```
237 0.237 0.378 0.429  0.54      C59  0.55; C58  1.12; C60  1.94; Fe4  2.25; C57  2.29; C61  2.61; C37  3.14;
238 0.638 0.937 0.104  0.54 void C59  2.65; C55  2.89; C32  2.99; C56  3.18;
239 0.604 0.191 0.241  0.54      C31  2.06; N5   2.21; N6   2.44; N1   2.55; C33  2.55; N2   2.57; C35  2.84; B1   2.88; C34  2.91;
240 0.824 0.079 0.354  0.54      Fe1  1.03; C8   1.54; C12  1.80; C7   1.88; C4   2.11; C11  2.16; C13  2.29; C6   2.52; C5   2.64;
241 0.517 0.531 0.139  0.54 void C19  2.89; C18  2.89; C31  3.09;
242 0.090 0.266 0.507  0.54      C38  2.46; C39  2.62; C57  3.06;
243 0.495 0.124 0.856  0.54      C14  1.52; C3   2.22; C15  2.28; C32  2.52; N2   2.63; C16  2.72; B1   2.81;
244 0.832 0.636 0.383  0.54      C64  2.25; C43  2.79; C38  2.95;
245 0.659 0.516 0.529  0.54      C59  2.56; C63  3.20;
246 0.374 0.798 0.298  0.54      N6   0.63; N5   0.77; C35  1.64; C33  1.77; B1   2.06; C34  2.11; Cr   2.45; N2   2.74; N1   2.78;
247 0.499 0.706 0.181  0.53      C16  1.42; C3   1.86; C14  1.92; N2   2.41; C2   2.62; C31  2.83; C15  3.13; B1   3.13;
248 0.418 0.379 0.674  0.53      C44  1.66; C18  2.49; C32  2.52; C19  2.73; C45  2.74; C43  2.76; C30  2.79; C31  2.94;
249 0.667 0.781 0.896  0.53      Fe3  0.99; C44  1.62; C37  1.78; C43  1.89; C38  1.96; C45  2.22; C36  2.36; C42  2.51; C39  2.57;
250 0.176 0.234 0.117  0.53      C43  2.12; C38  2.40; C42  2.50; C39  2.61; Fe3  2.61;
251 0.188 0.452 0.420  0.53      C60  0.93; C59  0.96; Fe4  2.07; C61  2.24; C58  2.25; C57  2.76; C55  3.10;
252 0.278 0.142 0.859  0.53      C56  1.87; C58  1.91; Fe4  2.00; C59  2.22; C55  2.37; C52  2.81; C57  2.91;
253 0.010 0.045 0.066  0.53      C50  2.35; C49  2.99; C60  3.02;
254 0.357 0.317 0.049  0.53      C36  0.80; C40  0.89; Fe3  1.61; C37  1.88; C39  1.93; C38  2.33; C41  2.93; C45  3.00;
255 0.922 0.455 0.594  0.53      C60  2.08; C61  2.90; C49  3.14;
256 0.266 0.313 0.083  0.53      C39  1.12; Fe3  1.21; C40  1.60; C38  1.85; C42  2.15; C36  2.36; C37  2.47; C41  2.52; C43  2.57;
257 0.377 0.235 0.593  0.53      Fe3  0.85; C36  1.59; C37  1.79; C45  1.87; C44  2.08; C40  2.13; C41  2.31; C38  2.37; C39  2.54;
258 0.582 0.824 0.008  0.53      C37  1.92; C15  2.16; C36  2.30;
259 0.469 0.738 0.930  0.53      C34  1.43; C33  2.39; C35  2.42; C36  2.58; C47  2.86; C45  3.10; C46  3.13;
260 0.064 0.173 0.517  0.53 void C39  2.68; C10  2.83;
261 0.923 0.648 0.321  0.53      C26  2.54; C27  2.55; C25  3.01; C28  3.03;
262 0.520 0.670 0.657  0.53      C14  0.91; C3   1.83; C16  1.88; C15  2.16; N2   2.37; B1   2.64; C2   3.14;
263 0.298 0.611 0.391  0.53      C48  1.09; C46  2.26; C47  2.88; C35  2.91;
264 0.590 0.530 0.272  0.53      C19  0.74; C18  0.99; N4   1.79; C30  1.83; C17  2.00; N3   2.35; C32  2.49; C31  2.62;
265 0.689 0.019 0.063  0.53      C59  2.54; C48  2.91; C60  3.16;
266 0.945 0.907 0.408  0.53      C7   1.93; C6   2.16;
267 0.280 0.438 0.727  0.53      C17  1.10; C29  1.45; C18  1.57; C28  2.18; N3   2.24; C25  2.64; C19  2.66; C64  2.91; N4   2.92;
268 0.373 0.048 0.507  0.53      C40  2.28; C22  2.83; C36  2.95;
269 0.666 0.330 0.022  0.53      C47  1.59; C46  2.86;
270 0.202 0.689 0.497  0.53      C63  2.30; C47  2.42; C9   2.88;
271 0.691 0.452 0.187  0.53      N3   1.65; C17  1.77; C21  2.33; C29  2.40; N4   2.47; C18  2.63; N6   2.76; Cr   2.83; Fe2  2.95;
272 0.597 0.920 0.944  0.53 void C37  2.63; C64  3.12;
273 0.943 0.284 0.013  0.53      C10  2.33; C9   2.33;
274 0.971 0.548 0.407  0.53      C50  2.25; C49  2.85; C51  3.12; C60  3.19;
275 0.189 0.330 0.493  0.52      C38  1.63; C58  2.14; C59  2.16; C37  2.42; C57  2.60; C60  2.66; C39  2.70; C61  2.89;
276 0.366 0.729 0.087  0.52      C2   0.67; C3   1.69; C1   1.97; C14  2.59; C15  2.65; N2   2.75; N1   2.87; C13  2.99;
277 0.637 0.922 0.063  0.52      C59  2.35; C58  2.99; C15  3.03;
278 0.543 0.578 0.033  0.52 void
279 0.581 0.903 0.602  0.52 void C16  2.82; C22  2.84;
280 0.094 0.420 0.351  0.52      Fe4  1.12; C61  1.41; C60  1.68; C53  2.05; C57  2.14; C54  2.15; C49  2.18; C59  2.43; C52  2.62;
281 0.982 0.436 0.655  0.52 void C26  2.89; C54  2.94;
282 0.141 0.065 0.145  0.52      C64  2.11; C51  2.69; C50  2.82; C25  2.84; C62  2.90; C29  2.96;
283 0.752 0.701 0.593  0.52      C58  0.82; C59  1.95; C57  2.04; Fe4  2.56; C60  3.06; C61  3.10; C37  3.11;
284 0.543 0.235 0.108  0.52      C34  0.56; C33  1.68; C35  1.86; C45  2.60; N5   2.69; N6   2.80; C46  2.87; C47  3.11; C36  3.18;
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285 0.846 0.497 0.619  0.52      C60  1.56; Fe4  2.08; C59  2.21; C54  2.23; C55  2.56; C61  2.59; C53  3.11; C48  3.11;
286 0.547 0.662 0.454  0.52      C37  2.09; C36  2.51; C34  2.84; C15  3.13;
287 0.350 0.911 0.975  0.52 void C63  2.62; C48  2.94; C47  3.14;
288 0.030 0.626 0.049  0.52      C10  1.16; C11  2.12; C9   2.28; Fe1  2.34; C6   2.81;
289 0.362 0.312 0.449  0.52      C15  2.20; C37  2.21; C58  2.51; C36  2.60; C59  2.79; C14  3.12; C38  3.17;
290 0.765 0.923 0.923  0.52      C64  1.11; C62  2.48; C38  2.81; C63  2.99; C37  3.15;
291 0.252 0.065 0.186  0.51      C17  1.95; C64  1.99; C29  2.07; C18  2.36; N3   2.73; C28  2.75; C62  2.83; C25  2.85; C43  3.04;
292 0.091 0.796 0.419  0.51 void
293 0.026 0.949 0.017  0.51      C50  1.89; C49  2.69; C61  3.09; C51  3.11; C60  3.19;
294 0.130 0.110 0.740  0.51      C52  0.79; C53  1.12; C56  1.83; C54  2.07; C55  2.34; Fe4  2.51;
295 0.340 0.377 0.512  0.51      C37  1.67; C38  2.51; C59  2.66; C36  2.91; C58  3.14;
296 0.073 0.340 0.713  0.51      C27  1.80; C26  2.00; C28  2.58; C25  2.82; C29  3.10;
297 0.167 0.878 0.304  0.51      Cl   1.76; Cr   2.20; C20  2.41; C25  2.72; C21  2.84; N6   3.05; N3   3.08; Fe2  3.12;
298 0.877 0.719 0.395  0.51 void C38  2.76; C43  2.94; C39  3.02;
299 0.062 0.893 0.025  0.51      C50  1.70; C49  2.46; C51  2.64; C63  3.04; C61  3.11;
300 0.566 0.809 0.875  0.51      C44  1.52; C45  1.83; C33  2.17; Fe3  2.23; C34  2.29; C37  2.59; C43  2.77; C36  2.90; C41  3.07;
301 0.906 0.669 0.577  0.51      C57  1.02; C61  1.09; C58  1.87; C60  1.94; C49  2.18; C59  2.27; Fe4  2.60; N8   3.06; C50  3.18;
302 0.439 0.515 0.617  0.51      C32  1.80; C30  2.98; C19  3.14; C64  3.15; C62  3.17;
303 0.842 0.905 0.639  0.51      Fe2  1.03; C23  1.34; C22  1.84; C24  1.87; C27  2.04; C28  2.30; C21  2.43; C20  2.45; C26  2.46;
304 0.419 0.093 0.929  0.51      C15  2.25; C14  2.89;
305 0.095 0.073 0.130  0.51 void C64  2.64; C50  2.70; C51  2.95; C25  3.17;
306 0.021 1.005 0.359  0.51      C24  1.60; C20  2.29; Fe2  2.64; C7   2.75; C23  2.80; C26  2.82; C11  3.00;
307 0.886 0.122 0.118  0.51      C48  2.31;
308 0.098 0.048 0.945  0.51      C60  0.97; C61  1.76; C59  2.17; C49  2.48; C50  2.81; C57  2.87; Fe4  2.96; C58  3.03;
309 0.047 0.237 0.415  0.51      C57  1.87; C10  2.18; C11  2.46; C61  2.56; C49  2.93; C58  2.98; N8   3.19;
310 0.164 0.252 0.076  0.51      C38  1.78; C39  1.83; Fe3  2.61; C43  2.88; C42  3.02; C37  3.12; C40  3.15;
