

Table 2. Hydrogen-bond parameters

$D-H\cdots A$	$D-H$ (Å)	$H\cdots A$ (Å)	$D\cdots A$ (Å)	$D-H\cdots A$ (°)
-173 °C				
N1—H1C \cdots O3 ⁱ	0.91	2.83	3.3170 (19)	114.6
N1—H1C \cdots O3 ⁱⁱ	0.91	2.14	2.9971 (15)	156.5
N1—H1B \cdots O3 ⁱⁱⁱ	0.91	2.26	2.9971 (15)	137.6
N1—H1A \cdots C11	0.91	2.50	3.3632 (17)	158.5
N2—H2C \cdots C11	0.91	2.92	3.3855 (13)	113.3
N2—H2B \cdots C11 ^{iv}	0.91	2.48	3.3598 (13)	163.4
N2—H2A \cdots O1 ⁱⁱ	0.91	2.41	3.2190 (17)	148.5
N2—H2C \cdots O3	0.91	2.32	3.0770 (16)	140.8
N3—H3C \cdots C11 ^{iv}	0.91	2.50	3.3841 (13)	163.4
N3—H3B \cdots C11 ^v	0.91	2.60	3.4921 (13)	167.3
N3—H3A \cdots O3 ⁱ	0.91	2.47	3.0356 (16)	120.9
N3—H3C \cdots O2 ^{vi}	0.91	2.63	3.0267 (16)	106.9
N3—H3A \cdots O4 ⁱⁱ	0.91	2.20	2.9500 (17)	139.7
-160 °C				
N1—H1C \cdots O3 ⁱ	0.91	2.83	3.320 (2)	114.9
N1—H1C \cdots O3 ⁱⁱ	0.91	2.14	2.9972 (16)	156.6
N1—H1B \cdots O3 ⁱⁱⁱ	0.91	2.26	2.9972 (16)	138.1
N1—H1A \cdots C11	0.91	2.50	3.3618 (18)	158.9
N2—H2C \cdots C11	0.91	2.92	3.3864 (14)	113.2
N2—H2B \cdots C11 ^{iv}	0.91	2.48	3.3620 (14)	163.4
N2—H2A \cdots O1 ⁱⁱ	0.91	2.41	3.2236 (17)	148.3
N2—H2C \cdots O3	0.91	2.32	3.0798 (17)	140.6
N3—H3C \cdots C11 ^{iv}	0.91	2.50	3.3887 (14)	164.5
N3—H3B \cdots C11 ^v	0.91	2.60	3.4950 (14)	169.2
N3—H3A \cdots O3 ⁱ	0.91	2.45	3.0370 (17)	122.9
N3—H3C \cdots O2 ^{vi}	0.91	2.64	3.0317 (17)	106.9
N3—H3A \cdots O4 ⁱⁱ	0.91	2.22	2.9516 (18)	137.3
-140 °C				
N1—H1C \cdots O3 ⁱ	0.91	2.84	3.321 (2)	114.6
N1—H1C \cdots O3 ⁱⁱ	0.91	2.14	2.9979 (16)	157.2
N1—H1B \cdots O3 ⁱⁱⁱ	0.91	2.26	2.9979 (16)	137.8
N1—H1A \cdots C11	0.91	2.50	3.3648 (19)	158.7
N2—H2C \cdots C11	0.91	2.95	3.3904 (14)	111.7
N2—H2B \cdots C11 ^{iv}	0.91	2.48	3.3617 (14)	164.6

N2—H2A···O1 ⁱⁱ	0.91	2.42	3.2281 (18)	148.0
N2—H2C···O3	0.91	2.32	3.0870 (17)	141.9
N3—H3C···C11 ^{iv}	0.91	2.51	3.3943 (15)	164.4
N3—H3B···C11 ^v	0.91	2.60	3.4989 (14)	169.2
N3—H3A···O3 ⁱ	0.91	2.44	3.0395 (18)	123.3
N3—H3C···O2 ^{vi}	0.91	2.64	3.0368 (18)	107.3
