

If the user has solved and refined their structure and finds that Z' is greater than 1, it is time to think seriously about the possibility of pseudosymmetry. That can be done in CRYSTALS with the MATCH routine, as described in our accompanying paper (for a complete description we suggest Collins, Cooper & Watkin, 2006, referenced in the paper and below). As well as handling native CRYSTALS format data, structures may usually be imported into CRYSTALS from the gift of a .cif or .res file, or the Cambridge Structural Database. Structure factors are not needed. CRYSTALS uses a different atom-naming format from SHELX, but can convert the names automatically. Once the atoms are present, they must be assigned residue numbers (residues are defined in the cif dictionary, but for molecular materials containing more than one independent molecule in the asymmetric unit, each molecule is usually a residue). This may simply be done by selecting *Allocate Residue Numbers* on the Structure menu in CRYSTALS. The process is automatic, and the residues are called *RESIDUE(1)* etc. To carry out an analysis on residues(1) and (2), we issue the command set:

```
\match
output punch=results
map resi(1)
onto resi(2)
end
```

In the \logs directory of the structure folder, a short-form results file (blue, below) will appear as bfile.pch. Many but not all of the features we'll be interested in appear in this file, so it is a quick indication of what we might learn.

```
CULD_0m in P2(1)      Internal_symmetry_2
Centroids      0.4156      0.4940      0.8313      0.4728      0.5121      0.3470
Axes of Inertia 308.10      211.86      20.66      344.71      199.12      16.12
Sum dev sq     10.5258      1.0515      13.2416      24.8189
RMS dev        0.6025      0.1904      0.6757      0.9251
RMS bond and tors dev 0.0070      15.1781
Min and Max bond dev 0.0003      0.0147
Min and Max tors dev 0.4492      63.4467
Max U & Uprime dev 0.0284      0.0593
Mean & Delta Centroids 0.4442      0.5031      0.5891      0.0571      0.0181      -0.4843
Transformation 0.274 0.448 -0.127 -2.066 0.218 -0.938 -0.251 0.003 0.914
Det and trace  1.0000      1.4055
Closeness to ideal rotation 0.21544
Closeness to group operator 0.09853
Combined measure of closeness 0.19297
Rworst & Raverage 0.554732323 0.386098921 4
Symmetry      none
Pseudo none
Operator      none S
No_Atoms      29
S.G.          P 1 21 1
```

Cell 9.5938 20.1903 10.1806 90.0000 104.6630 90.0000

The major findings are symmetry that is not a mirror or inversion, but although the title supplied by the MATCH procedure says symmetry 2, it is likely closer to 4 as we shall see below. The transformation matrix does not have any values particularly close to 0.5 or 1.0, so it appears initially that we may not find a supergroup. The determinant and trace add up to 2.405, nearer to a 4 than anything else, and the centroid difference between the two molecules is close to a one-half translation along c. The RMS torsion angle differences are small at 15.2 degrees, but the maximum entry is over 63 degrees. How hard will it be to find those? Read on...it's EASY!

If there are two instances of the same molecule in the asymmetric unit, we would normally expect equivalent bond lengths in each instance to be very similar, bond angles to show more variation, and see the greatest discrepancies in the torsion angles. The ADPs will be quite sensitive to crystal packing contacts and thus often show significant differences. CRYSTALS computes all of these metrics.

The long-form output appears in another file the log folder, bfile##.lis, where ## is usually a number which automatically increments with each new use of CRYSTALS (the first run it will be bfile.lis). In general, there may be several cycles/attempts before the final matching pair is chosen. What we usually do is go to the end of the file, and then look at the last run: there can be oodles of output. I have snipped out the early cycles in this run to leave the essential last cycle that was used in the paper.

```
#MATCH
Structure matching: measures of similarity and pseudosymmetry
A. Collins, R. I. Cooper and D. J. Watkin
Journal of Applied Crystallography 2006;39,842-849
```

CULD_0m in P2(1)

Date 31/03/21 Time 15:11:26

```
Input: mapping 29 atoms onto 29
Matching Permitting Improper Rotation (Method 4, Kabsch)
```

```
Matching atoms
WARNING - poor initial fit
Improving match
Improving: Mapping onto distance
```

Calculation of rotation matrix by Kabsch method

Rotation Matrix

```
-0.99549  -0.09276   0.01968
-0.09288   0.99567  -0.00491
-0.01914  -0.00671  -0.99979
```

Deviations in best plane system after fitting (Angstrom)
 "Angle" is the angular separation of the atoms as seen from
 the centre of gravity

The distance between MATCHed atoms appears in this list; we can get all, and easily scan for the maximum which is highlighted below. The list which follows this one shows the actual pairing.

