

Supplementary Material**Two-Dimensional Coordination Polymers in Rubidium and Caesium Complexes with Orphanic Acid***Graham Smith***Compound 1: CCDC 858092 [ORTHRB]**

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#-----  
# Reference: Smith (2012). Aust. J. Chem.  
# gs11gs29_ORTHRB_COMPOUND_(1)  
# CCDC reference: 858092  
#-----  
  
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poly[\m-aquatetrakis(\m-2-aminobenzenesulfonato)tetrarubidium]  
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'Rb' 'Rb' -0.9393 2.9676  
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_cell_length_c 11.3901(5)
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'SHELXL97 (Sheldrick, 2008) within WinGX (Farrugia, 1999) '
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_computing_publication_material 'PLATON'

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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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'calc w=1/[\s^2^(Fo^2^)+(0.0863P)^2^] where P=(Fo^2^+2Fc^2^)/3'
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Rb1 Rb Uani 0.44043(8) 0.24445(3) 0.48428(8) 1.000 0.0158(3) . .
Rb2 Rb Uani 0.70934(8) 0.24443(3) 0.32282(8) 1.000 0.0154(3) . .
Rb3 Rb Uani 0.07368(9) 0.15359(3) 0.40550(10) 1.000 0.0266(3) . .
Rb4 Rb Uani 0.07040(9) 0.25263(3) 0.16073(10) 1.000 0.0296(3) . .
S1A S Uani 0.7944(2) 0.18141(7) 0.0881(2) 1.000 0.0149(7) . .
S1B S Uani 0.3396(2) 0.17776(7) 0.2059(2) 1.000 0.0155(8) . .
S1C S Uani 0.3566(2) 0.18152(7) 0.7171(2) 1.000 0.0140(7) . .
S1D S Uani 0.7964(2) 0.17435(8) 0.5945(2) 1.000 0.0176(8) . .
O1W O Uani 0.0703(7) 0.2671(3) 0.4066(8) 1.000 0.058(4) . .
O11A O Uani 0.8732(6) 0.1917(2) 0.2136(5) 1.000 0.017(2) . .
O11B O Uani 0.4785(6) 0.1845(2) 0.2655(7) 1.000 0.036(3) . .
O11C O Uani 0.2747(6) 0.19270(19) 0.5940(6) 1.000 0.020(2) . .
O11D O Uani 0.6568(7) 0.1807(2) 0.5300(7) 1.000 0.041(3) . .
O12A O Uani 0.8712(7) 0.1862(2) 0.0017(6) 1.000 0.027(2) . .
O12B O Uani 0.2612(6) 0.1893(2) 0.2870(6) 1.000 0.023(2) . .
O12C O Uani 0.2866(6) 0.1874(2) 0.8074(6) 1.000 0.026(2) . .
O12D O Uani 0.8789(7) 0.1873(2) 0.5190(7) 1.000 0.027(3) . .
O13A O Uani 0.6706(6) 0.2047(2) 0.0500(7) 1.000 0.029(3) . .
O13B O Uani 0.2919(7) 0.1981(2) 0.0872(6) 1.000 0.031(3) . .
O13C O Uani 0.4827(6) 0.2029(2) 0.7497(6) 1.000 0.027(2) . .
O13D O Uani 0.8390(8) 0.1931(2) 0.7151(7) 1.000 0.041(3) . .
N2A N Uani 0.9879(7) 0.1072(3) 0.1392(8) 1.000 0.032(3) . .
N2B N Uani 0.3877(11) 0.1065(3) 0.4025(9) 1.000 0.053(4) . .
N2C N Uani 0.1517(7) 0.1108(3) 0.6756(8) 1.000 0.030(3) . .
N2D N Uani 0.7575(12) 0.1066(4) 0.3957(10) 1.000 0.051(5) . .
C1A C Uani 0.7550(9) 0.1264(3) 0.0905(9) 1.000 0.017(3) . .
C1B C Uani 0.3142(9) 0.1217(3) 0.1781(9) 1.000 0.015(3) . .
C1C C Uani 0.3871(8) 0.1259(3) 0.7136(8) 1.000 0.013(3) . .
C1D C Uani 0.8219(9) 0.1187(3) 0.6157(10) 1.000 0.022(3) . .
C2A C Uani 0.8554(9) 0.0953(3) 0.1129(9) 1.000 0.021(3) . .