N3—H3A···O4 ⁱⁱ	0.91	2.23	2.9545 (19)	136.4
-120 °C				
N1—H1C···O3 ⁱ	0.91	2.83	3.321 (2)	115.2
N1—H1C···O3 ⁱⁱ	0.91	2.14	2.9997 (17)	157.0
N1—H1B···O3 ⁱⁱⁱ	0.91	2.26	2.9997 (17)	138.4
N1—H1A···C11	0.91	2.50	3.370 (2)	159.2
N2—H2C···C11	0.91	2.92	3.3931 (15)	114.1
N2—H2B···C11 ^{iv}	0.91	2.48	3.3638 (15)	162.5
N2—H2A···O1 ⁱⁱ	0.91	2.43	3.2341 (19)	147.7
N2—H2C···O3	0.91	2.35	3.0931 (19)	139.2
N3—H3C···C11 ^{iv}	0.91	2.51	3.3984 (15)	165.0
N3—H3B···C11 ^v	0.91	2.61	3.5053 (15)	170.2
N3—H3A···O3 ⁱ	0.91	2.44	3.0444 (19)	124.4
N3—H3C···O2 ^{vi}	0.91	2.65	3.0445 (18)	107.3
N3—H3A···O4 ⁱⁱ	0.91	2.24	2.956 (2)	134.7
-100 °C				
N1—H1C···O3 ⁱ	0.91	2.85	3.325 (2)	114.0
N1—H1C···O3 ⁱⁱ	0.91	2.14	3.0003 (17)	158.3
N1—H1B···O3 ⁱⁱⁱ	0.91	2.27	3.0003 (17)	137.3
N1—H1A···C11	0.91	2.51	3.369 (2)	158.4
N2—H2C···C11	0.91	2.94	3.3954 (15)	112.3
N2—H2B···C11 ^{iv}	0.91	2.48	3.3655 (15)	164.0
N2—H2A···O1 ⁱⁱ	0.91	2.44	3.2407 (19)	147.5
N2—H2C···O3	0.91	2.34	3.0985 (19)	140.8
N3—H3C···C11 ^{iv}	0.91	2.52	3.4058 (16)	165.8
N3—H3B···C11 ^v	0.91	2.60	3.5089 (15)	172.3
N3—H3A···O3 ⁱ	0.91	2.41	3.0470 (19)	126.7
N3—H3C···O2 ^{vi}	0.91	2.65	3.0510 (19)	107.4
N3—H3A···O4 ⁱⁱ	0.91	2.27	2.959 (2)	132.0
-80 °C				
N1—H1C···O3 ⁱ	0.91	2.83	3.327 (2)	115.4
N1—H1C···O3 ⁱⁱ	0.91	2.14	3.0006 (18)	157.5
N1—H1B···O3 ⁱⁱⁱ	0.91	2.26	3.0006 (18)	138.7

N1—H1A…C11	0.91	2.51	3.373 (2)	159.5
N2—H2C…C11	0.91	2.87	3.3987 (16)	118.8
N2—H2B…C11 ^{iv}	0.91	2.51	3.3671 (16)	157.9
N2—H2A…O1 ⁱⁱ	0.91	2.45	3.246 (2)	146.8
N2—H2C…O3	0.91	2.40	3.104 (2)	134.1
N3—H3C…C11 ^{iv}	0.91	2.52	3.4111 (16)	165.8
N3—H3B…C11 ^v	0.91	2.61	3.5146 (16)	172.3
N3—H3A…O3 ⁱ	0.91	2.42	3.051 (2)	126.8
N3—H3C…O2 ^{vi}	0.91	2.66	3.0562 (19)	107.6
N3—H3A…O4 ⁱⁱ	0.91	2.28	2.960 (2)	131.5
-60 °C				
N1—H1C…O3 ⁱ	0.90	2.80	3.331 (3)	118.7
N1—H1C…O3 ⁱⁱ	0.90	2.16	3.003 (2)	155.5
N1—H1B…O3 ⁱⁱⁱ	0.90	2.24	3.003 (2)	142.2
N1—H1A…C11	0.90	2.50	3.370 (2)	161.9
N2—H2C…C11	0.90	2.88	3.3976 (18)	117.8
N2—H2B…C11 ^{iv}	0.90	2.51	3.3677 (18)	159.1
