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**Supporting information for article:**

**Crystal structure and pseudosymmetry analysis of the triclinic prodrug cloxazolam ( $Z = 4$ )**

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### **Supplementary Material Table Sm1**

**HalfSum and differences for I (MP run on the ( $a\ddagger$ ,  $b\ddagger$ ,  $c\ddagger$ ) reference frame).**

AB		Coordinates HalfSum			Coordinates Difference	
AB01	0.25300	-0.18299	0.00000	0.34240	-0.37373	0.18416
AB02	0.25326	-0.10108	-0.00467	-0.26209	-0.37698	0.11573
AB03	0.25021	0.05724	-0.00604	-0.05882	-0.37288	0.42268
AB04	0.24708	0.23903	-0.00879	-0.08560	-0.37870	0.18823
AB05	0.24995	0.05668	-0.00577	-0.22943	-0.37741	0.25066
AB06	0.24848	0.14152	-0.00901	0.09445	-0.37603	0.20650
AB07	0.25060	0.01164	-0.00542	-0.10578	-0.37497	0.31400
AB08	0.25148	-0.06560	-0.00476	-0.18091	-0.37527	0.35850
AB09	0.25107	-0.08688	-0.00465	-0.17357	-0.37376	0.48414
AB10	0.25274	-0.15691	-0.00441	-0.23766	-0.37494	0.52622
AB11	0.25438	-0.20653	-0.00444	-0.31388	-0.37751	0.44429
AB12	0.25444	-0.18649	-0.00437	-0.32492	-0.37863	0.31940
AB13	0.25291	-0.11770	-0.00471	-0.25629	-0.37732	0.27731
AB14	0.25028	0.11213	-0.00694	-0.18317	-0.37196	0.45163
AB15	0.24985	0.09628	-0.00618	-0.31183	-0.37579	0.35390
AB16	0.24843	0.10784	-0.00721	-0.17763	-0.38019	0.14893
AB17	0.24784	0.16856	-0.00874	-0.05382	-0.37800	0.18239
AB18	0.24935	0.06285	-0.00767	0.14548	-0.37558	0.20485
AB19	0.25057	-0.00082	-0.00541	0.05062	-0.37515	0.24307
AB20	0.25168	-0.07603	-0.00344	0.11481	-0.37487	0.23334
AB21	0.25168	-0.08728	-0.00353	0.26981	-0.37430	0.19287
AB22	0.25025	-0.02428	-0.00634	0.36562	-0.37418	0.16430
AB23	0.24908	0.05023	-0.00845	0.30358	-0.37488	0.16870
Mean:	0.25081	-0.00820	-0.00569	-0.05516	-0.37578	0.27982
Esd:	0.00196	0.12088	0.00206	0.21763	0.00198	0.11676

AC		Coordinates HalfSum			Coordinates Difference	
AC01	0.31271	0.06109	0.07115	0.22299	-0.86191	0.04185
AC02	0.31597	0.06341	0.04825	-0.38750	-0.70596	0.00990
AC03	0.30929	0.06455	0.19902	-0.17698	-0.38751	0.01256
AC04	0.30946	0.06182	0.08877	-0.21035	-0.02428	-0.00689
AC05	0.30977	0.06473	0.11387	-0.34907	-0.39351	0.01138
AC06	0.30888	0.06155	0.09329	-0.02634	-0.21610	0.00190
AC07	0.30888	0.06455	0.14491	-0.22233	-0.48079	0.01334
AC08	0.30826	0.06476	0.16797	-0.29446	-0.63600	0.01304
AC09	0.30498	0.06566	0.23055	-0.28137	-0.67883	0.01374

AC10	0.30806	0.06355	0.25336	-0.34831	-0.81586	0.01068
AC11	0.31447	0.06006	0.21404	-0.43407	-0.91069	0.00732
AC12	0.31646	0.06010	0.15172	-0.44896	-0.87181	0.00723
AC13	0.31320	0.06262	0.12887	-0.37688	-0.73796	0.01017
AC14	0.31243	0.07008	0.21542	-0.30747	-0.28785	0.00691
AC15	0.31156	0.06902	0.16616	-0.43524	-0.32127	0.00921
AC16	0.30917	0.06029	0.06480	-0.29909	-0.28508	0.00492
AC17	0.30937	0.06136	0.08331	-0.17687	-0.16360	-0.00172
AC18	0.30929	0.06162	0.08971	0.02560	-0.37312	0.01008
AC19	0.30955	0.06258	0.10849	-0.06735	-0.50193	0.01525
AC20	0.31097	0.06239	0.10075	-0.00376	-0.65170	0.02495
AC21	0.31209	0.06134	0.07812	0.14899	-0.67155	0.02956
AC22	0.31150	0.06087	0.06355	0.24313	-0.54449	0.02452
AC23	0.31020	0.06064	0.06845	0.18134	-0.39569	0.01490
Mean:	0.31072	0.06298	0.12802	-0.17497	-0.51815	0.01238
Esd:	0.00261	0.00259	0.05954	0.21736	0.24034	0.01008

