FIN

Table 1 Crystal data and structure refinement for FIN.

Identification code	FIN
Empirical formula	$C_{10}H_{26}N_5Na_2O_{15}P$
Formula weight	533.31
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.0139(3)
b/Å	21.2524(8)
c/Å	22.2753(8)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	4267.2(3)
Z	8
ρ_{calc}mg/mm^3	1.660
m/mm^{-1}	0.255
F(000)	2224.0
Crystal size/mm^3	0.319 × 0.229 × 0.0549
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.24 to 53.98°
Index ranges	$-9 \le h \le 11$, $-27 \le k \le 25$, $-28 \le l \le 28$
Reflections collected	26750
Independent reflections	9320 [R_{int} = 0.1005, R_{sigma} = 0.1267]
Data/restraints/parameters	9320/15/609
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0794, wR_2 = 0.1792
Final R indexes [all data]	R_1 = 0.1160, wR_2 = 0.2118
Largest diff. peak/hole / e Å^{-3}	1.13/-0.98
Flack parameter	0.2(2)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for FIN. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	3899(2)	5125.6(9)	6271.0(8)	13.6(4)
O1	2507(6)	4267(2)	7964(2)	16.7(12)
O2	6611(7)	1689(3)	7446(3)	25.4(14)
O3	5665(6)	4662(3)	8843(2)	18.6(12)
O4	3081(6)	5295(3)	8938(2)	17.8(12)
O5	3823(6)	5030(3)	6998(2)	16.4(12)
O6	5534(6)	5105(3)	6138(2)	18.4(12)
O7	3043(6)	4596(3)	5981(2)	18.2(12)

O8	3202(6)	5762(3)	6145(2)	17.8(12)
N1	4515(8)	3584(3)	7977(3)	17.5(14)
N2	5608(9)	3071(3)	7216(3)	23.8(16)
N3	5707(7)	1843(3)	8378(3)	16.4(14)
N4	4533(8)	2771(3)	8750(3)	17.4(15)
N5	4735(9)	1878(3)	9334(3)	25.8(17)
C1	4995(10)	3589(4)	7393(4)	22.2(19)
C2	5531(9)	2677(4)	7715(3)	16.3(17)
C3	5987(10)	2059(4)	7799(4)	20.5(18)
C4	4958(9)	2188(3)	8815(3)	14.9(16)
C5	4839(9)	2993(4)	8194(3)	16.7(17)
C6	3801(9)	4096(4)	8293(3)	13.9(15)
C7	4742(9)	4698(4)	8329(3)	16.5(17)
C8	3592(9)	5210(4)	8331(3)	16.6(17)
C9	2367(10)	4940(4)	7926(3)	16.3(17)
C10	2418(9)	5154(4)	7276(3)	16.4(16)
P2	8903(2)	5936.9(9)	8860.0(8)	14.1(4)
O21	7535(6)	6842(2)	7210(2)	17.6(12)
O22	11794(7)	9416(3)	7463(3)	24.8(14)
O23	10583(6)	6381(3)	6293(2)	20.1(13)
O24	7941(7)	5823(3)	6228(2)	22.6(13)
O25	8798(6)	6046(2)	8145(2)	13.9(11)
O26	10532(6)	5983(3)	8986(2)	16.4(12)
O27	8002(6)	6457(3)	9154(2)	18.1(12)
O28	8280(6)	5291(3)	8983(2)	17.1(12)
N24	9521(8)	8244(3)	6292(3)	17.0(14)
N31	9575(8)	7505(3)	7121(3)	15.3(14)
N38	10754(7)	9195(3)	6562(3)	16.1(14)
N44	9587(8)	9087(4)	5638(3)	23.8(17)
N53	10749(8)	8076(3)	7823(3)	19.9(15)
C21	10127(10)	7540(4)	7700(3)	20.2(18)
C22	10639(9)	8420(4)	7297(3)	15.6(17)
C23	11132(9)	9027(4)	7151(3)	17.6(17)
C24	9937(9)	8825(4)	6175(4)	16.9(17)
C25	9902(8)	8074(4)	6860(3)	14.2(16)
C26	8803(9)	6982(4)	6845(3)	14.6(16)
C27	9699(9)	6369(4)	6818(3)	14.2(16)
C28	8484(10)	5876(4)	6818(3)	19.7(18)
C29	7313(9)	6168(4)	7239(3)	14.1(16)
C30	7359(9)	5950(4)	7885(3)	17.1(17)
Na1	5903(4)	5792.4(15)	10502.8(13)	20.3(7)
Na2	8474(4)	7976.8(15)	10374.5(14)	19.4(7)
Na3	7202(4)	3071.9(15)	6350.3(13)	19.0(7)
Na4	5541(4)	4121.1(15)	10385.5(14)	22.9(8)
O1W	9132(7)	8748(3)	8820(2)	23.7(13)
O2W	9243(7)	7614(3)	9438(2)	24.0(14)
O3W	5139(6)	6167(3)	9506(2)	21.2(13)
O4W	7506(7)	4977(3)	10144(2)	22.2(13)
O5W	4088(6)	5017(3)	10222(2)	20.5(13)
O6W	7016(7)	6933(3)	10336(3)	24.7(13)

