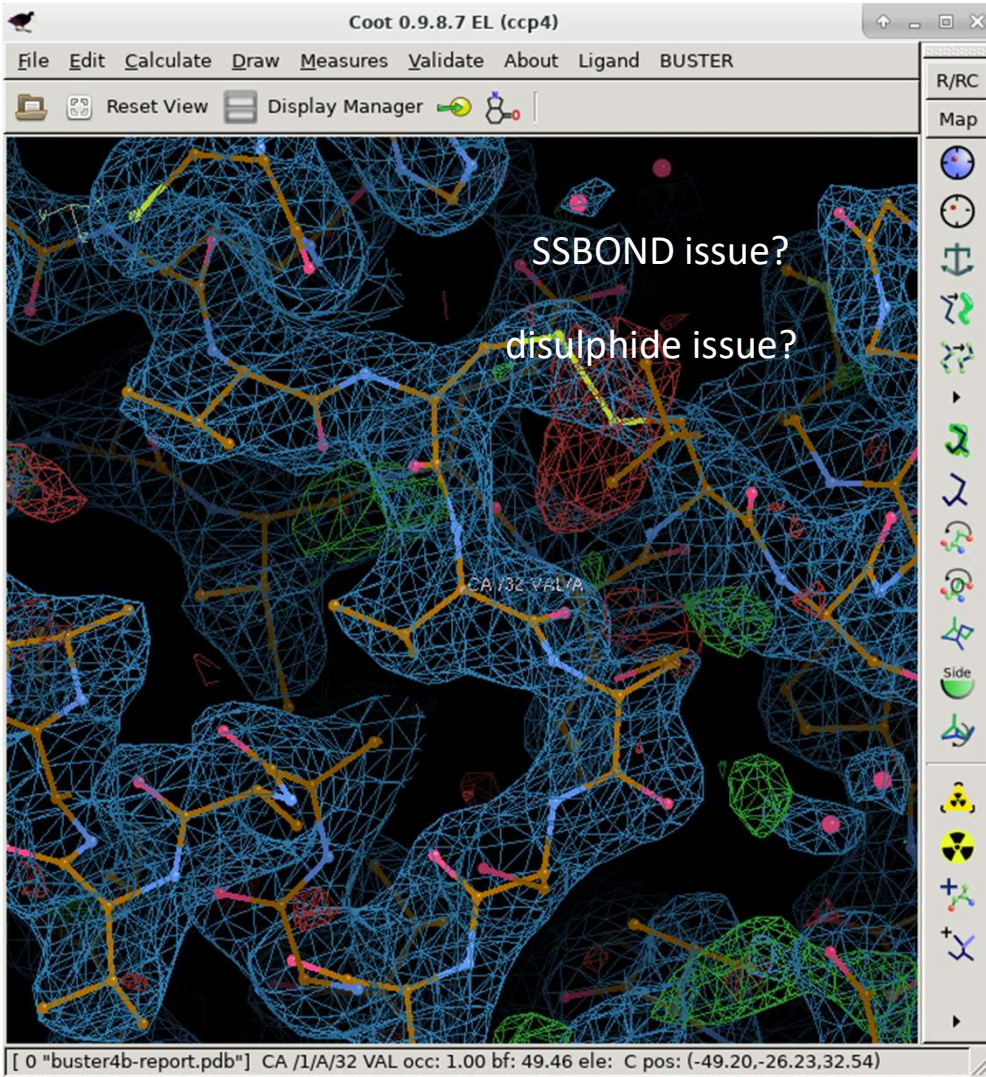
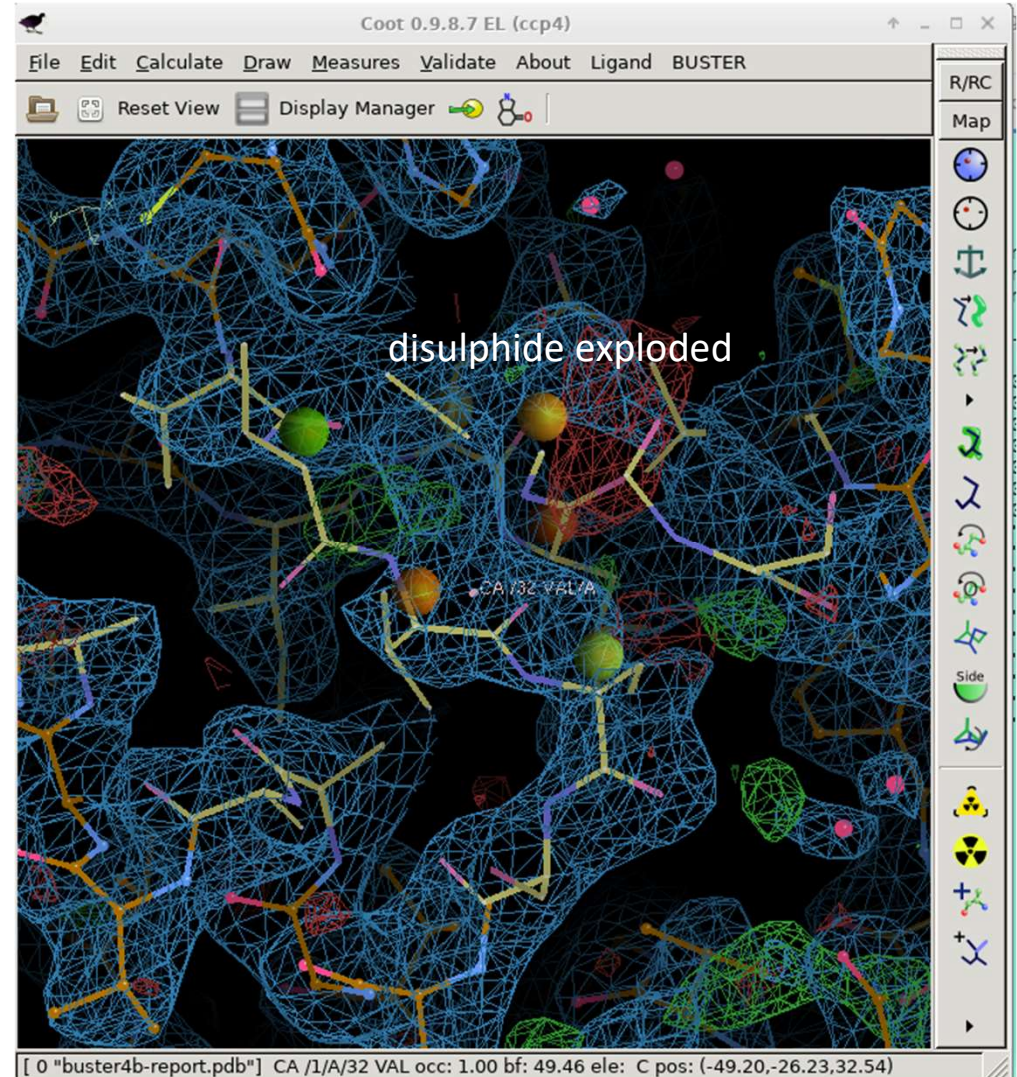


"R" refinement does not work in COOT

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

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!

The image displays two side-by-side screenshots of the COOT 0.9.8.7 EL (ccp4) software interface, illustrating the state of a protein model before and after refinement.

Left Screenshot (Before refinement): The interface shows the protein structure in stick representation overlaid on a blue mesh electron density map. The sequence is displayed at the top: Chain A: NGFLMEVCDVSVESAVNAERGGADRILELCSGLSEGGTTPSMGVLOVVKQSVQIPVFMIRPRGGDFL; Chain B: NGFLMEVCDVSVESAVNAERGGADRILELCSGLSEGGTTPSMGVLOVVKQSVQIPVFMIRPRGGDFL. The status bar at the bottom indicates: [0 "cutc-x31-1.pdb"] CA 1/A/32 VAL occ: 1.00 bf: 54.92 ele: C pos: (-49.26,-26.48,32.60).

Right Screenshot (After refinement – all OK!): The interface shows the same protein structure, but now with a green mesh electron density map. The status bar at the bottom indicates: [0 "cutc-x31-1.pdb"] CA 1/A/32 VAL occ: 1.00 bf: 54.92 ele: C pos: (-49.26,-26.48,32.60). A dialog box titled "Accept Refinement?" is open on the right, showing "Success". The dialog also displays quality metrics: Bonds: 0.646, Angles: 0.898, Planes: 0.692, Chirals: 1.010, Non-bonded: 0.000. The "Active Refinement" section includes buttons for "Flip This Peptide", "Flip Next Peptide", "Backrub Rotamer Fit", "Side-chain Flip 180°", and "Crankshaft Peptide Optimise". The "Accept" button is highlighted.

