
Crystal structure of C₂₀H₂₆O₂ — she1011

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Abstract

The crystal structure of C₂₀H₂₆O₂ is reported.

Comment

The crystallographic asymmetric unit consists of six molecules of C₂₀H₂₆O₂. The molecules are grouped into pairs: the coordinates of atoms of molecule two are very similar to the coordinates of the corresponding atoms of molecule one after a translation of 0.5 in x, and likewise for molecules four and three and for molecules six and five.

Experimental

The compound was prepared by MFS and was crystallised from dichloromethane/hexane. The sample ID is MFSB187-HPLC-F2.

Computing details

Data collection: *COLLECT* (Nonius, 2001).; cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-II* (Johnson 1976) in *TEXSAN* (MSC, 1992-1997); software used to prepare material for publication: *CRYSTALS* (Betteridge *et al.*, 2003).

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(she1011)

Crystal data

$C_{20}H_{26}O_2$	$Z = 12$
$M_r = 298.43$	$F(000) = 1944$
Triclinic, $P\bar{1}$	$D_x = 1.199 \text{ Mg m}^{-3}$
$a = 15.4327 (5) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 18.8275 (7) \text{ \AA}$	Cell parameters from 25482 reflections
$c = 19.7010 (6) \text{ \AA}$	$\theta = 2.6\text{--}25^\circ$
$\alpha = 65.4476 (19)^\circ$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 84.430 (2)^\circ$	$T = 200 \text{ K}$
$\gamma = 72.3229 (16)^\circ$	Needle, Colourless
$V = 4958.1 (3) \text{ \AA}^3$	$0.37 \times 0.10 \times 0.03 \text{ mm}$

Data collection

Area diffractometer	9783 reflections with $I > 2.0\sigma(I)$
graphite	$R_{\text{int}} = 0.109$
φ & ω scans	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.6^\circ$
Absorption correction: Multi-scan	$h = -18 \rightarrow 17$
<i>DENZO/SCALEPACK</i> (Otwinowski & Minor, 1997)	$k = -22 \rightarrow 22$
$T_{\text{min}} = 0.89$, $T_{\text{max}} = 1.00$	$l = -23 \rightarrow 23$
56272 measured reflections	
17519 independent reflections	

Refinement

Refinement on F^2	Primary atom site location: Structure-invariant direct methods
Least-squares matrix: Full	Hydrogen site location: Inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.069$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.176$	Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.05P)^2 + 4.94P]$, where $P = (\max(F_o^2, 0) + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{\text{max}} = 0.004$
17515 reflections	$\Delta\rho_{\text{max}} = 0.78 \text{ e \AA}^{-3}$
1239 parameters	$\Delta\rho_{\text{min}} = -0.63 \text{ e \AA}^{-3}$
33 restraints	

Special details

Refinement. The intensities of reflections with an even-value h index are systematically much stronger than those with h odd. As the structure is probably prone to stacking faults, two scales were used: one for h even and one for h odd. The final values were 1.023 and

0.945.

There is some disorder at C517 and C518 of molecule six, seemingly arising from the presence of two alternative orientations for this group. Additional sites (C527 and C528) were added as indicated in difference electron density maps and the relative populations of sites were refined. Restraints were imposed on bonded distances and angles so they should match values obtained in the rest of the structure. The displacement parameters of C517 and C527 were constrained to be equal as they are so close together and restraints were imposed on displacement parameters of bonded atoms in this section of this molecule so they would tend to be similar. Interestingly, the major component of the disorder is the one different from every other occurrence of this unit in the structure.

H atoms attached to C were included at calculated locations and ride on the atoms to which they are bonded. H attached to O were included at positions indicated in difference electron density maps and then their positional parameters were allowed to refine while maintaining restraints on the O—H distances and C—O—H angles.

The largest peaks in the final difference electron density map are located randomly through the structure and appear to have no chemical or structural significance.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O21	0.19329 (18)	0.40090 (15)	0.55220 (13)	0.0500	
O22	0.17347 (17)	0.36811 (15)	0.71042 (14)	0.0419	
O121	0.75960 (16)	0.40797 (14)	0.57159 (13)	0.0418	
O122	0.68461 (16)	0.36326 (15)	0.72076 (14)	0.0413	
O221	0.47546 (19)	0.43117 (19)	0.60218 (13)	0.0557	
O222	0.29460 (18)	0.46372 (15)	0.66651 (14)	0.0486	
O321	0.92829 (19)	0.43567 (19)	0.62046 (13)	0.0549	
O322	0.76904 (16)	0.47965 (15)	0.69591 (13)	0.0412	
O421	0.40457 (17)	0.47582 (15)	0.45832 (13)	0.0415	
O422	0.28462 (16)	0.39423 (15)	0.43538 (12)	0.0413	
O521	0.95375 (17)	0.47486 (15)	0.45175 (13)	0.0403	
O522	0.81542 (16)	0.40141 (15)	0.44036 (13)	0.0397	
C1	0.2574 (2)	0.0815 (2)	0.75353 (18)	0.0341	
C2	0.2151 (3)	0.0773 (2)	0.6872 (2)	0.0470	
C3	0.1662 (3)	0.0126 (3)	0.7139 (2)	0.0603	
C4	0.1049 (3)	0.0186 (2)	0.7750 (2)	0.0519	
C5	0.1074 (2)	0.0610 (2)	0.8142 (2)	0.0417	
C6	0.0421 (2)	0.0670 (2)	0.8743 (2)	0.0503	
C7	0.0918 (3)	0.0306 (3)	0.9498 (2)	0.0528	
C8	0.1732 (2)	0.0602 (2)	0.9427 (2)	0.0419	
C9	0.2140 (2)	0.0914 (2)	0.87951 (18)	0.0329	
C10	0.2917 (2)	0.1255 (2)	0.87520 (18)	0.0352	
C11	0.2726 (2)	0.2128 (2)	0.81560 (18)	0.0366	
C12	0.2326 (2)	0.2230 (2)	0.74243 (17)	0.0314	
C13	0.2940 (2)	0.1555 (2)	0.72073 (17)	0.0311	
C14	0.1437 (2)	0.19883 (19)	0.76049 (18)	0.0311	
C15	0.1786 (2)	0.1045 (2)	0.80381 (18)	0.0314	
C16	0.3673 (2)	0.1597 (2)	0.68056 (19)	0.0453	
C17	0.3309 (3)	0.0017 (2)	0.7897 (2)	0.0448	
C18	0.3285 (3)	-0.0617 (3)	0.8510 (2)	0.0602	
C19	0.2236 (2)	0.3093 (2)	0.68232 (18)	0.0357	
C20	0.1790 (3)	0.3276 (2)	0.60970 (18)	0.0422	
C101	0.7747 (2)	0.0855 (2)	0.74252 (19)	0.0354	

C102	0.7535 (3)	0.0885 (2)	0.6654 (2)	0.0437
C103	0.6973 (3)	0.0317 (2)	0.6728 (2)	0.0539
C104	0.6184 (3)	0.0416 (2)	0.7213 (2)	0.0507
C105	0.6113 (2)	0.0755 (2)	0.7696 (2)	0.0390
C106	0.5314 (3)	0.0807 (3)	0.8191 (2)	0.0517
C107	0.5619 (3)	0.0342 (3)	0.9008 (2)	0.0585
C108	0.6419 (2)	0.0565 (2)	0.9155 (2)	0.0470
C109	0.6967 (2)	0.0886 (2)	0.86329 (19)	0.0361
C110	0.7716 (2)	0.1142 (2)	0.88082 (19)	0.0404
C111	0.7672 (2)	0.2024 (2)	0.82801 (18)	0.0386
C112	0.7484 (2)	0.2205 (2)	0.74620 (18)	0.0329
C113	0.8169 (2)	0.1545 (2)	0.72688 (18)	0.0322
C114	0.6572 (2)	0.2045 (2)	0.74185 (18)	0.0328
C115	0.6831 (2)	0.1095 (2)	0.78052 (18)	0.0345
C116	0.8980 (2)	0.1566 (2)	0.7001 (2)	0.0455
C117	0.8387 (3)	0.0015 (2)	0.7853 (2)	0.0479
C118	0.8198 (3)	-0.0627 (3)	0.8353 (2)	0.0645
C119	0.7509 (2)	0.3070 (2)	0.69652 (18)	0.0360
C120	0.7349 (3)	0.3336 (2)	0.61417 (18)	0.0417
C201	0.4612 (2)	0.3878 (2)	0.89424 (18)	0.0324
C202	0.5438 (2)	0.3155 (2)	0.89590 (19)	0.0388
C203	0.5553 (2)	0.2406 (2)	0.9697 (2)	0.0446
C204	0.4667 (3)	0.2227 (2)	0.9940 (2)	0.0447
C205	0.3854 (2)	0.2744 (2)	0.96816 (18)	0.0394
C206	0.2984 (3)	0.2544 (3)	0.9988 (2)	0.0493
C207	0.2428 (3)	0.3154 (3)	1.0316 (2)	0.0546
C208	0.2340 (3)	0.4008 (3)	0.9770 (2)	0.0451
C209	0.2912 (2)	0.4223 (2)	0.92307 (19)	0.0398
C210	0.2768 (2)	0.5097 (2)	0.86780 (19)	0.0448
C211	0.2821 (2)	0.5178 (2)	0.7871 (2)	0.0428
C212	0.3648 (2)	0.4521 (2)	0.77772 (18)	0.0330
C213	0.4474 (2)	0.4528 (2)	0.81407 (18)	0.0337
C214	0.3522 (2)	0.3684 (2)	0.82963 (17)	0.0333
C215	0.3724 (2)	0.3609 (2)	0.90803 (17)	0.0300
C216	0.4985 (3)	0.5017 (2)	0.7818 (2)	0.0495
C217	0.4843 (2)	0.4169 (2)	0.94950 (19)	0.0397
C218	0.4578 (2)	0.4000 (2)	1.0182 (2)	0.0446
C219	0.3747 (2)	0.4666 (2)	0.69515 (19)	0.0395
C220	0.4543 (3)	0.4056 (2)	0.67971 (19)	0.0465
C301	0.9543 (2)	0.3834 (2)	0.91762 (17)	0.0300
C302	1.0344 (2)	0.3107 (2)	0.91622 (19)	0.0403
C303	1.0463 (3)	0.2361 (2)	0.9891 (2)	0.0531
C304	0.9567 (3)	0.2187 (2)	1.0142 (2)	0.0532
C305	0.8762 (3)	0.2717 (2)	0.98955 (18)	0.0412
C306	0.7881 (3)	0.2521 (3)	1.0188 (2)	0.0614
C307	0.7338 (3)	0.3105 (3)	1.0536 (2)	0.0690
C308	0.7285 (3)	0.3964 (3)	1.0039 (2)	0.0563
C309	0.7858 (2)	0.4199 (3)	0.9509 (2)	0.0420
C310	0.7737 (3)	0.5075 (2)	0.9002 (2)	0.0496
C311	0.7742 (2)	0.5209 (2)	0.8182 (2)	0.0445
C312	0.8523 (2)	0.4550 (2)	0.80417 (17)	0.0318
C313	0.9397 (2)	0.4504 (2)	0.83842 (18)	0.0336