N2—H2A…O1 ⁱⁱ	0.90	2.46	3.251 (2)	146.8
N2—H2C…O3	0.90	2.40	3.106 (2)	135.3
N3—H3C…C11 ^{iv}	0.90	2.54	3.4177 (18)	166.1
N3—H3B…C11 ^v	0.90	2.62	3.5151 (18)	173.1
N3—H3A…O3 ⁱ	0.90	2.41	3.050 (2)	127.9
N3—H3C…O2 ^{vi}	0.90	2.66	3.063 (2)	108.0
N3—H3A…O4 ⁱⁱ	0.90	2.30	2.961 (2)	130.1
-40 °C				
N1—H1C…O3 ⁱ	0.90	2.84	3.334 (3)	116.1
N1—H1C…O3 ⁱⁱ	0.90	2.15	3.006 (2)	157.8
N1—H1B…O3 ⁱⁱⁱ	0.90	2.26	3.006 (2)	139.6
N1—H1A…C11	0.90	2.51	3.375 (2)	160.1
N2—H2C…C11	0.90	2.88	3.4002 (18)	118.7
N2—H2B…C11 ^{iv}	0.90	2.52	3.3698 (18)	158.2
N2—H2A…O1 ⁱⁱ	0.90	2.47	3.255 (2)	146.5
N2—H2C…O3	0.90	2.42	3.113 (2)	134.4
N3—H3C…C11 ^{iv}	0.90	2.54	3.4222 (19)	166.3
N3—H3B…C11 ^v	0.90	2.63	3.5215 (18)	173.6
N3—H3A…O3 ⁱ	0.90	2.41	3.056 (2)	128.4
N3—H3C…O2 ^{vi}	0.90	2.67	3.069 (2)	108.0
N3—H3A…O4 ⁱⁱ	0.90	2.31	2.964 (2)	129.3
-20 °C				

N1—H1C···O3 ⁱ	0.89	2.86	3.337 (3)	115.2
N1—H1C···O3 ⁱⁱ	0.89	2.16	3.009 (2)	158.9
N1—H1B···O3 ⁱⁱⁱ	0.89	2.28	3.009 (2)	138.6
N1—H1A···C11	0.89	2.53	3.380 (2)	159.4
N2—H2C···C11	0.89	2.87	3.4027 (18)	120.1
N2—H2B···C11 ^{iv}	0.89	2.54	3.3726 (18)	156.9
N2—H2A···O1 ⁱⁱ	0.89	2.49	3.264 (2)	146.3
N2—H2C···O3	0.89	2.44	3.118 (2)	133.2
N3—H3C···C11 ^{iv}	0.89	2.56	3.4279 (19)	166.2
N3—H3B···C11 ^v	0.89	2.64	3.5268 (19)	173.0
N3—H3A···O3 ⁱ	0.89	2.43	3.062 (2)	128.1
N3—H3C···O2 ^{vi}	0.89	2.67	3.075 (2)	108.5
N3—H3A···O4 ⁱⁱ	0.89	2.32	2.967 (2)	129.8
0 °C				
N1—H1C···O3 ⁱ	0.89	2.86	3.343 (3)	115.6
N1—H1C···O3 ⁱⁱ	0.89	2.16	3.011 (2)	158.8
N1—H1B···O3 ⁱⁱⁱ	0.89	2.28	3.011 (2)	139.0
N1—H1A···C11	0.89	2.53	3.383 (3)	159.7
N2—H2C···C11	0.89	2.84	3.4070 (19)	123.3
N2—H2B···C11 ^{iv}	0.89	2.55	3.3734 (19)	153.5
N2—H2A···O1 ⁱⁱ	0.89	2.50	3.267 (2)	145.4
N2—H2C···O3	0.89	2.47	3.122 (3)	130.1
N3—H3C···C11 ^{iv}	0.89	2.56	3.433 (2)	166.2
N3—H3B···C11 ^v	0.89	2.65	3.5325 (19)	173.0
N3—H3A···O3 ⁱ	0.89	2.44	3.068 (3)	128.2
N3—H3C···O2 ^{vi}	0.89	2.68	3.083 (2)	108.6
N3—H3A···O4 ⁱⁱ	0.89	2.32	2.969 (3)	129.3
20 °C				
N1—H1C···O3 ⁱ	0.89	2.89	3.348 (3)	113.5
