

PLATON(V-311206)-Run for: char232 in C2/c

TIME: May 6 15:20:40 2009

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Crystal Data

Input Cell (Lattice Type: C)		Temp = 200K	Reduced Cell (Acta Cryst.(1976), A32, 297-298)	
a = 35.876(10) Angstrom	alpha = 90 Degree		a = 13.816	alpha = 96.26 V = 4352.5
b = 13.816(4)	beta = 96.715(5)		b = 17.684	beta = 111.06
c = 17.684(4)	gamma = 90		c = 19.222	gamma = 90.00
V = 8705(4) Cubic-Angstrom	d(100) = 35.6298 Angstrom		Niggli Values	
	d(010) = 13.8156		190.872	312.738 369.488
Lambda(MoKa) = 0.71073 Angstrom	d(001) = 17.5631		-37.093	-95.436 0.000

Orthogonalization Matrices

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

(X0) (35.87600 0 -2.06780) (X)	, (X) (0.02787 0 0.00328) (X0)	Orthogonal Axes A0, B0 and C0
(Y0) = (0 13.81600 0)*(Y)	, (Y) = (0 0.07238 0)*(Y0)	are defined as:
(Z0) (0 0 17.56269) (Z)	, (Z) (0 0 0.05694) (Z0)	A0 // A, C0 // C*, B0 // C0 X A0

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group C2/c No: 15, Laue: 2/m [Hall: -C 2yc]

Lattice Type mC, Centric, Monoclinic, Order 8(2) [Schoenflies: C2h^6]

Nr ***** Symmetry Operation(s) *****

1	X ,	Y ,	Z
2	- X ,	Y ,	1/2 - Z
3	- X ,	- Y ,	- Z
4	X ,	- Y ,	1/2 + Z
5	1/2 + X ,	1/2 + Y ,	Z
6	1/2 - X ,	1/2 + Y ,	1/2 - Z
7	1/2 - X ,	1/2 - Y ,	- Z
8	1/2 + X ,	1/2 - Y ,	1/2 + Z

(Not-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

Site = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
 ***** Move = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
 SYMBOLS: Type = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
 ***** El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
 ARU = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
 RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
 FLAGS : d = determined, c = calculated, R = riding G = group

Atom Types :	C	H	Cl	Co	N	O
Cov.Rad(Ang):	0.68	0.35	0.99	1.23	0.68	0.68
Atom Volume :	13.87	5.08	25.80	29.40	11.80	11.39
Atom Number :	6	1	17	27	7	8
Atom Weight :	12.010	1.008	35.45	58.93	14.01	16.00
Scat.Fact.f0:	5.999	1.000	17.001	26.989	6.995	7.999
Scat.Fact.f':	0.003	0.000	0.148	0.349	0.006	0.011
Scat.Fact.f":	0.002	0.000	0.159	0.972	0.003	0.006
Mu/Rho(MoKa):	0.58	0.37	11.52	40.98	0.84	1.22
Elem. Type :	--	--	HL	TR	--	--

Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
 - Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
 - Atomic Wt. : SHELXL97
 - Scat. Fact.: SHELXL97 (International Tables)
 - mu/rho : International Tables C, table 4.2.4.2, p193-199

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (X0,Y0,Z0)			Site	SSN*SSOF =	S.O.F	Move	Type
-	Co	0.11165	0.73236	0.12201	3.7533	10.1183	2.1429	1	1	1	-	Met
-	O(1)	0.15845	0.75061	0.06969	5.5404	10.3704	1.2239	1	1	1	-	D/A
-	O(2)	0.12756	0.72990	-0.04678	4.6731	10.0843	-0.8216	1	1	1	-	D/A
-	N(1)	0.05896	0.72680	0.17877	1.7456	10.0415	3.1397	1	1	1	-	D/A
-	N(2)	0.10250	0.58785	0.11300	3.4438	8.1218	1.9847	1	1	1	-	D/A
-	N(3)	0.13030	0.54145	0.00969	4.6548	7.4807	0.1701	1	1	1	-	D/A
-	N(4)	0.11771	0.42378	0.09476	4.0270	5.8549	1.6642	1	1	1	-	D/A
-	N(5)	0.08054	0.84456	0.06607	2.7528	11.6684	1.1603	1	1	1	-	D/A
-	N(6)	0.12240	0.96355	0.04566	4.2968	13.3124	0.8018	1	1	1	-	D/A
-	N(7)	0.06782	0.95854	-0.03033	2.4957	13.2431	-0.5327	1	1	1	-	D/A
-	N(8)	0.13215	0.77139	0.23163	4.2619	10.6576	4.0680	1	1	1	-	D/A
-	N(9)	0.19431	0.75643	0.22064	6.5149	10.4508	3.8751	1	1	1	-	D/A
-	N(10)	0.17729	0.77850	0.34082	5.6556	10.7558	5.9857	1	1	1	-	D/A
-	C(1)	0.11719	0.51860	0.07450	4.0503	7.1650	1.3084	1	1	1	-	-
-	C(2)	0.15511	0.48626	-0.03504	5.6372	6.7181	-0.6154	1	1	1	-	-
-	C(3)	0.13911	0.47808	-0.11396	5.2265	6.6051	-2.0014	1	1	1	-	-
-	C(4)	0.19570	0.53365	-0.02330	7.0691	7.3729	-0.4093	1	1	1	-	-
-	C(5)	0.13082	0.39448	0.17259	4.3363	5.4501	3.0312	1	1	1	-	-
-	C(6)	0.17119	0.34529	0.17038	5.7892	4.7705	2.9923	1	1	1	-	-

-	C(7)	0.10049	0.31795	0.20399	3.1833	4.3928	3.5827	1	1	1	-	-
-	C(8)	0.07424	0.55610	0.16639	2.3195	7.6831	2.9223	1	1	1	-	-
-	C(9)	0.04301	0.62606	0.16120	1.2097	8.6497	2.8310	1	1	1	-	-
-	C(10)	0.08938	0.91672	0.02833	3.1480	12.6653	0.4975	1	1	1	-	-
-	C(11)	0.13938	0.97604	0.12324	4.7454	13.4850	2.1644	1	1	1	-	-
-	C(12)	0.11918	1.04675	0.16423	3.9362	14.4618	2.8843	1	1	1	-	-
-	C(13)	0.17765	1.01353	0.12571	6.1136	14.0030	2.2079	1	1	1	-	-
-	C(14)	0.05067	0.90200	-0.09615	2.0166	12.4620	-1.6886	1	1	1	-	-
-	C(15)	0.07388	0.88917	-0.15866	2.9785	12.2848	-2.7865	1	1	1	-	-
-	C(16)	0.01111	0.94837	-0.12528	0.6578	13.1027	-2.2003	1	1	1	-	-
-	C(17)	0.03986	0.82059	0.06135	1.3031	11.3373	1.0775	1	1	1	-	-
-	C(18)	0.03404	0.79895	0.14792	0.9153	11.0383	2.5978	1	1	1	-	-
-	C(19)	0.16562	0.77027	0.26660	5.3907	10.6420	4.6822	1	1	1	-	-
-	C(20)	0.22520	0.68168	0.24336	7.5760	9.4181	4.2740	1	1	1	-	-
-	C(21)	0.25511	0.71081	0.18240	8.7751	9.8205	3.2035	1	1	1	-	-
-	C(22)	0.21151	0.57862	0.22974	7.1132	7.9942	4.0349	1	1	1	-	-
-	C(23)	0.20621	0.82583	0.38134	6.6093	11.4097	6.6973	1	1	1	-	-
-	C(24)	0.21754	0.80524	0.45059	6.8729	11.1252	7.9137	1	1	1	-	-
-	C(25)	0.19860	0.93181	0.36550	6.3690	12.8739	6.4192	1	1	1	-	-
-	C(26)	0.10163	0.81077	0.27064	3.0865	11.2016	4.7532	1	1	1	-	-
-	C(27)	0.07060	0.74038	0.25995	1.9953	10.2291	4.5654	1	1	1	-	-
-	C(28)	0.15497	0.76010	-0.00718	5.5746	10.5016	-0.1261	1	1	1	-	-
-	C(29)	0.18771	0.80110	-0.03982	6.8166	11.0680	-0.6994	1	1	1	-	-
-	H(2A)	0.15734	0.41933	-0.01345	5.6724	5.7935	-0.2363	1	1	1	-	-
-	H(3A)	0.12307	0.59815	-0.00941	4.4349	8.2641	-0.1652	1	1	1	-	D-H
-	H(3B)	0.11455	0.44641	-0.11661	4.3508	6.1676	-2.0479	1	1	1	-	-
-	H(3C)	0.15584	0.43951	-0.14205	5.8846	6.0722	-2.4947	1	1	1	-	-
-	H(3D)	0.13614	0.54279	-0.13655	5.1664	7.4992	-2.3982	1	1	1	-	-
-	H(4A)	0.11006	0.37956	0.06060	3.8234	5.2440	1.0644	1	1	1	-	D-H
-	H(4B)	0.21388	0.48911	-0.04177	7.7595	6.7576	-0.7336	1	1	1	-	-
-	H(4C)	0.20282	0.54660	0.03095	7.2124	7.5518	0.5435	1	1	1	-	-
-	H(4D)	0.19545	0.59450	-0.05184	7.1192	8.2136	-0.9105	1	1	1	-	-
-	H(5A)	0.13342	0.45287	0.20621	4.3601	6.2569	3.6216	1	1	1	-	-
-	H(6A)	0.13392	0.98718	0.00843	4.7871	13.6389	0.1481	1	1	1	-	D-H
-	H(6B)	0.18892	0.39375	0.15559	6.4561	5.4400	2.7326	1	1	1	-	-
-	H(6C)	0.16908	0.29231	0.13328	5.7902	4.0385	2.3407	1	1	1	-	-
-	H(6D)	0.18022	0.31977	0.22092	6.0088	4.4179	3.8799	1	1	1	-	-
-	H(7A)	0.06387	1.02136	-0.02930	2.3520	14.1111	-0.5145	1	1	1	-	D-H
-	H(7B)	0.07737	0.31701	0.16851	2.4271	4.3799	2.9595	1	1	1	-	-
-	H(7C)	0.09474	0.33872	0.25433	2.8730	4.6798	4.4668	1	1	1	-	-
-	H(7D)	0.11144	0.25289	0.20769	3.5685	3.4940	3.6475	1	1	1	-	-
-	H(8A)	0.06454	0.49080	0.15187	2.0016	6.7809	2.6672	1	1	1	-	-
-	H(8B)	0.08664	0.55317	0.21939	2.6545	7.6426	3.8531	1	1	1	-	-
-	H(9A)	0.19466	0.79056	0.17872	6.6140	10.9224	3.1387	1	1	1	-	D-H
-	H(9B)	0.02534	0.60873	0.19803	0.4995	8.4103	3.4779	1	1	1	-	-
-	H(9C)	0.02918	0.62478	0.10937	0.8207	8.6319	1.9209	1	1	1	-	-
-	H(10A)	0.16320	0.74632	0.36970	5.0905	10.3112	6.4929	1	1	1	-	D-H