311 0.877 0.390 0.265  0.51      N7   1.81; N8   1.91; Cl   2.01; Cr   2.04; C25  2.26; C51  2.94; C49  3.04; N3   3.07; C29  3.18;
312 0.037 0.125 0.857  0.51      C61  1.01; C49  1.22; N8   1.69; C57  1.79; Fe4  2.03; C60  2.20; C50  2.58; C53  2.67; C58  2.88;
313 0.856 0.500 0.164  0.51      Fe2  0.98; C20  1.35; C24  1.77; C21  1.88; C25  1.98; C26  2.22; C23  2.38; C22  2.43; C29  2.45;
314 0.247 0.925 0.936  0.51      C48  2.10; C63  2.86; C60  3.02; C59  3.06;
315 0.845 0.838 0.129  0.51      C57  0.95; C58  1.12; Fe4  1.22; C61  1.72; C59  1.87; C60  2.14; C52  2.64; C56  2.75; C53  2.98;
316 0.126 0.017 0.906  0.51      C60  0.87; C59  1.99; C61  2.01; Fe4  2.25; C49  2.83; C54  2.90; C58  3.02; C57  3.04;
317 0.768 0.594 0.730  0.51      C56  0.49; C55  1.27; C52  1.51; C54  2.10; C53  2.20; Fe4  2.34; C42  3.16;
318 0.801 0.891 0.180  0.51      Fe4  0.97; C56  1.06; C55  1.45; C52  1.54; C54  1.96; C53  2.01; C58  2.44; C59  2.58; C57  2.72;
319 0.109 0.547 0.466  0.51      C60  2.32; C63  2.96;
320 0.694 0.283 0.257  0.51      N1   1.38; Cr   1.40; N6   1.55; N5   2.04; N2   2.06; B1   2.34; C1   2.61; N3   2.72; C35  2.73;
321 0.049 0.391 0.487  0.51      C61  2.32; C60  2.44; C49  2.61; C50  2.61; C57  3.11;
322 0.843 0.953 0.704  0.51      Fe2  0.93; C25  1.16; C29  1.36; C26  1.42; C28  1.67; C27  1.72; C20  2.64; C21  2.69; C17  2.69;
323 0.253 0.756 0.914  0.51      C46  0.90; C47  0.92; C48  1.85; C35  2.29;
324 0.170 0.467 0.282  0.50      C54  0.59; C55  0.96; C53  1.41; C56  1.68; C52  1.91; Fe4  2.00;
325 0.701 0.046 0.492  0.50      C5   1.96; C4   2.48; C21  2.93; C22  2.99;
326 0.382 0.485 0.987  0.50 void C22  2.68; C40  3.02; C21  3.04;
327 0.308 0.238 0.061  0.50      C37  0.97; C38  1.06; Fe3  1.19; C36  1.63; C39  1.72; C40  1.98; C44  2.72; C43  2.77; C45  3.03;
328 0.378 0.302 0.623  0.50      C44  1.14; Fe3  1.60; C45  1.86; C43  2.04; C37  2.24; C33  2.72; C38  2.73; C36  2.75; C41  2.77;
329 0.207 0.468 0.499  0.50      C59  2.15; C60  2.20; C63  2.53; C64  2.62; C62  3.08;
330 0.691 0.891 0.913  0.50      C64  1.84; C37  2.34; C38  2.51; C44  2.75; Fe3  2.93; C43  3.05; C62  3.18;
331 0.536 0.265 0.652  0.50      C34  0.84; C33  0.86; N5   1.89; C35  1.92; C45  1.94; N6   2.36; C44  2.63;
332 0.730 0.315 0.976  0.50      C47  2.28; C9   2.45; C2   2.49; C13  2.93; C1   2.95; C5   3.08;
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333 0.908 0.077 0.014  0.50 void C50  2.64; C63  2.83; C60  3.08;
334 0.126 0.139 0.523  0.50      C39  1.93; C6   2.51; C40  2.93; C38  3.00; C23  3.00; C7   3.15; C5   3.18;
335 0.141 0.674 0.945  0.50 void C47  2.70; C20  2.80; C9   3.13; C46  3.20;
336 0.363 0.627 0.148  0.50      C2   2.04; C1   2.23; C31  2.41; C4   2.42; C3   2.75; C13  2.88; N1   2.96; C8   3.07; N2   3.20;
337 0.576 0.129 0.429  0.50      C2   2.40; C3   3.10;
338 0.582 0.530 0.615  0.50      C32  1.94;
339 0.568 0.080 0.517  0.00 void
340 0.949 0.769 0.832  0.00 void
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Unique Density Minima in Enhanced Difference Map (CutOff level = -0.50 eA-3)

#	x	y	z	(e/A^3)	Shortest Contacts within 3.2 Angstrom (Excl. H)
1	0.841	0.908	0.389	-0.99	C7 1.33; C6 1.92; C8 2.07; C5 2.71; C4 2.78; C42 2.88; C39 2.89;
2	0.668	0.217	0.399	-0.89	C2 0.50; C1 1.34; C3 1.88; C13 2.30; N1 2.42; N2 2.62; C9 2.89; C14 3.07;
3	0.844	0.405	0.655	-0.88	C48 1.89; C54 2.31; C55 2.87; C46 3.18;
4	0.836	0.042	0.665	-0.88	C20 1.21; Fe2 1.63; C21 1.69; C25 2.18; C24 2.21; C29 2.61; C22 2.68; C26 2.80; C23 2.90;
5	0.767	0.675	0.249	-0.87	C28 1.24; C27 2.13; C29 2.26; C43 2.52; C17 3.00; C18 3.10; C26 3.14;
6	0.663	0.780	0.398	-0.85	Fe3 0.16; C36 1.95; C40 1.98; C41 1.98; C45 1.98; C37 2.05; C44 2.06; C42 2.07; C39 2.10;
7	0.831	0.394	0.895	-0.79	Fe1 0.25; C13 1.83; C9 1.85; C12 1.94; C10 2.01; C4 2.04; C11 2.06; C5 2.10; C8 2.16;
8	0.236	0.672	0.742	-0.77	Cr 0.10; N6 2.11; N1 2.13; N7 2.18; N3 2.27; Cl 2.35; N5 2.99; N2 3.02; N8 3.04;
9	0.818	0.405	0.773	-0.75	C12 2.07; C54 2.57; C8 2.75; C11 2.86; C55 2.94; Fe1 2.94; C13 3.18;
10	0.453	0.184	0.155	-0.69	C44 1.34; C45 1.71; C33 1.96; C34 2.31; Fe3 2.69; C43 2.76; N5 3.08; C41 3.09; C32 3.16;
11	0.160	0.141	0.850	-0.69	Fe4 0.68; C57 1.54; C58 1.60; C61 1.98; C59 2.06; C52 2.08; C56 2.17; C60 2.26; C53 2.41;
12	0.171	0.088	0.850	-0.68	Fe4 0.36; C55 1.86; C59 1.87; C60 1.93; C54 1.96; C56 2.02; C58 2.09; C61 2.18; C53 2.19;
13	0.262	0.059	0.406	-0.67	C22 0.23; C21 1.47; C23 1.63; Fe2 2.09; C20 2.44; C24 2.50;
14	0.108	0.215	0.280	-0.65	C27 1.34; C28 2.26; C26 2.55; C52 2.69; C57 3.15;
15	0.513	0.325	0.031	-0.65	C36 2.33; C34 2.73;
16	0.983	0.545	0.327	-0.64	C26 2.38; C25 2.53; C54 3.04; C49 3.05; C50 3.14;
17	0.316	0.158	0.538	-0.63	C40 0.12; C36 1.36; C39 1.45; Fe3 1.94; C37 2.26; C38 2.30; C41 3.18;
18	0.840	0.969	0.659	-0.63	Fe2 0.41; C20 1.65; C24 1.78; C21 1.82; C23 2.01; C22 2.04; C25 2.09; C26 2.16; C29 2.26;
19	0.142	0.096	0.258	-0.63	C27 1.06; C26 1.16; C28 1.25; C25 1.41; C29 1.47; Fe2 2.00; C17 2.90;
20	0.768	0.703	0.341	-0.62	C43 1.12; C42 2.16; C44 2.32; Fe3 2.58; C38 3.05;
21	0.851	0.426	0.883	-0.62	Fe1 0.52; C7 1.64; C8 1.78; C6 1.92; C11 2.01; C12 2.10; C4 2.11; C5 2.19; C10 2.27;
22	0.310	0.439	0.249	-0.62	C56 1.86; C55 2.01; C42 2.88; C30 2.89; C8 2.89; C41 2.91; C52 2.97; C54 3.08;
23	0.735	0.346	0.233	-0.62	Cr 0.74; N6 1.60; N3 1.88; N5 2.52; N1 2.52; Cl 2.62; N4 2.71; C35 2.76; N7 2.78;
24	0.843	0.141	0.540	-0.61	C20 2.55; C47 2.88; C9 2.96; C5 3.04; C24 3.19; C21 3.19;
25	0.402	0.796	0.194	-0.60	N2 0.21; C3 1.39; B1 1.46; N1 1.51; C2 2.30; C1 2.32; N5 2.40; C14 2.47; N4 2.62;
26	0.718	0.015	0.305	-0.60	C8 1.40; C4 2.24; C7 2.69; C31 2.76; Fe1 2.99; C55 3.02;
27	0.419	0.813	0.343	-0.60	C33 1.18; N5 1.22; C34 1.38; N6 1.48; C35 1.52; C45 2.53; B1 2.66; C46 2.95;
28	0.157	0.500	0.049	-0.60	C6 0.56; C5 0.94; C7 1.85; C4 2.07; Fe1 2.14; C8 2.42;
29	0.860	0.190	0.569	-0.60	C47 2.57; C20 2.87; C46 2.89;
30	0.861	0.704	0.657	-0.60	C57 1.28; Fe4 1.78; C58 1.83; C52 2.27; C61 2.33; C56 2.75; C59 2.85; C53 2.92; C60 3.08;
31	0.020	0.309	0.015	-0.59	C10 2.45; C9 3.11;
32	0.751	0.955	0.198	-0.59	C55 0.35; C56 1.20; C54 1.73; Fe4 2.17; C52 2.34; C53 2.51;
33	0.331	0.862	0.637	-0.59	C2 1.83; C1 1.83; C4 2.23; C13 2.34; N1 2.75; C3 2.77; Fe1 2.79; C31 2.89; C8 2.92;
34	0.096	0.154	0.538	-0.58	C39 2.29; C6 2.70; C7 3.10; C38 3.16;
35	0.176	0.453	0.067	-0.58	C6 0.98; C5 1.43; C7 1.57; C4 2.05; C8 2.11; Fe1 2.65; C39 2.84; C40 3.09;
36	0.064	0.061	0.102	-0.58	C50 2.36; C64 2.90; C51 2.96; C49 3.12;
37	0.999	0.453	0.100	-0.58	C24 2.08; C7 2.29; C6 2.56; C20 2.57;
38	0.781	0.124	0.164	-0.58	C48 1.11; C46 2.39; C54 2.83; C55 2.95; C35 3.12;
39	0.970	0.518	0.380	-0.57	C50 1.93; C49 2.25; C51 2.72; C61 2.89; C60 2.94; N8 3.02;
40	0.751	0.735	0.249	-0.57	C43 2.17; C28 2.19; C42 2.55; C52 2.77; C27 2.82; C56 2.87; C44 3.17;
41	0.124	0.830	0.467	-0.57	C9 2.58; C10 3.00; C47 3.12; C20 3.15;
42	0.344	0.516	0.936	-0.57	C21 1.82; C22 1.96; C20 3.07;
43	0.272	0.093	0.203	-0.57	C17 1.88; C29 1.99; C18 2.02; C28 2.37; C64 2.53; C43 2.60; C44 2.89; N3 2.92; C25 3.02;