N1—H1C···O3 ⁱⁱ	0.89	2.16	3.014 (2)	160.6
N1—H1B···O3 ⁱⁱⁱ	0.89	2.30	3.014 (2)	136.9
N1—H1A···C11	0.89	2.54	3.386 (3)	158.0
N2—H2C···C11	0.89	2.81	3.4095 (19)	126.2
N2—H2B···C11 ^{iv}	0.89	2.57	3.3775 (19)	150.4
N2—H2A···O1 ⁱⁱ	0.89	2.51	3.275 (2)	144.4
N2—H2C···O3	0.89	2.51	3.128 (3)	127.2
N3—H3C···C11 ^{iv}	0.89	2.57	3.439 (2)	166.9
N3—H3B···C11 ^v	0.89	2.65	3.5376 (19)	175.7
N3—H3A···O3 ⁱ	0.89	2.42	3.074 (3)	130.7

N3—H3C…O2 ^{vi}	0.89	2.69	3.088 (2)	108.3
N3—H3A…O4 ⁱⁱ	0.89	2.35	2.972 (3)	126.6
30 °C				
N1—H1C…O3 ⁱ	0.89	2.88	3.352 (3)	114.5
N1—H1C…O3 ⁱⁱ	0.89	2.16	3.016 (2)	160.0
N1—H1B…O3 ⁱⁱⁱ	0.89	2.30	3.016 (2)	138.1
N1—H1A…C11	0.89	2.54	3.386 (3)	158.9
N2—H2C…C11	0.89	2.79	3.4109 (19)	128.4
N2—H2B…C11 ^{iv}	0.89	2.59	3.3811 (19)	148.1
N2—H2A…O1 ⁱⁱ	0.89	2.52	3.277 (2)	143.6
N2—H2C…O3	0.89	2.53	3.132 (3)	125.2
N3—H3C…C11 ^{iv}	0.89	2.57	3.444 (2)	166.1
N3—H3B…C11 ^v	0.89	2.66	3.5407 (19)	172.8
N3—H3A…O3 ⁱ	0.89	2.45	3.076 (3)	128.1
N3—H3C…O2 ^{vi}	0.89	2.69	3.093 (2)	108.9
N3—H3A…O4 ⁱⁱ	0.89	2.33	2.974 (3)	129.0
40 °C				
N1—H1C…O3 ⁱ	0.89	2.91	3.354 (3)	112.5
N1—H1C…O3 ⁱⁱ	0.89	2.16	3.018 (2)	161.6
N1—H1B…O3 ⁱⁱⁱ	0.89	2.31	3.018 (2)	136.1
N1—H1A…C11	0.89	2.55	3.387 (2)	157.3
N2—H2C…C11	0.89	2.85	3.4121 (18)	122.4
N2—H2B…C11 ^{iv}	0.89	2.56	3.3821 (19)	154.6
N2—H2A…O1 ⁱⁱ	0.89	2.51	3.279 (2)	145.3
N2—H2C…O3	0.89	2.48	3.136 (3)	131.0
N3—H3C…C11 ^{iv}	0.89	2.58	3.447 (2)	165.3
N3—H3B…C11 ^v	0.89	2.66	3.5428 (19)	170.9
N3—H3A…O3 ⁱ	0.89	2.46	3.078 (3)	126.5
N3—H3C…O2 ^{vi}	0.89	2.68	3.095 (2)	109.3
N3—H3A…O4 ⁱⁱ	0.89	2.32	2.977 (3)	130.6
50 °C				
N1—H1C…O3 ⁱ	0.89	2.91	3.357 (3)	113.1
N1—H1C…O3 ⁱⁱ	0.89	2.16	3.020 (2)	161.2
N1—H1B…O3 ⁱⁱⁱ	0.89	2.31	3.020 (2)	136.8
N1—H1A…C11	0.89	2.55	3.389 (3)	157.9
N2—H2C…C11	0.89	2.79	3.4126 (19)	127.9
N2—H2B…C11 ^{iv}	0.89	2.59	3.3839 (19)	148.7
N2—H2A…O1 ⁱⁱ	0.89	2.52	3.283 (2)	143.7
N2—H2C…O3	0.89	2.53	3.137 (3)	125.7

N3—H3C…C11 ^{iv}	0.89	2.58	3.449 (2)	165.7
N3—H3B…C11 ^v	0.89	2.66	3.546 (2)	171.9
N3—H3A…O3 ⁱ	0.89	2.46	3.081 (3)	127.3