C314	0.8384 (2)	0.3711 (2)	0.85304 (16)	0.0324	
C315	0.8644 (2)	0.3583 (2)	0.93230 (17)	0.0331	
C316	0.9930 (3)	0.4976 (2)	0.8060 (2)	0.0507	
C317	0.9819 (2)	0.4095 (2)	0.97299 (19)	0.0399	
C318	0.9545 (3)	0.3962 (2)	1.0409 (2)	0.0474	
C319	0.8564 (2)	0.4749 (2)	0.72040 (18)	0.0385	
C320	0.9291 (2)	0.4139 (2)	0.69942 (18)	0.0426	
C401	0.5575 (2)	0.2100 (2)	0.3929 (2)	0.0444	
C402	0.6191 (3)	0.2651 (3)	0.3494 (2)	0.0588	
C403	0.6516 (3)	0.2560 (3)	0.2770 (3)	0.0669	
C404	0.5768 (3)	0.2561 (3)	0.2339 (2)	0.0574	
C405	0.4979 (3)	0.2448 (2)	0.2617 (2)	0.0451	
C406	0.4282 (3)	0.2405 (3)	0.2165 (2)	0.0533	
C407	0.4133 (3)	0.1569 (3)	0.2524 (2)	0.0587	
C408	0.3967 (3)	0.1349 (3)	0.3335 (2)	0.0547	
C409	0.4230 (3)	0.1660 (2)	0.3745 (2)	0.0454	
C410	0.3987 (3)	0.1455 (2)	0.4549 (2)	0.0575	
C411	0.3597 (3)	0.2217 (2)	0.4715 (2)	0.0484	
C412	0.4147 (2)	0.2837 (2)	0.43454 (18)	0.0356	
C413	0.5142 (3)	0.2376 (2)	0.4554 (2)	0.0434	
C414	0.4103 (2)	0.3077 (2)	0.35042 (18)	0.0354	
C415	0.4746 (2)	0.2305 (2)	0.34189 (19)	0.0376	
C416	0.5583 (3)	0.2228 (3)	0.5162 (2)	0.0676	
C417	0.6170 (3)	0.1223 (3)	0.4236 (3)	0.0693	
C418	0.6336 (4)	0.0706 (3)	0.3944 (3)	0.0890	
C419	0.3790 (2)	0.3556 (2)	0.45796 (18)	0.0339	
C420	0.4300 (2)	0.4189 (2)	0.4242 (2)	0.0397	
C501	1.0711 (2)	0.2087 (2)	0.3871 (2)	0.0406	
C502	1.1334 (2)	0.2602 (2)	0.3372 (2)	0.0463	
C503	1.1580 (3)	0.2484 (3)	0.2654 (2)	0.0594	
C504	1.0771 (3)	0.2495 (2)	0.2286 (2)	0.0514	
C505	0.9993 (3)	0.2422 (2)	0.2608 (2)	0.0422	
C506	0.9237 (3)	0.2384 (2)	0.2211 (2)	0.0504	
C507	0.9063 (3)	0.1562 (3)	0.2622 (2)	0.0545	
C508	0.8950 (3)	0.1372 (2)	0.3432 (2)	0.0529	
C509	0.9275 (3)	0.1703 (2)	0.3797 (2)	0.0428	
C510	0.9098 (3)	0.1531 (2)	0.4608 (2)	0.0529	
C511	0.8790 (3)	0.2308 (2)	0.4752 (2)	0.0459	
C512	0.9368 (2)	0.2886 (2)	0.43284 (17)	0.0332	
C513	1.0373 (2)	0.2389 (2)	0.44863 (19)	0.0402	
C514	0.9251 (2)	0.3115 (2)	0.34886 (17)	0.0314	
C515	0.9816 (2)	0.2318 (2)	0.34109 (19)	0.0349	
C516	1.0877 (3)	0.2264 (3)	0.5051 (2)	0.0606	
C517	1.1218 (10)	0.1201 (4)	0.4055 (5)	0.0555	0.726 (10)
C518	1.1584 (5)	0.0640 (3)	0.4684 (4)	0.0766	0.726 (10)
C519	0.9117 (2)	0.3619 (2)	0.45391 (18)	0.0334	
C520	0.9624 (2)	0.4239 (2)	0.41267 (19)	0.0380	
C527	1.125 (3)	0.1199 (9)	0.4264 (17)	0.0555	0.274 (10)
C528	1.1315 (14)	0.0603 (8)	0.4071 (11)	0.0876	0.274 (10)
H21	0.1730	0.1288	0.6600	0.0565*	
H22	0.2623	0.0651	0.6555	0.0565*	
H31	0.2099	-0.0397	0.7314	0.0725*	

H32	0.1314	0.0192	0.6733	0.0725*
H41	0.0604	-0.0099	0.7872	0.0623*
H61	0.0104	0.1228	0.8622	0.0604*
H62	-0.0002	0.0383	0.8773	0.0604*
H71	0.0517	0.0464	0.9841	0.0634*
H72	0.1109	-0.0272	0.9677	0.0634*
H81	0.1976	0.0564	0.9870	0.0503*
H101	0.3006	0.1254	0.9223	0.0423*
H102	0.3452	0.0921	0.8633	0.0423*
H111	0.2305	0.2484	0.8343	0.0440*
H112	0.3280	0.2269	0.8054	0.0440*
H141	0.1066	0.2236	0.7907	0.0374*
H142	0.1105	0.2134	0.7162	0.0374*
H161	0.3856	0.2080	0.6621	0.0543*
H162	0.4017	0.1144	0.6701	0.0543*
H171	0.3865	-0.0030	0.7642	0.0538*
H181	0.2750	-0.0611	0.8793	0.0722*
H182	0.3803	-0.1083	0.8674	0.0722*
H191	0.2831	0.3153	0.6721	0.0429*
H201	0.1155	0.3349	0.6161	0.0506*
H202	0.2046	0.2833	0.5955	0.0506*
H1021	0.8093	0.0727	0.6431	0.0525*
H1022	0.7205	0.1428	0.6344	0.0525*
H1031	0.7349	-0.0231	0.6939	0.0647*
H1032	0.6755	0.0439	0.6246	0.0647*
H1041	0.5697	0.0223	0.7175	0.0608*
H1061	0.5021	0.1363	0.8095	0.0621*
H1062	0.4900	0.0579	0.8085	0.0621*
H1071	0.5131	0.0476	0.9308	0.0702*
H1072	0.5790	-0.0227	0.9131	0.0702*
H1081	0.6540	0.0469	0.9654	0.0564*
H1101	0.7663	0.1101	0.9307	0.0486*
H1102	0.8285	0.0790	0.8760	0.0486*
H1111	0.8237	0.2113	0.8315	0.0463*
H1112	0.7199	0.2384	0.8429	0.0463*
H1141	0.6116	0.2288	0.7681	0.0393*
H1142	0.6368	0.2243	0.6915	0.0393*
H1161	0.9190	0.2018	0.6921	0.0546*
H1162	0.9355	0.1128	0.6888	0.0546*
H1171	0.9012	-0.0051	0.7740	0.0575*
H1181	0.8672	-0.1120	0.8580	0.0774*
H1182	0.7587	-0.0604	0.8493	0.0774*
H1191	0.8092	0.3107	0.7033	0.0431*
H1201	0.7708	0.2918	0.5995	0.0500*
H1202	0.6724	0.3429	0.6046	0.0500*
H2021	0.5973	0.3324	0.8882	0.0466*
H2022	0.5356	0.3009	0.8567	0.0466*
H2031	0.5786	0.2503	1.0069	0.0536*
H2032	0.5969	0.1949	0.9637	0.0536*
H2041	0.4690	0.1699	1.0310	0.0537*
H2061	0.3124	0.2007	1.0370	0.0591*
H2062	0.2635	0.2578	0.9598	0.0591*

H2071	0.2727	0.3053	1.0760	0.0655*
H2072	0.1838	0.3084	1.0427	0.0655*
H2081	0.1838	0.4428	0.9813	0.0541*
H2101	0.3224	0.5294	0.8769	0.0537*
H2102	0.2186	0.5416	0.8746	0.0537*
H2111	0.2876	0.5703	0.7552	0.0513*
H2112	0.2281	0.5117	0.7738	0.0513*
H2141	0.2918	0.3674	0.8254	0.0400*
H2142	0.3939	0.3258	0.8189	0.0400*
H2161	0.5486	0.4982	0.8087	0.0593*
H2162	0.4853	0.5406	0.7316	0.0593*
H2171	0.5226	0.4515	0.9321	0.0477*
H2181	0.4770	0.4221	1.0475	0.0536*
H2182	0.4194	0.3656	1.0387	0.0536*
H2191	0.3819	0.5195	0.6679	0.0474*
H2201	0.5062	0.3977	0.7072	0.0558*
H2202	0.4402	0.3554	0.6959	0.0558*
H3021	1.0889	0.3264	0.9072	0.0484*
H3022	1.0230	0.2975	0.8770	0.0484*
H3031	1.0707	0.2451	1.0262	0.0638*
H3032	1.0872	0.1904	0.9824	0.0638*
H3041	0.9583	0.1657	1.0505	0.0638*
H3061	0.8014	0.1976	1.0556	0.0737*
H3062	0.7532	0.2577	0.9788	0.0737*
H3071	0.7626	0.2965	1.0997	0.0827*
H3072	0.6740	0.3053	1.0621	0.0827*
H3081	0.6799	0.4379	1.0107	0.0676*
H3101	0.8219	0.5239	0.9100	0.0595*
H3102	0.7172	0.5396	0.9097	0.0595*
H3111	0.7819	0.5731	0.7882	0.0534*
H3112	0.7178	0.5187	0.8049	0.0534*
H3141	0.8774	0.3297	0.8392	0.0389*
H3142	0.7770	0.3720	0.8500	0.0389*
H3161	1.0453	0.4911	0.8323	0.0609*
H3162	0.9791	0.5380	0.7564	0.0609*
H3171	1.0249	0.4397	0.9562	0.0480*
H3181	0.9777	0.4163	1.0701	0.0568*
H3182	0.9115	0.3665	1.0612	0.0568*
H3191	0.8664	0.5269	0.6950	0.0462*
H3201	0.9869	0.4114	0.7147	0.0511*
H3202	0.9192	0.3618	0.7244	0.0511*
H4021	0.6707	0.2507	0.3802	0.0706*
H4022	0.5855	0.3204	0.3377	0.0706*
H4031	0.6749	0.3001	0.2468	0.0803*
H4032	0.6985	0.2059	0.2887	0.0803*
H4041	0.5866	0.2650	0.1830	0.0689*
H4061	0.3725	0.2809	0.2144	0.0640*
H4062	0.4490	0.2500	0.1674	0.0640*
H4071	0.4657	0.1177	0.2466	0.0704*
H4072	0.3620	0.1575	0.2289	0.0704*
H4081	0.3649	0.0954	0.3578	0.0657*
H4101	0.4519	0.1119	0.4855	0.0690*

