

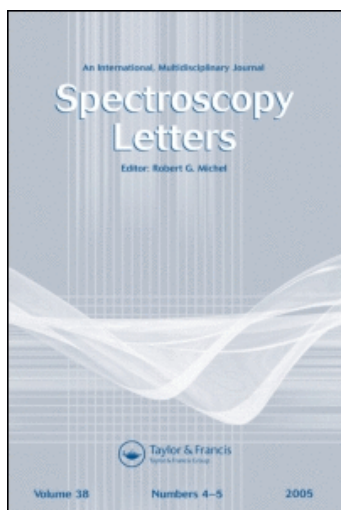
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Structure of 5-Allyl-2-hydroxy-3-methoxyazobenzene

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STRUCTURE OF

5 - ALLYL - 2 - HYDROXY - 3 - METHOXYAZOBENZENE

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ABSTRACT

5 - allyl - 2 - hydroxy - 3 - methoxyazobenzene was prepared by the reaction of 4 - allyl - 2 - methoxyphenol and benzenediazoniumchloride and crystallized from dimethylsulphoxide to yield crystals suitable for analysis. The molecular structure was identified by UV-VIS, IR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$ and elemental analysis. The crystal structure of the title compound was determined as monoclinic by single crystal X-Ray diffraction technique. The crystal parameters of this compound are as follows: monoclinic $P2_1/n$, $a=5.559(2)$ Å, $b=14.900(2)$ Å, $c=17.573(29)$ Å, $\beta=98.58(1)^\circ$, $V=1439.3(2)$ Å³, $Z=2$, $D_x=0.610$ g/cm³, $F(000)=284$, $\lambda(\text{MoK}\alpha)=0.71070$ Å, $\mu=0.041$ mm⁻¹. The structure was solved by SHELXS-86 and refined by SHELXL-93. $R=0.09$ for 1107 observed reflections with $I > 2\sigma(I)$.

INTRODUCTION

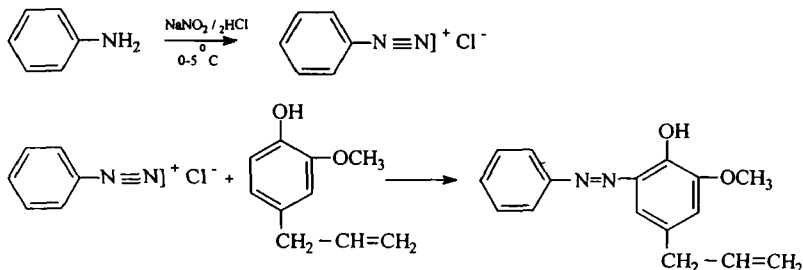
The relationship between molecular structure, solid state packing arrangements and dye performance characteristics has, over recent years, become an area of increasing investigation. The importance of molecular structure to molecular electronic properties such as colour has also been the subject of considerable study. Properties such as solubility and saturation value in the fibre are related to the free energy of the dye

molecule in the crystalline state. In class of the dye molecule, azo compounds are an important kind of organic colorants and consist of at least a conjugate chromophore azo ($\text{N}=\text{N}$) group and two or more aromatic rings. The colour of azo dyes is mainly due to the interaction of the $\text{N}=\text{N}$ group and incident light.

In this study, the molecular and crystal structure of 5-allyl-2-hydroxy-3-methoxyazobenzene was identified by the spectroscopic techniques such as UV-VIS, IR, ^1H -NMR, ^{13}C -NMR, and determined by X-Ray diffraction method.

EXPERIMENTAL

The solution of 0.041 mol aniline and 18 ml of distilled water was mixed with 8 ml concentrated HCl solution in a beaker to obtain anilinium chloride solution. Then the solution was placed in an ice bath and the cold solution of NaNO_2 and 7.5 ml of distilled water was added dropwise to the solution to give benzenediazonium chloride solution. 0.04 mol eugenol was dissolved in NaOH solution and this solution was slowly added to the solution of benzenediazonium chloride solution by stirring. The solution was stirred about 30 min. and the solid product formed was filtered off and washed with water. After that the solid product was dissolved in acetic acid and the brown coloured azo compound was precipitated by adding distilled water to the acetic acid solution. The azo dye, 5-allyl-2-hydroxy-3-methoxyazobenzene, was crystallized from dimethylsulphoxide to yield crystals suitable for analysis.



5 - allyl - 2- hydroxy - 3 - methoxyazobenzene:

Yield; 70 %, m.p.; 68.3° C,

IR(KBr): 3500 (OH), 3100 - 2850 (alkyl), 1640 (C = C), 1450 -1400 (N = N),
1380 (OCH₃) cm⁻¹.

UV-VIS (CHCl₃) λ_{max} (ε) : 3337.4 (13769.7), 242.7(15424.4), 215.7 (115.1) nm.

¹H-NMR (CDCl₃ -d₆) : δ 13.15 (s, 1H, -OH), 8.0 - 6.2 (m, 6H, arom.), 6.5 - 5.5 (m, 1H, =CH), 5.2 - 5.0 (m, 2H, =CH₂), 3.8 (s, 3H, -OCH₃), 3.6 - 3.3 (d, 2H, CH₂). ppm.