O7W	3377(7)	2388(3)	10409(3)	28.5(15)
O8W	1240(7)	1439(3)	10483(2)	25.2(14)
O9W	-2076(7)	1323(3)	9920(3)	26.2(14)
O10W	7593(6)	1948(3)	6320(2)	21.8(13)
O11W	7494(7)	4163(3)	6350(2)	22.6(13)
O12W	2842(13)	2438(5)	6609(4)	81(3)
O13W	4927(7)	2774(3)	5812(3)	25.4(14)
O14W	3415(6)	3645(3)	5097(3)	22.8(13)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for FIN. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
P1	15.5(10)	16.2(10)	8.9(9)	-0.6(7)	0.1(8)	-0.8(9)
O1	16(3)	17(3)	17(3)	3(2)	-3(2)	-3(2)
O2	39(4)	20(3)	17(3)	0(2)	12(3)	7(3)
O3	19(3)	23(3)	14(3)	2(2)	-3(2)	-1(3)
O4	16(3)	27(3)	11(3)	-2(2)	0(2)	4(3)
O5	17(3)	26(3)	6(2)	0.5(19)	3(2)	2(3)
O6	16(3)	25(3)	14(3)	1(2)	1(2)	-3(3)
O7	22(3)	19(3)	14(3)	-2(2)	0(2)	-3(3)
O8	21(3)	24(3)	9(3)	-3(2)	2(2)	-2(3)
N1	22(4)	15(3)	15(3)	0(2)	4(3)	2(3)
N2	40(4)	16(4)	15(4)	3(3)	3(3)	2(4)
N3	16(3)	19(4)	14(3)	1(3)	0(3)	4(3)
N4	21(4)	22(4)	9(3)	0(2)	-1(3)	1(3)
N5	43(5)	23(4)	12(3)	2(3)	6(3)	6(4)
C1	31(5)	22(5)	14(4)	5(3)	-1(4)	1(4)
C2	18(4)	25(4)	6(3)	-4(3)	6(3)	-3(4)
C3	18(4)	21(4)	23(4)	-3(3)	4(4)	1(4)
C4	17(4)	14(4)	14(4)	-1(3)	1(3)	1(3)
C5	22(4)	16(4)	12(4)	0(3)	4(3)	1(4)
C6	16(4)	16(4)	10(3)	1(3)	-2(3)	5(4)
C7	19(4)	26(4)	5(3)	1(3)	0(3)	1(4)
C8	24(4)	23(4)	3(3)	-2(3)	-2(3)	-2(4)
C9	21(4)	17(4)	11(4)	-1(3)	4(3)	2(4)
C10	20(4)	15(4)	14(4)	3(3)	-2(3)	2(4)
P2	15.4(10)	18.8(11)	8.1(9)	-0.7(7)	-0.1(8)	1.1(9)
O21	20(3)	16(3)	17(3)	1(2)	3(2)	0(3)
O22	34(4)	20(3)	21(3)	-1(2)	-6(3)	-8(3)
O23	21(3)	26(3)	13(3)	-4(2)	3(2)	2(3)
O24	26(3)	32(3)	11(3)	-3(2)	0(2)	-12(3)
O25	16(3)	23(3)	3(2)	0.9(18)	-1(2)	-1(2)
O26	13(3)	27(3)	9(3)	1(2)	1(2)	0(3)
O27	20(3)	19(3)	15(3)	-2(2)	0(2)	2(3)
O28	21(3)	23(3)	7(3)	-2(2)	-1(2)	-1(3)
N24	21(4)	17(4)	13(3)	0(2)	1(3)	-2(3)
N31	19(3)	18(3)	8(3)	2(2)	-1(3)	-4(3)
N38	19(3)	20(4)	10(3)	2(2)	-1(3)	-2(3)