44	0.320	0.032	0.313	-0.57	C17 1.43; C18 1.87; C29 1.87; N3 2.28; C28 2.42; C21 2.56; Fe2 2.58; C19 2.75; C22 2.78;

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 45 0.394 0.921 0.609 -0.56      C4   2.18; C2   2.75; C31  3.12; C5   3.17;
 46 0.143 0.999 0.188 -0.56      C25  1.69; C29  2.19; C51  2.21; N7   2.28; C26  2.69; C50  2.71; C17  2.75; N8   2.77; C64  2.81;
 47 0.948 0.625 0.302 -0.56      C26  1.90; C27  2.21; C25  2.57; C28  2.95; C29  3.14;
 48 0.202 0.408 0.696 -0.56      C29  1.80; C28  2.15; C25  2.35; C17  2.37; C64  2.60; C27  2.79; C26  2.88; C18  2.96; C43  2.96;
 49 0.882 0.292 0.226 -0.56      Cl   0.14; Cr   2.30; N8   2.91; N7   3.08;
 50 0.511 0.858 0.322 -0.56      C33  1.56; C45  1.70; N5   1.75; C41  1.82; B1   2.17; C34  2.72; N4   2.78; N6   2.92; C44  3.11;
 51 0.156 0.375 0.725 -0.56      C28  1.50; C27  1.62; C29  1.83; C26  1.98; C25  2.09; Fe2  2.95; C17  2.99;
 52 0.312 0.396 0.710 -0.55      C18  1.61; C17  1.95; C29  2.35; C43  2.43; C44  2.46; C28  2.60; C19  2.69; C64  2.84; N3   3.02;
 53 0.488 0.780 0.885 -0.55      C34  0.96; C33  1.57; C45  2.21; C35  2.32; C44  2.67; N5   2.77; C36  3.01; Fe3  3.03; N6   3.11;
 54 0.160 0.999 0.265 -0.55      C25  0.53; C29  1.27; C26  1.86; Fe2  1.94; C17  2.27; C28  2.37; C27  2.61; N3   2.71; C20  3.00;
 55 0.855 0.594 0.670 -0.55      Fe4  0.40; C53  1.65; C54  1.72; C52  1.80; C55  1.90; C56  1.93; C61  2.20; C60  2.26; C57  2.31;
 56 0.027 0.469 0.819 -0.55      C26  1.77; C24  2.19; Fe2  2.24; C25  2.53; C20  2.68; C27  2.69; C11  2.99; C23  3.06; C53  3.19;
 57 0.877 0.638 0.821 -0.55      C52  2.06; C53  2.53; C7   2.56; C42  2.85; C56  2.94; C8   3.14;
 58 0.770 0.262 0.780 -0.55      N1   1.73; Cr   1.75; C12  2.04; C1   2.29; C13  2.35; N6   2.66; Cl   2.70; N7   2.84; N2   2.99;
 59 0.406 0.017 0.640 -0.55      C4   2.39; C41  2.64; C8   2.91; C31  2.96; C30  3.15;
 60 0.396 0.784 0.587 -0.55      C2   1.00; C3   1.70; C14  2.34; C15  2.36; C1   2.37; N2   2.91; C16  3.09; N1   3.20;
 61 0.578 0.876 0.798 -0.55      C44  1.79; C18  2.00; C19  2.40; C31  2.56; C30  2.58; C32  2.70; C43  2.77; C45  2.82; C17  3.17;
 62 0.300 0.557 0.865 -0.55      C21  1.34; C20  2.42; C22  2.44; Fe2  2.83; N3   2.93; C17  2.96; N6   3.04; C29  3.18;
 63 0.143 0.675 0.350 -0.54      C48  1.77; C46  2.38; Cl   2.69;
 64 0.561 0.174 0.858 -0.54      C3   0.95; C14  1.33; N2   1.56; C2   2.15; C15  2.28; B1   2.45; C16  2.66; N1   2.66; C1   2.90;
 65 0.111 0.201 0.898 -0.54      C57  0.31; C61  1.53; C58  1.55; Fe4  2.35; C59  2.44; C60  2.45; C49  2.60; N8   3.15;
 66 0.312 0.985 0.304 -0.54      C17  1.28; N3   1.62; C29  1.97; C18  2.11; N4   2.43; C21  2.50; C19  2.66; Fe2  2.77; C25  2.91;
 67 0.516 0.668 0.215 -0.54      C16  2.05; C31  2.08; C18  2.66; C3   2.82; C14  2.93; N2   3.04; C44  3.12; C30  3.12; C19  3.17;
 68 0.521 0.298 0.235 -0.54      B1   1.23; N5   1.29; C33  1.74; C45  2.03; N2   2.12; N6   2.61; N4   2.69; C41  2.71; C44  2.96;
 69 0.375 0.172 0.447 -0.54      C36  2.14; C40  2.52; C22  2.89; C15  2.92; C37  3.03; C16  3.13;
 70 0.156 0.065 0.322 -0.54      Fe2  0.41; C27  1.66; C26  1.68; C28  1.78; C25  1.84; C29  1.90; C23  2.27; C24  2.29; C22  2.37;
 71 0.128 0.359 0.789 -0.54      C27  0.13; C28  1.38; C26  1.48; Fe2  1.97; C29  2.32; C25  2.35;
 72 0.169 0.235 0.662 -0.54      C43  2.05; C42  2.10; C52  3.08; Fe3  3.16;
 73 0.691 0.312 0.930 -0.54      C2   1.39; C1   1.99; C13  2.40; C9   2.57; C3   2.74; C4   2.98; Fe1  3.13; C47  3.19;
 74 0.502 0.639 0.336 -0.54      C32  2.21; C44  2.28; C34  2.42; C33  2.46; C31  2.62; C45  2.66; C30  2.78;
 75 0.026 0.670 0.795 -0.54      Cl   1.66; C53  2.77; C52  2.95;
 76 0.997 0.379 0.712 -0.54      C26  1.89; C27  2.45; C25  2.91;
 77 0.311 0.390 0.281 -0.54      C56  1.26; C55  1.96; C52  2.58; C42  2.96; Fe4  3.11; C54  3.18; C41  3.19;
 78 0.111 0.077 0.577 -0.54      C6   1.36; C7   1.49; C5   2.52; C8   2.64; C39  3.06; C4   3.09; Fe1  3.14;
 79 0.436 0.639 0.610 -0.54      C14  1.72; C3   1.76; C15  1.99; N2   2.43; C2   2.59; C63  3.08; B1   3.20;
 80 0.903 0.471 0.977 -0.53      C6   1.20; C5   1.81; Fe1  2.36; C7   2.51; C10  2.90; C4   3.04; C24  3.19;
 81 0.860 0.470 0.515 -0.53      C60  2.30; C63  2.48; C59  3.01; C50  3.02;
 82 0.360 0.030 0.530 -0.53      C40  2.35; C5   2.72; C4   2.73; C22  3.20;
 83 0.372 0.436 0.071 -0.53      C40  2.02; C4   2.56; C36  2.82; C41  2.91; C5   2.97; Fe3  3.03; C39  3.14;
 84 0.286 0.153 0.725 -0.53      C42  1.43; C56  2.00; C41  2.11; C43  2.39; C52  2.54; C55  3.01; C45  3.14;
 85 0.907 0.921 0.375 -0.53      C7   1.31; C6   2.16; C8   2.52;
 86 0.861 0.971 0.226 -0.53      C54  0.47; C53  1.07; C55  1.47; C52  1.94; C56  2.06; Fe4  2.14;
 87 0.043 0.345 0.343 -0.53      C61  1.42; C57  1.61; C49  1.71; N8   1.76; Fe4  2.03; C53  2.58; C60  2.65; C52  2.79; C58  2.81;
 88 0.033 0.139 0.671 -0.53 void C53  2.62; C52  2.66; Cl   3.07; C7   3.11;
 89 0.654 0.113 0.377 -0.53      C4   1.92; C2   2.12; C1   2.39; C13  2.82; C8   2.83; Fe1  2.92; C31  2.96; C5   2.97; C3   3.07;
 90 0.785 0.837 0.984 -0.53      C38  1.30; C37  2.04; C59  2.48; C39  2.59; C58  2.62; C60  3.06; Fe3  3.19;
 91 0.620 0.247 0.282 -0.53      N2   1.20; N1   1.36; B1   2.00; C3   2.10; N5   2.12; C1   2.21; N6   2.51; C2   2.57; Cr   2.87;
 92 0.734 0.940 0.352 -0.53      C8   1.27; C4   1.93; C7   2.09; C42  2.31; C41  2.41; C5   2.79; C6   2.86;
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381 0.503 0.062 0.973  0.00 void C15  2.71;
382 0.988 0.874 0.872  0.00 void
383 0.075 0.751 0.893  0.00 void Cl   3.08;
384 0.949 0.769 0.831  0.00 void
385 0.518 0.955 0.967  0.00 void
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Unique Density Minima in Enhanced Difference Map (CutOff level = -0.50 eA-3)

#	x	y	z	(e/A^3)	Shortest Contacts within 3.2 Angstrom (Excl. H)
1	0.841	0.908	0.389	-0.98	C7 1.33; C6 1.92; C8 2.07; C5 2.71; C4 2.78; C39 2.89; C42 2.89;
2	0.833	0.053	0.658	-0.89	C20 1.07; C21 1.61; Fe2 1.83; C24 2.21; C25 2.43; C22 2.69; C29 2.83; C23 2.95; C26 3.05;
3	0.157	0.907	0.842	-0.87	C48 1.92; C54 2.24; C55 2.80;
4	0.668	0.217	0.399	-0.87	C2 0.50; C1 1.34; C3 1.88; C13 2.30; N1 2.43; N2 2.63; C9 2.89; C14 3.07;
5	0.767	0.675	0.249	-0.85	C28 1.25; C27 2.13; C29 2.26; C43 2.51; C17 3.01; C18 3.11; C26 3.14;
6	0.662	0.780	0.399	-0.80	Fe3 0.17; C36 1.94; C40 1.98; C45 1.98; C41 1.99; C37 2.04; C44 2.06; C42 2.09; C39 2.10;
7	0.830	0.394	0.894	-0.77	Fe1 0.25; C13 1.82; C9 1.86; C12 1.94; C10 2.02; C4 2.04; C11 2.05; C5 2.11; C8 2.16;
8	0.236	0.828	0.243	-0.73	Cr 0.12; N6 2.08; N1 2.15; N7 2.21; N3 2.27; Cl 2.33; N5 2.97; N2 3.04; N8 3.07;
9	0.818	0.405	0.773	-0.72	C12 2.07; C54 2.58; C8 2.75; C11 2.86; Fe1 2.94; C55 2.94; C13 3.17;
10	0.547	0.689	0.344	-0.69	C44 1.31; C45 1.61; C33 1.89; C34 2.27; Fe3 2.64; C43 2.72; C41 3.00; N5 3.01;
11	0.263	0.059	0.406	-0.68	C22 0.23; C21 1.47; C23 1.63; Fe2 2.09; C20 2.45; C24 2.50;