¹³C-NMR (CDCl₃) : δ 150.37, 148.65, 141.59, 137.11, 136.91, 131.13, 130.61, 129.32, 123.89, 122.15, 116.20, 115.42, 56.39, 39.56 ppm.

Anal. Calcd. for C₁₆H₁₆N₂O₂ : % C : 71.64, % H : 5.97, % N : 10.44

Found : % C :71.84, % H : 6.00, % N : 10.44

x-ray diffraction:

Intensities were measured on an Enraf - Nonius CAD - 4 four - circle diffractometer (graphite - monochromated MoKα x-rays). Crystal dimensions approximately 0.4 x 0.3 x 0.15 mm³. Accurate unit - cell parameters and the orientation matrix determined by least squares using 25 reflections in the range 5.45° < θ < 11.10°. Data collection used w/2θ scan. A total of 1107 reflections (0 < h < 6, 0 < k < 17, -20 < l < 20) was considered non - zero at the 2σ (I) significance level out of 1669 possible reflections in the θ range 2.34° - 24.26°. Three standart reflections were checked with interval 120 min. for orientation.

Data were corrected for Lorentz, Polarization factors. This structure was solved by direct methods using SHELXS-86¹ and refined by full matrix least squares using SHELXL - 93². The title crystal was of poor quality so the R and wR indexes are not good enough. Final R = 0.09, wR = 0.26 with weighting scheme

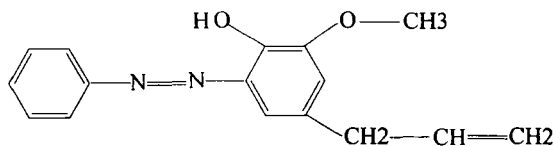


Fig.-1

$w^{-1} = [\sigma^2 (F_o) + (0.2426) P^2]$, $P = (F_o^2 + 2 F_c^2) / 3$. Max. and min. heights in final difference Fourier map 0.30 and $-0.46 \text{ e} \text{ \AA}^{-3}$. The C16 atom of the allyl group is disordered two sites (C16A, C16B to proportions 81:19). The H atoms of the C16 atom in the allyl group attached to major component C16A. H atoms isotropically, non-H atoms anisotropically refined. The temperature factors of C15, C16A and C16B atoms are only slightly larger than the other atoms.

RESULT AND DISCUSSION

The title structure in Fig.-1 is very similar to the previous works of the azo compounds³⁻⁵. Table-1 lists final atomic coordinates of non-H atoms and selected bond lengths and angles are given in Table-2. Also positional of Hydrogen atoms are given in Table-3. An ORTEP⁶ drawing of the molecule with atomic numbering scheme is shown Fig.-2. In the compound the unsubstituted phenyl ring and the other phenyl ring are trans. The lengths of the two C-N bonds are almost identical and average C-N bond length is $1.391(7) \text{ \AA}$. Also the average value of the C-N-N angles is $115.8(4)^\circ$. The N=N bond length is $1.278(6) \text{ \AA}$ in accordance with the expected value for aromatic azo compounds. The angle between the least-square planes through atoms C1 - C6 and C7-C12 is $5.00(1)^\circ$. The torsion angles N2-N1-C1-C6 and N2-N1-C1-C2

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for title compound.

	x	y	z	U(eq) *
O(1)	1058 (7)	7933 (3)	2001 (2)	70 (1)
C(9)	4394 (9)	8935 (4)	2243 (3)	60 (2)
N(1)	-765 (7)	7486 (3)	3221 (3)	58 (1)
N(2)	745 (8)	7979 (3)	3655 (3)	60 (1)
C(1)	-2429 (9)	7010 (4)	3595 (3)	56 (1)
C(8)	2585 (9)	8430 (3)	2506 (3)	53 (1)
C(7)	2421 (9)	8436 (4)	3299 (3)	57 (2)
O(2)	4408 (7)	8879 (3)	1458 (2)	77 (1)
C(12)	4074 (10)	8964 (4)	3795 (3)	64 (2)
C(10)	5983 (10)	9451 (5)	2737 (3)	69 (2)
C(6)	-2384 (12)	6975 (5)	4389 (4)	74 (2)
C(2)	-4202 (11)	6524 (4)	3124 (4)	68 (2)
C(4)	-5817 (13)	5981 (6)	4228 (4)	83 (2)
C(3)	-5882 (11)	6015 (5)	3447 (5)	79 (2)
C(13)	6234 (12)	9335 (7)	1140 (4)	82 (2)
C(11)	5842 (10)	9458 (4)	3537 (3)	65 (2)
C(14)	7656 (15)	10014 (6)	4079 (5)	88 (2)
C(5)	-4093 (13)	6477 (6)	4693 (5)	85 (2)
C(15)	7331 (18)	10971 (7)	4011 (4)	99 (3)
C(16A)	9013 (31)	11558 (11)	3975 (5)	149 (9)
C(16B)	9349 (31)	10638 (11)	3810 (5)	17 (5)

* U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2. Selected bond lengths [Å] and angles [deg] for title compound.

