
'good' → green (Z <1.5)
'unknown' → gray (Mogul does not find sufficient CSD equivalents).

| atoms | actual in ° | Mogul mean in ° | difference in ° | Mogul $\sigma$ in ° | Mogul # samples | Zscore |
|---|---|---|---|---|---|---|
| O40-C57-C40 | 113.8 | 109.2 | 4.7 | 2.6 | 216 | 1.82 |
| C1-C22-C20 | 112.7 | 114.3 | -1.7 | 1.1 | 16 | 1.52 |
| C42-C40-C57 | 114.0 | 111.7 | 2.2 | 1.5 | 19 | 1.49 |
| C36-C20-N15 | 113.4 | 111.1 | 2.3 | 1.7 | 15 | 1.33 |
| C22-C20-N15 | 114.3 | 113.0 | 1.3 | 1.2 | 35 | 1.05 |
| O41-C35-C57 | 119.0 | 120.0 | -1.0 | 1.1 | 77 | 0.90 |
| C22-C1-C6 | 112.9 | 111.7 | 1.2 | 1.5 | 102 | 0.78 |
| C20-N15-C21 | 117.9 | 118.7 | -0.8 | 1.0 | 16 | 0.78 |
| C42-C45-C47 | 112.5 | 111.3 | 1.2 | 1.6 | 13 | 0.76 |
| C20-C36-N38 | 114.9 | 116.1 | -1.2 | 1.7 | 205 | 0.75 |
| C2-C1-C6 | 110.2 | 109.3 | 0.9 | 1.2 | 441 | 0.70 |
| C31-C27-C32 | 110.6 | 111.5 | -0.9 | 1.4 | 2900 | 0.65 |
| C4-C3-C2 | 111.9 | 111.3 | 0.6 | 1.0 | 1280 | 0.64 |
| O41-C35-N36 | 122.5 | 123.2 | -0.7 | 1.1 | 1578 | 0.64 |
| C32-C27-C33 | 110.7 | 111.5 | -0.8 | 1.4 | 2900 | 0.54 |
| C27-O25-C24 | 121.3 | 120.8 | 0.5 | 0.9 | 1559 | 0.54 |
| O37-C36-C20 | 121.6 | 120.8 | 0.9 | 1.6 | 563 | 0.54 |
| C5-C6-C1 | 112.8 | 112.2 | 0.6 | 1.2 | 289 | 0.52 |
| C22-C20-C36 | 110.8 | 111.8 | -1.0 | 1.9 | 17 | 0.52 |
| C4-C5-C6 | 111.8 | 111.3 | 0.5 | 1.0 | 1280 | 0.50 |
| (table limited to 20 rows) | | | | | | |

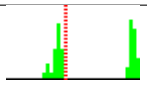
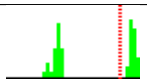
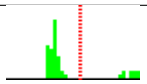
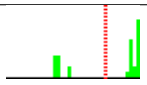
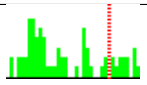
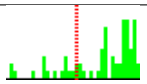
For help on "Ligand Mogul Analysis: Angles" see BUSTER wiki page
http://www.globalphasing.com/buster/wiki/index.cgi?BRLigandReportAfter201507#MogulAngles

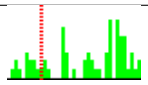
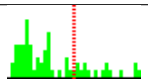
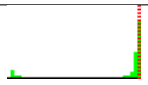
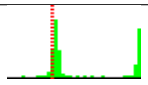
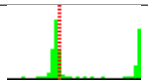
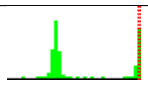
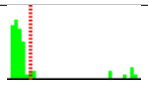
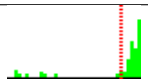
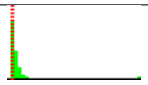
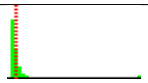
**Mogul dihedral results for OEW A 401**

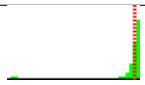
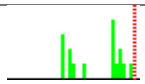
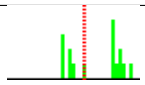
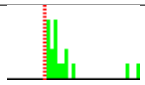
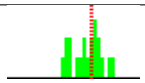
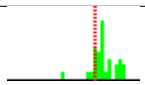



**Mogul dihedrals schematic**

'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).