-	H(11A)	0.13988	0.91245	0.15035	4.7074	12.6064	2.6406	1	1	1	-	-
-	H(12A)	0.12780	1.04270	0.21880	4.1326	14.4059	3.8427	1	1	1	-	-
-	H(12B)	0.09221	1.03311	0.15566	2.9863	14.2735	2.7338	1	1	1	-	-
-	H(12C)	0.12397	1.11194	0.14575	4.1460	15.3625	2.5598	1	1	1	-	-
-	H(13A)	0.19377	0.96423	0.10646	6.7316	13.3218	1.8697	1	1	1	-	-
-	H(13B)	0.18724	1.02977	0.17836	6.3487	14.2273	3.1324	1	1	1	-	-
-	H(13C)	0.17758	1.07171	0.09399	6.1764	14.8067	1.6507	1	1	1	-	-
-	H(14A)	0.04561	0.83585	-0.07676	1.7951	11.5482	-1.3481	1	1	1	-	-
-	H(15A)	0.09313	0.84007	-0.14436	3.6396	11.6064	-2.5353	1	1	1	-	-
-	H(15B)	0.08598	0.95069	-0.16869	3.4334	13.1348	-2.9626	1	1	1	-	-
-	H(15C)	0.05799	0.86821	-0.20460	2.5036	11.9952	-3.5933	1	1	1	-	-
-	H(16A)	0.00270	0.98872	-0.08497	0.2725	13.6601	-1.4923	1	1	1	-	-
-	H(16B)	-0.00721	0.89674	-0.13857	0.0278	12.3893	-2.4337	1	1	1	-	-
-	H(16C)	0.01343	0.98830	-0.17030	0.8341	13.6544	-2.9908	1	1	1	-	-
-	H(17A)	0.03372	0.76310	0.02886	1.1500	10.5429	0.5068	1	1	1	-	-
-	H(17B)	0.02417	0.87573	0.04094	0.7824	12.0991	0.7190	1	1	1	-	-
-	H(18A)	0.03829	0.85901	0.17824	1.0050	11.8680	3.1304	1	1	1	-	-
-	H(18B)	0.00789	0.77762	0.15064	-0.0285	10.7436	2.6457	1	1	1	-	-
-	H(20A)	0.23660	0.69120	0.29719	7.8737	9.5496	5.2195	1	1	1	-	-
-	H(21A)	0.28060	0.69280	0.20379	9.6454	9.5717	3.5791	1	1	1	-	-
-	H(21B)	0.25400	0.78071	0.17299	8.7548	10.7863	3.0381	1	1	1	-	-
-	H(21C)	0.24842	0.67615	0.13438	8.6344	9.3416	2.3601	1	1	1	-	-
-	H(22A)	0.20873	0.54773	0.27865	6.9123	7.5674	4.8939	1	1	1	-	-
-	H(22B)	0.22975	0.54233	0.20378	7.8211	7.4929	3.5788	1	1	1	-	-
-	H(22C)	0.18722	0.57917	0.19800	6.3073	8.0019	3.4775	1	1	1	-	-
-	H(23A)	0.22828	0.81108	0.35361	7.4587	11.2059	6.2104	1	1	1	-	-
-	H(24A)	0.24266	0.83238	0.46435	7.7455	11.5002	8.1552	1	1	1	-	-
-	H(24B)	0.21849	0.73477	0.45689	6.8937	10.1516	8.0243	1	1	1	-	-
-	H(24C)	0.20019	0.83275	0.48371	6.1817	11.5053	8.4952	1	1	1	-	-
-	H(25A)	0.21520	0.95542	0.32930	7.0397	13.2000	5.7835	1	1	1	-	-
-	H(25B)	0.20325	0.96850	0.41310	6.4376	13.3808	7.2551	1	1	1	-	-
-	H(25C)	0.17239	0.94032	0.34382	5.4737	12.9914	6.0385	1	1	1	-	-
-	H(26A)	0.09341	0.87421	0.24861	2.8372	12.0781	4.3663	1	1	1	-	-
-	H(26B)	0.11008	0.81968	0.32552	3.2761	11.3247	5.7171	1	1	1	-	-
-	H(27A)	0.07887	0.67777	0.28344	2.2435	9.3641	4.9780	1	1	1	-	-
-	H(27B)	0.04915	0.76424	0.28516	1.1735	10.5588	5.0082	1	1	1	-	-
-	H(29A)	0.17989	0.85860	-0.07005	6.5987	11.8624	-1.2303	1	1	1	-	-
-	H(29B)	0.19780	0.75271	-0.07248	7.2461	10.3995	-1.2729	1	1	1	-	-
-	H(29C)	0.20710	0.81913	0.00146	7.4270	11.3171	0.0257	1	1	1	-	-

Ordered Structure							Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)						
Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	Cl	Co	N	O
1	1	0.129	0.728	0.120	642.82	1	8	29	63	-	1	10	2
Unit Cell Weight =					5142.59			232	504	0	8	80	16
Calculated Analysis (Percent) =								54.2	9.9	0.0	9.2	21.8	5.0
Moiety_Formula =					C29 H63 Co N10 O2								
Sum_Formula =					C29 H63 Co N10 O2								
Formula_Weight =					642.82 [Note: Based on SHELXL97 Atomic Weights]								
Formula_Z =					8								
SpaceGroup_Z =					8 ==> Z' = 8 / 8 = 1.000								
Calculated Density =					0.9810(5) g cm-3 [= Mg m-3]				** WARNING **				
F(000) =					2800.0 [2803.49]				Please Check the Derived Crystal Data. They may be Incorrect for Disordered, Incomplete or Polymeric Structures.				
mu(MoKa) =					4.27 cm-1 = 0.427 mm-1								
Resonant Scattering =					2.76 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)								
Predicted Volume =					7139.6[7073.1] Ang**3, 298[200]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)								

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f,f' & f"

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6

van der Waals (or ion) Radii used in the Analysis

C	H	Cl	Co	N	O
1.70	1.20	1.75	2.03	1.55	1.52

:: Grid: Y-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.19
 :: Grid: X-Axis Step = 0.0056 = Points 180, Angstrom Step = 0.20
 :: Grid: Z-Axis Step = 0.0119 = Points 84, Angstrom Step = 0.21

:: Total Potential Solvent Area Vol 1499.7 Ang^3
 per Unit Cell Vol 8705.0 Ang^3 [17.2%]

Note: Expected volumes for solvent molecules are:
 A hydrogen bonded H2O-molecule 40 Ang^3
 Small molecules (e.g. Toluene) 100-300 Ang^3

Values below for gridpoints and volumes in []
 refer to areas where atom centers may reside.

Area	#GridPoint	VolPerc.	Vol(A^3)	X(av)	Y(av)	Z(av)	Eigenvector(frac)	Sig(Ang)
1	93774[20186]	9	750[161.4]	0.500	0.000	0.131	1 -0.004-0.239 1.000	5.27
							2 -0.005 1.000 0.144	2.83
							3 -1.000-0.027-0.256	2.34
2	93773[20186]	9	750[161.4]	0.000	0.500	0.115	1 -0.004-0.265 1.000	5.34
							2 -0.006 1.000 0.160	2.79
							3 -1.000-0.035-0.258	2.34

x y z Shortest Contacts within 4.5 Angstrom (Excl. H)

1	0.500	0.000	0.131	C9	2.35;	C8	2.78;	N1	3.82;	N2	3.92;	C18	4.31;	C1	4.44;	C7	4.46;	N4	4.47;
2	0.000	0.500	0.115	C9	2.41;	C8	2.82;	N2	3.88;	N1	3.88;	C18	4.33;	C1	4.35;	N4	4.41;		

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

Report the Distance from VOID-CG to Boundary in EV-Directions

Nr	MinEV1	MaxEV1	MinEV2	MaxEV2	MinEV3	MaxEV3	MaxDist (Ang)
1	-11.95	10.47	-6.49	5.36	-1.01	3.75	12.41
2	-12.29	10.92	-6.43	5.61	-1.23	3.75	12.35

(An)isotropic, Equivalent and Main Axes Displacement Parameters - Unusual Values Marked with a # - [Optional Coordinate Split-up]

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Co	0.07608	0.05596	0.06111	0.00226	0.02429	0.01434	0.06310	0.0435	0.0560	0.0898	2.06
		[0.1132	0.7362	0.1253]	[0.1101	0.7285	0.1188]					
2	O1	0.10912	0.06466	0.10637	0.00419	0.05923	0.00012	0.08970	0.0540	0.0655	0.1496	2.77
		[0.1608	0.7512	0.0775]	[0.1561	0.7500	0.0619]					
3	O2	0.17957	0.10085	0.08450	0.02324	0.04858	0.05387	0.11902	0.0678	0.0747	0.2146	3.16
		[0.1309	0.7405	-0.0419]	[0.1242	0.7193	-0.0516]					
4	N1	0.06410	0.10239	0.05929	0.00172	0.01762	0.02461	0.07444	0.0444	0.0643	0.1146	2.58
		[0.0597	0.7358	0.1795]	[0.0582	0.7178	0.1781]					
5	N2	0.08059	0.05669	0.06750	-0.00219	0.01869	0.00409	0.06747	0.0539	0.0633	0.0852	1.58
		[0.1037	0.5886	0.1155]	[0.1013	0.5871	0.1105]					
6	N3	0.12013	0.07986	0.08273	-0.01881	0.03872	0.00961	0.09212	0.0491	0.0959	0.1314	2.68
		[0.1332	0.5417	0.0157]	[0.1274	0.5412	0.0037]					
7	N4	0.14665	0.05696	0.10529	-0.02041	0.02244	0.00425	0.10236	0.0485	0.1112	0.1473	3.04
		[0.1221	0.4244	0.0987]	[0.1133	0.4232	0.0909]					
8	N5	0.13157	0.07372	0.07152	0.00908	0.02948	0.05128	0.09088	0.0429	0.0662	0.1635	3.81
		[0.0837	0.8558	0.0695]	[0.0774	0.8333	0.0627]					
9	N6	0.23485	0.06142	0.09106	-0.00800	0.04464	0.02211	0.12709	0.0533	0.0887	0.2393	4.49
		[0.1291	0.9686	0.0514]	[0.1157	0.9585	0.0399]					
10	N7	0.26764	0.08950	0.07316	0.01385	0.02011	0.08899	0.14342	0.0502	0.0753	0.3048	6.08
		[0.0742	0.9757	-0.0284]	[0.0615	0.9413	-0.0323]					
11	N8	0.07871	0.06524	0.06797	-0.00041	0.02360	0.00297	0.06945	0.0549	0.0655	0.0879	1.60
		[0.1333	0.7721	0.2345]	[0.1310	0.7707	0.2287]					
12	N9	0.08006	0.11877	0.13236	-0.02301	0.03372	-0.01893	0.10871	0.0676	0.1017	0.1569	2.32
		[0.1953	0.7497	0.2261]	[0.1933	0.7632	0.2152]					
13	N10	0.10170	0.22109	0.11287	-0.08017	0.00489	-0.04643	0.14583	0.0560	0.1126	0.2689	4.80
		[0.1762	0.7974	0.3349]	[0.1784	0.7596	0.3467]					
14	C1	0.10806	0.06982	0.06144	-0.01358	0.02390	-0.00111	0.07867	0.0479	0.0772	0.1109	2.32
		[0.1199	0.5168	0.0782]	[0.1145	0.5204	0.0708]					
15	C2	0.15980	0.11179	0.12328	-0.02623	0.07319	0.02326	0.12715	0.0516	0.1345	0.1953	3.78
		[0.1590	0.4876	-0.0249]	[0.1512	0.4849	-0.0452]					
16	C3	0.25010	0.28993	0.14820	-0.14160	0.07717	-0.02059	0.22516	0.0477	0.2416	0.3861	8.09
		[0.1371	0.5037	-0.1246]	[0.1412	0.4525	-0.1033]					
17	C4	0.14774	0.10913	0.16807	0.00546	0.08031	0.03270	0.13676	0.0718	0.1190	0.2194	3.05
		[0.1985	0.5382	-0.0135]	[0.1929	0.5291	-0.0332]					
18	C5	0.20890	0.05728	0.12831	0.00946	0.02612	0.01255	0.13099	0.0554	0.1276	0.2100	3.79
		[0.1369	0.3977	0.1761]	[0.1248	0.3912	0.1691]					
19	C6	0.16060	0.13613	0.32091	0.05118	-0.05085	0.00228	0.21212	0.1123	0.1506	0.3735	3.33
		[0.1708	0.3507	0.1853]	[0.1716	0.3399	0.1555]					
20	C7	0.26632	0.08908	0.16447	0.00719	0.08775	-0.00437	0.16835	0.0871	0.1284	0.2895	3.32
		[0.1057	0.3179	0.2140]	[0.0953	0.3179	0.1939]					
21	C8	0.10760	0.07449	0.08597	-0.00455	0.04339	-0.01926	0.08682	0.0543	0.0735	0.1326	2.44

48	H4A	0.12283	0.12283
49	H4B	0.20514	0.20514
50	H4C	0.20514	0.20514
51	H4D	0.20514	0.20514
52	H5A	0.15719	0.15719
53	H6A	0.15251	0.15251
54	H6B	0.31818	0.31818
55	H6C	0.31818	0.31818
56	H6D	0.31818	0.31818
57	H7A	0.17210	0.17210
58	H7B	0.25252	0.25252
59	H7C	0.25252	0.25252
60	H7D	0.25252	0.25252
61	H8A	0.10418	0.10418
62	H8B	0.10418	0.10418
63	H9A	0.13046	0.13046
64	H9B	0.11021	0.11021
65	H9C	0.11021	0.11021
66	H10A	0.17499	0.17499
67	H11A	0.14964	0.14964
68	H12A	0.23893	0.23893
69	H12B	0.23893	0.23893
70	H12C	0.23893	0.23893
71	H13A	0.27397	0.27397
72	H13B	0.27397	0.27397
73	H13C	0.27397	0.27397
74	H14A	0.16097	0.16097
75	H15A	0.19894	0.19894
76	H15B	0.19894	0.19894
77	H15C	0.19894	0.19894
78	H16A	0.26205	0.26205
79	H16B	0.26205	0.26205
80	H16C	0.26205	0.26205
81	H17A	0.13909	0.13909
82	H17B	0.13909	0.13909
83	H18A	0.12014	0.12014
84	H18B	0.12014	0.12014
85	H20A	0.14952	0.14952
86	H21A	0.22647	0.22647
87	H21B	0.22647	0.22647
88	H21C	0.22647	0.22647
89	H22A	0.19084	0.19084
90	H22B	0.19084	0.19084
91	H22C	0.19084	0.19084
92	H23A	0.22462	0.22462
93	H24A	0.46371	0.46371
94	H24B	0.46371	0.46371
95	H24C	0.46371	0.46371

