

# **Supporting Information for**

## **Multitasking pharmacophores support cabotegravir-based long-acting HIV Pre-Exposure Prophylaxis (PrEP)**

Zheng Wan<sup>1</sup>, Man Shi<sup>1</sup>, Yanqing Gong<sup>2</sup>, Massimo Lucci<sup>3</sup>, Jinjin Li<sup>4</sup>,  
Jiahai Zhou<sup>5</sup>, Xiao-Liang Yang<sup>\*6</sup>, Moreno Lelli<sup>3,7\*</sup>,  
Xiao He<sup>1,8\*</sup>, Jiafei Mao<sup>9,10\*</sup>

<sup>1</sup> Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, Shanghai Frontiers Science Center of Molecule Intelligent Syntheses, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, 200062, China

<sup>2</sup> State Key Laboratory of New Drug and Pharmaceutical Process, Shanghai Institute of Pharmaceutical Industry, China State Institute of Pharmaceutical Industry, 285 Gebaini Road, Shanghai, 201203, China

<sup>3</sup> C.I.R.M.M.P. - Consorzio Interuniversitario Risonanze Magnetiche di Metallo Proteine, Via L. Sacconi 6, 50019 Sesto Fiorentino, Firenze, Italy

<sup>4</sup> Key Laboratory for Thin Film and Microfabrication of Ministry of Education, Department of Micro/Nano-electronics, Shanghai Jiao Tong University, Shanghai, 200240, China

<sup>5</sup> CAS Key Laboratory of Quantitative Engineering Biology, Shenzhen Institute of Synthetic Biology, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen, 518055, China

<sup>6</sup> State Key Laboratory of Coordination Chemistry and Jiangsu Key Laboratory of Advanced Organic Materials, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, 210023, China

<sup>7</sup> Department of Chemistry “Ugo Schiff”, Magnetic Resonance Center (CERM) University of Florence, Via della Lastruccia 3, 50019 Sesto Fiorentino, Florence, Italy

<sup>8</sup> New York University–East China Normal University Center for Computational Chemistry, New York University Shanghai, Shanghai, 200062, China

<sup>9</sup> Beijing National Laboratory for Molecular Sciences (BNLMS), Institute of Chemistry, Chinese Academy of Sciences, Zhongguancun North First Street 2, 100190 Beijing, China

<sup>10</sup> Center for Physicochemical Analysis and Measurement, Institute of Chemistry, Chinese Academy of Science, Zhongguancun North First Street 2, 100190 Beijing, China

\*Correspondence to:

Jiafei Mao ([jmao2023@iccas.ac.cn](mailto:jmao2023@iccas.ac.cn)),  
Xiao He ([xiaohe@phy.ecnu.edu.cn](mailto:xiaohe@phy.ecnu.edu.cn)),  
Moreno Lelli ([moreno.elli@unifi.it](mailto:moreno.elli@unifi.it)),  
Xiaoliang Yang ([yxlnmr@nju.edu.cn](mailto:yxlnmr@nju.edu.cn))

**Table S1** The atomic coordinates ( $10^{-4}$  Å) and equivalent isotropic displacements ( $10^{-3}$  Å<sup>2</sup>) of GSK744 crystal.

Atom	x	y	z	U(eq)
F(1)	164(2)	-392(2)	5119(1)	44(1)
F(2)	-42(3)	5755(2)	5510(1)	57(1)
O(1)	-1161(2)	1631(2)	3527(1)	34(1)
O(2)	4639(2)	1466(2)	3560(1)	27(1)
O(3)	6588(2)	1690(2)	2881(1)	29(1)
O(4)	6537(2)	2725(2)	2062(1)	27(1)
O(5)	1411(2)	1559(2)	1347(1)	31(1)
N(1)	1344(2)	901(2)	3904(1)	26(1)
N(2)	1995(2)	2090(2)	2462(1)	22(1)
N(3)	4014(2)	1581(2)	1738(1)	23(1)
C(1)	241(2)	1844(3)	4596(1)	25(1)
C(2)	164(3)	1402(3)	5012(1)	28(1)
C(3)	88(3)	2672(3)	5326(1)	34(1)
C(4)	71(3)	4470(3)	5208(1)	34(1)
C(5)	151(3)	5022(3)	4802(1)	34(1)
C(6)	238(3)	3691(3)	4499(1)	28(1)
C(7)	306(3)	366(3)	4268(1)	30(1)
C(8)	523(3)	1441(3)	3554(1)	23(1)
C(9)	1775(2)	1742(2)	3194(1)	22(1)
C(10)	3732(3)	1673(2)	3232(1)	22(1)
C(11)	4756(3)	1839(2)	2848(1)	22(1)
C(12)	3908(2)	2040(3)	2474(1)	21(1)
C(13)	4951(3)	2162(2)	2073(1)	22(1)
C(14)	4603(3)	1931(3)	1307(1)	24(1)
C(15)	2939(3)	1167(3)	1080(1)	31(1)
C(16)	2039(3)	1151(3)	1749(1)	23(1)
C(17)	1089(3)	2367(3)	2059(1)	24(1)
C(18)	1001(3)	1959(3)	2810(1)	22(1)
C(19)	6398(3)	1031(3)	1185(1)	31(1)
H(3A)	6887	1716	3132	44
H(1A)	2549	869	3913	31
H(3B)	49	2318	5608	41
H(5A)	148	6286	4731	40
H(6A)	297	4052	4217	34
H(7A)	863	-750	4389	35
H(7B)	-961	58	4184	35
H(14A)	4686	3282	1259	29
H(15A)	2784	1773	809	37
H(15B)	3067	-169	1036	37
H(16A)	1835	-171	1816	28
H(17A)	1185	3666	1974	29
H(17B)	-225	2041	2079	29
H(18A)	-296	2019	2790	27
H(19A)	6683	1333	897	46
H(19B)	7382	1481	1364	46
H(19C)	6289	-300	1215	46