12	0.841	0.860	0.149	-0.68	Fe4 0.67; C57 1.52; C58 1.59; C61 1.95; C59 2.04; C52 2.10; C56 2.20; C60 2.22; C53 2.41;
13	0.108	0.215	0.280	-0.66	C27 1.33; C28 2.26; C26 2.55; C52 2.70; C57 3.16;
14	0.514	0.325	0.031	-0.66	C36 2.34; C34 2.73;
15	0.172	0.088	0.850	-0.65	Fe4 0.35; C55 1.86; C59 1.88; C60 1.93; C54 1.96; C56 2.02; C58 2.08; C61 2.18; C53 2.19;
16	0.142	0.096	0.259	-0.64	C27 1.05; C26 1.16; C28 1.25; C25 1.41; C29 1.47; Fe2 2.00; C17 2.90;
17	0.064	0.061	0.102	-0.63	C50 2.36; C64 2.90; C51 2.97; C49 3.12;
18	0.768	0.703	0.341	-0.63	C43 1.12; C42 2.16; C44 2.32; Fe3 2.58; C38 3.05;
19	0.860	0.189	0.569	-0.63	C47 2.58; C20 2.86; C46 2.90;
20	0.982	0.544	0.327	-0.62	C26 2.38; C25 2.52; C49 3.04; C54 3.04; C50 3.13;
21	0.317	0.158	0.538	-0.62	C40 0.12; C36 1.36; C39 1.46; Fe3 1.95; C37 2.26; C38 2.30; C41 3.18;
22	0.843	0.141	0.540	-0.61	C20 2.55; C47 2.88; C9 2.97; C5 3.04; C24 3.19; C21 3.19;
23	0.310	0.440	0.249	-0.61	C56 1.86; C55 2.01; C42 2.88; C30 2.89; C8 2.89; C41 2.91; C52 2.97; C54 3.08;
24	0.019	0.309	0.015	-0.61	C10 2.45; C9 3.10;
25	0.156	0.500	0.049	-0.60	C6 0.56; C5 0.94; C7 1.85; C4 2.08; Fe1 2.14; C8 2.42;
26	0.851	0.426	0.883	-0.60	Fe1 0.51; C7 1.65; C8 1.79; C6 1.92; C11 2.00; C12 2.09; C4 2.11; C5 2.19; C10 2.25;
27	0.718	0.015	0.305	-0.60	C8 1.41; C4 2.25; C7 2.69; C31 2.76; Fe1 3.00; C55 3.01;
28	0.840	0.969	0.660	-0.60	Fe2 0.40; C20 1.66; C24 1.79; C21 1.83; C23 2.01; C22 2.05; C25 2.08; C26 2.15; C29 2.26;
29	0.402	0.796	0.194	-0.59	N2 0.21; C3 1.39; B1 1.46; N1 1.51; C2 2.30; C1 2.32; N5 2.40; C14 2.47; N4 2.62;
30	0.331	0.862	0.637	-0.59	C2 1.83; C1 1.83; C4 2.23; C13 2.34; N1 2.75; C3 2.77; Fe1 2.79; C31 2.88; C8 2.92;
31	0.860	0.703	0.657	-0.58	C57 1.29; Fe4 1.78; C58 1.83; C52 2.27; C61 2.33; C56 2.74; C59 2.85; C53 2.92; C60 3.08;
32	0.736	0.346	0.233	-0.58	Cr 0.74; N6 1.60; N3 1.88; N5 2.52; N1 2.52; Cl 2.62; N4 2.72; C35 2.76; N7 2.78;
33	0.419	0.812	0.343	-0.58	C33 1.18; N5 1.23; C34 1.36; N6 1.48; C35 1.51; C45 2.54; B1 2.67; C46 2.94;
34	0.156	0.375	0.725	-0.58	C28 1.50; C27 1.62; C29 1.83; C26 1.98; C25 2.09; Fe2 2.95; C17 2.99;
35	0.751	0.735	0.249	-0.58	C43 2.16; C28 2.19; C42 2.55; C52 2.77; C27 2.82; C56 2.87; C44 3.17;
36	0.271	0.092	0.203	-0.58	C17 1.88; C29 1.98; C18 2.02; C28 2.37; C64 2.53; C43 2.61; C44 2.90; N3 2.92; C25 3.01;
37	0.781	0.124	0.164	-0.58	C48 1.11; C46 2.39; C54 2.83; C55 2.95; C35 3.12;
38	0.751	0.955	0.197	-0.58	C55 0.35; C56 1.21; C54 1.73; Fe4 2.16; C52 2.34; C53 2.51;
39	0.394	0.920	0.609	-0.57	C4 2.18; C2 2.74; C31 3.12; C5 3.16;
40	0.176	0.453	0.067	-0.57	C6 0.98; C5 1.44; C7 1.57; C4 2.06; C8 2.11; Fe1 2.65; C39 2.83; C40 3.10;
41	0.096	0.154	0.538	-0.57	C39 2.29; C6 2.70; C7 3.11; C38 3.16;
42	0.142	0.499	0.687	-0.57	C25 1.71; C51 2.21; C29 2.21; N7 2.31; C26 2.69; C50 2.70; C17 2.77; N8 2.79; C64 2.79;
43	0.124	0.829	0.467	-0.57	C9 2.57; C10 3.00; C47 3.11; C20 3.16;
44	0.970	0.518	0.380	-0.57	C50 1.93; C49 2.25; C51 2.72; C61 2.89; C60 2.94; N8 3.02;

45	0.999	0.453	0.100	-0.57		C24	2.08;	C7	2.30;	C6	2.57;	C20	2.57;								
46	0.344	0.515	0.936	-0.57		C21	1.82;	C22	1.97;	C20	3.07;										
47	0.360	0.030	0.530	-0.56		C40	2.35;	C5	2.71;	C4	2.72;										
48	0.877	0.637	0.821	-0.56		C52	2.05;	C53	2.52;	C7	2.56;	C42	2.85;	C56	2.93;	C8	3.14;				
49	0.027	0.469	0.819	-0.56		C26	1.77;	C24	2.18;	Fe2	2.23;	C25	2.53;	C20	2.67;	C27	2.68;	C11	3.00;	C23	3.05;	C53	3.19;
50	0.320	0.031	0.313	-0.56		C17	1.43;	C18	1.86;	C29	1.87;	N3	2.28;	C28	2.42;	C21	2.56;	Fe2	2.59;	C19	2.75;	C22	2.79;
51	0.936	0.310	0.478	-0.56		C9	2.53;	C50	2.65;	C10	2.77;	C49	2.90;										
52	0.948	0.625	0.302	-0.56		C26	1.90;	C27	2.21;	C25	2.57;	C28	2.95;	C29	3.14;								
53	0.202	0.408	0.696	-0.56		C29	1.80;	C28	2.15;	C25	2.35;	C17	2.37;	C64	2.61;	C27	2.79;	C26	2.88;	C18	2.96;	C43	2.97;
54	0.910	0.576	0.459	-0.56	void	C64	2.82;	C50	2.90;	C60	3.19;												
55	0.517	0.669	0.215	-0.56		C16	2.03;	C31	2.10;	C18	2.66;	C3	2.81;	C14	2.92;	N2	3.04;	C44	3.12;	C30	3.14;	C19	3.19;
56	0.301	0.557	0.865	-0.55		C21	1.35;	C20	2.43;	C22	2.44;	Fe2	2.84;	N3	2.93;	C17	2.96;	N6	3.05;	C29	3.19;		
57	0.436	0.639	0.609	-0.55		C14	1.72;	C3	1.76;	C15	1.99;	N2	2.43;	C2	2.59;	C63	3.08;						
58	0.312	0.391	0.281	-0.55		C56	1.27;	C55	1.96;	C52	2.59;	C42	2.96;	Fe4	3.11;	C54	3.18;	C41	3.19;				
59	0.579	0.877	0.798	-0.55		C44	1.79;	C18	1.99;	C19	2.39;	C31	2.56;	C30	2.57;	C32	2.70;	C43	2.78;	C45	2.83;	C17	3.16;
60	0.160	0.999	0.264	-0.55		C25	0.53;	C29	1.27;	C26	1.86;	Fe2	1.94;	C17	2.28;	C28	2.37;	C27	2.60;	N3	2.71;	C20	3.00;
61	0.373	0.327	0.944	-0.55		C36	2.21;	C40	2.58;	C22	2.86;	C15	2.91;	C16	3.06;	C37	3.07;						
62	0.512	0.859	0.322	-0.55		C33	1.57;	C45	1.70;	N5	1.76;	C41	1.82;	B1	2.17;	C34	2.73;	N4	2.78;	N6	2.93;	C44	3.11;
63	0.770	0.262	0.780	-0.55		N1	1.74;	Cr	1.75;	C12	2.03;	C1	2.29;	C13	2.35;	N6	2.66;	Cl	2.70;	N7	2.85;	N2	3.00;
64	0.653	0.687	0.244	-0.55		C43	2.21;	C16	2.32;	C44	2.33;	C18	2.39;	C28	2.60;	C42	3.03;	C17	3.12;	C45	3.16;		
65	0.520	0.298	0.235	-0.54		B1	1.24;	N5	1.30;	C33	1.74;	C45	2.03;	N2	2.13;	N6	2.62;	C41	2.70;	N4	2.70;	C44	2.96;
66	0.654	0.112	0.377	-0.54		C4	1.91;	C2	2.12;	C1	2.40;	C13	2.82;	C8	2.83;	Fe1	2.92;	C5	2.96;	C31	2.97;	C3	3.08;
67	0.621	0.248	0.282	-0.54		N2	1.20;	N1	1.34;	B1	2.00;	C3	2.11;	N5	2.12;	C1	2.20;	N6	2.50;	C2	2.57;	Cr	2.85;
68	0.997	0.378	0.712	-0.54		C26	1.90;	C27	2.45;	C25	2.92;												
69	0.025	0.670	0.794	-0.54		Cl	1.67;	C53	2.76;	C52	2.94;												
70	0.882	0.291	0.227	-0.54		Cl	0.15;	Cr	2.29;	N8	2.91;	N7	3.07;										
71	0.123	0.844	0.937	-0.54	void	C48	2.78;																
72	0.396	0.783	0.587	-0.54		C2	1.00;	C3	1.70;	C14	2.34;	C15	2.35;	C1	2.37;	N2	2.91;	C16	3.09;	N1	3.19;		
73	0.904	0.471	0.977	-0.54		C6	1.20;	C5	1.81;	Fe1	2.37;	C7	2.51;	C10	2.91;	C4	3.04;	C24	3.19;				
74	0.111	0.201	0.899	-0.54		C57	0.32;	C61	1.53;	C58	1.55;	Fe4	2.36;	C59	2.45;	C60	2.45;	C49	2.60;	N8	3.15;		
75	0.312	0.985	0.305	-0.54		C17	1.29;	N3	1.62;	C29	1.98;	C18	2.11;	N4	2.43;	C21	2.50;	C19	2.66;	Fe2	2.77;	C25	2.91;
76	0.312	0.397	0.710	-0.54		C18	1.60;	C17	1.94;	C29	2.34;	C43	2.44;	C44	2.46;	C28	2.60;	C19	2.69;	C64	2.83;	N3	3.01;
77	0.924	0.454	0.290	-0.54		C25	1.70;	N8	2.03;	N7	2.24;	C26	2.50;	C49	2.54;	C51	2.79;	C53	2.90;	C29	2.92;	C50	2.95;
78	0.406	0.017	0.640	-0.54		C4	2.39;	C41	2.64;	C8	2.92;	C31	2.96;	C30	3.14;								
79	0.488	0.780	0.885	-0.54		C34	0.96;	C33	1.57;	C45	2.20;	C35	2.33;	C44	2.67;	N5	2.77;	C36	3.00;	Fe3	3.03;	N6	3.11;
80	0.611	0.547	0.213	-0.54		C18	0.80;	C17	1.60;	C19	1.61;	N4	2.35;	N3	2.38;	C29	2.67;	C30	2.77;	C31	3.02;	C28	3.13;
81	0.561	0.174	0.858	-0.54		C3	0.95;	C14	1.33;	N2	1.56;	C2	2.15;	C15	2.28;	B1	2.45;	C16	2.66;	N1	2.66;	C1	2.90;
82	0.719	0.154	0.251	-0.53	void	C12	2.70;	N1	2.70;	C31	2.79;	N6	2.93;	C1	3.02;	C48	3.17;	C13	3.18;				
83	0.033	0.139	0.672	-0.53	void	C53	2.62;	C52	2.66;	Cl	3.06;	C7	3.12;										
84	0.785	0.823	0.536	-0.53		C39	1.82;	C40	2.12;	C23	2.14;	C38	2.44;	C22	2.64;	C36	2.79;	C58	2.92;	C37	2.95;	C57	3.18;
85	0.285	0.153	0.725	-0.53		C42	1.43;	C56	1.99;	C41	2.12;	C43	2.39;	C52	2.53;	C55	3.01;	C45	3.15;				