H4102	0.3546	0.1167	0.4664	0.0690*	
H4111	0.3613	0.2057	0.5240	0.0582*	
H4112	0.2985	0.2471	0.4529	0.0582*	
H4141	0.4317	0.3539	0.3237	0.0426*	
H4142	0.3501	0.3190	0.3335	0.0426*	
H4161	0.5271	0.2417	0.5523	0.0811*	
H4162	0.6211	0.1934	0.5239	0.0811*	
H4171	0.6459	0.1032	0.4709	0.0832*	
H4181	0.6727	0.0170	0.4200	0.1068*	
H4182	0.6069	0.0857	0.3471	0.1068*	
H4191	0.3841	0.3349	0.5108	0.0408*	
H4201	0.4936	0.3924	0.4320	0.0477*	
H4202	0.4159	0.4472	0.3721	0.0477*	
H5021	1.1880	0.2451	0.3649	0.0557*	
H5022	1.1026	0.3163	0.3248	0.0557*	
H5031	1.1817	0.2911	0.2321	0.0713*	
H5032	1.2030	0.1974	0.2765	0.0713*	
H5041	1.0820	0.2559	0.1780	0.0618*	
H5061	0.9404	0.2455	0.1715	0.0605*	
H5062	0.8700	0.2804	0.2199	0.0605*	
H5071	0.9564	0.1152	0.2562	0.0655*	
H5072	0.8525	0.1570	0.2418	0.0655*	
H5081	0.8626	0.0991	0.3708	0.0636*	
H5101	0.9643	0.1184	0.4894	0.0635*	
H5102	0.8636	0.1263	0.4762	0.0635*	
H5111	0.8849	0.2163	0.5272	0.0551*	
H5112	0.8171	0.2580	0.4591	0.0551*	
H5141	0.9487	0.3556	0.3194	0.0378*	
H5142	0.8630	0.3252	0.3350	0.0378*	
H5161	1.1503	0.1965	0.5097	0.0726*	
H5162	1.0614	0.2473	0.5411	0.0726*	
H5171	1.1274	0.1037	0.3654	0.0666*	0.726
H5181	1.1553	0.0763	0.5109	0.0917*	0.726
H5182	1.1885	0.0102	0.4724	0.0917*	0.726
H5191	0.9245	0.3421	0.5058	0.0401*	
H5201	1.0248	0.3966	0.4106	0.0456*	
H5202	0.9372	0.4562	0.3634	0.0456*	
H5271	1.1578	0.1060	0.4707	0.0666*	0.274
H5281	1.1678	0.0067	0.4367	0.1054*	0.274
H5282	1.1001	0.0703	0.3634	0.1054*	0.274
H9021	0.1509 (18)	0.4405 (13)	0.5512 (17)	0.0600*	
H9022	0.2045 (17)	0.3987 (17)	0.705 (2)	0.0500*	
H9121	0.7137 (14)	0.4472 (12)	0.5661 (18)	0.0500*	
H9122	0.7079 (17)	0.3988 (16)	0.718 (2)	0.0490*	
H9221	0.4287 (16)	0.438 (3)	0.5785 (13)	0.0670*	
H9222	0.2636 (19)	0.5105 (12)	0.6416 (19)	0.0590*	
H9321	0.8808 (17)	0.433 (3)	0.6086 (13)	0.0660*	
H9322	0.7542 (18)	0.5192 (16)	0.6559 (13)	0.0490*	
H9421	0.439 (2)	0.5053 (18)	0.4422 (18)	0.0500*	
H9422	0.2570 (15)	0.399 (2)	0.4717 (12)	0.0490*	
H9521	0.991 (2)	0.5009 (19)	0.4350 (17)	0.0490*	
H9522	0.7936 (15)	0.410 (2)	0.4771 (13)	0.0480*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O21	0.0582 (18)	0.0331 (15)	0.0373 (13)	-0.0016 (12)	0.0165 (12)	-0.0052 (12)
O22	0.0479 (16)	0.0342 (15)	0.0489 (15)	-0.0130 (12)	0.0064 (12)	-0.0220 (12)
O121	0.0449 (15)	0.0325 (14)	0.0393 (13)	-0.0073 (11)	0.0087 (12)	-0.0105 (12)
O122	0.0460 (15)	0.0358 (15)	0.0469 (14)	-0.0133 (12)	0.0090 (12)	-0.0221 (12)
O221	0.0596 (18)	0.083 (2)	0.0343 (14)	-0.0351 (17)	0.0086 (13)	-0.0248 (14)
O222	0.0562 (17)	0.0394 (15)	0.0463 (15)	-0.0177 (13)	-0.0206 (13)	-0.0064 (13)
O321	0.0608 (19)	0.091 (2)	0.0301 (13)	-0.0457 (17)	0.0122 (13)	-0.0262 (14)
O322	0.0434 (15)	0.0428 (15)	0.0337 (13)	-0.0157 (12)	-0.0108 (11)	-0.0073 (11)
O421	0.0456 (16)	0.0410 (16)	0.0431 (14)	-0.0156 (12)	0.0048 (12)	-0.0208 (12)
O422	0.0326 (14)	0.0488 (16)	0.0318 (13)	-0.0034 (12)	0.0027 (10)	-0.0126 (12)
O521	0.0497 (16)	0.0395 (15)	0.0420 (14)	-0.0191 (12)	0.0094 (12)	-0.0238 (12)
O522	0.0383 (14)	0.0423 (15)	0.0361 (13)	-0.0068 (12)	0.0042 (11)	-0.0178 (12)
C1	0.0324 (19)	0.031 (2)	0.0388 (19)	-0.0068 (15)	-0.0038 (15)	-0.0152 (16)
C2	0.054 (2)	0.043 (2)	0.047 (2)	-0.0081 (19)	-0.0097 (19)	-0.0228 (19)
C3	0.069 (3)	0.052 (3)	0.072 (3)	-0.021 (2)	-0.017 (2)	-0.031 (2)
C4	0.044 (2)	0.042 (2)	0.071 (3)	-0.0203 (19)	-0.015 (2)	-0.015 (2)
C5	0.030 (2)	0.039 (2)	0.047 (2)	-0.0123 (17)	-0.0083 (16)	-0.0061 (18)
C6	0.030 (2)	0.048 (2)	0.061 (3)	-0.0180 (18)	-0.0039 (18)	-0.005 (2)
C7	0.040 (2)	0.056 (3)	0.051 (2)	-0.018 (2)	0.0028 (18)	-0.008 (2)
C8	0.033 (2)	0.046 (2)	0.037 (2)	-0.0101 (17)	-0.0021 (16)	-0.0084 (17)
C9	0.0273 (18)	0.0334 (19)	0.0343 (19)	-0.0075 (15)	-0.0007 (15)	-0.0110 (16)
C10	0.0328 (19)	0.044 (2)	0.0336 (18)	-0.0139 (16)	-0.0010 (15)	-0.0175 (16)
C11	0.039 (2)	0.039 (2)	0.0376 (19)	-0.0162 (17)	0.0022 (16)	-0.0179 (17)
C12	0.0315 (18)	0.0319 (19)	0.0309 (17)	-0.0095 (15)	0.0006 (14)	-0.0128 (15)
C13	0.0258 (18)	0.034 (2)	0.0295 (17)	-0.0049 (15)	0.0000 (14)	-0.0114 (15)
C14	0.0274 (18)	0.0303 (19)	0.0314 (17)	-0.0078 (15)	0.0011 (14)	-0.0089 (15)
C15	0.0258 (17)	0.0305 (19)	0.0337 (18)	-0.0085 (15)	-0.0059 (14)	-0.0073 (15)
C16	0.042 (2)	0.042 (2)	0.043 (2)	-0.0033 (18)	0.0023 (18)	-0.0150 (18)
C17	0.041 (2)	0.037 (2)	0.053 (2)	-0.0044 (18)	-0.0040 (18)	-0.0189 (19)
C18	0.053 (3)	0.042 (3)	0.068 (3)	0.001 (2)	-0.008 (2)	-0.014 (2)
C19	0.037 (2)	0.032 (2)	0.0397 (19)	-0.0114 (16)	0.0077 (16)	-0.0158 (16)
C20	0.053 (2)	0.032 (2)	0.0361 (19)	-0.0074 (17)	0.0027 (17)	-0.0125 (16)
C101	0.0285 (18)	0.034 (2)	0.0395 (19)	-0.0029 (15)	-0.0020 (15)	-0.0142 (16)
C102	0.046 (2)	0.039 (2)	0.047 (2)	-0.0087 (18)	-0.0018 (17)	-0.0196 (18)
C103	0.060 (3)	0.046 (2)	0.063 (3)	-0.012 (2)	-0.010 (2)	-0.028 (2)
C104	0.042 (2)	0.046 (2)	0.067 (3)	-0.0154 (19)	-0.008 (2)	-0.022 (2)
C105	0.031 (2)	0.031 (2)	0.047 (2)	-0.0096 (16)	-0.0033 (16)	-0.0066 (17)
C106	0.037 (2)	0.054 (3)	0.059 (2)	-0.0212 (19)	0.0004 (19)	-0.012 (2)
C107	0.044 (2)	0.060 (3)	0.057 (3)	-0.022 (2)	0.004 (2)	-0.006 (2)
C108	0.039 (2)	0.047 (2)	0.044 (2)	-0.0086 (19)	-0.0053 (18)	-0.0084 (18)
C109	0.0273 (18)	0.033 (2)	0.0363 (19)	-0.0070 (15)	0.0003 (15)	-0.0044 (16)
C110	0.039 (2)	0.040 (2)	0.0332 (19)	-0.0105 (17)	-0.0057 (16)	-0.0053 (16)
C111	0.037 (2)	0.043 (2)	0.0386 (19)	-0.0139 (17)	-0.0003 (16)	-0.0178 (17)
C112	0.0287 (18)	0.036 (2)	0.0328 (18)	-0.0106 (15)	-0.0027 (14)	-0.0112 (16)
C113	0.0286 (19)	0.0282 (19)	0.0351 (18)	-0.0062 (15)	-0.0039 (15)	-0.0087 (15)
C114	0.0292 (18)	0.0310 (19)	0.0325 (18)	-0.0032 (15)	-0.0030 (14)	-0.0106 (15)
C115	0.0312 (19)	0.033 (2)	0.0350 (18)	-0.0072 (15)	-0.0059 (15)	-0.0097 (15)
C116	0.033 (2)	0.042 (2)	0.054 (2)	-0.0073 (17)	-0.0012 (18)	-0.0146 (19)
C117	0.034 (2)	0.033 (2)	0.065 (3)	-0.0009 (17)	-0.0068 (19)	-0.014 (2)

C118	0.059 (3)	0.037 (3)	0.072 (3)	0.002 (2)	-0.011 (2)	-0.006 (2)
C119	0.040 (2)	0.034 (2)	0.0339 (18)	-0.0108 (16)	0.0016 (15)	-0.0141 (16)
C120	0.054 (2)	0.032 (2)	0.039 (2)	-0.0131 (18)	0.0029 (17)	-0.0147 (17)
C201	0.0283 (18)	0.038 (2)	0.0345 (18)	-0.0122 (15)	-0.0001 (14)	-0.0160 (16)
C202	0.0292 (19)	0.041 (2)	0.046 (2)	-0.0087 (16)	0.0014 (16)	-0.0186 (17)
C203	0.036 (2)	0.039 (2)	0.049 (2)	-0.0014 (17)	-0.0059 (17)	-0.0134 (18)
C204	0.052 (2)	0.034 (2)	0.039 (2)	-0.0121 (19)	-0.0055 (18)	-0.0056 (17)
C205	0.042 (2)	0.051 (2)	0.0324 (18)	-0.0240 (19)	0.0059 (16)	-0.0172 (17)
C206	0.054 (2)	0.061 (3)	0.037 (2)	-0.031 (2)	0.0052 (18)	-0.0136 (19)
C207	0.044 (2)	0.088 (3)	0.045 (2)	-0.031 (2)	0.0114 (18)	-0.033 (2)
C208	0.037 (2)	0.062 (3)	0.045 (2)	-0.0150 (19)	0.0021 (18)	-0.029 (2)
C209	0.035 (2)	0.054 (2)	0.040 (2)	-0.0144 (18)	0.0002 (17)	-0.0267 (18)
C210	0.035 (2)	0.044 (2)	0.048 (2)	0.0007 (17)	-0.0009 (17)	-0.0205 (19)
C211	0.041 (2)	0.038 (2)	0.048 (2)	-0.0086 (17)	-0.0056 (17)	-0.0170 (18)
C212	0.0315 (19)	0.0326 (19)	0.0349 (18)	-0.0100 (15)	-0.0014 (15)	-0.0126 (15)
C213	0.0349 (19)	0.033 (2)	0.0353 (18)	-0.0110 (16)	-0.0010 (15)	-0.0145 (16)
C214	0.0320 (19)	0.038 (2)	0.0339 (18)	-0.0144 (16)	0.0022 (15)	-0.0159 (16)
C215	0.0291 (18)	0.0339 (19)	0.0310 (17)	-0.0119 (15)	0.0030 (14)	-0.0154 (15)
C216	0.054 (2)	0.049 (2)	0.047 (2)	-0.023 (2)	-0.0074 (19)	-0.0126 (19)
C217	0.036 (2)	0.044 (2)	0.043 (2)	-0.0155 (17)	-0.0032 (16)	-0.0180 (18)
C218	0.046 (2)	0.052 (2)	0.044 (2)	-0.0170 (19)	-0.0047 (18)	-0.0240 (19)
C219	0.046 (2)	0.036 (2)	0.0361 (19)	-0.0183 (18)	-0.0068 (17)	-0.0089 (16)
C220	0.053 (2)	0.054 (3)	0.0319 (19)	-0.023 (2)	0.0028 (17)	-0.0132 (18)
C301	0.0285 (18)	0.0342 (19)	0.0289 (17)	-0.0096 (15)	0.0003 (14)	-0.0139 (15)
C302	0.0297 (19)	0.046 (2)	0.043 (2)	-0.0068 (17)	0.0004 (16)	-0.0188 (18)
C303	0.052 (3)	0.041 (2)	0.059 (3)	0.001 (2)	-0.008 (2)	-0.021 (2)
C304	0.071 (3)	0.041 (2)	0.047 (2)	-0.024 (2)	-0.005 (2)	-0.0100 (19)
C305	0.053 (2)	0.048 (2)	0.0270 (18)	-0.026 (2)	0.0006 (17)	-0.0110 (17)
C306	0.070 (3)	0.079 (3)	0.042 (2)	-0.050 (3)	0.003 (2)	-0.012 (2)
C307	0.055 (3)	0.128 (5)	0.042 (2)	-0.050 (3)	0.014 (2)	-0.038 (3)
C308	0.040 (2)	0.095 (4)	0.046 (2)	-0.021 (2)	0.0062 (19)	-0.040 (3)
C309	0.0294 (19)	0.069 (3)	0.038 (2)	-0.0140 (19)	0.0052 (16)	-0.034 (2)
C310	0.042 (2)	0.058 (3)	0.051 (2)	0.0017 (19)	-0.0003 (18)	-0.035 (2)
C311	0.042 (2)	0.041 (2)	0.046 (2)	-0.0020 (18)	-0.0090 (17)	-0.0190 (18)
C312	0.0339 (19)	0.0312 (19)	0.0293 (17)	-0.0099 (15)	-0.0011 (14)	-0.0106 (15)
C313	0.0333 (19)	0.037 (2)	0.0330 (18)	-0.0112 (16)	0.0007 (15)	-0.0157 (16)
C314	0.0295 (18)	0.042 (2)	0.0299 (17)	-0.0133 (16)	0.0034 (14)	-0.0165 (16)
C315	0.0309 (18)	0.042 (2)	0.0289 (17)	-0.0117 (16)	0.0034 (14)	-0.0163 (16)
C316	0.058 (3)	0.060 (3)	0.040 (2)	-0.036 (2)	-0.0040 (19)	-0.0107 (19)
C317	0.039 (2)	0.044 (2)	0.039 (2)	-0.0139 (17)	-0.0051 (16)	-0.0167 (17)
C318	0.050 (2)	0.057 (3)	0.043 (2)	-0.014 (2)	-0.0058 (18)	-0.028 (2)
C319	0.042 (2)	0.042 (2)	0.0331 (18)	-0.0190 (17)	-0.0042 (16)	-0.0109 (16)
C320	0.045 (2)	0.062 (3)	0.0279 (18)	-0.024 (2)	0.0045 (16)	-0.0204 (18)
C401	0.036 (2)	0.036 (2)	0.054 (2)	0.0001 (17)	-0.0027 (17)	-0.0188 (18)
C402	0.041 (2)	0.059 (3)	0.079 (3)	-0.011 (2)	0.002 (2)	-0.033 (2)
C403	0.049 (3)	0.074 (3)	0.086 (3)	-0.024 (2)	0.022 (2)	-0.040 (3)
C404	0.062 (3)	0.058 (3)	0.059 (3)	-0.024 (2)	0.025 (2)	-0.031 (2)
C405	0.053 (3)	0.039 (2)	0.045 (2)	-0.0146 (19)	0.0079 (19)	-0.0201 (18)
C406	0.058 (3)	0.062 (3)	0.047 (2)	-0.015 (2)	0.005 (2)	-0.030 (2)
C407	0.059 (3)	0.068 (3)	0.069 (3)	-0.024 (2)	0.013 (2)	-0.045 (3)
C408	0.059 (3)	0.050 (3)	0.068 (3)	-0.025 (2)	0.012 (2)	-0.031 (2)
C409	0.052 (2)	0.036 (2)	0.049 (2)	-0.0150 (19)	0.0086 (18)	-0.0180 (18)