C2B C Uani 0.3424(10) 0.0932(3) 0.2797(10) 1.000 0.027(4) . .
C2C C Uani 0.2793(9) 0.0969(3) 0.6919(9) 1.000 0.022(3) . .
C2D C Uani 0.7967(11) 0.0906(3) 0.5121(12) 1.000 0.037(4) . .
C3A C Uani 0.8197(11) 0.0525(3) 0.1188(11) 1.000 0.036(4) . .
C3B C Uani 0.3153(10) 0.0495(3) 0.2531(11) 1.000 0.033(4) . .
C3C C Uani 0.3047(10) 0.0536(3) 0.6821(11) 1.000 0.035(4) . .
C3D C Uani 0.8319(14) 0.0472(4) 0.5347(17) 1.000 0.065(7) . .
C4A C Uani 0.6914(11) 0.0405(3) 0.1013(11) 1.000 0.037(4) . .
C4B C Uani 0.2638(11) 0.0358(3) 0.1334(12) 1.000 0.034(4) . .

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C4C	C	Uani	0.4290(11)	0.0388(3)	0.6919(13)	1.000	0.046(5)	. . .
C4D	C	Uani	0.8810(13)	0.0322(4)	0.6558(19)	1.000	0.069(7)	. . .
C5A	C	Uani	0.5927(11)	0.0710(4)	0.0754(11)	1.000	0.038(4)	. . .
C5B	C	Uani	0.2406(9)	0.0640(3)	0.0387(10)	1.000	0.029(4)	. . .
C5C	C	Uani	0.5328(10)	0.0674(3)	0.7115(12)	1.000	0.038(4)	. . .
C5D	C	Uani	0.8984(11)	0.0587(5)	0.7538(16)	1.000	0.060(6)	. . .
C6A	C	Uani	0.6256(10)	0.1137(3)	0.0702(10)	1.000	0.028(4)	. . .
C6B	C	Uani	0.2652(8)	0.1067(3)	0.0597(9)	1.000	0.019(3)	. . .
C6C	C	Uani	0.5116(9)	0.1106(3)	0.7239(9)	1.000	0.025(3)	. . .
C6D	C	Uani	0.8686(9)	0.1020(4)	0.7344(11)	1.000	0.036(4)	. . .
H3A	H	Uiso	0.88470	0.03150	0.13490	1.000	0.0430	calc R
H3B	H	Uiso	0.33220	0.02960	0.31700	1.000	0.0400	calc R
H3C	H	Uiso	0.23580	0.03400	0.66850	1.000	0.0420	calc R
H3D	H	Uiso	0.82260	0.02840	0.46910	1.000	0.0780	calc R
H4A	H	Uiso	0.67090	0.01170	0.10700	1.000	0.0450	calc R
H4B	H	Uiso	0.24470	0.00690	0.11720	1.000	0.0400	calc R
H4C	H	Uiso	0.44330	0.00960	0.68540	1.000	0.0550	calc R
H4D	H	Uiso	0.90210	0.00330	0.66940	1.000	0.0830	calc R
H5A	H	Uiso	0.50530	0.06290	0.06160	1.000	0.0460	calc R
H5B	H	Uiso	0.20730	0.05410	-0.04170	1.000	0.0350	calc R
H5C	H	Uiso	0.61670	0.05740	0.71620	1.000	0.0450	calc R
H5D	H	Uiso	0.93020	0.04800	0.83340	1.000	0.0720	calc R
H6A	H	Uiso	0.55940	0.13430	0.05280	1.000	0.0340	calc R
H6B	H	Uiso	0.24890	0.12570	-0.00620	1.000	0.0220	calc R
H6C	H	Uiso	0.58200	0.12970	0.73940	1.000	0.0290	calc R
H6D	H	Uiso	0.87990	0.12010	0.80160	1.000	0.0430	calc R
H11W	H	Uiso	0.01060	0.25300	0.43460	1.000	0.0700	. R
H12W	H	Uiso	0.14060	0.27800	0.46360	1.000	0.0700	. R
