

Supporting Information

Formation of quaternary centres by copper catalysed asymmetric conjugate addition to β -substituted cyclopentenones with the aid of a quantitative structure-selectivity relationship

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Table 1. Crystal data and structure refinement for 6797.

| | | |
|-----------------------------------|--|-----------------------|
| Identification code | 6797 | |
| Empirical formula | C ₄₂ H _{36.34} N O _{2.17} P | |
| Formula weight | 620.79 | |
| Temperature | 150 K | |
| Wavelength | 1.54184 Å | |
| Crystal system | Orthorhombic | |
| Space group | P 21 21 21 | |
| Unit cell dimensions | a = 13.9558(3) Å | $\alpha = 90^\circ$. |
| | b = 15.4622(3) Å | $\beta = 90^\circ$. |
| | c = 30.6296(6) Å | $\gamma = 90^\circ$. |
| Volume | 6609.5(2) Å ³ | |
| Z | 8 | |
| Density (calculated) | 1.248 Mg/m ³ | |
| Absorption coefficient | 1.030 mm ⁻¹ | |
| F(000) | 2621.600 | |
| Crystal size | 0.31 x 0.20 x 0.09 mm ³ | |
| Theta range for data collection | 3.480 to 76.542°. | |
| Index ranges | -17 ≤ h ≤ 14, -19 ≤ k ≤ 18, -30 ≤ l ≤ 38 | |
| Reflections collected | 51019 | |
| Independent reflections | 13718 [R(int) = 0.042] | |
| Completeness to theta = 75.011° | 99.7 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.91 and 0.82 | |
| Refinement method | Full-matrix least-squares on F ² | |
| Data / restraints / parameters | 13717 / 0 / 888 | |
| Goodness-of-fit on F ² | 0.9994 | |
| Final R indices [I > 2σ(I)] | R1 = 0.0323, wR2 = 0.0789 | |
| R indices (all data) | R1 = 0.0359, wR2 = 0.0822 | |
| Absolute structure parameter | 0.001(7) | |
| Largest diff. peak and hole | 0.24 and -0.26 e.Å ⁻³ | |

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6797. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

| | x | y | z | $U(\text{eq})$ |
|-------|----------|---------|---------|----------------|
| P(1) | 10013(1) | 4657(1) | 3403(1) | 21 |
| O(2) | 9484(1) | 4940(1) | 3871(1) | 22 |
| C(3) | 8684(1) | 5466(1) | 3809(1) | 21 |
| C(4) | 8808(1) | 6368(1) | 3831(1) | 26 |
| C(5) | 8038(1) | 6894(1) | 3763(1) | 29 |
| C(6) | 7119(1) | 6542(1) | 3671(1) | 26 |
| C(7) | 6313(2) | 7086(1) | 3602(1) | 35 |
| C(8) | 5438(2) | 6751(1) | 3504(1) | 40 |
| C(9) | 5324(1) | 5846(1) | 3461(1) | 38 |
| C(10) | 6086(1) | 5304(1) | 3527(1) | 29 |
| C(11) | 7002(1) | 5628(1) | 3644(1) | 23 |
| C(12) | 7817(1) | 5082(1) | 3725(1) | 21 |
| C(13) | 7765(1) | 4127(1) | 3696(1) | 21 |
| C(14) | 7104(1) | 3628(1) | 3953(1) | 22 |
| C(15) | 6575(1) | 4000(1) | 4301(1) | 26 |
| C(16) | 5967(1) | 3502(1) | 4549(1) | 32 |
| C(17) | 5853(1) | 2608(1) | 4460(1) | 34 |
| C(18) | 6364(1) | 2235(1) | 4134(1) | 30 |
| C(19) | 7009(1) | 2724(1) | 3875(1) | 25 |
| C(20) | 7572(1) | 2330(1) | 3544(1) | 28 |
| C(21) | 8251(1) | 2797(1) | 3327(1) | 28 |
| C(22) | 8373(1) | 3685(1) | 3416(1) | 22 |
| O(23) | 9093(1) | 4105(1) | 3190(1) | 24 |
| N(24) | 10772(1) | 3933(1) | 3605(1) | 24 |
| C(25) | 11802(1) | 4039(1) | 3506(1) | 26 |
| C(26) | 10493(1) | 3208(1) | 3896(1) | 28 |
| C(27) | 10987(1) | 3253(1) | 4341(1) | 34 |
| C(28) | 10664(2) | 2323(1) | 3693(1) | 41 |
| C(31) | 11836(2) | 2658(2) | 2458(1) | 55 |
| C(32) | 12734(2) | 2318(2) | 2464(1) | 53 |
| C(33) | 13400(2) | 2571(2) | 2791(1) | 37 |
| C(34) | 14346(2) | 2244(2) | 2793(1) | 45 |

| | | | | |
|-------|----------|----------|---------|----|
| C(43) | 12095(1) | 4990(1) | 3483(1) | 28 |
| C(44) | 12506(1) | 5350(1) | 3110(1) | 34 |
| C(45) | 12797(1) | 6213(2) | 3105(1) | 39 |
| C(46) | 12675(1) | 6705(1) | 3477(1) | 39 |
| C(47) | 12244(1) | 6377(1) | 3854(1) | 36 |
| C(48) | 11965(1) | 5508(1) | 3851(1) | 32 |
| C(49) | 13226(2) | 6606(2) | 2699(1) | 54 |
| C(50) | 12060(2) | 6944(2) | 4245(1) | 52 |
| P(51) | 7520(1) | -707(1) | 3967(1) | 23 |
| O(52) | 7003(1) | 146(1) | 3732(1) | 22 |
| C(53) | 6218(1) | -87(1) | 3476(1) | 26 |
| C(54) | 6373(1) | -244(2) | 3026(1) | 38 |
| C(55) | 5616(2) | -448(2) | 2766(1) | 49 |
| C(56) | 4680(2) | -529(2) | 2942(1) | 41 |
| C(57) | 3881(2) | -729(2) | 2671(1) | 55 |
| C(58) | 2989(2) | -828(2) | 2842(1) | 57 |
| C(59) | 2852(2) | -772(2) | 3298(1) | 46 |
| C(60) | 3606(1) | -583(1) | 3568(1) | 35 |
| C(61) | 4536(1) | -419(1) | 3399(1) | 30 |
| C(62) | 5336(1) | -170(1) | 3668(1) | 23 |
| C(63) | 5255(1) | -46(1) | 4148(1) | 22 |
| C(64) | 4570(1) | 539(1) | 4340(1) | 24 |
| C(65) | 4021(1) | 1124(1) | 4083(1) | 30 |
| C(66) | 3377(1) | 1678(1) | 4276(1) | 39 |
| C(67) | 3242(2) | 1674(1) | 4730(1) | 44 |
| C(68) | 3768(1) | 1135(1) | 4987(1) | 40 |
| C(69) | 4455(1) | 558(1) | 4802(1) | 30 |
| C(70) | 5018(1) | 2(1) | 5064(1) | 34 |
| C(71) | 5719(1) | -492(1) | 4882(1) | 30 |
| C(72) | 5858(1) | -490(1) | 4425(1) | 24 |
| O(73) | 6584(1) | -1015(1) | 4269(1) | 28 |
| N(74) | 8266(1) | -201(1) | 4301(1) | 24 |
| C(75) | 9299(1) | -411(1) | 4265(1) | 22 |
| C(76) | 8002(1) | 506(1) | 4607(1) | 27 |
| C(77) | 8517(1) | 1352(1) | 4503(1) | 34 |
| C(78) | 8166(2) | 253(1) | 5082(1) | 38 |
| C(79) | 9639(1) | -1100(1) | 4584(1) | 23 |
| C(80) | 9036(1) | -1705(1) | 4759(1) | 29 |