96	H25A	0.27342	0.27342
97	H25B	0.27342	0.27342
98	H25C	0.27342	0.27342
99	H26A	0.09577	0.09577
100	H26B	0.09577	0.09577
101	H27A	0.09763	0.09763
102	H27B	0.09763	0.09763
103	H29A	0.28278	0.28278
104	H29B	0.28278	0.28278
105	H29C	0.28278	0.28278

U(i, j) -Average	0.1573	0.1183	0.1134	-0.0124	0.0266	0.0140	0.1288	0.0962	0.1282	0.1620	1.68
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The Displacement Factor has the Form of $\text{Exp}(-T)$

where

$$T = 8 \cdot (\pi^2) \cdot U_{\text{iso}} \cdot \sin(\theta/\lambda)^2, \text{ for Isotropic Atoms,}$$
$$T = 2 \cdot (\pi^2) \cdot (U_{11} \cdot (h \cdot a_s)^2 + U_{22} \cdot (k \cdot b_s)^2 + U_{33} \cdot (l \cdot c_s)^2 + 2 \cdot U_{23} \cdot k \cdot l \cdot b_s \cdot c_s + 2 \cdot U_{13} \cdot h \cdot l \cdot a_s \cdot c_s + 2 \cdot U_{12} \cdot h \cdot k \cdot a_s \cdot b_s), \text{ for Anisotr. Atoms}$$
$$U_{eq} = 1/3 \sum(i,j) (U_{ij} * a_s(i) * a_s(j) * a(i) . a(j))$$

U1, U2, U3 are the three Main Axes Components of U_{ij}

Reference U(eq): R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	Cl	Co	N	O
Average	0.1288	0.1420	0.2185	0.0000	0.0631	0.1022	0.1044
Minimum	0.0631	0.0787	0.0958	0.0000	0.0631	0.0675	0.0897
Maximum	0.3091	0.3091	0.4637	0.0000	0.0631	0.1458	0.1190
Ratio	4.8994	3.9296	4.8417	0.0000	1.0000	2.1615	1.3269
Number	42	29	63	0	1	10	2

```
:: Reflection Data are READ from File : char232s.hkl - ( OBS-Data)
```

```

:: TRMX =      1.00      0.00      0.00      0.00      1.00      0.00      0.00      0.00      1.00

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```
:: Nr. of Eliminated Reflections (Theta Limit = 27.5 Deg) = 2759
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SQUEEZE - Procedure (cf. BYPASS-procedure - P. van der Sluis & A.L. Spek (1990). Acta Cryst. A46, 194-201)

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:: # Accepted Reflns      Hmax Kmax Lmax
::           48290        46   17   22

:: A,  B,  C (Angstrom) =    35.876    13.816    17.684
:: NX, NY, NZ (SOLV-MAP) =      180       72       84
:: NX, NY, NZ (FFT-MAP)  =      128       64       64
:: Resolution (FFT-MAP)  =      0.28     0.22     0.28 Angstrom