86	0.371	0.436	0.071	-0.53		C40	2.01;	C4	2.56;	C36	2.81;	C41	2.91;	C5	2.97;	Fe3	3.02;	C39	3.13;				
87	0.734	0.940	0.352	-0.53		C8	1.27;	C4	1.93;	C7	2.09;	C42	2.31;	C41	2.41;	C5	2.79;	C6	2.86;				
88	0.872	0.894	0.430	-0.53		C6	1.77;	C7	1.94;	C39	2.48;	C5	2.71;	C8	2.89;								
89	0.169	0.235	0.663	-0.53		C43	2.04;	C42	2.09;	C52	3.07;	Fe3	3.15;										
90	0.078	0.624	0.945	-0.53		C20	2.57;	C24	2.83;														
91	0.011	0.657	0.057	-0.53		C10	0.98;	C11	1.94;	C9	2.29;	Fe1	2.70;	C12	3.13;								
92	0.361	0.547	0.358	-0.53		C32	2.15;	C48	2.63;	C55	2.73;	C30	3.19;										

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 93 0.109 0.422 0.081 -0.53      C6   1.42; C7   1.45; C5   2.59; C8   2.62; C39  3.11; C4   3.12; Fe1  3.15;
 94 0.861 0.471 0.515 -0.53      C60  2.29; C63  2.49; C59  3.01; C50  3.03;
 95 0.737 0.077 0.954 -0.53      C63  0.30; C62  1.67; C64  2.47; C51  2.71;
 96 0.561 0.157 0.104 -0.53      C34  1.66; C35  2.42; C33  2.72; C48  2.91; C46  2.95; C32  3.09;
 97 0.827 0.674 0.368 -0.53      C43  2.26; C64  2.86; C38  2.92; C42  3.13;
 98 0.371 0.045 0.338 -0.53      C18  2.08; C17  2.21; C29  2.76; C22  2.80; C19  2.80; C21  2.80; N3   2.94; C28  3.02;
 99 0.331 0.703 0.806 -0.52      N6   0.11; C35  1.33; N5   1.50; Cr   2.08; C34  2.29; C33  2.35; C46  2.44; B1   2.66; N3   2.86;
100 0.644 0.828 0.689 -0.52      C16  1.61; C28  2.43; C18  2.54; C14  3.13; C17  3.13; C29  3.15;
101 0.690 0.312 0.930 -0.52      C2   1.39; C1   1.99; C13  2.41; C9   2.58; C3   2.73; C4   2.99; Fe1  3.13; C47  3.18;
102 0.861 0.971 0.227 -0.52      C54  0.48; C53  1.07; C55  1.47; C52  1.93; C56  2.05; Fe4  2.15;
103 0.502 0.639 0.336 -0.52      C32  2.21; C44  2.28; C34  2.42; C33  2.45; C31  2.62; C45  2.66; C30  2.78;
104 0.169 0.342 0.126 -0.52      C42  2.13; C7   2.46; C39  2.60; C43  2.85; Fe3  2.94; C8   2.97; C6   3.08;
105 0.117 0.127 0.054 -0.52 void C64  2.78; C38  2.78;
106 0.128 0.359 0.789 -0.52      C27  0.13; C28  1.38; C26  1.48; Fe2  1.98; C29  2.32; C25  2.35;
107 0.796 0.311 0.635 -0.52      C48  0.96; C46  1.41; C47  2.50; C35  2.65; Cl   2.96;
108 0.042 0.156 0.844 -0.52      C61  1.41; C57  1.62; C49  1.68; N8   1.74; Fe4  2.06; C53  2.60; C60  2.65; C58  2.82; C52  2.82;
109 0.797 0.299 0.741 -0.52      Cl   2.25; C12  2.37; Cr   2.44; N6   2.81; C48  2.89; N1   2.95; C46  3.12; C35  3.16;
110 0.090 0.940 0.140 -0.52      C50  1.20; C51  1.32; C49  1.44; N8   1.61; N7   1.62; C62  2.67; C61  2.77; C25  3.07; C64  3.15;
111 0.285 0.500 0.843 -0.52      C21  1.45; C22  2.04; Fe2  2.04; C17  2.20; C29  2.21; C20  2.53; N3   2.68; C28  2.80; C25  2.94;
112 0.218 0.501 0.445 -0.52      C59  1.79; C60  1.81; C63  3.03; Fe4  3.08; C58  3.20;
113 0.091 0.830 0.508 -0.52      C9   1.76; C10  1.82; Fe1  2.78; C13  3.16; C11  3.18;
114 0.906 0.921 0.375 -0.52      C7   1.31; C6   2.17; C8   2.51;
115 0.517 0.130 0.603 -0.52      C33  2.23; C34  2.33; N5   2.79; C45  2.80; C35  2.93; C36  3.04; C41  3.07; N6   3.19;
116 0.150 0.061 0.325 -0.52      Fe2  0.39; C26  1.67; C27  1.72; C25  1.86; C28  1.91; C29  2.01; C24  2.18; C23  2.22; C20  2.29;
117 0.909 0.907 0.404 -0.52      C7   1.59; C6   1.90; C8   2.82; C5   3.11;
118 0.188 0.502 0.086 -0.52      C6   0.96; C5   1.05; C7   1.26; C4   1.35; C8   1.46; Fe1  1.75;
119 0.315 0.015 0.711 -0.51      C8   1.98; C31  2.59; C30  2.72; C4   2.74; C55  2.82; C41  2.92; C56  2.95; C42  3.15;
120 0.926 0.637 0.843 -0.51      C7   2.55; C52  2.69; C53  2.86;
121 0.797 0.988 0.234 -0.51      C55  0.99; C54  1.18; C56  1.84; C53  2.05; C52  2.36; Fe4  2.69; C8   3.05;
122 0.030 0.506 0.657 -0.51      C49  2.06; C50  2.23; N8   2.47; C25  2.69; C51  2.73; C61  2.75; N7   2.88; C26  3.00; C60  3.06;
123 0.749 0.594 0.760 -0.51      C56  1.26; C55  1.89; C52  1.97; C42  2.48; C54  2.66; C53  2.70; C8   2.85; C41  3.04; Fe4  3.18;
124 0.126 0.973 0.641 -0.51      C7   1.01; Fe1  1.62; C8   1.62; C6   2.03; C11  2.42; C4   2.58; C12  2.65; C5   2.76; C10  3.04;
125 0.356 0.654 0.251 -0.51      C31  1.83; N1   2.68; N6   2.87; N5   2.98; N2   3.06; C1   3.07; C30  3.11; C35  3.16;
126 0.270 0.612 0.241 -0.51 void C12  2.67; C31  2.69; C8   3.01; C55  3.11;
127 0.854 0.594 0.670 -0.51      Fe4  0.40; C53  1.65; C54  1.72; C52  1.79; C55  1.90; C56  1.92; C61  2.21; C60  2.27; C57  2.31;
128 0.361 0.218 0.951 -0.51      C37  2.10; C36  2.23; C15  2.23; C58  2.62; C38  3.03; C59  3.11; C14  3.17; C40  3.18;
129 0.813 0.094 0.541 -0.51      C20  2.05; C21  2.44; C5   2.54; C24  2.62; C22  3.13; C47  3.16;
130 0.173 0.325 0.920 -0.51      C23  1.67; C22  2.46; C57  2.58; C58  2.70; C24  2.92; C39  2.92; Fe2  2.99;
131 0.779 0.223 0.000 -0.51      C47  2.03; C9   2.62; C63  2.70; C46  3.15;
132 0.735 0.294 0.211 -0.51      N6   1.15; Cr   1.36; C35  1.98; Cl   2.37; N5   2.44; C46  2.47; N1   2.72; N3   2.87;
133 0.656 0.467 0.572 -0.51 void C48  2.79; C59  3.07;
134 0.764 0.690 0.147 -0.51      C28  2.05; C27  2.40; Fe2  2.67; C22  2.71; C23  2.81; C58  2.82; C57  3.07;
135 0.701 0.201 0.821 -0.51      N1   0.45; N2   1.43; C1   1.47; Cr   2.05; C3   2.30; C2   2.32; C13  2.50; B1   2.53; N7   2.63;
136 0.843 0.469 0.273 -0.51      C25  1.15; C29  1.83; N7   2.23; C17  2.38; N3   2.47; C26  2.50; Cr   2.69; C51  2.73; N8   2.74;
137 0.122 0.188 0.641 -0.51 void C42  2.68; C7   3.02; C43  3.05; C52  3.11;
138 0.841 0.643 0.954 -0.51      C39  1.50; C6   2.48; C40  2.50; C38  2.68; C7   2.87; C5   3.04; Fe3  3.15;
139 0.216 0.642 0.249 -0.51      C12  2.24; C48  3.01; C54  3.17; C13  3.17;
140 0.786 0.836 0.984 -0.51      C38  1.30; C37  2.04; C59  2.48; C39  2.59; C58  2.62; C60  3.06; Fe3  3.19;
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141 0.970 0.177 0.335 -0.51      C11  1.12; C12  1.91; C10  2.32; C27  3.00; C13  3.06; Fe1  3.11; C26  3.15;
142 0.035 0.219 0.264 -0.51      C27  1.97; C26  2.64; Cl   2.74; C52  3.10; C28  3.20;
143 0.797 0.748 0.711 -0.50      C52  2.16; C28  2.22; C27  2.32; C56  2.47; Fe4  3.02; C58  3.18; C57  3.19;
144 0.886 0.564 0.000 -0.50      C6   1.82; C5   2.38; C23  2.38; C24  2.57; C39  2.98; C7   3.01;
145 0.060 0.280 0.212 -0.50      C52  2.25; Cl   2.83; C53  2.88; C27  3.07;
146 0.045 0.956 0.380 -0.50      C24  1.54; C20  1.75; Fe2  2.92; C23  2.93; C7   3.01; C21  3.12;
147 0.823 0.640 0.802 -0.50      C52  1.76; C42  2.18; C56  2.27; C53  2.58; C7   2.81; C8   2.97; C43  3.04; C55  3.10;
148 0.297 0.234 0.609 -0.50      Fe3  0.59; C43  1.66; C42  1.77; C38  1.92; C39  1.98; C44  2.03; C41  2.19; C37  2.26; C45  2.34;
149 0.833 0.215 0.117 -0.50      C46  1.75; C48  1.76; C47  2.41; Cl   2.89; C35  3.17;
150 0.880 0.108 0.789 -0.50      N7   1.30; N8   1.45; Cr   2.13; C51  2.38; C25  2.41; Cl   2.41; C49  2.53; C50  2.96; N3   3.11;
151 0.119 0.277 0.006 -0.50      C39  1.93; C38  2.21;
152 0.107 0.685 0.119 -0.50      C11  0.93; C10  1.11; C12  1.21; C9   1.45; C13  1.50; Fe1  1.87; C1   2.95;
153 0.860 0.095 0.559 -0.50      C20  1.75; C24  2.25; C21  2.60; C5   3.02; C23  3.17;