**Table S2** The measured bond lengths (Å) and angles (degree) for the GSK744 crystal.

Atoms	Bond length	Atoms	Bond length
F(1)-C(2)	1.355(2)	C(5)-C(6)	1.381(3)
F(2)-C(4)	1.357(2)	C(5)-H(5A)	0.9500
O(1)-C(8)	1.240(2)	C(6)-H(6A)	0.9500
O(2)-C(10)	1.260(2)	C(7)-H(7A)	0.9900
O(3)-C(11)	1.346(2)	C(7)-H(7B)	0.9900
O(3)-H(3A)	0.8400	C(8)-C(9)	1.495(2)
O(4)-C(13)	1.229(2)	C(9)-C(18)	1.374(2)
O(5)-C(16)	1.409(2)	C(9)-C(10)	1.435(3)
O(5)-C(15)	1.440(2)	C(10)-C(11)	1.454(3)
N(1)-C(8)	1.340(2)	C(11)-C(12)	1.365(3)
N(1)-C(7)	1.455(2)	C(12)-C(13)	1.507(3)
N(1)-H(1A)	0.8800	C(14)-C(19)	1.518(3)
N(2)-C(18)	1.342(2)	C(14)-C(15)	1.525(3)
N(2)-C(12)	1.397(2)	C(14)-H(14A)	1.0000
N(2)-C(17)	1.476(2)	C(15)-H(15A)	0.9900
N(3)-C(13)	1.350(2)	C(15)-H(15B)	0.9900
N(3)-C(16)	1.476(2)	C(16)-C(17)	1.509(3)
N(3)-C(14)	1.481(2)	C(16)-H(16A)	1.0000
C(1)-C(6)	1.384(3)	C(17)-H(17A)	0.9900
C(1)-C(2)	1.385(3)	C(17)-H(17B)	0.9900
C(1)-C(7)	1.513(3)	C(18)-H(18A)	0.9500
C(2)-C(3)	1.375(3)	C(19)-H(19A)	0.9800
C(3)-C(4)	1.367(3)	C(19)-H(19B)	0.9800
C(3)-H(3B)	0.9500	C(19)-H(19C)	0.9800
C(4)-C(5)	1.376(3)		
Atoms	Angle	Atoms	Angle
C(11)-O(3)-H(3A)	109.5	C(3)-C(2)-C(1)	124.17(19)
C(16)-O(5)-C(15)	105.01(14)	C(4)-C(3)-C(2)	116.26(18)
C(8)-N(1)-C(7)	122.03(17)	C(4)-C(3)-H(3B)	121.9
C(8)-N(1)-H(1A)	119.0	C(2)-C(3)-H(3B)	121.9
C(7)-N(1)-H(1A)	119.0	F(2)-C(4)-C(3)	117.69(19)
C(18)-N(2)-C(12)	121.00(15)	F(2)-C(4)-C(5)	119.2(2)
C(18)-N(2)-C(17)	120.50(15)	C(3)-C(4)-C(5)	123.14(19)
C(12)-N(2)-C(17)	118.45(15)	C(4)-C(5)-C(6)	118.23(19)
C(13)-N(3)-C(16)	122.86(15)	C(4)-C(5)-H(5A)	120.9
C(13)-N(3)-C(14)	123.66(15)	C(6)-C(5)-H(5A)	120.9
C(16)-N(3)-C(14)	110.05(14)	C(5)-C(6)-C(1)	121.68(18)
C(6)-C(1)-C(2)	116.53(18)	C(5)-C(6)-H(6A)	119.2
C(6)-C(1)-C(7)	122.45(17)	C(1)-C(6)-H(6A)	119.2
C(2)-C(1)-C(7)	121.02(18)	N(1)-C(7)-C(1)	113.07(16)
F(1)-C(2)-C(3)	117.55(17)	N(1)-C(7)-H(7A)	109.0
F(1)-C(2)-C(1)	118.28(17)	C(1)-C(7)-H(7A)	109.0
N(1)-C(7)-H(7B)	109.0	O(5)-C(15)-C(14)	104.82(14)
C(1)-C(7)-H(7B)	109.0	O(5)-C(15)-H(15A)	110.8
H(7A)-C(7)-H(7B)	107.8	C(14)-C(15)-H(15A)	110.8
O(1)-C(8)-N(1)	122.36(17)	O(5)-C(15)-H(15B)	110.8
O(1)-C(8)-C(9)	122.38(16)	C(14)-C(15)-H(15B)	110.8
N(1)-C(8)-C(9)	115.22(16)	H(15A)-C(15)-H(15B)	108.9

C(18)-C(9)-C(10)	119.29(16)	O(5)-C(16)-N(3)	104.53(14)
C(18)-C(9)-C(8)	117.93(16)	O(5)-C(16)C(17)	109.83(15)
C(10)-C(9)-C(8)	122.61(16)	N(3)-C(16)-C(17)	109.84(15)
O(2)-C(10)-C(9)	126.72(17)	O(5)-C(16)-H(16A)	110.8
O(2)-C(10)-C(11)	117.33(16)	N(3)-C(16)-H(16A)	110.8
C(9)-C(10)-C(11)	115.94(16)	C(17)-C(16)-H(16A)	110.8
O(3)-C(11)-C(12)	121.99(16)	N(2)-C(17)-C(16)	107.51(15)
O(3)-C(11)-C(10)	115.84(15)	N(2)-C(17)-H(17A)	110.2
C(12)-C(11)-C(10)	122.09(17)	C(16)-C(17)-H(17A)	110.2
C(11)-C(12)-N(2)	118.73(16)	N(2)-C(17)-H(17B)	110.2
C(11)-C(12)-C(13)	122.64(17)	C(16)-C(17)H(17B)	110.2
N(2)-C(12)-C(13)	118.62(16)	H(17A)-C(17)-H(17B)	108.5
O(4)-C(13)-N(3)	123.93(17)	N(2)-C(18)-C(9)	122.95(17)
O(4)-C(13)-C(12)	121.41(16)	N(2)-C(18)-H(18A)	118.5
N(3)-C(13)-C(12)	114.65(16)	C(9)-C(18)-H(18A)	118.5
N(3)-C(14)-C(19)	114.89(15)	C(14)-C(19)-H(19A)	109.5
N(3)-C(14)-C(15)	99.11(14)	C(14)-C(19)-H(19B)	109.5
C(19)-C(14)-H(14A)	113.85(16)	H(19A)-C(19)-H(19B)	109.5
N(3)-C(14)H(14A)	109.5	C(14)-C(19)-H(19C)	109.5
C(19)-C(14)-H(14A)	109.5	H(19A)-C(19)-H(19C)	109.5
C(15)-C(14)-H(14A)	109.5	H(19B)-C(19)-H(19C)	109.5

**Table S3** The measured torsional angles [degree] for the GSK744 crystal.

C(6)-C(1)-C(2)-F(1)	180.00(19)
C(7)-C(1)-C(2)-F(1)	0.6(3)
C(6)-C(1)-C(2)-C(3)	-0.1(3)
C(7)-C(1)-C(2)-C(3)	-179.5(2)
F(1)-C(2)-C(3)-C(4)	-179.4(2)
C(1)-C(2)-C(3)-C(4)	0.7(4)
C(2)-C(3)-C(4)-F(2)	178.7(2)
C(2)-C(3)-C(4)-C(5)	-0.9(4)
F(2)-C(4)-C(5)-C(6)	-179.0(2)
C(3)-C(4)-C(5)-C(6)	0.5(4)
C(4)-C(5)-C(6)-C(1)	0.1(4)
C(2)-C(1)-C(6)-C(5)	-0.3(3)
C(7)-C(1)-C(6)-C(5)	179.0(2)
C(8)-N(1)-C(7)-C(1)	-101.8(2)
C(6)-C(1)-C(7)-N(1)	32.6(3)
C(2)-C(1)-C(7)-N(1)	-148.08(19)
C(7)-N(1)-C(8)-O(1)	4.7(3)
C(7)-N(1)-C(8)-C(9)	-173.43(16)
O(1)-C(8)-C(9)-C(18)	-10.1(3)
N(1)-C(8)-C(9)-C(18)	168.05(17)
O(1)-C(8)-C(9)-C(10)	174.70(19)
N(1)-C(8)-C(9)-C(10)	-7.2(3)
C(18)-C(9)-C(10)-O(2)	-179.37(18)
C(8)-C(9)-C(10)-O(2)	-4.2(3)
C(18)-C(9)-C(10)-C(11)	-0.2(3)
C(8)-C(9)-C(10)-C(11)	174.96(16)
O(2)-C(10)-C(11)-O(3)	2.2(2)
C(9)-C(10)-C(11)-O(3)	-177.07(16)
O(2)-C(10)-C(11)-C(12)	179.00(18)
C(9)-C(10)-C(11)-C(12)	-0.3(3)
O(3)-C(11)-C(12)-N(2)	176.70(17)
C(10)-C(11)-C(12)-N(2)	0.1(3)
O(3)-C(11)-C(12)-C(13)	-1.7(3)
C(10)-C(11)-C(12)-C(13)	-178.30(16)
C(18)-N(2)-C(12)-C(11)	0.6(3)
C(17)-N(2)-C(12)-C(11)	178.06(16)
C(18)-N(2)-C(12)-C(13)	179.01(16)
C(17)-N(2)-C(12)-C(13)	-3.5(2)
C(16)-N(3)-C(13)-O(4)	-171.40(17)
C(14)-N(3)-C(13)-O(4)	-14.4(3)
C(16)-N(3)-C(13)-C(12)	9.7(3)
C(14)-N(3)-C(13)-C(12)	166.71(16)
C(11)-C(12)-C(13)-O(4)	-26.0(3)
N(2)-C(12)-C(13)-O(4)	155.58(18)
C(11)-C(12)-C(13)-N(3)	152.89(18)
N(2)-C(12)-C(13)-N(3)	-25.5(2)
C(13)-N(3)-C(14)-C(19)	64.4(2)
C(16)-N(3)-C(14)-C(19)	-136.01(17)
C(13)-N(3)-C(14)-C(15)	-173.83(18)
C(16)-N(3)-C(14)-C(15)	-14.28(19)

