

**Table S 1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) of  $\beta'$ -BiSeO<sub>3</sub>Cl**

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Bi1	0.83058 (11)	0.94300 (3)	0.73001 (15)	0.0177 (4)
Bi2	1.07566 (13)	0.94440 (3)	0.46808 (18)	0.0264 (5)
Bi3	0.70037 (11)	0.97961 (3)	0.20999 (16)	0.0220 (4)
Bi4	1.06773 (11)	0.64526 (3)	-0.03419 (15)	0.0228 (4)
Bi5	1.33606 (11)	0.64057 (2)	0.24423 (15)	0.0212 (4)
Bi6	0.20161 (11)	0.97967 (3)	0.98544 (15)	0.0225 (4)
Bi7	1.07824 (11)	0.93894 (3)	0.97991 (15)	0.0193 (4)
Bi8	1.46187 (12)	0.69444 (2)	0.24901 (16)	0.0203 (4)
Bi9	0.81348 (12)	0.94041 (2)	0.97290 (16)	0.0195 (4)
Bi10	1.32491 (11)	0.72959 (3)	0.23065 (16)	0.0230 (4)
Bi11	0.56859 (11)	0.94315 (3)	0.70624 (16)	0.0226 (5)
Bi12	0.60026 (12)	0.72966 (3)	0.00583 (16)	0.0227 (4)
Bi13	1.71596 (11)	0.69307 (3)	0.49162 (16)	0.0189 (4)
Bi14	0.57719 (11)	0.93881 (3)	0.96639 (15)	0.0182 (4)
Bi15	0.46336 (12)	0.69460 (2)	-0.25002 (17)	0.0205 (4)
Bi16	0.71410 (11)	0.89270 (2)	0.96130 (15)	0.0214 (4)
Bi17	0.19496 (12)	0.89061 (2)	0.96828 (16)	0.0227 (4)
Bi18	0.93629 (11)	0.98330 (2)	0.21303 (15)	0.0208 (4)
Bi19	0.57328 (14)	0.94379 (3)	0.47180 (18)	0.0284 (5)
Bi20	0.33122 (11)	0.94270 (3)	0.72515 (15)	0.0175 (4)
Bi21	0.59311 (11)	0.64301 (3)	0.00160 (16)	0.0228 (4)
Bi22	0.47572 (12)	0.69188 (2)	-0.48591 (16)	0.0200 (4)
Bi23	1.44964 (12)	0.69202 (2)	-0.01131 (16)	0.0202 (4)
Bi24	0.94820 (12)	0.69029 (2)	0.24077 (16)	0.0205 (4)
Bi25	1.43687 (11)	0.98320 (2)	0.45218 (15)	0.0216 (4)
Bi26	0.56673 (11)	0.94148 (2)	0.22464 (16)	0.0194 (4)
Bi27	1.06752 (11)	0.94354 (2)	0.22051 (16)	0.0209 (4)
Bi28	0.31955 (12)	0.94413 (3)	0.96752 (17)	0.0217 (4)
Bi29	0.06782 (11)	0.94169 (3)	0.70155 (16)	0.0192 (4)
Bi30	1.20987 (12)	0.69290 (3)	0.48564 (16)	0.0198 (5)
Bi31	0.86148 (11)	0.64257 (2)	0.25664 (15)	0.0216 (4)
Bi32	0.81983 (12)	0.94446 (3)	0.46690 (17)	0.0223 (4)
Bi33	0.59420 (12)	0.65299 (2)	-0.23989 (16)	0.0236 (4)
Bi34	1.21683 (11)	0.89518 (3)	0.25882 (16)	0.0233 (4)
Bi35	0.71694 (13)	0.69409 (3)	-0.24904 (18)	0.0272 (5)
Bi36	1.31605 (12)	0.94072 (3)	0.44967 (17)	0.0220 (4)
Bi37	0.83292 (11)	0.73328 (2)	0.00286 (15)	0.0213 (4)
Bi38	0.97632 (12)	0.69085 (2)	-0.23281 (16)	0.0215 (4)
Bi39	0.95534 (13)	0.69348 (2)	-0.00543 (16)	0.0220 (4)
Bi40	1.33195 (11)	0.65284 (2)	0.00054 (15)	0.0230 (4)
Bi41	1.97117 (13)	0.69324 (3)	0.50905 (17)	0.0234 (5)
Bi42	0.43823 (11)	0.90224 (2)	1.21751 (15)	0.0244 (4)
Bi43	0.94066 (11)	0.90340 (2)	0.44939 (15)	0.0210 (4)
Bi44	1.71996 (11)	0.68922 (3)	0.24888 (16)	0.0206 (4)
Bi45	0.09225 (11)	0.73326 (2)	-0.23850 (15)	0.0208 (4)
Bi46	0.69651 (11)	0.89252 (2)	0.21257 (15)	0.0226 (4)
Bi47	0.20934 (13)	0.69421 (3)	-0.25626 (18)	0.0279 (5)
Bi48	1.20802 (11)	0.68897 (3)	0.23673 (15)	0.0208 (5)
Se1	0.6006 (3)	0.71982 (6)	-0.2450 (4)	0.0175 (9)
Se2	1.4514 (3)	0.96971 (6)	0.2349 (4)	0.0178 (10)
Se3	0.3584 (3)	0.72290 (6)	-0.2470 (4)	0.0178 (10)
Se4	0.3243 (3)	0.71976 (6)	-0.0211 (4)	0.0159 (9)
Se5	0.6831 (3)	0.97129 (6)	0.7010 (4)	0.0178 (10)
Se6	1.5675 (3)	0.72283 (6)	0.4630 (4)	0.0162 (10)
Se7	1.4418 (3)	0.91766 (6)	0.4442 (4)	0.0152 (9)

Se8	1.1859 (3)	0.97145 (6)	0.4595 (4)	0.0162 (10)
Se9	0.6850 (3)	0.91496 (6)	0.4568 (4)	0.0179 (10)
Se10	1.5892 (3)	0.66495 (6)	0.5095 (4)	0.0162 (9)
Se11	0.1035 (3)	0.71812 (6)	-0.0159 (3)	0.0164 (9)
Se12	0.8577 (3)	0.66381 (6)	-0.2466 (4)	0.0154 (9)
Se13	0.1849 (3)	0.91498 (6)	0.7046 (4)	0.0160 (9)
Se14	0.7102 (3)	0.91368 (6)	0.7519 (4)	0.0193 (10)
Se15	0.0905 (3)	0.72137 (6)	-0.4878 (3)	0.0145 (9)
Se16	0.2123 (3)	0.97271 (6)	0.7549 (4)	0.0161 (10)
Se17	1.0629 (3)	0.72135 (6)	0.2128 (4)	0.0155 (9)
Se18	1.2106 (3)	0.91382 (6)	0.4604 (4)	0.0158 (9)
Se19	0.9402 (3)	0.91799 (6)	0.2301 (4)	0.0188 (9)
Se20	0.9522 (3)	0.96977 (6)	0.4615 (4)	0.0194 (10)
Se21	1.0679 (3)	0.66369 (6)	0.4640 (4)	0.0182 (10)
Se22	1.3324 (3)	0.72079 (6)	0.4516 (4)	0.0182 (10)
Se23	0.7109 (3)	0.97280 (6)	0.4615 (4)	0.0160 (10)
Se24	0.4860 (2)	0.97070 (6)	1.0009 (3)	0.0128 (9)
Se25	1.2252 (3)	0.96822 (6)	0.2314 (3)	0.0164 (9)
Se26	0.8337 (3)	0.72145 (6)	-0.2452 (4)	0.0138 (9)
Se27	0.3371 (3)	0.66498 (6)	-0.2430 (4)	0.0161 (10)
Se28	0.9573 (3)	0.97157 (6)	1.0029 (3)	0.0169 (10)
Se29	1.5631 (3)	0.66412 (6)	0.2150 (4)	0.0156 (9)
Se30	1.0847 (3)	0.66319 (6)	0.2089 (4)	0.0154 (9)
Se31	0.1068 (3)	0.66777 (5)	-0.2272 (4)	0.0166 (9)
Se32	0.4823 (3)	0.91309 (6)	0.7490 (4)	0.0169 (10)
Se33	0.8188 (3)	0.66766 (6)	-0.0164 (4)	0.0224 (11)
Se34	1.8634 (3)	0.72154 (6)	0.5122 (3)	0.0150 (9)
Se35	0.9542 (3)	0.91420 (6)	0.7006 (4)	0.0163 (9)
Se36	0.8230 (3)	0.71815 (6)	0.2031 (4)	0.0178 (10)
Se37	1.5939 (3)	0.72089 (6)	0.2138 (4)	0.0184 (10)
Se38	0.3624 (3)	0.66400 (6)	-0.4850 (4)	0.0152 (9)
Se39	0.4572 (3)	0.97135 (6)	0.7028 (4)	0.0190 (10)
Se40	0.7812 (2)	0.93444 (5)	0.2323 (3)	0.0150 (8)
Se41	1.8414 (3)	0.66332 (6)	0.4651 (4)	0.0172 (9)
Se42	0.7250 (3)	0.96818 (6)	0.0116 (4)	0.0175 (10)
Se43	0.9863 (3)	0.97088 (6)	0.7640 (3)	0.0150 (9)
Se44	0.4531 (3)	0.91378 (6)	0.9988 (4)	0.0182 (10)
Se45	0.2812 (3)	0.93386 (6)	1.1231 (4)	0.0199 (9)
Se46	0.6584 (3)	0.68454 (5)	-0.0166 (3)	0.0179 (9)
Se47	0.9832 (3)	0.91322 (6)	1.0068 (4)	0.0171 (10)
Se48	1.2675 (3)	0.68405 (6)	0.0926 (3)	0.0181 (9)
Cl1	1.2203 (7)	0.63687 (15)	-0.0152 (9)	0.022 (2)*
Cl2	1.2218 (8)	0.74843 (17)	0.2307 (11)	0.035 (3)*
Cl3	0.3422 (7)	0.88815 (15)	0.9989 (10)	0.022 (3)*
Cl4	0.9444 (8)	0.75008 (16)	0.2008 (11)	0.035 (3)*
Cl5	0.8350 (8)	0.88790 (16)	0.9798 (11)	0.028 (3)*
Cl6	0.2023 (8)	0.75092 (17)	-0.0340 (11)	0.034 (3)*
Cl7	0.0885 (8)	0.88932 (17)	0.7398 (11)	0.033 (3)*
Cl8	0.9708 (8)	0.63797 (16)	-0.2603 (10)	0.027 (3)*
Cl9	0.5978 (7)	0.88771 (13)	0.7417 (9)	0.019 (2)*
Cl10	-0.0219 (8)	0.74981 (17)	-0.2656 (11)	0.034 (3)*
Cl11	0.7055 (9)	0.74831 (18)	0.2136 (12)	0.039 (3)*
Cl12	0.7230 (8)	0.75087 (16)	-0.0132 (10)	0.031 (3)*
Cl13	0.4782 (7)	0.63944 (14)	-0.2578 (9)	0.020 (2)*
Cl14	1.4385 (8)	0.74860 (16)	0.4523 (11)	0.035 (3)*
Cl15	0.7021 (7)	0.63785 (16)	-0.0263 (10)	0.026 (3)*
Cl16	0.9658 (7)	0.63849 (15)	-0.0243 (10)	0.027 (2)*
Cl17	0.7048 (7)	0.85959 (16)	0.2259 (10)	0.026 (3)*
Cl18	0.4714 (8)	0.63940 (17)	-0.0122 (11)	0.032 (3)*
Cl19	0.3378 (6)	0.88694 (13)	1.2263 (8)	0.016 (2)*