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|--------|-----------|----------|----------|-----|
| C(81) | 9356(2) | -2295(1) | 5080(1) | 36 |
| C(82) | 10277(2) | -2262(1) | 5228(1) | 35 |
| C(83) | 10931(1) | -1660(1) | 5052(1) | 29 |
| C(84) | 11893(2) | -1622(1) | 5198(1) | 37 |
| C(85) | 12519(1) | -1038(1) | 5028(1) | 40 |
| C(86) | 12227(1) | -478(1) | 4692(1) | 36 |
| C(87) | 11301(1) | -500(1) | 4541(1) | 29 |
| C(88) | 10621(1) | -1080(1) | 4720(1) | 24 |
| C(93) | 9594(1) | -575(1) | 3789(1) | 23 |
| C(94) | 9505(2) | 108(1) | 3495(1) | 32 |
| C(95) | 9796(2) | 21(1) | 3063(1) | 37 |
| C(96) | 10176(1) | -767(1) | 2928(1) | 33 |
| C(97) | 10249(1) | -1466(1) | 3212(1) | 28 |
| C(98) | 9963(1) | -1361(1) | 3647(1) | 25 |
| C(99) | 9698(3) | 772(2) | 2749(1) | 62 |
| C(100) | 10630(2) | -2320(1) | 3052(1) | 41 |
| C(234) | 14507(17) | 2850(20) | 2688(8) | 45 |
| C(30) | 11537(2) | 3230(2) | 2794(1) | 41 |
| C(35) | 14995(2) | 2499(2) | 3099(1) | 43 |
| C(235) | 15050(20) | 2880(20) | 3025(10) | 43 |
| C(29) | 12147(2) | 3471(2) | 3123(1) | 27 |
| C(236) | 14590(40) | 3260(40) | 3400(20) | 32 |
| C(36) | 14732(3) | 3115(3) | 3417(2) | 32 |
| C(37) | 13811(3) | 3432(2) | 3425(1) | 25 |
| C(237) | 13750(40) | 3620(30) | 3465(17) | 25 |
| C(38) | 13112(2) | 3174(2) | 3119(1) | 27 |
| C(229) | 12140(20) | 3740(20) | 3079(11) | 27 |
| C(230) | 11632(18) | 3670(20) | 2730(8) | 41 |
| C(231) | 11981(18) | 3320(20) | 2340(8) | 55 |
| C(232) | 12891(18) | 2990(20) | 2330(8) | 53 |
| C(233) | 13534(15) | 3123(19) | 2686(7) | 37 |
| C(238) | 13130(20) | 3475(18) | 3057(9) | 27 |
| O(101) | 1931(11) | 630(13) | 2331(4) | 77 |
| O(103) | 7120(20) | 6244(13) | 1935(6) | 114 |
| O(104) | 8140(20) | 5750(20) | 1713(14) | 139 |

Table 3. Bond lengths [\AA] and angles [$^\circ$] for 6797.

| | | | |
|--------------|------------|--------------|------------|
| P(1)-O(2) | 1.6709(11) | C(19)-C(20) | 1.420(2) |
| P(1)-O(23) | 1.6739(12) | C(20)-C(21) | 1.364(3) |
| P(1)-N(24) | 1.6601(14) | C(20)-H(201) | 0.934 |
| O(2)-C(3) | 1.3950(19) | C(21)-C(22) | 1.411(2) |
| C(3)-C(4) | 1.407(2) | C(21)-H(211) | 0.943 |
| C(3)-C(12) | 1.373(2) | C(22)-O(23) | 1.3835(19) |
| C(4)-C(5) | 1.363(3) | N(24)-C(25) | 1.478(2) |
| C(4)-H(41) | 0.971 | N(24)-C(26) | 1.485(2) |
| C(5)-C(6) | 1.422(3) | C(25)-C(43) | 1.528(3) |
| C(5)-H(51) | 0.945 | C(25)-H(251) | 0.980 |
| C(6)-C(7) | 1.420(2) | C(25)-C(29) | 1.540(3) |
| C(6)-C(11) | 1.426(2) | C(25)-C(43) | 1.528(3) |
| C(7)-C(8) | 1.359(3) | C(25)-H(251) | 0.980 |
| C(7)-H(71) | 0.961 | C(25)-C(229) | 1.47(3) |
| C(8)-C(9) | 1.415(3) | C(26)-C(27) | 1.529(2) |
| C(8)-H(81) | 0.928 | C(26)-C(28) | 1.523(3) |
| C(9)-C(10) | 1.369(3) | C(26)-H(261) | 0.998 |
| C(9)-H(91) | 0.951 | C(27)-H(271) | 0.976 |
| C(10)-C(11) | 1.420(2) | C(27)-H(272) | 0.977 |
| C(10)-H(101) | 0.965 | C(27)-H(273) | 0.970 |
| C(11)-C(12) | 1.437(2) | C(28)-H(283) | 0.997 |
| C(12)-C(13) | 1.480(2) | C(28)-H(282) | 0.984 |
| C(13)-C(14) | 1.438(2) | C(28)-H(281) | 0.958 |
| C(13)-C(22) | 1.386(2) | C(31)-C(32) | 1.360(4) |
| C(14)-C(15) | 1.418(2) | C(31)-H(311) | 0.936 |
| C(14)-C(19) | 1.424(2) | C(31)-C(30) | 1.421(3) |
| C(15)-C(16) | 1.375(2) | C(32)-C(33) | 1.420(3) |
| C(15)-H(151) | 0.924 | C(32)-H(321) | 0.951 |
| C(16)-C(17) | 1.417(3) | C(33)-C(34) | 1.414(3) |
| C(16)-H(161) | 0.940 | C(33)-C(38) | 1.429(3) |
| C(17)-C(18) | 1.357(3) | C(34)-H(341) | 0.926 |
| C(17)-H(171) | 0.925 | C(34)-C(35) | 1.363(4) |
| C(18)-C(19) | 1.418(2) | C(43)-C(44) | 1.395(2) |
| C(18)-H(181) | 0.924 | C(43)-C(48) | 1.394(3) |

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|--------------|------------|--------------|----------|
| C(44)-C(45) | 1.395(3) | C(62)-C(63) | 1.486(2) |
| C(44)-H(441) | 0.945 | C(63)-C(64) | 1.440(2) |
| C(45)-C(46) | 1.379(3) | C(63)-C(72) | 1.378(2) |
| C(45)-C(49) | 1.509(3) | C(64)-C(65) | 1.422(2) |
| C(46)-C(47) | 1.397(3) | C(64)-C(69) | 1.425(2) |
| C(46)-H(461) | 0.925 | C(65)-C(66) | 1.375(3) |
| C(47)-C(48) | 1.399(3) | C(65)-H(651) | 0.938 |
| C(47)-C(50) | 1.507(3) | C(66)-C(67) | 1.403(3) |
| C(48)-H(481) | 0.941 | C(66)-H(661) | 0.945 |
| C(49)-H(493) | 0.943 | C(67)-C(68) | 1.361(3) |
| C(49)-H(492) | 0.960 | C(67)-H(671) | 0.949 |
| C(49)-H(491) | 0.944 | C(68)-C(69) | 1.428(3) |
| C(50)-H(501) | 0.976 | C(68)-H(681) | 0.936 |
| C(50)-H(502) | 0.963 | C(69)-C(70) | 1.416(3) |
| C(50)-H(503) | 0.972 | C(70)-C(71) | 1.362(3) |
| P(51)-O(52) | 1.6668(11) | C(70)-H(701) | 0.926 |
| P(51)-O(73) | 1.6693(13) | C(71)-C(72) | 1.413(2) |
| P(51)-N(74) | 1.6555(14) | C(71)-H(711) | 0.936 |
| O(52)-C(53) | 1.394(2) | C(72)-O(73) | 1.383(2) |
| C(53)-C(54) | 1.416(2) | N(74)-C(75) | 1.482(2) |
| C(53)-C(62) | 1.371(2) | N(74)-C(76) | 1.486(2) |
| C(54)-C(55) | 1.362(3) | C(75)-C(79) | 1.522(2) |
| C(54)-H(541) | 0.947 | C(75)-C(93) | 1.534(2) |
| C(55)-C(56) | 1.419(3) | C(75)-H(751) | 0.989 |
| C(55)-H(551) | 0.939 | C(76)-C(77) | 1.526(2) |
| C(56)-C(57) | 1.424(3) | C(76)-C(78) | 1.524(2) |
| C(56)-C(61) | 1.424(2) | C(76)-H(761) | 1.004 |
| C(57)-C(58) | 1.360(3) | C(77)-H(773) | 0.945 |
| C(57)-H(571) | 0.947 | C(77)-H(772) | 0.975 |
| C(58)-C(59) | 1.410(3) | C(77)-H(771) | 0.961 |
| C(58)-H(581) | 0.960 | C(78)-H(781) | 0.975 |
| C(59)-C(60) | 1.371(3) | C(78)-H(782) | 0.963 |
| C(59)-H(591) | 0.948 | C(78)-H(783) | 0.960 |
| C(60)-C(61) | 1.420(3) | C(79)-C(80) | 1.368(2) |
| C(60)-H(601) | 0.925 | C(79)-C(88) | 1.433(2) |
| C(61)-C(62) | 1.439(2) | C(80)-C(81) | 1.415(3) |