C(16)-O(5)-C(15)-C(14)	-42.22(19)
N(3)-C(14)-C(15)-O(5)	33.47(18)
C(19)-C(14)-C(15)-O(5)	155.95(16)
C(15)-O(5)-C(16)-N(3)	31.90(19)
C(15)-O(5)-C(16)-C(17)	149.68(16)
C(13)-N(3)-C(16)-O(5)	149.70(17)
C(14)-N(3)-C(16)-O(5)	-10.0(2)
C(13)-N(3)-C(16)-C(17)	31.9(2)
C(14)-N(3)-C(16)-C(17)	-127.83(16)
C(18)-N(2)-C(17)-C(16)	-138.09(17)
C(12)-N(2)-C(17)-C(16)	44.4(2)
O(5)-C(16)-C(17)-N(2)	-171.32(14)
N(3)-C(16)-C(17)-N(2)	-56.88(19)
C(12)-N(2)-C(18)-C(9)	-1.0(3)
C(17)-N(2)-C(18)-C(9)	-178.51(17)
C(10)-C(9)-C(18)-N(2)	0.8(3)

**Table S4** The measured hydrogen bonds for the GSK744 crystal.

<b>D-H...A</b>	<b>d(D-H) (Å)</b>	<b>d(H...A) (Å)</b>	<b>d(D...A) (Å)</b>	<b>&lt;(DHA) (degree)</b>
O(3)-H(3A)...O(1)	0.84	1.92	2.6587(18)	146.8
O(3)-H(3A)...O(2)	0.84	2.16	2.6215(18)	114.9
N(1)-H(1A)...O(2)	0.88	1.96	2.682(2)	138.8

**Table S5** The comparison of calculated and observed chemical shifts for  $^{13}\text{C}$  atoms. All values are in ppm.

Atom	Chemical shift (crystal, SSNMR)	Chemical shift (crystal, AF-QM/MM)	Chemical shift (solution, NMR)	Chemical shift (solution, DFT)
<b>C2</b>	74.5	76.5	72.4	74.5
<b>C3</b>	56.1	57.1	52.9	57.0
<b>C5</b>	155.8	154.2	158.9	155.3
<b>C6</b>	152.0	152.0	153.1	149.0
<b>C7</b>	172.6	170.5	170.4	168.1
<b>C8</b>	114.8	117.1	114.9	114.7
<b>C9</b>	139.2	137.7	141.5	139.2
<b>C10a</b>	118.9	119.9	117.4	118.8
<b>C11</b>	53.7	58.1	51.4	59.0
<b>C11a</b>	84.0	85.9	81.7	86.6
<b>C12</b>	14.0	17.5	16.6	16.7
<b>C13</b>	166.7	165.1	163.6	163.8
<b>C15</b>	34.3	39.7	35.8	38.6
<b>C16</b>	122.8	123.2	122.4	123.2
<b>C17</b>	158.6	157.6	160.2	158.9
<b>C18</b>	103.2	104.3	103.8	102.9
<b>C19</b>	161.4	160.2	161.5	160.6
<b>C20</b>	110.2	109.2	111.4	109.9
<b>C21</b>	129.3	127.8	130.8	127.9

**Table S6** The comparison of calculated and observed chemical shifts for  $^1\text{H}$  atoms. All values are in ppm.

<b>Atom</b>	<b>Chemical shift (crystal, SSNMR)</b>	<b>Chemical shift (crystal, AF-QM/MM)</b>	<b>Chemical shift (solution, NMR)</b>	<b>Chemical shift (solution, DFT)</b>
<b>H2</b>	4.20	4.27	4.03 (3.66,4.4)	4.28
<b>H3</b>	3.97	4.88	4.30	4.32
<b>H9</b>	8.80	8.90	8.47	8.34
<b>H11</b>	4.76	4.37	4.45 (4.01,4.89)	4.32
<b>H11a</b>	5.79	5.82	5.39	5.62
<b>H12</b>	1.64	1.66	1.35	1.68
<b>H14</b>	11.45	12.14	10.30	11.08
<b>H15</b>	4.99	5.22	4.55	4.84
<b>H18</b>	6.73	6.74	7.07	7.22
<b>H20</b>	7.04	7.33	7.24	7.29
<b>H21</b>	7.46	7.90	7.40	7.80



**Table S7** The performance of AF-QM/MM calculated  $^{13}\text{C}$  chemical shifts for the carbon set using different density functionals with the 6-31G\*\* basis set as compared to experimental results. MaxD denotes the maximum deviation. All values are in ppm.

<b>Density functional</b>	<b>RMSE</b>	<b>MUE</b>	<b>MaxD</b>	<b>Ref.</b>
<b>B3LYP</b>	2.6	2.3	4.2	191.7
<b>B3PW91</b>	2.4	2.0	5.0	194.9
<b>mPW1PW91</b>	2.1	1.6	5.1	196.2
<b>M06-L</b>	8.7	8.3	14.6	193.7
<b>M06-2X</b>	11.5	10.5	15.4	196.7
<b>OB98</b>	7.2	6.3	13.3	192.0
<b>OPBE</b>	7.3	6.1	13.4	195.5

**Table S8** The performance of AF-QM/MM calculated  $^1\text{H}$  chemical shifts for the carbon set using different density functionals with the 6-31G\*\* basis set as compared to experimental results. MaxD denotes the maximum deviation. All values are in ppm.

<b>Density functional</b>	<b>RMSE</b>	<b>MUE</b>	<b>MaxD</b>	<b>Ref.</b>
<b>B3LYP</b>	0.38	0.26	0.85	31.75
<b>B3PW91</b>	0.41	0.30	0.83	31.70
<b>mPW1PW91</b>	0.44	0.34	0.86	31.75
<b>M06-L</b>	0.83	0.74	1.39	31.97
<b>M06-2X</b>	0.94	0.81	1.90	31.87
<b>OB98</b>	0.38	0.31	0.73	31.64
<b>OPBE</b>	0.38	0.33	0.62	31.53

**Table S9** Comparison of  $^{13}\text{C}$  chemical shifts between solid-state and solution samples and between experiments and DFT calculations at the mPW1PW91/6-31G\*\* level, and considering the Influence of DMSO Solvent Effects to Ensure Consistency with Experimental Conditions. The chemical shift differences are in ppm.