CI20	0.9616 (9)	0.63774 (18)	0.2365 (12)	0.038 (3)*
CI21	0.0855 (7)	0.88734 (15)	0.9730 (10)	0.024 (2)*
CI22	0.4835 (8)	0.74876 (16)	-0.0040 (10)	0.032 (3)*
CI23	0.2040 (8)	0.85810 (17)	0.9732 (11)	0.030 (3)*
CI24	1.3371 (8)	0.60863 (17)	0.2333 (11)	0.029 (3)*
CI25	0.8356 (7)	0.61035 (16)	0.2289 (10)	0.026 (3)*
CI26	0.7153 (8)	0.85961 (19)	0.9856 (12)	0.038 (3)*
CI27	0.5891 (7)	0.88808 (16)	-0.0097 (10)	0.025 (3)*
CI28	1.4476 (7)	0.63901 (15)	0.2133 (9)	0.022 (2)*
CI29	0.7059 (8)	0.63807 (18)	0.2208 (11)	0.035 (3)*
CI30	0.5973 (8)	0.99811 (17)	0.0039 (11)	0.034 (3)*
CI31	0.5946 (8)	0.49836 (15)	0.7640 (10)	0.030 (3)*
CI32	1.4547 (7)	0.63925 (15)	0.4691 (10)	0.027 (2)*
CI33	1.2171 (7)	0.63797 (15)	0.2297 (10)	0.025 (2)*
CI34	1.2091 (7)	0.86071 (16)	0.2284 (10)	0.025 (3)*
CI35	1.3300 (7)	0.88723 (14)	0.4703 (10)	0.023 (2)*
CI36	0.5847 (7)	0.61036 (15)	-0.0220 (9)	0.022 (2)*
CI37	0.5921 (8)	0.99879 (17)	0.2158 (11)	0.039 (3)*
CI38	0.8420 (6)	0.88698 (14)	0.2402 (9)	0.018 (2)*
CI39	0.8435 (9)	1.00126 (19)	0.2294 (12)	0.040 (3)*
CI40	0.9596 (8)	0.63859 (16)	0.4735 (10)	0.029 (3)*
CI41	1.3414 (9)	1.00095 (19)	0.2497 (12)	0.041 (3)*
CI42	0.8491 (7)	1.00016 (15)	0.0147 (10)	0.030 (3)*
CI43	0.8391 (7)	0.88829 (14)	0.4706 (9)	0.023 (2)*
CI44	0.5927 (7)	0.89013 (14)	0.2269 (9)	0.023 (2)*
CI45	1.0885 (6)	0.61103 (14)	-0.0217 (9)	0.018 (2)*
CI46	1.3521 (8)	1.00044 (17)	0.4807 (11)	0.038 (3)*
CI47	1.0932 (6)	0.88796 (13)	0.2324 (8)	0.016 (2)*
CI48	0.1005 (9)	0.9987 (2)	0.9883 (12)	0.043 (4)*
O1	1.3423 (16)	0.6703 (3)	0.118 (2)	0.012 (6)*
O2	0.0907 (19)	0.7161 (4)	-0.137 (3)	0.030 (8)*
O3	0.589 (2)	0.6707 (4)	-0.137 (3)	0.027 (8)*
O4	1.8401 (18)	0.6696 (4)	0.364 (3)	0.024 (7)*
O5	0.8377 (18)	0.7166 (4)	0.110 (3)	0.027 (7)*
O6	1.3358 (18)	0.7141 (4)	0.350 (3)	0.024 (7)*
O7	0.2172 (16)	0.7164 (3)	-0.137 (2)	0.016 (6)*
O8	0.7183 (16)	0.7136 (3)	0.116 (2)	0.012 (6)*
O9	0.837 (2)	0.6764 (4)	-0.352 (3)	0.030 (8)*
O10	1.0826 (18)	0.9196 (4)	1.099 (2)	0.022 (6)*
O11	0.0791 (19)	0.9221 (4)	0.599 (3)	0.023 (7)*
O12	0.7136 (19)	0.6708 (4)	-0.133 (3)	0.025 (7)*
O13	0.5801 (16)	0.9218 (3)	0.347 (2)	0.015 (6)*
O14	0.8359 (18)	0.9220 (4)	0.106 (2)	0.022 (7)*
O15	0.4597 (17)	0.7164 (4)	-0.148 (2)	0.019 (6)*
O16	0.4585 (18)	0.9566 (4)	0.896 (2)	0.024 (6)*
O17	0.9566 (17)	0.7156 (3)	0.101 (2)	0.015 (6)*
O18	1.6735 (15)	0.7079 (3)	0.322 (2)	0.010 (5)*
O19	0.9599 (18)	0.9591 (4)	0.652 (2)	0.026 (7)*
O20	0.5825 (18)	0.9195 (4)	0.853 (2)	0.019 (7)*
O21	1.0950 (18)	0.6692 (4)	0.117 (3)	0.026 (7)*
O22	1.0897 (15)	0.7081 (3)	0.156 (2)	0.009 (5)*
O23	0.7102 (16)	0.9586 (4)	0.643 (2)	0.019 (6)*
O24	0.5401 (18)	0.9252 (4)	1.054 (2)	0.023 (6)*
O25	0.9571 (17)	0.9259 (3)	0.896 (2)	0.016 (6)*
O26	0.3346 (16)	0.7098 (3)	-0.356 (2)	0.014 (6)*
O27	1.5960 (18)	0.7100 (4)	0.408 (3)	0.017 (7)*
O28	0.827 (2)	0.9203 (5)	0.348 (3)	0.033 (9)*
O29	1.0407 (17)	0.9586 (3)	1.059 (2)	0.014 (6)*
O30	1.090 (2)	0.9634 (5)	0.863 (3)	0.039 (9)*
O31	1.3469 (17)	0.6947 (3)	0.227 (2)	0.015 (6)*

---

O32	0.7032 (18)	0.7170 (4)	-0.154 (3)	0.022 (7)*
O33	0.9194 (15)	0.7096 (3)	-0.184 (2)	0.009 (5)*
O34	1.2119 (17)	0.9197 (4)	0.359 (2)	0.012 (6)*
O35	1.4608 (19)	0.6713 (4)	0.105 (3)	0.021 (6)*
O36	1.4620 (17)	0.7158 (3)	0.356 (2)	0.020 (6)*
O37	0.3322 (17)	0.6751 (4)	-0.600 (2)	0.020 (6)*
O38	0.073 (2)	0.6961 (4)	-0.023 (3)	0.037 (8)*
O39	0.6279 (16)	0.9263 (3)	0.643 (2)	0.016 (6)*
O40	0.9538 (17)	0.9214 (4)	0.350 (2)	0.018 (6)*
O41	0.3408 (18)	0.7178 (4)	0.098 (3)	0.025 (7)*
O42	0.7195 (17)	0.9665 (4)	0.369 (2)	0.019 (7)*
O43	1.5947 (18)	0.7135 (4)	0.111 (3)	0.025 (7)*
O44	1.5043 (18)	0.6777 (4)	0.400 (2)	0.019 (6)*
O45	0.2150 (17)	0.9275 (4)	0.817 (2)	0.022 (6)*
O46	1.2095 (19)	0.9592 (4)	0.400 (3)	0.025 (7)*
O47	0.963 (2)	0.6699 (4)	0.357 (3)	0.030 (8)*
O48	0.3262 (18)	0.9204 (4)	1.091 (2)	0.022 (7)*
O49	1.4524 (19)	0.9207 (4)	0.350 (3)	0.018 (7)*
O50	0.2935 (17)	0.9599 (3)	0.808 (2)	0.013 (6)*
O51	0.6835 (19)	0.6709 (4)	0.084 (3)	0.020 (7)*
O52	0.5749 (17)	0.6986 (4)	-0.294 (2)	0.020 (6)*
O53	1.0927 (15)	0.6767 (3)	0.402 (2)	0.011 (5)*
O54	0.2042 (15)	0.7144 (3)	0.100 (2)	0.008 (5)*
O55	0.9637 (15)	0.9212 (3)	0.609 (2)	0.008 (5)*
O56	0.4623 (18)	0.9211 (3)	1.112 (3)	0.023 (6)*
O57	0.7089 (17)	0.9212 (4)	0.129 (2)	0.018 (6)*
O58	0.4648 (16)	0.6717 (3)	-0.390 (2)	0.010 (5)*
O59	0.5909 (18)	0.7176 (4)	-0.157 (2)	0.026 (7)*
O60	1.1684 (18)	0.6750 (4)	0.317 (3)	0.025 (7)*
O61	0.9642 (17)	0.9667 (3)	0.370 (2)	0.018 (6)*
O62	1.9244 (17)	0.6742 (4)	0.577 (2)	0.021 (6)*
O63	0.9523 (17)	0.9248 (3)	1.060 (2)	0.020 (6)*
O64	1.0818 (17)	0.9647 (4)	0.354 (2)	0.019 (6)*
O65	1.9659 (17)	0.7155 (3)	0.612 (2)	0.016 (6)*
O66	0.5792 (17)	0.9639 (4)	0.592 (2)	0.018 (6)*
O67	0.712 (2)	0.9593 (4)	0.816 (3)	0.024 (8)*
O68	0.4602 (18)	0.9655 (4)	0.602 (3)	0.023 (7)*
O69	1.2096 (16)	0.9588 (3)	0.568 (2)	0.017 (6)*
O70	0.7275 (18)	0.9457 (4)	0.255 (2)	0.018 (7)*
O71	1.2015 (19)	0.9471 (4)	0.240 (3)	0.025 (7)*
O72	1.4633 (17)	0.9657 (4)	0.355 (2)	0.021 (6)*
O73	0.6267 (18)	0.9610 (4)	0.402 (2)	0.023 (7)*
O74	0.8617 (17)	0.6971 (3)	0.265 (2)	0.014 (6)*
O75	0.7949 (16)	0.9263 (3)	0.813 (2)	0.012 (6)*
O76	0.8719 (16)	0.9596 (3)	0.891 (2)	0.015 (6)*
O77	1.5868 (17)	0.6724 (3)	0.609 (2)	0.018 (6)*
O78	0.005 (2)	0.7092 (4)	-0.600 (3)	0.043 (8)*
O79	0.2553 (18)	0.6766 (4)	-0.351 (2)	0.022 (7)*
O80	0.4542 (16)	0.9255 (3)	0.806 (2)	0.013 (6)*
O81	0.2157 (18)	0.9654 (4)	0.864 (3)	0.026 (7)*
O82	0.2018 (16)	0.9207 (3)	1.078 (2)	0.014 (6)*
O83	1.349 (2)	0.9676 (4)	0.114 (3)	0.033 (8)*
O84	1.4797 (19)	0.9487 (4)	0.238 (3)	0.029 (7)*
O85	1.5113 (17)	0.7096 (4)	0.159 (2)	0.022 (6)*
O86	1.5934 (16)	0.7112 (3)	0.573 (2)	0.016 (6)*
O87	0.7086 (16)	0.9270 (3)	0.563 (2)	0.015 (6)*
O88	0.8356 (17)	0.6755 (4)	-0.183 (2)	0.017 (6)*
O89	0.0932 (17)	0.6717 (4)	-0.141 (2)	0.020 (6)*
O90	0.0921 (15)	0.6761 (3)	-0.425 (2)	0.010 (5)*
O91	0.7062 (16)	0.9641 (4)	0.098 (2)	0.015 (6)*