H21A	H	Uiso	0.99820	0.12530	0.08120	1.000	0.0380	. R
H21B	H	Uiso	0.40000	0.13480	0.40470	1.000	0.0630	. R
H21C	H	Uiso	0.14850	0.13020	0.73320	1.000	0.0350	. R
H21D	H	Uiso	0.69340	0.12640	0.38440	1.000	0.0800	. R
H22A	H	Uiso	1.03810	0.08380	0.14060	1.000	0.0380	. R
H22B	H	Uiso	0.46390	0.09340	0.43870	1.000	0.0630	. R
H22C	H	Uiso	0.09820	0.08860	0.67810	1.000	0.0350	. R
H22D	H	Uiso	0.73250	0.08580	0.33850	1.000	0.0800	. R

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Rb1	0.0112(5)	0.0236(5)	0.0114(5)	0.0010(4)	0.0018(4)	-0.0003(4)		
Rb2	0.0111(5)	0.0239(5)	0.0103(5)	0.0006(4)	0.0019(4)	0.0025(4)		
Rb3	0.0182(5)	0.0457(6)	0.0126(5)	0.0005(5)	-0.0002(4)	-0.0024(5)		
Rb4	0.0184(5)	0.0349(6)	0.0292(6)	0.0153(5)	-0.0022(4)	-0.0049(4)		
S1A	0.0125(12)	0.0193(13)	0.0113(13)	0.0010(10)	0.0013(10)	-0.0003(9)		
S1B	0.0176(13)	0.0189(13)	0.0101(13)	-0.0023(10)	0.0042(10)	-0.0046(10)		
S1C	0.0123(12)	0.0191(13)	0.0084(13)	-0.0023(10)	-0.0004(10)	-0.0018(9)		
S1D	0.0203(13)	0.0221(13)	0.0108(13)	0.0032(10)	0.0052(11)	0.0059(10)		
O1W	0.025(5)	0.106(8)	0.039(5)	-0.002(5)	0.004(4)	-0.015(5)		
O11A	0.017(4)	0.029(4)	0.010(3)	-0.003(3)	0.005(3)	-0.002(3)		
O11B	0.016(4)	0.035(5)	0.054(6)	-0.011(4)	0.005(4)	-0.012(3)		
O11C	0.022(4)	0.017(4)	0.017(4)	0.004(3)	0.001(3)	-0.001(3)		
O11D	0.020(4)	0.046(5)	0.051(6)	0.018(4)	0.004(4)	0.014(3)		

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O12A 0.035(4) 0.035(4) 0.017(4) 0.002(3) 0.017(3) -0.004(3)
O12B 0.030(4) 0.030(4) 0.013(4) -0.004(3) 0.013(3) 0.004(3)
O12C 0.035(4) 0.033(4) 0.015(4) -0.002(3) 0.015(3) 0.004(3)
O12D 0.035(4) 0.022(4) 0.033(5) 0.002(3) 0.024(4) 0.000(3)
O13A 0.015(4) 0.021(4) 0.045(5) 0.008(3) -0.001(3) 0.005(3)
O13B 0.056(5) 0.024(4) 0.013(4) 0.005(3) 0.012(4) -0.001(3)
O13C 0.013(4) 0.033(4) 0.027(4) -0.003(3) -0.007(3) -0.010(3)
O13D 0.068(6) 0.040(5) 0.016(4) -0.006(4) 0.015(4) 0.013(4)
N2A 0.014(5) 0.040(6) 0.040(6) 0.000(5) 0.006(4) 0.012(4)
N2B 0.089(9) 0.038(6) 0.025(6) 0.008(5) 0.008(6) 0.023(6)
N2C 0.019(4) 0.027(5) 0.054(7) 0.005(4) 0.011(4) -0.004(4)
N2D 0.059(10) 0.058(8) 0.034(8) -0.021(6) 0.013(7) -0.020(7)
C1A 0.016(5) 0.020(5) 0.013(5) -0.005(4) 0.001(4) 0.002(4)
C1B 0.017(5) 0.017(5) 0.016(6) 0.004(4) 0.012(4) 0.002(4)