N44	34(4)	27(4)	11(3)	6(3)	-5(3)	-1(4)
N53	28(4)	19(4)	12(3)	5(2)	-4(3)	-5(3)
C21	32(5)	22(4)	7(4)	3(3)	-2(4)	-1(4)
C22	18(4)	24(4)	5(3)	1(3)	0(3)	5(4)
C23	18(4)	22(4)	13(4)	-4(3)	1(3)	-2(4)
C24	11(4)	25(4)	14(4)	-2(3)	-4(3)	4(4)
C25	11(4)	20(4)	11(4)	-1(3)	0(3)	-6(4)
C26	14(4)	22(4)	8(3)	0(3)	3(3)	-6(4)
C27	13(4)	21(4)	9(4)	-2(3)	2(3)	0(4)
C28	31(5)	19(4)	9(4)	2(3)	-2(3)	3(4)
C29	13(4)	17(4)	12(4)	1(3)	0(3)	-4(3)
C30	21(4)	21(4)	9(4)	4(3)	1(3)	-2(4)
Na1	22.8(17)	26.4(18)	11.8(15)	-1.2(12)	-1.1(14)	0.5(16)
Na2	22.0(17)	22.6(17)	13.5(16)	-0.1(12)	0.7(13)	-0.4(15)
Na3	24.3(17)	23.4(18)	9.2(15)	-0.3(11)	0.5(13)	1.0(16)
Na4	29.3(18)	29.3(19)	10.1(15)	-0.9(12)	1.7(14)	4.4(17)
O1W	31(3)	25(3)	14(3)	-2(2)	0(3)	3(3)
O2W	35(4)	22(3)	15(3)	-2(2)	-2(3)	3(3)
O3W	22(3)	28(3)	13(3)	-1(2)	0(2)	-1(3)
O4W	24(3)	38(4)	6(3)	4(2)	1(2)	1(3)
O5W	20(3)	26(3)	15(3)	2(2)	-3(2)	3(3)
O6W	29(3)	33(3)	12(3)	1(2)	-6(3)	-9(3)
O7W	34(4)	31(4)	21(3)	4(2)	-2(3)	0(3)
O8W	30(3)	33(4)	12(3)	1(2)	-5(3)	-5(3)
O9W	35(4)	29(3)	15(3)	-2(2)	3(3)	-2(3)
O10W	28(3)	26(3)	12(3)	0(2)	1(2)	0(3)
O11W	29(3)	27(3)	11(3)	1(2)	-3(3)	4(3)
O12W	99(8)	102(8)	43(6)	1(5)	-6(6)	-1(7)
O13W	28(3)	32(4)	17(3)	5(2)	2(3)	9(3)
O14W	31(3)	26(3)	12(3)	-2(2)	2(3)	-1(3)

Table 4 Bond Lengths for FIN.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
P1	O5	1.633(5)	P2	O25	1.612(5)
P1	O6	1.504(6)	P2	O26	1.498(6)
P1	O7	1.511(6)	P2	O27	1.521(6)
P1	O8	1.517(6)	P2	O28	1.509(6)
O1	C6	1.425(9)	O21	C26	1.434(9)
O1	C9	1.439(9)	O21	C29	1.447(9)
O2	C3	1.245(10)	O22	C23	1.234(10)
O3	C7	1.417(9)	O23	C27	1.414(9)
O4	C8	1.440(9)	O24	C28	1.408(9)
O5	C10	1.434(10)	O25	C30	1.434(9)
N1	C1	1.371(10)	N24	C24	1.316(10)
N1	C5	1.376(10)	N24	C25	1.360(10)
N1	C6	1.448(10)	N31	C21	1.385(10)
N2	C1	1.293(11)	N31	C25	1.374(10)
N2	C2	1.394(10)	N31	C26	1.448(10)