---

O92	1.336 (2)	0.9202 (4)	0.352 (3)	0.023 (7)*
O93	0.5385 (17)	0.9583 (3)	0.810 (2)	0.012 (6)*
O94	0.1773 (17)	0.7097 (4)	-0.427 (2)	0.021 (6)*
O95	1.2923 (17)	0.9254 (3)	0.562 (2)	0.018 (6)*
O96	0.7923 (17)	0.9602 (3)	0.565 (2)	0.017 (6)*
O97	0.2104 (19)	0.6709 (4)	-0.136 (3)	0.026 (7)*
O98	0.4562 (17)	0.9592 (3)	1.057 (2)	0.016 (6)*
O99	1.8351 (15)	0.7087 (3)	0.402 (2)	0.009 (5)*
O100	1.0408 (16)	0.9252 (3)	0.817 (2)	0.012 (6)*
O101	1.5912 (16)	0.6771 (3)	0.325 (2)	0.014 (6)*
O102	0.4555 (19)	0.9252 (4)	0.638 (3)	0.019 (7)*
O103	1.1288 (15)	0.9264 (3)	0.405 (2)	0.007 (5)*
O104	1.4187 (16)	0.7102 (3)	0.568 (2)	0.015 (6)*
O105	1.6697 (16)	0.6772 (3)	0.566 (2)	0.014 (6)*
O106	0.2114 (15)	0.9275 (3)	0.649 (2)	0.011 (6)*
O107	0.7100 (15)	0.9275 (3)	0.396 (2)	0.012 (6)*
O108	1.2102 (16)	0.9633 (4)	0.114 (2)	0.014 (6)*
O109	0.9627 (19)	0.9651 (4)	1.113 (3)	0.021 (6)*
O110	1.5970 (18)	0.6751 (4)	0.162 (3)	0.021 (7)*
O111	0.0828 (18)	0.6889 (4)	-0.289 (2)	0.021 (7)*
O112	0.8480 (16)	0.6887 (3)	-0.020 (2)	0.011 (6)*
O113	1.8368 (18)	0.7101 (4)	0.570 (2)	0.025 (7)*
O114	0.3729 (14)	0.9270 (3)	0.8940 (18)	0.001 (5)*
O115	0.7536 (16)	0.7094 (3)	-0.353 (2)	0.017 (6)*
O116	0.7094 (17)	0.9199 (4)	0.860 (2)	0.021 (6)*
O117	1.0032 (19)	0.6745 (4)	0.158 (3)	0.030 (8)*
O118	0.8382 (17)	0.7143 (4)	-0.139 (2)	0.016 (6)*
O119	0.699 (2)	0.9476 (4)	-0.053 (3)	0.021 (8)*
O120	0.8750 (17)	0.9266 (3)	0.648 (2)	0.018 (6)*
O121	1.2356 (16)	0.6709 (3)	0.136 (2)	0.010 (5)*
O122	0.9617 (17)	0.6697 (3)	-0.145 (2)	0.016 (6)*
O123	0.0931 (15)	0.7146 (3)	-0.385 (2)	0.009 (5)*
O124	0.9804 (18)	0.9383 (4)	0.240 (3)	0.024 (7)*
O125	1.2492 (15)	0.7075 (3)	0.397 (2)	0.008 (5)*
O126	0.8390 (17)	0.6711 (4)	0.104 (2)	0.018 (6)*
O127	0.9749 (15)	0.9487 (3)	0.510 (2)	0.007 (5)*
O128	0.3414 (16)	0.6719 (3)	-0.136 (2)	0.013 (6)*
O129	1.0905 (15)	0.7101 (3)	0.323 (2)	0.015 (6)*
O130	1.7569 (15)	0.6756 (3)	0.409 (2)	0.012 (5)*
O131	0.4248 (15)	0.6773 (3)	-0.181 (2)	0.008 (5)*
O132	0.9588 (18)	0.9583 (4)	0.820 (2)	0.021 (6)*
O133	0.3424 (17)	0.6765 (3)	-0.422 (2)	0.020 (6)*
O134	0.8502 (18)	0.9674 (4)	0.371 (2)	0.020 (6)*
O135	0.1282 (16)	0.9608 (3)	0.644 (2)	0.016 (6)*
O136	0.832 (2)	0.9660 (5)	0.100 (3)	0.036 (9)*
O137	0.3342 (17)	0.7110 (3)	-0.186 (2)	0.020 (6)*
O138	1.3313 (18)	0.9657 (4)	0.348 (2)	0.022 (7)*
O139	0.3482 (17)	0.6976 (4)	-0.023 (2)	0.020 (6)*
O140	1.4721 (17)	0.9383 (3)	0.495 (2)	0.016 (6)*
O141	0.3758 (16)	0.9591 (3)	0.646 (2)	0.017 (6)*
O142	0.585 (2)	0.6946 (4)	-0.036 (3)	0.032 (8)*
O143	0.5877 (18)	0.9629 (4)	1.104 (2)	0.024 (7)*
O144	0.2230 (18)	0.9445 (4)	0.990 (2)	0.022 (7)*

**Table S 2. Atomic displacement parameters ( $\text{\AA}^2$ ) of  $\beta'$ -BiSeO<sub>3</sub>Cl**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Bi1	0.0089 (9)	0.0283 (12)	0.0123 (10)	0.0010 (8)	0.0062 (9)	0.0014 (8)
Bi2	0.0247 (12)	0.0304 (13)	0.0290 (12)	-0.0001 (9)	0.0207 (11)	-0.0009 (9)
Bi3	0.0124 (9)	0.0321 (11)	0.0163 (9)	-0.0045 (8)	0.0082 (8)	-0.0034 (8)
Bi4	0.0140 (9)	0.0317 (12)	0.0202 (9)	-0.0020 (8)	0.0112 (8)	-0.0020 (8)
Bi5	0.0179 (10)	0.0263 (11)	0.0185 (9)	0.0022 (8)	0.0125 (9)	0.0014 (8)
Bi6	0.0136 (9)	0.0325 (12)	0.0203 (9)	-0.0023 (8)	0.0116 (9)	-0.0007 (8)
Bi7	0.0141 (10)	0.0264 (11)	0.0178 (10)	-0.0006 (7)	0.0114 (9)	-0.0003 (7)
Bi8	0.0178 (10)	0.0246 (10)	0.0171 (10)	-0.0014 (8)	0.0118 (9)	-0.0006 (8)
Bi9	0.0114 (10)	0.0255 (10)	0.0170 (10)	0.0002 (7)	0.0084 (9)	0.0000 (7)
Bi10	0.0179 (10)	0.0324 (12)	0.0226 (10)	-0.0016 (8)	0.0157 (9)	0.0014 (8)
Bi11	0.0135 (10)	0.0303 (12)	0.0207 (11)	-0.0039 (8)	0.0109 (10)	-0.0050 (8)
Bi12	0.0191 (10)	0.0277 (11)	0.0181 (9)	0.0028 (8)	0.0120 (9)	0.0039 (8)
Bi13	0.0157 (11)	0.0237 (11)	0.0176 (11)	0.0001 (7)	0.0118 (10)	0.0002 (7)
Bi14	0.0172 (10)	0.0233 (11)	0.0150 (9)	-0.0005 (7)	0.0117 (9)	0.0001 (7)
Bi15	0.0192 (10)	0.0247 (10)	0.0194 (10)	0.0017 (8)	0.0142 (10)	0.0022 (8)
Bi16	0.0182 (10)	0.0298 (11)	0.0187 (9)	-0.0009 (8)	0.0139 (9)	-0.0003 (7)
Bi17	0.0181 (10)	0.0239 (11)	0.0206 (10)	-0.0009 (8)	0.0117 (9)	-0.0020 (8)
Bi18	0.0188 (10)	0.0266 (10)	0.0197 (9)	-0.0006 (8)	0.0146 (9)	-0.0020 (7)
Bi19	0.0287 (12)	0.0275 (13)	0.0259 (12)	0.0029 (9)	0.0182 (11)	0.0021 (8)
Bi20	0.0109 (10)	0.0292 (12)	0.0119 (10)	-0.0003 (8)	0.0078 (9)	-0.0015 (7)
Bi21	0.0182 (10)	0.0262 (11)	0.0238 (9)	-0.0022 (8)	0.0148 (9)	-0.0001 (8)
Bi22	0.0185 (11)	0.0261 (11)	0.0157 (10)	0.0003 (8)	0.0122 (10)	-0.0015 (8)
Bi23	0.0177 (10)	0.0262 (10)	0.0171 (10)	-0.0003 (8)	0.0124 (9)	-0.0011 (7)
Bi24	0.0191 (11)	0.0264 (11)	0.0182 (10)	0.0020 (8)	0.0140 (10)	0.0008 (7)
Bi25	0.0157 (10)	0.0261 (10)	0.0218 (10)	0.0001 (8)	0.0128 (9)	0.0003 (8)
Bi26	0.0112 (10)	0.0298 (11)	0.0173 (9)	0.0001 (7)	0.0101 (9)	0.0014 (7)
Bi27	0.0136 (10)	0.0270 (11)	0.0186 (10)	-0.0023 (8)	0.0102 (9)	0.0007 (8)
Bi28	0.0145 (10)	0.0315 (11)	0.0184 (10)	-0.0023 (8)	0.0113 (9)	-0.0009 (8)
Bi29	0.0126 (10)	0.0269 (11)	0.0155 (10)	-0.0003 (7)	0.0089 (9)	-0.0021 (8)
Bi30	0.0178 (11)	0.0221 (12)	0.0207 (11)	0.0001 (8)	0.0141 (10)	-0.0011 (7)
Bi31	0.0134 (9)	0.0298 (11)	0.0196 (9)	0.0001 (8)	0.0109 (9)	0.0002 (7)
Bi32	0.0142 (10)	0.0329 (12)	0.0193 (10)	-0.0014 (9)	0.0117 (9)	-0.0031 (9)
Bi33	0.0209 (10)	0.0293 (11)	0.0208 (10)	-0.0008 (8)	0.0148 (9)	-0.0005 (8)
Bi34	0.0195 (10)	0.0296 (11)	0.0233 (9)	-0.0011 (8)	0.0160 (9)	-0.0010 (8)
Bi35	0.0240 (12)	0.0234 (12)	0.0284 (12)	-0.0002 (8)	0.0164 (11)	-0.0021 (8)
Bi36	0.0136 (10)	0.0280 (11)	0.0213 (10)	0.0015 (8)	0.0112 (9)	0.0018 (8)
Bi37	0.0206 (10)	0.0243 (10)	0.0212 (9)	0.0002 (8)	0.0155 (9)	0.0010 (7)
Bi38	0.0173 (11)	0.0282 (11)	0.0175 (10)	-0.0021 (8)	0.0117 (10)	-0.0022 (8)
Bi39	0.0235 (11)	0.0245 (11)	0.0177 (10)	-0.0019 (8)	0.0144 (10)	-0.0020 (7)
Bi40	0.0211 (10)	0.0262 (11)	0.0224 (10)	0.0000 (8)	0.0156 (9)	-0.0016 (8)
Bi41	0.0250 (12)	0.0247 (11)	0.0259 (11)	0.0028 (8)	0.0199 (11)	0.0028 (8)
Bi42	0.0149 (10)	0.0346 (11)	0.0200 (9)	-0.0002 (8)	0.0110 (9)	0.0007 (8)
Bi43	0.0133 (9)	0.0303 (11)	0.0152 (9)	0.0011 (8)	0.0085 (8)	0.0010 (7)
Bi44	0.0133 (10)	0.0276 (12)	0.0168 (10)	0.0002 (8)	0.0092 (9)	-0.0004 (8)
Bi45	0.0192 (10)	0.0248 (10)	0.0222 (9)	0.0013 (8)	0.0160 (9)	0.0016 (7)
Bi46	0.0196 (10)	0.0247 (11)	0.0196 (9)	-0.0006 (8)	0.0124 (9)	0.0024 (8)
Bi47	0.0262 (12)	0.0218 (12)	0.0265 (12)	-0.0007 (8)	0.0154 (11)	-0.0034 (8)
Bi48	0.0148 (10)	0.0291 (12)	0.0183 (10)	0.0010 (8)	0.0116 (10)	0.0006 (7)
Se1	0.015 (2)	0.018 (2)	0.019 (2)	0.0055 (19)	0.012 (2)	0.0058 (19)
Se2	0.015 (2)	0.028 (3)	0.010 (2)	-0.002 (2)	0.009 (2)	-0.0045 (19)
Se3	0.016 (3)	0.020 (3)	0.014 (2)	0.000 (2)	0.009 (2)	0.0012 (18)
Se4	0.010 (2)	0.020 (2)	0.013 (2)	0.0002 (19)	0.006 (2)	0.0015 (18)
Se5	0.014 (3)	0.025 (3)	0.020 (2)	-0.002 (2)	0.014 (2)	-0.002 (2)
Se6	0.011 (2)	0.018 (3)	0.018 (2)	-0.0006 (19)	0.010 (2)	0.0013 (19)
Se7	0.012 (2)	0.024 (2)	0.014 (2)	-0.0016 (18)	0.011 (2)	0.0009 (18)
Se8	0.015 (2)	0.022 (3)	0.014 (2)	-0.0028 (19)	0.011 (2)	-0.0036 (18)
Se9	0.009 (2)	0.027 (3)	0.008 (2)	0.0023 (19)	0.003 (2)	0.0015 (18)