```

Missing Reflections below $\sin(\theta)/\lambda=0.3$

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N	H	K	L	Theta
1	2	0	0	1.14

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:: Number of Removed Systematic Extinctions =    1017
:: Number of Non-extinction   Reflections =   47273
:: Number of Missing Low Order Reflections =      1

```

:: Fo-scale =0.662847E+00 - SinT/L-Min = 0.20 for Fo/Fc-Scaling

:: Cycle = 1, R(F) = 0.35, Nref(Hemi) = 19552, R(F > 4SIGF) = 0.19 Nref = 4603

Unique Density Maxima in Enhanced Difference Map (CutOff level = 0.50 eA-3)

#	x	y	z	(e/A^3)	Shortest Contacts within 3.2 Angstrom (Excl. H)																		
1	0.609	0.370	0.447	2.96	void	N7	2.85;	N6	2.89;														
2	0.616	0.293	0.482	2.90	void																		
3	0.885	0.262	0.533	2.49	void	N4	3.17;																
4	0.404	0.291	0.027	2.48	void																		
5	0.499	0.136	0.609	1.94	void																		
6	0.480	0.119	0.686	1.86	void																		
7	0.062	0.229	-0.002	1.81	void																		
8	0.516	0.136	0.843	1.80	void																		
9	0.956	0.411	0.092	1.71	void																		
10	0.361	0.245	0.982	1.68	void	N4	2.84;	C6	3.07;														
11	0.469	0.031	0.562	1.65	void																		
12	0.950	0.501	0.143	1.58	void	C3	3.19;																
13	0.545	0.045	0.842	1.15	void																		
14	1.000	0.501	0.001	0.79	void																		
15	0.218	0.251	0.737	0.77		N9	0.87;	C20	0.97;	C21	1.81;	C19	2.03;	C22	2.37;	N10	2.51;	C23	2.85;	N8	3.08;		
16	0.697	0.267	0.265	0.69		N9	0.79;	C19	1.13;	N10	1.60;	C20	1.63;	C23	2.20;	N8	2.33;	C22	2.74;	C21	2.79;	C25	2.89;
17	0.877	0.031	0.765	0.68		C12	1.64;	C11	2.13;	C26	2.43;	N8	2.76;	C13	2.97;	C19	3.16;						
18	0.377	0.531	0.765	0.68		C12	1.64;	C11	2.13;	C26	2.43;	N8	2.76;	C13	2.97;	C19	3.16;						
19	0.352	0.480	0.763	0.67		C12	1.59;	C11	2.08;	C13	2.34;	C25	3.00;										
20	0.759	0.189	0.256	0.65		C20	1.21;	C21	1.33;	C22	2.30;	N9	2.51;										
21	0.312	0.226	0.246	0.65		N9	0.77;	C19	1.06;	C20	1.50;	N10	1.78;	N8	2.10;	C22	2.27;	C23	2.66;	C21	2.85;		
22	0.735	0.261	0.765	0.63		C21	1.04;	C20	1.67;	N9	2.55;	C22	2.94;	C6	3.04;								
23	0.910	0.014	0.786	0.62		C12	1.67;	C11	2.53;	C26	2.63;	C15	2.95;										
24	0.718	0.126	0.344	0.62		C20	1.98;	C22	2.11;	N10	2.57;	N9	2.88;	C23	2.88;	C19	2.97;	C24	3.11;				
25	0.905	0.215	0.906	0.62		Co	1.02;	N5	1.08;	C17	2.07;	C10	2.16;	N1	2.24;	O1	2.40;	C18	2.50;	N8	2.63;	N2	2.75;
26	0.287	0.320	0.487	0.61		C29	1.26;	C28	2.23;	O1	2.49;												
27	0.648	0.144	0.236	0.60		N8	1.85;	C19	1.91;	N9	2.30;	C22	2.45;	Co	2.58;	N2	2.68;	N10	2.75;	C20	2.79;	C26	2.96;
28	0.860	0.447	0.300	0.60		C5	0.92;	C6	1.92;	N4	1.97;	C7	2.28;	C1	2.48;	N2	2.73;	C8	2.79;	C22	3.15;		
29	0.883	0.035	0.235	0.60		C12	1.80;	C15	2.41;	C11	2.84;	C26	3.14;										
30	0.333	0.250	0.138	0.59		N10	0.69;	C19	1.70;	C23	1.76;	C24	2.39;	N8	2.50;	C25	2.76;	N9	2.79;	C26	2.80;		
31	0.678	0.484	0.845	0.59		C25	1.39;	C23	2.85;														
32	0.140	0.388	0.754	0.59		N8	2.25;	C19	2.37;	C3	2.65;	C22	2.68;	N2	2.71;	C8	2.78;	N9	2.89;	Co	2.95;	N10	2.99;
33	0.351	0.354	0.706	0.58	void	C12	2.77;	C15	2.94;	C29	3.20;												
34	0.370	0.015	0.252	0.58		C5	2.13;	C8	2.39;	C3	2.43;	N2	2.67										

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45	0.656	0.201	0.186	0.54	N8	1.57; N9	1.63; C19	1.71; Co	1.89; O1	2.19; C20	2.59; C22	2.67; N2	2.69; N10	2.95;
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Unique Density Minima in Enhanced Difference Map (CutOff level = -0.50 eA-3)

#	x	y	z	(e/A^3)	Shortest Contacts within 3.2 Angstrom (Excl. H)																	
1	0.886	0.264	0.877	-2.15	Co	0.09;	O1	1.96;	N8	2.02;	N2	2.09;	N5	2.10;	N1	2.31;	C26	2.89;	C28	2.89;	C17	2.99;
2	0.248	0.221	0.330	-0.84	C21	0.26;	C20	1.79;	N9	2.41;	C22	2.73;										
3	0.132	0.276	0.464	-0.72	O2	0.25;	C28	1.04;	O1	2.02;	C29	2.27;	N3	2.65;	Co	2.97;	N5	3.19;				
4	0.133	0.231	0.733	-0.69	C19	1.27;	C26	1.48;	Co	2.07;	N9	2.26;	N10	2.35;	C27	2.36;	N1	2.76;	O1	3.14;		
5	0.896	0.410	0.909	-0.66	N2	0.39;	C1	1.15;	C8	1.86;	N3	1.93;	Co	2.05;	N4	2.35;	C9	2.69;	O1	3.01;	N1	3.03;
6	0.993	0.051	0.121	-0.65	C16	0.17;	C14	1.70;	N7	2.56;	C15	2.69;										
7	0.939	0.244	0.828	-0.65	N1	0.43;	C18	1.17;	C27	1.56;	C9	1.91;	Co	2.14;	C17	2.21;	C26	2.26;	N5	2.42;	N8	2.65;
8	0.218	0.186	0.955	-0.64	C24	0.14;	C23	1.33;	C25	2.32;	N10	2.40;	C24	3.15;								
9	0.402	0.315	0.252	-0.64	C26	0.42;	N8	1.42;	C27	1.45;	N1	2.12;	C19	2.49;	Co	2.59;	C18	2.73;	N10	3.16;		
10	0.319	0.260	0.174	-0.62	N10	0.40;	C19	1.14;	C23	1.55;	N9	1.98;	N8	2.28;	C24	2.51;	C20	2.53;	C25	2.54;	C26	2.98;
11	0.577	0.249	0.248	-0.62	C27	0.35;	C26	1.25;	N1	1.36;	N8	2.05;	C18	2.32;	C9	2.52;	Co	2.69;	C8	3.03;	C19	3.16;
12	0.338	0.278	0.235	-0.61	C19	0.17;	N8	1.17;	N10	1.38;	N9	1.51;	C26	2.23;	C23	2.53;	C20	2.70;	C25	2.97;	Co	3.00;
13	0.860	0.467	0.611	-0.60	C3	0.16;	C2	1.42;	N3	2.44;	C4	2.56;										
14	0.791	0.433	0.781	-0.59	C22	0.26;	C20	1.72;	N9	2.67;	C21	2.70;										
15	0.807	0.216	0.050	-0.58	C29	0.37;	C28	1.69;	O2	2.49;	O1	2.63;	C21	3.14;								
16	0.382	0.449	0.846	-0.58	C12	0.19;	C11	1.44;	N6	2.29;	C13	2.33;	C10	2.98;								
17	0.409	0.205	0.793	-0.58	C7	0.47;	C5	2.12;	N4	2.90;	C6	3.10;										
18	0.923	0.153	0.952	-0.57	N5	0.33;	C10	1.13;	C17	1.43;	N7	2.07;	N6	2.29;	Co	2.32;	C18	2.56;	C14	2.72;	N1	2.98;
19	0.463	0.326	0.466	-0.55	C17	0.49;	N5	1.63;	C18	2.06;	C10	2.28;	N7	2.49;	C14	2.63;	N1	2.93;				
20	0.710	0.029	0.000	-0.55	C4	0.64;	C2	2.09;	N3	2.91;	C3	3.15;										
21	0.609	0.243	0.608	-0.54	C7	1.95;	C5	2.31;	N4	2.34;	C6	2.68;	C12	3.08;								
22	0.962	0.382	0.856	-0.54	C9	0.35;	C8	1.57;	N1	1.77;	N2	2.49;	C18	2.51;	C27	2.81;	Co	3.16;	C17	3.17;		
23	0.110	0.137	0.784	-0.53	C26	0.80;	N8	1.82;	C27	2.21;	C19	2.44;	N10	2.78;	N1	3.09;						
24	0.962	0.195	0.845	-0.53	C18	0.19;	N1	1.35;	C17	1.67;	C27	2.26;	N5	2.38;	C9	2.48;	C26	2.89;	Co	2.94;		
25	0.706	0.300	0.363	-0.52	C23	0.48;	N10	1.10;	C24	1.55;	C25	1.84;	C19	2.15;	N9	2.58;	C20	2.83;				
26	0.131	0.435	0.097	-0.52	N4	0.48;	C1	1.29;	C5	1.45;	N3	2.13;	C6	2.21;	N2	2.37;	C2	2.69;	C7	2.80;	C8	2.99;
27	1.000	0.018	0.655	-0.52	C16	1.14;	C14	2.55;	C18	2.82;	N7	3.19;	C15	3.20;								
28	0.302	0.280	0.060	-0.52	C24	0.79;	C23	1.29;	N10	1.83;	C25	2.48;	C19	3.16;								
29	0.923	0.146	0.152	-0.52	C15	0.51;	C14	1.60;	N7	2.65;	C16	2.80;	O2	2.98;								
30	0.431	0.056	0.346	-0.51	C8	0.27;	C9	1.36;	N2	1.54;	C1	2.41;	N1	2.43;	N4	2.82;	Co	2.96;	C5	3.14;	C27	3.15;
31	0.485	0.497	0.564	-0.51	C16	1.27;	C14	1.96;	N7	1.99;	C10	3.16;										
32	0.069	0.018	0.487	-0.51	N7	0.45;	C10	1.32;	C14	1.90;	N6	2.07;	N5	2.36;	C16	2.75;	C17	2.85;	C15	2.91;		
33	0.361	0.188	0.327	-0.50	Co	1.40;	N8	1.58;	N2	2.12;	C19	2.13;	O1	2.21;	N9	2.26;	C26	2.86;	N1	2.94;	C8	2.95;

Void X(av) Y(av) Z(av) Volume Ang³ El-Count (e-) Vol/Electron Vol/Atom

1	0.500	0.000	0.131	747	201	3.7	30
2	0.000	0.500	0.115	747	201	3.7	30

Total (Positive) Electron Count in Voids/Cell = 402

Total (Fo-Fc)map Electron Count in Unit Cell = 397

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VOID-Fo-Fc-Map: Rho(min) = -0.48, Rho(max) = 4.20, RhoCutoff = 0.00
PeaksCloseToAtoms: Rho(min) = -2.15, Rho(max) = 0.78, RhoCutoff = 0.50

:: Fo-scale =0.683651E+00 - SinT/L-Min = 0.20 for Fo/Fc-Scaling

:: Cycle = 5, R(F) = 0.23, Nref(Hemi) = 19552, R(F > 4SIGF) = 0.09 Nref = 4603

Unique Density Maxima in Enhanced Difference Map (CutOff level = 0.50 eA-3)

#	x	y	z	(e/A^3)	Shortest Contacts within 3.2 Angstrom (Excl. H)
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[illegible]

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45 0.556 0.350 0.511 0.69 void N7 2.80;
46 0.915 0.287 0.579 0.67 void C27 2.86; C26 3.10;
47 0.932 0.442 0.124 0.67 void C3 2.76; N3 3.06;
48 0.523 0.103 0.980 0.65 void
49 0.940 0.325 0.160 0.65 void C7 2.95; C15 2.99; O2 3.04;
50 0.074 0.403 0.347 0.65 void C3 2.87; C7 3.03; O2 3.13;
51 0.235 0.220 0.268 0.64 C21 0.92; C20 1.55; N9 2.57; C22 2.73;
52 0.454 0.082 0.013 0.63 void N4 3.01; C1 3.14;
53 0.448 0.329 0.942 0.62 void C16 3.15;
54 1.002 0.291 0.031 0.62 C17 2.59;
55 0.204 0.205 0.986 0.62 C24 0.84; C23 1.91; N10 2.65; C25 2.85;
56 0.961 0.277 0.194 0.62 void C15 2.66; C14 3.03; C7 3.07;
57 0.695 0.238 0.248 0.62 N9 0.55; C19 1.23; C20 1.34; N10 1.91; N8 2.29; C22 2.32; C21 2.59; C23 2.63;
58 0.977 0.495 0.216 0.62 void C9 2.98; C8 3.06;
59 0.039 0.159 0.022 0.61 void C17 3.05; C16 3.09; N7 3.13;
60 0.024 0.394 0.970 0.61 void C9 3.15;
61 0.082 0.505 0.329 0.61 C3 2.19; C8 2.94;
62 0.417 0.220 0.404 0.60 Co 1.09; N1 1.78; N5 1.80; N2 1.97; C17 2.11; C9 2.33; C18 2.33; C8 2.62; O1 2.84;
63 0.827 0.475 0.516 0.60 C2 0.70; C4 1.18; N3 1.88; C3 1.99; C1 2.76; N4 3.02;
64 0.626 0.196 0.676 0.60 C7 1.11; C5 1.26; C6 1.72; N4 2.18;
65 0.439 0.261 0.080 0.59 void C27 2.91;
66 0.566 0.157 0.913 0.59 O2 2.45; N3 3.14;
67 0.308 0.031 0.982 0.58 C4 1.17; C2 1.54; N3 2.40; C3 2.83; C1 3.03; N4 3.18;
68 0.441 0.359 0.111 0.58 void C26 2.82; C27 2.88; N7 2.90; C16 3.16;