```
$ 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 reftmac 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

/proj/xray/users/x_marmo/targets/cutC/CutC-x31/ccp4i/cutC-x31-1.pdb											
ATOM	ID	Element	Type	Chain	Res	X	Y	Z	Occupancy	B-factor	Label
ATOM	3759	CA	VAL	C	30	-26.035	-30.334	1.200	1.00	40.10	C
ATOM	3760	CB	VAL	C	30	-25.901	-31.826	0.840	1.00	41.38	C
ATOM	3761	CG1	VAL	C	30	-25.875	-32.695	2.087	1.00	39.38	C
ATOM	3762	CG2	VAL	C	30	-27.002	-32.271	-0.121	1.00	41.44	C
ATOM	3763	C	VAL	C	30	-24.825	-29.846	1.997	1.00	42.26	C
ATOM	3764	O	VAL	C	30	-23.730	-29.823	1.425	1.00	38.66	O
ATOM	3765	N	CYS	C	31	-25.034	-29.452	3.261	1.00	48.61	N
ATOM	3766	CA	CYS	C	31	-23.972	-29.172	4.271	1.00	53.91	C
ATOM	3767	CB	CYS	C	31	-24.540	-28.543	5.551	1.00	59.78	C
ATOM	3768	SG	CYS	C	31	-23.654	-27.127	6.296	1.00	77.35	S
ATOM	3769	C	CYS	C	31	-23.360	-30.532	4.620	1.00	48.54	C
ATOM	3770	O	CYS	C	31	-24.125	-31.485	4.806	1.00	46.00	O
ATOM	3771	N	VAL	C	32	-22.044	-30.589	4.736	1.00	44.98	N
ATOM	3772	CA	VAL	C	32	-21.269	-31.847	4.825	1.00	43.76	C
ATOM	3773	CB	VAL	C	32	-20.932	-32.290	3.400	1.00	44.63	C
ATOM	3774	CG1	VAL	C	32	-19.460	-32.438	3.078	1.00	44.22	C
ATOM	3775	CG2	VAL	C	32	-21.765	-33.480	3.128	1.00	47.39	C
ATOM	3776	C	VAL	C	32	-20.038	-31.626	5.685	1.00	45.93	C
ATOM	3777	O	VAL	C	32	-19.555	-30.484	5.733	1.00	47.46	O
ATOM	3778	N	ASP	C	33	-19.563	-32.651	6.398	1.00	53.09	N
ATOM	3779	CA	ASP	C	33	-18.444	-32.430	7.380	1.00	56.21	C
ATOM	3780	CB	ASP	C	33	-18.877	-32.542	8.847	1.00	65.77	C
ATOM	3781	CG	ASP	C	33	-19.460	-33.892	9.191	1.00	77.62	C
ATOM	3782	OD1	ASP	C	33	-20.097	-33.991	10.228	1.00	82.55	O
ATOM	3783	OD2	ASP	C	33	-19.262	-34.822	8.413	1.00	86.79	O
ATOM	3784	C	ASP	C	33	-17.224	-33.285	7.074	1.00	51.59	C
ATOM	3785	O	ASP	C	33	-16.187	-33.014	7.668	1.00	56.21	O
ATOM	3786	N	SER	C	34	-17.319	-34.217	6.132	1.00	50.71	N
ATOM	3787	CA	SER	C	34	-16.289	-35.248	5.855	1.00	51.17	C
ATOM	3788	CB	SER	C	34	-16.575	-36.474	6.663	1.00	57.97	C
ATOM	3789	CG	SER	C	34	-17.764	-37.120	6.190	1.00	64.77	O
ATOM	3790	C	SER	C	34	-16.275	-35.587	4.366	1.00	47.13	C
ATOM	3791	O	SER	C	34	-17.231	-35.197	3.659	1.00	44.12	O
ATOM	3792	N	VAL	C	35	-15.264	-36.329	3.925	1.00	44.96	N
ATOM	3793	CA	VAL	C	35	-15.175	-36.792	2.514	1.00	50.53	C
ATOM	3794	CB	VAL	C	35	-13.791	-37.382	2.182	1.00	51.87	C
ATOM	3795	CG1	VAL	C	35	-13.728	-37.890	0.747	1.00	55.11	C
ATOM	3796	CG2	VAL	C	35	-12.685	-36.361	2.388	1.00	57.96	C
ATOM	3797	C	VAL	C	35	-16.309	-37.801	2.268	1.00	53.22	C
ATOM	3798	O	VAL	C	35	-16.931	-37.735	1.183	1.00	55.57	O