N3—H3C…O2 ^{vi}	0.89	2.69	3.098 (2)	109.2
N3—H3A…O4 ⁱⁱ	0.89	2.33	2.978 (3)	129.5
60 °C				
N1—H1C…O3 ⁱ	0.89	2.93	3.360 (3)	111.7
N1—H1C…O3 ⁱⁱ	0.89	2.16	3.022 (2)	162.3
N1—H1B…O3 ⁱⁱⁱ	0.89	2.32	3.022 (2)	135.3
N1—H1A…C11	0.89	2.55	3.390 (3)	156.6
N2—H2C…C11	0.89	2.83	3.4134 (19)	124.2
N2—H2B…C11 ^{iv}	0.89	2.57	3.3857 (19)	152.7
N2—H2A…O1 ⁱⁱ	0.89	2.52	3.285 (2)	144.7
N2—H2C…O3	0.89	2.50	3.141 (3)	129.2
N3—H3C…C11 ^{iv}	0.89	2.59	3.454 (2)	164.4
N3—H3B…C11 ^v	0.89	2.67	3.5480 (19)	169.3
N3—H3A…O3 ⁱ	0.89	2.49	3.084 (3)	125.0
N3—H3C…O2 ^{vi}	0.89	2.69	3.103 (2)	109.7
N3—H3A…O4 ⁱⁱ	0.89	2.31	2.980 (3)	131.8
70 °C				
N1—H1C…O3 ⁱ	0.89	2.92	3.364 (3)	112.2
N1—H1C…O3 ⁱⁱ	0.89	2.16	3.023 (2)	162.0
N1—H1B…O3 ⁱⁱⁱ	0.89	2.32	3.023 (2)	135.8
N1—H1A…C11	0.89	2.55	3.392 (3)	157.1
N2—H2C…C11	0.89	2.79	3.415 (2)	128.0
N2—H2B…C11 ^{iv}	0.89	2.60	3.388 (2)	148.5
N2—H2A…O1 ⁱⁱ	0.89	2.53	3.289 (3)	143.5
N2—H2C…O3	0.89	2.54	3.140 (3)	125.5
N3—H3C…C11 ^{iv}	0.89	2.59	3.456 (2)	166.2
N3—H3B…C11 ^v	0.89	2.67	3.551 (2)	173.0
N3—H3A…O3 ⁱ	0.89	2.45	3.086 (3)	128.4
N3—H3C…O2 ^{vi}	0.89	2.70	3.105 (2)	109.2
N3—H3A…O4 ⁱⁱ	0.89	2.35	2.980 (3)	128.2
80 °C				
N1—H1C…O3 ⁱ	0.89	2.92	3.364 (3)	112.5
N1—H1C…O3 ⁱⁱ	0.89	2.17	3.025 (2)	161.8
N1—H1B…O3 ⁱⁱⁱ	0.89	2.32	3.025 (2)	136.1
N1—H1A…C11	0.89	2.56	3.396 (3)	157.3
N2—H2C…C11	0.89	2.82	3.417 (2)	126.1

N2—H2B…C11 ^{iv}	0.89	2.58	3.389 (2)	150.6
N2—H2A…O1 ⁱⁱ	0.89	2.53	3.292 (3)	144.1
N2—H2C…O3	0.89	2.52	3.145 (3)	127.4
N3—H3C…C11 ^{iv}	0.89	2.59	3.460 (2)	166.2
N3—H3B…C11 ^v	0.89	2.67	3.554 (2)	173.0
N3—H3A…O3 ⁱ	0.89	2.46	3.090 (3)	128.3
N3—H3C…O2 ^{vi}	0.89	2.70	3.110 (2)	109.3
N3—H3A…O4 ⁱⁱ	0.89	2.35	2.983 (3)	128.1
90 °C				
N1—H1C…O3 ⁱ	0.89	2.92	3.369 (3)	112.9
N1—H1C…O3 ⁱⁱ	0.89	2.17	3.028 (2)	161.7
N1—H1B…O3 ⁱⁱⁱ	0.89	2.32	3.028 (2)	136.5
N1—H1A…C11	0.89	2.56	3.398 (3)	157.7
N2—H2C…C11	0.89	2.77	3.4197 (19)	131.2
N2—H2B…C11 ^{iv}	0.89	2.62	3.3892 (19)	145.1
N2—H2A…O1 ⁱⁱ	0.89	2.55	3.296 (3)	142.1