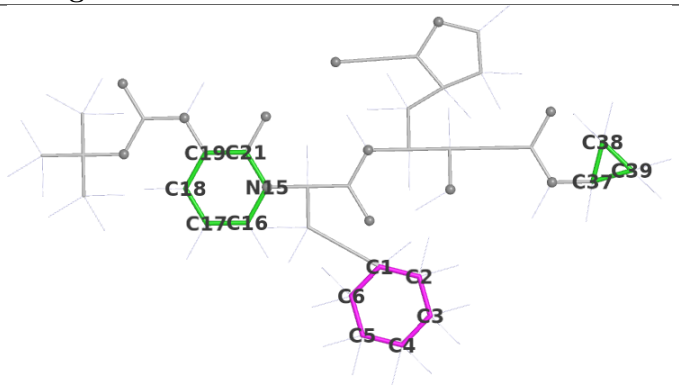
| atoms | actual torsion angle in ° | Mogul histogram | Mogul # samples | classification or % Mogul population within ± 10° |
|---|---|---|---|---|
| ...-C1-C22-... | | | | rare |
| C2-C1-C22-C20 | 79.8 |  | 56 | 30% |
| C6-C1-C22-C20 | -154.9 |  | 56 | 4% |
| ...-C20-C22-... | | | | unusual |
| N15-C20-C22-C1 | -96.0 |  | 51 | 0% |
| C36-C20-C22-C1 | 134.4 |  | 31 | 0% |
| ...-C20-C36-... | | | | rare |
| N15-C20-C36-N38 | 139.0 |  | 69 | 9% |
| C22-C20-C36-N38 | -90.9 |  | 70 | 10% |

| atoms | actual torsion angle in ° | Mogul histogram | Mogul # samples | classification or % Mogul population within ± 10° |
|---|---|---|---|---|
| N15-C20-C36-O37 | -44.0 |  | 69 | 10% |
| C22-C20-C36-O37 | 86.1 |  | 70 | 11% |
| ...-C24-N23-... | | | | common |
| O26-C24-N23-C19 | 1.9 |  | 59 | 86% |
| O25-C24-N23-C19 | -178.5 |  | 59 | 86% |
| ...-C24-O25-... | | | | common |
| O26-C24-O25-C27 | -6.0 |  | 1568 | 98% |
| N23-C24-O25-C27 | 174.4 |  | 1491 | 99% |
| ...-C27-O25-... | | | | common |
| C31-C27-O25-C24 | -56.2 |  | 4576 | 64% |
| C33-C27-O25-C24 | 65.5 |  | 4576 | 64% |
| C32-C27-O25-C24 | -175.2 |  | 4576 | 34% |
| ...-C35-C57-... | | | | common |
| N36-C35-C57-O40 | 25.4 |  | 72 | 22% |
| O41-C35-C57-O40 | -153.8 |  | 77 | 17% |
| ...-C35-N36-... | | | | common |
| C57-C35-N36-C37 | -174.5 |  | 90 | 100% |
| O41-C35-N36-C37 | 4.6 |  | 1546 | 97% |
| ...-C36-N38-... | | | | common |
| O37-C36-N38-C40 | -6.3 |  | 1546 | 99% |

| atoms | actual torsion angle in ° | Mogul histogram | Mogul # samples | classification or % Mogul population within ± 10° |
|---|---|---|---|---|
| C20-C36-N38-C40 | 170.6 |  | 1158 | 98% |
| ...-C37-N36-... | | | | rare |
| C39-C37-N36-C35 | -174.2 |  | 16 | 6% |
| C38-C37-N36-C35 | -104.7 |  | 16 | 6% |
| ...-C40-C42-... | | | | common |
| N38-C40-C42-C45 | -47.2 |  | 17 | 35% |
| ...-C40-N38-... | | | | common |
| C57-C40-N38-C36 | -113.7 |  | 20 | 50% |
| C42-C40-N38-C36 | 119.5 |  | 32 | 62% |

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 ° |
|---|---|---|
| C1-C6-C5-C4-C3-C2 | 113 | 67.9 |
| C37-C39-C38 | 190 | 0.0 |
| N15-C21-C19-C18-C17-C16 | 18 | 0.8 |

‡'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 | 0.3178 | K_MISS | 1.0000 |
| B_IMPF_FRAG | 1.7990 | B_MISS | 0.0000 |
| K_SOLV | 0.7920 | K_IMPF_MISS | 1.0000 |
| B_SOLV | 71.5719 | B_IMPF_MISS | 0.0000 |
| B_IMPF_SOLV | 29.2381 | K_IMPF_SOLV | 1.0000 |
| B_11 | 3.0594 | B_OVER | 0.0000 |
| B_22 | -0.4905 | B_12 | 0.0000 |
| B_13 | -0.7208 | B_23 | 0.0000 |
| B_33 | -2.5689 | | |
| Anisotropic ratio | 0.12 | | |