O(1)-C(8)	1.353(6)
C(9)-O(2)	1.382(6)
N(1)-N(2)	1.278(6)
N(1)-C(1)	1.404(7)
N(2)-C(7)	1.378(7)
O(2)-C(13)	1.405(8)
C(11)-C(14)	1.524(9)
C(14)-C(15)	1.441(12)
C(15)-C(16A)	1.288(13)
C(15)-C(16B)	1.32(2)
O(2)-C(9)-C(8)	114.3(4)
N(2)-N(1)-C(1)	115.5(4)
N(1)-N(2)-C(7)	116.2(4)
C(6)-C(1)-N(1)	125.0(5)
C(2)-C(1)-N(1)	116.3(5)
O(1)-C(8)-C(9)	119.5(5)
O(1)-C(8)-C(7)	121.6(5)
N(2)-C(7)-C(8)	126.4(5)
N(2)-C(7)-C(12)	114.7(5)

Table 3. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for title compound.

	x	y	z	U(eq)
H(1)	-67(11)	766(5)	236(4)	101(23)
H(12)	382(10)	888(4)	437(4)	77(17)
H(10)	713(9)	993(4)	252(3)	60(15)
H(6)	-124(11)	731(4)	472(4)	84(21)
H(2)	-420(9)	664(3)	257(3)	53(14)
H(4)	-694(9)	559(4)	443(3)	61(16)
H(3)	-678(12)	575(4)	311(4)	73(20)
H(13A)	611(19)	945(7)	57(7)	185(40)
H(13B)	780(10)	895(4)	138(3)	60(14)
H(13C)	616(9)	996(4)	124(3)	57(17)
H(14A)	74(2)	993(6)	462(3)	14(3)
H(14B)	917(19)	969(11)	402(9)	297(8)
H(5)	-411(12)	644(4)	5180(40)	83(22)
H(15)	561(7)	1125(4)	396(4)	81(20)
H(16A)	1062(3)	11375(11)	3993(5)	566(30)
H(16B)	862(3)	12164(11)	3932(5)	185(61)

are $-6.5(7)^\circ$ and $175.3(5)^\circ$, respectively. Thus the benzene ring skeleton and the azo group are almost coplanar.

The planarity of the molecule facilitates an intramolecular hydrogen bond, completing the six membered ring, in which the hydroxyl group (O1-H1) adjacent to the -N=N- bond serves as the donor to the N1 atom. The O1-H1.....N1 angle is $150.7(6)^\circ$

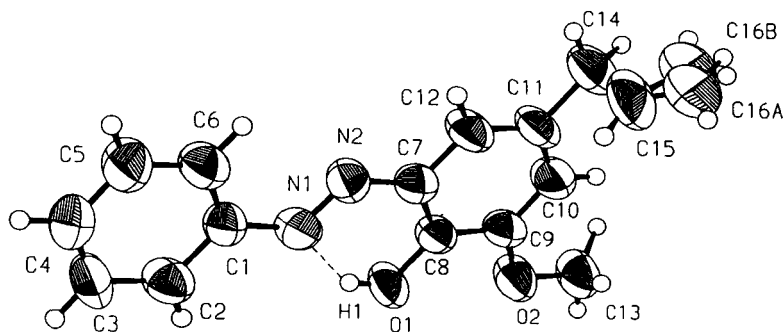


Fig.-2

and the length of the hydrogen bond (O1-H1....N1) in the molecule is 1.634(1) Å, whereas the length of O1- N1 bond is 2.592(1) Å which is shorter than a typical hydrogen bond⁷ (N....O-H = 2.78 (10) Å). This shows the presence of a very strong intramolecular interaction in the molecule, the strong intramolecular hydrogen bonding was also confirmed by IR and ¹H-NMR spectroscopy. In the IR spectra of the title compound the broadening of the OH band was observed in the range of 3500 - 3200 cm⁻¹ while the OH resonance in the ¹H - NMR spectra was greatly shifted to downfield. ¹H-NMR spectra of the starting compound, eugenol, which does not exist a strong intramolecular hydrogen bonding, the OH resonance occurs in the range of δ 6.0 - 5.0 ppm. However in the title compound this resonance shifts to 13.15 ppm due to the presence of the hydrogen bond. It is evident that this strong intramolecular hydrogen bond tend to keep the molecule planar. However, there is no intermolecular interaction other than van der Waals contacts between the molecules which are therefore present as isolated individuals within the crystal.

There is evidence of some disorder in the position of atom C16 of the Allyl group. The disordered C16 atom was recognized in a proportion of 81:19 s.o.f's. C15-C16A and C15-C16B double bond lengths (1.29(1), 1.32(2) respectively) are shorter than literature since this moiety have disorder.

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The authors wish to acknowledge for the use of the CAD - 4 diffractometer (purchased under Grant DPT/TBAG1 of the Scientific and Technical Research Council of Turkey) of Physics Engineering Dept., Hacettepe University, Turkey.

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Supplementary Table 1. Bond lengths [$\text{\AA}$] and angles [deg] for title compound.