C410	0.081 (3)	0.040 (2)	0.054 (2)	-0.030 (2)	0.015 (2)	-0.017 (2)
C411	0.057 (3)	0.051 (3)	0.040 (2)	-0.026 (2)	0.0115 (18)	-0.0162 (19)
C412	0.0349 (19)	0.036 (2)	0.0327 (18)	-0.0092 (16)	0.0013 (15)	-0.0122 (16)
C413	0.043 (2)	0.035 (2)	0.045 (2)	-0.0025 (17)	-0.0067 (18)	-0.0142 (17)
C414	0.0316 (19)	0.034 (2)	0.0366 (19)	-0.0084 (16)	-0.0001 (15)	-0.0108 (16)
C415	0.036 (2)	0.035 (2)	0.0401 (19)	-0.0101 (16)	0.0050 (16)	-0.0149 (17)
C416	0.061 (3)	0.065 (3)	0.065 (3)	0.013 (2)	-0.025 (2)	-0.031 (2)
C417	0.076 (3)	0.057 (3)	0.065 (3)	0.007 (3)	-0.008 (2)	-0.031 (3)
C418	0.095 (4)	0.062 (3)	0.092 (4)	0.006 (3)	-0.008 (3)	-0.031 (3)
C419	0.0343 (19)	0.037 (2)	0.0281 (17)	-0.0101 (16)	0.0028 (14)	-0.0113 (15)
C420	0.038 (2)	0.037 (2)	0.047 (2)	-0.0093 (17)	0.0068 (16)	-0.0230 (18)
C501	0.039 (2)	0.035 (2)	0.045 (2)	-0.0045 (17)	-0.0013 (17)	-0.0175 (17)
C502	0.035 (2)	0.045 (2)	0.062 (2)	-0.0144 (18)	0.0017 (18)	-0.023 (2)
C503	0.048 (3)	0.069 (3)	0.078 (3)	-0.025 (2)	0.024 (2)	-0.047 (3)
C504	0.054 (3)	0.058 (3)	0.055 (2)	-0.022 (2)	0.016 (2)	-0.034 (2)
C505	0.049 (2)	0.039 (2)	0.050 (2)	-0.0145 (18)	0.0072 (18)	-0.0285 (19)
C506	0.057 (3)	0.055 (3)	0.052 (2)	-0.023 (2)	0.004 (2)	-0.029 (2)
C507	0.056 (3)	0.064 (3)	0.065 (3)	-0.026 (2)	0.009 (2)	-0.043 (2)
C508	0.059 (3)	0.046 (3)	0.067 (3)	-0.027 (2)	0.012 (2)	-0.030 (2)
C509	0.052 (2)	0.030 (2)	0.052 (2)	-0.0173 (18)	0.0088 (18)	-0.0195 (18)
C510	0.070 (3)	0.042 (2)	0.054 (2)	-0.030 (2)	0.009 (2)	-0.019 (2)
C511	0.060 (3)	0.040 (2)	0.041 (2)	-0.0195 (19)	0.0050 (18)	-0.0155 (18)
C512	0.037 (2)	0.0313 (19)	0.0317 (18)	-0.0101 (16)	0.0023 (15)	-0.0137 (15)
C513	0.038 (2)	0.031 (2)	0.042 (2)	-0.0032 (16)	-0.0081 (17)	-0.0093 (16)
C514	0.0314 (18)	0.033 (2)	0.0328 (18)	-0.0097 (15)	0.0016 (14)	-0.0161 (15)
C515	0.036 (2)	0.030 (2)	0.0399 (19)	-0.0100 (16)	0.0026 (16)	-0.0152 (16)
C516	0.053 (3)	0.061 (3)	0.061 (3)	0.001 (2)	-0.017 (2)	-0.027 (2)
C517	0.055 (3)	0.042 (3)	0.069 (7)	0.002 (2)	-0.009 (5)	-0.030 (3)
C518	0.090 (5)	0.036 (4)	0.088 (5)	0.008 (3)	-0.031 (4)	-0.022 (3)
C519	0.0318 (19)	0.036 (2)	0.0323 (18)	-0.0087 (15)	0.0017 (14)	-0.0143 (15)
C520	0.042 (2)	0.036 (2)	0.045 (2)	-0.0153 (17)	0.0105 (16)	-0.0233 (17)
C527	0.055 (3)	0.042 (3)	0.069 (7)	0.002 (2)	-0.009 (5)	-0.030 (3)
C528	0.129 (19)	0.029 (10)	0.087 (15)	-0.001 (10)	0.000 (13)	-0.021 (9)

Geometric parameters (Å, °)

O21—C20	1.440 (4)	C216—H2162	0.950
O21—H9021	0.824 (18)	C217—C218	1.308 (5)
O22—C19	1.428 (4)	C217—H2171	0.950
O22—H9022	0.826 (18)	C218—H2181	0.950
O121—C120	1.448 (4)	C218—H2182	0.950
O121—H9121	0.831 (18)	C219—C220	1.510 (5)
O122—C119	1.436 (4)	C219—H2191	0.950
O122—H9122	0.833 (18)	C220—H2201	0.950
O221—C220	1.435 (4)	C220—H2202	0.950
O221—H9221	0.842 (18)	C301—C302	1.549 (5)
O222—C219	1.433 (4)	C301—C313	1.529 (4)
O222—H9222	0.822 (18)	C301—C315	1.563 (5)
O321—C320	1.435 (4)	C301—C317	1.508 (4)
O321—H9321	0.810 (18)	C302—C303	1.512 (5)
O322—C319	1.440 (4)	C302—H3021	0.950

O322—H9322	0.819 (18)	C302—H3022	0.950
O421—C420	1.432 (4)	C303—C304	1.508 (6)
O421—H9421	0.828 (18)	C303—H3031	0.950
O422—C419	1.436 (4)	C303—H3032	0.950
O422—H9422	0.821 (18)	C304—C305	1.318 (5)
O521—C520	1.432 (4)	C304—H3041	0.950
O521—H9521	0.820 (18)	C305—C306	1.515 (5)
O522—C519	1.440 (4)	C305—C315	1.514 (5)
O522—H9522	0.822 (18)	C306—C307	1.527 (6)
C1—C2	1.557 (4)	C306—H3061	0.950
C1—C13	1.528 (5)	C306—H3062	0.950
C1—C15	1.565 (5)	C307—C308	1.484 (6)
C1—C17	1.511 (5)	C307—H3071	0.950
C2—C3	1.509 (6)	C307—H3072	0.950
C2—H21	0.950	C308—C309	1.320 (5)
C2—H22	0.950	C308—H3081	0.950
C3—C4	1.478 (6)	C309—C310	1.493 (5)
C3—H31	0.950	C309—C315	1.537 (5)
C3—H32	0.950	C310—C311	1.528 (5)
C4—C5	1.331 (5)	C310—H3101	0.950
C4—H41	0.950	C310—H3102	0.950
C5—C6	1.498 (5)	C311—C312	1.543 (5)
C5—C15	1.512 (5)	C311—H3111	0.950
C6—C7	1.525 (5)	C311—H3112	0.950
C6—H61	0.950	C312—C313	1.530 (4)
C6—H62	0.950	C312—C314	1.539 (5)
C7—C8	1.496 (5)	C312—C319	1.532 (4)
C7—H71	0.950	C313—C316	1.320 (5)
C7—H72	0.950	C314—C315	1.551 (4)
C8—C9	1.325 (5)	C314—H3141	0.950
C8—H81	0.950	C314—H3142	0.950
C9—C10	1.502 (5)	C316—H3161	0.950
C9—C15	1.535 (4)	C316—H3162	0.950
C10—C11	1.528 (5)	C317—C318	1.307 (5)
C10—H101	0.950	C317—H3171	0.950
C10—H102	0.950	C318—H3181	0.950
C11—C12	1.538 (4)	C318—H3182	0.950
C11—H111	0.950	C319—C320	1.508 (5)
C11—H112	0.950	C319—H3191	0.950
C12—C13	1.528 (4)	C320—H3201	0.950
C12—C14	1.538 (4)	C320—H3202	0.950
C12—C19	1.536 (5)	C401—C402	1.554 (6)
C13—C16	1.319 (5)	C401—C413	1.546 (5)
C14—C15	1.557 (4)	C401—C415	1.557 (5)
C14—H141	0.950	C401—C417	1.515 (5)
C14—H142	0.950	C402—C403	1.526 (6)
C16—H161	0.950	C402—H4021	0.950
C16—H162	0.950	C402—H4022	0.950
C17—C18	1.306 (5)	C403—C404	1.495 (6)
C17—H171	0.950	C403—H4031	0.950
C18—H181	0.950	C403—H4032	0.950
C18—H182	0.950	C404—C405	1.326 (5)

C19—C20	1.509 (5)	C404—H4041	0.950
C19—H191	0.950	C405—C406	1.501 (5)
C20—H201	0.950	C405—C415	1.515 (5)
C20—H202	0.950	C406—C407	1.514 (6)
C101—C102	1.559 (5)	C406—H4061	0.950
C101—C113	1.534 (5)	C406—H4062	0.950
C101—C115	1.565 (5)	C407—C408	1.492 (6)
C101—C117	1.514 (5)	C407—H4071	0.950
C102—C103	1.524 (5)	C407—H4072	0.950
C102—H1021	0.950	C408—C409	1.327 (5)
C102—H1022	0.950	C408—H4081	0.950
C103—C104	1.489 (6)	C409—C410	1.505 (5)
C103—H1031	0.950	C409—C415	1.535 (5)
C103—H1032	0.950	C410—C411	1.534 (5)
C104—C105	1.328 (5)	C410—H4101	0.950
C104—H1041	0.950	C410—H4102	0.950
C105—C106	1.500 (5)	C411—C412	1.546 (5)
C105—C115	1.510 (5)	C411—H4111	0.950
C106—C107	1.519 (5)	C411—H4112	0.950
C106—H1061	0.950	C412—C413	1.516 (5)
C106—H1062	0.950	C412—C414	1.528 (4)
C107—C108	1.506 (5)	C412—C419	1.538 (5)
C107—H1071	0.950	C413—C416	1.320 (5)
C107—H1072	0.950	C414—C415	1.555 (5)
C108—C109	1.327 (5)	C414—H4141	0.950
C108—H1081	0.950	C414—H4142	0.950
C109—C110	1.498 (5)	C416—H4161	0.950
C109—C115	1.530 (5)	C416—H4162	0.950
C110—C111	1.533 (5)	C417—C418	1.275 (6)
C110—H1101	0.950	C417—H4171	0.950
C110—H1102	0.950	C418—H4181	0.950
C111—C112	1.540 (4)	C418—H4182	0.950
C111—H1111	0.950	C419—C420	1.514 (5)
C111—H1112	0.950	C419—H4191	0.950
C112—C113	1.524 (5)	C420—H4201	0.950
C112—C114	1.543 (4)	C420—H4202	0.950
C112—C119	1.523 (5)	C501—C502	1.556 (5)
C113—C116	1.315 (5)	C501—C513	1.528 (5)
C114—C115	1.560 (5)	C501—C515	1.571 (5)
C114—H1141	0.950	C501—C517	1.512 (6)
C114—H1142	0.950	C501—C527	1.513 (9)
C116—H1161	0.950	C502—C503	1.518 (5)
C116—H1162	0.950	C502—H5021	0.950
C117—C118	1.299 (6)	C502—H5022	0.950
C117—H1171	0.950	C503—C504	1.495 (5)
C118—H1181	0.950	C503—H5031	0.950
C118—H1182	0.950	C503—H5032	0.950
C119—C120	1.507 (4)	C504—C505	1.320 (5)
C119—H1191	0.950	C504—H5041	0.950
C120—H1201	0.950	C505—C506	1.501 (5)
C120—H1202	0.950	C505—C515	1.519 (5)
C201—C202	1.548 (5)	C506—C507	1.515 (5)