AD	Coordinates HalfSum			Coordinates Difference		
AD01	0.35565	0.25094	0.01020	0.13710	-1.24160	0.16376
AD02	0.05195	0.25243	-0.00595	0.14055	-1.08400	0.11830
AD03	0.15834	0.24973	-0.00129	0.12492	-0.75786	0.41318
AD04	0.14197	0.24906	-0.00801	0.12462	-0.39877	0.18666
AD05	0.07160	0.25133	-0.00248	0.12728	-0.76673	0.24408
AD06	0.23284	0.25001	-0.00510	0.12574	-0.59303	0.19868
AD07	0.13474	0.25101	-0.00200	0.12594	-0.85370	0.30716
AD08	0.09853	0.25028	-0.00369	0.12500	-1.00703	0.35636
AD09	0.10543	0.24978	-0.00365	0.11773	-1.04709	0.48213
AD10	0.07260	0.24734	-0.00601	0.12263	-1.18344	0.52942
AD11	0.02985	0.24515	-0.00869	0.13518	-1.28087	0.45279
AD12	0.02163	0.24667	-0.00849	0.14071	-1.24493	0.32765
AD13	0.05733	0.24931	-0.00610	0.13487	-1.11135	0.28010
AD14	0.09417	0.25354	-0.00347	0.12905	-0.65478	0.44469
AD15	0.02938	0.25387	-0.00331	0.12912	-0.69097	0.34816
AD16	0.09644	0.24803	-0.00475	0.12636	-0.66056	0.14402
AD17	0.15811	0.24898	-0.00658	0.12564	-0.53884	0.17806
AD18	0.25824	0.25029	-0.00167	0.12771	-0.75046	0.19284
AD19	0.21161	0.25060	-0.00054	0.12855	-0.87799	0.23332
AD20	0.24310	0.25071	0.00302	0.13198	-1.02833	0.22043
AD21	0.31915	0.25068	0.00582	0.13486	-1.05023	0.17416
AD22	0.36611	0.25081	0.00510	0.13390	-0.92436	0.14142
AD23	0.33560	0.25021	0.00140	0.13053	-0.77485	0.14900
Mean:	0.15845	0.25003	-0.00245	0.12956	-0.89225	0.27332
Esd:	0.10801	0.00195	0.00473	0.00565	0.24016	0.12092

<b>BC</b>	<b>Coordinates HalfSum</b>			<b>Coordinates Difference</b>		
BC01	0.14151	0.24796	-0.02092	-0.11941	-0.48818	-0.14231
BC02	0.44702	0.25190	-0.00962	-0.12541	-0.32898	-0.10583
BC03	0.33870	0.25099	-0.01232	-0.11816	-0.01463	-0.41012
BC04	0.35225	0.25117	-0.00535	-0.12475	0.35442	-0.19512
BC05	0.42449	0.25343	-0.01146	-0.11964	-0.01610	-0.23928
BC06	0.26166	0.24957	-0.00996	-0.12079	0.15993	-0.20460
BC07	0.36177	0.25204	-0.01209	-0.11655	-0.10582	-0.30066
BC08	0.39871	0.25240	-0.01128	-0.11355	-0.26073	-0.34546
BC09	0.39176	0.25254	-0.01152	-0.10780	-0.30507	-0.47040
BC10	0.42689	0.25102	-0.00975	-0.11065	-0.44092	-0.51554
BC11	0.47141	0.24881	-0.00810	-0.12019	-0.53318	-0.43697
BC12	0.47892	0.24942	-0.00798	-0.12404	-0.49318	-0.31217
BC13	0.44135	0.25128	-0.00979	-0.12059	-0.36064	-0.26714
BC14	0.40401	0.25605	-0.01039	-0.12430	0.08411	-0.44472
BC15	0.46747	0.25691	-0.01078	-0.12341	0.05452	-0.34469
BC16	0.39798	0.25038	-0.00967	-0.12146	0.09511	-0.14401
BC17	0.33627	0.25036	-0.00789	-0.12305	0.21440	-0.18411
BC18	0.23655	0.24941	-0.01272	-0.11988	0.00246	-0.19477
BC19	0.28425	0.25015	-0.01304	-0.11797	-0.12678	-0.22782
BC20	0.25357	0.24983	-0.01591	-0.11857	-0.27683	-0.20839
BC21	0.17718	0.24849	-0.01831	-0.12082	-0.29725	-0.16331
BC22	0.12868	0.24796	-0.01860	-0.12249	-0.17031	-0.13978
BC23	0.15841	0.24808	-0.01590	-0.12224	-0.02081	-0.15380
Mean:	0.33830	0.25088	-0.01189	-0.11981	-0.14237	-0.26743
Esd:	0.10922	0.00229	0.00372	0.00428	0.24064	0.11846