Position	Type	Serial	old(x)	old(y)	old(z)	new(x)	new(y)	new(z)	d(x)	d(y)	d(z)	Distance	Angle
1	O	4.	-4.022	4.155	0.369	-3.910	3.905	1.157	0.112	-0.250	0.788	0.834	8.319
2	O	8.	3.212	4.548	-0.362	4.237	4.253	-1.317	1.024	-0.296	-0.956	1.432	12.810
3	C	7.	-4.027	2.785	0.240	-4.012	2.580	0.810	0.014	-0.205	0.570	0.606	6.320
4	C	16.	3.397	3.198	-0.247	4.196	3.041	-0.682	0.799	-0.158	-0.435	0.923	9.596
5	O	3.	-2.861	3.023	-1.865	-3.662	3.247	-1.476	-0.801	0.224	0.389	0.918	9.723
6	O	7.	3.415	3.571	2.092	2.006	3.631	0.162	-1.410	0.059	-1.931	2.391	24.734
7	C	6.	-3.451	2.235	-0.904	-3.847	2.272	-0.544	-0.396	0.036	0.360	0.537	6.239
8	C	15.	3.456	2.669	1.046	3.054	2.755	0.069	-0.402	0.086	-0.977	1.060	12.418
9	C	8.	-4.580	1.951	1.192	-4.250	1.570	1.735	0.330	-0.381	0.542	0.741	7.760
10	C	17.	3.510	2.339	-1.336	5.198	2.089	-0.779	1.688	-0.250	0.557	1.795	18.029
11	C	5.	-3.411	0.859	-1.064	-3.864	0.941	-0.951	-0.452	0.082	0.112	0.473	5.951
12	C	14.	3.542	1.302	1.242	2.937	1.533	0.702	-0.605	0.232	-0.540	0.844	11.249
13	C	9.	-4.504	0.566	1.046	-4.287	0.247	1.313	0.217	-0.319	0.266	0.469	5.348
14	C	18.	3.650	0.970	-1.136	5.055	0.840	-0.181	1.405	-0.130	0.954	1.703	18.742
15	C	4.	-3.921	-0.001	-0.081	-4.070	-0.079	-0.022	-0.149	-0.078	0.059	0.178	2.220
16	C	13.	3.638	0.429	0.152	3.918	0.538	0.565	0.280	0.109	0.413	0.511	6.644
17	N	1.	-1.292	-1.384	-0.367	-1.452	-1.307	-0.435	-0.160	0.077	-0.069	0.190	3.796
18	N	2.	1.599	-1.374	-0.884	1.459	-1.059	-0.115	-0.140	0.315	0.769	0.843	17.743
19	C	3.	-3.786	-1.502	-0.208	-3.959	-1.528	-0.442	-0.172	-0.026	-0.234	0.292	3.732
20	C	12.	3.697	-1.062	0.415	3.657	-0.864	1.062	-0.040	0.198	0.647	0.678	8.738
21	C	2.	-2.443	-1.979	0.353	-2.615	-2.096	0.027	-0.172	-0.118	-0.326	0.387	5.708
22	C	11.	2.961	-1.896	-0.657	2.826	-1.620	0.020	-0.135	0.275	0.677	0.743	10.712
23	CU	1.	0.253	-2.570	-0.101	0.123	-2.487	-0.233	-0.130	0.082	-0.132	0.202	3.593
24	O	1.	-1.050	-3.931	0.303	-1.146	-3.922	-0.444	-0.096	0.008	-0.747	0.753	9.590
25	O	5.	1.728	-3.788	0.180	1.581	-3.684	0.155	-0.147	0.104	-0.025	0.182	2.263
26	O	6.	3.923	-4.013	-0.090	3.778	-3.768	0.461	-0.145	0.246	0.551	0.620	6.019
27	O	2.	-3.241	-4.252	0.478	-3.322	-4.334	-0.510	-0.081	-0.083	-0.988	0.995	9.538
28	C	1.	-2.269	-3.505	0.358	-2.367	-3.558	-0.352	-0.098	-0.053	-0.710	0.719	8.386
29	C	10.	2.877	-3.345	-0.168	2.739	-3.134	0.246	-0.139	0.211	0.414	0.485	5.741

	x	y	z	over-all
Total squared deviations	10.526	1.051	13.242	Total 24.819
RMS deviations	0.602	0.190	0.676	Mean 0.925

Maximum distance O 7 2.391
 Maximum angle O 7 24.734

The following compares the ADPs of pairs of atoms that have been MATCHed in the common reference system.