Void  X(av) Y(av) Z(av) Volume Ang^3 El-Count (e-) Vol/Electron Vol/Atom
=============================================================================
   1  0.005 0.210 0.089          160       40               4.0       32
   2  0.005 0.290 0.589          160       40               4.0       32
   3 -0.005 0.710 0.411          160       39               4.1       32
   4 -0.005 0.790 0.911          160       40               4.0       32
   5  0.500 0.500 0.000          180       37               4.8       39
   6  0.500 1.000 0.500          180       37               4.8       38
   7  0.500 0.500 0.500          104       27               3.8       30
   8  0.500 1.000 1.000          104       28               3.7       30

Total (Positive) Electron Count in Voids/Cell =   289

Total (Fo-Fc)map Electron Count in  Unit Cell =   288

VOID-Fo-Fc-Map:    Rho(min) =     -0.66, Rho(max) =      4.47, RhoCutOff =  0.00
PeaksCloseToAtoms: Rho(min) =     -0.98, Rho(max) =      0.76, RhoCutOff =  0.50

:: Fo-scale =0.575070E+00 - SinT/L-Min = 0.20 for Fo/Fc-Scaling


:: Cycle =  5, R(F) = 0.11, Nref(Hemi) = 32559, R(F > 4SIGF) = 0.04 Nref = 12308
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Unique Density Maxima in Enhanced Difference Map (CutOff level = 0.50 eA-3)

#	x	y	z	(e/A^3)	Shortest Contacts within 3.2 Angstrom (Excl. H)
1	0.982	0.314	0.542	4.55	void
2	0.035	0.296	0.631	4.50	void
3	0.032	0.873	0.933	4.04	void
4	0.016	0.751	0.920	3.98	void
5	0.502	1.003	0.500	3.66	void
6	1.000	0.885	0.930	3.39	void
7	0.480	0.986	0.397	3.31	void
8	0.987	0.873	0.872	3.25	void
9	0.564	0.014	0.029	2.86	void
10	0.474	0.544	0.954	2.63	void
11	0.499	0.470	0.946	2.59	void
12	0.492	1.002	0.439	2.28	void
13	0.547	0.531	0.484	2.08	void
14	0.588	0.966	-0.001	2.00	void
15	0.587	0.550	0.498	1.94	void
16	0.472	0.081	0.013	1.87	void C15 3.04;
17	0.518	0.954	0.967	1.86	void
18	0.520	1.003	0.964	1.47	void
19	0.467	0.542	0.480	1.44	void
20	0.443	1.001	0.515	1.41	void
21	1.005	0.690	0.916	1.40	void
22	0.549	0.439	0.537	1.38	void
23	0.011	0.294	0.592	1.33	void
24	0.070	0.798	0.969	1.29	void C9 3.11;
25	0.510	0.562	0.074	1.29	void
26	0.928	0.637	0.395	1.27	void
27	0.973	0.313	0.502	1.23	void C50 3.04; C9 3.10; C10 3.14;
28	0.054	0.265	0.593	1.23	void
29	0.894	0.733	0.365	1.23	void C43 2.98;
30	0.528	0.535	0.438	1.22	void C32 2.68;
31	0.404	0.504	0.430	1.18	void C32 2.91;
32	0.985	0.682	0.498	1.15	void C61 3.08; C49 3.14; C50 3.14;
33	0.061	0.236	0.050	1.12	void C38 3.02; C39 3.08;
34	0.515	0.128	0.007	1.10	C15 2.33;
35	0.515	0.986	0.048	1.10	void C32 3.03;
36	0.546	0.535	0.068	1.09	void
37	0.619	0.999	0.055	1.09	void C59 3.11;
38	0.572	0.989	0.952	1.06	void C32 3.12;
39	0.032	0.201	0.625	1.05	void
40	0.503	0.062	0.973	1.04	void C15 2.71;
41	0.938	0.328	0.635	1.01	void C48 3.00;
42	0.950	0.769	0.831	1.00	void
43	0.488	0.422	0.972	1.00	void
44	0.473	0.591	0.418	0.99	C32 2.57; C34 2.96;

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 45 0.471 0.891 0.503  0.98 void
 46 0.563 0.053 0.982  0.97 void C15  3.11;
 47 0.034 0.781 0.885  0.96 void
 48 0.036 0.278 0.033  0.95 void C10  3.03; C39  3.16;
 49 0.375 0.989 0.983  0.94 void C63  3.09;
 50 0.423 0.967 0.562  0.93 void C4   2.84;
 51 0.109 0.848 0.970  0.93 void C63  3.02;
 52 0.950 0.222 0.006  0.91 void C9   2.62; C10  2.74;
 53 0.940 0.787 0.411  0.91 void
 54 0.556 1.004 0.923  0.89      C32  2.45;
 55 0.075 0.751 0.893  0.88 void Cl   3.07;
 56 0.442 0.500 0.929  0.88 void C22  3.14; C21  3.17;
 57 0.527 1.000 0.081  0.87      C32  2.23;
 58 0.017 0.124 0.168  0.87 void C26  2.60; C27  3.04; C25  3.19;
 59 0.114 0.359 0.610  0.86 void C64  2.85;
 60 0.543 0.575 0.438  0.86 void C32  2.89; C37  3.15;
 61 0.601 0.454 0.517  0.85 void C63  3.17;
 62 0.503 0.372 0.955  0.85 void C15  3.00;
 63 0.590 1.004 0.603  0.84 void C21  2.66; C22  2.81;
 64 0.593 0.064 0.517  0.84 void
 65 0.109 0.344 0.630  0.84 void C64  3.18;
 66 0.474 0.921 0.015  0.84 void C15  2.61;
 67 0.591 1.004 0.486  0.83 void
 68 0.015 0.941 0.873  0.83 void C60  2.93; C50  2.95; C49  3.04;
 69 0.419 0.637 0.476  0.81 void C15  2.79; C47  2.90;
 70 0.458 0.968 0.931  0.80      C32  2.57;
 71 0.411 0.581 0.479  0.80 void
 72 0.953 0.573 0.460  0.80 void C50  2.85;
 73 0.569 0.044 0.092  0.80      C32  2.24;
 74 0.483 0.449 0.443  0.79 void C15  2.71; C32  3.01;
 75 0.138 0.437 0.339  0.78      Fe4  0.77; C54  1.51; C53  1.80; C55  1.91; C60  1.95; C61  2.13; C52  2.29; C56  2.31; C59  2.34;
 76 0.957 0.898 0.960  0.77 void
 77 0.467 0.544 0.111  0.77 void C4   3.16;
 78 0.562 0.954 0.620  0.77 void C18  3.06; C22  3.18;
 79 0.017 0.874 0.985  0.76 void C50  2.77;
 80 0.926 0.824 0.967  0.76 void C38  2.85;
 81 0.910 0.216 0.128  0.76 void Cl   2.74; C48  2.79; C46  2.93;
 82 0.841 0.217 0.579  0.75      C47  2.17; C46  2.34; C48  3.03; C20  3.19;
 83 0.521 0.905 0.582  0.75 void C16  3.12;
 84 0.107 0.688 0.524  0.75      C9   2.31; C50  2.70; C10  2.91; C63  2.92; C51  3.03; C49  3.17;
 85 0.455 0.450 0.063  0.75 void C40  2.93;
 86 0.453 0.893 0.423  0.75 void C34  2.83; C33  3.05; C35  3.16;
 87 0.045 0.175 0.582  0.75 void C7   3.18;
 88 0.526 0.874 0.516  0.75 void C36  2.61; C40  3.09;
 89 0.088 0.373 0.526  0.75 void C38  3.03; C60  3.06; C61  3.17;
 90 0.472 0.936 0.051  0.74      C15  2.56;
 91 0.575 0.623 0.505  0.74      C37  2.44; C15  2.52; C36  3.12;
 92 0.597 0.488 0.130  0.74 void C21  2.68; C22  3.00; C18  3.01; C17  3.02;
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 93 0.985 0.346 0.056  0.74 void
 94 0.572 0.389 0.494  0.74      C15  2.50; C63  3.18;
 95 0.928 0.796 0.379  0.74 void
 96 0.965 0.045 0.088  0.74      C60  2.44; C50  2.72; C49  2.91; C61  3.00;
 97 0.896 0.919 0.938  0.74      C64  2.48; C50  2.82;
 98 0.920 0.826 0.016  0.74      C61  2.34; C57  2.50; C60  2.74; C38  2.89; C49  2.94; C58  2.96; C59  3.07;
 99 0.576 0.908 0.046  0.74      C15  2.36;
100 0.894 0.660 0.422  0.73 void C38  2.84; C64  3.15;
101 0.917 0.231 0.087  0.73 void
102 0.550 0.699 0.126  0.73      C16  1.07; C14  1.74; C15  2.16; C3   2.54; C2   3.09;
103 0.126 0.107 0.131  0.73      C64  2.46;
104 0.077 0.706 0.925  0.72 void
105 0.940 0.564 0.508  0.72      C60  2.31; C61  2.60; C50  2.73; C49  2.89;
106 0.514 0.892 0.437  0.72 void C36  2.62; C40  2.87; C34  3.13; C33  3.17;
107 0.974 0.783 0.334  0.72 void Cl   2.81; C52  3.14;
108 0.886 0.783 0.820  0.71 void C27  2.85; C43  2.92; C28  3.12;
109 0.899 0.677 0.329  0.71 void C27  2.80; C26  3.06; C28  3.10;
110 0.533 0.107 0.533  0.71 void C36  3.16;
111 0.439 0.061 0.445  0.71 void C22  2.97;
112 0.095 0.049 0.102  0.71      C50  2.14; C64  2.39; C51  2.57; C62  2.98; C49  3.08;
113 0.891 0.376 0.543  0.71 void C63  3.07;
114 0.591 0.531 0.572  0.71 void C32  2.93;
115 0.626 0.014 0.936  0.71      C63  2.27; C64  2.60; C62  2.64;
116 0.059 0.575 0.457  0.71 void C60  2.92;
117 0.558 0.405 0.026  0.71 void
118 0.987 0.326 0.123  0.70 void Cl   3.18;
119 0.689 0.106 0.140  0.70      C48  1.35; C46  2.47; C35  2.76; C55  3.06; C34  3.13;