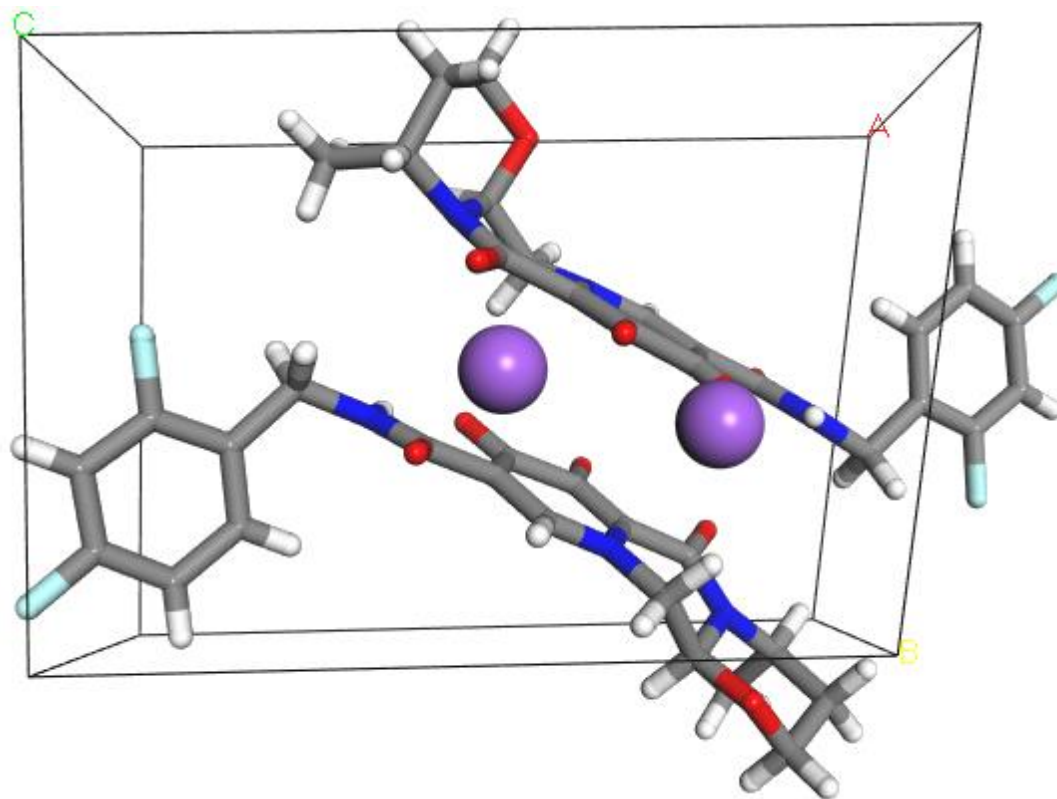
<b>Atom</b>	<b><math>\Delta\delta(^{13}\text{C})</math> (solution/exp vs. crystal/exp)</b>	<b><math>\Delta\delta(^{13}\text{C})</math> (crystal/exp vs. crystal/calc)</b>	<b><math>\Delta\delta(^{13}\text{C})</math> (solution/exp vs. solution/calc)</b>	<b><math>\Delta\delta(^{13}\text{C})</math> (solution/calc vs. crystal/calc)</b>
<b>C2</b>	-2.1	-2	-2.1	-2.0
<b>C3</b>	-3.2	-1	-4.1	-0.1
<b>C5</b>	3.1	1.6	3.6	1.0
<b>C6</b>	1.1	0	4.1	-3.0
<b>C7</b>	-2.2	2.1	2.3	-2.4
<b>C8</b>	0.1	-2.3	0.2	-2.5
<b>C9</b>	2.3	1.5	2.3	1.4
<b>C10a</b>	-1.5	-1	-1.4	-1.1
<b>C11</b>	-2.3	-4.4	-7.6	0.9
<b>C11a</b>	-2.3	-1.9	-4.9	0.7
<b>C12</b>	2.6	-3.5	-0.1	-0.7
<b>C13</b>	-3.1	1.6	-0.2	-1.3
<b>C15</b>	1.5	-5.4	-2.8	-1.1
<b>C16</b>	-0.4	-0.4	-0.8	0.0
<b>C17</b>	1.6	1	1.3	1.3
<b>C18</b>	0.6	-1.1	0.9	-1.4
<b>C19</b>	0.1	1.2	0.9	0.4
<b>C20</b>	1.2	1	1.5	0.7
<b>C21</b>	1.5	1.5	2.9	0.1

**Table S10** Comparison of  $^1\text{H}$  chemical shifts between solid-state and solution samples and between experiments and DFT calculations at the B3LYP/6-31G\*\* level, and considering the Influence of DMSO Solvent Effects to Ensure Consistency with Experimental Conditions. The chemical shift differences are in ppm.

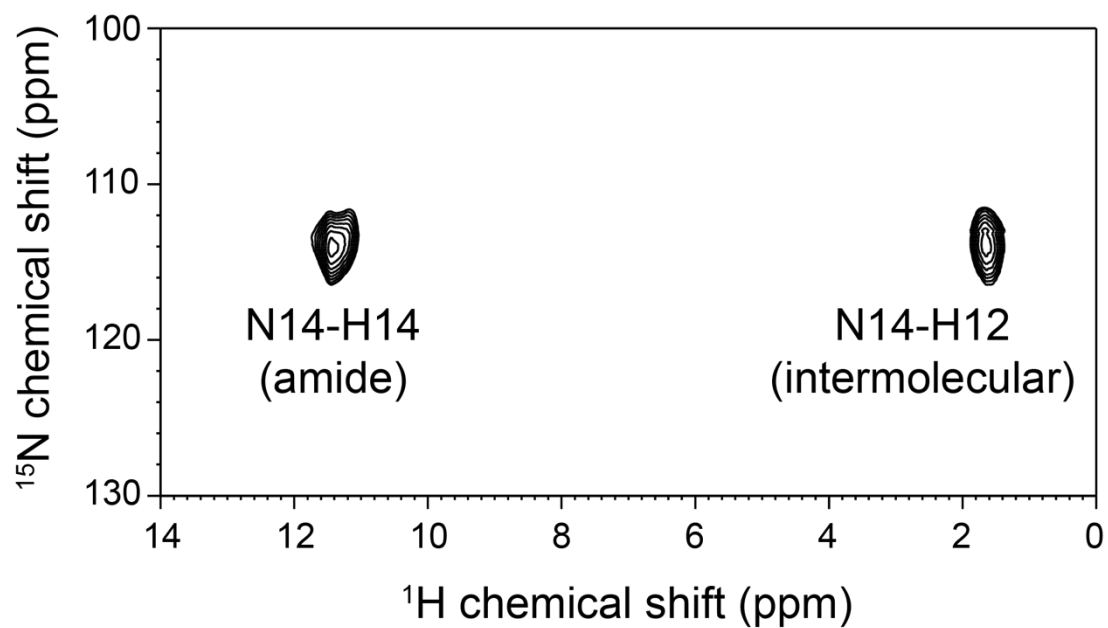
<b>Atom</b>	<b><math>\Delta\delta(^1\text{H})</math> (solution/exp vs. crystal/exp)</b>	<b><math>\Delta\delta(^1\text{H})</math> (crystal/exp vs. crystal/calc)</b>	<b><math>\Delta\delta(^1\text{H})</math> (solution/exp vs. solution/calc)</b>	<b><math>\Delta\delta(^1\text{H})</math> (solution/calc vs. crystal/calc)</b>
<b>H2</b>	-0.17	-0.07	-0.25	0.01
<b>H3</b>	0.33	-0.91	-0.02	-0.55
<b>H9</b>	-0.33	-0.1	0.13	-0.56
<b>H11</b>	-0.31	0.39	0.13	-0.05
<b>H11a</b>	-0.4	-0.03	-0.23	-0.19
<b>H12</b>	-0.29	-0.02	-0.33	0.01
<b>H14</b>	-1.15	-0.69	-0.78	-1.06
<b>H15</b>	-0.44	-0.23	-0.29	-0.37
<b>H18</b>	0.34	-0.01	-0.15	0.48
<b>H20</b>	0.2	-0.29	-0.05	-0.04
<b>H21</b>	-0.06	-0.44	-0.4	-0.10

