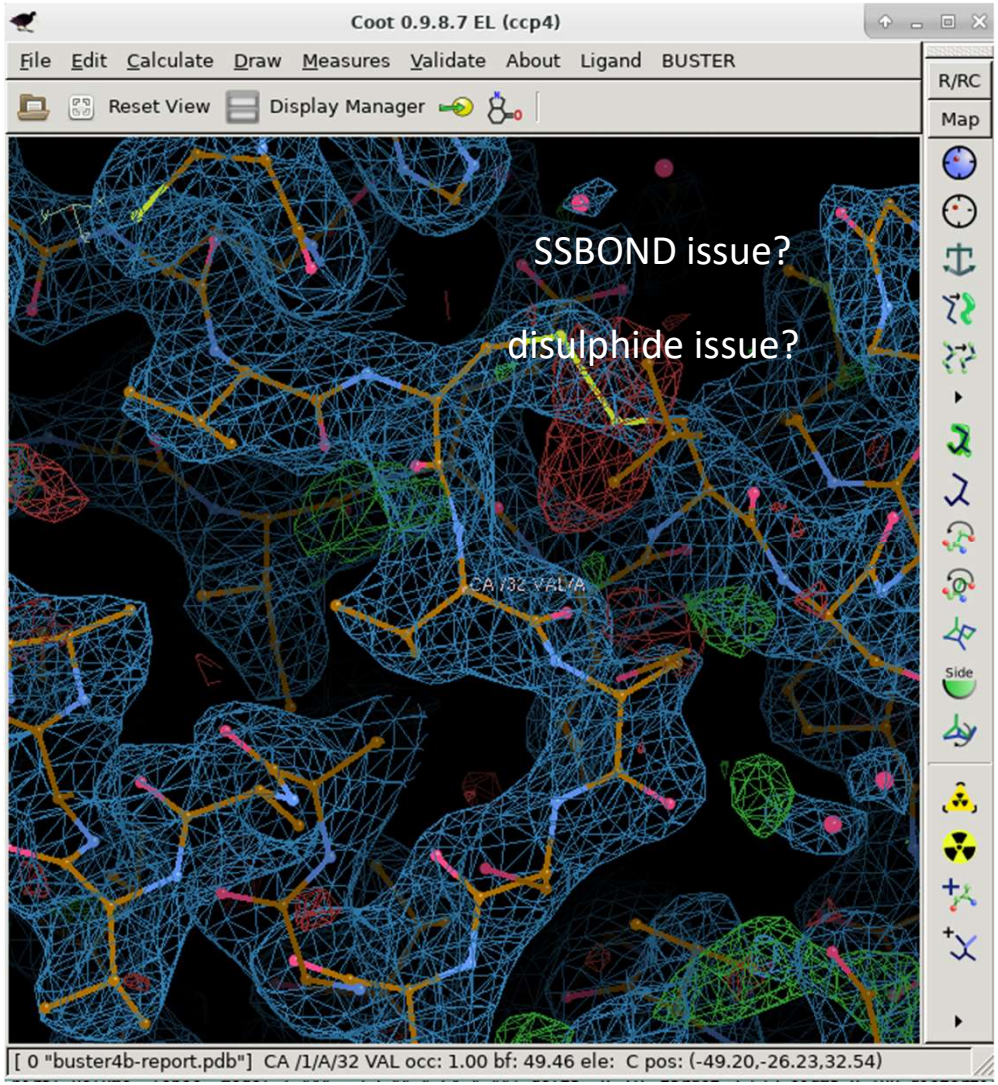