---

Se10	0.013 (2)	0.016 (2)	0.017 (2)	-0.0013 (18)	0.010 (2)	-0.0023 (18)
Se11	0.010 (2)	0.023 (3)	0.009 (2)	0.0055 (18)	0.005 (2)	0.0021 (17)
Se12	0.012 (2)	0.024 (3)	0.016 (2)	0.0013 (19)	0.012 (2)	0.0004 (18)
Se13	0.011 (2)	0.024 (3)	0.013 (2)	0.0041 (19)	0.009 (2)	0.0025 (18)
Se14	0.017 (3)	0.015 (3)	0.023 (3)	0.0015 (19)	0.014 (2)	-0.001 (2)
Se15	0.011 (2)	0.025 (3)	0.009 (2)	-0.0004 (18)	0.008 (2)	-0.0001 (18)
Se16	0.011 (2)	0.025 (3)	0.006 (2)	0.0009 (19)	0.004 (2)	-0.0014 (18)
Se17	0.006 (2)	0.029 (3)	0.017 (2)	0.0026 (18)	0.010 (2)	0.0035 (19)
Se18	0.017 (2)	0.022 (3)	0.012 (2)	0.0003 (19)	0.012 (2)	0.0018 (18)
Se19	0.012 (2)	0.020 (2)	0.013 (2)	0.0016 (18)	0.005 (2)	0.0017 (18)
Se20	0.012 (2)	0.023 (3)	0.025 (3)	0.000 (2)	0.014 (2)	-0.001 (2)
Se21	0.020 (3)	0.015 (3)	0.014 (2)	0.003 (2)	0.010 (2)	0.0024 (18)
Se22	0.016 (3)	0.019 (2)	0.017 (2)	0.0013 (19)	0.011 (2)	-0.0009 (18)
Se23	0.009 (2)	0.021 (3)	0.018 (2)	-0.0021 (18)	0.009 (2)	-0.0038 (19)
Se24	0.002 (2)	0.022 (2)	0.007 (2)	0.0018 (17)	0.0004 (19)	0.0026 (17)
Se25	0.005 (2)	0.030 (3)	0.007 (2)	0.0027 (18)	0.002 (2)	-0.0002 (18)
Se26	0.007 (2)	0.024 (3)	0.014 (2)	0.0004 (18)	0.009 (2)	0.0006 (18)
Se27	0.012 (2)	0.020 (3)	0.015 (2)	-0.0010 (18)	0.009 (2)	0.0011 (18)
Se28	0.009 (2)	0.034 (3)	0.0015 (19)	0.000 (2)	0.0015 (19)	-0.0013 (18)
Se29	0.017 (2)	0.016 (2)	0.015 (2)	0.0001 (19)	0.012 (2)	-0.0005 (17)
Se30	0.014 (2)	0.021 (2)	0.014 (2)	0.0017 (18)	0.011 (2)	0.0019 (17)
Se31	0.020 (3)	0.014 (2)	0.023 (2)	0.0003 (18)	0.017 (2)	0.0026 (18)
Se32	0.014 (2)	0.019 (2)	0.020 (2)	0.0000 (18)	0.013 (2)	-0.0009 (18)
Se33	0.022 (3)	0.021 (3)	0.014 (2)	-0.001 (2)	0.009 (2)	-0.0004 (18)
Se34	0.010 (2)	0.022 (2)	0.007 (2)	0.0003 (19)	0.005 (2)	0.0013 (17)
Se35	0.014 (2)	0.028 (3)	0.015 (2)	-0.0008 (19)	0.013 (2)	0.0019 (18)
Se36	0.009 (2)	0.027 (3)	0.016 (2)	-0.0010 (19)	0.009 (2)	-0.0026 (19)
Se37	0.021 (3)	0.018 (2)	0.020 (2)	0.0027 (19)	0.016 (2)	-0.0004 (18)
Se38	0.010 (2)	0.022 (2)	0.017 (2)	-0.0001 (18)	0.010 (2)	0.0000 (19)
Se39	0.016 (2)	0.028 (3)	0.020 (2)	0.001 (2)	0.015 (2)	-0.001 (2)
Se40	0.004 (2)	0.024 (2)	0.012 (2)	0.0027 (17)	0.0039 (19)	-0.0003 (17)
Se41	0.018 (2)	0.016 (2)	0.019 (2)	0.0010 (18)	0.013 (2)	0.0008 (18)
Se42	0.013 (2)	0.026 (3)	0.011 (2)	0.0029 (19)	0.007 (2)	0.0010 (18)
Se43	0.010 (2)	0.022 (2)	0.009 (2)	0.0014 (18)	0.006 (2)	0.0006 (17)
Se44	0.015 (2)	0.023 (3)	0.016 (2)	-0.001 (2)	0.011 (2)	-0.0011 (19)
Se45	0.015 (2)	0.029 (3)	0.019 (2)	0.0016 (19)	0.013 (2)	0.0002 (18)
Se46	0.014 (2)	0.026 (2)	0.011 (2)	0.0014 (19)	0.008 (2)	-0.0002 (17)
Se47	0.009 (2)	0.024 (3)	0.019 (2)	-0.0023 (18)	0.010 (2)	-0.0025 (19)
Se48	0.012 (2)	0.028 (3)	0.016 (2)	0.0032 (18)	0.010 (2)	0.0019 (18)