**Table S11**  $^1\text{H}$  chemical shifts of cabotegravir in different solvents as obtained by NMR experiments.

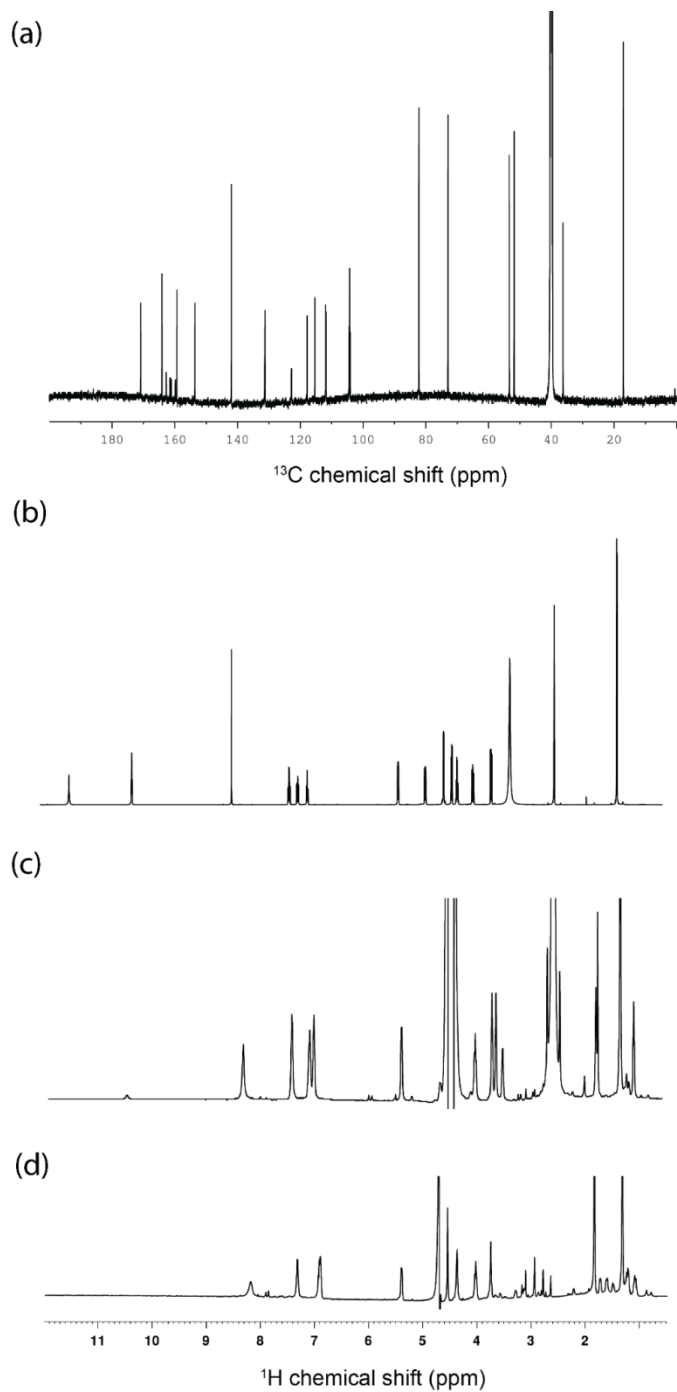
Atom	$\delta(^1\text{H})$ (DMSO)	$\delta(^1\text{H})$ (DMSO /D <sub>2</sub> O)	$\delta(^1\text{H})$ (D <sub>2</sub> O)	$\Delta\delta(^1\text{H})$ (DMSO/D <sub>2</sub> O vs. DMSO)	$\Delta\delta(^1\text{H})$ (D <sub>2</sub> O vs. DMSO)	$\Delta\delta(^1\text{H})$ (D <sub>2</sub> O vs. (DMSO/D <sub>2</sub> O)
<b>H2</b>	4.03 (3.66, 4.4)	3.65 (3.65, -)	4.065 (3.75,4.38)	-	0.035	-
<b>H3</b>	4.3	-	-	-	-	-
<b>H9</b>	8.47	8.24	8.2	-0.23	-0.27	-0.04
<b>H11</b>	4.45 (4.01, 4.89)	3.95 (3.95, -)	4.04 (4.04, -)	-	-	-
<b>H11a</b>	5.39	5.32	5.41	-0.07	0.02	0.09
<b>H12</b>	1.35	1.27	1.33	-0.08	-0.02	0.06
<b>H14</b>	10.3	10.38	-	0.08	-	-
<b>H15</b>	4.55	4.6	4.56	0.05	0.01	-0.04
<b>H18</b>	7.07	6.93	6.92	-0.14	-0.15	-0.01
<b>H20</b>	7.24	7.01	-	-0.23	-	-
<b>H21</b>	7.4	7.34	7.33	-0.06	-0.07	-0.01



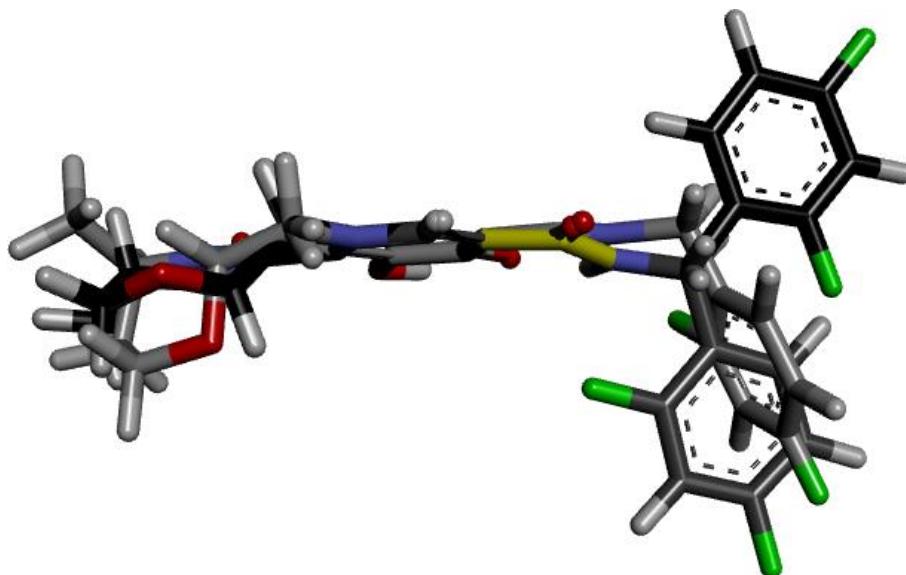
**Figure S1.** Crystal structure of sodium salt of dolutegravir (CSD Entry: KILNEA).



**Figure S2.**  $^1\text{H}$ - $^{15}\text{N}$  HSQC SSNMR spectra of cabotegravir microcrystalline powder acquired under VFMAS.



**Figure S3.**  $^{13}\text{C}$  and  $^1\text{H}$  solution NMR spectra of cabotegravir in different solvents: (a) DMSO solution, (b) DMSO solution, (c) DMSO/ $\text{D}_2\text{O}$  solution, (d) aqueous solution.



**Figure S4.** The comparison of the crystal structure of cabotegravir (dark gray), the best computed cabotegravir structural model in aqueous solution (middle gray) and the crystal structure of dolutegravir (light gray).

#### 570.CIF

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 C17 0.0248(9) 0.0305(10) 0.0182(9) 0.0019(7) -0.0019(7) 0.0027(8)  
 C18 0.0218(9) 0.0249(9) 0.0208(9) 0.0000(8) 0.0025(7) 0.0016(7)  
 C19 0.0342(11) 0.0369(11) 0.0206(9) 0.0000(8) 0.0056(8) 0.0024(9)

\_geom\_special\_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)  
 are estimated using the full covariance matrix. The cell esds are taken  
 into account individually in the estimation of esds in distances, angles  
 and torsion angles; correlations between esds in cell parameters are only  
 used when they are defined by crystal symmetry. An approximate (isotropic)  
 treatment of cell esds is used for estimating esds involving l.s. planes.

;

loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

F1 C2 1.355(2) . ?

F2 C4 1.357(2) . ?

O1 C8 1.240(2) . ?

O2 C10 1.260(2) . ?

O3 C11 1.346(2) . ?

O3 H3A 0.8400 . ?

O4 C13 1.229(2) . ?

O5 C16 1.409(2) . ?

O5 C15 1.440(2) . ?