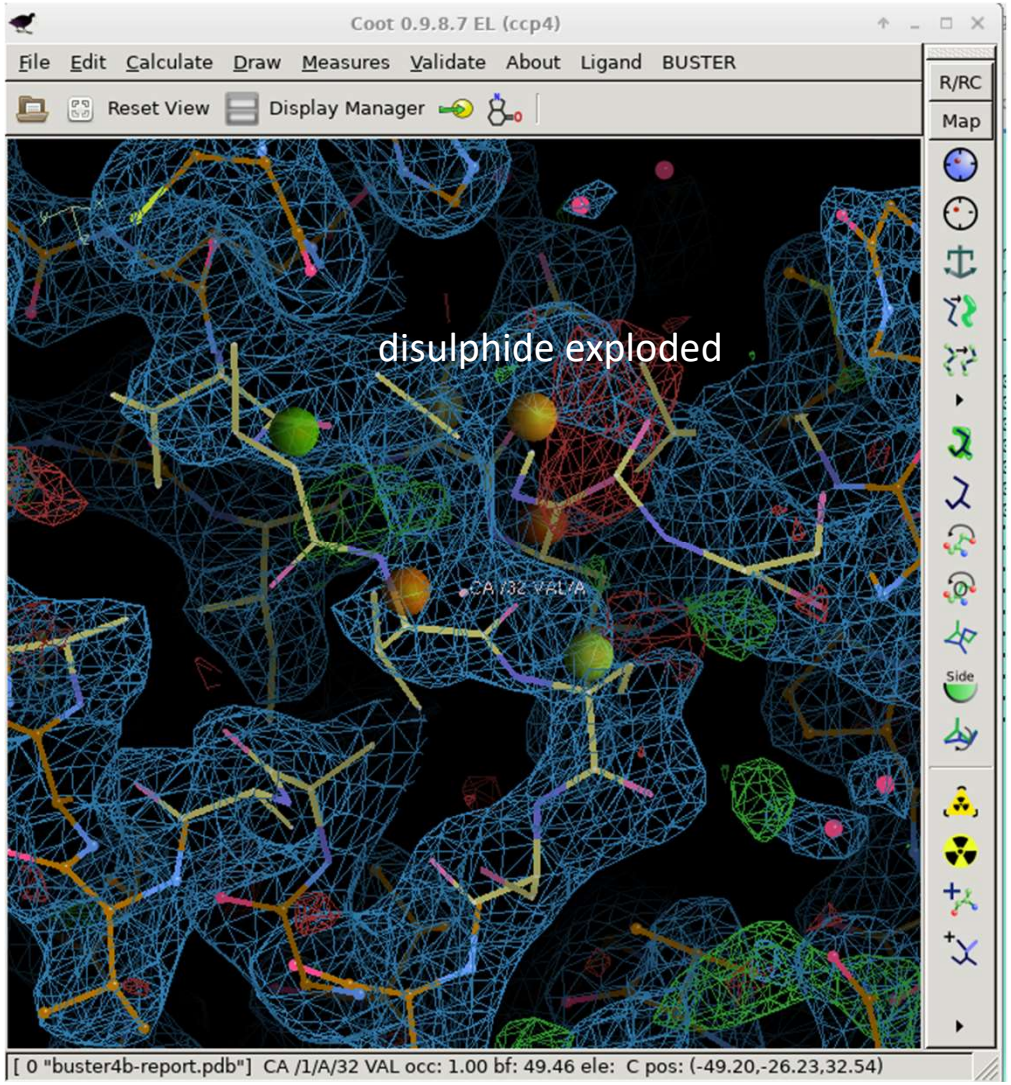
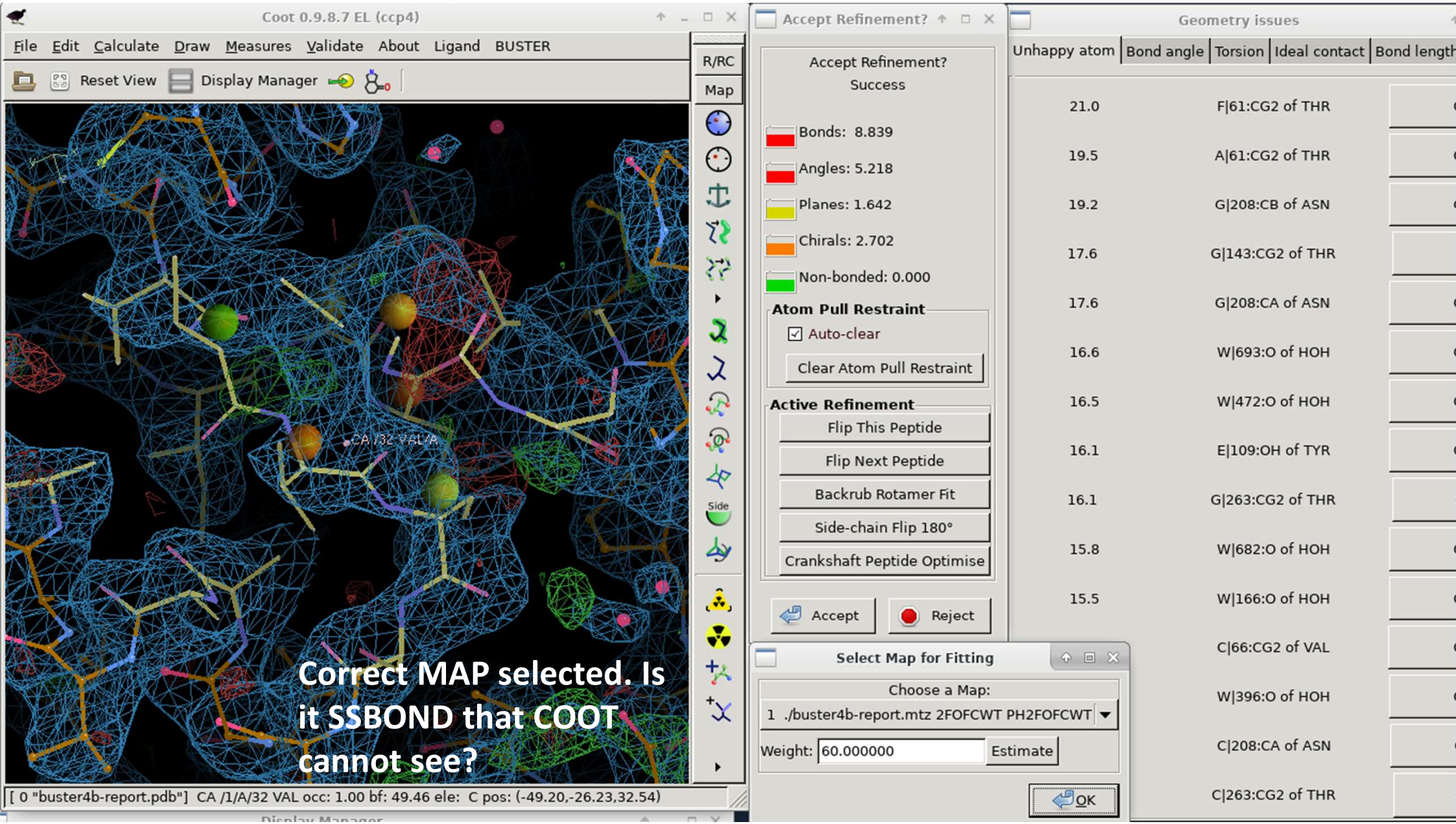
”R” refinement does not work in COOT