C1C 0.009(5) 0.022(5) 0.007(5) 0.001(4) 0.000(4) 0.001(4)
C1D 0.007(5) 0.027(6) 0.030(7) 0.003(5) 0.005(5) 0.003(4)
C2A 0.020(5) 0.024(6) 0.017(6) -0.008(4) 0.005(4) 0.005(4)
C2B 0.027(6) 0.022(6) 0.031(7) 0.003(5) 0.009(5) 0.005(4)
C2C 0.016(5) 0.022(6) 0.025(6) 0.007(5) 0.001(5) 0.001(4)
C2D 0.047(8) 0.025(6) 0.043(8) -0.006(6) 0.019(6) -0.013(5)
C3A 0.037(7) 0.026(6) 0.043(8) -0.003(5) 0.011(6) 0.011(5)
C3B 0.041(7) 0.025(6) 0.037(8) 0.012(5) 0.017(6) 0.010(5)
C3C 0.030(7) 0.022(6) 0.054(9) -0.002(6) 0.013(6) -0.005(5)
C3D 0.059(10) 0.037(9) 0.110(15) -0.023(9) 0.042(10) -0.009(7)
C4A 0.051(8) 0.020(6) 0.048(8) -0.009(5) 0.026(7) -0.009(5)
C4B 0.033(7) 0.019(6) 0.053(9) -0.005(6) 0.019(6) 0.000(5)
C4C 0.042(8) 0.016(6) 0.082(11) 0.000(6) 0.022(7) 0.007(5)
C4D 0.044(9) 0.021(8) 0.142(19) 0.021(10) 0.028(11) 0.004(6)
C5A 0.024(6) 0.038(7) 0.055(9) -0.012(6) 0.016(6) -0.009(5)
C5B 0.028(6) 0.027(6) 0.030(7) -0.013(5) 0.004(5) -0.003(5)
C5C 0.019(6) 0.029(7) 0.066(9) 0.009(6) 0.014(6) 0.012(5)
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C6A 0.018(6) 0.027(6) 0.038(7) -0.002(5) 0.007(5) 0.004(4)
C6B 0.017(5) 0.031(6) 0.008(5) -0.005(4) 0.004(4) -0.006(4)
C6C 0.007(5) 0.038(6) 0.024(6) 0.008(5) -0.002(4) 0.005(4)
C6D 0.009(5) 0.047(8) 0.049(8) 0.025(6) 0.006(5) 0.003(5)

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Bond distances, angles etc. have been calculated using the
rounded fractional coordinates. All su's are estimated
from the variances of the (full) variance-covariance matrix.
The cell esds are taken into account in the estimation of
distances, angles and torsion angles

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Rb1      O11B      3.234(7)      .      .      yes
Rb1      O11C      2.931(7)      .      .      yes
Rb1      O11D      2.965(7)      .      .      yes
Rb1      O12B      3.010(7)      .      .      yes
Rb1      O13C      3.193(7)      .      .      yes

```

Rb1	O12C	3.042 (6)	.	4_554	yes
Rb1	O13A	2.822 (7)	.	4_555	yes
Rb1	O13B	2.861 (7)	.	4_555	yes
Rb2	O11A	2.930 (6)	.	.	yes
Rb2	O11B	2.996 (7)	.	.	yes
Rb2	O12D	2.998 (7)	.	.	yes
Rb2	O13C	2.827 (7)	.	4_554	yes
Rb2	O13D	2.865 (8)	.	4_554	yes
Rb2	O12A	3.110 (7)	.	4_555	yes
Rb2	O13A	3.164 (7)	.	4_555	yes