Uij in Best Match Coordinate System

Uprime = U(max).U(min)/U(min), Watkin, Acta Cryst (2000) B56 747-749

Position	Type	Serial	Old U[ij]						Old Principal Axes			Uprime	Ugeom
			New U[ij]						New Principal Axes				
			delta U[ij]						delta Principal Axes				
1	O	108.	0.035	0.009	0.014	-0.002	-0.001	0.004	0.008	0.014	0.036	0.065	0.016
		4.	0.020	0.011	0.022	-0.006	0.002	0.000	0.008	0.019	0.025	0.059	0.016
			0.015	-0.002	-0.008	0.004	-0.003	0.004	-0.001	-0.005	0.010	0.007	-0.000
2	O	104.	0.023	0.012	0.019	0.003	0.002	0.001	0.011	0.019	0.025	0.042	0.017
		8.	0.019	0.016	0.039	0.008	0.008	0.001	0.013	0.017	0.044	0.058	0.021
			0.004	-0.004	-0.020	-0.005	-0.005	-0.000	-0.002	0.002	-0.020	-0.016	-0.004
3	C	116.	0.018	0.010	0.017	-0.001	-0.004	0.002	0.009	0.014	0.022	0.035	0.014
		7.	0.012	0.011	0.022	-0.003	-0.003	0.001	0.010	0.011	0.024	0.027	0.014
			0.007	-0.001	-0.005	0.002	-0.001	0.001	-0.001	0.003	-0.002	0.008	0.000
4	C	107.	0.012	0.013	0.020	0.001	0.001	-0.001	0.011	0.014	0.020	0.026	0.014
		16.	0.016	0.012	0.026	0.001	-0.000	-0.001	0.012	0.016	0.026	0.034	0.017
			-0.004	0.001	-0.006	0.000	0.002	-0.001	-0.001	-0.002	-0.006	-0.008	-0.003
5	O	107.	0.029	0.007	0.024	0.002	0.010	0.002	0.007	0.016	0.038	0.086	0.016
		3.	0.026	0.011	0.022	0.001	0.004	0.002	0.011	0.019	0.029	0.051	0.018
			0.003	-0.004	0.002	0.002	0.006	0.000	-0.004	-0.003	0.009	0.035	-0.002
6	O	103.	0.021	0.015	0.017	-0.002	0.001	-0.003	0.013	0.017	0.023	0.031	0.017
		7.	0.017	0.010	0.048	0.005	0.010	0.003	0.009	0.015	0.052	0.090	0.019
			0.003	0.005	-0.031	-0.007	-0.009	-0.006	0.004	0.002	-0.028	-0.059	-0.002
7	C	115.	0.014	0.010	0.017	0.003	-0.001	-0.000	0.009	0.014	0.018	0.027	0.013
		6.	0.010	0.011	0.021	-0.000	-0.001	0.001	0.010	0.012	0.021	0.024	0.014
			0.003	-0.002	-0.004	0.003	0.001	-0.001	-0.001	0.002	-0.004	0.003	-0.001
8	C	106.	0.012	0.014	0.018	-0.001	-0.000	-0.002	0.011	0.015	0.019	0.027	0.014
		15.	0.014	0.011	0.025	-0.003	0.001	-0.001	0.011	0.014	0.026	0.033	0.016
			-0.002	0.003	-0.007	0.002	-0.001	-0.002	-0.000	0.001	-0.007	-0.006	-0.001
9	C	117.	0.023	0.016	0.013	-0.002	0.003	0.004	0.010	0.017	0.025	0.042	0.016
		8.	0.018	0.019	0.019	-0.001	-0.000	0.001	0.017	0.018	0.021	0.022	0.019
			0.005	-0.003	-0.006	-0.001	0.003	0.003	-0.007	-0.002	0.005	0.019	-0.002
10	C	108.	0.018	0.014	0.018	0.002	0.002	-0.001	0.013	0.018	0.020	0.028	0.017
		17.	0.014	0.017	0.033	-0.002	0.003	-0.001	0.014	0.017	0.033	0.042	0.020
			0.004	-0.003	-0.014	0.004	-0.001	-0.000	-0.001	0.000	-0.013	-0.014	-0.003

11	C	114.	0.015	0.011	0.014	-0.001	0.001	0.001	0.010	0.014	0.015	0.021	0.013
	C	5.	0.015	0.015	0.020	-0.004	-0.002	0.003	0.012	0.014	0.023	0.028	0.016
			0.000	-0.005	-0.006	0.003	0.003	-0.002	-0.002	-0.001	-0.008	-0.007	-0.003
12	C	105.	0.014	0.016	0.018	0.002	-0.002	-0.002	0.013	0.015	0.021	0.024	0.016
	C	14.	0.016	0.014	0.019	-0.003	0.001	-0.003	0.011	0.016	0.021	0.030	0.016
			-0.002	0.002	-0.001	0.005	-0.003	0.001	0.002	-0.001	-0.000	-0.006	0.000
13	C	118.	0.021	0.013	0.014	0.003	0.001	-0.001	0.010	0.016	0.021	0.034	0.015
	C	9.	0.018	0.014	0.025	0.003	-0.001	0.001	0.013	0.018	0.026	0.037	0.018
			0.003	-0.001	-0.012	0.000	0.002	-0.001	-0.003	-0.002	-0.005	-0.002	-0.003
14	C	109.	0.018	0.014	0.019	-0.001	0.001	-0.002	0.013	0.018	0.020	0.026	0.017
	C	18.	0.014	0.016	0.031	-0.002	-0.001	0.004	0.011	0.019	0.032	0.053	0.019
			0.003	-0.002	-0.012	0.001	0.002	-0.006	0.002	-0.001	-0.012	-0.026	-0.002
15	C	113.	0.012	0.010	0.016	-0.000	-0.002	0.001	0.009	0.011	0.017	0.021	0.012
	C	4.	0.013	0.010	0.025	-0.003	-0.004	0.002	0.009	0.012	0.027	0.038	0.014
			-0.001	-0.000	-0.009	0.003	0.002	-0.001	0.001	-0.001	-0.010	-0.017	-0.002
16	C	104.	0.015	0.011	0.021	0.002	-0.001	0.000	0.011	0.014	0.022	0.029	0.015
	C	13.	0.017	0.011	0.019	-0.002	-0.005	-0.001	0.010	0.014	0.023	0.034	0.015
			-0.003	0.000	0.002	0.004	0.004	0.001	0.001	0.000	-0.001	-0.005	0.000
17	N	102.	0.015	0.008	0.015	0.001	-0.001	-0.001	0.008	0.014	0.016	0.027	0.012
	N	1.	0.016	0.008	0.025	-0.001	-0.000	-0.001	0.008	0.017	0.025	0.051	0.015
			-0.002	0.000	-0.010	0.001	-0.000	0.000	0.000	-0.002	-0.009	-0.024	-0.003
18	N	101.	0.016	0.014	0.024	0.006	-0.004	-0.001	0.011	0.014	0.029	0.039	0.016
	N	2.	0.015	0.008	0.026	0.001	-0.002	0.001	0.008	0.015	0.026	0.050	0.015
			0.000	0.006	-0.001	0.005	-0.002	-0.002	0.003	-0.001	0.002	-0.011	0.002
19	C	112.	0.014	0.010	0.018	0.002	-0.000	0.001	0.009	0.014	0.018	0.030	0.013
	C	3.	0.016	0.011	0.028	-0.003	-0.005	0.001	0.011	0.014	0.030	0.040	0.016
			-0.002	-0.002	-0.010	0.005	0.005	0.000	-0.002	0.001	-0.012	-0.010	-0.003
20	C	103.	0.021	0.011	0.022	0.002	-0.004	-0.001	0.010	0.018	0.026	0.045	0.017
	C	12.	0.019	0.011	0.019	-0.000	-0.005	-0.001	0.011	0.015	0.024	0.032	0.016
			0.002	-0.000	0.003	0.003	0.001	0.000	-0.001	0.003	0.002	0.013	0.001
21	C	111.	0.015	0.009	0.013	0.002	-0.001	0.001	0.008	0.013	0.016	0.026	0.012
	C	2.	0.014	0.009	0.018	-0.001	-0.002	-0.000	0.009	0.014	0.019	0.028	0.013
			0.001	-0.001	-0.005	0.002	0.000	0.001	-0.001	-0.000	-0.003	-0.001	-0.001
22	C	102.	0.015	0.012	0.018	0.003	-0.000	0.000	0.011	0.015	0.019	0.026	0.014
	C	11.	0.013	0.007	0.016	0.001	0.000	-0.001	0.007	0.013	0.016	0.029	0.012
			0.001	0.004	0.002	0.002	-0.000	0.001	0.003	0.001	0.003	-0.004	0.003
23	CU	101.	0.012	0.008	0.021	0.004	-0.002	-0.000	0.007	0.012	0.022	0.038	0.012
	CU	1.	0.012	0.007	0.023	0.001	-0.000	-0.000	0.007	0.012	0.023	0.040	0.013