C201—C213	1.529 (5)	C506—H5061	0.950
C201—C215	1.562 (4)	C506—H5062	0.950
C201—C217	1.517 (4)	C507—C508	1.489 (5)
C202—C203	1.525 (5)	C507—H5071	0.950
C202—H2021	0.950	C507—H5072	0.950
C202—H2022	0.950	C508—C509	1.336 (5)
C203—C204	1.493 (5)	C508—H5081	0.950
C203—H2031	0.950	C509—C510	1.508 (5)
C203—H2032	0.950	C509—C515	1.533 (5)
C204—C205	1.324 (5)	C510—C511	1.530 (5)
C204—H2041	0.950	C510—H5101	0.950
C205—C206	1.506 (5)	C510—H5102	0.950
C205—C215	1.530 (5)	C511—C512	1.539 (5)
C206—C207	1.543 (5)	C511—H5111	0.950
C206—H2061	0.950	C511—H5112	0.950
C206—H2062	0.950	C512—C513	1.534 (5)
C207—C208	1.489 (6)	C512—C514	1.541 (4)
C207—H2071	0.950	C512—C519	1.530 (4)
C207—H2072	0.950	C513—C516	1.317 (5)
C208—C209	1.323 (5)	C514—C515	1.550 (4)
C208—H2081	0.950	C514—H5141	0.950
C209—C210	1.510 (5)	C514—H5142	0.950
C209—C215	1.525 (5)	C516—H5161	0.950
C210—C211	1.529 (5)	C516—H5162	0.950
C210—H2101	0.950	C517—C518	1.287 (7)
C210—H2102	0.950	C517—H5171	0.950
C211—C212	1.542 (5)	C518—H5181	0.950
C211—H2111	0.950	C518—H5182	0.950
C211—H2112	0.950	C519—C520	1.509 (5)
C212—C213	1.528 (4)	C519—H5191	0.950
C212—C214	1.541 (5)	C520—H5201	0.950
C212—C219	1.534 (5)	C520—H5202	0.950
C213—C216	1.316 (5)	C527—C528	1.302 (9)
C214—C215	1.545 (4)	C527—H5271	0.950
C214—H2141	0.950	C528—H5281	0.950
C214—H2142	0.950	C528—H5282	0.950
C216—H2161	0.950		
O21…O422	2.608 (4)	O321…O521	3.103 (4)
O21…O521 ⁱ	2.699 (3)	O321…C520 ⁱⁱ	3.365 (5)
O21…C419	3.345 (4)	O322…O422 ⁱ	2.671 (3)
O21…O222	3.596 (5)	O322…C119	3.341 (5)
O22…O222	2.814 (4)	O322…C420 ⁱ	3.574 (4)
O22…O521 ⁱ	3.556 (3)	O421…C120 ⁱ	3.346 (4)
O121…O522	2.685 (4)	O422…C319 ⁱ	3.461 (4)
O121…O421 ⁱ	2.721 (3)	O422…C20	3.550 (4)
O121…O321	3.115 (5)	O521…O521 ⁱⁱ	3.065 (7)
O121…O322	3.283 (4)	O521…C20 ⁱ	3.407 (4)
O121…C519	3.319 (4)	O521…C320 ⁱⁱ	3.549 (4)
O121…O422 ⁱ	3.522 (4)	O522…C120	3.377 (4)
O122…O322	2.731 (4)	C3…C507 ⁱⁱⁱ	3.520 (9)
O122…C220	3.496 (5)	C4…C116 ^{iv}	3.437 (5)

O221...O421 ⁱ	2.779 (4)	C7...C7 ^v	3.503 (9)
O221...O421	2.828 (4)	C16...C106	3.429 (5)
O221...C420 ⁱ	3.391 (6)	C102...C528 ^{vi}	3.59 (2)
O222...O522 ⁱ	2.720 (3)	C103...C528 ^{vi}	3.34 (2)
O222...C19	3.296 (5)	C208...C310 ^{vii}	3.484 (7)
O321...O521 ⁱⁱ	2.747 (4)		
C20—O21—H9021	109.3 (17)	H2201—C220—H2202	109.5
C19—O22—H9022	107.6 (16)	C302—C301—C313	107.4 (3)
C120—O121—H9121	108.1 (16)	C302—C301—C315	109.2 (3)
C119—O122—H9122	107.3 (16)	C313—C301—C315	103.9 (2)
C220—O221—H9221	107.4 (17)	C302—C301—C317	106.5 (3)
C219—O222—H9222	109.2 (17)	C313—C301—C317	112.6 (3)
C320—O321—H9321	108.3 (17)	C315—C301—C317	116.9 (3)
C319—O322—H9322	108.7 (16)	C301—C302—C303	112.0 (3)
C420—O421—H9421	106.6 (16)	C301—C302—H3021	108.8
C419—O422—H9422	107.3 (16)	C303—C302—H3021	108.8
C520—O521—H9521	107.8 (16)	C301—C302—H3022	108.8
C519—O522—H9522	109.1 (16)	C303—C302—H3022	108.8
C2—C1—C13	106.9 (3)	H3021—C302—H3022	109.5
C2—C1—C15	108.4 (3)	C302—C303—C304	111.1 (3)
C13—C1—C15	103.9 (3)	C302—C303—H3031	109.0
C2—C1—C17	106.8 (3)	C304—C303—H3031	109.0
C13—C1—C17	113.1 (3)	C302—C303—H3032	109.1
C15—C1—C17	117.3 (3)	C304—C303—H3032	109.1
C1—C2—C3	111.7 (3)	H3031—C303—H3032	109.5
C1—C2—H21	108.9	C303—C304—C305	124.7 (4)
C3—C2—H21	108.9	C303—C304—H3041	117.7
C1—C2—H22	108.9	C305—C304—H3041	117.7
C3—C2—H22	108.9	C304—C305—C306	122.6 (4)
H21—C2—H22	109.5	C304—C305—C315	122.8 (4)
C2—C3—C4	111.4 (3)	C306—C305—C315	114.6 (3)
C2—C3—H31	109.0	C305—C306—C307	109.9 (3)
C4—C3—H31	109.0	C305—C306—H3061	109.4
C2—C3—H32	109.0	C307—C306—H3061	109.4
C4—C3—H32	109.0	C305—C306—H3062	109.3
H31—C3—H32	109.5	C307—C306—H3062	109.4
C3—C4—C5	124.8 (4)	H3061—C306—H3062	109.5
C3—C4—H41	117.6	C306—C307—C308	111.4 (3)
C5—C4—H41	117.6	C306—C307—H3071	109.0
C4—C5—C6	122.9 (4)	C308—C307—H3071	109.0
C4—C5—C15	122.9 (4)	C306—C307—H3072	109.0
C6—C5—C15	114.2 (3)	C308—C307—H3072	109.0
C5—C6—C7	111.1 (3)	H3071—C307—H3072	109.5
C5—C6—H61	109.1	C307—C308—C309	125.3 (4)
C7—C6—H61	109.1	C307—C308—H3081	117.4
C5—C6—H62	109.1	C309—C308—H3081	117.4
C7—C6—H62	109.1	C308—C309—C310	122.4 (4)
H61—C6—H62	109.5	C308—C309—C315	122.0 (4)
C6—C7—C8	110.5 (3)	C310—C309—C315	115.3 (3)
C6—C7—H71	109.2	C309—C310—C311	111.5 (3)
C8—C7—H71	109.2	C309—C310—H3101	109.0

C6—C7—H72	109.2	C311—C310—H3101	109.0
C8—C7—H72	109.2	C309—C310—H3102	109.0
H71—C7—H72	109.5	C311—C310—H3102	109.0
C7—C8—C9	125.1 (3)	H3101—C310—H3102	109.5
C7—C8—H81	117.4	C310—C311—C312	111.1 (3)
C9—C8—H81	117.5	C310—C311—H3111	109.1
C8—C9—C10	122.5 (3)	C312—C311—H3111	109.1
C8—C9—C15	122.5 (3)	C310—C311—H3112	109.1
C10—C9—C15	114.7 (3)	C312—C311—H3112	109.1
C9—C10—C11	111.4 (3)	H3111—C311—H3112	109.5
C9—C10—H101	109.0	C311—C312—C313	107.5 (3)
C11—C10—H101	109.0	C311—C312—C314	108.2 (3)
C9—C10—H102	109.0	C313—C312—C314	102.5 (2)
C11—C10—H102	109.0	C311—C312—C319	109.6 (3)
H101—C10—H102	109.5	C313—C312—C319	114.1 (3)
C10—C11—C12	112.5 (3)	C314—C312—C319	114.5 (3)
C10—C11—H111	108.7	C312—C313—C301	108.8 (3)
C12—C11—H111	108.7	C312—C313—C316	126.0 (3)
C10—C11—H112	108.7	C301—C313—C316	125.2 (3)
C12—C11—H112	108.7	C312—C314—C315	102.2 (3)
H111—C11—H112	109.5	C312—C314—H3141	111.3
C11—C12—C13	107.4 (3)	C315—C314—H3141	111.3
C11—C12—C14	107.8 (3)	C312—C314—H3142	111.3
C13—C12—C14	102.1 (3)	C315—C314—H3142	111.3
C11—C12—C19	110.2 (3)	H3141—C314—H3142	109.5
C13—C12—C19	113.5 (3)	C309—C315—C314	104.1 (3)
C14—C12—C19	115.3 (3)	C309—C315—C301	112.2 (3)
C12—C13—C1	109.1 (3)	C314—C315—C301	101.5 (3)
C12—C13—C16	125.8 (3)	C309—C315—C305	111.8 (3)
C1—C13—C16	125.1 (3)	C314—C315—C305	113.0 (3)
C12—C14—C15	102.5 (2)	C301—C315—C305	113.4 (3)
C12—C14—H141	111.2	C313—C316—H3161	120.0
C15—C14—H141	111.2	C313—C316—H3162	120.0
C12—C14—H142	111.2	H3161—C316—H3162	120.0
C15—C14—H142	111.2	C301—C317—C318	128.7 (4)
H141—C14—H142	109.5	C301—C317—H3171	115.6
C9—C15—C14	104.7 (3)	C318—C317—H3171	115.7
C9—C15—C1	112.3 (2)	C317—C318—H3181	120.0
C14—C15—C1	101.3 (3)	C317—C318—H3182	120.0
C9—C15—C5	110.9 (3)	H3181—C318—H3182	120.0
C14—C15—C5	114.4 (3)	C312—C319—O322	107.7 (3)
C1—C15—C5	112.7 (3)	C312—C319—C320	114.8 (3)
C13—C16—H161	120.0	O322—C319—C320	108.8 (3)
C13—C16—H162	120.0	C312—C319—H3191	108.5
H161—C16—H162	120.0	O322—C319—H3191	108.5
C1—C17—C18	129.0 (4)	C320—C319—H3191	108.5
C1—C17—H171	115.5	C319—C320—O321	111.8 (3)
C18—C17—H171	115.5	C319—C320—H3201	108.9
C17—C18—H181	120.0	O321—C320—H3201	108.9
C17—C18—H182	120.0	C319—C320—H3202	108.9
H181—C18—H182	120.0	O321—C320—H3202	108.9
C12—C19—O22	109.6 (3)	H3201—C320—H3202	109.5