N2—H2C…O3	0.89	2.58	3.147 (3)	122.6
N3—H3C…C11 ^{iv}	0.89	2.59	3.461 (2)	166.1
N3—H3B…C11 ^v	0.89	2.67	3.557 (2)	172.7
N3—H3A…O3 ⁱ	0.89	2.47	3.096 (3)	128.1
N3—H3C…O2 ^{vi}	0.89	2.70	3.112 (2)	109.3
N3—H3A…O4 ⁱⁱ	0.89	2.35	2.984 (3)	128.3
100 °C				
N1—H1C…O3 ⁱ	0.89	2.93	3.371 (3)	112.5
N1—H1C…O3 ⁱⁱ	0.89	2.17	3.030 (3)	162.0
N1—H1B…O3 ⁱⁱⁱ	0.89	2.33	3.030 (3)	136.1
N1—H1A…C11	0.89	2.56	3.398 (3)	157.3
N2—H2C…C11	0.89	2.74	3.420 (2)	134.5
N2—H2B…C11 ^{iv}	0.89	2.65	3.391 (2)	141.5
N2—H2A…O1 ⁱⁱ	0.89	2.56	3.300 (3)	140.6
N2—H2C…O3	0.89	2.61	3.146 (3)	119.5
N3—H3C…C11 ^{iv}	0.89	2.59	3.464 (2)	166.1
N3—H3B…C11 ^v	0.89	2.67	3.559 (2)	172.8
N3—H3A…O3 ⁱ	0.89	2.47	3.097 (3)	128.1
N3—H3C…O2 ^{vi}	0.89	2.71	3.115 (3)	109.3
N3—H3A…O4 ⁱⁱ	0.89	2.35	2.985 (3)	128.1
110 °C				
N1—H1C…O3 ⁱ	0.89	2.94	3.372 (3)	111.7
N1—H1C…O3 ⁱⁱ	0.89	2.17	3.031 (3)	162.7

N1—H1B…O3 ⁱⁱⁱ	0.89	2.33	3.031 (3)	135.3
N1—H1A…C11	0.89	2.56	3.399 (3)	156.7
N2—H2C…C11	0.89	2.82	3.421 (2)	126.3
N2—H2B…C11 ^{iv}	0.89	2.59	3.393 (2)	150.4
N2—H2A…O1 ⁱⁱ	0.89	2.54	3.301 (3)	143.8
N2—H2C…O3	0.89	2.53	3.153 (3)	127.2
N3—H3C…C11 ^{iv}	0.89	2.60	3.467 (2)	165.7
N3—H3B…C11 ^v	0.89	2.68	3.560 (2)	171.9
N3—H3A…O3 ⁱ	0.89	2.48	3.100 (3)	127.4
N3—H3C…O2 ^{vi}	0.89	2.71	3.118 (3)	109.5
N3—H3A…O4 ⁱⁱ	0.89	2.35	2.987 (3)	128.8
120 °C				
N1—H1C…O3 ⁱ	0.89	2.93	3.375 (3)	113.1
N1—H1C…O3 ⁱⁱ	0.89	2.17	3.033 (3)	161.7
N1—H1B…O3 ⁱⁱⁱ	0.89	2.32	3.033 (3)	136.6
N1—H1A…C11	0.89	2.56	3.403 (3)	157.8
N2—H2C…C11	0.89	2.77	3.421 (2)	131.5
N2—H2B…C11 ^{iv}	0.89	2.63	3.396 (2)	144.8
N2—H2A…O1 ⁱⁱ	0.89	2.56	3.306 (3)	141.9
N2—H2C…O3	0.89	2.59	3.152 (3)	122.3
N3—H3C…C11 ^{iv}	0.89	2.60	3.470 (2)	166.7
N3—H3B…C11 ^v	0.89	2.68	3.563 (2)	174.6
N3—H3A…O3 ⁱ	0.89	2.46	3.103 (3)	129.8
N3—H3C…O2 ^{vi}	0.89	2.71	3.121 (3)	109.2
N3—H3A…O4 ⁱⁱ	0.89	2.38	2.989 (3)	126.1

Symmetry code(s): (i) $x-1/2, y, -z+3/2$; (ii) $-x+1/2, -y, z-1/2$; (iii) $-x+1/2, y+1/2, z-1/2$; (iv) $-x+1/2, -y, z+1/2$; (v) $x-1/2, -y+1/2, -z+3/2$; (vi) $-x, y-1/2, -z+2$.