Rb3	O11C	2.812 (7)	.	.	yes
Rb3	O12B	2.942 (7)	.	.	yes
Rb3	N2C	3.224 (9)	.	.	yes
Rb3	O11A	2.817 (6)	.	1_455	yes
Rb3	O12D	2.946 (8)	.	1_455	yes
Rb3	N2A	3.233 (9)	.	1_455	yes
Rb4	O1W	2.837 (9)	.	.	yes
Rb4	O12B	2.885 (7)	.	.	yes
Rb4	O13B	3.213 (7)	.	.	yes
Rb4	O11A	3.020 (6)	.	1_455	yes
Rb4	O12A	3.121 (7)	.	1_455	yes
Rb4	O12D	2.877 (7)	.	4_454	yes
Rb4	O13D	3.196 (8)	.	4_454	yes
Rb4	O1W	2.959 (9)	.	4_554	yes
Rb4	O11C	3.032 (7)	.	4_554	yes
Rb4	O12C	3.043 (7)	.	4_554	yes
S1A	O11A	1.459 (6)	.	.	no
S1A	O12A	1.464 (8)	.	.	no
S1A	O13A	1.451 (7)	.	.	no
S1A	C1A	1.765 (10)	.	.	no
S1B	O11B	1.445 (7)	.	.	no
S1B	O12B	1.463 (7)	.	.	no
S1B	O13B	1.440 (7)	.	.	no
S1B	C1B	1.779 (10)	.	.	no
S1C	O11C	1.453 (7)	.	.	no
S1C	O12C	1.451 (7)	.	.	no
S1C	O13C	1.443 (7)	.	.	no
S1C	C1C	1.764 (10)	.	.	no
S1D	O11D	1.460 (8)	.	.	no
S1D	O12D	1.458 (8)	.	.	no
S1D	O13D	1.435 (8)	.	.	no
S1D	C1D	1.759 (10)	.	.	no
O1W	H12W	0.9000	.	.	no
O1W	H11W	0.9100	.	.	no
N2A	C2A	1.401 (13)	.	.	no
N2B	C2B	1.398 (15)	.	.	no
N2C	C2C	1.384 (13)	.	.	no
N2D	C2D	1.359 (17)	.	.	no
N2A	H21A	0.9000	.	.	no
N2A	H22A	0.9000	.	.	no
N2B	H22B	0.8900	.	.	no
N2B	H21B	0.8900	.	.	no
N2C	H21C	0.9000	.	.	no
N2C	H22C	0.9000	.	.	no
N2D	H21D	0.9000	.	.	no
N2D	H22D	0.9000	.	.	no
C1A	C6A	1.384 (15)	.	.	no
C1A	C2A	1.407 (14)	.	.	no

C1B	C2B	1.417 (14)	.	.		no
C1B	C6B	1.373 (14)	.	.		no
C1C	C6C	1.379 (13)	.	.		no
C1C	C2C	1.422 (13)	.	.		no
C1D	C2D	1.428 (16)	.	.		no
C1D	C6D	1.393 (16)	.	.		no
C2A	C3A	1.392 (13)	.	.		no
C2B	C3B	1.404 (13)	.	.		no
C2C	C3C	1.386 (13)	.	.		no
C2D	C3D	1.405 (16)	.	.		no
C3A	C4A	1.371 (17)	.	.		no
C3B	C4B	1.376 (17)	.	.		no
C3C	C4C	1.373 (17)	.	.		no
C3D	C4D	1.40 (3)	.	.		no
C4A	C5A	1.380 (17)	.	.		no
C4B	C5B	1.355 (16)	.	.		no
C4C	C5C	1.384 (16)	.	.		no
C4D	C5D	1.36 (2)	.	.		no
C5A	C6A	1.380 (16)	.	.		no
C5B	C6B	1.362 (13)	.	.		no
C5C	C6C	1.378 (13)	.	.		no
C5D	C6D	1.39 (2)	.	.		no
C3A	H3A	0.9300	.	.		no
C3B	H3B	0.9300	.	.		no
C3C	H3C	0.9300	.	.		no
C3D	H3D	0.9300	.	.		no
C4A	H4A	0.9300	.	.		no
C4B	H4B	0.9300	.	.		no
C4C	H4C	0.9300	.	.		no
C4D	H4D	0.9300	.	.		no
C5A	H5A	0.9300	.	.		no
C5B	H5B	0.9300	.	.		no
C5C	H5C	0.9300	.	.		no
C5D	H5D	0.9300	.	.		no
C6A	H6A	0.9300	.	.		no
C6B	H6B	0.9300	.	.		no
C6C	H6C	0.9300	.	.		no
C6D	H6D	0.9300	.	.		no