C12—C19—C20	114.4 (3)	C402—C401—C413	106.9 (3)
O22—C19—C20	108.9 (3)	C402—C401—C415	109.4 (3)
C12—C19—H191	107.9	C413—C401—C415	103.7 (3)
O22—C19—H191	107.9	C402—C401—C417	107.8 (3)
C20—C19—H191	107.9	C413—C401—C417	112.4 (3)
C19—C20—O21	110.0 (3)	C415—C401—C417	116.4 (3)
C19—C20—H201	109.3	C401—C402—C403	112.4 (3)
O21—C20—H201	109.3	C401—C402—H4021	108.7
C19—C20—H202	109.4	C403—C402—H4021	108.7
O21—C20—H202	109.4	C401—C402—H4022	108.7
H201—C20—H202	109.5	C403—C402—H4022	108.7
C102—C101—C113	107.1 (3)	H4021—C402—H4022	109.5
C102—C101—C115	109.2 (3)	C402—C403—C404	112.4 (3)
C113—C101—C115	104.4 (3)	C402—C403—H4031	108.7
C102—C101—C117	106.6 (3)	C404—C403—H4031	108.7
C113—C101—C117	113.1 (3)	C402—C403—H4032	108.7
C115—C101—C117	116.2 (3)	C404—C403—H4032	108.7
C101—C102—C103	112.1 (3)	H4031—C403—H4032	109.5
C101—C102—H1021	108.8	C403—C404—C405	124.7 (4)
C103—C102—H1021	108.8	C403—C404—H4041	117.6
C101—C102—H1022	108.8	C405—C404—H4041	117.6
C103—C102—H1022	108.8	C404—C405—C406	121.8 (4)
H1021—C102—H1022	109.5	C404—C405—C415	122.4 (4)
C102—C103—C104	111.5 (3)	C406—C405—C415	115.7 (3)
C102—C103—H1031	109.0	C405—C406—C407	109.8 (3)
C104—C103—H1031	109.0	C405—C406—H4061	109.4
C102—C103—H1032	109.0	C407—C406—H4061	109.4
C104—C103—H1032	109.0	C405—C406—H4062	109.4
H1031—C103—H1032	109.5	C407—C406—H4062	109.4
C103—C104—C105	124.6 (4)	H4061—C406—H4062	109.5
C103—C104—H1041	117.7	C406—C407—C408	110.0 (3)
C105—C104—H1041	117.7	C406—C407—H4071	109.4
C104—C105—C106	122.0 (3)	C408—C407—H4071	109.3
C104—C105—C115	123.1 (3)	C406—C407—H4072	109.3
C106—C105—C115	114.9 (3)	C408—C407—H4072	109.3
C105—C106—C107	110.8 (3)	H4071—C407—H4072	109.5
C105—C106—H1061	109.1	C407—C408—C409	125.1 (4)
C107—C106—H1061	109.1	C407—C408—H4081	117.5
C105—C106—H1062	109.1	C409—C408—H4081	117.5
C107—C106—H1062	109.1	C408—C409—C410	122.5 (4)
H1061—C106—H1062	109.5	C408—C409—C415	122.5 (4)
C106—C107—C108	110.3 (3)	C410—C409—C415	114.8 (3)
C106—C107—H1071	109.3	C409—C410—C411	112.6 (3)
C108—C107—H1071	109.3	C409—C410—H4101	108.7
C106—C107—H1072	109.3	C411—C410—H4101	108.7
C108—C107—H1072	109.3	C409—C410—H4102	108.7
H1071—C107—H1072	109.5	C411—C410—H4102	108.7
C107—C108—C109	124.4 (3)	H4101—C410—H4102	109.5
C107—C108—H1081	117.8	C410—C411—C412	111.7 (3)
C109—C108—H1081	117.8	C410—C411—H4111	108.9
C108—C109—C110	121.7 (3)	C412—C411—H4111	108.9
C108—C109—C115	123.1 (3)	C410—C411—H4112	108.9

C110—C109—C115	115.0 (3)	C412—C411—H4112	108.9
C109—C110—C111	111.6 (3)	H4111—C411—H4112	109.5
C109—C110—H1101	108.9	C411—C412—C413	107.4 (3)
C111—C110—H1101	108.9	C411—C412—C414	107.1 (3)
C109—C110—H1102	108.9	C413—C412—C414	103.1 (3)
C111—C110—H1102	108.9	C411—C412—C419	110.2 (3)
H1101—C110—H1102	109.5	C413—C412—C419	113.9 (3)
C110—C111—C112	112.1 (3)	C414—C412—C419	114.6 (3)
C110—C111—H1111	108.8	C401—C413—C412	108.7 (3)
C112—C111—H1111	108.8	C401—C413—C416	124.7 (3)
C110—C111—H1112	108.8	C412—C413—C416	126.7 (4)
C112—C111—H1112	108.8	C412—C414—C415	102.9 (3)
H1111—C111—H1112	109.5	C412—C414—H4141	111.1
C111—C112—C113	108.0 (3)	C415—C414—H4141	111.1
C111—C112—C114	108.1 (3)	C412—C414—H4142	111.1
C113—C112—C114	102.6 (3)	C415—C414—H4142	111.1
C111—C112—C119	109.3 (3)	H4141—C414—H4142	109.5
C113—C112—C119	114.4 (3)	C409—C415—C414	105.2 (3)
C114—C112—C119	114.1 (3)	C409—C415—C401	111.9 (3)
C101—C113—C112	108.4 (3)	C414—C415—C401	101.3 (3)
C101—C113—C116	125.4 (3)	C409—C415—C405	110.5 (3)
C112—C113—C116	126.1 (3)	C414—C415—C405	113.3 (3)
C112—C114—C115	101.9 (2)	C401—C415—C405	114.1 (3)
C112—C114—H1141	111.3	C413—C416—H4161	120.0
C115—C114—H1141	111.3	C413—C416—H4162	120.0
C112—C114—H1142	111.3	H4161—C416—H4162	120.0
C115—C114—H1142	111.3	C401—C417—C418	128.8 (4)
H1141—C114—H1142	109.5	C401—C417—H4171	115.6
C109—C115—C114	104.8 (3)	C418—C417—H4171	115.6
C109—C115—C101	112.6 (3)	C417—C418—H4181	120.0
C114—C115—C101	101.1 (3)	C417—C418—H4182	120.0
C109—C115—C105	110.7 (3)	H4181—C418—H4182	120.0
C114—C115—C105	113.2 (3)	C412—C419—O422	108.8 (3)
C101—C115—C105	113.6 (3)	C412—C419—C420	113.2 (3)
C113—C116—H1161	120.0	O422—C419—C420	108.7 (3)
C113—C116—H1162	120.0	C412—C419—H4191	108.7
H1161—C116—H1162	120.0	O422—C419—H4191	108.7
C101—C117—C118	128.8 (4)	C420—C419—H4191	108.7
C101—C117—H1171	115.6	C419—C420—O421	110.2 (3)
C118—C117—H1171	115.6	C419—C420—H4201	109.3
C117—C118—H1181	120.0	O421—C420—H4201	109.3
C117—C118—H1182	120.0	C419—C420—H4202	109.3
H1181—C118—H1182	120.0	O421—C420—H4202	109.3
C112—C119—O122	109.2 (3)	H4201—C420—H4202	109.5
C112—C119—C120	115.6 (3)	C502—C501—C513	107.3 (3)
O122—C119—C120	108.7 (3)	C502—C501—C515	108.9 (3)
C112—C119—H1191	107.7	C513—C501—C515	103.2 (3)
O122—C119—H1191	107.7	C502—C501—C517	107.1 (7)
C120—C119—H1191	107.7	C513—C501—C517	121.2 (4)
C119—C120—O121	110.4 (3)	C515—C501—C517	108.6 (5)
C119—C120—H1201	109.2	C502—C501—C527	111 (2)
O121—C120—H1201	109.2	C513—C501—C527	105.9 (12)

C119—C120—H1202	109.2	C515—C501—C527	119.5 (13)
O121—C120—H1202	109.2	C501—C502—C503	113.4 (3)
H1201—C120—H1202	109.5	C501—C502—H5021	108.5
C202—C201—C213	107.5 (3)	C503—C502—H5021	108.5
C202—C201—C215	109.6 (3)	C501—C502—H5022	108.5
C213—C201—C215	103.5 (2)	C503—C502—H5022	108.5
C202—C201—C217	106.4 (3)	H5021—C502—H5022	109.5
C213—C201—C217	113.1 (3)	C502—C503—C504	111.6 (3)
C215—C201—C217	116.4 (3)	C502—C503—H5031	108.9
C201—C202—C203	112.7 (3)	C504—C503—H5031	109.0
C201—C202—H2021	108.7	C502—C503—H5032	108.9
C203—C202—H2021	108.7	C504—C503—H5032	108.9
C201—C202—H2022	108.6	H5031—C503—H5032	109.5
C203—C202—H2022	108.7	C503—C504—C505	125.1 (4)
H2021—C202—H2022	109.5	C503—C504—H5041	117.4
C202—C203—C204	111.3 (3)	C505—C504—H5041	117.5
C202—C203—H2031	109.0	C504—C505—C506	121.5 (3)
C204—C203—H2031	109.0	C504—C505—C515	123.3 (3)
C202—C203—H2032	109.0	C506—C505—C515	115.1 (3)
C204—C203—H2032	109.0	C505—C506—C507	109.4 (3)
H2031—C203—H2032	109.5	C505—C506—H5061	109.5
C203—C204—C205	125.3 (3)	C507—C506—H5061	109.5
C203—C204—H2041	117.3	C505—C506—H5062	109.5
C205—C204—H2041	117.3	C507—C506—H5062	109.5
C204—C205—C206	122.7 (4)	H5061—C506—H5062	109.5
C204—C205—C215	122.6 (3)	C506—C507—C508	110.8 (3)
C206—C205—C215	114.7 (3)	C506—C507—H5071	109.1
C205—C206—C207	110.0 (3)	C508—C507—H5071	109.1
C205—C206—H2061	109.4	C506—C507—H5072	109.1
C207—C206—H2061	109.3	C508—C507—H5072	109.2
C205—C206—H2062	109.3	H5071—C507—H5072	109.5
C207—C206—H2062	109.3	C507—C508—C509	124.3 (4)
H2061—C206—H2062	109.5	C507—C508—H5081	117.8
C206—C207—C208	110.4 (3)	C509—C508—H5081	117.8
C206—C207—H2071	109.2	C508—C509—C510	122.6 (4)
C208—C207—H2071	109.2	C508—C509—C515	122.4 (3)
C206—C207—H2072	109.2	C510—C509—C515	114.9 (3)
C208—C207—H2072	109.2	C509—C510—C511	112.6 (3)
H2071—C207—H2072	109.5	C509—C510—H5101	108.7
C207—C208—C209	124.6 (4)	C511—C510—H5101	108.7
C207—C208—H2081	117.7	C509—C510—H5102	108.7
C209—C208—H2081	117.7	C511—C510—H5102	108.7
C208—C209—C210	122.1 (3)	H5101—C510—H5102	109.5
C208—C209—C215	123.2 (4)	C510—C511—C512	111.4 (3)
C210—C209—C215	114.6 (3)	C510—C511—H5111	109.0
C209—C210—C211	112.0 (3)	C512—C511—H5111	109.0
C209—C210—H2101	108.8	C510—C511—H5112	109.0
C211—C210—H2101	108.8	C512—C511—H5112	109.0
C209—C210—H2102	108.8	H5111—C511—H5112	109.5
C211—C210—H2102	108.8	C511—C512—C513	108.0 (3)
H2101—C210—H2102	109.5	C511—C512—C514	107.6 (3)
C210—C211—C212	111.0 (3)	C513—C512—C514	102.2 (3)