O(1)-C(8)	1.353(6)
C(9)-C(10)	1.378(8)
C(9)-O(2)	1.382(6)
C(9)-C(8)	1.389(7)
N(1)-N(2)	1.278(6)
N(1)-C(1)	1.404(7)
N(2)-C(7)	1.378(7)
C(1)-C(6)	1.392(8)
C(1)-C(2)	1.392(8)
C(8)-C(7)	1.410(7)
C(7)-C(12)	1.409(8)
O(2)-C(13)	1.405(8)
C(12)-C(11)	1.358(8)
C(10)-C(11)	1.419(8)
C(6)-C(5)	1.375(10)
C(2)-C(3)	1.389(9)
C(4)-C(3)	1.368(10)
C(4)-C(5)	1.377(10)
C(11)-C(14)	1.524(9)
C(14)-C(16B)	1.45(2)
C(14)-C(15)	1.441(12)
C(15)-C(16A)	1.288(13)
C(15)-C(16B)	1.32(2)
C(10)-C(9)-O(2)	124.4(5)
C(10)-C(9)-C(8)	121.3(5)

O(2) - C(9) - C(8)	114.3(4)
N(2) - N(1) - C(1)	115.5(4)
N(1) - N(2) - C(7)	116.2(4)
C(6) - C(1) - C(2)	118.8(6)
C(6) - C(1) - N(1)	125.0(5)
C(2) - C(1) - N(1)	116.3(5)
O(1) - C(8) - C(9)	119.5(5)
O(1) - C(8) - C(7)	121.6(5)
C(9) - C(8) - C(7)	118.8(5)
N(2) - C(7) - C(8)	126.4(5)
N(2) - C(7) - C(12)	114.7(5)
C(8) - C(7) - C(12)	118.8(5)
C(9) - O(2) - C(13)	118.6(5)
C(11) - C(12) - C(7)	122.3(6)
C(9) - C(10) - C(11)	120.3(6)
C(5) - C(6) - C(1)	120.0(7)
C(3) - C(2) - C(1)	120.1(6)
C(3) - C(4) - C(5)	119.2(7)
C(4) - C(3) - C(2)	120.7(7)
C(12) - C(11) - C(10)	118.4(5)
C(12) - C(11) - C(14)	122.0(6)
C(10) - C(11) - C(14)	119.6(6)
C(16B) - C(14) - C(15)	54.4(9)
C(16B) - C(14) - C(11)	123.0(7)
C(15) - C(14) - C(11)	115.0(6)
C(6) - C(5) - C(4)	121.2(7)
C(16A) - C(15) - C(14)	126.4(11)
C(16B) - C(15) - C(14)	63.2(8)
C(15) - C(16B) - C(14)	62.4(8)

Supplementary Table 2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for title compound.

	U11	U22	U33	U23	U13	U12
O(1)	64(2)	91(3)	52(2)	-7(2)	-3(2)	-17(2)
C(9)	57(3)	77(4)	43(3)	3(3)	-3(3)	3(3)
N(1)	55(3)	66(3)	53(3)	1(2)	4(2)	15(2)
N(2)	57(3)	63(3)	58(3)	1(2)	2(2)	7(2)
C(1)	45(3)	68(3)	55(3)	10(3)	11(2)	9(3)
C(8)	48(3)	56(3)	52(3)	-1(3)	1(2)	9(3)
C(7)	54(3)	68(4)	49(3)	5(3)	6(3)	7(3)
O(2)	70(3)	109(4)	50(2)	3(2)	9(2)	-19(2)
C(12)	55(3)	85(4)	48(3)	-9(3)	-2(3)	0(3)
C(10)	56(3)	89(4)	61(4)	9(3)	3(3)	6(3)
C(6)	66(4)	99(5)	56(4)	5(4)	5(3)	3(4)
C(2)	62(4)	82(4)	60(4)	-1(3)	6(3)	14(3)
C(4)	64(4)	101(6)	86(5)	20(4)	19(4)	2(4)
C(3)	51(4)	98(5)	86(6)	1(4)	5(4)	-9(4)
C(13)	63(4)	112(7)	72(4)	12(5)	19(3)	-8(4)
C(11)	53(3)	74(4)	61(4)	-12(3)	-11(3)	3(3)
C(14)	89(5)	96(6)	72(5)	-11(4)	-13(4)	-7(4)
C(5)	75(4)	120(6)	64(5)	9(4)	22(4)	-3(4)
C(15)	131(8)	92(7)	70(5)	-18(4)	-3(5)	-23(6)
C(16A)	245(19)	114(13)	68(7)	3(6)	-41(8)	-78(11)
C(16B)	212(70)	209(94)	92(35)	57(42)	79(39)	128(68)

The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 \cdot [h^2 \cdot a^{*2} \cdot U_{11} + \dots + 2 \cdot h \cdot k \cdot a^* \cdot b^* \cdot U_{12}]$

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Supplementary Table 3. Observed and calculated structure factors for title compound.