			0.000	0.001	-0.003	0.003	-0.002	0.000	0.000	-0.000	-0.001	-0.003	-0.000
24	O	105.	0.014	0.008	0.022	0.003	0.001	0.001	0.007	0.014	0.023	0.042	0.013
	O	1.	0.014	0.009	0.033	-0.001	-0.002	0.000	0.009	0.014	0.034	0.054	0.016
			-0.001	-0.001	-0.012	0.004	0.002	0.001	-0.001	-0.000	-0.011	-0.012	-0.003
25	O	101.	0.014	0.012	0.029	0.006	-0.001	-0.000	0.010	0.014	0.031	0.045	0.016
	O	5.	0.014	0.008	0.026	0.002	0.000	-0.000	0.008	0.014	0.026	0.045	0.014
			0.000	0.003	0.004	0.004	-0.002	-0.000	0.002	0.000	0.005	-0.001	0.002
26	O	102.	0.019	0.015	0.025	0.004	0.003	0.004	0.012	0.018	0.028	0.042	0.018
	O	6.	0.016	0.011	0.029	0.001	-0.001	0.003	0.010	0.017	0.029	0.050	0.017
			0.003	0.004	-0.003	0.003	0.004	0.001	0.003	0.002	-0.001	-0.008	0.002
27	O	106.	0.017	0.012	0.029	0.006	0.002	-0.002	0.009	0.017	0.031	0.058	0.017
	O	2.	0.016	0.010	0.027	0.001	-0.003	-0.003	0.009	0.016	0.028	0.049	0.016
			0.001	0.002	0.002	0.006	0.005	0.001	0.000	0.001	0.003	0.008	0.001
28	C	110.	0.017	0.010	0.014	0.002	-0.000	-0.001	0.009	0.015	0.017	0.029	0.013
	C	1.	0.017	0.010	0.016	0.002	-0.001	0.000	0.009	0.016	0.018	0.032	0.014
			0.000	0.000	-0.003	0.000	0.001	-0.001	-0.000	-0.001	-0.001	-0.003	-0.001
29	C	101.	0.017	0.012	0.015	0.002	-0.000	-0.001	0.011	0.015	0.017	0.024	0.014
	C	10.	0.016	0.009	0.016	-0.001	0.002	0.000	0.009	0.014	0.019	0.030	0.013
			0.001	0.003	-0.001	0.003	-0.003	-0.001	0.002	0.001	-0.001	-0.006	0.001

If the MATCHing was chemically sensible, the bonds should be very similar, of course!

Bond length deviations

O108-C116	O4-C7	0.002
O104-C107	O8-C16	0.002
C116-C117	C7-C8	0.008
C107-C108	C16-C17	0.007
O107-C115	O3-C6	0.013
O103-C106	O7-C15	0.013
C115-C116	C6-C7	0.004
C106-C107	C15-C16	0.001
C117-C118	C8-C9	0.005
C108-C109	C17-C18	0.001
C114-C115	C5-C6	0.006
C105-C106	C14-C15	0.004
C113-C114	C4-C5	0.007
C113-C118	C4-C9	0.001
C104-C105	C13-C14	0.004
C104-C109	C13-C18	0.004
N102-C111	N1-C2	0.003
N101-C102	N2-C11	0.008
C112-C113	C3-C4	0.001
C103-C104	C12-C13	0.005
C111-C112	C2-C3	0.000

C102-C103	C11-C12	0.012
CU101-O101	CU1-O5	0.008
CU101-O105	CU1-O1	0.000
CU101-N101	CU1-N2	0.004
CU101-N102	CU1-N1	0.013
O105-C110	O1-C1	0.015
O101-C101	O5-C10	0.004
O102-C101	O6-C10	0.007
O106-C110	O2-C1	0.009
C110-C111	C1-C2	0.006
C101-C102	C10-C11	0.001

The following table will allow us to find the maximum torsion angle deviation EASILY, by simple inspection...I have highlighted it below. Torsions having A-B-C or B-C-D angles within 5-10 degrees (depending on CRYSTALS version) of linear will be omitted from the statistics and have a STATUS of SKIPPED, otherwise OK.