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_geom_angle_publ_flag						
O11B	Rb1	O11C	104.02 (17)	.	.	yes
O11B	Rb1	O11D	58.59 (19)	.	.	yes
O11B	Rb1	O12B	45.07 (18)	.	.	yes
O11B	Rb1	O13C	118.76 (17)	.	.	yes
O11B	Rb1	O12C	93.38 (17)	.	4_554	yes
O11B	Rb1	O13A	103.19 (19)	.	4_555	yes
O11B	Rb1	O13B	152.72 (19)	.	4_555	yes
O11C	Rb1	O11D	95.31 (19)	.	.	yes
O11C	Rb1	O12B	71.18 (18)	.	.	yes
O11C	Rb1	O13C	46.01 (18)	.	.	yes

O11C	Rb1	O12C	113.11 (18)	.	.	4_554	yes
O11C	Rb1	O13A	141.3 (2)	.	.	4_555	yes
O11C	Rb1	O13B	72.02 (18)	.	.	4_555	yes
O11D	Rb1	O12B	91.95 (19)	.	.	.	yes
O11D	Rb1	O13C	71.43 (19)	.	.	.	yes
O11D	Rb1	O12C	144.88 (19)	.	.	4_554	yes
O11D	Rb1	O13A	76.25 (19)	.	.	4_555	yes
O11D	Rb1	O13B	147.4 (2)	.	.	4_555	yes
O12B	Rb1	O13C	110.69 (17)	.	.	.	yes
O12B	Rb1	O12C	78.98 (17)	.	.	4_554	yes
O12B	Rb1	O13A	145.4 (2)	.	.	4_555	yes
O12B	Rb1	O13B	110.99 (19)	.	.	4_555	yes
O12C	Rb1	O13C	143.51 (17)	4_554	.	.	yes
O13A	Rb1	O13C	96.42 (19)	4_555	.	.	yes
O13B	Rb1	O13C	78.65 (17)	4_555	.	.	yes
O12C	Rb1	O13A	92.08 (19)	4_554	.	4_555	yes
O12C	Rb1	O13B	65.29 (18)	4_554	.	4_555	yes
O13A	Rb1	O13B	94.8 (2)	4_555	.	4_555	yes
O11A	Rb2	O11B	96.45 (18)	.	.	.	yes
O11A	Rb2	O12D	71.49 (18)	.	.	.	yes
O11A	Rb2	O13C	139.79 (18)	.	.	4_554	yes
O11A	Rb2	O13D	76.92 (19)	.	.	4_554	yes
O11A	Rb2	O12A	112.57 (19)	.	.	4_555	yes
O11A	Rb2	O13A	150.20 (17)	.	.	4_555	yes
O11B	Rb2	O12D	93.66 (19)	.	.	.	yes
O11B	Rb2	O13C	74.08 (18)	.	.	4_554	yes
O11B	Rb2	O13D	143.0 (2)	.	.	4_554	yes
O11B	Rb2	O12A	146.3 (2)	.	.	4_555	yes
O11B	Rb2	O13A	100.95 (18)	.	.	4_555	yes
O12D	Rb2	O13C	146.4 (2)	.	.	4_554	yes
O12D	Rb2	O13D	117.5 (2)	.	.	4_554	yes
O12A	Rb2	O12D	80.36 (18)	4_555	.	.	yes
O12D	Rb2	O13A	83.36 (19)	.	.	4_555	yes
O13C	Rb2	O13D	87.6 (2)	4_554	.	4_554	yes
O12A	Rb2	O13C	92.64 (19)	4_555	.	4_554	yes
O13A	Rb2	O13C	69.00 (18)	4_555	.	4_554	yes
O12A	Rb2	O13D	64.29 (19)	4_555	.	4_554	yes
O13A	Rb2	O13D	102.04 (19)	4_555	.	4_554	yes
O12A	Rb2	O13A	45.53 (18)	4_555	.	4_555	yes
O11C	Rb3	O12B	73.83 (19)	.	.	.	yes
O11C	Rb3	N2C	62.1 (2)	.	.	.	yes
O11A	Rb3	O11C	129.45 (18)	1_455	.	.	yes
O11C	Rb3	O12D	89.1 (2)	.	.	1_455	yes
O11C	Rb3	N2A	147.7 (2)	.	.	1_455	yes
O12B	Rb3	N2C	125.31 (19)	.	.	.	yes
O11A	Rb3	O12B	86.85 (18)	1_455	.	.	yes
O12B	Rb3	O12D	136.92 (18)	.	.	1_455	yes