C210—C211—H2111	109.1	C511—C512—C519	110.7 (3)
C212—C211—H2111	109.1	C513—C512—C519	113.5 (3)
C210—C211—H2112	109.1	C514—C512—C519	114.3 (3)
C212—C211—H2112	109.1	C512—C513—C501	109.4 (3)
H2111—C211—H2112	109.5	C512—C513—C516	125.3 (3)
C211—C212—C213	107.3 (3)	C501—C513—C516	125.2 (3)
C211—C212—C214	107.2 (3)	C512—C514—C515	102.4 (3)
C213—C212—C214	102.2 (2)	C512—C514—H5141	111.2
C211—C212—C219	110.2 (3)	C515—C514—H5141	111.2
C213—C212—C219	114.7 (3)	C512—C514—H5142	111.2
C214—C212—C219	114.7 (3)	C515—C514—H5142	111.2
C201—C213—C212	109.2 (3)	H5141—C514—H5142	109.5
C201—C213—C216	125.3 (3)	C509—C515—C514	105.7 (3)
C212—C213—C216	125.5 (3)	C509—C515—C505	110.9 (3)
C212—C214—C215	102.9 (3)	C514—C515—C505	113.8 (3)
C212—C214—H2141	111.1	C509—C515—C501	111.5 (3)
C215—C214—H2141	111.1	C514—C515—C501	101.7 (2)
C212—C214—H2142	111.1	C505—C515—C501	112.7 (3)
C215—C214—H2142	111.1	C513—C516—H5161	120.0
H2141—C214—H2142	109.5	C513—C516—H5162	120.0
C214—C215—C205	112.6 (3)	H5161—C516—H5162	120.0
C214—C215—C209	105.1 (3)	C501—C517—C518	128.6 (6)
C205—C215—C209	111.7 (3)	C501—C517—H5171	115.7
C214—C215—C201	101.0 (2)	C518—C517—H5171	115.7
C205—C215—C201	113.0 (3)	C517—C518—H5181	120.0
C209—C215—C201	112.8 (3)	C517—C518—H5182	120.0
C213—C216—H2161	120.0	H5181—C518—H5182	120.0
C213—C216—H2162	120.0	C512—C519—O522	108.7 (3)
H2161—C216—H2162	120.0	C512—C519—C520	114.5 (3)
C201—C217—C218	127.9 (4)	O522—C519—C520	109.1 (3)
C201—C217—H2171	116.1	C512—C519—H5191	108.1
C218—C217—H2171	116.1	O522—C519—H5191	108.1
C217—C218—H2181	120.0	C520—C519—H5191	108.1
C217—C218—H2182	120.0	C519—C520—O521	108.6 (3)
H2181—C218—H2182	120.0	C519—C520—H5201	109.7
C212—C219—O222	110.4 (3)	O521—C520—H5201	109.7
C212—C219—C220	114.5 (3)	C519—C520—H5202	109.7
O222—C219—C220	106.9 (3)	O521—C520—H5202	109.7
C212—C219—H2191	108.3	H5201—C520—H5202	109.5
O222—C219—H2191	108.3	C501—C527—C528	128.0 (9)
C220—C219—H2191	108.3	C501—C527—H5271	116.0
C219—C220—O221	113.2 (3)	C528—C527—H5271	116.0
C219—C220—H2201	108.5	C527—C528—H5281	120.0
O221—C220—H2201	108.5	C527—C528—H5282	120.0
C219—C220—H2202	108.5	H5281—C528—H5282	120.0
O221—C220—H2202	108.5		
O21—C20—C19—O22	70.8 (4)	C213—C212—C214—C215	39.4 (3)
O21—C20—C19—C12	-166.2 (3)	C213—C212—C219—C220	58.5 (4)
O22—C19—C12—C11	-53.4 (3)	C214—C212—C213—C216	162.7 (4)
O22—C19—C12—C13	-173.8 (3)	C214—C212—C219—C220	-59.4 (4)
O22—C19—C12—C14	68.9 (4)	C214—C215—C201—C217	159.2 (2)

O121—C120—C119—O122	70.3 (4)	C215—C201—C213—C216	169.2 (4)
O121—C120—C119—C112	-166.6 (3)	C215—C201—C217—C218	23.0 (4)
O122—C119—C112—C111	-58.0 (3)	C215—C214—C212—C219	164.1 (2)
O122—C119—C112—C113	-179.2 (3)	C216—C213—C201—C217	42.3 (5)
O122—C119—C112—C114	63.1 (4)	C216—C213—C212—C219	38.0 (5)
O221—C220—C219—O222	71.7 (4)	C301—C302—C303—C304	48.0 (5)
O221—C220—C219—C212	-165.6 (4)	C301—C313—C312—C311	94.0 (3)
O222—C219—C212—C211	-59.6 (4)	C301—C313—C312—C314	-20.0 (4)
O222—C219—C212—C213	179.2 (3)	C301—C313—C312—C319	-144.2 (3)
O222—C219—C212—C214	61.4 (3)	C301—C315—C305—C304	-11.4 (6)
O321—C320—C319—O322	58.5 (4)	C301—C315—C305—C306	165.9 (4)
O321—C320—C319—C312	179.2 (3)	C301—C315—C309—C308	-138.6 (4)
O322—C319—C312—C311	-57.6 (4)	C301—C315—C309—C310	47.0 (5)
O322—C319—C312—C313	-178.2 (3)	C301—C315—C314—C312	-45.8 (3)
O322—C319—C312—C314	64.2 (3)	C302—C301—C313—C312	107.4 (3)
O421—C420—C419—O422	69.3 (4)	C302—C301—C313—C316	-74.1 (5)
O421—C420—C419—C412	-169.7 (2)	C302—C301—C315—C305	40.0 (4)
O422—C419—C412—C411	-59.3 (3)	C302—C301—C315—C309	167.9 (3)
O422—C419—C412—C413	-180.0 (2)	C302—C301—C315—C314	-81.4 (3)
O422—C419—C412—C414	61.7 (3)	C302—C301—C317—C318	-104.2 (4)
O521—C520—C519—O522	74.8 (3)	C302—C303—C304—C305	-18.0 (6)
O521—C520—C519—C512	-163.1 (2)	C303—C302—C301—C313	-171.8 (4)
O522—C519—C512—C511	-55.4 (3)	C303—C302—C301—C315	-59.7 (4)
O522—C519—C512—C513	-177.1 (2)	C303—C302—C301—C317	67.4 (4)
O522—C519—C512—C514	66.3 (3)	C303—C304—C305—C306	-177.6 (4)
C1—C2—C3—C4	48.1 (4)	C303—C304—C305—C315	-0.5 (7)
C1—C13—C12—C11	92.0 (3)	C304—C305—C306—C307	119.5 (4)
C1—C13—C12—C14	-21.2 (3)	C304—C305—C315—C309	-139.6 (4)
C1—C13—C12—C19	-146.0 (3)	C304—C305—C315—C314	103.3 (5)
C1—C15—C5—C4	-10.2 (4)	C305—C306—C307—C308	47.7 (5)
C1—C15—C5—C6	167.6 (2)	C305—C315—C301—C313	154.4 (3)
C1—C15—C9—C8	-139.5 (3)	C305—C315—C301—C317	-81.0 (4)
C1—C15—C9—C10	47.3 (4)	C305—C315—C309—C308	-9.8 (6)
C1—C15—C14—C12	-45.4 (4)	C305—C315—C309—C310	175.8 (4)
C2—C1—C13—C12	107.7 (3)	C305—C315—C314—C312	-167.6 (3)
C2—C1—C13—C16	-72.7 (4)	C306—C305—C315—C309	37.7 (5)
C2—C1—C15—C5	41.0 (3)	C306—C305—C315—C314	-79.3 (4)
C2—C1—C15—C9	167.0 (3)	C306—C307—C308—C309	-22.4 (7)
C2—C1—C15—C14	-81.8 (3)	C307—C306—C305—C315	-57.8 (4)
C2—C1—C17—C18	-102.1 (6)	C307—C308—C309—C310	176.8 (5)
C2—C3—C4—C5	-15.2 (5)	C307—C308—C309—C315	2.8 (8)
C3—C2—C1—C13	-172.9 (3)	C308—C309—C310—C311	-126.1 (5)
C3—C2—C1—C15	-61.5 (4)	C308—C309—C315—C314	112.4 (5)
C3—C2—C1—C17	65.8 (4)	C309—C310—C311—C312	-45.2 (4)
C3—C4—C5—C6	178.3 (3)	C309—C315—C301—C313	-77.7 (3)
C3—C4—C5—C15	-4.1 (5)	C309—C315—C301—C317	46.9 (3)
C4—C5—C6—C7	118.1 (4)	C309—C315—C314—C312	70.9 (3)
C4—C5—C15—C9	-137.1 (3)	C310—C309—C315—C314	-61.9 (5)
C4—C5—C15—C14	104.9 (4)	C310—C311—C312—C313	-50.1 (4)
C5—C6—C7—C8	46.3 (5)	C310—C311—C312—C314	60.0 (4)
C5—C15—C1—C13	154.5 (2)	C310—C311—C312—C319	-174.6 (3)
C5—C15—C1—C17	-79.9 (4)	C311—C310—C309—C315	48.3 (5)

C5—C15—C9—C8	-12.4 (4)	C311—C312—C313—C316	-84.5 (4)
C5—C15—C9—C10	174.3 (3)	C311—C312—C314—C315	-73.0 (3)
C5—C15—C14—C12	-167.0 (3)	C311—C312—C319—C320	-178.9 (3)
C6—C5—C15—C9	40.7 (3)	C312—C313—C301—C315	-8.3 (4)
C6—C5—C15—C14	-77.3 (4)	C312—C313—C301—C317	-135.6 (3)
C6—C7—C8—C9	-19.8 (6)	C313—C301—C315—C314	32.9 (3)
C7—C6—C5—C15	-59.7 (4)	C313—C301—C317—C318	138.3 (3)
C7—C8—C9—C10	175.6 (3)	C313—C312—C314—C315	40.5 (3)
C7—C8—C9—C15	2.9 (5)	C313—C312—C319—C320	60.5 (4)
C8—C9—C10—C11	-125.9 (3)	C314—C312—C313—C316	161.5 (4)
C8—C9—C15—C14	111.4 (4)	C314—C312—C319—C320	-57.1 (4)
C9—C10—C11—C12	-44.4 (4)	C314—C315—C301—C317	157.5 (2)
C9—C15—C1—C13	-79.6 (3)	C315—C301—C313—C316	170.2 (4)
C9—C15—C1—C17	46.1 (5)	C315—C301—C317—C318	18.2 (4)
C9—C15—C14—C12	71.5 (3)	C315—C314—C312—C319	164.5 (2)
C10—C9—C15—C14	-61.8 (3)	C316—C313—C301—C317	42.9 (5)
C10—C11—C12—C13	-50.4 (3)	C316—C313—C312—C319	37.3 (5)
C10—C11—C12—C14	58.9 (3)	C401—C402—C403—C404	44.6 (5)
C10—C11—C12—C19	-174.5 (2)	C401—C413—C412—C411	93.8 (4)
C11—C10—C9—C15	47.3 (4)	C401—C413—C412—C414	-19.2 (4)
C11—C12—C13—C16	-87.6 (4)	C401—C413—C412—C419	-143.9 (3)
C11—C12—C14—C15	-71.9 (3)	C401—C415—C405—C404	-13.6 (5)
C11—C12—C19—C20	-176.1 (3)	C401—C415—C405—C406	162.9 (3)
C12—C13—C1—C15	-6.8 (3)	C401—C415—C409—C408	-134.2 (4)
C12—C13—C1—C17	-135.1 (3)	C401—C415—C409—C410	50.1 (4)
C13—C1—C15—C14	31.7 (3)	C401—C415—C414—C412	-45.1 (3)
C13—C1—C17—C18	140.7 (5)	C402—C401—C413—C412	106.8 (3)
C13—C12—C14—C15	41.0 (3)	C402—C401—C413—C416	-73.0 (5)
C13—C12—C19—C20	63.5 (4)	C402—C401—C415—C405	40.8 (4)
C14—C12—C13—C16	159.2 (3)	C402—C401—C415—C409	167.1 (3)
C14—C12—C19—C20	-53.7 (4)	C402—C401—C415—C414	-81.3 (4)
C14—C15—C1—C17	157.3 (4)	C402—C401—C417—C418	-92.8 (7)
C15—C1—C13—C16	172.8 (3)	C402—C403—C404—C405	-15.9 (7)
C15—C1—C17—C18	19.7 (8)	C403—C402—C401—C413	-168.8 (3)
C15—C14—C12—C19	164.6 (3)	C403—C402—C401—C415	-57.2 (4)
C16—C13—C1—C17	44.5 (5)	C403—C402—C401—C417	70.2 (5)
C16—C13—C12—C19	34.4 (5)	C403—C404—C405—C406	-176.1 (4)
C101—C102—C103—C104	47.6 (4)	C403—C404—C405—C415	0.2 (7)
C101—C113—C112—C111	92.0 (3)	C404—C405—C406—C407	116.8 (4)
C101—C113—C112—C114	-22.0 (3)	C404—C405—C415—C409	-140.7 (4)
C101—C113—C112—C119	-146.2 (3)	C404—C405—C415—C414	101.7 (4)
C101—C115—C105—C104	-11.9 (4)	C405—C406—C407—C408	49.9 (5)
C101—C115—C105—C106	166.6 (2)	C405—C415—C401—C413	154.5 (3)
C101—C115—C109—C108	-138.4 (3)	C405—C415—C401—C417	-81.6 (4)
C101—C115—C109—C110	47.1 (4)	C405—C415—C409—C408	-5.8 (5)
C101—C115—C114—C112	-45.6 (4)	C405—C415—C409—C410	178.4 (3)
C102—C101—C113—C112	109.4 (3)	C405—C415—C414—C412	-167.8 (3)
C102—C101—C113—C116	-69.6 (4)	C406—C405—C415—C409	35.8 (4)
C102—C101—C115—C105	39.2 (3)	C406—C405—C415—C414	-81.8 (4)
C102—C101—C115—C109	166.2 (3)	C406—C407—C408—C409	-23.1 (6)
C102—C101—C115—C114	-82.5 (4)	C407—C406—C405—C415	-59.7 (4)
C102—C101—C117—C118	-97.4 (6)	C407—C408—C409—C410	175.8 (4)