120 0.441 0.861 0.459  0.70 void C34  2.89; C47  2.92;
121 0.142 0.404 0.303  0.70      Fe4  1.01; C53  1.12; C52  1.21; C54  1.48; C56  1.59; C55  1.73; C61  2.75; C57  2.77; C60  2.92;
122 0.402 0.999 0.486  0.70 void C22  2.96; C21  3.17;
123 0.908 0.535 0.219  0.70      C26  0.75; C25  1.07; Fe2  1.65; C27  1.90; C29  2.14; C28  2.45; C20  2.87; C24  2.89;
124 0.030 0.347 0.475  0.70      C61  2.22; C49  2.39; C50  2.57; C57  2.77; C60  2.78;
125 0.371 0.485 0.938  0.70      C22  2.06; C21  2.28;
126 0.606 0.048 0.553  0.70 void C21  2.63; C22  2.94;
127 0.380 0.959 0.915  0.69 void C32  2.86; C48  2.89;
128 0.935 0.312 0.052  0.69 void C9   3.10; C10  3.18;
129 0.968 0.869 0.982  0.69 void C50  3.10; C61  3.15;
130 0.341 0.499 0.413  0.69 void C59  2.69; C55  3.05; C48  3.14;
131 1.001 0.219 0.682  0.69      Cl   2.22; C52  3.15;
132 0.457 0.061 0.536  0.68 void C40  2.84; C36  2.98;
133 0.033 0.640 0.339  0.68 void C26  3.11;
134 0.500 0.140 0.082  0.68      C34  2.32; C37  3.03; C32  3.07; C33  3.14;
135 0.485 0.903 0.598  0.68 void C16  3.05; C2   3.18;
136 0.097 0.630 0.390  0.68 void C48  2.61;
137 1.002 0.327 0.038  0.67 void C10  2.86;
138 0.554 0.971 0.528  0.67 void
139 0.066 0.470 0.555  0.67      C50  1.99; C51  2.85; C64  2.91; C49  3.05;
140 0.546 0.497 0.885  0.67 void C4   2.97;
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141 0.220 0.656 0.688  0.67      N7   1.19; Cr   1.29; N1   1.85; C51  2.12; N8   2.39; N3   2.48; C1   2.58; C62  2.67; N2   2.83;
142 0.875 0.541 0.628  0.67      C60  1.20; Fe4  1.43; C61  1.79; C59  2.03; C54  2.14; C53  2.59; C55  2.59; C57  2.64; C49  2.67;
143 0.614 0.391 0.049  0.67 void C47  2.74; C21  2.97;
144 0.455 0.297 0.882  0.67      C16  1.21; C14  1.69; C15  1.99; C3   2.49; C2   3.01;
145 0.136 0.675 0.421  0.67      C48  2.38; C46  2.77; C47  2.86;
146 0.787 0.654 0.727  0.66      C56  0.88; C52  1.03; C55  2.17; Fe4  2.27; C53  2.31; C54  2.75; C42  3.01;
147 0.026 0.062 0.123  0.66 void C50  2.65; C49  3.03;
148 0.393 0.032 0.398  0.66      C22  2.35; C21  2.53;
149 0.042 0.669 0.522  0.66      C50  2.40; C49  2.63; C9   2.97; C61  3.04; C10  3.09; C51  3.19;
150 0.469 0.059 0.632  0.66      C41  2.58; C33  3.06; C45  3.10;
151 0.140 0.193 0.130  0.66      C43  2.58; C38  3.11;
152 0.348 0.440 0.529  0.66 void C37  2.71; C64  2.79; C59  3.07; C63  3.09;
153 0.212 0.094 0.865  0.66      Fe4  0.93; C59  1.50; C58  1.78; C55  1.91; C56  2.02; C60  2.06; C57  2.40; C54  2.41; C61  2.53;
154 0.405 0.189 0.681  0.66      C41  0.76; C45  0.82; C42  1.78; C44  1.83; C33  2.04; Fe3  2.19; C43  2.21; N5   2.75; B1   2.99;
155 0.494 0.861 0.954  0.66 void C34  2.78; C37  3.03; C15  3.07;
156 0.932 0.168 0.552  0.66 void C9   3.13; C10  3.18; C20  3.18;
157 0.049 0.065 0.180  0.66      C26  2.11; C25  2.25; C27  2.92; C29  3.09;
158 0.357 0.739 0.453  0.65      C47  1.05; C46  1.98; C35  2.43; C34  2.50; C48  2.75;
159 0.581 0.904 0.601  0.65 void C22  2.83; C16  2.84;
160 0.466 0.971 0.082  0.65      C32  2.35; C15  3.17;
161 0.660 0.454 0.542  0.65 void C63  2.97; C48  2.98;
162 0.646 0.500 0.957  0.65      C4   2.25; C5   2.39; C40  2.82;
163 0.425 0.219 0.149  0.65      C44  0.95; C45  1.11; C33  1.83; Fe3  2.00; C43  2.26; C41  2.39; C34  2.43; C42  2.82; C37  2.99;
164 0.506 0.011 0.651  0.65      C19  2.59; C18  2.94; C30  2.99; N4   3.05; C31  3.07;
165 0.037 0.845 0.830  0.65 void Cl   3.07; C26  3.10;
166 0.687 0.017 0.063  0.65      C59  2.53; C48  2.96; C60  3.16;
167 0.648 1.002 0.982  0.64      C63  2.42; C64  3.07;
168 0.843 0.387 0.930  0.64      Fe1  0.92; C9   1.55; C10  1.81; C5   1.84; C6   2.11; C13  2.13; C4   2.29; C11  2.40; C12  2.56;
169 0.379 0.887 0.925  0.64      C48  2.30; C46  2.84; C34  2.87; C47  2.95; C35  3.09;
170 0.139 0.283 0.172  0.64      C42  2.49; C52  2.62; C43  2.63;
171 0.082 0.890 0.972  0.63 void C50  3.01; C63  3.12;
172 0.984 0.688 0.540  0.63      C61  2.27; C49  2.33; C57  2.56; C50  2.69; C10  2.86; C60  3.14; N8   3.18;
173 0.923 0.637 0.327  0.63      C26  2.57; C27  2.68; C25  2.95; C28  3.11;
174 0.866 0.919 0.897  0.63      C64  1.95; C50  2.82; C51  2.95; C62  2.96;
175 0.496 0.844 0.569  0.63      C15  2.45; C16  2.75; C14  2.83; C2   2.95; C3   3.14;
176 0.057 0.765 0.478  0.63      C9   2.57; C10  2.66;
177 0.504 0.064 0.095  0.63      C32  2.03;
178 0.389 0.909 0.972  0.63 void C63  3.15; C48  3.16;
179 0.698 0.187 0.703  0.63      N6   0.63; Cr   1.60; C35  1.74; N5   1.88; N3   2.53; C46  2.57; B1   2.79; N1   2.80; C34  2.81;
180 0.402 0.968 0.036  0.63 void C63  2.63;
181 0.813 0.386 0.569  0.63      C48  2.02; C46  2.94; C47  3.02; C63  3.04;
182 0.751 0.249 0.375  0.63      C1   0.69; C13  1.12; N1   1.69; C2   1.81; C9   2.06; C12  2.38; N2   2.65; C3   2.71; N7   2.94;
183 0.091 0.266 0.507  0.62      C38  2.45; C39  2.61; C57  3.07;
184 0.856 0.295 0.499  0.62      C9   2.39; C63  2.85; C47  3.11;
185 0.360 0.924 0.437  0.62      C21  2.26; C22  2.90; C47  3.10;
186 0.973 0.422 0.509  0.62      C50  2.45; C49  3.18;
187 0.273 0.781 0.206  0.62      N1   0.80; Cr   1.45; C1   1.85; N2   2.02; C13  2.49; N6   2.49; N7   2.54; C12  2.76; B1   2.81;
188 0.896 0.313 0.653  0.62      C48  2.40; Cl   2.52; C46  2.84;
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189 0.957 0.561 0.347  0.62 void C26  2.77; C25  2.78; C50  2.89; C49  3.13;
190 0.435 0.235 0.187  0.62      C45  0.87; C44  1.02; C33  1.72; C41  2.11; C43  2.19; Fe3  2.53; N5   2.61; C42  2.62; C34  2.75;
191 0.206 0.483 0.389  0.62      C59  1.67; C60  1.69; Fe4  1.94; C55  2.27; C54  2.46; C58  2.79; C61  2.83; C56  3.08; C48  3.15;
192 0.421 0.093 0.930  0.62      C15  2.24; C14  2.88;
193 0.469 0.845 0.453  0.61      C34  2.59; C36  2.69; C47  3.14; C33  3.17; C35  3.18;
194 0.654 0.530 0.268  0.61      C18  0.78; C17  1.04; C19  1.49; N3   1.74; N4   1.90; C29  2.31; C30  2.85; C28  3.13; C64  3.17;
195 0.160 0.060 0.879  0.61      Fe4  1.13; C60  1.13; C59  1.47; C61  1.86; C58  2.21; C54  2.30; C57  2.38; C55  2.40; C53  2.76;
196 0.656 0.541 0.509  0.61      C59  2.57; C63  3.19; C37  3.20;
197 0.989 0.185 0.646  0.61 void Cl   2.70;
198 0.957 0.041 0.131  0.61      C60  2.50; C49  2.88; C54  2.90; C61  2.93; C50  3.04;
199 0.375 0.048 0.507  0.61      C40  2.30; C22  2.84; C36  2.96;
200 0.589 0.046 0.620  0.61 void C21  2.76;
201 0.998 0.486 0.821  0.61      C26  2.22; C24  2.38; Fe2  2.74; C53  2.86; C20  2.87; C7   2.91; C25  2.93; C11  2.97;
202 0.140 0.861 0.476  0.61      C9   2.56; C5   2.82; C20  2.89; C10  2.98;
203 0.674 0.675 0.397  0.61      Fe3  1.76; C44  1.80; C37  1.89; C38  2.07; C43  2.12; C45  2.74; C64  2.83; C36  2.83; C39  3.04;
204 0.422 0.623 0.068  0.61      C2   2.51; C4   3.18;
205 0.874 0.563 0.106  0.60      C23  0.81; C24  0.83; Fe2  1.71; C20  1.94; C22  1.95; C21  2.37; C27  3.01; C26  3.07;
206 0.139 0.064 0.145  0.60      C64  2.13; C51  2.68; C50  2.81; C25  2.82; C62  2.91; C29  2.96;