Before refinement



After ”R” refinement

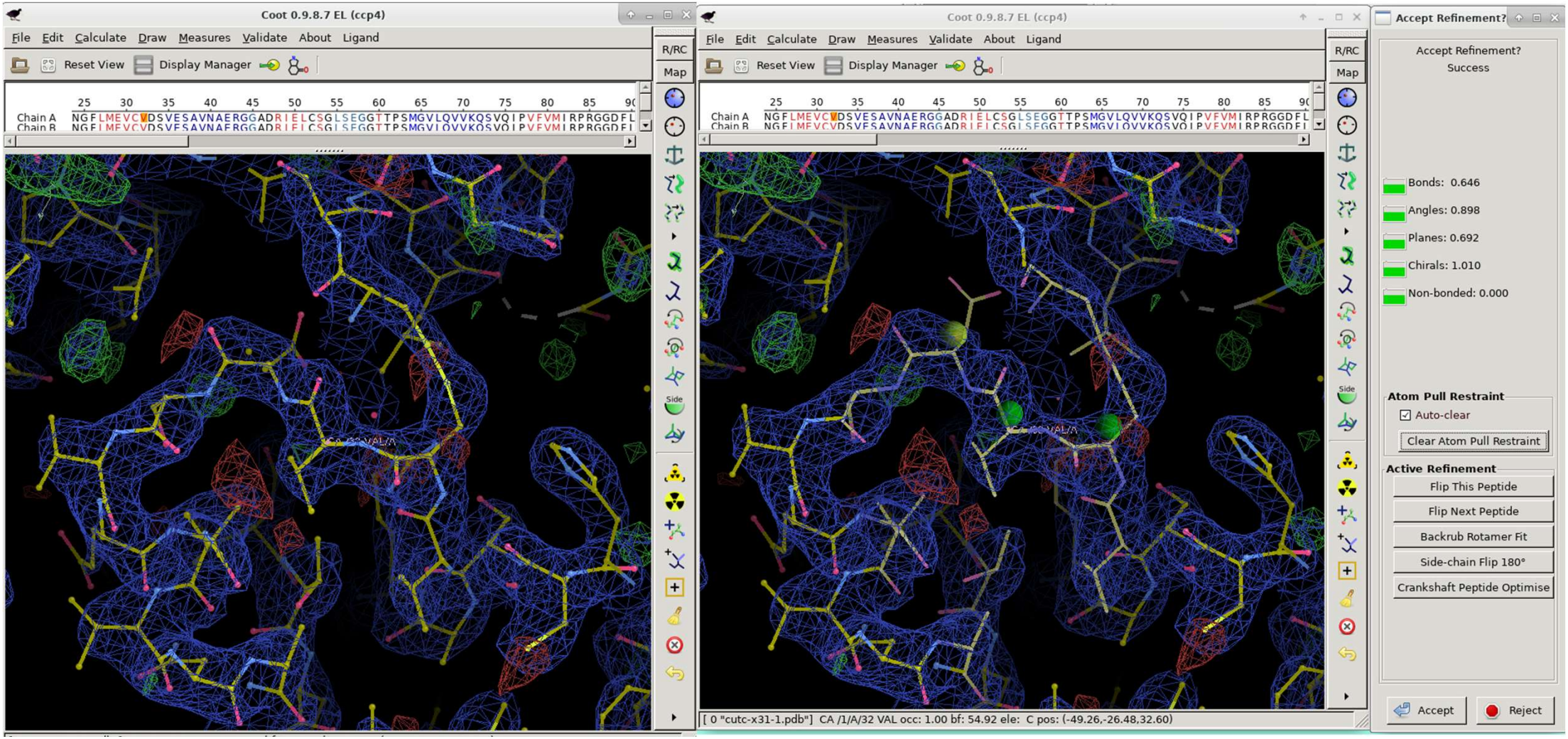



Coot 0.9.8.7 EL (ccp4)
File Edit Calculate Draw Measures Validate About Ligand BUSTER
Reset View
Display Manager
R/RC
Map
Side
CA /32 VAL/A
Correct MAP selected. Is it SSBOND that COOT cannot see?
[0 "buster4b-report.pdb"] CA /1/A/32 VAL occ: 1.00 bf: 49.46 ele: C pos: (-49.20,-26.23,32.54)
Accept Refinement?
Accept Refinement?
Success
Bonds: 8.839
Angles: 5.218
Planes: 1.642
Chirals: 2.702
Non-bonded: 0.000
Atom Pull Restraint
Auto-clear
Clear Atom Pull Restraint
Active Refinement
Flip This Peptide
Flip Next Peptide
Backrub Rotamer Fit
Side-chain Flip 180°
Crankshaft Peptide Optimise
Accept
Reject
Select Map for Fitting
Choose a Map:
1 ./buster4b-report.mtz 2FOFCWT PH2FOFCWT
Weight: 60.000000
Estimate
OK
Geometry issues
Unhappy atom
Bond angle
Torsion
Ideal contact
Bond length
21.0 F|61:CG2 of THR
19.5 A|61:CG2 of THR
19.2 G|208:CB of ASN
17.6 G|143:CG2 of THR
17.6 G|208:CA of ASN
16.6 W|693:O of HOH
16.5 W|472:O of HOH
16.1 E|109:OH of TYR
16.1 G|263:CG2 of THR
15.8 W|682:O of HOH
15.5 W|166:O of HOH
C|66:CG2 of VAL
W|396:O of HOH
C|208:CA of ASN
C|263:CG2 of THR

When PDB file never seen BUSTER, COOT ”R” is OK?

Before refinement

After refinement – all OK!