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|----------------|----------|------------------|------------|
| C(80)-H(801) | 0.944 | C(234)-C(235) | 1.28(4) |
| C(81)-C(82) | 1.363(3) | C(234)-H(2341) | 0.932 |
| C(81)-H(811) | 0.932 | C(234)-C(233) | 1.42(3) |
| C(82)-C(83) | 1.411(3) | C(30)-C(29) | 1.372(4) |
| C(82)-H(821) | 0.958 | C(35)-C(36) | 1.411(6) |
| C(83)-C(84) | 1.415(3) | C(235)-C(236) | 1.43(7) |
| C(83)-C(88) | 1.424(2) | C(235)-H(2351) | 0.932 |
| C(84)-C(85) | 1.361(3) | C(29)-C(38) | 1.423(3) |
| C(84)-H(841) | 0.948 | C(236)-C(237) | 1.32(6) |
| C(85)-C(86) | 1.407(3) | C(236)-H(2361) | 0.933 |
| C(85)-H(851) | 0.942 | C(36)-C(37) | 1.375(5) |
| C(86)-C(87) | 1.372(2) | C(37)-C(38) | 1.411(5) |
| C(86)-H(861) | 0.937 | C(237)-H(2371) | 0.934 |
| C(87)-C(88) | 1.417(2) | C(237)-C(238) | 1.54(6) |
| C(87)-H(871) | 0.959 | H(2321)-C(232) | 0.932 |
| C(93)-C(94) | 1.394(2) | H(2311)-C(231) | 0.932 |
| C(93)-C(98) | 1.389(2) | H(2301)-C(230) | 0.929 |
| C(94)-C(95) | 1.388(3) | C(229)-C(230) | 1.29(4) |
| C(94)-H(941) | 0.957 | C(229)-C(238) | 1.43(4) |
| C(95)-C(96) | 1.391(3) | C(230)-C(231) | 1.40(3) |
| C(95)-C(99) | 1.515(3) | C(231)-C(232) | 1.37(4) |
| C(96)-C(97) | 1.392(3) | C(232)-C(233) | 1.43(3) |
| C(96)-H(961) | 0.955 | C(233)-C(238) | 1.38(3) |
| C(97)-C(98) | 1.401(2) | O(101)-H(1012) | 0.924 |
| C(97)-C(100) | 1.505(3) | O(101)-H(1011) | 0.950 |
| C(98)-H(981) | 0.933 | O(103)-H(1031) | 0.950 |
| C(99)-H(993) | 0.961 | O(103)-H(1032) | 0.950 |
| C(99)-H(992) | 0.989 | O(104)-H(1041) | 0.950 |
| C(99)-H(991) | 0.978 | O(104)-H(1042) | 0.950 |
| C(100)-H(1003) | 0.973 | | |
| C(100)-H(1002) | 0.953 | O(2)-P(1)-O(23) | 97.44(6) |
| C(100)-H(1001) | 0.945 | O(2)-P(1)-N(24) | 97.95(6) |
| H(301)-C(30) | 0.939 | O(23)-P(1)-N(24) | 106.94(7) |
| H(351)-C(35) | 0.944 | P(1)-O(2)-C(3) | 112.90(9) |
| H(361)-C(36) | 0.940 | O(2)-C(3)-C(4) | 118.25(14) |
| H(371)-C(37) | 0.961 | O(2)-C(3)-C(12) | 118.63(14) |

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|--------------------|------------|--------------------|------------|
| C(4)-C(3)-C(12) | 123.12(15) | C(16)-C(15)-H(151) | 119.4 |
| C(3)-C(4)-C(5) | 119.17(16) | C(15)-C(16)-C(17) | 120.62(17) |
| C(3)-C(4)-H(41) | 119.5 | C(15)-C(16)-H(161) | 119.8 |
| C(5)-C(4)-H(41) | 121.3 | C(17)-C(16)-H(161) | 119.6 |
| C(4)-C(5)-C(6) | 120.85(15) | C(16)-C(17)-C(18) | 119.78(17) |
| C(4)-C(5)-H(51) | 119.7 | C(16)-C(17)-H(171) | 118.9 |
| C(6)-C(5)-H(51) | 119.5 | C(18)-C(17)-H(171) | 121.3 |
| C(5)-C(6)-C(7) | 121.18(16) | C(17)-C(18)-C(19) | 121.30(17) |
| C(5)-C(6)-C(11) | 119.60(15) | C(17)-C(18)-H(181) | 119.2 |
| C(7)-C(6)-C(11) | 119.22(17) | C(19)-C(18)-H(181) | 119.5 |
| C(6)-C(7)-C(8) | 121.21(18) | C(14)-C(19)-C(18) | 119.21(16) |
| C(6)-C(7)-H(71) | 118.5 | C(14)-C(19)-C(20) | 119.29(15) |
| C(8)-C(7)-H(71) | 120.3 | C(18)-C(19)-C(20) | 121.49(16) |
| C(7)-C(8)-C(9) | 119.93(17) | C(19)-C(20)-C(21) | 120.34(15) |
| C(7)-C(8)-H(81) | 121.3 | C(19)-C(20)-H(201) | 119.2 |
| C(9)-C(8)-H(81) | 118.8 | C(21)-C(20)-H(201) | 120.5 |
| C(8)-C(9)-C(10) | 120.31(18) | C(20)-C(21)-C(22) | 120.30(16) |
| C(8)-C(9)-H(91) | 118.5 | C(20)-C(21)-H(211) | 120.1 |
| C(10)-C(9)-H(91) | 121.2 | C(22)-C(21)-H(211) | 119.6 |
| C(9)-C(10)-C(11) | 121.38(17) | C(21)-C(22)-C(13) | 121.75(15) |
| C(9)-C(10)-H(101) | 120.5 | C(21)-C(22)-O(23) | 116.53(14) |
| C(11)-C(10)-H(101) | 118.2 | C(13)-C(22)-O(23) | 121.60(14) |
| C(6)-C(11)-C(10) | 117.88(15) | C(22)-O(23)-P(1) | 126.87(10) |
| C(6)-C(11)-C(12) | 118.86(15) | P(1)-N(24)-C(25) | 118.00(11) |
| C(10)-C(11)-C(12) | 123.24(15) | P(1)-N(24)-C(26) | 124.46(11) |
| C(11)-C(12)-C(3) | 118.37(15) | C(25)-N(24)-C(26) | 117.48(13) |
| C(11)-C(12)-C(13) | 122.50(14) | N(24)-C(25)-C(43) | 112.02(14) |
| C(3)-C(12)-C(13) | 119.04(14) | N(24)-C(25)-H(251) | 106.2 |
| C(12)-C(13)-C(14) | 122.32(14) | C(43)-C(25)-H(251) | 105.8 |
| C(12)-C(13)-C(22) | 119.90(14) | N(24)-C(25)-C(29) | 113.44(16) |
| C(14)-C(13)-C(22) | 117.78(14) | C(43)-C(25)-C(29) | 115.50(15) |
| C(13)-C(14)-C(15) | 121.83(14) | H(251)-C(25)-C(29) | 102.7 |
| C(13)-C(14)-C(19) | 119.68(15) | N(24)-C(25)-C(43) | 112.02(14) |
| C(15)-C(14)-C(19) | 118.41(15) | N(24)-C(25)-H(251) | 106.2 |
| C(14)-C(15)-C(16) | 120.64(16) | C(43)-C(25)-H(251) | 105.8 |
| C(14)-C(15)-H(151) | 119.9 | N(24)-C(25)-C(229) | 117.7(14) |