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

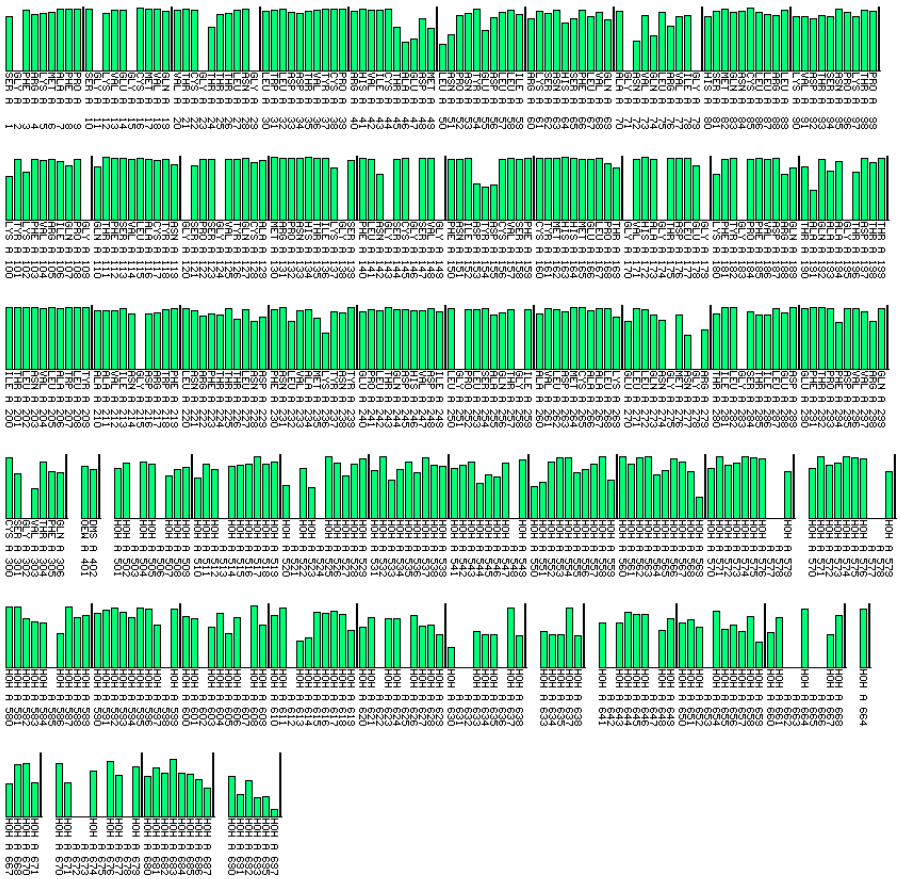
## 5.2 Wilson plots

### 5.2.1 Wilson plot at start of refinement

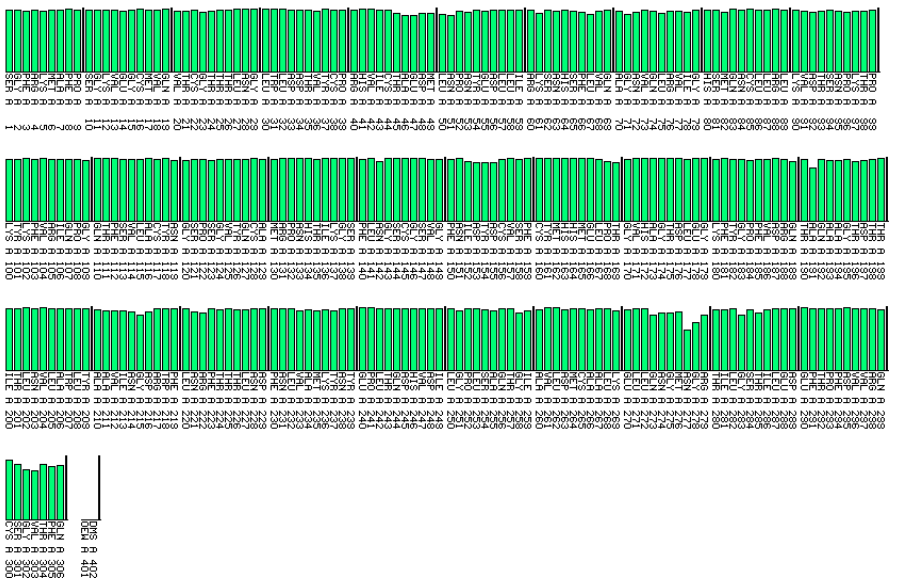

### 5.2.2 Wilson plot at end of refinement

# 6 Real-space correlations

## 6.1 Side chains of chain A



## 6.2 Mainchain of chain A



## 6.3 Side chains of chain W