Torsion angles are omitted from the statistics if angles C-A-B or A-B-D are within 5 degrees of co-linearity		Angles, Difference & Status		
Torsion angle deviations				
C115-C116-C117-C118	C6-C7-C8-C9	3.25	1.67	1.58 OK
O108-C116-C117-C118	O4-C7-C8-C9	-176.95	-177.42	0.47 OK
C106-C107-C108-C109	C15-C16-C17-C18	1.40	2.51	-1.12 OK
O104-C107-C108-C109	O8-C16-C17-C18	-177.72	-175.60	-2.12 OK
C114-C115-C116-O108	C5-C6-C7-O4	178.80	176.40	2.40 OK
C114-C115-C116-C117	C5-C6-C7-C8	-1.39	-2.75	1.35 OK
O107-C115-C116-O108	O3-C6-C7-O4	1.66	-3.31	4.97 OK
O107-C115-C116-C117	O3-C6-C7-C8	-178.53	177.55	3.92 OK
C105-C106-C107-O104	C14-C15-C16-O8	175.22	178.17	-2.94 OK
C105-C106-C107-C108	C14-C15-C16-C17	-3.95	-0.07	-3.88 OK
O103-C106-C107-O104	O7-C15-C16-O8	-4.37	0.84	-5.21 OK
O103-C106-C107-C108	O7-C15-C16-C17	176.46	-177.39	-6.15 OK
C116-C117-C118-C113	C7-C8-C9-C4	-2.62	0.94	-3.55 OK
C107-C108-C109-C104	C16-C17-C18-C13	1.98	-2.20	4.17 OK
C113-C114-C115-O107	C4-C5-C6-O3	176.09	-179.05	-4.86 OK
C113-C114-C115-C116	C4-C5-C6-C7	-1.14	1.24	-2.38 OK
C104-C105-C106-O103	C13-C14-C15-O7	-177.28	174.69	8.03 OK
C104-C105-C106-C107	C13-C14-C15-C16	3.16	-2.74	5.90 OK
C112-C113-C114-C115	C3-C4-C5-C6	-175.41	-174.22	-1.19 OK
C118-C113-C114-C115	C9-C4-C5-C6	1.78	1.33	0.45 OK
C112-C113-C118-C117	C3-C4-C9-C8	177.29	173.12	4.17 OK
C114-C113-C118-C117	C5-C4-C9-C8	0.09	-2.43	2.52 OK
C103-C104-C105-C106	C12-C13-C14-C15	-178.55	-169.21	-9.34 OK
C109-C104-C105-C106	C18-C13-C14-C15	0.21	3.03	-2.82 OK
C103-C104-C109-C108	C12-C13-C18-C17	175.93	171.61	4.32 OK
C105-C104-C109-C108	C14-C13-C18-C17	-2.78	-0.56	-2.22 OK
CU101-N102-C111-C110	CU1-N1-C2-C1	-30.12	-34.21	4.09 OK
CU101-N102-C111-C112	CU1-N1-C2-C3	-156.97	-162.39	5.42 OK
CU101-N101-C102-C101	CU1-N2-C11-C10	12.74	-8.80	21.54 OK
CU101-N101-C102-C103	CU1-N2-C11-C12	-106.77	-137.31	30.54 OK
C111-C112-C113-C114	C2-C3-C4-C5	86.01	102.53	-16.52 OK
C111-C112-C113-C118	C2-C3-C4-C9	-91.10	-72.98	-18.11 OK

C102-C103-C104-C105	C11-C12-C13-C14	144.39	80.94	63.45	OK
C102-C103-C104-C109	C11-C12-C13-C18	-34.31	-91.04	56.73	OK
C110-C111-C112-C113	C1-C2-C3-C4	175.69	-179.21	-5.09	OK
N102-C111-C112-C113	N1-C2-C3-C4	-60.74	-54.82	-5.92	OK
C101-C102-C103-C104	C10-C11-C12-C13	-170.37	167.52	22.11	OK
N101-C102-C103-C104	N2-C11-C12-C13	-50.23	-66.78	16.55	OK
O105-CU101-O101-C101	O1-CU1-O5-C10	170.63	173.22	-2.58	OK
N101-CU101-O101-C101	N2-CU1-O5-C10	2.68	-3.67	6.34	OK
N102-CU101-O101-C101	N1-CU1-O5-C10	174.08	-114.89	-71.03	SKIPPED 177.9
O101-CU101-O105-C110	O5-CU1-O1-C1	173.77	161.27	12.50	OK
N101-CU101-O105-C110	N2-CU1-O1-C1	-107.51	-125.99	18.48	OK
N102-CU101-O105-C110	N1-CU1-O1-C1	-6.10	-12.76	6.65	OK
O101-CU101-N101-C102	O5-CU1-N2-C11	-8.99	7.10	-16.09	OK
O105-CU101-N101-C102	O1-CU1-N2-C11	-88.44	-65.85	-22.59	OK
N102-CU101-N101-C102	N1-CU1-N2-C11	171.33	-178.78	-9.90	OK
O101-CU101-N102-C111	O5-CU1-N1-C2	17.59	-45.65	63.24	SKIPPED 177.9
O105-CU101-N102-C111	O1-CU1-N1-C2	21.04	26.69	-5.65	OK
N101-CU101-N102-C111	N2-CU1-N1-C2	-171.04	-156.32	-14.72	OK
CU101-O105-C110-O106	CU1-O1-C1-O2	172.91	177.23	-4.32	OK
CU101-O105-C110-C111	CU1-O1-C1-C2	-10.80	-5.20	-5.60	OK
CU101-O101-C101-O102	CU1-O5-C10-O6	-177.90	-178.39	0.49	OK
CU101-O101-C101-C102	CU1-O5-C10-C11	4.43	-0.79	5.23	OK
O105-C110-C111-N102	O1-C1-C2-N1	27.89	27.42	0.47	OK
O105-C110-C111-C112	O1-C1-C2-C3	153.60	154.70	-1.10	OK
O106-C110-C111-N102	O2-C1-C2-N1	-155.72	-154.94	-0.78	OK
O106-C110-C111-C112	O2-C1-C2-C3	-30.02	-27.66	-2.36	OK
O101-C101-C102-N101	O5-C10-C11-N2	-11.59	6.51	-18.10	OK
O101-C101-C102-C103	O5-C10-C11-C12	109.41	133.48	-24.07	OK
O102-C101-C102-N101	O6-C10-C11-N2	170.64	-175.78	-13.59	OK
O102-C101-C102-C103	O6-C10-C11-C12	-68.37	-48.81	-19.56	OK