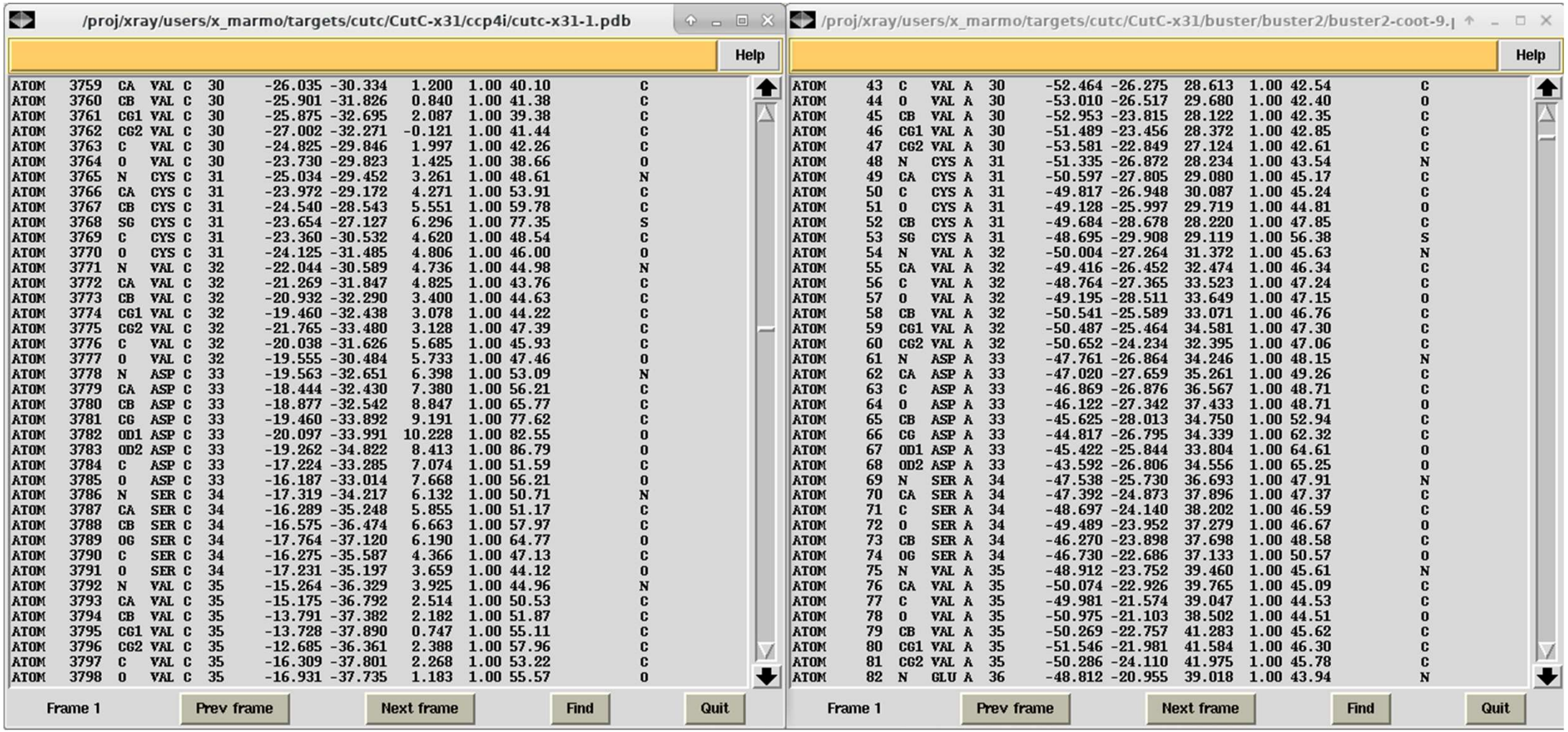


```
$ grep SSBOND cutc-x31-1.pdb
SSBOND   1 CYS A   31    CYS A   52
SSBOND   2 CYS B   31    CYS B   52
SSBOND   3 CYS C   31    CYS C   52
SSBOND   4 CYS D   31    CYS D   52
SSBOND   5 CYS E   31    CYS E   52
SSBOND   6 CYS F   31    CYS F   52
SSBOND   7 CYS G   31    CYS G   52
SSBOND   8 CYS H   31    CYS H   52
```

This did not matter when trying to add SSBOND as in refmac into buster4b_edit.pdb

```
 $ grep SSBOND buster4b_edit.pdb
 SSBOND   1 CYS A   31    CYS A   52                          1555   1555  2.04
 SSBOND   2 CYS B   31    CYS B   52                          1555   1555  2.05
 SSBOND   3 CYS C   31    CYS C   52                          1555   1555  2.05
 SSBOND   4 CYS D   31    CYS D   52                          1555   1555  2.04
 SSBOND   5 CYS E   31    CYS E   52                          1555   1555  2.04
 SSBOND   6 CYS F   31    CYS F   52                          1555   1555  2.05
 SSBOND   7 CYS G   31    CYS G   52                          1555   1555  2.05
 SSBOND   8 CYS H   31    CYS H   52                          1555   1555  2.05
```

CYS atom order differs refmac vs buster



N-CA-CB-SG-C-O refmac style

N-CA-C-O-CB-SG buster style