/proj/xray/users/x_marmo/targets/cutC/CutC-x31/buster/buster2/buster2-coot-9.1											
ATOM	ID	Element	Type	Chain	Res	X	Y	Z	Occupancy	B-factor	Label
ATOM	43	C	VAL	A	30	-52.464	-26.275	28.613	1.00	42.54	C
ATOM	44	O	VAL	A	30	-53.010	-26.517	29.680	1.00	42.40	O
ATOM	45	CB	VAL	A	30	-52.953	-23.815	28.122	1.00	42.35	C
ATOM	46	CG1	VAL	A	30	-51.489	-23.456	28.372	1.00	42.85	C
ATOM	47	CG2	VAL	A	30	-53.581	-22.849	27.124	1.00	42.61	C
ATOM	48	N	CYS	A	31	-51.335	-26.872	28.234	1.00	43.54	N
ATOM	49	CA	CYS	A	31	-50.597	-27.805	29.080	1.00	45.17	C
ATOM	50	C	CYS	A	31	-49.817	-26.948	30.087	1.00	45.24	C
ATOM	51	O	CYS	A	31	-49.128	-25.997	29.719	1.00	44.81	O
ATOM	52	CB	CYS	A	31	-49.684	-28.678	28.220	1.00	47.85	C
ATOM	53	SG	CYS	A	31	-48.695	-29.908	29.119	1.00	56.38	S
ATOM	54	N	VAL	A	32	-50.004	-27.264	31.372	1.00	45.63	N
ATOM	55	CA	VAL	A	32	-49.416	-26.452	32.474	1.00	46.34	C
ATOM	56	C	VAL	A	32	-48.764	-27.365	33.523	1.00	47.24	C
ATOM	57	O	VAL	A	32	-49.195	-28.511	33.649	1.00	47.15	O
ATOM	58	CB	VAL	A	32	-50.541	-25.589	33.071	1.00	46.76	C
ATOM	59	CG1	VAL	A	32	-50.487	-25.464	34.581	1.00	47.30	C
ATOM	60	CG2	VAL	A	32	-50.652	-24.234	32.395	1.00	47.06	C
ATOM	61	N	ASP	A	33	-47.761	-26.864	34.246	1.00	48.15	N
ATOM	62	CA	ASP	A	33	-47.020	-27.659	35.261	1.00	49.26	C
ATOM	63	C	ASP	A	33	-46.869	-26.876	36.567	1.00	48.71	C
ATOM	64	O	ASP	A	33	-46.122	-27.342	37.433	1.00	48.71	O
ATOM	65	CB	ASP	A	33	-45.625	-28.013	34.750	1.00	52.94	C
ATOM	66	CG	ASP	A	33	-44.817	-26.795	34.339	1.00	62.32	C
ATOM	67	OD1	ASP	A	33	-45.422	-25.844	33.804	1.00	64.61	O
ATOM	68	OD2	ASP	A	33	-43.592	-26.806	34.556	1.00	65.25	O
ATOM	69	N	SER	A	34	-47.538	-25.730	36.693	1.00	47.91	N
ATOM	70	CA	SER	A	34	-47.392	-24.873	37.896	1.00	47.37	C
ATOM	71	C	SER	A	34	-48.697	-24.140	38.202	1.00	46.59	C
ATOM	72	O	SER	A	34	-49.489	-23.952	37.279	1.00	46.67	O
ATOM	73	CB	SER	A	34	-46.270	-23.898	37.698	1.00	48.58	C
ATOM	74	CG	SER	A	34	-46.730	-22.686	37.133	1.00	50.57	O
ATOM	75	N	VAL	A	35	-48.912	-23.752	39.460	1.00	45.61	N
ATOM	76	CA	VAL	A	35	-50.074	-22.926	39.765	1.00	45.09	C
ATOM	77	C	VAL	A	35	-49.981	-21.574	39.047	1.00	44.53	C
ATOM	78	O	VAL	A	35	-50.975	-21.103	38.502	1.00	44.51	O
ATOM	79	CB	VAL	A	35	-50.269	-22.757	41.283	1.00	45.62	C
ATOM	80	CG1	VAL	A	35	-51.546	-21.981	41.584	1.00	46.30	C
ATOM	81	CG2	VAL	A	35	-50.286	-24.110	41.975	1.00	45.78	C
ATOM	82	N	GLU	A	36	-48.812	-20.955	39.018	1.00	43.94	N

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

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