N3	C3	1.392(10)	N38	C23	1.401(10)
N3	C4	1.392(10)	N38	C24	1.379(10)
N4	C4	1.305(10)	N44	C24	1.356(10)
N4	C5	1.355(10)	N53	C21	1.298(10)
N5	C4	1.346(10)	N53	C22	1.384(9)
C2	C3	1.389(12)	C22	C23	1.404(12)
C2	C5	1.405(10)	C22	C25	1.388(10)
C6	C7	1.537(11)	C26	C27	1.534(11)
C7	C8	1.503(11)	C27	C28	1.515(11)
C8	C9	1.536(11)	C28	C29	1.543(11)
C9	C10	1.520(10)	C29	C30	1.513(10)

Table 5 Bond Angles for FIN.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O6	P1	O5	103.5(3)	O26	P2	O25	103.5(3)
O6	P1	O7	113.2(3)	O26	P2	O27	113.3(3)
O6	P1	O8	113.3(3)	O26	P2	O28	113.0(3)
O7	P1	O5	108.1(3)	O27	P2	O25	106.8(3)
O7	P1	O8	111.9(3)	O28	P2	O25	106.7(3)
O8	P1	O5	106.1(3)	O28	P2	O27	112.7(3)
C6	O1	C9	110.8(6)	C26	O21	C29	109.9(6)
C10	O5	P1	116.2(5)	C30	O25	P2	115.5(4)
C1	N1	C5	105.9(6)	C24	N24	C25	111.3(7)
C1	N1	C6	126.5(7)	C21	N31	C26	127.6(6)
C5	N1	C6	127.6(7)	C25	N31	C21	105.6(6)
C1	N2	C2	104.3(7)	C25	N31	C26	126.8(6)
C3	N3	C4	124.3(7)	C24	N38	C23	124.8(7)
C4	N4	C5	111.9(7)	C21	N53	C22	104.7(7)
N2	C1	N1	114.6(7)	N53	C21	N31	113.5(7)
N2	C2	C5	109.8(7)	N53	C22	C23	131.2(7)
C3	C2	N2	131.4(7)	N53	C22	C25	110.3(7)
C3	C2	C5	118.8(7)	C25	C22	C23	118.4(7)
O2	C3	N3	117.4(7)	O22	C23	N38	118.4(7)
O2	C3	C2	130.2(8)	O22	C23	C22	129.6(8)
C2	C3	N3	112.4(7)	N38	C23	C22	111.9(7)
N4	C4	N3	124.3(7)	N24	C24	N38	124.2(7)
N4	C4	N5	121.1(7)	N24	C24	N44	119.6(7)
N5	C4	N3	114.6(7)	N44	C24	N38	116.2(7)
N1	C5	C2	105.3(7)	N24	C25	N31	125.0(7)
N4	C5	N1	126.6(7)	N24	C25	C22	129.1(7)
N4	C5	C2	128.1(8)	N31	C25	C22	105.9(6)
O1	C6	N1	107.8(6)	O21	C26	N31	107.5(6)
O1	C6	C7	105.5(6)	O21	C26	C27	105.4(6)
N1	C6	C7	114.0(6)	N31	C26	C27	114.5(6)
O3	C7	C6	108.7(6)	O23	C27	C26	108.3(6)
O3	C7	C8	116.3(6)	O23	C27	C28	114.8(6)
C8	C7	C6	102.9(6)	C28	C27	C26	101.9(6)
O4	C8	C7	108.2(6)	O24	C28	C27	107.9(6)