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|---------------------|------------|---------------------|------------|
| C(43)-C(25)-C(229) | 100.2(12) | C(43)-C(44)-H(441) | 120.2 |
| H(251)-C(25)-C(229) | 114.4 | C(45)-C(44)-H(441) | 119.2 |
| N(24)-C(26)-C(27) | 112.52(15) | C(44)-C(45)-C(46) | 118.95(17) |
| N(24)-C(26)-C(28) | 113.13(15) | C(44)-C(45)-C(49) | 120.6(2) |
| C(27)-C(26)-C(28) | 109.58(15) | C(46)-C(45)-C(49) | 120.5(2) |
| N(24)-C(26)-H(261) | 105.0 | C(45)-C(46)-C(47) | 122.30(19) |
| C(27)-C(26)-H(261) | 107.2 | C(45)-C(46)-H(461) | 119.4 |
| C(28)-C(26)-H(261) | 109.1 | C(47)-C(46)-H(461) | 118.3 |
| C(26)-C(27)-H(271) | 109.8 | C(46)-C(47)-C(48) | 117.58(19) |
| C(26)-C(27)-H(272) | 112.1 | C(46)-C(47)-C(50) | 121.26(19) |
| H(271)-C(27)-H(272) | 109.6 | C(48)-C(47)-C(50) | 121.14(18) |
| C(26)-C(27)-H(273) | 110.4 | C(47)-C(48)-C(43) | 121.41(17) |
| H(271)-C(27)-H(273) | 106.9 | C(47)-C(48)-H(481) | 119.6 |
| H(272)-C(27)-H(273) | 107.9 | C(43)-C(48)-H(481) | 118.9 |
| C(26)-C(28)-H(283) | 110.6 | C(45)-C(49)-H(493) | 108.7 |
| C(26)-C(28)-H(282) | 111.7 | C(45)-C(49)-H(492) | 109.8 |
| H(283)-C(28)-H(282) | 108.7 | H(493)-C(49)-H(492) | 111.4 |
| C(26)-C(28)-H(281) | 111.6 | C(45)-C(49)-H(491) | 108.9 |
| H(283)-C(28)-H(281) | 108.1 | H(493)-C(49)-H(491) | 109.3 |
| H(282)-C(28)-H(281) | 105.9 | H(492)-C(49)-H(491) | 108.8 |
| C(32)-C(31)-H(311) | 119.2 | C(47)-C(50)-H(501) | 111.7 |
| C(32)-C(31)-C(30) | 120.1(2) | C(47)-C(50)-H(502) | 110.4 |
| H(311)-C(31)-C(30) | 120.6 | H(501)-C(50)-H(502) | 107.8 |
| C(31)-C(32)-C(33) | 120.5(2) | C(47)-C(50)-H(503) | 109.2 |
| C(31)-C(32)-H(321) | 120.0 | H(501)-C(50)-H(503) | 110.3 |
| C(33)-C(32)-H(321) | 119.5 | H(502)-C(50)-H(503) | 107.5 |
| C(32)-C(33)-C(34) | 121.1(2) | O(52)-P(51)-O(73) | 97.18(6) |
| C(32)-C(33)-C(38) | 119.4(2) | O(52)-P(51)-N(74) | 99.55(6) |
| C(34)-C(33)-C(38) | 119.5(2) | O(73)-P(51)-N(74) | 106.59(7) |
| C(33)-C(34)-H(341) | 119.0 | P(51)-O(52)-C(53) | 112.29(10) |
| C(33)-C(34)-C(35) | 121.3(2) | O(52)-C(53)-C(54) | 118.13(15) |
| H(341)-C(34)-C(35) | 119.7 | O(52)-C(53)-C(62) | 119.23(14) |
| C(25)-C(43)-C(44) | 122.06(17) | C(54)-C(53)-C(62) | 122.63(16) |
| C(25)-C(43)-C(48) | 118.81(15) | C(53)-C(54)-C(55) | 119.48(17) |
| C(44)-C(43)-C(48) | 119.11(18) | C(53)-C(54)-H(541) | 118.5 |
| C(43)-C(44)-C(45) | 120.61(19) | C(55)-C(54)-H(541) | 121.9 |

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|--------------------|------------|--------------------|------------|
| C(54)-C(55)-C(56) | 120.69(17) | C(66)-C(67)-C(68) | 120.24(19) |
| C(54)-C(55)-H(551) | 120.6 | C(66)-C(67)-H(671) | 121.6 |
| C(56)-C(55)-H(551) | 118.7 | C(68)-C(67)-H(671) | 118.2 |
| C(55)-C(56)-C(57) | 121.13(18) | C(67)-C(68)-C(69) | 120.95(18) |
| C(55)-C(56)-C(61) | 119.64(17) | C(67)-C(68)-H(681) | 121.8 |
| C(57)-C(56)-C(61) | 119.23(19) | C(69)-C(68)-H(681) | 117.2 |
| C(56)-C(57)-C(58) | 121.1(2) | C(68)-C(69)-C(64) | 118.95(18) |
| C(56)-C(57)-H(571) | 119.0 | C(68)-C(69)-C(70) | 121.74(17) |
| C(58)-C(57)-H(571) | 119.9 | C(64)-C(69)-C(70) | 119.30(16) |
| C(57)-C(58)-C(59) | 119.8(2) | C(69)-C(70)-C(71) | 120.40(15) |
| C(57)-C(58)-H(581) | 119.6 | C(69)-C(70)-H(701) | 120.2 |
| C(59)-C(58)-H(581) | 120.5 | C(71)-C(70)-H(701) | 119.4 |
| C(58)-C(59)-C(60) | 120.5(2) | C(70)-C(71)-C(72) | 120.31(17) |
| C(58)-C(59)-H(591) | 119.4 | C(70)-C(71)-H(711) | 121.4 |
| C(60)-C(59)-H(591) | 120.1 | C(72)-C(71)-H(711) | 118.3 |
| C(59)-C(60)-C(61) | 121.32(18) | C(71)-C(72)-C(63) | 121.75(16) |
| C(59)-C(60)-H(601) | 119.8 | C(71)-C(72)-O(73) | 116.22(15) |
| C(61)-C(60)-H(601) | 118.9 | C(63)-C(72)-O(73) | 121.82(14) |
| C(56)-C(61)-C(60) | 117.73(16) | C(72)-O(73)-P(51) | 126.67(10) |
| C(56)-C(61)-C(62) | 119.02(16) | P(51)-N(74)-C(75) | 117.45(11) |
| C(60)-C(61)-C(62) | 123.24(16) | P(51)-N(74)-C(76) | 125.56(11) |
| C(61)-C(62)-C(53) | 118.40(14) | C(75)-N(74)-C(76) | 116.74(13) |
| C(61)-C(62)-C(63) | 122.78(15) | N(74)-C(75)-C(79) | 114.07(13) |
| C(53)-C(62)-C(63) | 118.74(14) | N(74)-C(75)-C(93) | 111.65(13) |
| C(62)-C(63)-C(64) | 122.26(14) | C(79)-C(75)-C(93) | 114.21(13) |
| C(62)-C(63)-C(72) | 119.80(15) | N(74)-C(75)-H(751) | 103.5 |
| C(64)-C(63)-C(72) | 117.92(14) | C(79)-C(75)-H(751) | 107.0 |
| C(63)-C(64)-C(65) | 122.17(15) | C(93)-C(75)-H(751) | 105.3 |
| C(63)-C(64)-C(69) | 119.47(16) | N(74)-C(76)-C(77) | 112.47(14) |
| C(65)-C(64)-C(69) | 118.32(16) | N(74)-C(76)-C(78) | 112.09(14) |
| C(64)-C(65)-C(66) | 120.77(18) | C(77)-C(76)-C(78) | 110.39(15) |
| C(64)-C(65)-H(651) | 118.7 | N(74)-C(76)-H(761) | 106.1 |
| C(66)-C(65)-H(651) | 120.5 | C(77)-C(76)-H(761) | 107.5 |
| C(65)-C(66)-C(67) | 120.7(2) | C(78)-C(76)-H(761) | 108.0 |
| C(65)-C(66)-H(661) | 118.9 | C(76)-C(77)-H(773) | 109.2 |
| C(67)-C(66)-H(661) | 120.3 | C(76)-C(77)-H(772) | 111.5 |