Some of the best & important things are here:

Summary of Deviations

	position	bond	torsion	
rms deviations	0.9251	0.0070	15.1781	
max deviations	2.3912	0.0147	63.4467	maximum positional and torsion angle
	Ugeom(max)	Uprime(max)	U[ij] (old-new)	
Old	0.018	0.086		
New	0.021	0.090		
Individual Delta	0.059	0.028	O103	- 07

Average and difference of centroids (in crystal fractions)

0.44420 0.50309 0.58912 0.05713 0.01809 -0.48432

The centroids of the two molecules differ by (0, 0, ½)

– i.e, along the c axis!

Transformation matrix relating new and old coordinates

In best plane system

In orthogonal system

In crystal system

-0.995494	-0.092763	0.019682	0.213812	0.975893	0.043789	0.273643	0.447839	-0.127021
-0.092876	0.995665	-0.004907	-0.949736	0.218156	-0.224522	-2.066021	0.218156	-0.938110
-0.019142	-0.006712	-0.999794	-0.228662	0.006418	0.973485	-0.250817	0.003236	0.913654

Note that the trace for the orthogonal and crystal system matrices are the same. We examine the crystal system matrix to look for a possible supercell and/or an alternative pseudo-space group.

Trace = 1.405 Determinant = 1.000 Tr+Det = 2.405

see Giacovazzo, Sect 1.D

Element: 1 2 3 4 6 -1 -2 -3 -4 -6

Tr_det: 4 0 1 2 3 -4 0 -1 -2 -3

Looking at this little table is very enlightening! We are closest to a 4 axis, and the molecular translation, as noted above, is (0, 0, .5)...looks like a pseudo 4₂ axis!

New atom coordinates in crystal fractions

O	4.	0.0578	0.6288	1.1060
O	8.	0.6030	0.2904	1.2908
C	7.	0.1201	0.6484	1.0048
C	16.	0.5689	0.2902	1.1518
O	3.	0.3407	0.6651	1.1773
O	7.	0.3882	0.3736	1.1542
C	6.	0.2662	0.6651	1.0443
C	15.	0.4587	0.3327	1.0851
C	8.	0.0452	0.6512	0.8689
C	17.	0.6398	0.2521	1.0760
C	5.	0.3379	0.6817	0.9459
C	14.	0.4221	0.3362	0.9451
C	9.	0.1173	0.6690	0.7718
C	18.	0.6063	0.2575	0.9352
C	4.	0.2640	0.6831	0.8089
C	13.	0.4972	0.2999	0.8673
N	1.	0.4344	0.5773	0.7306
N	2.	0.5085	0.4358	0.7487
C	3.	0.3445	0.6948	0.7011
C	12.	0.4728	0.3136	0.7173
C	2.	0.3639	0.6290	0.6331
C	11.	0.5613	0.3743	0.6976
CU	1.	0.5037	0.5093	0.6221

O	1.	0.5106	0.5814	0.4997
O	5.	0.5507	0.4439	0.5026
O	6.	0.6069	0.3379	0.4891
O	2.	0.4439	0.6860	0.4576
C	1.	0.4461	0.6338	0.5227
C	10.	0.5727	0.3851	0.5517

Comparison of group number 1 completed

Next we go to the Omni Calculator on the web, and plug in the 3 x 3 pseudosymmetry matrix to get the eigenvector and eigenvalues. The link is in the paper, here also: <https://www.omnicalculator.com/math/eigenvalue-eigenvector>

First row	
a_1	0.274
a_2	0.448
a_3	-0.127

Second row	
b_1	-2.066
b_2	0.218
b_3	-0.938

Third row	
c_1	-.251
c_2	0.003
c_3	.914

Result

Your eigenvalues are:

$$\lambda_1 = 1, \lambda_2 = 0.2+0.98i, \lambda_3 = 0.2-0.98i.$$

The real eigenvectors are:

$$v_1 = (-0.35, -0.28, 1).$$

The complex eigenvectors are:

$$v_2 = (2.73-3.62i, 7.76+6.56i, 1), v_3 = (2.73+3.62i, 7.76-6.56i, 1).$$

Hmm...looks like it's close to a -1 -1 3 reciprocal direction [closest integer to (-0.35, -0.28, 1)] – we can test how close we got with that guess by downloading CTOOL at <http://people.brandeis.edu/~foxman1/ctool.exe> and looking at the difference in direction.