---

**Table S 3. Selected Bi-O distances ( $\text{\AA}$ ) in  $\beta$ -BiSeO<sub>3</sub>Cl ( $d_{\max}=3\text{\AA}$ )**

Atom1	Atom2	d, $\text{\AA}$	Atom1	Atom2	d, $\text{\AA}$	Atom1	Atom2	d, $\text{\AA}$		
Bi1	O23	2.336(33)	Bi9	O14	2.299(44)	Bi15	O131	2.264(39)		
	O75	2.366(40)		O116	2.301(35)		O15	2.383(21)		
	O76	2.399(32)		O67	2.356(27)		O26	2.402(45)		
	O87	2.423(21)		O119	2.387(33)		O142	2.453(40)		
	O132	2.448(36)		O75	2.531(44)		O133	2.525(38)		
	O120	2.492(42)		O136	2.643(24)		O104	2.609(32)		
	O25	2.501(22)		O63	2.663(28)		O3	2.734(25)		
	O96	2.502(33)		O76	2.849(36)		O59	2.760(38)		
	Bi2	O103		2.472(39)	Bi10		O6	2.115(28)	Bi16	O58
O69		2.479(31)	O54	2.268(29)		O116	2.602(38)			
O64		2.482(39)	O36	2.450(53)		O20	2.973(38)			
O61		2.486(28)	Bi11	O41	2.562(37)	Bi17	O82	2.842(29)		
O135		2.494(31)		O31	2.733(47)		Bi18	O136	2.142(30)	
O40		2.636(30)		O102	2.390(35)			O61	2.473(21)	
O106		2.639(20)		O140	2.436(41)	O109		2.500(33)		
O124		2.666(40)		O68	2.445(49)	Bi19	O64	2.739(34)		
O11		2.668(48)		O93	2.490(23)		O66	2.399(35)		
O127		2.822(43)		O39	2.539(29)		O72	2.441(36)		
Bi3		O143		2.220(31)	Bi12	O66	2.565(55)	Bi20	O39	2.465(10)
		O91		2.236(40)		O67	2.670(25)		O73	2.528(15)
	O42	2.480(39)	O119	2.765(21)		O23	2.536(22)			
	O134	2.588(28)	O20	2.809(40)		O140	2.607(35)			
	O70	2.655(31)	O116	2.888(25)		O87	2.623(14)			
Bi4	O122	2.535(13)	Bi13	O43	2.169(31)	Bi21	O49	2.629(20)		
	O21	2.743(20)		O8	2.265(42)		O13	2.706(14)		
	O89	2.965(25)		O15	2.485(41)		O84	2.733(30)		
Bi5	O121	2.836(12)	Bi14	O59	2.636(40)	Bi22	O106	2.356(34)		
Bi6	O30	2.192(14)		O142	2.736(39)		O69	2.381(35)		
	O108	2.303(44)		O115	2.347(32)		O16	2.410(53)		
Bi7	O81	2.446(14)		O27	2.395(38)		O50	2.419(13)		
	O83	2.559(20)		O9	2.396(28)		O141	2.457(23)		
	O144	2.735(11)		O105	2.404(50)		O114	2.463(29)		
	O25	2.267(24)		O18	2.435(27)		O80	2.469(38)		
	O100	2.352(33)	O113	2.436(26)	O95	2.476(29)				
	O10	2.366(38)	O101	2.443(41)	O51	2.590(30)				
	O82	2.462(54)	O130	2.482(32)	O52	2.241(45)				
	O29	2.478(36)	O80	2.304(14)	O58	2.317(23)				
	O132	2.512(32)	O24	2.334(32)	O77	2.342(46)				
Bi8	O30	2.797(23)	O20	2.415(37)	O104	2.446(32)				
	O108	2.826(12)	O16	2.469(28)	O44	2.576(44)				
	O44	2.270(34)	O93	2.489(41)	O86	2.580(36)				
	O31	2.372(34)	O57	2.559(32)	O37	2.682(41)				
	O36	2.373(39)	O143	2.759(37)	O6	2.848(31)				
	O27	2.495(29)	O91	2.840(21)	O36	2.965(21)				
	O101	2.610(40)								
	O85	2.644(25)								
	O1	2.675(51)								
	O41	2.689(28)								
O35	2.902(34)									



*Table S 4. Continued*

Atom1	Atom2	d, Å	Atom1	Atom2	d, Å	Atom1	Atom2	d, Å	
Bi23	O139	2.215(24)	Bi29	O127	2.242(42)	Bi36	O34	2.334(24)	
	O35	2.326(41)		O55	2.303(55)		O46	2.402(41)	
	O128	2.340(41)		O11	2.373(31)		O71	2.441(51)	
	O85	2.418(30)		O19	2.380(21)		O92	2.479(50)	
	O137	2.543(32)		O135	2.583(36)		O95	2.509(33)	
	O131	2.616(33)		O100	2.649(37)		O102	2.656(23)	
	O110	2.732(13)		O45	2.651(29)		O138	2.694(18)	
	O43	2.877(12)		O30	2.811(27)		O141	2.779(12)	
Bi24	O47	2.271(32)	Bi30	O53	2.318(54)	Bi37	O68	2.999(37)	
	O74	2.314(22)		O94	2.375(40)		O5	2.084(11)	
	O126	2.333(21)		O79	2.384(24)		O17	2.440(37)	
	O78	2.376(23)		O125	2.423(30)		O32	2.468(16)	
	O53	2.558(36)		O129	2.430(48)		O118	2.776(13)	
	O117	2.671(29)		O26	2.447(36)		Bi38	O122	2.322(36)
	O5	2.708(40)		O60	2.550(37)			O33	2.405(27)
	O129	2.576(44)		O133	2.555(35)		O89	2.417(47)	
Bi25	O138	2.163(34)	Bi31	O47	2.657(38)	O38	2.424(31)		
	O72	2.433(33)		O4	2.948(44)	O9	2.518(37)		
	O68	2.472(28)		Bi32	O107	2.279(27)	O2	2.687(20)	
O66	2.724(44)	O42	2.337(24)		O62	2.694(41)			
Bi26	O84	2.202(46)	O96		2.391(26)	O113	2.840(47)		
	O56	2.297(23)	O70	2.428(50)	Bi39	O112	2.306(21)		
	O13	2.321(31)	O120	2.599(39)		O17	2.394(33)		
	O98	2.417(21)	O19	2.617(40)		O22	2.471(25)		
	O107	2.579(36)	O134	2.728(40)		O117	2.481(42)		
	O73	2.593(27)	O28	2.747(33)		O118	2.483(31)		
	O24	2.662(33)	O55	2.920(24)		O88	2.543(43)		
	O143	2.825(46)	Bi33	O3		2.206(30)	O33	2.666(32)	
Bi27	O124	2.245(46)		O12		2.363(42)	O38	2.883(51)	
	O109	2.361(26)		O58	2.548(34)	O21	2.929(41)		
	O63	2.454(40)	O77	2.749(40)	O122	2.971(26)			
	O29	2.489(22)	Bi34	O34	2.529(20)	O1	2.186(39)		
	O64	2.520(56)		O92	2.743(21)	O97	2.406(31)		
	O103	2.572(29)	Bi35	O10	2.886(45)	O35	2.538(48)		
	O46	2.647(30)		O32	2.488(33)	O128	2.766(31)		
	O71	2.841(42)		O118	2.496(13)	Bi41	O111	2.330(27)	
O10	2.871(48)	O88		2.525(13)	O65		2.438(12)		
O34	2.955(21)	O86		2.535(26)	O62		2.467(20)		
Bi28	O45	2.235(15)		O115	2.611(32)		O90	2.505(40)	
	O81	2.334(29)	O12	2.621(30)	O99		2.529(36)		
	O144	2.459(56)	O112	2.661(30)	O123		2.567(38)		
	O50	2.496(26)	O105	2.673(41)	O78	2.655(33)			
	O114	2.570(34)	O77	2.679(26)	O4	2.788(37)			
	O98	2.593(21)	O52	2.782(31)	O74	2.802(36)			
	O48	2.617(21)			O47	2.926(34)			
	O83	2.646(32)			Bi42	O48	2.288(34)		
O56	2.895(38)			O49		2.381(24)			
				O56		2.563(42)			
						O13	2.736(34)		

*Table S 5. Continued*

Atom1	Atom2	d, Å
Bi43	O28	2.248(21)
	O40	2.284(43)
	O55	2.610(27)
	O11	2.652(24)
Bi44	O130	2.314(34)
	O110	2.325(58)
	O4	2.449(35)
	O99	2.455(29)
	O18	2.509(35)
	O51	2.563(10)
	O43	2.750(18)
	O8	2.818(38)
Bi45	O2	2.115(21)
	O7	2.417(35)
	O65	2.473(42)
	O123	2.765(32)
Bi46	O57	2.694(29)
	O28	2.991(26)
Bi47	O123	2.444(56)
	O7	2.473(29)
	O90	2.483(26)
	O137	2.539(28)
	O111	2.560(48)
	O94	2.576(50)
	O97	2.620(16)
	O139	2.709(13)
	O128	2.732(27)
	O79	2.733(37)
Bi48	O60	2.292(40)
	O37	2.346(35)
	O21	2.368(29)
	O125	2.473(11)
	O22	2.476(19)
	O121	2.522(33)
	O6	2.826(37)
	O54	2.892(31)
	O99	2.455(21)
	O18	2.509(38)
	O51	2.563(46)
	O43	2.750(29)
O8	2.818(35)	

**Table S 6. Selected Bi-Cl distances (Å) in  $\beta'$ -BiSeO<sub>3</sub>Cl ( $d_{max}=4\text{Å}$ )**

Atom1	Atom2	d, Å	Atom1	Atom2	d, Å	Atom1	Atom2	d, Å
Bi1	Cl24	3.966(14)	Bi25	Cl46	2.628(21)	Bi48	Cl33	3.927(12)
Bi3	Cl30	2.738(13)		Cl41	2.676(15)			
	Cl37	2.922(21)		Cl37	3.341(12)			
	Cl39	3.461(23)		Cl30	3.425(20)			
	Cl42	3.794(12)	Bi26	Cl44	3.983(12)			
Bi4	Cl16	2.483(20)	Bi31	Cl40	2.493(13)			
	Cl45	2.652(12)		Cl25	2.509(13)			
	Cl8	2.653(14)		Cl20	2.538(26)			
	Cl33	3.075(11)		Cl29	3.169(22)			
	Cl1	3.317(19)		Cl15	3.259(11)			
Bi5	Cl24	2.460(14)	Bi33	Cl13	2.650(18)			
	Cl33	2.548(20)		Cl15	2.690(12)			
	Cl32	2.560(11)		Cl34	3.168(20)			
	Cl28	2.905(20)		Cl47	3.173(11)			
	Cl1	2.977(12)		Cl32	3.472(12)			
Bi6	Cl48	2.747(23)	Bi34	Cl35	2.484(11)			
	Cl31	2.897(12)		Cl47	2.584(16)			
	Cl41	3.422(14)		Cl34	2.674(13)			
	Cl46	3.790(22)		Cl19	3.199(17)			
Bi7	Cl21	3.970(12)		Cl21	3.312(13)			
Bi10	Cl2	2.751(21)	Bi37	Cl4	2.607(12)			
	Cl14	2.910(13)		Cl12	2.684(20)			
	Cl6	3.430(14)		Cl14	3.329(22)			
	Cl10	3.780(21)		Cl2	3.442(15)			
Bi12	Cl11	2.760(14)	Bi40	Cl28	2.648(10)			
	Cl22	2.933(20)		Cl1	2.661(18)			
	Cl12	3.421(21)		Cl43	3.215(12)			
	Cl4	3.798(13)		Cl17	3.270(13)			
Bi13	Cl23	3.935(14)		Cl18	3.469(22)			
Bi14	Cl27	3.904(13)	Bi42	Cl19	2.655(16)			
Bi16	Cl9	2.528(10)		Cl3	2.725(13)			
	Cl26	2.568(15)		Cl8	3.136(13)			
	Cl5	2.569(22)		Cl45	3.165(10)			
	Cl27	3.202(21)		Cl44	3.525(19)			
	Cl38	3.208(12)	Bi43	Cl38	2.693(11)			
Bi17	Cl23	2.501(14)		Cl43	2.807(19)			
	Cl21	2.550(20)		Cl36	3.144(18)			
	Cl7	2.603(14)		Cl18	3.325(14)			
	Cl19	2.961(90)		Cl7	3.471(13)			
	Cl3	3.020(19)	Bi44	Cl29	3.940(14)			
Bi18	Cl42	2.612(13)	Bi45	Cl10	2.631(20)			
	Cl39	2.680(23)		Cl6	2.695(13)			
	Cl31	3.377(19)		Cl22	3.360(14)			
	Cl48	3.471(13)		Cl11	3.462(25)			
Bi21	Cl29	2.519(13)	Bi46	Cl44	2.530(20)			
	Cl36	2.522(12)		Cl17	2.533(13)			
	Cl18	2.624(22)		Cl27	2.549(12)			
	Cl15	2.835(21)		Cl43	2.965(10)			
	Cl13	2.977(12)		Cl38	3.034(17)			