h	k	l	10fo	10fc	10s	h	k	l	10fo	10fc	10s	h	k	l	10fo	10fc	10s
2	0	0	181	160	2	-1	3	1	892	795	2	-1	16	1	75	67	4
4	0	0	93	96	2	0	3	1	399	482	91	0	16	1	11	21	10
6	0	0	233	262	3	1	3	1	1683	1772	2	1	16	1	33	31	9
1	1	0	251	224	2	2	3	1	53	52	2	-1	17	1	25	21	14
2	1	0	163	133	2	3	3	1	50	44	3	0	17	1	22	8	21
3	1	0	8	7	7	4	3	1	90	91	2	-2	0	2	58	51	2
5	1	0	23	28	22	5	3	1	144	147	2	0	0	2	854	807	31
6	1	0	16	47	16	6	3	1	29	29	28	2	0	2	466	451	3
0	2	0	263	254	1	-5	4	1	62	58	4	4	0	2	89	99	2
1	2	0	1031	953	2	-4	4	1	24	12	8	6	0	2	99	113	4
4	2	0	67	68	3	-3	4	1	19	9	8	-6	1	2	78	83	4
5	2	0	163	166	2	-2	4	1	150	150	2	-4	1	2	69	61	3
6	2	0	39	39	7	-1	4	1	855	786	2	-3	1	2	144	139	2
1	3	0	701	674	2	0	4	1	188	178	38	-2	1	2	142	125	2
2	3	0	208	205	2	1	4	1	93	120	1	-1	1	2	584	572	2
3	3	0	59	53	2	2	4	1	72	65	2	0	1	2	701	772	165
4	3	0	94	91	2	3	4	1	120	129	1	1	1	2	80	72	1
5	3	0	126	131	2	4	4	1	122	124	2	3	1	2	110	100	1
0	4	0	755	744	2	5	4	1	153	154	2	5	1	2	65	70	4
1	4	0	962	1047	2	-6	5	1	26	20	13	6	1	2	106	117	3
2	4	0	231	205	2	-4	5	1	150	140	2	-5	2	2	103	108	3
3	4	0	203	204	2	-3	5	1	107	96	2	-3	2	2	42	45	3
5	4	0	87	96	3	-2	5	1	19	25	18	-2	2	2	29	26	3

(continued)

2	12	0	73	57	3	2	8	1	189	177	2	3	4	2	131	130	1	-2	1	3	59	58	2	4	10	3	24	38	24
3	12	0	53	40	5	3	8	1	72	56	3	4	4	2	100	100	2	-1	1	3	265	309	2	-4	11	3	16	25	15
4	12	0	24	21	15	4	8	1	162	147	2	6	4	2	29	45	28	0	1	3	25	21	4	-3	11	3	86	79	3
1	13	0	54	49	4	5	8	1	22	12	17	-6	5	2	24	7	23	1	1	3	293	253	2	-1	11	3	44	42	4
2	13	0	95	139	3	-4	9	1	50	40	5	-5	5	2	64	74	4	2	1	3	149	154	1	0	11	3	63	52	3
4	13	0	88	90	4	-3	9	1	159	129	2	-4	5	2	9	9	9	3	1	3	141	133	1	1	11	3	13	12	13
1	16	0	28	26	11	0	9	1	43	39	3	-3	5	2	81	84	2	5	1	3	36	30	6	2	11	3	46	44	5
2	16	0	20	24	20	1	9	1	12	8	11	-2	5	2	103	95	1	-5	2	3	23	20	22	3	11	3	74	73	4
1	17	0	50	50	7	2	9	1	78	62	2	-1	5	2	584	578	3	-4	2	3	205	202	3	4	11	3	20	19	19
-5	0	1	27	31	26	3	9	1	153	142	2	0	5	2	94	95	15	-3	2	3	100	90	1	-4	12	3	24	19	17
-3	0	1	83	91	2	5	9	1	20	10	19	1	5	2	18	27	7	-2	2	3	31	32	3	-3	12	3	26	5	25
-1	0	1	22	19	3	-3	10	1	401	353	5	2	5	2	329	287	3	-1	2	3	124	149	2	-1	12	3	25	11	25
1	0	1	207	210	2	-2	10	1	51	54	4	3	5	2	41	38	4	0	2	3	689	732	179	0	12	3	17	16	17
3	0	1	134	139	2	-1	10	1	19	30	10	5	5	2	132	132	2	1	2	3	390	350	2	1	12	3	50	55	5
5	0	1	122	129	2	0	10	1	34	31	4	-5	6	2	65	71	4	2	2	3	462	417	3	3	12	3	19	47	18
-6	1	1	44	48	7	1	10	1	34	33	5	-4	6	2	144	132	2	3	2	3	4	26	4	-4	13	3	49	35	6
-4	1	1	74	74	3	2	10	1	40	55	5	-3	6	2	18	22	11	5	2	3	26	26	10	-2	13	3	18	28	17
-3	1	1	20	23	7	-3	11	1	54	46	5	-1	6	2	141	148	2	6	2	3	62	64	5	-1	13	3	56	47	4
-2	1	1	431	408	3	-2	11	1	16	2	15	0	6	2	67	61	5	-6	3	3	31	42	10	0	13	3	39	27	6
-1	1	1	359	319	2	-1	11	1	18	1	19	1	6	2	145	262	1	-5	3	3	54	53	4	-3	14	3	35	18	9
1	1	1	158	151	1	1	11	1	43	51	4	2	6	2	325	337	4	-4	3	3	31	28	6	-2	14	3	37	25	7
2	1	1	25	26	4	2	11	1	73	68	3	3	6	2	26	32	7	-3	3	3	47	39	3	-1	14	3	71	56	3
3	1	1	61	63	2	3	11	1	129	127	2	4	6	2	22	10	21	-2	3	3	157	139	2	0	14	3	24	31	24
4	1	1	63	62	3	-3	12	1	81	76	3	-5	7	2	15	16	15	-1	3	3	376	445	2	1	14	3	7	14	7

(continued)

