



BIOLOGICAL  
CRYSTALLOGRAPHY

Volume 71 (2015)

**Supporting information for article:**

**ANS complex of St John's wort PR-10 protein with 28 copies in the asymmetric unit: a fiendish combination of pseudosymmetry with tetartohedral twinning**

**Joanna Sliwiak, Zbigniew Dauter, Marcin Kowiel, Airlie J. McCoy, Randy J. Read and Mariusz Jaskolski**

**Table S1** Scale and *R* factors in seven L=mod(*l*,7) groups, calculated in different resolution ranges (in Å) for FC\_ALL\_LS structure factors from REFMAC output.

## scales on FP\*FP/FC\_ALL\_LS\*FC\_ALL\_LS

Resolution	5.250	4.170	3.640	3.310	3.070	2.890	2.740	2.620	2.520	2.430	All
0	0.951	0.996	1.026	1.069	1.009	0.906	0.840	0.800	0.790	0.784	0.978
1	0.983	0.933	1.000	1.020	1.015	0.835	0.810	0.782	0.765	0.796	0.953
2	0.630	1.078	1.246	1.373	1.361	1.117	1.032	0.975	0.965	0.885	1.095
3	1.139	0.974	1.052	1.092	1.069	0.925	0.878	0.846	0.820	0.804	1.035
4	1.062	0.944	1.050	1.029	1.003	0.914	0.825	0.792	0.800	0.789	0.993
5	0.553	1.079	1.292	1.306	1.278	1.051	0.949	0.892	0.882	0.869	1.079
6	0.999	1.054	1.095	1.124	1.106	0.943	0.870	0.876	0.844	0.846	1.045
All	0.996	0.977	1.054	1.077	1.049	0.922	0.856	0.824	0.815	0.809	1.061

## scales on FP/FC\_ALL\_LS

Resolution	5.250	4.170	3.640	3.310	3.070	2.890	2.740	2.620	2.520	2.430	All
0	1.000	1.001	1.005	1.018	1.003	0.949	0.908	0.894	0.897	0.904	0.985
1	0.969	0.969	1.000	1.019	1.024	0.921	0.907	0.904	0.902	0.918	0.968
2	0.785	1.054	1.141	1.208	1.244	1.086	1.059	1.046	1.054	0.984	1.066
3	1.065	0.988	1.029	1.042	1.043	0.961	0.938	0.931	0.915	0.919	1.007
4	1.020	0.978	1.020	1.008	0.999	0.943	0.904	0.891	0.891	0.905	0.982
5	0.739	1.052	1.166	1.179	1.188	1.052	1.011	1.001	1.001	0.970	1.046

6	0.976	1.029	1.064	1.080	1.093	0.989	0.956	0.971	0.963	0.953	1.022
All	0.987	0.998	1.038	1.052	1.054	0.970	0.940	0.933	0.932	0.930	1.024

## R factor on FP/FC\_ALL\_LS

Resolution	5.250	4.170	3.640	3.310	3.070	2.890	2.740	2.620	2.520	2.430	All
------------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----

0	0.2733	0.1770	0.1954	0.2162	0.2362	0.2137	0.2131	0.1913	0.1741	0.0740	0.2194
1	0.3318	0.2293	0.2406	0.2542	0.2727	0.2145	0.2130	0.2015	0.1799	0.0815	0.2445
2	0.4529	0.3105	0.3064	0.3170	0.3538	0.2295	0.2226	0.2230	0.2270	0.1053	0.3120
3	0.2145	0.1781	0.1927	0.2092	0.2386	0.2015	0.1957	0.1898	0.1763	0.0798	0.2018
4	0.2148	0.1639	0.1740	0.1973	0.2371	0.2070	0.1993	0.1824	0.1752	0.0778	0.1932
5	0.4810	0.3091	0.3075	0.3226	0.3430	0.2311	0.2146	0.2171	0.2055	0.1013	0.3102
6	0.3343	0.2269	0.2522	0.2592	0.2975	0.2243	0.2223	0.2056	0.1895	0.0918	0.2509
All	0.2869	0.2014	0.2174	0.2376	0.2691	0.2167	0.2118	0.2002	0.1881	0.0871	0.2304

**Table S2** Tables of CC<sub>1/2</sub>, CC\*, CC<sub>work</sub> and CC<sub>free</sub> (on intensities) calculated in seven L=mod(*l*,7) groups and different resolution (Å) ranges.CC<sub>1/2</sub>