**Table S 7. Selected Se-O distances (Å) in  $\beta'$ -BiSeO<sub>3</sub>Cl**

Atom1	Atom2	d, Å	Atom1	Atom2	d, Å	Atom1	Atom2	d, Å
Se1	O59	1.585(46)	Se17	O129	1.643(32)	Se33	O126	1.662(39)
	O32	1.672(33)		O22	1.737(39)		O12	1.716(28)
	O52	1.722(31)		O17	1.765(27)		O112	1.762(28)
Se2	O83	1.679(28)	Se18	O95	1.617(23)	Se34	O113	1.670(44)
	O84	1.724(35)		O103	1.684(30)		O99	1.705(31)
	O72	1.774(41)		O34	1.709(43)		O65	1.710(29)
Se3	O137	1.689(42)	Se19	O14	1.733(25)	Se35	O120	1.645(33)
	O15	1.702(29)		O40	1.740(41)		O100	1.696(21)
	O26	1.740(33)		O124	1.756(36)		O55	1.716(41)
Se4	O41	1.675(54)	Se20	O134	1.658(33)	Se36	O8	1.740(31)
	O7	1.745(24)		O61	1.688(45)		O5	1.750(59)
	O139	1.793(33)		O127	1.709(24)		O74	1.771(23)
Se5	O67	1.724(46)	Se21	O90	1.732(33)	Se37	O85	1.646(36)
	O23	1.733(42)		O47	1.751(32)		O18	1.685(21)
	O66	1.764(27)		O53	1.759(39)		O43	1.757(55)
Se6	O86	1.671(33)	Se22	O104	1.678(21)	Se38	O133	1.673(41)
	O27	1.725(52)		O125	1.742(30)		O37	1.678(35)
	O36	1.778(27)		O6	1.762(56)		O58	1.751(28)
Se7	O140	1.690(24)	Se23	O96	1.665(23)	Se39	O141	1.658(31)
	O49	1.706(59)		O73	1.675(36)		O93	1.698(22)
	O92	1.724(37)		O42	1.699(44)		O68	1.726(56)
Se8	O46	1.675(53)	Se24	O98	1.705(42)	Se40	O57	1.622(25)
	O69	1.715(33)		O16	1.706(34)		O28	1.726(41)
	O64	1.750(28)		O143	1.740(29)		O70	1.730(45)
Se9	O87	1.660(33)	Se25	O108	1.704(39)	Se41	O62	1.640(24)
	O107	1.727(39)		O138	1.723(27)		O4	1.673(55)
	O13	1.766(25)		O71	1.744(36)		O130	1.714(31)
Se10	O105	1.644(31)	Se26	O115	1.646(21)	Se42	O91	1.743(44)
	O44	1.724(26)		O33	1.696(30)		O119	1.748(34)
	O77	1.733(42)		O118	1.724(42)		O136	1.752(39)
Se11	O54	1.660(22)	Se27	O79	1.643(25)	Se43	O19	1.699(36)
	O2	1.757(55)		O128	1.733(40)		O132	1.709(44)
	O38	1.800(35)		O131	1.745(30)		O30	1.763(35)
Se12	O88	1.680(43)	Se28	O76	1.705(21)	Se44	O114	1.687(20)
	O9	1.701(47)		O29	1.725(33)		O24	1.726(38)
	O122	1.730(28)		O109	1.754(55)		O56	1.767(53)
Se13	O106	1.685(39)	Se29	O101	1.710(32)	Se45	O82	1.717(33)
	O45	1.704(34)		O110	1.718(54)		O144	1.729(28)
	O11	1.785(31)		O35	1.737(29)		O48	1.766(44)
Se14	O39	1.694(21)	Se30	O117	1.645(41)	Se46	O51	1.652(44)
	O75	1.712(31)		O60	1.668(27)		O142	1.654(50)
	O116	1.812(43)		O21	1.712(57)		O3	1.744(30)
Se15	O123	1.691(39)	Se31	O89	1.644(45)	Se47	O10	1.673(32)
	O94	1.708(35)		O97	1.692(35)		O63	1.690(42)
	O78	1.715(28)		O111	1.774(31)		O25	1.724(33)
Se16	O135	1.687(21)	Se32	O20	1.684(29)	Se48	O121	1.656(39)
	O50	1.694(33)		O102	1.696(46)		O31	1.754(21)
	O81	1.788(55)		O80	1.725(40)		O1	1.784(36)

*Table S 8. Selected Se-O angles in  $\beta'$ -BiSeO<sub>3</sub>Cl*

A1	A2	A3	$\wedge$ (°)	A1	A2	A3	$\wedge$ (°)	A1	A2	A3	$\wedge$ (°)
			A2-A1-A3				A2-A1-A3				A2-A1-A3
Se1	O59	O32	105.2	Se17	O129	O22	105.0	Se33	O12	O126	104.9
	O59	O52	94.8		O129	O17	99.1		O12	O112	94.6
	O32	O52	94.1		O22	O17	92.1		O126	O112	95.2
Se2	O72	O84	93.0	Se18	O95	O103	105.3	Se34	O99	O113	102.8
	O72	O83	105.4		O95	O34	92.4		O99	O65	93.8
	O84	O83	99.3		O103	O34	97.3		O113	O65	98.2
Se3	O15	O137	94.4	Se19	O40	O14	108.5	Se35	O120	O100	105.0
	O15	O26	91.3		O40	O124	93.7		O120	O55	97.5
	O137	O26	104.9		O14	O124	99.6		O100	O55	94.2
Se4	O41	O7	103.8	Se20	O127	O134	93.0	Se36	O8	O5	104.5
	O41	O139	96.2		O127	O61	96.1		O8	O74	96.5
	O7	O139	91.2		O134	O61	101.6		O5	O74	94.6
Se5	O67	O23	105.2	Se21	O90	O47	94.5	Se37	O85	O18	105.0
	O67	O66	97.9		O90	O53	107.1		O85	O43	93.2
	O23	O66	91.9		O47	O53	92.5		O18	O43	94.8
Se6	O86	O27	104.7	Se22	O104	O125	104.8	Se38	O37	O133	105.7
	O86	O36	97.1		O104	O6	96.9		O37	O58	90.1
	O27	O36	94.1		O125	O6	94.7		O133	O58	93.5
Se7	O140	O92	98.2	Se23	O73	O96	104.2	Se39	O141	O93	104.8
	O140	O49	93.0		O73	O42	98.2		O141	O68	95.7
	O92	O49	105.2		O96	O42	89.0		O93	O68	94.3
Se8	O69	O46	106.5	Se24	O16	O98	102.6	Se40	O57	O70	102.1
	O69	O64	94.0		O16	O143	90.4		O57	O28	94.6
	O46	O64	93.6		O98	O143	92.4		O70	O28	93.3
Se9	O87	O107	106.7	Se25	O71	O138	96.5	Se41	O62	O4	97.7
	O87	O13	95.3		O71	O108	93.5		O62	O130	108.7
	O107	O13	92.7		O138	O108	103.1		O4	O130	94.6
Se10	O105	O44	105.8	Se26	O115	O33	107.7	Se42	O119	O136	95.8
	O105	O77	95.1		O115	O118	94.3		O119	O91	97.0
	O44	O77	90.4		O33	O118	93.0		O136	O91	107.4
Se11	O54	O2	106.4	Se27	O79	O128	98.9	Se43	O132	O19	107.5
	O54	O38	97.7		O79	O131	105.9		O132	O30	91.8
	O2	O38	93.5		O128	O131	90.4		O19	O30	92.1
Se12	O88	O9	107.2	Se28	O76	O29	105.6	Se44	O114	O24	104.1
	O88	O122	95.1		O76	O109	94.4		O114	O56	95.8
	O9	O122	92.2		O29	O109	93.8		O24	O56	91.2
Se13	O106	O45	102.2	Se29	O110	O101	105.4	Se45	O144	O82	94.6
	O106	O11	95.3		O110	O35	93.8		O144	O48	92.4
	O45	O11	93.7		O101	O35	94.9		O82	O48	99.0
Se14	O75	O39	105.0	Se30	O60	O117	108.1	Se46	O51	O3	95.6
	O75	O116	92.7		O60	O21	88.9		O51	O142	97.6
	O39	O116	94.1		O117	O21	101.4		O3	O142	93.9
Se15	O78	O123	96.3	Se31	O89	O97	101.0	Se47	O63	O25	103.0
	O78	O94	107.0		O89	O111	98.2		O63	O10	101.1
	O123	O94	94.5		O97	O111	91.8		O25	O10	92.6
Se16	O135	O81	95.7	Se32	O102	O20	97.4	Se48	O121	O31	97.7
	O135	O50	104.4		O102	O80	104.2		O121	O1	98.8
	O81	O50	90.5		O20	O80	93.4		O31	O1	92.5

*Table S 9. Bond sum valence values of selected atoms in  $\beta'$ -BiSeO<sub>3</sub>Cl*