To use CTOOL, we only need the cell constants for our crystal, and the directions, real and/or reciprocal, that we'd like to get some angle information on:

DIRECT CELL CONSTANTS: 9.5939 20.1903 10.1806 90.0000 104.6630 90.0000

CALCULATION OF ANGLE BETWEEN A R.L. VECTOR OR DIRECT SPACE PLANE

AND A DIRECT SPACE DIRECTION

THIS IS ALSO EQUIVALENT TO AN OBLIQUITY CALCULATION

h1	k1	l1	[h2	k2	l2]	ANGLE	(obliquity)
-1.00	-1.00	3.00	0.00	0.00	1.00	11.179	

So, the angle between -1 -1 3 and the c-axis, i.e., [1 0 0] is 11.18 degrees. The pseudosymmetry is in fact disrupted by rotations about the CH₂-C(ips0) bonds, as explained, and discovered, by running MATCH with fewer atoms! (refer to the accompanying paper). This comes from an “rd” calculation in CTOOL (reciprocal direction to direct direction).

CALCULATION OF ANGLE BETWEEN TWO R.L. VECTORS OR TWO DIRECT SPACE PLANES

h1	k1	l1	h2	k2	l2	ANGLE
-1.00	-1.00	3.00	-0.35	-0.28	1.00	1.826

And, we can check how good our guess about -1 -1 3 was...not bad, a tad below 2 degrees! This comes from an “rr” calculation in CTOOL (reciprocal direction to reciprocal direction).

Now, we'd like to see a picture of the overlap! We right-click on atom Cu(1), for example, and the popup has a variety of options....we want "Map fragment containing Cu(1) onto another", and when we go to that we get three more options at the left...select "Compare geometries" and click.

The screenshot displays the Crystals software interface. The main window shows a 3D ball-and-stick model of a molecular structure. A context menu is open over atom Cu(1), listing various actions. The 'Map fragment containing Cu(1) onto another' option is highlighted, and a sub-menu is visible on the left with 'Compare geometries' selected. The background features a terminal window with the following text:

```
The R-factor is 3.410 %, the ratio Fo/Fc is 0.9994
* Deciding on the best course of action...
Very low R factor - Begin to tidy up
Recommended: Locate or place all hydrogen atoms.
Other options: Refine positions and Uanisot.
View the structure.
```

Id	Type	Se...	x	y	z	occ
1	CU	1	0.513	0.503	0.114	1.000
2	CU	101	0.498	0.502	0.609	1.000
3	O	1	0.662	0.530	0.028	1.000
4	O	2	0.868	0.585	0.067	1.000
5	O	3	0.037	0.544	0.086	1.000
6	O	4	0.037	0.544	0.086	1.000
7	O	5	0.037	0.544	0.086	1.000

At the bottom of the terminal window, a table of refinement statistics is shown:

Refinement	Cell/Sym	Weights	Constrain	Restrain	Files	Crystal	Reflns	Twin
Results of last cycle:								
R	3.41 %		Parameters	622.		Flack	-0.006	
Rw	6.81 %		Reflections	11278.		Extinction	0.	
Goof	0.995		max Δ/σ	0.0008				
$\chi^2 =$	$\sum [F_o^2 - F_c^2]^2$		$F^2/\sigma(F^2) >$	none				

Then we select, in the new popup on the left, “Show molecules overlaid in Cameron” CAMERON is the CRYSTALS graphic engine.

The screenshot shows the Crystals software interface. The main window displays a 3D ball-and-stick model of a molecule with a copper atom (CU(101)) highlighted. The interface includes a menu bar (File, Data, Solve, Structure, Fourier, Refinement, Analyse, Results, Graphics, Appearance, Tools, Help) and a toolbar. A dialog box titled "Map ... Onto..." is open, showing a list of atoms and checkboxes for "Show molecules overlaid in Cameron" and "Allow Inversion".

The "Map ... Onto..." dialog box contains the following content:

Map ... Onto...

Show molecules overlaid in Cameron

Allow Inversion

Click an atom in the residue to compare with the first.

Cancel

The list currently contains:

CU 1	CU 101	O 4	O 5
O 6	O 7	O 101	O 102
O 103	O 104	O 108	N 1
N 2	N 101	C 3	C 4
C 5	C 6	C 10	C 11
C 12	C 13	C 17	C 18
C 101	C 102	C 106	C 107
C 108	C 109	C 113	C 114
C 115	C 116		

The list currently contains:

CU 1	CU 101	O 4	O 5
O 6	O 7	O 101	O 102
O 103	O 104	O 105	O 106
N 2	N 101	N 102	C 1
C 5	C 6	C 7	C 8
C 12	C 13	C 14	C 15
C 101	C 102	C 103	C 104
C 108	C 109	C 110	C 111
C 115	C 116	C 117	C 118
		C 107	C 108
		C 9	C 10
		C 16	C 17
		C 105	C 106
		C 112	C 113