69 0.537 0.198 0.933 0.58 void C17 2.83; C14 2.92;
70 0.866 0.219 0.573 0.57 N10 2.31; C23 2.87; C26 2.91; C24 3.00; C19 3.19;
71 0.993 0.447 0.241 0.56 void
72 0.624 0.170 0.131 0.56 Co 0.97; N2 1.39; O1 2.07; N8 2.25; C1 2.32; C8 2.51; N1 2.68; N3 2.82; C19 3.01;
73 0.470 0.260 0.077 0.56 C18 2.54; C17 2.69;
74 0.459 0.172 0.033 0.56 void
75 0.353 0.361 0.967 0.56 C13 2.55; N6 2.60; C11 2.79; C12 2.93; C24 3.15;
76 0.990 0.299 0.267 0.55 void
77 0.925 0.187 0.924 0.55 N5 0.52; C17 1.26; C10 1.77; Co 1.84; C18 2.07; N1 2.31; N7 2.74; N6 2.78; O1 3.13;
78 0.401 0.280 0.409 0.55 Co 0.93; N5 1.17; C10 2.20; C17 2.21; O1 2.23; N1 2.37; N8 2.63; C18 2.67; N2 2.69;
79 0.620 0.398 0.516 0.55 N6 1.98; C11 2.61; C12 2.74; N7 2.77; C10 2.80; C13 2.94;
80 0.983 0.392 0.265 0.54 void
81 0.022 0.344 0.063 0.54 void
82 0.228 0.185 0.922 0.53 C24 0.70; C23 1.01; C25 2.11; N10 2.25;
83 0.999 0.448 0.953 0.53 C9 2.59; C8 3.18;
84 0.681 0.507 0.840 0.53 C25 1.12; C23 2.56; N10 2.97;
85 0.555 0.044 0.294 0.52 C8 2.45; C9 2.60; C27 2.85;
86 0.668 0.433 0.407 0.52 C25 1.39; C23 2.10; N10 2.48; C24 2.56;
87 0.672 0.275 0.110 0.52 O1 0.88; N9 2.04; C28 2.10; Co 2.28; N8 2.72; C29 2.79; C19 2.81; C11 3.04; O2 3.10;
88 0.036 0.359 0.271 0.52 void C7 2.77;
89 0.698 0.468 0.388 0.52 C25 0.64; C23 2.00; C24 2.58; N10 2.82;
90 0.647 0.303 0.577 0.51 void C6 2.70; C12 2.83; C13 2.86; C11 3.18;
91 0.479 0.253 0.655 0.51 C14 2.49; C15 2.67; C16 2.78;
92 0.920 0.396 0.513 0.51 N4 2.24; C1 2.56; N3 2.69; C2 3.03; C3 3.13;
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93 0.343 0.203 0.315 0.51      N9  1.59; N8  1.59; C19 1.71; Co  1.91; O1  2.15; C20 2.56; C22 2.65; N2  2.72; N10 2.95;
94 0.309 0.505 0.120 0.51      C25 1.09; C23 2.54; C29 3.04; C24 3.13;
95 0.698 0.435 0.407 0.50      C25 0.73; C23 1.61; C24 2.05; N10 2.53;
96 0.999 0.475 0.403 0.50 void C9  2.75; C8  3.00;
97 0.563 0.260 0.505 0.00 void
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Unique Density Minima in Enhanced Difference Map (CutOff level = -0.50 eA-3)

#	x	y	z	(e/A^3)	Shortest Contacts within 3.2 Angstrom (Excl. H)																	
1	0.886	0.264	0.877	-1.97	Co	0.09;	O1	1.96;	N8	2.01;	N2	2.09;	N5	2.10;	N1	2.30;	C26	2.89;	C28	2.90;	C17	2.99;
2	0.248	0.221	0.330	-0.86	C21	0.27;	C20	1.79;	N9	2.41;	C22	2.73;										
3	0.632	0.228	0.966	-0.70	O2	0.26;	C28	1.00;	O1	1.99;	C29	2.25;	N3	2.70;	Co	2.93;	N5	3.14;				
4	0.896	0.411	0.908	-0.65	N2	0.39;	C1	1.14;	C8	1.86;	N3	1.93;	Co	2.05;	N4	2.34;	C9	2.69;	O1	3.01;	N1	3.03;
5	0.367	0.272	0.267	-0.65	C19	1.24;	C26	1.49;	Co	2.09;	N9	2.24;	N10	2.34;	C27	2.40;	N1	2.79;	O1	3.13;		
6	0.218	0.186	0.955	-0.63	C24	0.14;	C23	1.33;	C25	2.32;	N10	2.40;	C24	3.15;								
7	0.939	0.244	0.827	-0.61	N1	0.43;	C18	1.17;	C27	1.55;	C9	1.91;	Co	2.15;	C17	2.21;	C26	2.26;	N5	2.42;	N8	2.65;
8	0.902	0.190	0.745	-0.61	C26	0.29;	C27	1.38;	N8	1.45;	N1	2.16;	C19	2.48;	Co	2.68;	C18	2.80;	N10	3.10;		
9	0.319	0.260	0.175	-0.61	N10	0.41;	C19	1.13;	C23	1.56;	N9	1.97;	N8	2.27;	C20	2.51;	C24	2.52;	C25	2.54;	C26	2.98;
10	0.577	0.249	0.248	-0.61	C27	0.36;	C26	1.25;	N1	1.36;	N8	2.04;	C18	2.32;	C9	2.52;	Co	2.68;	C8	3.03;	C19	3.16;
11	0.993	0.052	0.120	-0.61	C16	0.18;	C14	1.70;	N7	2.55;	C15	2.69;										
12	0.338	0.278	0.235	-0.60	C19	0.16;	N8	1.17;	N10	1.39;	N9	1.50;	C26	2.23;	C23	2.53;	C20	2.69;	C25	2.97;	Co	3.00;
13	0.860	0.467	0.611	-0.59	C3	0.17;	C2	1.42;	N3	2.43;	C4	2.56;										
14	0.506	0.469	0.635	-0.59	C16	0.68;	C14	2.26;	N7	3.05;	C15	3.14;										
15	0.806	0.216	0.051	-0.59	C29	0.38;	C28	1.70;	O2	2.50;	O1	2.64;	C21	3.13;								
16	0.409	0.205	0.793	-0.57	C7	0.46;	C5	2.11;	N4	2.91;	C6	3.09;										
17	0.791	0.432	0.782	-0.57	C22	0.26;	C20	1.72;	N9	2.67;	C21	2.70;										
18	0.609	0.242	0.608	-0.56	C7	1.95;	C5	2.30;	N4	2.33;	C6	2.67;	C12	3.09;								
19	0.109	0.138	0.784	-0.55	C26	0.79;	N8	1.81;	C27	2.20;	C19	2.43;	N10	2.78;	N1	3.07;						
20	0.383	0.449	0.846	-0.55	C12	0.19;	C11	1.45;	N6	2.29;	C13	2.34;	C10	2.98;								
21	0.963	0.171	0.970	-0.54	C17	0.57;	N5	1.64;	C18	2.14;	C10	2.25;	N7	2.42;	C14	2.55;	N1	3.01;				
22	0.922	0.145	0.153	-0.54	C15	0.50;	C14	1.61;	N7	2.65;	C16	2.80;	O2	2.99;								
23	0.923	0.153	0.952	-0.54	N5	0.33;	C10	1.13;	C17	1.43;	N7	2.07;	N6	2.29;	Co	2.32;	C18	2.57;	C14	2.73;	N1	2.98;
24	0.711	0.029	0.000	-0.53	C4	0.64;	C2	2.10;	N3	2.92;	C3	3.15;										
25	0.962	0.194	0.846	-0.53	C18	0.20;	N1	1.36;	C17	1.66;	C27	2.27;	N5	2.36;	C9	2.49;	C26	2.88;	Co	2.94;		
26	0.302	0.280	0.059	-0.51	C24	0.79;	C23	1.29;	N10	1.83;	C25	2.48;	C19	3.16;								
27	0.706	0.301	0.364	-0.51	C23	0.47;	N10	1.10;	C24	1.55;	C25	1.83;	C19	2.15;	N9	2.59;	C20	2.84;				
28	0.963	0.382	0.856	-0.51	C9	0.36;	C8	1.59;	N1	1.76;	N2	2.50;	C18	2.50;	C27	2.81;	Co	3.16;	C17	3.16;		
29	1.000	0.018	0.655	-0.51	C16	1.14;	C14	2.56;	C18	2.81;	N7	3.20;										
30	0.013	0.013	0.287	-0.51	C16	1.64;	C14	2.60;	C15	2.65;	C16	2.94;										
31	0.130	0.435	0.097	-0.51	N4	0.48;	C1	1.30;	C5	1.44;	N3	2.14;	C6	2.21;	N2	2.37;	C2	2.69;	C7	2.79;	C8	2.99;
32	0.023	0.377	-0.002	-0.51	void																	
33	0.409	0.205	0.793	0.00	C7	0.46;	C5	2.11;	N4	2.91;	C6	3.09;										

 Void X(av) Y(av) Z(av) Volume Ang³ El-Count (e-) Vol/Electron Vol/Atom

1	0.500	0.000	0.131	747	202	3.7	30
2	0.000	0.500	0.115	747	202	3.7	30

Total (Positive) Electron Count in Voids/Cell = 404

Total (Fo-Fc)map Electron Count in Unit Cell = 402

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VOID-Fo-Fc-Map: Rho(min) = -0.51, Rho(max) = 4.28, RhoCutOff = 0.00
PeaksCloseToAtoms: Rho(min) = -1.97, Rho(max) = 0.77, RhoCutOff = 0.50

:: Fo-scale = 0.687828E+00 - SinT/L-Min = 0.20 for Fo/Fc-Scaling

:: Cycle = 6, R(F) = 0.22, Nref(Hemi) = 19552, R(F > 4SIGF) = 0.09 Nref = 4603

:: Reflection Data are READ from File : char232s.hkl - (OBS-Data)

:: TRMX = 1.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 1.00

:: Nr. of Eliminated Reflections (Theta Limit = 27.5 Deg) = 2759

:: Reflection Data are READ from File : char232s.hkl - (OBS-Data)

:: TRMX = 1.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 1.00

H	K	L	Sinth/l	F(obs)	F(mod)	F(solv)	F(tot)	D(F^2)/S	I	Sig(I)
-4	0	0	0.06	674.19	722.83	16.00	707.17	2.57	454536.66	17705.08
-4	0	0	0.06	667.44	722.83	16.00	707.17	3.04	445473.31	17983.27
6	0	0	0.08	52.85	91.67	3.36	89.28	22.94	2792.75	225.67
-6	0	0	0.08	50.87	91.67	3.36	89.28	22.05	2587.42	244.12
6	0	0	0.08	55.28	91.67	3.36	89.28	24.10	3056.27	203.91
-6	0	0	0.08	47.81	91.67	3.36	89.28	29.74	2286.05	191.14
8	0	0	0.11	91.65	45.47	62.12	107.52	6.52	8400.02	484.93
-8	0	0	0.11	97.08	45.47	62.12	107.52	4.53	9423.82	471.21
8	0	0	0.11	96.27	45.47	62.12	107.52	4.77	9267.22	481.15
-8	0	0	0.11	96.72	45.47	62.12	107.52	3.98	9355.69	554.01
10	0	0	0.14	130.12	146.31	1.72	147.98	6.51	16930.61	762.65
10	0	0	0.14	126.02	146.31	1.72	147.98	7.73	15881.26	778.26
-10	0	0	0.14	113.73	146.31	1.72	147.98	11.34	12933.80	790.56
-10	0	0	0.14	127.15	146.31	1.72	147.98	7.74	16166.54	740.41
1	1	0	0.04	71.06	76.67	143.27	66.80	2.57	5049.47	228.51
-1	-1	0	0.04	70.91	76.67	143.27	66.80	2.35	5027.71	240.34
-1	1	0	0.04	76.18	76.67	143.50	67.18	5.27	5803.13	244.60
1	-1	0	0.04	71.18	76.67	143.50	67.18	2.38	5066.50	232.77
3	1	0	0.06	7.87	186.56	159.13	27.43	13.77	61.98	50.15
-3	-1	0	0.06	3.30	186.56	159.13	27.43	16.67	10.88	44.47
3	1	0	0.06	11.30	186.56	159.13	27.43	12.45	127.74	50.15
3	-1	0	0.06	8.28	186.56	158.90	28.44	16.30	68.60	45.42
-3	1	0	0.06	2.18	186.56	158.90	28.44	17.00	4.73	47.31
-3	1	0	0.06	9.15	186.56	158.90	28.44	14.33	83.74	50.62
-3	-1	0	0.06	8.56	186.56	159.13	27.43	23.53	73.33	28.86
3	1	0	0.06	4.30	186.56	159.13	27.43	33.00	18.45	22.24
-5	-1	0	0.08	13.48	111.61	116.16	5.91	2.79	181.67	52.51
5	1	0	0.08	14.74	111.61	116.16	5.91	2.24	217.16	81.37
-5	1	0	0.08	14.35	111.61	115.13	4.38	4.70	205.80	39.74
5	-1	0	0.08	15.13	111.61	115.13	4.38	2.53	228.98	82.79
5	1	0	0.08	15.73	111.61	116.16	5.91	2.29	247.43	92.73
-5	1	0	0.08	14.57	111.61	115.13	4.38	2.33	212.43	82.79
5	1	0	0.08	12.53	111.61	116.16	5.91	2.81	157.07	43.53
7	1	0	0.10	150.89	102.20	22.59	124.61	7.39	22768.28	980.28
7	-1	0	0.10	142.76	102.20	21.90	124.08	5.34	20379.09	932.49
7	1	0	0.10	144.33	102.20	22.59	124.61	5.70	20830.43	931.07
7	-1	0	0.10	148.10	102.20	21.90	124.08	7.38	21933.71	886.13
-7	-1	0	0.10	151.05	102.20	22.59	124.61	8.29	22817.48	879.98
-7	1	0	0.10	151.08	102.20	21.90	124.08	7.77	22825.05	955.68
-7	-1	0	0.10	133.44	102.20	22.59	124.61	2.37	17804.91	961.83
-7	1	0	0.10	133.41	102.20	21.90	124.08	2.50	17799.23	961.83
9	-1	0	0.13	55.39	106.40	34.41	72.00	10.33	3068.57	204.86
-9	1	0	0.13	53.50	106.40	34.41	72.00	8.93	2861.82	260.21
9	1	0	0.13	55.53	106.40	34.92	71.51	7.14	3083.24	284.34
-9	-1	0	0.13	47.19	106.40	34.92	71.51	10.78	2226.91	267.78
-9	1	0	0.13	54.79	106.40	34.41	72.00	7.18	3002.34	303.73

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9	1	0	0.13	53.56	106.40	34.92	71.51	8.20	2868.92	273.93
9	-1	0	0.13	54.28	106.40	34.41	72.00	7.92	2946.51	282.44