Supplementary Table 3. Continued

h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s		h k l 10Fo 10Fc 10s			
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-2	2	4	376	327	3	2	12	4	8	4	7	5	7	5	30	26	30	4	4	6	114	119	2	-5	2	7	25	10	25
-1	2	4	121	148	1	-4	13	4	20	30	20	5	8	5	59	49	5	-4	5	6	58	56	4	-4	2	7	125	132	2
0	2	4	176	195	43	-2	13	4	66	60	4	-3	8	5	62	58	3	-3	5	6	108	107	2	-3	2	7	74	72	2
1	2	4	37	39	2	-1	13	4	85	70	3	-1	8	5	165	203	2	-2	5	6	184	199	2	-2	2	7	19	22	19
2	2	4	310	278	3	0	13	4	25	28	24	0	8	5	71	64	2	-1	5	6	88	127	2	-1	2	7	407	441	3
3	2	4	94	85	2	1	13	4	14	58	14	1	8	5	111	155	2	0	5	6	94	107	28	0	2	7	237	234	9
4	2	4	55	51	3	-3	14	4	23	3	22	2	8	5	18	36	17	1	5	6	40	37	3	1	2	7	31	39	4
6	2	4	24	13	23	-1	14	4	11	5	10	4	8	5	35	23	7	2	5	6	55	54	3	2	2	7	174	176	2
-5	3	4	22	15	12	0	14	4	20	11	20	5	8	5	43	48	7	3	5	6	24	26	23	3	2	7	9	21	8
-4	3	4	112	108	2	1	14	4	42	50	6	-4	9	5	30	4	29	5	5	6	20	20	19	4	2	7	29	22	8
-3	3	4	16	11	15	3	14	4	26	10	26	-3	9	5	29	32	28	-5	6	6	68	60	4	5	2	7	65	67	4
-2	3	4	419	366	3	-1	15	4	11	24	11	0	9	5	211	178	7	-3	6	6	46	45	4	-6	3	7	19	15	19
-1	3	4	30	36	3	0	15	4	14	1	14	1	9	5	26	29	25	-1	6	6	147	196	2	-3	3	7	92	89	2
0	3	4	91	75	24	-2	16	4	20	2	20	2	9	5	62	57	3	0	6	6	44	52	12	-2	3	7	21	30	29
1	3	4	30	27	3	-1	16	4	16	10	16	-4	10	5	11	6	10	1	6	6	298	307	4	-1	3	7	104	116	1
2	3	4	28	32	4	1	16	4	21	17	21	-3	10	5	105	84	3	2	6	6	49	44	3	0	3	7	244	240	28
3	3	4	19	2	18	-5	0	5	56	58	4	-2	10	5	9	29	9	3	6	6	5	18	5	1	3	7	39	41	3
4	3	4	52	49	4	-3	0	5	275	269	3	-1	10	5	117	115	2	5	6	6	68	73	5	3	3	7	53	63	4
-5	4	4	21	29	20	-1	0	5	236	251	3	1	10	5	17	31	16	-5	7	6	38	23	7	4	3	7	37	42	6
-4	4	4	180	168	2	1	0	5	517	452	3	2	10	5	27	24	27	-4	7	6	22	18	12	-5	4	7	28	26	9
-3	4	4	11	37	11	3	0	5	8	6	8	3	10	5	71	72	3	-3	7	6	146	139	2	-4	4	7	19	13	18
-2	4	4	139	125	2	5	0	5	35	38	7	4	10	5	19	22	19	-2	7	6	83	76	2	-3	4	7	60	55	3
-1	4	4	121	162	1	-4	1	5	9	20	8	-3	11	5	23	6	12	-1	7	6	185	208	2	-2	4	7	169	208	2
0	4	4	124	159	37	-3	1	5	500	452	4	0	11	5	38	35	17	1	7	6	177	162	2	0	4	7	87	78	14

(continued)

Supplementary Table 3. Continued

h		1		102c		10s		h		k		1		102c		10s		h		k		1		102c		10s		h		k		1		102c		10s					
2	4	4	359	312	3	-1	1	5	513	562	2	1	11	5	24	21	9	2	7	6	98	85	2	1	4	7	85	79	2	1	4	7	85	79	2	1	4	7	85	79	2
3	4	4	78	79	2	0	1	5	479	441	12	2	11	5	64	51	4	3	7	6	126	108	2	2	4	7	96	92	2	2	4	7	96	92	2	2	4	7	96	92	2
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-2	5	4	286	251	3	-6	2	5	15	3	15	2	12	5	29	23	9	0	8	6	22	27	22	-3	5	7	33	30	5	-3	5	7	33	30	5	-3	5	7	33	30	5
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-2	6	4	67	63	2	4	2	5	64	72	3	2	14	5	16	20	15	4	9	6	25	6	24	-2	6	7	143	153	1	-2	6	7	143	153	1	-2	6	7	143	153	1
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1	6	4	273	335	3	-2	3	5	302	253	3	-2	16	5	51	36	6	-2	10	6	82	74	3	2	6	7	53	49	3	2	6	7	53	49	3	2	6	7	53	49	3
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-2	7	4	264	223	3	4	3	5	149	155	2	2	0	6	324	300	3	-4	11	6	71	60	4	-1	7	7	32	38	5	-1	7	7	32	38	5	-1	7	7	32	38	5