<b>Atom</b>	<b>BVS</b>	<b>Atom</b>	<b>BVS</b>	<b>Atom</b>	<b>BVS</b>	<b>Atom</b>	<b>BVS</b>
<b>Bi1</b>	3.31(19)	<b>Bi25</b>	3.20(17)	<b>Se1</b>	4.7(5)	<b>Se25</b>	4.0(4)
<b>Bi2</b>	2.69(15)	<b>Bi26</b>	3.2(2)	<b>Se2</b>	3.2(3)	<b>Se26</b>	3.8(4)
<b>Bi3</b>	3.04(17)	<b>Bi27</b>	2.80(16)	<b>Se3</b>	4.2(4)	<b>Se27</b>	3.6(3)
<b>Bi4</b>	3.28(13)	<b>Bi28</b>	2.90(19)	<b>Se4</b>	3.4(4)	<b>Se28</b>	3.4(3)
<b>Bi5</b>	3.55(12)	<b>Bi29</b>	3.06(19)	<b>Se5</b>	3.7(4)	<b>Se29</b>	3.8(4)
<b>Bi6</b>	3.3(2)	<b>Bi30</b>	3.4(2)	<b>Se6</b>	3.9(4)	<b>Se30</b>	4.1(4)
<b>Bi7</b>	3.1(2)	<b>Bi31</b>	3.26(13)	<b>Se7</b>	3.5(4)	<b>Se31</b>	3.9(5)
<b>Bi8</b>	3.08(18)	<b>Bi32</b>	2.99(17)	<b>Se8</b>	3.4(3)	<b>Se32</b>	4.3(4)
<b>Bi9</b>	2.89(17)	<b>Bi33</b>	3.17(16)	<b>Se9</b>	3.7(4)	<b>Se33</b>	3.8(3)
<b>Bi10</b>	3.2(2)	<b>Bi34</b>	3.04(11)	<b>Se10</b>	3.9(4)	<b>Se34</b>	4.2(5)
<b>Bi11</b>	2.86(17)	<b>Bi35</b>	2.70(14)	<b>Se11</b>	3.7(3)	<b>Se35</b>	3.9(3)
<b>Bi12</b>	3.1(2)	<b>Bi36</b>	2.74(17)	<b>Se12</b>	4.1(5)	<b>Se36</b>	3.5(5)
<b>Bi13</b>	3.18(19)	<b>Bi37</b>	3.4(3)	<b>Se13</b>	3.7(4)	<b>Se37</b>	4.0(4)
<b>Bi14</b>	3.0(2)	<b>Bi38</b>	2.9(2)	<b>Se14</b>	4.0(3)	<b>Se38</b>	4.1(4)
<b>Bi15</b>	3.00(17)	<b>Bi39</b>	2.82(18)	<b>Se15</b>	4.4(4)	<b>Se39</b>	3.7(3)
<b>Bi16</b>	3.06(10)	<b>Bi40</b>	3.24(16)	<b>Se16</b>	3.8(4)	<b>Se40</b>	4.2(4)
<b>Bi17</b>	3.16(11)	<b>Bi41</b>	2.98(17)	<b>Se17</b>	4.1(4)	<b>Se41</b>	3.6(3)
<b>Bi18</b>	3.6(2)	<b>Bi42</b>	3.16(17)	<b>Se18</b>	3.9(4)	<b>Se42</b>	3.5(3)
<b>Bi19</b>	2.89(15)	<b>Bi43</b>	3.09(16)	<b>Se19</b>	3.3(3)	<b>Se43</b>	4.1(5)
<b>Bi20</b>	3.33(18)	<b>Bi44</b>	3.03(19)	<b>Se20</b>	3.8(4)	<b>Se44</b>	3.5(3)
<b>Bi21</b>	3.26(11)	<b>Bi45</b>	3.3(2)	<b>Se21</b>	3.7(3)	<b>Se45</b>	3.4(4)
<b>Bi22</b>	3.05(18)	<b>Bi46</b>	3.33(11)	<b>Se22</b>	3.9(4)	<b>Se46</b>	4.0(3)
<b>Bi23</b>	3.4(3)	<b>Bi47</b>	2.79(17)	<b>Se23</b>	4.3(4)	<b>Se47</b>	4.3(5)
<b>Bi24</b>	3.05(19)	<b>Bi48</b>	2.92(18)	<b>Se24</b>	4.0(4)	<b>Se48</b>	3.9(3)

**Table S 10. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) of  $\text{Bi}_6(\text{SeO}_3)_4\text{Cl}_{10}$**

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Bi1a	0.48273 (2)	0.34082 (5)	0.36920 (3)	0.01344 (12)	0.960 (2)
Bi1b	0.5189 (5)	0.4141 (18)	0.1366 (8)	0.025 (4)	0.040 (2)
Se3a	0.51770 (5)	0.43441 (13)	0.19264 (8)	0.01236 (19)*	0.9604
Se3b	0.4825 (11)	0.331 (3)	0.3145 (16)	0.005 (4)*	0.0396
Bi2	0.853973 (19)	1.11560 (5)	0.57426 (3)	0.01572 (12)	
Bi3	0.95274 (2)	0.83971 (5)	0.84829 (3)	0.01647 (12)	
Bi4	0.66931 (2)	0.61536 (6)	0.37377 (3)	0.02098 (13)	
Bi5	0.86877 (2)	0.62396 (5)	0.58018 (3)	0.01797 (12)	
Bi6	0.66324 (2)	1.12862 (5)	0.34402 (3)	0.01840 (12)	
Se1	0.73099 (5)	1.34197 (12)	0.56176 (7)	0.0113 (3)	
Se2	1.01931 (5)	0.93685 (12)	0.69363 (7)	0.0109 (3)	
Se4	0.72380 (5)	0.84150 (12)	0.55349 (7)	0.0124 (3)	
Cl1	0.84786 (13)	0.6432 (3)	0.74343 (18)	0.0175 (7)	
Cl2	1.06902 (13)	0.8894 (4)	1.00701 (18)	0.0180 (7)	
Cl3	0.55971 (17)	0.6180 (4)	0.4501 (2)	0.0263 (10)	
Cl4	0.86972 (16)	1.1267 (4)	0.75028 (19)	0.0233 (9)	
Cl5	0.92933 (14)	0.6500 (3)	0.98585 (18)	0.0186 (8)	
Cl6	0.79082 (14)	0.6136 (4)	0.38048 (19)	0.0221 (8)	
Cl7	0.79039 (13)	1.1190 (4)	0.37837 (19)	0.0211 (8)	
Cl8	0.57275 (15)	0.1470 (4)	0.4788 (2)	0.0259 (9)	
Cl9	0.66974 (17)	0.3475 (5)	0.2228 (2)	0.0324 (11)	
Cl10	0.66601 (15)	0.8907 (5)	0.2209 (2)	0.0313 (11)	
O1	0.5591 (4)	0.3434 (10)	0.2993 (6)	0.017 (2)	
O2	0.7435 (4)	1.1414 (9)	0.5547 (6)	0.016 (3)	
O3	0.8129 (4)	1.3825 (9)	0.5756 (6)	0.017 (2)	
O4	0.7267 (5)	0.6416 (10)	0.5358 (6)	0.020 (3)	
O5	0.8063 (4)	0.8702 (9)	0.5658 (6)	0.016 (2)	
O6	1.0442 (4)	0.9601 (10)	0.8133 (5)	0.015 (2)	
O7	0.9458 (4)	0.8439 (10)	0.6870 (5)	0.016 (2)	
O8	0.6905 (4)	0.3686 (9)	0.4441 (5)	0.014 (2)	
O9	0.4469 (4)	0.4603 (12)	0.2189 (6)	0.021 (3)	
O10	0.9888 (4)	1.1233 (10)	0.6566 (5)	0.015 (2)	
O11	0.4453 (4)	0.1178 (10)	0.2828 (6)	0.020 (2)	
O12	0.6821 (4)	0.8812 (11)	0.4383 (6)	0.018 (2)	

**Table S 9. Atomic displacement parameters ( $\text{\AA}^2$ ) of  $\text{Bi}_6(\text{SeO}_3)_4\text{Cl}_{10}$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Bi1a	0.01377 (18)	0.01563 (19)	0.01177 (19)	-0.00004 (13)	0.00556 (13)	-0.00031 (13)
Bi1b	0.004 (4)	0.047 (8)	0.025 (6)	0.006 (4)	0.005 (4)	0.003 (5)
Bi2	0.01209 (16)	0.01578 (18)	0.01791 (18)	-0.00019 (13)	0.00359 (13)	-0.00043 (14)
Bi3	0.01887 (18)	0.01502 (18)	0.01827 (18)	0.00109 (14)	0.00996 (14)	-0.00113 (14)
Bi4	0.01430 (18)	0.0215 (2)	0.0221 (2)	-0.00059 (15)	0.00018 (15)	0.00140 (16)
Bi5	0.02051 (19)	0.01522 (18)	0.01863 (18)	0.00105 (15)	0.00744 (15)	0.00117 (14)
Bi6	0.01736 (18)	0.01718 (19)	0.01796 (18)	-0.00022 (14)	0.00287 (14)	0.00045 (15)
Se1	0.0126 (4)	0.0113 (4)	0.0120 (4)	-0.0002 (3)	0.0069 (3)	-0.0006 (3)
Se2	0.0122 (4)	0.0127 (4)	0.0082 (4)	-0.0001 (3)	0.0041 (3)	0.0006 (3)
Se4	0.0139 (4)	0.0118 (4)	0.0123 (4)	0.0012 (3)	0.0058 (3)	-0.0004 (3)
Cl1	0.0170 (11)	0.0231 (12)	0.0134 (10)	-0.0039 (9)	0.0064 (9)	-0.0034 (9)
Cl2	0.0158 (11)	0.0257 (13)	0.0116 (10)	-0.0023 (10)	0.0036 (8)	0.0000 (9)
Cl3	0.0315 (15)	0.0270 (15)	0.0253 (14)	-0.0046 (12)	0.0162 (12)	-0.0074 (11)
Cl4	0.0295 (14)	0.0265 (14)	0.0145 (11)	0.0063 (11)	0.0086 (10)	0.0026 (10)
Cl5	0.0221 (12)	0.0229 (13)	0.0148 (11)	0.0014 (10)	0.0116 (9)	0.0031 (9)
Cl6	0.0156 (11)	0.0343 (15)	0.0168 (11)	-0.0004 (11)	0.0063 (9)	0.0013 (11)
Cl7	0.0140 (11)	0.0334 (15)	0.0157 (11)	0.0009 (10)	0.0049 (9)	-0.0010 (10)
Cl8	0.0228 (13)	0.0334 (16)	0.0182 (12)	0.0072 (12)	0.0032 (10)	0.0061 (11)
Cl9	0.0288 (15)	0.048 (2)	0.0249 (14)	0.0100 (14)	0.0148 (12)	0.0150 (14)
Cl10	0.0196 (13)	0.048 (2)	0.0287 (15)	-0.0069 (13)	0.0113 (11)	-0.0183 (14)
O1	0.013 (3)	0.018 (4)	0.020 (4)	0.005 (3)	0.005 (3)	0.007 (3)
O2	0.015 (3)	0.007 (3)	0.032 (4)	0.002 (3)	0.014 (3)	0.001 (3)
O3	0.008 (3)	0.010 (3)	0.026 (4)	0.000 (3)	0.000 (3)	0.001 (3)
O4	0.032 (5)	0.008 (3)	0.022 (4)	-0.002 (3)	0.013 (3)	-0.004 (3)
O5	0.010 (3)	0.009 (3)	0.025 (4)	-0.001 (3)	0.001 (3)	-0.001 (3)
O6	0.018 (4)	0.017 (4)	0.011 (3)	-0.009 (3)	0.008 (3)	0.000 (3)
O7	0.015 (3)	0.019 (4)	0.016 (3)	-0.006 (3)	0.006 (3)	-0.001 (3)
O8	0.018 (3)	0.013 (3)	0.012 (3)	0.002 (3)	0.006 (3)	-0.006 (3)
O9	0.014 (4)	0.035 (5)	0.017 (4)	0.004 (3)	0.007 (3)	0.011 (3)
O10	0.012 (3)	0.014 (3)	0.015 (3)	-0.003 (3)	0.001 (3)	-0.001 (3)
O11	0.013 (3)	0.015 (4)	0.021 (4)	0.000 (3)	-0.007 (3)	-0.004 (3)
O12	0.013 (3)	0.022 (4)	0.016 (4)	-0.002 (3)	0.001 (3)	-0.001 (3)