-9	-1	0	0.13	52.37	106.40	34.92	71.51	11.52	2742.13	205.80
2	2	0	0.08	93.93	87.77	22.74	110.44	8.32	8822.50	405.45
-2	-2	0	0.08	95.88	87.77	22.74	110.44	6.94	9193.42	432.89
-2	2	0	0.08	95.41	87.77	22.98	110.48	7.22	9103.05	429.58
2	2	0	0.08	95.93	87.77	22.74	110.44	6.32	9201.93	473.58
-2	2	0	0.08	96.04	87.77	22.98	110.48	6.33	9222.75	471.69
2	-2	0	0.08	94.20	87.77	22.98	110.48	8.00	8874.54	416.33
2	2	0	0.08	92.98	87.77	22.74	110.44	7.49	8644.61	474.05
-6	2	0	0.11	91.21	59.34	43.37	102.59	4.27	8318.64	516.63
-6	-2	0	0.11	94.42	59.34	42.91	101.94	2.76	8914.76	535.56
-8	2	0	0.13	50.78	24.43	51.27	27.45	6.47	2578.43	281.97
8	2	0	0.13	50.40	24.43	50.59	28.34	7.20	2540.11	241.28
-8	-2	0	0.13	46.74	24.43	50.59	28.34	5.22	2184.34	264.47
-8	-2	0	0.13	50.36	24.43	50.59	28.34	9.49	2535.85	182.62
-8	2	0	0.13	51.72	24.43	51.27	27.45	6.76	2674.95	284.34
8	-2	0	0.13	52.90	24.43	51.27	27.45	7.69	2798.90	265.89
8	2	0	0.13	54.32	24.43	50.59	28.34	6.93	2950.30	309.89
-1	-3	0	0.11	73.12	29.53	49.07	78.56	2.41	5346.58	342.06
1	-3	0	0.11	71.81	29.53	49.34	78.83	3.65	5157.34	290.01
-1	3	0	0.11	70.01	29.53	49.34	78.83	3.76	4901.86	349.15
-1	3	0	0.11	74.04	29.53	49.34	78.83	2.10	5481.89	349.63
3	3	0	0.12	51.53	39.78	33.37	73.10	10.29	2655.55	261.16
-3	3	0	0.12	53.67	39.78	33.11	72.86	9.43	2880.75	257.37
3	3	0	0.12	56.23	39.78	33.37	73.10	7.45	3161.77	292.85
3	3	0	0.12	55.18	39.78	33.37	73.10	11.33	3044.44	202.96
-3	-3	0	0.12	55.76	39.78	33.37	73.10	9.52	3108.79	234.66
-3	3	0	0.12	56.81	39.78	33.11	72.86	8.82	3227.06	236.08
3	-3	0	0.12	56.09	39.78	33.11	72.86	9.56	3146.16	226.15
0	4	0	0.14	478.89	484.53	18.34	502.86	2.49	229336.75	9444.64
2	-4	0	0.15	136.61	140.47	9.13	149.48	3.86	18663.60	952.36
2	4	0	0.15	141.58	140.47	7.88	148.33	2.29	20044.60	852.54
2	4	0	0.15	138.69	140.47	7.88	148.33	2.80	19235.59	989.27
2	4	0	0.15	137.08	140.47	7.88	148.33	3.29	18789.92	976.02
-2	4	0	0.15	137.35	140.47	9.13	149.48	3.54	18865.14	983.59
-9	-1	1	0.13	66.57	48.20	13.92	60.31	2.17	4432.07	367.13
-9	-1	1	0.13	65.77	48.20	13.92	60.31	3.09	4326.09	223.31
7	-1	-1	0.11	224.39	75.57	125.45	200.83	4.96	50352.31	2019.69
-7	-1	1	0.11	223.56	79.72	125.33	204.98	3.97	49977.61	2006.92
7	1	-1	0.11	223.88	79.72	125.33	204.98	4.00	50120.96	2027.26
-7	-1	1	0.11	224.24	79.72	125.33	204.98	3.93	50281.34	2102.96
7	1	-1	0.11	224.77	79.72	125.33	204.98	4.24	50519.31	2004.55
7	-1	-1	0.11	224.43	75.57	125.45	200.83	4.95	50368.39	2025.84
7	1	-1	0.11	227.45	79.72	125.33	204.98	4.61	51731.89	2109.58
5	1	-1	0.08	125.10	15.25	103.93	118.91	2.19	15649.43	690.26
5	-1	-1	0.08	123.38	13.42	103.82	117.04	2.23	15221.75	684.59
-5	1	1	0.08	128.40	13.42	103.82	117.04	3.81	16486.36	731.90

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-5	-1	1	0.08	125.55	15.25	103.93	118.91	2.25	15762.98	722.91
1	1	-1	0.05	141.77	104.39	51.69	156.08	4.73	20099.95	900.32
1	-1	-1	0.05	141.17	104.02	52.23	156.07	4.85	19929.63	913.10
-1	1	1	0.05	150.17	104.02	52.23	156.07	2.02	22550.17	892.75
1	1	1	0.05	416.55	595.00	155.13	439.87	2.79	173517.69	7155.74
-1	-1	-1	0.05	421.72	595.00	155.13	439.87	2.23	177847.08	7008.61
3	-1	1	0.06	10.13	211.99	198.84	15.99	2.49	102.66	61.50
5	1	1	0.09	19.04	31.89	25.19	6.70	3.15	362.40	100.77
5	1	1	0.09	18.48	31.89	25.19	6.70	3.04	341.58	97.46
-5	-1	-1	0.09	22.74	31.89	25.19	6.70	4.73	517.11	99.83
5	-1	1	0.09	23.54	36.47	26.90	17.48	2.21	554.01	112.60
-5	1	-1	0.09	34.05	36.47	26.90	17.48	5.22	1159.59	163.70
-7	-1	-1	0.11	98.03	175.24	63.23	112.05	4.91	9609.75	599.90
7	1	1	0.11	106.18	175.24	63.23	112.05	2.21	11273.19	579.56
-7	1	-1	0.11	106.44	178.32	63.05	115.28	3.19	11330.44	615.04
9	-1	1	0.14	131.47	147.95	7.34	154.99	8.08	17284.96	834.09
9	-1	1	0.14	130.17	147.95	7.34	154.99	9.44	16943.38	749.87
-9	1	-1	0.14	131.53	147.95	7.34	154.99	7.70	17300.11	872.88
-9	-1	-1	0.14	130.88	144.40	9.16	151.69	6.72	17129.31	875.25
-9	-1	-1	0.14	127.23	144.40	9.16	151.69	8.79	16187.36	776.37
9	1	1	0.14	128.72	144.40	9.16	151.69	7.90	16568.68	815.64
-9	1	-1	0.14	137.30	147.95	7.34	154.99	6.00	18850.95	862.47
9	1	1	0.14	131.69	144.40	9.16	151.69	6.77	17341.27	837.40
-8	-2	1	0.13	25.58	62.47	33.68	28.79	2.64	654.31	66.23
8	2	-1	0.13	23.93	62.47	33.68	28.79	4.34	572.46	59.14
6	2	-1	0.11	159.56	110.37	37.34	147.63	3.29	25459.31	1115.59
-6	-2	1	0.11	163.01	110.37	37.34	147.63	4.56	26571.11	1048.41
-6	2	1	0.11	161.45	110.51	38.10	148.57	3.37	26065.83	1186.08
6	-2	-1	0.11	161.13	110.51	38.10	148.57	3.38	25961.28	1148.70
6	2	-1	0.11	163.99	110.37	37.34	147.63	4.21	26892.82	1212.10
6	-2	-1	0.11	159.42	110.51	38.10	148.57	3.02	25415.31	1107.07
-6	-2	1	0.11	159.35	110.37	37.34	147.63	3.06	25393.55	1175.20
4	2	-1	0.09	158.44	295.28	113.14	182.24	7.10	25104.48	1141.13
4	2	-1	0.09	157.00	295.28	113.14	182.24	8.16	24647.46	1049.35
-4	-2	1	0.09	160.27	295.28	113.14	182.24	7.39	25685.45	1019.07
-4	-2	1	0.09	158.89	295.28	113.14	182.24	7.22	25244.99	1103.29
4	-2	-1	0.09	156.04	295.91	113.63	182.31	8.62	24347.51	1031.37
4	-2	-1	0.09	159.30	295.91	113.63	182.31	7.20	25375.09	1091.93
-4	2	1	0.09	155.94	295.91	113.63	182.31	8.04	24317.70	1109.44
0	2	1	0.08	91.06	27.75	100.31	72.57	6.89	8292.15	439.52
0	2	-1	0.08	90.88	26.97	100.55	73.60	7.06	8259.50	402.61
0	2	-1	0.08	93.12	26.97	100.55	73.60	7.48	8670.63	435.26
0	-2	-1	0.08	92.63	27.75	100.31	72.57	7.67	8580.27	431.95
0	2	-1	0.08	92.67	26.97	100.55	73.60	7.23	8587.84	438.57
0	2	-1	0.08	92.75	26.97	100.55	73.60	7.33	8602.98	434.79
-4	-2	-1	0.10	13.79	10.91	12.11	3.34	2.09	190.19	85.63
-4	2	-1	0.10	16.28	11.36	11.56	3.65	3.45	264.94	72.86
-4	-2	-1	0.10	17.56	10.91	12.11	3.34	2.77	308.47	107.40

4	2	1	0.10	15.35	10.91	12.11	3.34	2.51	235.61	89.42
-4	2	-1	0.10	17.75	11.36	11.56	3.65	2.54	315.09	118.75
4	-2	1	0.10	14.13	11.36	11.56	3.65	3.10	199.65	60.08
-6	2	-1	0.12	176.82	135.39	30.34	165.53	2.68	31266.22	1444.87
6	-2	1	0.12	186.51	135.39	30.34	165.53	5.26	34787.56	1405.60
6	2	1	0.12	182.50	134.11	29.93	163.82	4.42	33305.79	1464.74
-6	-2	-1	0.12	183.29	134.11	29.93	163.82	4.94	33593.91	1368.70
6	2	1	0.12	177.01	134.11	29.93	163.82	3.31	31333.88	1359.71
-6	-2	-1	0.12	182.99	134.11	29.93	163.82	4.55	33486.52	1461.90
-8	2	-1	0.14	127.82	100.74	20.27	120.93	2.03	16338.75	843.55
8	-2	1	0.14	132.55	100.74	20.27	120.93	3.62	17569.30	814.69
8	2	1	0.14	128.08	100.86	20.01	120.88	2.15	16404.04	834.56
-8	-2	-1	0.14	132.98	100.86	20.01	120.88	4.06	17684.74	757.44
-8	2	-1	0.14	133.41	100.74	20.27	120.93	3.72	17797.34	852.54
-7	3	1	0.15	136.87	131.68	22.45	154.12	4.73	18732.20	1061.65
7	3	-1	0.15	147.14	135.68	22.86	158.53	3.48	21649.85	1000.62
-7	-3	1	0.15	150.44	135.68	22.86	158.53	2.31	22633.44	1083.42
5	-3	-1	0.13	189.48	126.21	52.12	178.32	2.66	35903.15	1543.28
5	3	-1	0.13	187.51	124.77	52.37	177.02	2.61	35161.32	1467.10
-5	-3	1	0.13	189.85	124.77	52.37	177.02	3.25	36041.29	1448.18
5	-3	-1	0.13	189.87	126.21	52.12	178.32	2.92	36049.81	1454.80
-5	3	1	0.13	189.19	126.21	52.12	178.32	2.54	35793.86	1571.19
-3	-3	1	0.12	18.91	128.13	124.96	7.26	2.54	357.67	120.17
3	3	-1	0.12	22.85	128.13	124.96	7.26	2.73	522.31	172.21
1	3	1	0.11	404.12	381.94	3.63	378.72	3.28	163308.98	6063.81
-1	-3	-1	0.11	394.99	381.94	3.63	378.72	2.09	156016.03	6035.90
-1	-3	-1	0.11	396.07	381.94	3.63	378.72	2.22	156873.30	6064.29
-5	3	-1	0.13	300.36	310.71	3.43	314.02	2.24	90217.25	3751.27
-5	3	-1	0.13	299.99	310.71	3.43	314.02	2.28	89993.95	3781.07
2	4	-1	0.15	124.48	117.11	20.43	137.51	4.76	15494.73	717.23
2	4	-1	0.15	128.01	117.11	20.43	137.51	3.04	16385.59	828.88
2	4	-1	0.15	128.66	117.11	20.43	137.51	2.84	16553.07	828.88
-2	4	1	0.15	128.18	115.69	20.12	135.62	2.35	16430.06	835.03
2	-4	-1	0.15	123.69	115.69	20.12	135.62	4.65	15300.28	665.19
-2	4	1	0.15	123.38	115.69	20.12	135.62	4.10	15222.69	772.58
-2	-4	1	0.15	120.93	117.11	20.43	137.51	5.70	14624.21	751.29
2	-4	-1	0.15	123.64	115.69	20.12	135.62	3.90	15286.09	795.77
0	4	-1	0.15	167.47	181.76	4.76	177.15	2.56	28046.73	1303.88
0	4	1	0.15	167.47	182.92	5.44	177.80	2.76	28045.79	1294.89
0	-4	-1	0.15	166.21	182.92	5.44	177.80	3.13	27624.25	1274.08
0	4	-1	0.15	169.59	181.76	4.76	177.15	2.17	28760.65	1207.84
0	4	-1	0.15	166.49	181.76	4.76	177.15	2.79	27717.45	1311.93
0	-4	-1	0.15	171.22	182.92	5.44	177.80	2.01	29316.08	1144.45
-10	0	2	0.15	113.49	145.81	47.91	97.93	4.75	12879.39	692.16
10	0	-2	0.15	104.56	145.81	47.91	97.93	2.14	10932.08	627.34
10	0	-2	0.15	110.04	145.81	47.91	97.93	4.52	12108.70	557.79
10	0	-2	0.15	111.94	145.81	47.91	97.93	4.56	12531.66	644.84
8	0	-2	0.12	48.11	29.75	14.06	18.83	8.01	2314.44	244.60

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-8	0	2	0.12	48.21	29.75	14.06	18.83	7.69	2323.90	255.95
8	0	-2	0.12	47.55	29.75	14.06	18.83	10.33	2260.98	184.51
4	0	-2	0.08	134.36	127.21	228.51	101.31	10.53	18051.40	739.47
4	0	-2	0.08	128.49	127.21	228.51	101.31	8.26	16510.96	756.03
-4	0	2	0.08	134.00	127.21	228.51	101.31	9.95	17956.30	773.53
-2	0	2	0.06	508.96	516.62	36.59	480.35	2.82	259043.61	10050.21
2	0	-2	0.06	503.39	516.62	36.59	480.35	2.33	253396.59	9715.25