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0	7	4	69	82	6	-5	4	5	25	14	12	-5	1	6	42	49	5	-2	11	6	10	3	9	1	7	7	127	117	2
1	7	4	127	133	1	-5	4	5	26	25	10	-2	1	6	20	20	6	0	11	6	208	169	5	2	7	7	102	94	2
2	7	4	130	134	2	-4	4	5	69	69	3	-1	1	6	109	105	1	2	11	6	92	85	3	3	7	7	46	43	5
3	7	4	30	34	7	-3	4	5	110	103	1	0	1	6	58	52	2	3	11	6	38	36	6	-3	8	7	158	151	2
4	7	4	56	61	4	-2	4	5	482	457	3	2	1	6	67	69	2	4	11	6	31	16	30	-1	8	7	24	2	23
5	7	4	49	42	6	-1	4	5	66	80	2	3	1	6	103	108	2	-4	12	6	50	37	6	0	8	7	28	19	6
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1	9	4	104	126	1	4	4	5	91	86	2	-4	2	6	53	48	4	-3	13	6	27	28	27	-4	9	7	87	80	3
2	8	4	31	36	6	-6	5	5	22	12	22	-3	2	6	179	168	2	-2	13	6	32	40	9	-3	9	7	63	67	4
3	8	4	67	61	3	-5	5	5	9	3	8	-2	2	6	305	288	3	-1	13	6	12	34	12	-2	9	7	53	36	4
4	8	4	26	3	9	-4	5	5	143	143	2	-1	2	6	28	30	4	0	13	6	18	36	17	-1	9	7	43	32	4
5	9	4	39	30	8	-3	5	5	15	34	14	0	2	6	471	449	24	1	13	6	36	33	7	0	9	7	9	9	9
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0	9	4	175	168	11	3	5	5	43	50	4	-2	3	6	51	48	3	0	16	6	8	15	8	0	10	7	19	16	19
1	9	4	21	26	20	4	5	5	13	20	13	-2	3	6	10	11	10	-5	0	7	23	26	11	1	10	7	103	107	2
2	9	4	56	62	3	-5	6	5	44	50	6	-1	3	6	70	92	2	-3	0	7	189	147	2	2	10	7	10	35	10

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Supplementary Table 3. Continued

h	k	I	10Fo	10Fc	10s	h	k	I	10Fo	10Fc	10s	h	k	I	10Fo	10Fc	10s	h	k	I	10Fo	10Fc	10s	h	k	I	10Fo	10Fc	10s
4	9	4	25	10	10	-3	6	5	23	6	8	0	3	6	331	342	56	-1	0	7	174	170	2	3	10	7	11	3	10
-5	10	4	30	14	10	-2	6	5	95	86	2	1	3	6	144	134	2	1	0	7	419	412	3	4	10	7	23	5	23
-3	10	4	45	47	5	-1	6	5	158	220	2	2	3	6	77	69	2	3	0	7	147	145	2	-4	11	7	39	32	8
-2	10	4	39	40	5	1	6	5	276	309	2	3	3	6	59	52	3	5	0	7	70	74	4	-3	11	7	66	63	4
-1	10	4	41	45	4	2	6	5	45	45	3	4	3	6	38	42	6	-6	1	7	22	32	22	-1	11	7	14	10	13
0	10	4	233	211	8	3	6	5	26	34	8	5	3	6	25	26	24	-5	1	7	27	15	27	1	11	7	35	46	7
2	11	7	45	49	5	-1	8	8	27	29	7	2	7	9	67	66	3	-5	7	10	31	36	30	-2	8	11	57	46	4
3	11	7	37	48	7	0	8	8	66	59	10	4	7	9	39	42	7	-4	7	10	54	59	5	-1	8	11	53	43	5
4	11	7	17	8	16	1	8	8	19	18	13	-4	8	9	19	43	18	-3	7	10	10	12	9	0	8	11	226	203	6
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0	12	7	22	29	22	3	8	8	69	61	3	-1	8	9	118	120	2	-1	7	10	55	54	4	-4	9	11	32	2	32
1	12	7	33	39	7	-2	9	8	27	23	9	1	8	9	81	64	3	0	7	10	137	127	4	-2	9	11	42	19	6
2	12	7	22	17	13	-1	9	8	44	53	5	2	8	9	138	126	2	1	7	10	52	42	4	-1	9	11	89	88	3
3	12	7	15	30	15	0	9	8	9	33	8	3	8	9	47	46	5	2	7	10	114	113	2	0	9	11	116	102	2
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1	13	7	26	32	26	-3	10	8	43	29	6	-3	9	9	70	73	4	4	7	10	28	8	28	2	9	11	38	31	6
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1	14	7	45	46	6	1	10	8	27	13	7	0	9	9	86	64	6	-2	8	10	87	80	3	-3	10	11	15	29	15
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0	0	8	184	192	4	3	11	8	34	30	9	-1	10	9	38	37	6	4	8	10	31	32	30	0	11	11	38	47	15
2	0	8	216	196	2	-3	12	8	61	66	5	0	10	9	47	33	5	-2	9	10	50	40	5	1	11	11	59	42	4