O4	C8	C9	111.6(6)	O24	C28	C29	111.2(7)
C7	C8	C9	102.9(6)	C27	C28	C29	102.5(6)
O1	C9	C8	106.0(6)	O21	C29	C28	106.0(6)
O1	C9	C10	110.4(6)	O21	C29	C30	110.0(6)
C10	C9	C8	115.2(7)	C30	C29	C28	115.9(7)
O5	C10	C9	112.5(6)	O25	C30	C29	111.4(6)

Table 6 Hydrogen Bonds for FIN.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O3	H3	O28	1.08(8)	1.78(8)	2.727(8)	144(6)
O4	H4	O26[1]	0.82	1.91	2.725(8)	173.4
N3	H3A	O8[2]	0.91(9)	1.82(9)	2.717(9)	168(8)
N5	H5B	O7W	0.77	2.13	2.899(10)	177.4
C6	H6	N4	0.98	2.69	3.067(10)	103.4
O23	H23	O8[3]	0.82	1.97	2.723(8)	152.5
O24	H24	O6	0.82	1.88	2.660(8)	157.3
N38	H38	O28[4]	0.86	1.91	2.766(8)	170.7
N44	H44A	O9W[5]	0.85	2.05	2.904(10)	174.9
C26	H26	N24	0.98	2.63	3.022(10)	104.2
C30	H30A	O27	0.97	2.69	3.080(9)	104.6
O1W	H1WA	N53	0.85	2.22	3.017(9)	155.4
O1W	H1WB	O7[6]	0.85	1.90	2.699(8)	156.5
O2W	H2WA	O27	0.85	1.93	2.774(8)	172.4
O2W	H2WB	O1W	0.85	2.08	2.778(8)	138.7
O2W	H2WB	O12W[6]	0.85	2.54	3.019(12)	116.9
O3W	H3WA	O4	0.85	2.16	2.913(8)	147.9
O3W	H3WB	O27	0.85	1.93	2.766(8)	170.1
O4W	H4WA	O6[7]	0.85	2.01	2.837(8)	162.5
O4W	H4WB	O28	0.85	1.94	2.762(7)	162.5
O5W	H5WA	O4W	0.85	2.34	3.087(8)	147.4
O5W	H5WB	O4	0.85	2.22	3.059(8)	168.9
O5W	H5WB	O3W	0.85	2.61	3.068(8)	115.0
O6W	H6WA	O27	0.85	2.25	2.957(8)	140.8
O6W	H6WA	O3W	0.85	2.28	2.987(8)	141.0
O6W	H6WB	O13W[7]	0.85	2.67	3.018(9)	106.0
O7W	H7WA	O8W	0.85	1.94	2.793(9)	175.3
O7W	H7WB	N24[7]	0.85	2.25	3.043(9)	156.4
O8W	H8WB	O3[8]	0.85	2.28	2.827(8)	122.2
O9W	H9WA	O8[9]	0.85	2.01	2.842(8)	167.1
O9W	H9WA	O23[2]	0.85	2.51	3.022(8)	119.7
O9W	H9WB	O7W[8]	0.85	2.05	2.866(8)	160.3
O10W	H10C	O26[10]	0.85	1.91	2.745(8)	168.3
O10W	H10D	O2	0.85	1.89	2.716(8)	165.2
O11W	H11A	O6	0.86	1.86	2.710(8)	168.1
O11W	H11B	O22[10]	1.03	1.76	2.773(8)	166.3
O12W	H12A	O27[2]	0.85	2.17	2.796(12)	130.0
O12W	H12B	N2	0.84	2.40	3.139(14)	147.2
O13W	H13A	O12W	0.85	1.87	2.682(12)	160.7

O13W	H13B	O14W	0.85	2.06	2.798(8)	144.5
O14W	H14A	O26[11]	0.85	2.05	2.766(8)	141.8
O14W	H14B	O7	0.85	2.20	2.840(8)	132.0

[1]-1+X,+Y,+Z; [2]1-X,-1/2+Y,3/2-Z; [3]1+X,+Y,+Z; [4]2-X,1/2+Y,3/2-Z; [5]1/2-X,1-Y,-1/2+Z; [6]1-X,1/2+Y,3/2-Z; [7]3/2-X,1-Y,1/2+Z; [8]-1/2+X,1/2-Y,2-Z; [9]-X,-1/2+Y,3/2-Z; [10]2-X,-1/2+Y,3/2-Z; [11]3/2-X,1-Y,-1/2+Z

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for FIN.