O12B	Rb3	N2A	77.2 (2)	.	.	1_455	yes
O11A	Rb3	N2C	146.34 (19)	1_455	.	.	yes
O12D	Rb3	N2C	75.0 (2)	1_455	.	.	yes
N2A	Rb3	N2C	129.1 (2)	1_455	.	.	yes
O11A	Rb3	O12D	73.85 (19)	1_455	.	1_455	yes
O11A	Rb3	N2A	61.7 (2)	1_455	.	1_455	yes
O12D	Rb3	N2A	122.2 (2)	1_455	.	1_455	yes
O1W	Rb4	O12B	79.9 (2)	.	.	.	yes
O1W	Rb4	O13B	124.0 (2)	.	.	.	yes
S1A	Rb4	O1W	94.76 (18)	1_455	.	.	yes
O1W	Rb4	O11A	72.3 (2)	.	.	1_455	yes

O1W	Rb4	O12A	118.5 (2)	.	.	1_455	yes
S1D	Rb4	O1W	82.30 (18)	4_454	.	.	yes
O1W	Rb4	O12D	103.9 (2)	.	.	4_454	yes
O1W	Rb4	O13D	59.7 (2)	.	.	4_454	yes
S1C	Rb4	O1W	89.12 (18)	4_554	.	.	yes
O1W	Rb4	O1W	177.2 (3)	.	.	4_554	yes
O1W	Rb4	O11C	111.8 (2)	.	.	4_554	yes
O1W	Rb4	O12C	65.5 (2)	.	.	4_554	yes
O12B	Rb4	O13B	46.17 (17)	.	.	.	yes
O11A	Rb4	O12B	84.19 (18)	1_455	.	.	yes
O12A	Rb4	O12B	95.19 (18)	1_455	.	.	yes
O12B	Rb4	O12D	176.0 (2)	.	.	4_454	yes
O12B	Rb4	O13D	137.08 (19)	.	.	4_454	yes
O1W	Rb4	O12B	98.0 (2)	4_554	.	.	yes
O11C	Rb4	O12B	93.33 (18)	4_554	.	.	yes
O12B	Rb4	O12C	80.94 (18)	.	.	4_554	yes
O11A	Rb4	O13B	109.18 (17)	1_455	.	.	yes
O12A	Rb4	O13B	85.55 (18)	1_455	.	.	yes
O12D	Rb4	O13B	130.4 (2)	4_454	.	.	yes
O13B	Rb4	O13D	176.22 (18)	.	.	4_454	yes
O1W	Rb4	O13B	54.6 (2)	4_554	.	.	yes
O11C	Rb4	O13B	66.02 (17)	4_554	.	.	yes
O12C	Rb4	O13B	88.52 (18)	4_554	.	.	yes
O11A	Rb4	O12A	46.24 (17)	1_455	.	1_455	yes
O11A	Rb4	O12D	95.88 (19)	1_455	.	4_454	yes
O11A	Rb4	O13D	70.81 (18)	1_455	.	4_454	yes
O1W	Rb4	O11A	105.6 (2)	4_554	.	1_455	yes
O11A	Rb4	O11C	174.79 (17)	1_455	.	4_554	yes
O11A	Rb4	O12C	137.03 (17)	1_455	.	4_554	yes
O12A	Rb4	O12D	82.05 (19)	1_455	.	4_454	yes
O12A	Rb4	O13D	91.95 (19)	1_455	.	4_454	yes
O1W	Rb4	O12A	59.6 (2)	4_554	.	1_455	yes
O11C	Rb4	O12A	129.75 (18)	4_554	.	1_455	yes
O12A	Rb4	O12C	174.06 (19)	1_455	.	4_554	yes
O12D	Rb4	O13D	46.2 (2)	4_454	.	4_454	yes
O1W	Rb4	O12D	78.1 (2)	4_554	.	4_454	yes
O11C	Rb4	O12D	86.28 (19)	4_554	.	4_454	yes
O12C	Rb4	O12D	101.59 (18)	4_554	.	4_454	yes
O1W	Rb4	O13D	121.7 (2)	4_554	.	4_454	yes
O11C	Rb4	O13D	113.84 (17)	4_554	.	4_454	yes
O12C	Rb4	O13D	93.96 (18)	4_554	.	4_454	yes
O1W	Rb4	O11C	70.2 (2)	4_554	.	4_554	yes
O1W	Rb4	O12C	116.3 (2)	4_554	.	4_554	yes
O11C	Rb4	O12C	46.57 (17)	4_554	.	4_554	yes
O11A	S1A	O12A	111.3 (4)	.	.	.	no