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| H(773)-C(77)-H(772) | 107.3 | C(88)-C(87)-H(871) | 120.4 |
| C(76)-C(77)-H(771) | 111.9 | C(79)-C(88)-C(83) | 119.07(16) |
| H(773)-C(77)-H(771) | 108.5 | C(79)-C(88)-C(87) | 122.79(15) |
| H(772)-C(77)-H(771) | 108.2 | C(83)-C(88)-C(87) | 118.14(16) |
| C(76)-C(78)-H(781) | 110.3 | C(75)-C(93)-C(94) | 117.69(14) |
| C(76)-C(78)-H(782) | 110.0 | C(75)-C(93)-C(98) | 122.76(14) |
| H(781)-C(78)-H(782) | 107.9 | C(94)-C(93)-C(98) | 119.53(15) |
| C(76)-C(78)-H(783) | 113.2 | C(93)-C(94)-C(95) | 121.09(17) |
| H(781)-C(78)-H(783) | 108.0 | C(93)-C(94)-H(941) | 119.4 |
| H(782)-C(78)-H(783) | 107.2 | C(95)-C(94)-H(941) | 119.5 |
| C(75)-C(79)-C(80) | 122.63(15) | C(94)-C(95)-C(96) | 118.62(17) |
| C(75)-C(79)-C(88) | 118.05(14) | C(94)-C(95)-C(99) | 120.35(19) |
| C(80)-C(79)-C(88) | 119.24(15) | C(96)-C(95)-C(99) | 121.03(18) |
| C(79)-C(80)-C(81) | 121.33(17) | C(95)-C(96)-C(97) | 121.51(16) |
| C(79)-C(80)-H(801) | 118.6 | C(95)-C(96)-H(961) | 120.9 |
| C(81)-C(80)-H(801) | 120.0 | C(97)-C(96)-H(961) | 117.6 |
| C(80)-C(81)-C(82) | 120.28(18) | C(96)-C(97)-C(98) | 118.87(16) |
| C(80)-C(81)-H(811) | 119.9 | C(96)-C(97)-C(100) | 120.29(17) |
| C(82)-C(81)-H(811) | 119.9 | C(98)-C(97)-C(100) | 120.85(17) |
| C(81)-C(82)-C(83) | 120.60(17) | C(97)-C(98)-C(93) | 120.34(16) |
| C(81)-C(82)-H(821) | 120.1 | C(97)-C(98)-H(981) | 121.4 |
| C(83)-C(82)-H(821) | 119.3 | C(93)-C(98)-H(981) | 118.2 |
| C(82)-C(83)-C(84) | 121.38(17) | C(95)-C(99)-H(993) | 110.8 |
| C(82)-C(83)-C(88) | 119.38(17) | C(95)-C(99)-H(992) | 106.0 |
| C(84)-C(83)-C(88) | 119.24(18) | H(993)-C(99)-H(992) | 107.7 |
| C(83)-C(84)-C(85) | 121.03(18) | C(95)-C(99)-H(991) | 111.4 |
| C(83)-C(84)-H(841) | 117.3 | H(993)-C(99)-H(991) | 109.7 |
| C(85)-C(84)-H(841) | 121.7 | H(992)-C(99)-H(991) | 111.2 |
| C(84)-C(85)-C(86) | 120.18(18) | C(97)-C(100)-H(1003) | 115.2 |
| C(84)-C(85)-H(851) | 119.7 | C(97)-C(100)-H(1002) | 111.3 |
| C(86)-C(85)-H(851) | 120.1 | H(1003)-C(100)-H(1002) | 108.2 |
| C(85)-C(86)-C(87) | 120.32(19) | C(97)-C(100)-H(1001) | 109.8 |
| C(85)-C(86)-H(861) | 119.5 | H(1003)-C(100)-H(1001) | 104.9 |
| C(87)-C(86)-H(861) | 120.1 | H(1002)-C(100)-H(1001) | 106.8 |
| C(86)-C(87)-C(88) | 121.05(18) | C(235)-C(234)-H(2341) | 118.0 |
| C(86)-C(87)-H(871) | 118.5 | C(235)-C(234)-C(233) | 124(2) |

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| H(2341)-C(234)-C(233) | 118.1 | C(33)-C(38)-C(29) | 118.9(2) |
| C(31)-C(30)-H(301) | 119.8 | C(33)-C(38)-C(37) | 117.3(2) |
| C(31)-C(30)-C(29) | 121.3(2) | C(29)-C(38)-C(37) | 123.8(2) |
| H(301)-C(30)-C(29) | 118.9 | C(25)-C(229)-C(230) | 126(3) |
| H(351)-C(35)-C(34) | 120.3 | C(25)-C(229)-C(238) | 116(3) |
| H(351)-C(35)-C(36) | 119.8 | C(230)-C(229)-C(238) | 118(3) |
| C(34)-C(35)-C(36) | 119.9(3) | H(2301)-C(230)-C(229) | 118.5 |
| C(234)-C(235)-C(236) | 113(3) | H(2301)-C(230)-C(231) | 118.4 |
| C(234)-C(235)-H(2351) | 123.4 | C(229)-C(230)-C(231) | 123(3) |
| C(236)-C(235)-H(2351) | 123.4 | C(230)-C(231)-H(2311) | 120.3 |
| C(25)-C(29)-C(30) | 121.3(2) | C(230)-C(231)-C(232) | 119(2) |
| C(25)-C(29)-C(38) | 119.1(2) | H(2311)-C(231)-C(232) | 120.6 |
| C(30)-C(29)-C(38) | 119.5(2) | H(2321)-C(232)-C(231) | 119.7 |
| C(235)-C(236)-C(237) | 134(5) | H(2321)-C(232)-C(233) | 119.6 |
| C(235)-C(236)-H(2361) | 112.7 | C(231)-C(232)-C(233) | 121(2) |
| C(237)-C(236)-H(2361) | 113.3 | C(232)-C(233)-C(234) | 124(2) |
| C(35)-C(36)-H(361) | 119.6 | C(232)-C(233)-C(238) | 115(2) |
| C(35)-C(36)-C(37) | 119.8(4) | C(234)-C(233)-C(238) | 120(2) |
| H(361)-C(36)-C(37) | 120.6 | C(237)-C(238)-C(229) | 118(3) |
| H(371)-C(37)-C(36) | 118.8 | C(237)-C(238)-C(233) | 119(3) |
| H(371)-C(37)-C(38) | 119.0 | C(229)-C(238)-C(233) | 123(3) |
| C(36)-C(37)-C(38) | 122.2(3) | H(1012)-O(101)-H(1011) | 99.2 |
| C(236)-C(237)-H(2371) | 125.7 | H(1031)-O(103)-H(1032) | 109.5 |
| C(236)-C(237)-C(238) | 109(4) | H(1041)-O(104)-H(1042) | 109.5 |
| H(2371)-C(237)-C(238) | 125.8 | | |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6797. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