<b>BD</b>	<b>Coordinates HalfSum</b>			<b>Coordinates Difference</b>		
BD01	0.18445	0.43780	-0.08188	-0.20530	-0.86787	-0.02040
BD02	0.18299	0.44092	-0.06381	0.40264	-0.70702	0.00257
BD03	0.18775	0.43617	-0.21263	0.18374	-0.38498	-0.00950
BD04	0.18477	0.43841	-0.10213	0.21022	-0.02007	-0.00157
BD05	0.18632	0.44004	-0.12781	0.35671	-0.38932	-0.00658
BD06	0.18562	0.43803	-0.10835	0.03129	-0.21700	-0.00782
BD07	0.18763	0.43850	-0.15900	0.23172	-0.47873	-0.00684
BD08	0.18898	0.43791	-0.18294	0.30591	-0.63176	-0.00214
BD09	0.19221	0.43666	-0.24571	0.29130	-0.67333	-0.00201
BD10	0.19142	0.43481	-0.26912	0.36029	-0.80850	0.00320
BD11	0.18679	0.43390	-0.23084	0.44906	-0.90336	0.00850
BD12	0.18409	0.43598	-0.16819	0.46563	-0.86630	0.00825
BD13	0.18547	0.43797	-0.14476	0.39116	-0.73403	0.00279
BD14	0.18575	0.43952	-0.22928	0.31222	-0.28282	-0.00694
BD15	0.18530	0.44176	-0.18026	0.44095	-0.31518	-0.00574
BD16	0.18525	0.43813	-0.07922	0.30399	-0.28037	-0.00491
BD17	0.18502	0.43798	-0.09777	0.17946	-0.16084	-0.00433

BD18	0.18549	0.43808	-0.10409	-0.01777	-0.37488	-0.01201
BD19	0.18630	0.43818	-0.12207	0.07793	-0.50284	-0.00975
BD20	0.18569	0.43814	-0.11366	0.01717	-0.65346	-0.01291
BD21	0.18425	0.43783	-0.09062	-0.13495	-0.67593	-0.01871
BD22	0.18330	0.43790	-0.07705	-0.23172	-0.55018	-0.02288
BD23	0.18382	0.43766	-0.08295	-0.17305	-0.39997	-0.01970
Mean:	0.18603	0.43793	-0.14235	0.18472	-0.51647	-0.00650
Esd:	0.00227	0.00169	0.06010	0.21711	0.24045	0.00848

CD	Coordinates HalfSum			Coordinates Difference		
CD01	0.24415	0.68190	-0.01073	-0.08589	-0.37969	0.12191
CD02	0.24570	0.60541	-0.01090	0.52805	-0.37804	0.10840
CD03	0.24683	0.44349	-0.00757	0.30190	-0.37035	0.40062
CD04	0.24714	0.26120	-0.00457	0.33497	-0.37449	0.19355
CD05	0.24613	0.44809	-0.00817	0.47635	-0.37322	0.23270
CD06	0.24601	0.35807	-0.00605	0.15208	-0.37693	0.19678
CD07	0.24591	0.49141	-0.00867	0.34827	-0.37291	0.29382
CD08	0.24576	0.56827	-0.01021	0.41946	-0.37103	0.34332
CD09	0.24611	0.58920	-0.01051	0.39910	-0.36826	0.46839
CD10	0.24675	0.65527	-0.01135	0.47094	-0.36758	0.51874
CD11	0.24689	0.70049	-0.01235	0.56925	-0.37018	0.44547
CD12	0.24610	0.68257	-0.01211	0.58967	-0.37312	0.32042
CD13	0.24577	0.61830	-0.01118	0.51175	-0.37339	0.26993
CD14	0.24790	0.39746	-0.00692	0.43652	-0.36693	0.43778
CD15	0.24700	0.41450	-0.00791	0.56436	-0.36970	0.33895
CD16	0.24599	0.39057	-0.00721	0.42545	-0.37548	0.13910
CD17	0.24655	0.33078	-0.00572	0.30251	-0.37524	0.17978
CD18	0.24543	0.43685	-0.00671	0.10211	-0.37734	0.18276
CD19	0.24528	0.50157	-0.00817	0.19590	-0.37606	0.21807
CD20	0.24498	0.57656	-0.00946	0.13574	-0.37663	0.19548
CD21	0.24466	0.58646	-0.00896	-0.01413	-0.37868	0.14460
CD22	0.24455	0.52305	-0.00716	-0.10923	-0.37987	0.11690
CD23	0.24494	0.44806	-0.00605	-0.05081	-0.37916	0.13410
Mean:	0.24594	0.50911	-0.00864	0.30454	-0.37410	0.26094
Esd:	0.00090	0.11954	0.00216	0.21689	0.00389	0.12300

<b>AB Pseudo Operation</b>	0.50162-X, -0.37578+Y, -0.01138-Z
<b>CD Pseudo Operation</b>	0.50162-X, -0.37578+Y, -0.01138-Z

<b>AC Pseudo Operation</b>	0.62144-X, 0.12596-Y, Z
<b>BD Pseudo Operation</b>	0.37206-X, 0.87586-Y, Z

<b>AD Pseudo Operation</b>	0.12956+X, 0.50006-Y, -0.00490-Z
<b>BC Pseudo Operation</b>	-0.11981+X, 0.50176-Y, -0.02378-Z

Supplementary Material Fig.SM2: symmetry schemes for S.G.'s #55 to #60