**Table S 102. Selected interatomic distances ( $\text{\AA}$ ) in  $\text{Bi}_6(\text{SeO}_3)_4\text{Cl}_{10}$**

<b>Atom1</b>	<b>Atom2</b>	<b>d</b>	<b>Atom1</b>	<b>Atom2</b>	<b>d</b>
<b>Bi1a</b>	O1	2.252(11)	Se1	O2	1.7157(77)
	O11	2.2718(82)		O8	1.7193(69)
	O9	2.3797(90)		O3	1.7285(88)
	Cl8	2.6305(29)	Se2	O10	1.7154(82)
	Cl3	2.8716(32)		O7	1.7308(88)
	Cl10	3.0273(30)	Se4	O6	1.7323(74)
	Cl3	3.2263(37)		O4	1.7058(85)
<b>Bi1b</b>	O11	2.092(16)	Se3a	O12	1.7084(82)
	O9	2.347(17)		O5	1.7299(89)
	O1	2.410(15)	O11	1.7133(83)	
	Cl8	2.894(13)	O9	1.7174(99)	
	Cl3	3.037(14)	O1	1.7394(81)	
	Cl8	3.071(14)	Se3b	O1	1.7429(278)
	Cl9	3.086(11)		O9	1.7674(246)
<b>Bi2</b>	O5	2.2848(78)	O11	O11	1.9515(258)
	O2	2.2926(88)			
	O3	2.4120(78)			
	Cl4	2.6015(31)			
	Cl7	2.8282(27)			
	Cl5	3.3134(31)			
	Cl2	3.3208(33)			
	<b>Bi3</b>	O10	2.2252(87)		
		O7	2.4255(81)		
		O6	2.4302(92)		
		Cl1	2.7975(24)		
		Cl5	2.8268(30)		
Cl2		2.8363(23)			
Cl4		3.0592(31)			
Cl2		3.3246(33)			
<b>Bi4</b>		O8	2.3070(75)		
		O4	2.3629(82)		
	O12	2.4189(92)			
	Cl6	2.5732(32)			
	O11	2.7663(72)			
	Cl3	2.9739(40)			
	Cl9	3.2312(38)			
	Cl10	3.2766(38)			
	<b>Bi5</b>	O3	2.3448(80)		
O6		2.4293(73)			
O5		2.4325(79)			
O7		2.6309(75)			
Cl1		2.6997(31)			
O4		2.884(11)			
Cl6		2.9283(26)			
Cl2		2.9516(33)			
Cl5		2.9519(31)			
<b>Bi6</b>		O8	2.4759(74)		
	O12	2.4825(91)			
	Cl7	2.5916(28)			
	O9	2.6286(86)			
	Cl9	2.6533(38)			
	O1	2.7641(83)			
	Cl10	2.7647(38)			
	Cl8	3.3012(37)			

*Table S 13. Bond sum valence values of selected atoms in  $PbBi_{10}(SeO_3)_{12}Cl_8$*

<b>Atom</b>	<b>BVS</b>
<b>Bi1</b>	3.45(9)
<b>Bi2</b>	2.77(7)
<b>Pb2</b>	2.90(7)
<b>Bi3</b>	2.59(7)
<b>Pb3</b>	2.72(7)
<b>Bi4</b>	2.86(8)
<b>Pb4</b>	3.00(8)
<b>Bi5</b>	2.47(7)
<b>Pb5</b>	2.67(7)
<b>Se1</b>	4.28(19)
<b>Se2</b>	3.76(17)
<b>Se3</b>	3.84(16)

**Table S 11. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) in  $\text{PbBi}_{10}(\text{SeO}_3)_{12}\text{Cl}_8$**

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Bi1	0.5	0	0	0.0157 (10)	
Bi2	0.25	0	0.25	0.0390 (10)	0.9
Pb2	0.25	0	0.25	0.0390 (10)	0.1
Bi3	0.5	0	0.26397 (19)	0.0359 (11)	0.9
Pb3	0.5	0	0.26397 (19)	0.0359 (11)	0.1
Bi4	0.2407 (2)	0	0	0.0279 (9)	0.9
Pb4	0.2407 (2)	0	0	0.0279 (9)	0.1
Bi5	0.61813 (12)	-0.17735 (7)	0.38264 (13)	0.0278 (5)	0.9
Pb5	0.61813 (12)	-0.17735 (7)	0.38264 (13)	0.0278 (5)	0.1
Se1	0.3767 (2)	0.12635 (19)	0.1494 (2)	0.0090 (9)	
Se2	0.6504 (3)	0.1232 (2)	0.1218 (2)	0.0197 (11)	
Se3	0.3905 (3)	-0.11306 (18)	0.3900 (2)	0.0184 (11)	
Cl1	0.5	-0.2528 (7)	0.5	0.041 (6)	
Cl2	0.75	0.25	0.2359 (9)	0.046 (7)	
Cl3	0	0.25	0.25	0.072 (11)	
Cl4	0.75	0.25	0.0086 (11)	0.044 (7)	
O1	0.7551 (18)	0.0913 (16)	0.1223 (17)	0.017 (5)*	
O2	0.2930 (17)	0.0761 (14)	0.1235 (16)	0.013 (5)*	
O3	0.4605 (19)	0.0742 (17)	0.1230 (18)	0.021 (6)*	
O4	0.6216 (17)	0.0715 (16)	0.2073 (17)	0.016 (6)*	
O5	0.371 (2)	-0.098 (2)	0.4956 (19)	0.026 (9)*	
O6	0.6236 (17)	0.0679 (15)	0.0364 (17)	0.014 (5)*	
O7	0.4953 (16)	-0.099 (2)	0.3767 (18)	0.013 (6)*	
O8	0.3779 (17)	0.1014 (16)	0.2539 (19)	0.021 (6)*	
O9	0.3631 (18)	-0.0214 (12)	0.3627 (18)	0.018 (5)*	

**Table S 15. Atomic displacement parameters ( $\text{\AA}^2$ ) in  $\text{PbBi}_{10}(\text{SeO}_3)_{12}\text{Cl}_8$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Bi1	0.025 (2)	0.0130 (10)	0.0091 (16)	0	0	0
Bi2	0.065 (2)	0.0204 (9)	0.0315 (15)	0.0145 (12)	0.0253 (11)	0.0127 (10)
Pb2	0.065 (2)	0.0204 (9)	0.0315 (15)	0.0145 (12)	0.0253 (11)	0.0127 (10)
Bi3	0.057 (2)	0.0246 (15)	0.0259 (16)	-0.0132 (12)	0	0
Pb3	0.057 (2)	0.0246 (15)	0.0259 (16)	-0.0132 (12)	0	0
Bi4	0.0326 (19)	0.0227 (14)	0.0283 (13)	0	0	-0.0011 (9)
Pb4	0.0326 (19)	0.0227 (14)	0.0283 (13)	0	0	-0.0011 (9)
Bi5	0.0300 (10)	0.0128 (6)	0.0408 (11)	-0.0002 (7)	0.0060 (6)	-0.0006 (7)
Pb5	0.0300 (10)	0.0128 (6)	0.0408 (11)	-0.0002 (7)	0.0060 (6)	-0.0006 (7)
Se1	0.0087 (16)	0.0137 (16)	0.0045 (14)	-0.0002 (12)	-0.0052 (12)	0.0030 (12)
Se2	0.033 (2)	0.0054 (15)	0.0203 (19)	-0.0021 (15)	-0.0042 (17)	0.0022 (13)
Se3	0.038 (2)	0.0120 (14)	0.0057 (17)	-0.0012 (17)	0.0059 (13)	-0.0012 (13)
Cl1	0.082 (16)	0.014 (5)	0.028 (9)	0	-0.010 (8)	0
Cl2	0.099 (18)	0.025 (6)	0.012 (7)	-0.023 (9)	0	0
Cl3	0.12 (3)	0.018 (10)	0.080 (17)	0.009 (11)	0.051 (16)	-0.001 (13)
Cl4	0.083 (17)	0.021 (9)	0.027 (9)	-0.003 (12)	0	0

*Table S 126. Selected interatomic distances (Å) in PbBi<sub>10</sub>(SeO<sub>3</sub>)<sub>12</sub>Cl<sub>8</sub>*

atom1	atom2	d, Å	atom1	atom2	d, Å
Bi1	4xO6	2.372(27)	Se1	1xO2	1.650(27)
	4xO3	2.440(30)		1xO3	1.670(31)
Bi2 Pb2	2xO4	2.490(28)	Se2	1xO8	1.720(31)
	2xO2	2.520(26)		1xO4	1.700(28)
	2xO9	2.560(29)		1xO6	1.730(28)
	2xO1	2.600(28)		1xO1	1.750(29)
	2xO8	2.720(28)		1xO7	1.690(27)
Bi3 Pb3	2xO4	2.480(28)	Se3	1xO5	1.720(31)
	2xO7	2.520(33)		1xO9	1.750(23)
	2xO8	2.650(28)		1xO2	2.980(28)
	2xO3	2.670(30)		1xO4	3.000(28)
	2xO9	2.700(29)		Bi5 Pb5	1xCl1
Bi4 Pb4	2xO5	2.490(34)	Bi5 Pb5	1xCl4	3.002(2)
	2xO2	2.520(26)		1xCl2	3.094(9)
	2xO6	2.530(27)		1xCl3	3.099(2)
	2xO1	2.540(28)			
	2xO9	2.750(29)			
Bi5 Pb5	1xO7	2.400(30)			
	1xO5	2.400(33)			
	1xO8	2.450(30)			
	1xO1	2.530(29)			

*Table S 17. Bond sum valence values of selected atoms in Bi<sub>6</sub>(SeO<sub>3</sub>)<sub>4</sub>Cl<sub>10</sub>*

Atom	BVS
<b>Bi1a</b>	3.10(3)
<b>Bi1b</b>	2.88(5)
<b>Bi2</b>	3.17(2)
<b>Bi3</b>	3.06(2)
<b>Bi4</b>	2.96(2)
<b>Bi5</b>	3.072(18)
<b>Bi6</b>	3.113(17)
<b>Se1</b>	3.83(5)
<b>Se2</b>	3.77(5)
<b>Se3a</b>	3.81(5)

---

<b>Se3b</b>	3.01(12)
<b>Se4</b>	3.89(5)

---