| | U^{11} | U^{22} | U^{33} | U^{23} | U^{13} | U^{12} |
|-------|----------|----------|----------|----------|----------|----------|
| P(1) | 17(1) | 29(1) | 18(1) | 2(1) | 1(1) | 0(1) |
| O(2) | 18(1) | 27(1) | 19(1) | -1(1) | 0(1) | 2(1) |
| C(3) | 20(1) | 25(1) | 19(1) | -1(1) | 1(1) | 0(1) |
| C(4) | 23(1) | 25(1) | 31(1) | -2(1) | 0(1) | -4(1) |
| C(5) | 32(1) | 21(1) | 35(1) | -4(1) | 2(1) | 0(1) |
| C(6) | 28(1) | 26(1) | 25(1) | -3(1) | 1(1) | 4(1) |
| C(7) | 37(1) | 30(1) | 39(1) | -4(1) | -4(1) | 10(1) |
| C(8) | 31(1) | 39(1) | 50(1) | -6(1) | -8(1) | 15(1) |
| C(9) | 25(1) | 45(1) | 44(1) | -4(1) | -9(1) | 5(1) |
| C(10) | 24(1) | 32(1) | 31(1) | -1(1) | -4(1) | 2(1) |
| C(11) | 22(1) | 26(1) | 21(1) | -1(1) | 0(1) | 3(1) |
| C(12) | 21(1) | 23(1) | 19(1) | -1(1) | 2(1) | -1(1) |
| C(13) | 17(1) | 23(1) | 21(1) | -1(1) | -2(1) | 1(1) |
| C(14) | 17(1) | 24(1) | 24(1) | 1(1) | -3(1) | -1(1) |
| C(15) | 21(1) | 32(1) | 25(1) | -1(1) | 0(1) | -4(1) |
| C(16) | 26(1) | 44(1) | 27(1) | 1(1) | 4(1) | -4(1) |
| C(17) | 28(1) | 41(1) | 32(1) | 12(1) | -2(1) | -11(1) |
| C(18) | 27(1) | 26(1) | 37(1) | 7(1) | -6(1) | -4(1) |
| C(19) | 19(1) | 24(1) | 30(1) | 3(1) | -5(1) | -1(1) |
| C(20) | 25(1) | 23(1) | 36(1) | -3(1) | -6(1) | 2(1) |
| C(21) | 24(1) | 29(1) | 30(1) | -8(1) | -3(1) | 4(1) |
| C(22) | 18(1) | 27(1) | 21(1) | -1(1) | 0(1) | 0(1) |
| O(23) | 19(1) | 35(1) | 19(1) | -4(1) | 1(1) | -1(1) |
| N(24) | 18(1) | 32(1) | 23(1) | 2(1) | 3(1) | 4(1) |
| C(25) | 16(1) | 42(1) | 19(1) | 2(1) | 1(1) | 3(1) |
| C(26) | 22(1) | 30(1) | 31(1) | 4(1) | 2(1) | 3(1) |
| C(27) | 38(1) | 36(1) | 27(1) | 6(1) | 4(1) | 5(1) |
| C(28) | 41(1) | 34(1) | 49(1) | -5(1) | -1(1) | 0(1) |
| C(31) | 31(1) | 102(2) | 31(1) | -25(1) | -9(1) | 10(1) |
| C(32) | 33(1) | 93(2) | 32(1) | -29(1) | 0(1) | 10(1) |
| C(33) | 23(1) | 61(2) | 28(1) | -9(1) | 3(1) | 4(1) |
| C(34) | 30(1) | 66(2) | 38(1) | -16(1) | 4(1) | 14(1) |

| | | | | | | |
|-------|-------|-------|-------|--------|--------|--------|
| C(43) | 14(1) | 44(1) | 26(1) | 7(1) | -1(1) | 1(1) |
| C(44) | 21(1) | 53(1) | 29(1) | 10(1) | 5(1) | 4(1) |
| C(45) | 20(1) | 56(1) | 40(1) | 21(1) | 4(1) | 2(1) |
| C(46) | 26(1) | 41(1) | 49(1) | 16(1) | -6(1) | -4(1) |
| C(47) | 35(1) | 40(1) | 34(1) | 6(1) | -8(1) | -5(1) |
| C(48) | 30(1) | 42(1) | 23(1) | 8(1) | -3(1) | -4(1) |
| C(49) | 47(1) | 62(1) | 55(1) | 25(1) | 19(1) | -1(1) |
| C(50) | 77(2) | 39(1) | 41(1) | 0(1) | -6(1) | -8(1) |
| P(51) | 20(1) | 20(1) | 28(1) | -4(1) | -2(1) | 1(1) |
| O(52) | 18(1) | 25(1) | 24(1) | 1(1) | 0(1) | 0(1) |
| C(53) | 23(1) | 33(1) | 22(1) | -1(1) | 0(1) | 1(1) |
| C(54) | 28(1) | 63(1) | 24(1) | -5(1) | 6(1) | -4(1) |
| C(55) | 40(1) | 86(2) | 21(1) | -11(1) | 4(1) | -7(1) |
| C(56) | 33(1) | 65(1) | 26(1) | -8(1) | -2(1) | -6(1) |
| C(57) | 45(1) | 90(2) | 31(1) | -12(1) | -7(1) | -13(1) |
| C(58) | 39(1) | 91(2) | 41(1) | -11(1) | -14(1) | -16(1) |
| C(59) | 29(1) | 66(1) | 43(1) | -11(1) | -1(1) | -13(1) |
| C(60) | 28(1) | 47(1) | 30(1) | -7(1) | 2(1) | -7(1) |
| C(61) | 25(1) | 39(1) | 26(1) | -5(1) | -1(1) | -5(1) |
| C(62) | 24(1) | 26(1) | 20(1) | -2(1) | 0(1) | -2(1) |
| C(63) | 20(1) | 24(1) | 21(1) | -1(1) | 1(1) | -5(1) |
| C(64) | 20(1) | 28(1) | 25(1) | -4(1) | 3(1) | -6(1) |
| C(65) | 22(1) | 32(1) | 35(1) | -3(1) | 3(1) | -1(1) |
| C(66) | 25(1) | 35(1) | 57(1) | -6(1) | 2(1) | 1(1) |
| C(67) | 29(1) | 44(1) | 60(1) | -24(1) | 11(1) | -3(1) |
| C(68) | 31(1) | 53(1) | 37(1) | -21(1) | 13(1) | -13(1) |
| C(69) | 24(1) | 40(1) | 25(1) | -10(1) | 6(1) | -12(1) |
| C(70) | 35(1) | 48(1) | 19(1) | -3(1) | 3(1) | -18(1) |
| C(71) | 29(1) | 38(1) | 24(1) | 8(1) | -3(1) | -10(1) |
| C(72) | 23(1) | 24(1) | 25(1) | 1(1) | 2(1) | -6(1) |
| O(73) | 24(1) | 22(1) | 36(1) | 5(1) | 0(1) | -1(1) |
| N(74) | 19(1) | 25(1) | 27(1) | -4(1) | -3(1) | 3(1) |
| C(75) | 18(1) | 24(1) | 25(1) | -1(1) | -1(1) | 0(1) |
| C(76) | 24(1) | 29(1) | 29(1) | -8(1) | 0(1) | 4(1) |
| C(77) | 36(1) | 26(1) | 40(1) | -7(1) | -3(1) | 3(1) |
| C(78) | 41(1) | 44(1) | 29(1) | -6(1) | 4(1) | 1(1) |
| C(79) | 22(1) | 25(1) | 23(1) | -1(1) | -1(1) | 3(1) |
| C(80) | 24(1) | 30(1) | 34(1) | 3(1) | -2(1) | -1(1) |