N1 C8 1.340(2) . ?

N1 C7 1.455(2) . ?

N1 H1A 0.8800 . ?

N2 C18 1.342(2) . ?

N2 C12 1.397(2) . ?

N2 C17 1.476(2) . ?

N3 C13 1.350(2) . ?  
 N3 C16 1.476(2) . ?  
 N3 C14 1.481(2) . ?  
 C1 C6 1.384(3) . ?  
 C1 C2 1.385(3) . ?  
 C1 C7 1.513(3) . ?  
 C2 C3 1.375(3) . ?  
 C3 C4 1.367(3) . ?  
 C3 H3B 0.9500 . ?  
 C4 C5 1.376(3) . ?  
 C5 C6 1.381(3) . ?  
 C5 H5A 0.9500 . ?  
 C6 H6A 0.9500 . ?  
 C7 H7A 0.9900 . ?  
 C7 H7B 0.9900 . ?  
 C8 C9 1.495(2) . ?  
 C9 C18 1.374(2) . ?  
 C9 C10 1.435(3) . ?  
 C10 C11 1.454(3) . ?  
 C11 C12 1.365(3) . ?  
 C12 C13 1.507(3) . ?  
 C14 C19 1.518(3) . ?  
 C14 C15 1.525(3) . ?  
 C14 H14A 1.0000 . ?  
 C15 H15A 0.9900 . ?  
 C15 H15B 0.9900 . ?  
 C16 C17 1.509(3) . ?  
 C16 H16A 1.0000 . ?  
 C17 H17A 0.9900 . ?  
 C17 H17B 0.9900 . ?  
 C18 H18A 0.9500 . ?  
 C19 H19A 0.9800 . ?  
 C19 H19B 0.9800 . ?  
 C19 H19C 0.9800 . ?

loop\_  
 \_geom\_angle\_atom\_site\_label\_1  
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 \_geom\_angle\_site\_symmetry\_1  
 \_geom\_angle\_site\_symmetry\_3  
 \_geom\_angle\_publ\_flag  
 C11 O3 H3A 109.5 . . ?  
 C16 O5 C15 105.01(14) . . ?  
 C8 N1 C7 122.03(17) . . ?  
 C8 N1 H1A 119.0 . . ?  
 C7 N1 H1A 119.0 . . ?  
 C18 N2 C12 121.00(15) . . ?  
 C18 N2 C17 120.50(15) . . ?  
 C12 N2 C17 118.45(15) . . ?  
 C13 N3 C16 122.86(15) . . ?  
 C13 N3 C14 123.66(15) . . ?  
 C16 N3 C14 110.05(14) . . ?

C6 C1 C2 116.53(18) . . ?  
 C6 C1 C7 122.45(17) . . ?  
 C2 C1 C7 121.02(18) . . ?  
 F1 C2 C3 117.55(17) . . ?  
 F1 C2 C1 118.28(17) . . ?  
 C3 C2 C1 124.17(19) . . ?  
 C4 C3 C2 116.26(18) . . ?  
 C4 C3 H3B 121.9 . . ?  
 C2 C3 H3B 121.9 . . ?  
 F2 C4 C3 117.69(19) . . ?  
 F2 C4 C5 119.2(2) . . ?  
 C3 C4 C5 123.14(19) . . ?  
 C4 C5 C6 118.23(19) . . ?  
 C4 C5 H5A 120.9 . . ?  
 C6 C5 H5A 120.9 . . ?  
 C5 C6 C1 121.68(18) . . ?  
 C5 C6 H6A 119.2 . . ?  
 C1 C6 H6A 119.2 . . ?  
 N1 C7 C1 113.07(16) . . ?  
 N1 C7 H7A 109.0 . . ?  
 C1 C7 H7A 109.0 . . ?  
 N1 C7 H7B 109.0 . . ?  
 C1 C7 H7B 109.0 . . ?  
 H7A C7 H7B 107.8 . . ?  
 O1 C8 N1 122.36(17) . . ?  
 O1 C8 C9 122.38(16) . . ?  
 N1 C8 C9 115.22(16) . . ?  
 C18 C9 C10 119.29(16) . . ?  
 C18 C9 C8 117.93(16) . . ?  
 C10 C9 C8 122.61(16) . . ?  
 O2 C10 C9 126.72(17) . . ?  
 O2 C10 C11 117.33(16) . . ?  
 C9 C10 C11 115.94(16) . . ?  
 O3 C11 C12 121.99(16) . . ?  
 O3 C11 C10 115.84(15) . . ?  
 C12 C11 C10 122.09(17) . . ?  
 C11 C12 N2 118.73(16) . . ?  
 C11 C12 C13 122.64(17) . . ?  
 N2 C12 C13 118.62(16) . . ?  
 O4 C13 N3 123.93(17) . . ?  
 O4 C13 C12 121.41(16) . . ?  
 N3 C13 C12 114.65(16) . . ?  
 N3 C14 C19 114.89(15) . . ?  
 N3 C14 C15 99.11(14) . . ?  
 C19 C14 C15 113.85(16) . . ?  
 N3 C14 H14A 109.5 . . ?  
 C19 C14 H14A 109.5 . . ?  
 C15 C14 H14A 109.5 . . ?  
 O5 C15 C14 104.82(14) . . ?  
 O5 C15 H15A 110.8 . . ?  
 C14 C15 H15A 110.8 . . ?  
 O5 C15 H15B 110.8 . . ?  
 C14 C15 H15B 110.8 . . ?  
 H15A C15 H15B 108.9 . . ?

O5 C16 N3 104.53(14) . . ?  
 O5 C16 C17 109.83(15) . . ?  
 N3 C16 C17 109.84(15) . . ?  
 O5 C16 H16A 110.8 . . ?  
 N3 C16 H16A 110.8 . . ?  
 C17 C16 H16A 110.8 . . ?  
 N2 C17 C16 107.51(15) . . ?  
 N2 C17 H17A 110.2 . . ?  
 C16 C17 H17A 110.2 . . ?  
 N2 C17 H17B 110.2 . . ?  
 C16 C17 H17B 110.2 . . ?  
 H17A C17 H17B 108.5 . . ?  
 N2 C18 C9 122.95(17) . . ?  
 N2 C18 H18A 118.5 . . ?  
 C9 C18 H18A 118.5 . . ?  
 C14 C19 H19A 109.5 . . ?  
 C14 C19 H19B 109.5 . . ?  
 H19A C19 H19B 109.5 . . ?  
 C14 C19 H19C 109.5 . . ?  
 H19A C19 H19C 109.5 . . ?  
 H19B C19 H19C 109.5 . . ?

loop\_

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 \_geom\_torsion\_atom\_site\_label\_2  
 \_geom\_torsion\_atom\_site\_label\_3  
 \_geom\_torsion\_atom\_site\_label\_4  
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 \_geom\_torsion\_site\_symmetry\_1  
 \_geom\_torsion\_site\_symmetry\_2  
 \_geom\_torsion\_site\_symmetry\_3  
 \_geom\_torsion\_site\_symmetry\_4  
 \_geom\_torsion\_publ\_flag  
 C6 C1 C2 F1 180.00(19) . . . . ?  
 C7 C1 C2 F1 0.6(3) . . . . ?  
 C6 C1 C2 C3 -0.1(3) . . . . ?  
 C7 C1 C2 C3 -179.5(2) . . . . ?  
 F1 C2 C3 C4 -179.4(2) . . . . ?  
 C1 C2 C3 C4 0.7(4) . . . . ?  
 C2 C3 C4 F2 178.7(2) . . . . ?  
 C2 C3 C4 C5 -0.9(4) . . . . ?  
 F2 C4 C5 C6 -179.0(2) . . . . ?  
 C3 C4 C5 C6 0.5(4) . . . . ?  
 C4 C5 C6 C1 0.1(4) . . . . ?  
 C2 C1 C6 C5 -0.3(3) . . . . ?  
 C7 C1 C6 C5 179.0(2) . . . . ?  
 C8 N1 C7 C1 -101.8(2) . . . . ?  
 C6 C1 C7 N1 32.6(3) . . . . ?  
 C2 C1 C7 N1 -148.08(19) . . . . ?  
 C7 N1 C8 O1 4.7(3) . . . . ?  
 C7 N1 C8 C9 -173.43(16) . . . . ?  
 O1 C8 C9 C18 -10.1(3) . . . . ?  
 N1 C8 C9 C18 168.05(17) . . . . ?  
 O1 C8 C9 C10 174.70(19) . . . . ?