0	0	-2	0.06	243.70	2.76	215.18	212.45	6.11	59391.02	2333.84
0	0	-2	0.06	240.46	2.76	215.18	212.45	5.50	57821.73	2305.92
-2	0	-2	0.07	255.43	458.73	181.81	276.97	4.28	65242.88	2676.37
-2	0	-2	0.07	263.28	458.73	181.81	276.97	2.77	69317.75	2666.43
2	0	2	0.07	256.65	458.73	181.81	276.97	4.13	65870.70	2624.80
-4	0	-2	0.08	393.76	433.82	19.88	414.21	2.67	155044.75	6199.59
-4	0	-2	0.08	396.50	433.82	19.88	414.21	2.35	157213.00	6105.92
4	0	2	0.08	395.54	433.82	19.88	414.21	2.50	156455.55	6054.82
9	-1	-2	0.14	142.76	57.43	69.43	126.78	4.62	20379.09	932.02
9	1	-2	0.14	142.85	57.43	69.57	127.00	4.37	20405.11	978.86
-9	1	2	0.14	139.82	57.43	69.43	126.78	3.55	19550.20	979.80
9	1	-2	0.14	140.39	57.43	69.57	127.00	4.41	19710.59	812.32
9	1	-2	0.14	139.06	57.43	69.57	127.00	3.95	19338.72	811.85
9	-1	-2	0.14	140.42	57.43	69.43	126.78	4.07	19716.74	896.06
-9	-1	2	0.14	144.61	57.43	69.57	127.00	4.85	20910.86	986.43
9	1	-2	0.14	141.94	57.43	69.57	127.00	4.28	20146.32	939.12
7	-1	-2	0.11	53.77	151.49	85.71	66.03	5.80	2890.68	253.11
-7	-1	2	0.11	54.83	151.49	85.26	66.23	8.87	3006.12	155.65
7	1	-2	0.11	51.27	151.49	85.26	66.23	11.05	2629.06	158.96
-7	1	2	0.11	57.00	151.49	85.71	66.03	3.79	3248.83	293.33
7	1	-2	0.11	56.66	151.49	85.26	66.23	4.27	3210.50	275.35
-7	-1	2	0.11	49.72	151.49	85.26	66.23	7.22	2472.46	264.94
7	1	-2	0.11	58.45	151.49	85.26	66.23	3.14	3416.31	308.47
7	-1	-2	0.11	51.77	151.49	85.71	66.03	6.92	2679.68	242.70
-5	1	2	0.09	125.19	198.20	49.21	148.99	9.09	15672.14	718.18
5	1	-2	0.09	124.75	198.20	48.17	150.19	11.09	15561.44	630.65
5	1	-2	0.09	121.64	198.20	48.17	150.19	10.63	14797.37	729.53
5	1	-2	0.09	122.03	198.20	48.17	150.19	11.05	14891.04	693.57
5	-1	-2	0.09	123.42	198.20	49.21	148.99	10.17	15232.15	685.06
-5	-1	2	0.09	116.90	198.20	48.17	150.19	12.74	13666.64	697.83
-5	-1	2	0.09	121.22	198.20	48.17	150.19	12.67	14694.70	620.24
5	-1	-2	0.09	121.48	198.20	49.21	148.99	11.04	14757.63	674.18
-3	1	2	0.08	20.24	15.36	19.04	34.37	8.58	409.71	89.89
3	-1	-2	0.08	23.16	15.36	19.04	34.37	6.19	536.50	104.08
3	1	-2	0.08	25.75	15.36	18.57	33.83	4.42	663.30	108.81
3	1	-2	0.08	21.24	15.36	18.57	33.83	6.18	451.34	112.13
-3	-1	2	0.08	19.89	15.36	18.57	33.83	9.42	395.52	79.48
3	-1	-2	0.08	24.43	15.36	19.04	34.37	6.33	597.06	92.26
3	1	-2	0.08	26.60	15.36	18.57	33.83	4.62	707.30	94.62
1	1	-2	0.07	18.19	29.34	19.35	10.00	3.78	330.70	61.03
1	1	-2	0.07	17.39	29.34	19.35	10.00	2.50	302.32	80.90

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1	-1	-2	0.07	19.38	29.34	19.87	11.14	3.07	375.65	81.85
-1	1	2	0.07	16.88	29.34	19.87	11.14	2.46	284.81	65.29
1	1	-2	0.07	17.88	29.34	19.35	10.00	2.67	319.82	82.32
1	-1	-2	0.07	18.33	29.34	19.87	11.14	3.44	335.91	61.50
-1	-1	-2	0.07	162.99	167.62	12.35	156.02	2.04	26567.33	1088.62
-5	-1	-2	0.10	40.38	198.32	131.01	67.37	15.10	1630.33	192.55
5	-1	2	0.10	44.68	198.32	130.98	67.58	11.97	1996.04	214.79
-5	1	-2	0.10	44.33	198.32	130.98	67.58	10.96	1964.81	237.50
-5	1	-2	0.10	42.55	198.32	130.98	67.58	14.38	1810.58	191.61
5	1	2	0.10	41.52	198.32	131.01	67.37	15.34	1723.53	183.57
-5	-1	-2	0.10	45.91	198.32	131.01	67.37	11.52	2108.17	211.01
-9	1	-2	0.15	159.81	133.63	33.94	167.55	2.04	25539.74	1241.43
8	2	-2	0.14	89.73	40.41	58.74	99.11	3.40	8051.81	520.42
8	-2	-2	0.14	91.48	40.41	59.81	100.02	3.49	8368.32	468.38
8	2	-2	0.14	89.26	40.41	58.74	99.11	4.01	7968.07	462.70
-8	-2	2	0.14	89.10	40.41	58.74	99.11	3.82	7938.74	492.98
-8	2	2	0.14	85.82	40.41	59.81	100.02	5.38	7365.33	490.61
8	-2	-2	0.14	85.80	40.41	59.81	100.02	6.00	7362.02	439.99
-4	2	2	0.10	175.99	271.38	69.96	201.85	7.31	30971.01	1336.05
4	2	-2	0.10	169.97	271.38	69.90	201.53	8.61	28888.86	1362.55
-4	-2	2	0.10	174.02	271.38	69.90	201.53	7.85	30283.11	1316.66
4	2	-2	0.10	179.02	271.38	69.90	201.53	6.80	32049.69	1259.41
4	-2	-2	0.10	174.36	271.38	69.96	201.85	7.87	30401.86	1314.76
4	2	-2	0.10	168.91	271.38	69.90	201.53	9.42	28529.30	1283.07
4	-2	-2	0.10	179.42	271.38	69.96	201.85	6.82	32193.04	1252.79
2	-2	-2	0.09	103.38	54.61	11.16	64.83	12.04	10688.43	538.87
2	2	-2	0.09	99.85	54.61	9.99	64.50	11.38	9970.73	510.48
2	2	-2	0.09	102.39	54.61	9.99	64.50	12.39	10484.05	510.48
-2	2	2	0.09	102.70	54.61	11.16	64.83	12.02	10547.45	527.99
2	-2	-2	0.09	102.20	54.61	11.16	64.83	13.89	10445.26	449.45
2	2	-2	0.09	101.57	54.61	9.99	64.50	11.18	10315.63	550.70
2	2	-2	0.09	101.42	54.61	9.99	64.50	11.88	10285.35	515.69
0	2	2	0.09	219.32	305.11	95.17	210.02	2.08	48101.27	1919.87
0	2	-2	0.09	221.25	305.11	94.87	210.25	2.37	48952.38	2000.30
0	-2	-2	0.09	224.52	305.11	95.17	210.02	3.26	50410.03	1929.80

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5	-3	-2	0.14	227.05	239.84	27.51	212.41	3.17	51552.58	2028.21
-5	3	2	0.14	230.52	239.84	27.51	212.41	3.68	53140.33	2180.55
5	3	-2	0.14	223.09	239.84	26.85	213.02	2.12	49768.49	2072.68
5	3	-2	0.14	223.51	239.84	26.85	213.02	2.25	49957.26	2036.25
3	-3	-2	0.13	121.89	83.97	20.20	104.14	5.55	14856.03	722.43
3	-3	-2	0.13	121.02	83.97	20.20	104.14	6.31	14646.45	602.27
3	3	-2	0.13	113.12	83.97	20.33	104.29	2.75	12797.07	696.89
3	3	-2	0.13	117.77	83.97	20.33	104.29	4.48	13870.55	667.55
3	3	-2	0.13	113.73	83.97	20.33	104.29	3.11	12935.22	660.93
3	3	-2	0.13	119.26	83.97	20.33	104.29	4.49	14223.96	746.09
-3	3	2	0.13	118.31	83.97	20.20	104.14	4.38	13997.34	718.65
1	3	-2	0.12	86.28	173.65	57.27	116.38	14.51	7443.39	420.59
1	-3	-2	0.12	86.02	173.65	57.21	116.44	19.20	7399.87	320.77
-1	3	2	0.12	85.23	173.65	57.21	116.44	19.74	7263.61	318.87
1	3	-2	0.12	89.81	173.65	57.27	116.38	11.44	8065.53	478.78
1	3	-2	0.12	87.32	173.65	57.27	116.38	13.28	7625.54	445.67
-1	3	2	0.12	90.36	173.65	57.21	116.44	11.34	8164.88	475.47
1	3	-2	0.12	84.71	173.65	57.27	116.38	14.37	7175.61	443.30
1	-3	-2	0.12	86.71	173.65	57.21	116.44	13.44	7518.14	449.45
-3	3	-2	0.13	36.09	69.08	38.53	30.56	2.21	1302.46	167.01
-5	-3	-2	0.14	44.28	41.91	7.98	49.28	2.11	1960.56	221.89
5	-3	2	0.14	39.43	41.91	7.67	49.20	4.07	1555.10	212.90
5	3	2	0.14	43.09	41.91	7.98	49.28	3.48	1856.95	164.17
-5	3	-2	0.14	41.58	41.91	7.67	49.20	2.62	1729.21	263.52
-5	-3	-2	0.14	35.61	41.91	7.98	49.28	5.68	1268.40	204.38
-5	3	-2	0.14	42.32	41.91	7.67	49.20	3.89	1791.18	161.80
-5	3	-2	0.14	42.12	41.91	7.67	49.20	2.94	1773.68	219.99
9	1	-3	0.15	199.61	159.72	59.57	219.03	4.75	39845.55	1712.65
9	-1	-3	0.15	201.26	155.98	60.26	216.23	3.68	40505.06	1700.35
9	1	-3	0.15	198.31	159.72	59.57	219.03	5.42	39327.50	1596.26
-9	-1	3	0.15	196.70	159.72	59.57	219.03	5.31	38690.22	1750.02
9	-1	-3	0.15	201.48	155.98	60.26	216.23	3.68	40594.95	1673.85
9	1	-3	0.15	201.76	159.72	59.57	219.03	4.08	40708.50	1780.30
-9	1	3	0.15	199.56	155.98	60.26	216.23	3.93	39825.20	1761.38
7	-1	-3	0.13	104.65	81.74	39.51	121.23	6.77	10952.43	553.06
-7	1	3	0.13	102.78	81.74	39.51	121.23	7.03	10563.06	588.07
7	-1	-3	0.13	104.39	81.74	39.51	121.23	6.73	10898.02	564.89
7	1	-3	0.13	101.25	79.12	40.35	119.01	6.89	10251.28	568.20
-7	-1	3	0.13	107.09	79.12	40.35	119.01	4.50	11467.64	598.95
7	1	-3	0.13	107.13	79.12	40.35	119.01	5.35	11477.10	502.44
5	1	-3	0.11	80.12	140.18	51.29	88.90	3.59	6418.64	413.02
-3	1	3	0.10	154.71	59.51	88.79	148.10	2.02	23934.01	992.58
-1	1	3	0.09	98.80	18.64	106.79	90.69	3.51	9762.09	437.62
-1	-1	3	0.09	96.21	23.35	106.95	84.98	5.00	9257.29	407.35
1	-1	-3	0.09	97.85	18.64	106.79	90.69	3.05	9574.74	442.36
1	1	-3	0.09	93.95	23.35	106.95	84.98	3.36	8827.23	477.36
1	1	-3	0.09	92.44	23.35	106.95	84.98	2.84	8544.79	466.48
-1	-1	-3	0.10	54.02	114.31	74.36	39.95	6.84	2918.60	193.50

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-1	1	-3	0.10	50.17	113.41	73.92	39.60	5.93	2517.40	159.91
1	1	3	0.10	50.89	114.31	74.36	39.95	5.53	2590.26	179.78
-1	1	-3	0.10	52.95	113.41	73.92	39.60	4.92	2804.11	251.22
-1	1	-3	0.10	51.85	113.41	73.92	39.60	5.02	2688.67	223.31
-1	-1	-3	0.10	50.90	114.31	74.36	39.95	4.49	2591.21	221.41
-3	-1	-3	0.11	239.28	42.91	173.10	215.62	4.60	57257.30	2339.04
3	1	3	0.11	238.27	42.91	173.10	215.62	4.50	56774.74	2286.05
-3	1	-3	0.11	241.69	38.19	173.53	211.28	5.92	58416.42	2327.69
-3	-1	-3	0.11	240.62	42.91	173.10	215.62	4.85	57896.00	2351.34
-3	1	-3	0.11	237.19	38.19	173.53	211.28	4.91	56257.63	2364.59
-7	-1	-3	0.14	132.67	143.08	8.32	151.23	6.24	17601.00	844.97
-7	1	-3	0.14	125.97	139.20	8.06	147.26	6.74	15868.01	862.47
-7	-1	-3	0.14	133.13	143.08	8.32	151.23	6.07	17724.01	847.33
-7	1	-3	0.14	132.06	139.20	8.06	147.26	5.09	17438.72	835.03
7	-1	3	0.14	132.12	139.20	8.06	147.26	5.02	17454.81	842.60
7	1	3	0.14	129.54	143.08	8.32	151.23	7.58	16780.16	803.81
-6	-2	3	0.13	172.86	108.10	55.35	163.44	2.49	29879.55	1270.77
4	-2	-3	0.12	37.40	54.72	9.76	45.45	4.27	1398.98	156.13
-4	-2	3	0.12	37.44	54.22	10.34	44.70	3.51	1401.82	169.85
4	2	-3	0.12	39.10	54.22	10.34	44.70	2.27	1529.08	206.75
4	2	-3	0.12	39.30	54.22	10.34	44.70	2.48	1544.69	182.62
2	-2	-3	0.11	103.16	164.96	72.87	92.10	4.65	10642.54	464.59
-2	2	3	0.11	99.23	164.96	72.87	92.10	2.62	9846.30	519.94
2	2	-3	0.11	99.47	163.86	72.60	91.59	2.72	9893.61	552.59
2	2	-3	0.11	99.40	163.86	72.60	91.59	2.84	9881.31	524.68