4	0	8	41	32	6	-1	12	8	36	7	3	10	9	42	52	6	-1	9	10	86	80	3	2	11	11	32	31	33	
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-5	1	8	10	28	10	1	12	8	51	42	5	-1	11	9	27	23	26	1	9	10	28	41	27	-1	12	11	75	92	4
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2	1	8	8	32	8	2	14	8	12	31	11	0	13	9	39	31	38	-3	11	10	20	24	20	0	0	12	18	30	18
3	1	9	55	52	3	-1	15	8	33	4	32	2	13	9	28	33	11	-1	11	10	42	60	7	2	0	12	321	326	3
4	1	8	23	23	11	1	15	8	31	17	31	-2	14	9	26	43	25	0	11	10	42	48	12	-5	1	12	50	50	6
5	1	8	74	79	4	-5	0	9	81	73	3	-1	14	9	16	26	16	2	11	10	12	23	11	-4	1	12	93	91	3
-6	2	8	29	28	11	-1	0	9	10	29	10	1	14	9	13	0	13	-3	12	10	25	7	16	-3	1	12	224	235	3
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1	2	8	146	127	2	-1	1	9	70	58	2	-5	1	10	23	30	12	1	14	10	25	20	14	3	1	12	161	169	2
2	2	8	20	19	8	0	1	9	218	208	4	-4	1	10	20	14	19	-5	0	11	19	12	18	-5	2	12	36	0	7
3	2	8	24	19	24	1	1	9	258	245	3	-2	1	10	129	128	1	1	0	11	144	143	2	-4	2	12	23	15	23
4	2	8	68	82	4	3	1	9	9	9	9	-1	1	10	93	81	2	-5	1	11	22	26	22	-3	2	12	246	247	4
5	2	8	53	53	6	4	1	9	22	13	12	0	1	10	160	157	2	-4	1	11	130	132	2	-1	2	12	89	82	2

(continued)

Supplementary Table 3. Continued

h	k	1	10 ²⁰	10 ²⁰ c	10 ⁵ s	h	k	1	10 ²⁰	10 ²⁰ c	10 ⁵ s	h	k	1	10 ²⁰	10 ²⁰ c	10 ⁵ s	h	k	1	10 ²⁰	10 ²⁰ c	10 ⁵ s	h	k	1	10 ²⁰	10 ²⁰ c	10 ⁵ s
-5	3	8	22	28	12	5	1	9	16	19	16	1	1	10	146	138	2	-3	1	11	133	127	2	0	2	12	51	47	3
-4	3	8	48	55	4	-6	2	9	17	20	17	2	1	10	123	117	2	-2	1	11	45	46	4	1	2	12	108	109	2
-3	3	8	23	40	22	-5	2	9	28	3	28	3	1	10	22	14	11	-1	1	11	171	147	2	3	2	12	101	106	3
-2	3	8	82	82	2	-3	2	9	76	78	2	4	1	10	34	35	7	0	1	11	108	101	2	-5	3	12	14	20	13
-1	3	8	216	241	2	-1	2	9	74	80	2	5	1	10	29	24	11	1	1	11	58	58	3	-4	3	12	88	86	3
0	3	8	61	59	2	0	2	9	393	365	4	-4	2	10	141	139	2	2	1	11	145	147	2	-3	3	12	45	50	5
1	3	8	99	98	1	1	2	9	140	138	2	-3	2	10	123	115	2	3	1	11	100	102	2	-2	3	12	32	30	6
2	3	8	27	25	6	2	2	9	114	122	2	-2	2	10	120	109	1	4	1	11	52	41	5	-1	3	12	11	3	10
3	3	8	43	43	5	3	2	9	110	107	2	-1	2	10	67	52	2	-4	2	11	161	166	2	1	3	12	119	115	2
4	3	8	65	69	4	4	2	9	6	1	5	0	2	10	25	30	14	-2	2	11	89	85	2	2	3	12	40	46	6
-4	4	8	46	44	5	-5	3	9	15	39	15	1	2	10	14	8	14	-1	2	11	139	127	2	3	3	12	21	37	20
-3	4	8	33	30	6	-4	3	9	14	18	13	2	2	10	198	200	3	0	2	11	16	28	16	-5	4	12	45	51	7
-2	4	8	21	22	20	-3	3	9	49	50	4	3	2	10	85	82	3	1	2	11	24	29	24	-3	4	12	24	28	23
-1	4	8	120	129	1	-2	3	9	161	163	2	4	2	10	73	72	3	2	2	11	170	178	2	-2	4	12	122	129	2
0	4	8	191	197	21	-1	3	9	154	156	2	5	2	10	32	48	31	3	2	11	57	59	4	-1	4	12	69	62	3
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2	8	12	39	38	7	1	6	13	124	119	2	0	5	14	59	54	4	-3	6	15	19	9	19	0	3	17	96	93	3
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0	9	12	152	138	2	-2	7	13	37	36	7	3	5	14	113	118	3	-4	7	15	29	5	28	-3	4	17	25	18	25

(continued)

Supplementary Table 3. Continued

h k l 10Fo 10Fc 10s			h k l 10Fo 10Fc 10s			h k l 10Fo 10Fc 10s			h k l 10Fo 10Fc 10s			h k l 10Fo 10Fc 10s			h k l 10Fo 10Fc 10s														
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1	12	12	10	25	10	-1	10	13	85	98	4	0	8	14	93	76	6	-3	1	16	58	64	4	0	8	17	14	11	14
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