207 0.193 0.313 0.430  0.60      C58  0.63; C57  1.40; C59  1.59; C61  2.28; C60  2.36; Fe4  2.53; C38  2.73; C37  3.07;
208 0.098 0.312 0.260  0.60      C52  1.19; C53  1.98; C56  2.54; Fe4  2.58; C27  3.07; C57  3.13; C54  3.20;
209 0.599 0.954 0.415  0.60      C40  2.59; C4   2.62; C41  2.94;
210 0.427 0.922 0.514  0.60 void
211 0.473 0.406 0.469  0.60      C15  2.21;
212 0.453 0.032 0.097  0.60      C32  1.98;
213 0.983 0.933 0.990  0.60 void C50  2.67; C60  3.14; C49  3.18; C50  3.18;
214 0.102 0.317 0.086  0.60      C39  2.55; C7   3.03; C38  3.15;
215 0.187 0.386 0.447  0.60      C59  0.78; C60  1.34; C58  1.49; C61  2.04; C57  2.09; Fe4  2.49; C38  3.00;
216 0.380 0.250 0.618  0.60      Fe3  0.95; C45  1.40; C44  1.43; C41  2.05; C43  2.09; C37  2.21; C36  2.24; C42  2.37; C33  2.39;
217 0.517 0.532 0.139  0.60 void C18  2.88; C19  2.89; C31  3.08;
218 1.003 0.908 0.414  0.60 void C7   2.64; C24  2.64; C6   2.77; C20  2.81;
219 0.654 0.531 0.228  0.59      C18  0.80; C17  0.83; C19  1.76; N3   1.79; C29  2.02; N4   2.13; C28  2.75; C30  3.16;
220 0.896 0.409 0.610  0.59 void C48  2.71; C60  2.82;
221 0.907 0.566 0.343  0.59      C25  2.52; C26  2.75; C50  2.90; C64  2.94; C29  3.00; C51  3.01;
222 0.054 0.950 0.976  0.59 void C50  2.80; C60  2.85;
223 0.266 0.235 0.601  0.59      Fe3  1.00; C38  1.66; C39  1.70; C43  1.82; C42  1.92; C37  2.32; C40  2.35; C44  2.42; C41  2.55;
224 0.201 0.470 0.632  0.59      C64  0.99; C62  1.79; C51  2.10; C50  2.69; N7   3.03; C63  3.06; C17  3.16; C29  3.20;
225 0.972 0.549 0.407  0.59      C50  2.27; C49  2.86; C51  3.14; C60  3.18;
226 0.239 0.358 0.467  0.59      C59  1.26; C58  1.54; C38  2.28; C60  2.33; C37  2.34; C57  2.58; C61  2.93; Fe4  3.12;
227 0.893 0.723 0.874  0.59 void C42  3.02; C43  3.09;
228 0.372 0.452 0.866  0.59      C22  2.36; C21  2.53; C18  2.76; C17  2.82; C29  3.18;
229 0.659 0.516 0.529  0.59      C59  2.56; C63  3.18;
230 0.834 0.637 0.383  0.59      C64  2.26; C43  2.81; C38  2.95;
231 0.910 0.078 0.014  0.59 void C50  2.62; C63  2.85; C60  3.11;
232 0.596 0.920 0.943  0.59 void C37  2.63; C64  3.12;
233 0.123 0.939 0.633  0.59      Fe1  1.14; C7   1.48; C11  1.87; C8   1.89; C6   2.11; C12  2.14; C10  2.45; C4   2.58; C5   2.69;
234 0.441 0.483 0.057  0.58 void C40  3.18;
235 0.236 0.874 0.907  0.58      C48  1.04; C46  2.18; C47  2.60;
236 0.986 0.376 0.105  0.58 void C20  2.74; C24  2.93; C7   3.05;
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237 0.010 0.045 0.065  0.58      C50  2.35; C49  3.00; C60  3.03;
238 0.076 0.127 0.549  0.58      C6   2.30; C7   2.66; C39  2.80;
239 0.349 0.911 0.975  0.58 void C63  2.61; C48  2.93; C47  3.13;
240 0.856 0.581 0.947  0.58      C6   1.36; C7   1.98; C5   2.13; C39  2.47; C8   2.80; C4   2.88; C40  3.07;
241 0.279 0.141 0.858  0.58      C56  1.86; C58  1.93; Fe4  2.01; C59  2.24; C55  2.36; C52  2.81; C57  2.93;
242 0.566 0.749 0.383  0.58      C45  1.34; Fe3  1.72; C33  1.73; C44  1.80; C34  2.05; C36  2.29; C41  2.38; C37  2.49; C43  2.82;
243 0.016 0.313 0.992  0.58      C10  1.97; C9   2.81; C11  3.17;
244 0.406 0.736 0.667  0.58      C3   0.68; N2   0.89; C2   1.53; N1   1.72; C1   1.96; C14  2.02; B1   2.30; C16  2.73; C15  3.13;
245 0.043 0.748 0.354  0.58      Cl   2.46;
246 0.282 0.264 0.171  0.58      C43  0.59; C42  0.87; C44  1.82; Fe3  1.95; C41  1.99; C45  2.37;
247 0.081 0.808 0.054  0.57      C9   2.17; C50  2.29; C49  2.42; C10  2.47; C51  2.69; N8   2.85; C13  2.98; N7   3.04; C61  3.15;
248 0.646 0.957 0.032  0.57      C59  2.47;
249 0.700 0.859 0.963  0.57      C37  1.38; C38  1.74; C36  2.80; Fe3  2.82; C64  2.84; C59  2.91; C39  3.10;
250 0.813 0.516 0.135  0.57      Fe2  0.96; C21  1.15; C20  1.24; C22  1.50; C24  1.61; C23  1.74; C29  2.68; C25  2.68; C28  2.87;
251 0.934 0.985 0.867  0.57      C50  1.86; C49  2.32; C51  2.32; N8   2.85; N7   2.90; C25  2.98; C64  3.02;
252 0.174 0.267 0.608  0.57      C38  2.23; C43  2.26; C39  2.45; Fe3  2.59; C42  2.63;
253 0.671 0.141 0.078  0.57      C48  1.56; C46  2.07; C47  2.21; C35  2.70; C34  2.88;
254 0.921 0.455 0.593  0.57      C60  2.07; C61  2.91; C49  3.15;
255 0.140 0.924 0.298  0.57      C25  1.92; C20  2.13; Cl   2.37; Fe2  2.40; C21  2.69; C29  2.71; Cr   2.75; C26  2.84; C24  3.10;
256 0.945 0.907 0.408  0.57      C7   1.93; C6   2.17;
257 0.777 0.217 0.261  0.57      Cr   2.05; C12  2.13; N1   2.27; Cl   2.50; N6   2.62; C13  2.74; C1   2.79;
258 0.889 0.751 0.891  0.57 void C39  3.00; C38  3.01; C43  3.06;
259 0.796 0.988 0.683  0.57      Fe2  1.03; C29  1.51; C25  1.73; C21  1.83; C20  2.12; C28  2.17; C17  2.33; C22  2.35; C26  2.41;
260 0.046 0.579 0.610  0.57      C49  0.72; C50  0.77; N8   1.70; C51  1.79; C61  1.97; N7   2.19; C60  2.79; C62  3.16;
261 0.343 0.784 0.332  0.57      N6   0.68; C35  0.69; N5   1.71; C34  1.75; C46  1.96; C33  2.15; Cr   2.68; C48  2.94; C47  3.03;
262 0.894 0.419 0.906  0.57      Fe1  0.89; C10  1.72; C6   1.79; C11  1.79; C7   1.94; C9   2.29; C5   2.31; C12  2.38; C8   2.49;
263 0.454 0.487 0.153  0.57 void C31  2.74; C30  2.77; C19  2.81; C41  2.89; C4   3.11;
264 0.878 0.094 0.085  0.56 void C48  2.69; C60  2.77;
265 0.847 0.706 0.350  0.56      C43  2.27; C42  2.87;
266 0.404 0.278 0.876  0.56      C16  1.07; C14  1.87; C15  2.13; C3   3.05;
267 0.068 0.608 0.505  0.56      C50  2.17; C49  2.98; C63  3.02; C51  3.02;
268 0.168 0.878 0.305  0.56      Cl   1.78; Cr   2.19; C20  2.41; C25  2.71; C21  2.83; N6   3.04; N3   3.06; Fe2  3.12;
269 0.982 0.436 0.656  0.56 void C26  2.87; C54  2.92;
270 0.656 0.735 0.771  0.56      C43  1.57; C42  1.71; C44  1.94; C41  2.10; C45  2.23; C16  2.82; Fe3  3.08;
271 0.192 0.747 0.210  0.56      C12  1.75; Cr   1.79; N1   2.08; C13  2.21; Cl   2.40; N7   2.45; C1   2.47; N8   2.85; C11  2.93;
272 0.160 0.340 0.774  0.56      C27  0.76; C28  1.00; C26  2.01; C29  2.20; Fe2  2.41; C25  2.58;
273 0.215 0.985 0.923  0.56      C60  1.90; C59  1.98; C48  2.84; Fe4  2.86; C55  3.16;
274 0.894 0.265 0.538  0.56 void C9   2.89; C47  3.11;
275 0.604 0.190 0.241  0.56      C31  2.06; N5   2.22; N6   2.44; N1   2.55; C33  2.56; N2   2.58; C35  2.84; B1   2.89; C34  2.91;
276 0.891 0.543 0.181  0.56      Fe2  0.96; C26  1.37; C25  1.75; C27  1.93; C24  2.03; C20  2.21; C29  2.38; C28  2.45; C23  2.47;
277 0.420 0.527 0.579  0.56 void C32  2.65; C63  2.79; C62  3.07; C64  3.15;
278 0.513 0.406 0.120  0.56      C33  2.51; N5   2.80; C34  2.91; C41  2.92; C45  2.95;
279 0.907 0.357 0.666  0.56      C48  2.56; Cl   2.99; C54  3.11;
280 0.052 0.646 0.852  0.55      Cl   2.45; C20  2.49; C24  3.19;
281 0.534 0.370 0.528  0.55 void C15  2.75; C34  3.13;
282 0.207 0.613 0.093  0.55      Fe1  0.90; C4   1.72; C13  1.79; C9   1.83; C5   1.85; C8   2.28; C12  2.35; C10  2.42; C6   2.43;
283 0.712 0.028-0.001  0.55      C63  1.81; C62  2.91; C59  2.97; C64  3.01;
284 0.841 0.905 0.639  0.55      Fe2  1.03; C23  1.34; C22  1.83; C24  1.87; C27  2.03; C28  2.30; C21  2.43; C20  2.2.35; C10  2.4;
260 0.0465.370 6;
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