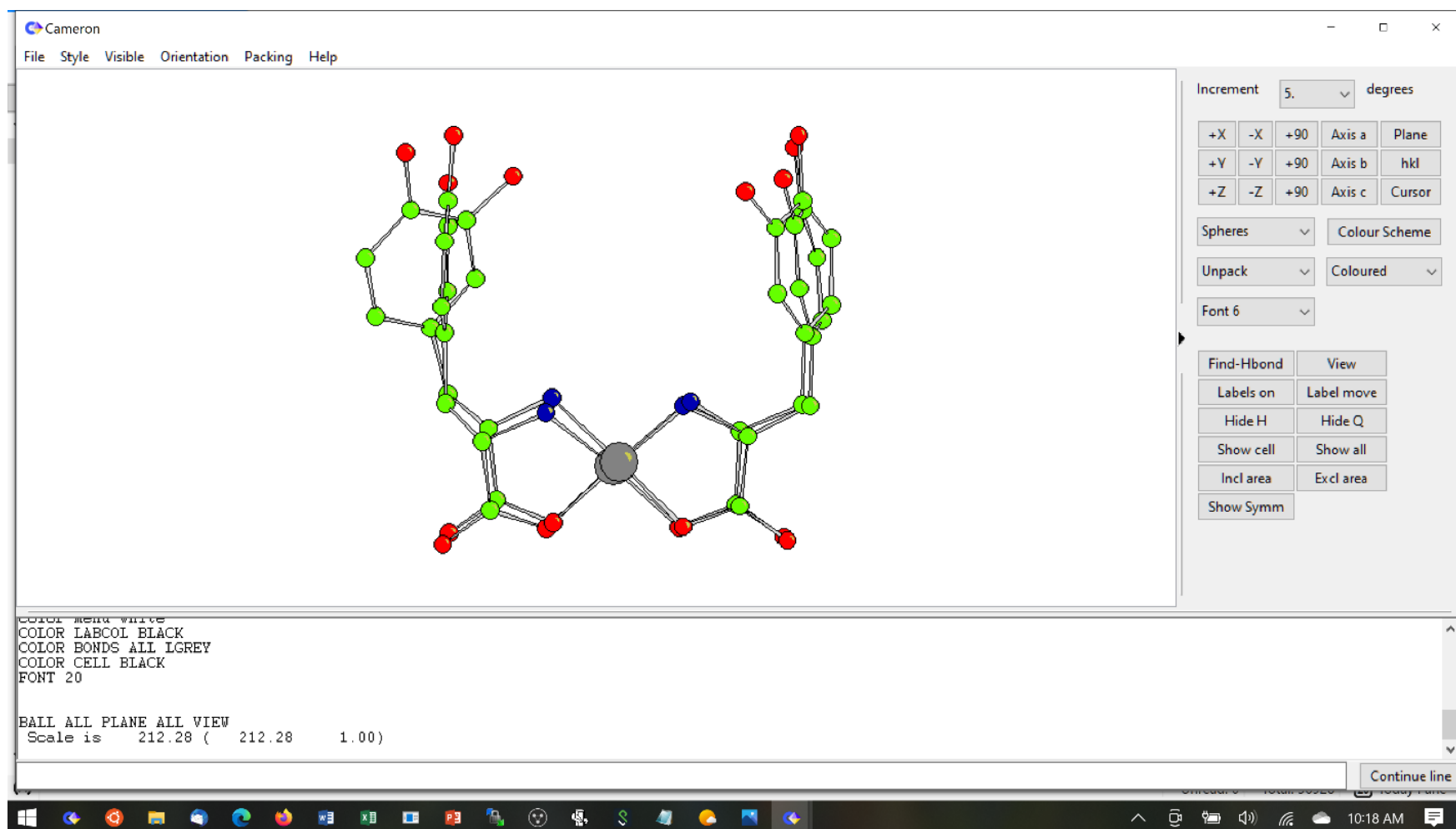
Results of last cycle:

R	3.41 %	Parameters	622.	Flack	-0.006
Rw	6.81 %	Reflections	11278.	Extinction	0.
Goof	0.995	max Δ/σ	0.0008		
χ² =	Σ[Fo² - Fc²]²	F²/σ(F²) >	none		

Refinement Cell/Sym Weights Constrain Restrain Files Crystal Reflns Twin

Id	Type	Se...	x	y	z	occ	Type	Ueq	Spare	Res...	Asse...	Gr...	F...
1	CU	1	0.513	0.503	0.114	1.000	Aniso	0.014	29.306	1	0	0	
2	CU	101	0.498	0.502	0.609	1.000	Aniso	0.014	29.306	2	0	0	
3	O	1	0.662	0.530	0.028	1.000	Aniso	0.019	8.010	1	0	0	
4	O	2	0.868	0.585	0.067	1.000	Aniso	0.018	8.010	1	0	0	
5	O	3	0.837	0.541	0.806	1.000	Aniso	0.020	8.010	1	0	0	
6	O	4	0.700	0.657	0.828	1.000	Aniso	0.018	8.010	1	0	0	
7	O	5	0.378	0.483	-0.056	1.000	Aniso	0.016	8.010	1	0	0	

And here is the result!!! We can get atom identities by click on those we are interested in, or, alternatively, in the lower instruction window, type label and then click on the desired atom(s), hit return, then type view, return, or hit the view button on the right.



The screenshot displays the Cameron software interface. The main window shows a ball-and-stick model of a complex organic molecule with a central grey atom, green and red atoms, and blue atoms. The interface includes a menu bar (File, Style, Visible, Orientation, Packing, Help) and a control panel on the right with various buttons and dropdown menus. At the bottom, a command window shows the following text:

```
COLOR MENU WHITE  
COLOR LABCOL BLACK  
COLOR BONDS ALL LGREY  
COLOR CELL BLACK  
FONT 20  
  
BALL ALL PLANE ALL VIEW  
Scale is 212.28 ( 212.28 1.00)
```

The control panel on the right includes the following elements:

- Increment: 5. degrees
- Buttons: +X, -X, +90, Axis a, Plane; +Y, -Y, +90, Axis b, hkl; +Z, -Z, +90, Axis c, Cursor
- Dropdowns: Spheres, Unpack, Font 6
- Buttons: Colour Scheme, Coloured
- Buttons: Find-Hbond, View
- Buttons: Labels on, Label move
- Buttons: Hide H, Hide Q
- Buttons: Show cell, Show all
- Buttons: Incl area, Excl area
- Button: Show Symm

The Windows taskbar at the bottom shows the time as 10:18 AM.