2	2	-3	0.11	99.73	163.86	72.60	91.59	3.14	9946.60	496.29
2	-2	-3	0.11	98.88	164.96	72.87	92.10	2.43	9778.18	533.66
2	2	-3	0.11	99.12	163.86	72.60	91.59	2.72	9824.54	528.46
0	-2	-3	0.11	124.24	33.89	77.70	111.57	4.68	15436.06	638.69
0	2	3	0.11	121.29	33.89	77.70	111.57	3.21	14711.74	706.35
0	2	-3	0.11	123.21	34.65	76.85	111.49	3.81	15179.64	722.43
0	2	-3	0.11	124.50	34.65	76.85	111.49	4.47	15500.41	687.42
0	2	-3	0.11	120.40	34.65	76.85	111.49	2.79	14496.00	739.47
0	-2	-3	0.11	120.45	33.89	77.70	111.57	2.82	14507.36	729.53
-2	-2	-3	0.12	29.34	56.17	20.14	36.03	2.51	861.05	174.10
4	-2	3	0.13	160.56	160.81	10.54	170.83	2.82	25780.55	1207.37
-3	3	3	0.14	197.85	116.13	69.51	185.56	2.77	39145.82	1699.40
3	-3	-3	0.14	197.52	116.13	69.51	185.56	2.72	39012.88	1685.21
3	3	-3	0.14	196.06	117.26	69.48	186.73	2.18	38439.95	1642.15
3	-3	-3	0.14	203.03	116.13	69.51	185.56	4.36	41219.92	1554.63
1	3	-3	0.14	206.31	145.67	70.82	216.46	2.33	42564.97	1838.02
1	3	-3	0.14	204.13	145.67	70.82	216.46	2.79	41668.43	1861.20
1	3	-3	0.14	204.84	145.67	70.82	216.46	2.58	41959.86	1896.69
-1	3	-3	0.14	75.99	92.30	1.92	90.88	6.01	5774.74	413.02
-1	3	-3	0.14	74.45	92.30	1.92	90.88	7.28	5542.92	373.28
1	3	3	0.14	77.16	92.78	2.91	90.42	5.69	5953.58	390.31
1	3	3	0.14	74.63	92.78	2.91	90.42	10.07	5569.89	258.79
-1	3	-3	0.14	78.34	92.30	1.92	90.88	5.72	6136.67	370.92

1	3	3	0.14	74.28	92.78	2.91	90.42	10.07	5517.85	263.99
-1	-3	-3	0.14	76.00	92.78	2.91	90.42	6.08	5775.69	394.57
-1	3	-3	0.14	72.54	92.30	1.92	90.88	8.28	5262.37	361.93
4	0	-4	0.12	28.86	167.65	146.49	22.03	2.11	833.14	165.11
-4	0	4	0.12	29.29	167.65	146.49	22.03	2.89	857.74	128.69
4	0	-4	0.12	29.54	167.65	146.49	22.03	2.30	872.88	168.43
2	0	-4	0.11	383.52	253.80	95.79	349.59	4.25	147084.25	5858.48
2	0	-4	0.11	381.39	253.80	95.79	349.59	4.02	145461.02	5784.21
2	0	-4	0.11	387.56	253.80	95.79	349.59	4.87	150199.19	5751.09
-2	0	4	0.11	382.57	253.80	95.79	349.59	4.11	146358.97	5870.31
0	0	-4	0.11	130.68	201.05	62.04	139.49	2.97	17076.80	802.39
-2	0	-4	0.12	53.32	89.43	63.36	26.29	11.32	2843.37	190.19
-2	0	-4	0.12	54.21	89.43	63.36	26.29	7.54	2938.47	298.06
-2	0	-4	0.12	51.58	89.43	63.36	26.29	8.23	2660.28	239.39
4	0	4	0.13	13.30	27.12	48.57	22.94	2.59	176.94	134.84
-4	0	-4	0.13	13.44	27.12	48.57	22.94	3.50	180.73	98.88
-6	0	-4	0.15	54.26	158.21	70.31	88.24	14.92	2943.67	324.55
6	0	4	0.15	55.71	158.21	70.31	88.24	16.77	3104.06	279.13
-6	0	-4	0.15	56.35	158.21	70.31	88.24	17.78	3175.49	259.26
-7	-1	4	0.15	74.10	52.14	17.10	68.82	2.11	5490.41	357.20
-5	-1	4	0.13	243.73	236.41	8.08	228.45	2.97	59405.68	2428.93
-5	1	4	0.13	250.43	236.41	9.14	227.84	4.41	62715.07	2451.64
5	1	-4	0.13	243.61	236.41	8.08	228.45	2.99	59347.50	2397.71
5	-1	-4	0.13	243.73	236.41	9.14	227.84	3.12	59403.32	2401.49
3	1	-4	0.12	123.79	111.26	6.38	117.30	2.15	15324.88	727.64
-1	-1	4	0.12	135.00	99.24	42.28	141.43	2.35	18225.97	755.55
1	1	-4	0.12	129.71	99.24	42.28	141.43	3.80	16824.16	836.45
-1	-1	4	0.12	135.62	99.24	42.28	141.43	2.14	18392.98	754.13
1	-1	-4	0.12	129.28	99.24	42.14	141.37	3.87	16713.93	845.44
-1	-1	-4	0.12	52.88	114.32	67.52	46.92	2.15	2796.54	277.24
-1	1	-4	0.12	54.72	114.32	66.95	47.46	2.52	2994.29	294.75
-3	1	-4	0.13	54.82	37.33	30.70	68.01	5.18	3004.70	312.72
3	1	4	0.13	56.09	37.33	31.89	69.09	6.14	3146.64	264.94
-3	-1	-4	0.13	51.77	37.33	31.89	69.09	9.06	2680.62	230.88
-3	1	-4	0.13	58.03	37.33	30.70	68.01	5.85	3367.58	214.79
-3	-1	-4	0.13	55.74	37.33	31.89	69.09	5.99	3106.42	278.19
-5	1	-4	0.15	266.19	253.77	26.45	280.21	2.54	70858.66	3009.91
-5	-1	-4	0.15	268.49	253.77	25.75	279.51	2.03	72086.38	2975.37
4	-2	-4	0.14	14.35	31.40	66.01	35.16	9.23	205.80	111.65
-4	2	4	0.14	7.05	31.40	66.01	35.16	12.86	49.68	92.26
4	2	-4	0.14	8.08	31.40	66.14	35.36	13.46	65.29	88.00
4	-2	-4	0.14	13.36	31.40	66.01	35.16	11.29	178.36	93.68
4	2	-4	0.14	8.14	31.40	66.14	35.36	10.60	66.23	111.65
-4	-2	4	0.14	13.10	31.40	66.14	35.36	11.87	171.74	90.84
2	2	-4	0.14	80.21	63.73	3.36	61.44	6.43	6434.26	413.50
-2	2	4	0.14	78.38	63.73	5.16	60.71	6.52	6143.30	377.07
2	-2	-4	0.14	80.26	63.73	5.16	60.71	6.57	6440.88	419.65
2	-2	-4	0.14	82.16	63.73	5.16	60.71	8.67	6750.29	353.41

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2	2	-4	0.14	77.55	63.73	3.36	61.44	5.51	6014.61	406.40
0	2	-4	0.13	180.27	58.50	96.67	154.96	5.62	32498.67	1510.63
0	-2	-4	0.13	187.42	58.50	96.88	155.02	7.20	35125.83	1540.44
0	2	-4	0.13	185.97	58.50	96.67	154.96	6.83	34586.49	1547.06
0	2	-4	0.13	190.64	58.50	96.67	154.96	8.36	36342.19	1475.15
0	-2	-4	0.13	188.94	58.50	96.88	155.02	8.09	35699.71	1442.50
0	2	4	0.13	192.49	58.50	96.88	155.02	8.60	37050.91	1513.94
2	2	4	0.14	12.44	15.91	54.68	38.90	12.43	154.71	109.29
2	2	4	0.14	13.69	15.91	54.68	38.90	13.67	187.35	96.99
-2	2	-4	0.14	18.53	15.91	55.18	39.57	9.75	343.48	125.37
-2	2	-4	0.14	12.01	15.91	55.18	39.57	16.33	144.30	87.05
-2	2	-4	0.14	16.49	15.91	55.18	39.57	8.41	272.04	153.76
-2	-2	-4	0.14	9.15	15.91	54.68	38.90	12.91	83.74	110.71
-1	-1	5	0.15	145.17	9.05	112.86	121.91	7.19	21073.13	863.89
-1	1	5	0.15	144.80	9.01	112.91	121.90	6.84	20967.16	892.75
1	-1	-5	0.15	144.46	9.01	112.91	121.90	6.03	20869.22	996.84
1	1	-5	0.15	141.10	9.05	112.86	121.91	5.18	19909.29	974.60
1	1	-5	0.15	145.56	9.05	112.86	121.91	6.33	21187.15	998.73
1	-1	-5	0.15	143.08	9.01	112.91	121.90	5.95	20472.76	943.38

:: Nr. of Eliminated Reflections (Theta Limit = 27.5 Deg) = 2759

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SQUEEZE Statistics on the Difference Map Phasing

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FcMod = Average contribution to Fc from discrete model
 FcSolv = Average contribution to Fc from solvent region
 FcTot = Average Fc total (= model + solvent contrib.)
 DelMS = Average Phase difference between model and solvent contrib.
 DelMT = Average Phase difference between model and combined contrib.
 N = Number of reflections in Sin(Theta)/Lambda range
 R(Mod) = SIGMA(ABS(ABS(FcMod) - Fo)) / SIGMA(Fo)
 R(Tot) = SIGMA(ABS(ABS(FcTot) - Fo)) / SIGMA(Fo)

SinT/L	<FcMod>	<FcSolv>	<FcTot>	<Fo>	<DelMS>	<DelMT>	N	R(Mod)	R(Tot)
0.05	298.79	99.51	237.30	233.48	147.71	18.73	70.	0.405	0.047
0.10	129.19	65.84	130.40	131.75	95.90	19.64	378.	0.502	0.091
0.15	94.55	31.19	104.51	102.70	75.85	22.77	788.	0.263	0.094
0.20	76.01	18.02	76.88	74.66	96.02	20.20	1365.	0.227	0.104
0.25	57.58	12.07	58.89	57.51	93.01	15.83	2227.	0.215	0.113
0.30	45.04	8.13	45.50	43.79	90.19	12.63	3125.	0.201	0.127
0.35	37.86	5.43	38.08	36.11	92.87	9.43	4235.	0.202	0.146
0.40	24.72	4.13	25.14	23.57	89.72	12.61	4896.	0.274	0.229
0.45	17.79	3.09	18.27	17.43	86.79	12.61	5662.	0.354	0.326
0.50	14.21	2.66	14.67	13.95	88.47	14.42	6409.	0.470	0.447
0.55	10.19	2.72	10.93	11.07	85.91	19.43	6925.	0.645	0.621
0.60	6.50	2.90	7.50	9.13	86.34	27.52	7414.	0.853	0.821
0.65	4.81	2.43	5.86	8.45	81.94	28.33	3779.	0.932	0.898

Comments on and Analysis of the SQUEEZE run

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- Significant Residual Density Excursion(s) in the
 Ordered part of the Structure: -2.0 0.8

Note on how to Proceed after SQUEEZE:

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- The file .hkp now contains solvent free reflection data.
 - Rename this file .hkp to .hkl
 - Use this new .hkl file to continue SHELXL refinement with a solvent-free .ins.
 - After L.S.-convergence, run PLATON with the new .hkl and .res files
 with the instruction 'CALC FCF' to produce a final FoFc-CIF on .hkp
 - Rename this .hkp file to .fcf.
 - Append the .sqf file produced by PLATON (detailing the SQUEEZE results)
 to the .cif produced by SHELXL
- =====

```

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***** N O T I C E *****
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- PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13
- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow
- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)
- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.
- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.
- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl
- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl
- More INFO can be found on <http://www.cryst.chem.uu.nl/platon/>

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Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

=====

N: No S.U.'s (esd) on observed/calculated parameters.

W: Low density (check!) of 0.981 gcm-3
 N: Number of Ignored Lines on INPUT 4
 of which blank in column 1 4
 W: Number of unusual anisotropic displacement parameters 1
 N: Total Potential Solvent Accessible Void Vol 1499.7 Ang^3
 N: Electron Count / Cell = 404 - To be included in D(calc), F000 & Mol.Wght.

=====

:: Input Xtal Data from File char232s.ins - Data Type RES

:: NORMAL END of PLATON : 45 Pages on:
 :: char232s.lis (ASCII, 132 Characters Wide)
 :: char232s.lps (PostScript Version of .lis)
 :: char232s.pdf (PDF Version of .lis)

:: SQUEEZE xyz on :char232s.sqz
 :: SQUEEZE CIF on :char232s.sqf