N1 C8 C9 C10 -7.2(3) . . . . ?  
 C18 C9 C10 O2 -179.37(18) . . . . ?  
 C8 C9 C10 O2 -4.2(3) . . . . ?  
 C18 C9 C10 C11 -0.2(3) . . . . ?  
 C8 C9 C10 C11 174.96(16) . . . . ?  
 O2 C10 C11 O3 2.2(2) . . . . ?  
 C9 C10 C11 O3 -177.07(16) . . . . ?  
 O2 C10 C11 C12 179.00(18) . . . . ?  
 C9 C10 C11 C12 -0.3(3) . . . . ?  
 O3 C11 C12 N2 176.70(17) . . . . ?  
 C10 C11 C12 N2 0.1(3) . . . . ?  
 O3 C11 C12 C13 -1.7(3) . . . . ?  
 C10 C11 C12 C13 -178.30(16) . . . . ?  
 C18 N2 C12 C11 0.6(3) . . . . ?  
 C17 N2 C12 C11 178.06(16) . . . . ?  
 C18 N2 C12 C13 179.01(16) . . . . ?  
 C17 N2 C12 C13 -3.5(2) . . . . ?  
 C16 N3 C13 O4 -171.40(17) . . . . ?  
 C14 N3 C13 O4 -14.4(3) . . . . ?  
 C16 N3 C13 C12 9.7(3) . . . . ?  
 C14 N3 C13 C12 166.71(16) . . . . ?  
 C11 C12 C13 O4 -26.0(3) . . . . ?  
 N2 C12 C13 O4 155.58(18) . . . . ?  
 C11 C12 C13 N3 152.89(18) . . . . ?  
 N2 C12 C13 N3 -25.5(2) . . . . ?  
 C13 N3 C14 C19 64.4(2) . . . . ?  
 C16 N3 C14 C19 -136.01(17) . . . . ?  
 C13 N3 C14 C15 -173.83(18) . . . . ?  
 C16 N3 C14 C15 -14.28(19) . . . . ?  
 C16 O5 C15 C14 -42.22(19) . . . . ?  
 N3 C14 C15 O5 33.47(18) . . . . ?  
 C19 C14 C15 O5 155.95(16) . . . . ?  
 C15 O5 C16 N3 31.90(19) . . . . ?  
 C15 O5 C16 C17 149.68(16) . . . . ?  
 C13 N3 C16 O5 149.70(17) . . . . ?  
 C14 N3 C16 O5 -10.0(2) . . . . ?  
 C13 N3 C16 C17 31.9(2) . . . . ?  
 C14 N3 C16 C17 -127.83(16) . . . . ?  
 C18 N2 C17 C16 -138.09(17) . . . . ?  
 C12 N2 C17 C16 44.4(2) . . . . ?  
 O5 C16 C17 N2 -171.32(14) . . . . ?  
 N3 C16 C17 N2 -56.88(19) . . . . ?  
 C12 N2 C18 C9 -1.0(3) . . . . ?  
 C17 N2 C18 C9 -178.51(17) . . . . ?  
 C10 C9 C18 N2 0.8(3) . . . . ?  
 C8 C9 C18 N2 -174.53(17) . . . . ?

loop\_

\_geom\_hbond\_atom\_site\_label\_D  
 \_geom\_hbond\_atom\_site\_label\_H  
 \_geom\_hbond\_atom\_site\_label\_A  
 \_geom\_hbond\_distance\_DH  
 \_geom\_hbond\_distance\_HA  
 \_geom\_hbond\_distance\_DA

```

_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
O3 H3A O1 0.84 1.92 2.6587(18) 146.8 1_655 yes
O3 H3A O2 0.84 2.16 2.6215(18) 114.9 . yes
N1 H1A O2 0.88 1.96 2.682(2) 138.8 . yes

_refine_diff_density_max 0.157
_refine_diff_density_min -0.172
_refine_diff_density_rms 0.036

_shelx_res_file
;
TITL GSK744 in P2(1)2(1)2(1)
570.res
created by SHELXL-2018/3 at 13:58:58 on 02-Jan-2019
CELL 1.54178 7.3002 7.3002 32.3426 90.000 90.000 90.000
ZERR 4.000 0.0005 0.0001 0.0021 0.000 0.000 0.000
LATT -1
SYMM 1/2-X, -Y, 1/2+Z
SYMM -X, 1/2+Y, 1/2-Z
SYMM 1/2+X, 1/2-Y, -Z
SFAC C H N O F
UNIT 76 68 12 20 8
TEMP -90.730
L.S. 4

ACTA
BOND $H
CONF
EQUIV $1 x+1, y, z
HTAB O3 O1_$1
HTAB O3 O2
HTAB N1 O2
SIZE 0.08 0.14 0.26
FMAP 2
PLAN 10
WGHT 0.040300 0.350200
FVAR 0.93199
F1 5 0.016443 -0.039173 0.511896 11.00000 0.07714 0.02946 =
0.02657 0.00817 0.00840 0.00455
F2 5 -0.004212 0.575509 0.551009 11.00000 0.09829 0.04096 =
0.03100 -0.01336 -0.00023 0.00232
O1 4 -0.116125 0.163073 0.352701 11.00000 0.02276 0.05649 =
0.02118 0.00203 0.00184 0.00035
O2 4 0.463921 0.146615 0.355974 11.00000 0.02647 0.03521 =
0.01872 0.00042 -0.00251 0.00180
O3 4 0.658824 0.169045 0.288085 11.00000 0.02031 0.04843 =
0.01931 0.00174 -0.00197 0.00149
AFIX 83
H3A 2 0.688729 0.171634 0.313157 11.00000 -1.50000
AFIX 0
O4 4 0.653674 0.272540 0.206158 11.00000 0.02351 0.03526 =
0.02345 0.00105 0.00160 -0.00560