Resolution	5.250	4.170	3.640	3.310	3.070	2.890	2.740	2.620	2.520	2.430	All
0	0.9944	0.9980	0.9982	0.9968	0.9956	0.9938	0.9839	0.9696	0.9428	0.8673	0.9967
1	0.9988	0.9983	0.9966	0.9921	0.9895	0.9760	0.9452	0.8904	0.8423	0.6747	0.9967
2	0.9967	0.9954	0.9902	0.9857	0.9701	0.9426	0.8896	0.7834	0.6627	0.4506	0.9862
3	0.9991	0.9972	0.9978	0.9970	0.9958	0.9926	0.9838	0.9669	0.9539	0.8195	0.9984
4	0.9988	0.9985	0.9980	0.9968	0.9955	0.9943	0.9872	0.9774	0.9431	0.8781	0.9987
5	0.9890	0.9901	0.9903	0.9841	0.9744	0.9443	0.8732	0.7275	0.6567	0.4017	0.9845
6	0.9975	0.9957	0.9972	0.9936	0.9857	0.9777	0.9370	0.8737	0.7679	0.6463	0.9959
All	0.9965	0.9985	0.9983	0.9971	0.9955	0.9918	0.9786	0.9558	0.9166	0.7907	0.9994

## CC\*

Resolution	5.250	4.170	3.640	3.310	3.070	2.890	2.740	2.620	2.520	2.430	All
0	0.9986	0.9995	0.9995	0.9992	0.9989	0.9984	0.9959	0.9923	0.9852	0.9638	0.9992
1	0.9997	0.9996	0.9991	0.9980	0.9974	0.9939	0.9858	0.9706	0.9563	0.8977	0.9992
2	0.9992	0.9989	0.9975	0.9964	0.9924	0.9851	0.9704	0.9373	0.8928	0.7882	0.9965
3	0.9998	0.9993	0.9994	0.9993	0.9990	0.9981	0.9959	0.9915	0.9881	0.9491	0.9996
4	0.9997	0.9996	0.9995	0.9992	0.9989	0.9986	0.9968	0.9943	0.9852	0.9670	0.9997
5	0.9972	0.9975	0.9976	0.9960	0.9935	0.9856	0.9656	0.9177	0.8904	0.7571	0.9961
6	0.9994	0.9989	0.9993	0.9984	0.9964	0.9943	0.9836	0.9657	0.9320	0.8861	0.9990
All	0.9991	0.9996	0.9996	0.9993	0.9989	0.9979	0.9946	0.9886	0.9780	0.9397	0.9998

## FP/FC\_ALL\_LS on Intensities

## CCwork

Resolution	5.250	4.170	3.640	3.310	3.070	2.890	2.740	2.620	2.520	2.430	All
0	0.611	0.895	0.907	0.916	0.880	0.862	0.857	0.896	0.906	0.987	0.814
1	0.792	0.899	0.880	0.862	0.832	0.830	0.828	0.867	0.906	0.985	0.896
2	0.649	0.807	0.830	0.811	0.764	0.854	0.856	0.873	0.876	0.976	0.822
3	0.885	0.929	0.922	0.917	0.879	0.866	0.876	0.894	0.916	0.985	0.934
4	0.900	0.899	0.938	0.920	0.875	0.873	0.872	0.918	0.930	0.991	0.933
5	0.481	0.817	0.829	0.791	0.772	0.844	0.826	0.862	0.891	0.974	0.821
6	0.829	0.895	0.879	0.871	0.806	0.855	0.833	0.867	0.905	0.980	0.905
All	0.774	0.925	0.938	0.927	0.893	0.885	0.879	0.912	0.921	0.988	0.875

## CCfree

Resolution	5.250	4.170	3.640	3.310	3.070	2.890	2.740	2.620	2.520	2.430	All
0	-	0.749	-	-	-	-	-	-	0.779	-	0.819
1	-	0.779	-	-	-	-	-	-	0.733	-	0.853
2	-	0.693	-	-	-	-	-	-	0.694	-	0.783
3	-	0.889	-	-	-	-	-	-	0.704	-	0.926
4	-	0.888	-	-	-	-	-	-	0.782	-	0.934
5	-	0.674	-	-	-	-	-	-	0.733	-	0.761
6	-	0.695	-	-	-	-	-	-	0.800	-	0.794
All	-	0.857	-	-	-	-	-	-	0.794	-	0.884