C102—C103—C104—C105	-18.9 (4)	C407—C408—C409—C415	0.4 (6)
C103—C102—C101—C113	-170.8 (3)	C408—C409—C410—C411	-130.8 (4)
C103—C102—C101—C115	-58.3 (4)	C408—C409—C415—C414	116.7 (4)
C103—C102—C101—C117	67.8 (4)	C409—C410—C411—C412	-43.7 (5)
C103—C104—C105—C106	-177.6 (3)	C409—C415—C401—C413	-79.2 (4)
C103—C104—C105—C115	0.8 (4)	C409—C415—C401—C417	44.7 (4)
C104—C105—C106—C107	118.8 (5)	C409—C415—C414—C412	71.5 (3)
C104—C105—C115—C109	-139.8 (3)	C410—C409—C415—C414	-59.0 (4)
C104—C105—C115—C114	102.8 (4)	C410—C411—C412—C413	-50.5 (4)
C105—C106—C107—C108	47.8 (6)	C410—C411—C412—C414	59.6 (3)
C105—C115—C101—C113	153.4 (2)	C410—C411—C412—C419	-175.0 (3)
C105—C115—C101—C117	-81.2 (4)	C411—C410—C409—C415	44.9 (5)
C105—C115—C109—C108	-9.9 (4)	C411—C412—C413—C416	-86.4 (5)
C105—C115—C109—C110	175.6 (3)	C411—C412—C414—C415	-73.4 (3)
C105—C115—C114—C112	-167.6 (3)	C411—C412—C419—C420	179.7 (3)
C106—C105—C115—C109	38.7 (3)	C412—C413—C401—C415	-8.7 (4)
C106—C105—C115—C114	-78.8 (4)	C412—C413—C401—C417	-135.2 (4)
C106—C107—C108—C109	-21.2 (6)	C413—C401—C415—C414	32.4 (3)
C107—C106—C105—C115	-59.7 (5)	C413—C401—C417—C418	149.8 (6)
C107—C108—C109—C110	176.1 (3)	C413—C412—C414—C415	39.7 (4)
C107—C108—C109—C115	2.0 (5)	C413—C412—C419—C420	59.0 (3)
C108—C109—C110—C111	-127.7 (3)	C414—C412—C413—C416	160.7 (4)
C108—C109—C115—C114	112.6 (4)	C414—C412—C419—C420	-59.4 (4)
C109—C110—C111—C112	-43.7 (4)	C414—C415—C401—C417	156.3 (3)
C109—C115—C101—C113	-79.6 (3)	C415—C401—C413—C416	171.5 (4)
C109—C115—C101—C117	45.7 (5)	C415—C401—C417—C418	30.5 (7)
C109—C115—C114—C112	71.5 (3)	C415—C414—C412—C419	164.0 (3)
C110—C109—C115—C114	-61.9 (3)	C416—C413—C401—C417	45.0 (6)
C110—C111—C112—C113	-51.5 (3)	C416—C413—C412—C419	35.9 (5)
C110—C111—C112—C114	58.8 (3)	C501—C502—C503—C504	44.3 (4)
C110—C111—C112—C119	-176.4 (2)	C501—C513—C512—C511	93.7 (3)
C111—C110—C109—C115	46.8 (4)	C501—C513—C512—C514	-19.7 (4)
C111—C112—C113—C116	-89.1 (4)	C501—C513—C512—C519	-143.2 (3)
C111—C112—C114—C115	-72.1 (3)	C501—C515—C505—C504	-14.5 (5)
C111—C112—C119—C120	179.2 (3)	C501—C515—C505—C506	161.9 (3)
C112—C113—C101—C115	-6.3 (3)	C501—C515—C509—C508	-131.9 (4)
C112—C113—C101—C117	-133.5 (3)	C501—C515—C509—C510	51.0 (4)
C113—C101—C115—C114	31.7 (3)	C501—C515—C514—C512	-45.9 (3)
C113—C101—C117—C118	145.1 (5)	C502—C501—C513—C512	106.6 (3)
C113—C112—C114—C115	41.9 (3)	C502—C501—C513—C516	-71.3 (4)
C113—C112—C119—C120	58.0 (4)	C502—C501—C515—C505	41.3 (4)
C114—C112—C113—C116	156.9 (3)	C502—C501—C515—C509	166.8 (3)
C114—C112—C119—C120	-59.7 (4)	C502—C501—C515—C514	-81.0 (3)
C114—C115—C101—C117	157.1 (4)	C502—C501—C517—C518	109 (1)
C115—C101—C113—C116	174.7 (3)	C502—C501—C527—C528	-98 (4)
C115—C101—C117—C118	24.4 (7)	C502—C503—C504—C505	-15.0 (6)
C115—C114—C112—C119	166.1 (3)	C503—C502—C501—C513	-169.2 (2)
C116—C113—C101—C117	47.5 (5)	C503—C502—C501—C515	-58.0 (4)
C116—C113—C112—C119	32.8 (5)	C503—C502—C501—C517	59.1 (6)
C201—C202—C203—C204	46.1 (5)	C503—C502—C501—C527	75 (2)
C201—C213—C212—C211	94.9 (3)	C503—C504—C505—C506	-175.9 (4)
C201—C213—C212—C214	-17.6 (4)	C503—C504—C505—C515	0.2 (6)

C201—C213—C212—C219	-142.3 (3)	C504—C505—C506—C507	116.3 (4)
C201—C215—C205—C204	-13.1 (6)	C504—C505—C515—C509	-140.3 (3)
C201—C215—C205—C206	163.5 (4)	C504—C505—C515—C514	100.7 (4)
C201—C215—C209—C208	-135.4 (4)	C505—C506—C507—C508	50.6 (4)
C201—C215—C209—C210	48.9 (4)	C505—C515—C501—C513	155.1 (3)
C201—C215—C214—C212	-46.1 (3)	C505—C515—C501—C517	-75.0 (5)
C202—C201—C213—C212	105.3 (3)	C505—C515—C501—C527	-88 (2)
C202—C201—C213—C216	-74.9 (5)	C505—C515—C509—C508	-5.3 (4)
C202—C201—C215—C205	40.5 (4)	C505—C515—C509—C510	177.6 (3)
C202—C201—C215—C209	168.3 (3)	C505—C515—C514—C512	-167.4 (3)
C202—C201—C215—C214	-80.1 (3)	C506—C505—C515—C509	36.0 (4)
C202—C201—C217—C218	-99.4 (3)	C506—C505—C515—C514	-83.0 (4)
C202—C203—C204—C205	-17.0 (6)	C506—C507—C508—C509	-22.8 (5)
C203—C202—C201—C213	-170.5 (3)	C507—C506—C505—C515	-60.0 (4)
C203—C202—C201—C215	-58.6 (4)	C507—C508—C509—C510	176.3 (3)
C203—C202—C201—C217	68.1 (4)	C507—C508—C509—C515	-0.6 (6)
C203—C204—C205—C206	-175.8 (4)	C508—C509—C510—C511	-132.6 (4)
C203—C204—C205—C215	0.6 (7)	C508—C509—C515—C514	118.5 (4)
C204—C205—C206—C207	118.9 (4)	C509—C510—C511—C512	-44.0 (5)
C204—C205—C215—C209	-141.4 (4)	C509—C515—C501—C513	-79.3 (4)
C204—C205—C215—C214	100.6 (5)	C509—C515—C501—C517	50.6 (6)
C205—C206—C207—C208	49.9 (5)	C509—C515—C501—C527	38 (2)
C205—C215—C201—C213	155.0 (3)	C509—C515—C514—C512	70.6 (3)
C205—C215—C201—C217	-80.2 (4)	C510—C509—C515—C514	-58.6 (4)
C205—C215—C209—C208	-7.0 (6)	C510—C511—C512—C513	-49.5 (4)
C205—C215—C209—C210	177.3 (3)	C510—C511—C512—C514	60.3 (3)
C205—C215—C214—C212	-167.0 (2)	C510—C511—C512—C519	-174.3 (3)
C206—C205—C215—C209	35.2 (5)	C511—C510—C509—C515	44.6 (5)
C206—C205—C215—C214	-82.8 (4)	C511—C512—C513—C516	-88.4 (5)
C206—C207—C208—C209	-24.3 (7)	C511—C512—C514—C515	-73.4 (3)
C207—C206—C205—C215	-57.7 (4)	C511—C512—C519—C520	-177.7 (3)
C207—C208—C209—C210	177.9 (5)	C512—C513—C501—C515	-8.3 (3)
C207—C208—C209—C215	2.5 (8)	C512—C513—C501—C517	-130.0 (7)
C208—C209—C210—C211	-128.6 (4)	C512—C513—C501—C527	-135 (2)
C208—C209—C215—C214	115.4 (4)	C513—C501—C515—C514	32.9 (3)
C209—C210—C211—C212	-45.7 (4)	C513—C501—C517—C518	-15 (2)
C209—C215—C201—C213	-77.3 (4)	C513—C501—C527—C528	146 (3)
C209—C215—C201—C217	47.5 (3)	C513—C512—C514—C515	40.3 (3)
C209—C215—C214—C212	71.2 (3)	C513—C512—C519—C520	60.7 (3)
C210—C209—C215—C214	-60.2 (4)	C514—C512—C513—C516	158.2 (4)
C210—C211—C212—C213	-48.6 (4)	C514—C512—C519—C520	-56.0 (4)
C210—C211—C212—C214	60.5 (4)	C514—C515—C501—C517	162.8 (5)
C210—C211—C212—C219	-174.1 (3)	C514—C515—C501—C527	150 (2)
C211—C210—C209—C215	47.1 (4)	C515—C501—C513—C516	173.8 (4)
C211—C212—C213—C216	-84.8 (4)	C515—C501—C517—C518	-134 (1)
C211—C212—C214—C215	-73.3 (3)	C515—C501—C527—C528	30 (4)
C211—C212—C219—C220	179.7 (3)	C515—C514—C512—C519	163.2 (3)
C212—C213—C201—C215	-10.6 (4)	C516—C513—C501—C517	52.1 (9)
C212—C213—C201—C217	-137.5 (3)	C516—C513—C501—C527	47 (2)
C213—C201—C215—C214	34.4 (3)	C516—C513—C512—C519	34.7 (5)
C213—C201—C217—C218	142.7 (3)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y, -z+1$; (iv) $x-1, y, z$; (v) $-x, -y, -z+2$; (vi) $-x+2, -y, -z+1$; (vii) $-x+1, -y+1, -z+2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O21—H9021 \cdots O521 ⁱ	0.82 (3)	1.88 (3)	2.699 (6)	174 (3)
O22—H9022 \cdots O222	0.83 (3)	2.02 (3)	2.814 (6)	162 (3)
O121—H9121 \cdots O421 ⁱ	0.83 (3)	1.91 (3)	2.721 (6)	165 (3)
O122—H9122 \cdots O322	0.83 (3)	1.91 (3)	2.731 (6)	170 (3)
O221—H9221 \cdots O421	0.84 (3)	2.21 (3)	2.828 (6)	131 (3)
O222—H9222 \cdots O522 ⁱ	0.82 (3)	1.94 (3)	2.720 (6)	157 (3)
O321—H9321 \cdots O121	0.81 (3)	2.31 (3)	3.115 (6)	171 (3)
O322—H9322 \cdots O422 ⁱ	0.82 (3)	1.85 (3)	2.671 (6)	176 (3)
O421—H9421 \cdots O221 ⁱ	0.83 (3)	1.95 (3)	2.779 (6)	174 (3)
O422—H9422 \cdots O21	0.82 (3)	1.79 (3)	2.608 (6)	174 (3)
O521—H9521 \cdots O321 ⁱⁱ	0.82 (3)	1.93 (3)	2.747 (6)	170 (3)
O522—H9522 \cdots O121	0.82 (3)	1.87 (3)	2.685 (6)	169 (3)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, -y+1, -z+1$.