```

O5 4 0.141079 0.155907 0.134745 11.00000 0.02835 0.04792 =  
 0.01615 -0.00279 -0.00195 0.00081  
 N1 3 0.134435 0.090094 0.390379 11.00000 0.02757 0.03379 =  
 0.01725 0.00151 0.00099 0.00183  
 AFIX 43  
 H1A 2 0.254861 0.086895 0.391341 11.00000 -1.20000  
 AFIX 0  
 N2 3 0.199543 0.209005 0.246231 11.00000 0.02353 0.02547 =  
 0.01641 0.00053 -0.00033 0.00103  
 N3 3 0.401392 0.158117 0.173796 11.00000 0.02267 0.02832 =  
 0.01740 -0.00029 0.00172 -0.00133  
 C1 1 0.024147 0.184408 0.459584 11.00000 0.02247 0.03133 =  
 0.01993 0.00240 0.00210 -0.00044  
 C2 1 0.016379 0.140236 0.501178 11.00000 0.03218 0.02815 =  
 0.02337 0.00464 0.00306 0.00193  
 C3 1 0.008757 0.267174 0.532556 11.00000 0.04514 0.03979 =  
 0.01738 0.00314 0.00150 0.00432  
 AFIX 43  
 H3B 2 0.004873 0.231832 0.560811 11.00000 -1.20000  
 AFIX 0  
 C4 1 0.007085 0.446980 0.520810 11.00000 0.04372 0.03477 =  
 0.02320 -0.00656 0.00041 0.00148  
 C5 1 0.015142 0.502212 0.480184 11.00000 0.04329 0.02758 =  
 0.03035 0.00216 0.00125 0.00088  
 AFIX 43  
 H5A 2 0.014757 0.628551 0.473144 11.00000 -1.20000  
 AFIX 0  
 C6 1 0.023807 0.369077 0.449904 11.00000 0.03410 0.03124 =  
 0.01994 0.00516 0.00116 0.00065  
 AFIX 43  
 H6A 2 0.029683 0.405185 0.421715 11.00000 -1.20000  
 AFIX 0  
 C7 1 0.030610 0.036564 0.426837 11.00000 0.03859 0.03064 =  
 0.01922 0.00292 0.00421 -0.00318  
 AFIX 23  
 H7A 2 0.086339 -0.075021 0.438853 11.00000 -1.20000  
 H7B 2 -0.096104 0.005798 0.418428 11.00000 -1.20000  
 AFIX 0  
 C8 1 0.052294 0.144122 0.355379 11.00000 0.02618 0.02576 =  
 0.01738 -0.00384 0.00075 -0.00048  
 C9 1 0.177526 0.174164 0.319446 11.00000 0.02414 0.02205 =  
 0.01922 -0.00160 0.00038 0.00020  
 C10 1 0.373247 0.167317 0.323160 11.00000 0.02605 0.02066 =  
 0.01874 -0.00172 -0.00171 0.00190  
 C11 1 0.475635 0.183925 0.284768 11.00000 0.02234 0.02191 =  
 0.02195 -0.00186 0.00003 0.00062  
 C12 1 0.390837 0.204031 0.247433 11.00000 0.02101 0.02140 =  
 0.02051 0.00049 0.00171 0.00036  
 C13 1 0.495054 0.216248 0.207301 11.00000 0.02636 0.02028 =  
 0.01994 0.00091 -0.00003 0.00090  
 C14 1 0.460328 0.193111 0.130693 11.00000 0.03041 0.02576 =  
 0.01621 0.00142 0.00280 -0.00078  
 AFIX 13  
 H14A 2 0.468605 0.328174 0.125884 11.00000 -1.20000

```

AFIX 0
C15 1 0.293948 0.116719 0.108014 11.00000 0.03186 0.04192 =
      0.01898 -0.00331 0.00104 -0.00252
AFIX 23
H15A 2 0.278383 0.177317 0.080857 11.00000 -1.20000
H15B 2 0.306680 -0.016874 0.103606 11.00000 -1.20000
AFIX 0
C16 1 0.203863 0.115080 0.174880 11.00000 0.02392 0.02784 =
      0.01841 0.00008 -0.00092 -0.00222
AFIX 13
H16A 2 0.183536 -0.017098 0.181576 11.00000 -1.20000
AFIX 0
C17 1 0.108864 0.236734 0.205935 11.00000 0.02478 0.03053 =
      0.01817 0.00194 -0.00190 0.00274
AFIX 23
H17A 2 0.118517 0.366621 0.197408 11.00000 -1.20000
H17B 2 -0.022478 0.204078 0.207874 11.00000 -1.20000
AFIX 0
C18 1 0.100119 0.195894 0.281023 11.00000 0.02180 0.02492 =
      0.02078 0.00002 0.00252 0.00155
AFIX 43
H18A 2 -0.029564 0.201907 0.278994 11.00000 -1.20000
AFIX 0
C19 1 0.639831 0.103147 0.118489 11.00000 0.03421 0.03693 =
      0.02062 0.00002 0.00555 0.00236
AFIX 33
H19A 2 0.668298 0.133257 0.089668 11.00000 -1.50000
H19B 2 0.738163 0.148102 0.136449 11.00000 -1.50000
H19C 2 0.628918 -0.029997 0.121472 11.00000 -1.50000

AFIX 0
HKL 4

```

```

REM GSK744 in P2(1)2(1)2(1)
REM wR2 = 0.0730, GooF = S = 1.059, Restrained GooF = 1.059 for all data
REM R1 = 0.0274 for 3114 Fo > 4sig(Fo) and 0.0279 for all 3165 data
REM 262 parameters refined using 0 restraints

```

END

```

WGHT 0.0403 0.3502

```

```

REM Highest difference peak 0.157, deepest hole -0.172, 1-sigma level 0.036
Q1 1 0.4407 0.1689 0.1538 11.00000 0.05 0.16
Q2 1 0.4416 0.2155 0.2299 11.00000 0.05 0.15
Q3 1 0.1538 0.1690 0.1924 11.00000 0.05 0.15
Q4 1 0.6253 0.0833 0.0827 11.00000 0.05 0.14
Q5 1 0.0577 0.1639 0.4779 11.00000 0.05 0.13
Q6 1 0.7250 0.2382 0.1735 11.00000 0.05 0.13
Q7 1 0.2560 0.1247 0.3217 11.00000 0.05 0.13
Q8 1 0.0728 0.4627 0.5002 11.00000 0.05 0.13

```

```

Q9  1  0.1242 0.1580 0.3344 11.00000 0.05  0.13
Q10 1  0.0809 0.2655 0.4547 11.00000 0.05  0.12
;
_shelx_res_checksum  51281
;
_shelx_hkl_checksum  2642

```

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 570

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

## Datablock: 570

---

Bond precision:	C-C = 0.0029 Å	Wavelength=1.54178
Cell:	a=7.3002 (5) alpha=90	b=7.3002 (1) beta=90
Temperature:	c=32.343 (2) gamma=90	182 K

	Calculated	Reported
Volume	1723.65 (16)	1723.63 (16)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C19 H17 F2 N3 O5	C19 H17 F2 N3 O5
Sum formula	C19 H17 F2 N3 O5	C19 H17 F2 N3 O5
Mr	405.36	405.35
Dx, g cm <sup>-3</sup>	1.562	1.562
Z	4	4
Mu (mm <sup>-1</sup> )	1.103	1.103
F000	840.0	840.0
F000'	843.17	
h, k, lmax	8, 8, 39	8, 8, 39
Nref	3185 [ 1877]	3165
Tmin, Tmax	0.831, 0.916	0.637, 0.753
Tmin'	0.751	

Correction method= # Reported T Limits: Tmin=0.637 Tmax=0.753  
AbsCorr = MULTI-SCAN

Data completeness= 1.69/0.99                      Theta(max)= 68.809

R(reflections)= 0.0274( 3114)

wR2(reflections)=  
0.0730( 3165)

S = 1.059

Npar= 262

---

The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

---

### Alert level B

SYMMS02\_ALERT\_1\_B The unit-cell lengths a and b should not be equal for anorthorhombic cell

Cell	7.3002	7.3002	32.3430
Angles	90.0000	90.0000	90.0000

---

### Alert level C

PLAT089\_ALERT\_3\_C Poor Data / Parameter Ratio (Zmax < 18) .....

7.11 Note PLAT911\_ALERT\_3\_C

Missing FCF Refl Between Thmin & STh/L=

0.600

10 Report

PLAT913\_ALERT\_3\_C Missing # of Very Strong Reflections in FCF ....

6 Note

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### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report PLAT398\_ALERT\_2\_G Deviating C-O-C Angle From 120 for O5 . 105.0 Degree PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL

2019/3 Note

PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min).

1 Note

PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600

1 Note

PLAT955\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Lmax Differ by .

1 Units

PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density.

10 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

8 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

2 ALERT type 2 Indicator that the structure model may be wrong or deficient

4 ALERT type 3 Indicator that the structure quality may be low

2 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

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PLATON version of 06/07/2023; check.def file  
version of 30/06/2023

**Datablock 570** - ellipsoid plot