| | | | | | | |
|--------|---------|---------|---------|---------|---------|---------|
| C(81) | 40(1) | 28(1) | 38(1) | 8(1) | 2(1) | -1(1) |
| C(82) | 45(1) | 31(1) | 30(1) | 4(1) | -4(1) | 9(1) |
| C(83) | 31(1) | 32(1) | 24(1) | -5(1) | -2(1) | 8(1) |
| C(84) | 37(1) | 44(1) | 31(1) | -8(1) | -10(1) | 14(1) |
| C(85) | 23(1) | 54(1) | 42(1) | -17(1) | -10(1) | 7(1) |
| C(86) | 22(1) | 46(1) | 39(1) | -13(1) | -1(1) | -3(1) |
| C(87) | 23(1) | 36(1) | 29(1) | -5(1) | 0(1) | -1(1) |
| C(88) | 21(1) | 29(1) | 22(1) | -5(1) | 1(1) | 3(1) |
| C(93) | 20(1) | 26(1) | 24(1) | -3(1) | -2(1) | -2(1) |
| C(94) | 45(1) | 26(1) | 26(1) | -3(1) | -2(1) | 0(1) |
| C(95) | 55(1) | 30(1) | 26(1) | -2(1) | -2(1) | -5(1) |
| C(96) | 36(1) | 41(1) | 24(1) | -8(1) | -1(1) | -5(1) |
| C(97) | 18(1) | 35(1) | 30(1) | -8(1) | -2(1) | 1(1) |
| C(98) | 20(1) | 26(1) | 28(1) | -1(1) | -2(1) | 2(1) |
| C(99) | 122(3) | 39(1) | 26(1) | 2(1) | 2(1) | 5(1) |
| C(100) | 38(1) | 47(1) | 38(1) | -13(1) | -3(1) | 15(1) |
| C(234) | 30(1) | 66(2) | 38(1) | -16(1) | 4(1) | 14(1) |
| C(30) | 22(1) | 72(2) | 28(1) | -8(1) | -1(1) | 9(1) |
| C(35) | 23(1) | 68(2) | 39(1) | -2(1) | 3(1) | 16(1) |
| C(235) | 23(1) | 68(2) | 39(1) | -2(1) | 3(1) | 16(1) |
| C(29) | 20(1) | 41(2) | 21(1) | 2(1) | 2(1) | 6(1) |
| C(236) | 18(2) | 45(2) | 33(1) | 3(1) | -4(1) | 4(1) |
| C(36) | 18(2) | 45(2) | 33(1) | 3(1) | -4(1) | 4(1) |
| C(37) | 21(1) | 30(2) | 23(1) | 0(1) | 1(1) | 3(1) |
| C(237) | 21(1) | 30(2) | 23(1) | 0(1) | 1(1) | 3(1) |
| C(38) | 20(1) | 41(1) | 20(1) | 3(1) | 3(1) | 2(1) |
| C(229) | 20(1) | 41(2) | 21(1) | 2(1) | 2(1) | 6(1) |
| C(230) | 22(1) | 72(2) | 28(1) | -8(1) | -1(1) | 9(1) |
| C(231) | 31(1) | 102(2) | 31(1) | -25(1) | -9(1) | 10(1) |
| C(232) | 33(1) | 93(2) | 32(1) | -29(1) | 0(1) | 10(1) |
| C(233) | 23(1) | 61(2) | 28(1) | -9(1) | 3(1) | 4(1) |
| C(238) | 20(1) | 41(1) | 20(1) | 3(1) | 3(1) | 2(1) |
| O(101) | 58(9) | 144(16) | 29(5) | -14(8) | 0(5) | -52(10) |
| O(103) | 200(30) | 74(12) | 73(12) | 15(9) | -94(15) | -51(15) |
| O(104) | 62(16) | 100(20) | 250(50) | 120(30) | -40(20) | -46(16) |

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 6797.

| | x | y | z | U(eq) |
|--------|-------|------|------|-------|
| H(41) | 9432 | 6603 | 3906 | 32 |
| H(51) | 8115 | 7500 | 3778 | 36 |
| H(71) | 6398 | 7701 | 3624 | 42 |
| H(81) | 4905 | 7104 | 3472 | 49 |
| H(91) | 4712 | 5628 | 3380 | 44 |
| H(101) | 6014 | 4688 | 3489 | 35 |
| H(151) | 6647 | 4579 | 4366 | 31 |
| H(161) | 5632 | 3753 | 4783 | 38 |
| H(171) | 5421 | 2292 | 4624 | 41 |
| H(181) | 6289 | 1651 | 4079 | 36 |
| H(201) | 7486 | 1743 | 3483 | 33 |
| H(211) | 8633 | 2530 | 3112 | 34 |
| H(251) | 12149 | 3796 | 3755 | 30 |
| H(261) | 9792 | 3287 | 3947 | 33 |
| H(271) | 10665 | 2866 | 4546 | 50 |
| H(272) | 11666 | 3102 | 4323 | 49 |
| H(273) | 10939 | 3832 | 4461 | 50 |
| H(283) | 10420 | 1856 | 3888 | 62 |
| H(282) | 11348 | 2220 | 3635 | 61 |
| H(281) | 10349 | 2269 | 3416 | 62 |
| H(301) | 10911 | 3453 | 2792 | 50 |
| H(311) | 11410 | 2489 | 2237 | 66 |
| H(321) | 12921 | 1910 | 2248 | 63 |
| H(341) | 14522 | 1842 | 2583 | 54 |
| H(351) | 15620 | 2268 | 3099 | 51 |
| H(361) | 15190 | 3310 | 3619 | 37 |
| H(371) | 13640 | 3845 | 3646 | 29 |
| H(441) | 12575 | 5014 | 2854 | 41 |
| H(461) | 12874 | 7275 | 3478 | 46 |
| H(481) | 11672 | 5268 | 4099 | 38 |

| | | | | |
|--------|-------|-------|------|----|
| H(493) | 13402 | 7182 | 2760 | 81 |
| H(492) | 13767 | 6270 | 2607 | 82 |
| H(491) | 12761 | 6601 | 2475 | 82 |
| H(501) | 11380 | 6969 | 4318 | 79 |
| H(502) | 12397 | 6726 | 4497 | 78 |
| H(503) | 12303 | 7522 | 4187 | 78 |
| H(541) | 6997 | -162 | 2912 | 46 |
| H(551) | 5701 | -531 | 2464 | 60 |
| H(571) | 3974 | -773 | 2366 | 66 |
| H(581) | 2458 | -948 | 2652 | 68 |
| H(591) | 2231 | -854 | 3415 | 55 |
| H(601) | 3514 | -570 | 3867 | 43 |
| H(651) | 4112 | 1131 | 3780 | 36 |
| H(661) | 3025 | 2063 | 4098 | 46 |
| H(671) | 2784 | 2039 | 4867 | 54 |
| H(681) | 3684 | 1114 | 5290 | 47 |
| H(701) | 4918 | -24 | 5363 | 41 |
| H(711) | 6122 | -837 | 5053 | 36 |
| H(751) | 9619 | 135 | 4347 | 25 |
| H(761) | 7297 | 608 | 4565 | 33 |
| H(773) | 8210 | 1811 | 4652 | 51 |
| H(772) | 9181 | 1339 | 4602 | 51 |
| H(771) | 8512 | 1477 | 4196 | 50 |
| H(781) | 7937 | 708 | 5276 | 56 |
| H(782) | 8840 | 174 | 5136 | 55 |
| H(783) | 7852 | -276 | 5163 | 56 |
| H(801) | 8389 | -1710 | 4668 | 35 |
| H(811) | 8933 | -2703 | 5195 | 42 |
| H(821) | 10481 | -2639 | 5458 | 43 |
| H(841) | 12079 | -2018 | 5419 | 45 |
| H(851) | 13147 | -1003 | 5140 | 48 |
| H(861) | 12672 | -99 | 4566 | 44 |
| H(871) | 11122 | -110 | 4311 | 33 |
| H(941) | 9240 | 645 | 3592 | 39 |
| H(961) | 10392 | -846 | 2635 | 40 |
| H(981) | 10013 | -1811 | 3849 | 30 |