Atom	***x***	***y***	***z***	**U(eq)**
H3	6390(90)	5060(40)	8890(40)	10(20)
H4	2350	5525	8939	27
H3A	6170(100)	1480(40)	8490(40)	20(20)
H5A	4945	1442	9345	30
H5B	4369	2025	9616	30(30)
H1	4887	3937	7144	27
H6	3522	3960	8697	17
H7	5357	4735	7968	20
H8	3991	5603	8166	20
H9	1404	5060	8095	20
H10A	1645	4939	7052	20
H10B	2216	5602	7258	20
H23	11216	6105	6314	30
H24	7088	5689	6236	34
H38	11052	9554	6432	19
H44A	8857	8943	5435	20(20)
H44B	9803	9467	5578	0(19)
H21	10059	7212	7975	24
H26	8479	7099	6440	18
H27	10323	6326	7176	17
H28	8843	5471	6970	24
H29	6328	6073	7077	17
H30A	6625	6180	8116	20
H30B	7109	5506	7904	20
H1WA	9497	8659	8479	36
H1WB	8421	9007	8776	36
H2WA	8940	7244	9358	36
H2WB	8772	7878	9224	36
H3WA	4574	6026	9232	32
H3WB	5976	6263	9356	32
H4WA	8106	5038	10433	33
H4WB	7932	5067	9815	33
H5WA	4944	4854	10256	31
H5WB	3931	5113	9858	31
H6WA	6833	6779	9992	37
H6WB	7402	7295	10297	37
H7WA	2764	2084	10425	43

H7WB	4090	2318	10650	43
H8WA	397	1278	10405	38
H8WB	1619	1252	10783	38
H9WA	-2294	1180	9574	39
H9WB	-2034	1722	9906	39
H10C	8063	1619	6218	33
H10D	7134	1881	6647	33
H11A	6790	4422	6261	34
H11B	7918	4234	6776	34
H12A	3097	2077	6481	122
H12B	3293	2637	6877	122
H13A	4224	2601	6006	38
H13B	4665	3141	5705	38
H14A	3689	3573	4739	34
H14B	3571	4030	5181	34

Experimental

Refinement model description

Number of restraints - 15, number of constraints - unknown.

Details:

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1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups, All N(H) groups
 At 1.5 times of:
  All O(H) groups, All O(H,H) groups
2. Restrained distances
 O11W-H11A = O11W-H11B = O12W-H12B
 0.85 with sigma of 0.002
3. Uiso/Uaniso restraints and constraints
Uanis(C2) ≈ Ueq, Uanis(O25) ≈ Ueq: with sigma of 0.01 and sigma for
terminal atoms of 0.05
4. Others
 Fixed Uiso: H5A(0.03)
5.a Riding coordinates:
 N5(H5A,H5B), N44(H44A,H44B), O1W(H1WA,H1WB), O2W(H2WA,H2WB), O3W(H3WA,H3WB),
 O4W(H4WA,H4WB), O5W(H5WA,H5WB), O6W(H6WA,H6WB), O7W(H7WA,H7WB), O8W(H8WA,H8WB),
  O9W(H9WA,H9WB), O10W(H10C,H10D), O11W(H11A,H11B), O12W(H12A,H12B), O13W(H13A,
 H13B), O14W(H14A,H14B)
5.b Ternary CH refined with riding coordinates:
 C6(H6), C7(H7), C8(H8), C9(H9), C26(H26), C27(H27), C28(H28), C29(H29)
5.c Secondary CH2 refined with riding coordinates:
 C10(H10A,H10B), C30(H30A,H30B)
5.d Aromatic/amide H refined with riding coordinates:
 C1(H1), N38(H38), C21(H21)
5.e Idealised tetrahedral OH refined as rotating group:
 O4(H4), O23(H23), O24(H24)
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