| | | | | |
|---------|-------|-------|------|-----|
| H(993) | 9492 | 574 | 2466 | 93 |
| H(992) | 10349 | 1016 | 2715 | 94 |
| H(991) | 9249 | 1206 | 2858 | 94 |
| H(1003) | 10773 | -2741 | 3279 | 62 |
| H(1002) | 11190 | -2244 | 2878 | 63 |
| H(1001) | 10169 | -2592 | 2872 | 64 |
| H(2321) | 13087 | 2657 | 2091 | 63 |
| H(2311) | 11600 | 3316 | 2090 | 66 |
| H(2341) | 14763 | 2629 | 2430 | 53 |
| H(2301) | 11003 | 3867 | 2738 | 49 |
| H(2351) | 15682 | 2683 | 3027 | 52 |
| H(2361) | 14979 | 3247 | 3647 | 38 |
| H(2371) | 13561 | 3911 | 3718 | 30 |
| H(1012) | 1556 | 1122 | 2319 | 94 |
| H(1011) | 2504 | 878 | 2442 | 94 |
| H(1041) | 8037 | 6351 | 1747 | 130 |
| H(1042) | 7641 | 5438 | 1855 | 130 |
| H(1031) | 7684 | 6575 | 1900 | 110 |
| H(1032) | 7279 | 5664 | 2004 | 110 |

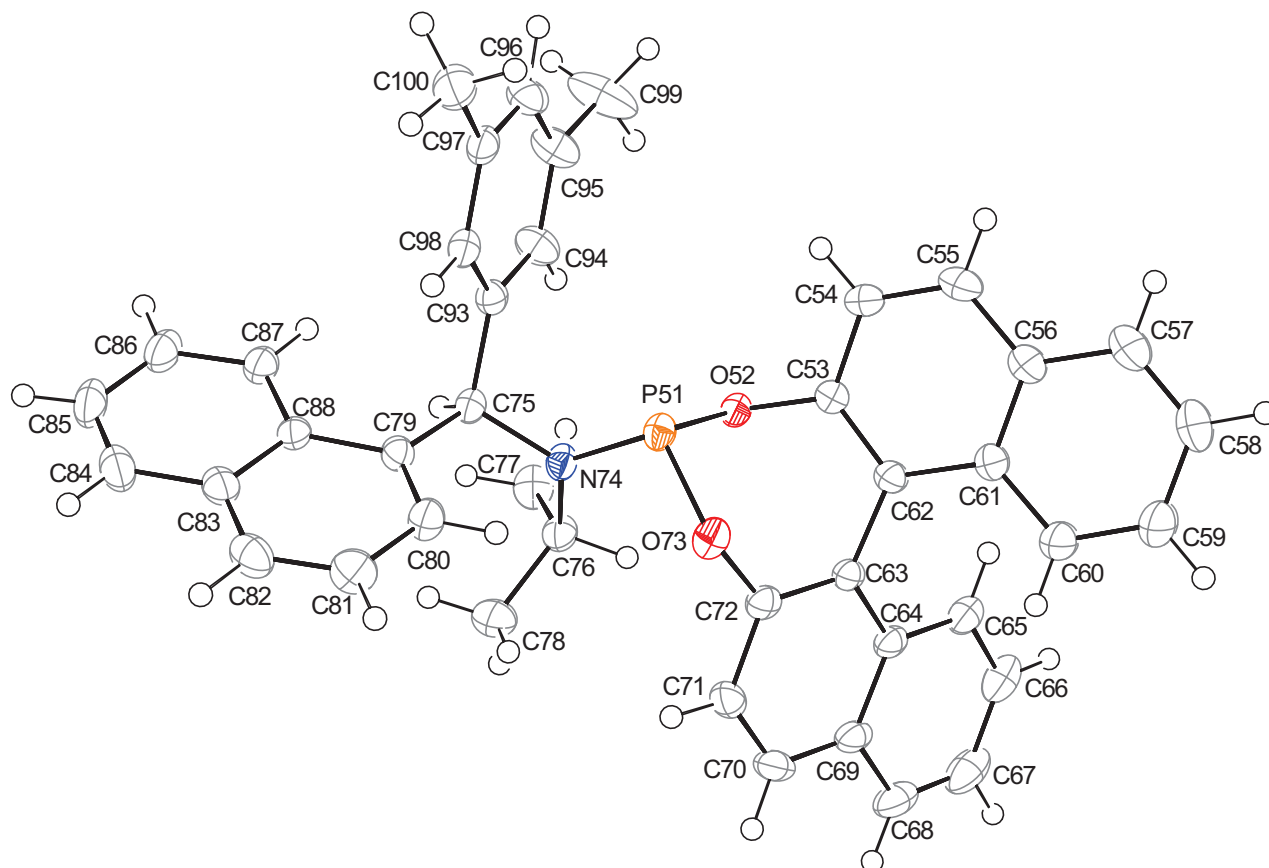
Table 6. Hydrogen bonds for 6797 [\AA and $^\circ$].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | $\angle(\text{DHA})$ |
|---------------------------|--------|----------|----------|----------------------|
| C(44)-H(441)...C(230) | 0.95 | 2.49 | 3.094(8) | 122 |
| C(70)-H(701)...O(2)#1 | 0.93 | 2.43 | 3.347(8) | 172 |
| C(99)-H(992)...O(101)#2 | 0.99 | 2.57 | 3.376(8) | 138 |
| C(232)-H(2321)...C(7)#3 | 0.93 | 2.45 | 3.366(8) | 168 |
| O(101)-H(1012)...C(31)#4 | 0.92 | 2.44 | 3.162(8) | 135 |
| O(101)-H(1011)...C(32)#4 | 0.95 | 2.25 | 2.869(8) | 122 |
| O(101)-H(1011)...O(103)#5 | 0.95 | 2.06 | 2.779(8) | 131 |
| O(104)-H(1042)...C(58)#6 | 0.95 | 2.34 | 3.205(8) | 151 |
| O(104)-H(1042)...C(59)#6 | 0.95 | 2.05 | 2.728(8) | 127 |
| O(103)-H(1032)...C(58)#6 | 0.95 | 2.38 | 3.279(8) | 157 |
| O(103)-H(1032)...C(59)#6 | 0.95 | 2.41 | 3.199(8) | 140 |

Symmetry transformations used to generate equivalent atoms:

#1 $x-1/2, -y+1/2, -z+1$ #2 $x+1, y, z$ #3 $-x+2, y-1/2, -z+1/2$

#4 $x-1, y, z$ #5 $-x+1, y-1/2, -z+1/2$ #6 $-x+1, y+1/2, -z+1/2$



This structure is a $Z'=2$ and therefore contain two unique molecules in the asymmetric unit. These two molecules are offset by 50 in the numbering scheme – only one molecule is drawn here for clarity.