O11A	S1A	O13A	112.7 (4)	.	.	.	no
O11A	S1A	C1A	105.5 (4)	.	.	.	no
O12A	S1A	O13A	112.9 (4)	.	.	.	no
O12A	S1A	C1A	107.0 (4)	.	.	.	no
O13A	S1A	C1A	106.9 (4)	.	.	.	no
O11B	S1B	O12B	111.4 (4)	.	.	.	no
O11B	S1B	O13B	113.6 (4)	.	.	.	no
O11B	S1B	C1B	107.8 (4)	.	.	.	no
O12B	S1B	O13B	112.2 (4)	.	.	.	no
O12B	S1B	C1B	105.6 (4)	.	.	.	no
O13B	S1B	C1B	105.8 (4)	.	.	.	no
O11C	S1C	O12C	111.5 (4)	.	.	.	no
O11C	S1C	O13C	112.3 (4)	.	.	.	no

O11C	S1C	C1C	105.9(4)	.	.	.	no
O12C	S1C	O13C	113.3(4)	.	.	.	no
O12C	S1C	C1C	106.1(4)	.	.	.	no
O13C	S1C	C1C	107.2(4)	.	.	.	no
O11D	S1D	O12D	111.6(4)	.	.	.	no
O11D	S1D	O13D	114.1(5)	.	.	.	no
O11D	S1D	C1D	107.1(4)	.	.	.	no
O12D	S1D	O13D	112.3(5)	.	.	.	no
O12D	S1D	C1D	104.9(4)	.	.	.	no
O13D	S1D	C1D	106.1(5)	.	.	.	no
Rb4	O1W	Rb4	158.9(4)	.	.	4_555	no
Rb2	O11A	S1A	107.4(3)	.	.	.	no
Rb2	O11A	Rb3	108.36(18)	.	.	1_655	no
Rb2	O11A	Rb4	105.71(19)	.	.	1_655	no
Rb3	O11A	S1A	138.3(4)	1_655	.	.	no
Rb4	O11A	S1A	99.9(3)	1_655	.	.	no
Rb3	O11A	Rb4	90.54(18)	1_655	.	1_655	no
Rb1	O11B	Rb2	75.95(16)	.	.	.	no
Rb1	O11B	S1B	95.7(3)	.	.	.	no
Rb2	O11B	S1B	148.1(4)	.	.	.	no
Rb1	O11C	Rb3	109.2(2)	.	.	.	no
Rb1	O11C	S1C	106.2(3)	.	.	.	no
Rb1	O11C	Rb4	111.54(19)	.	.	4_555	no
Rb3	O11C	S1C	137.0(4)	.	.	.	no
Rb3	O11C	Rb4	89.77(19)	.	.	4_555	no
Rb4	O11C	S1C	99.2(3)	4_555	.	.	no
Rb1	O11D	S1D	143.0(4)	.	.	.	no
Rb4	O12A	S1A	95.5(3)	1_655	.	.	no
Rb2	O12A	S1A	101.5(3)	4_554	.	.	no
Rb2	O12A	Rb4	93.80(17)	4_554	.	1_655	no
Rb1	O12B	Rb3	103.8(2)	.	.	.	no
Rb1	O12B	Rb4	100.13(19)	.	.	.	no
Rb1	O12B	S1B	104.9(3)	.	.	.	no
Rb3	O12B	Rb4	90.80(19)	.	.	.	no
Rb3	O12B	S1B	142.3(4)	.	.	.	no
Rb4	O12B	S1B	107.6(3)	.	.	.	no
Rb1	O12C	S1C	105.6(3)	4_555	.	.	no
Rb4	O12C	S1C	98.8(3)	4_555	.	.	no
Rb1	O12C	Rb4	95.95(18)	4_555	.	4_555	no
Rb2	O12D	S1D	105.6(4)	.	.	.	no
Rb2	O12D	Rb3	103.3(2)	.	.	1_655	no
Rb2	O12D	Rb4	101.49(19)	.	.	4_655	no
Rb3	O12D	S1D	142.0(4)	1_655	.	.	no
Rb4	O12D	S1D	107.4(4)	4_655	.	.	no
Rb3	O12D	Rb4	90.3(2)	1_655	.	4_655	no
Rb1	O13A	S1A	175.7(4)	4_554	.	.	no
Rb2	O13A	S1A	99.5(3)	4_554	.	.	no
Rb1	O13A	Rb2	79.54(17)	4_554	.	4_554	no
Rb4	O13B	S1B	93.8(3)	.	.	.	no
Rb1	O13B	Rb4	108.40(19)	4_554	.	.	no
Rb1	O13B	S1B	125.3(4)	4_554	.	.	no
Rb1	O13C	S1C	95.0(3)	.	.	.	no
Rb1	O13C	Rb2	84.79(17)	.	.	4_555	no
Rb2	O13C	S1C	171.3(4)	4_555	.	.	no
Rb2	O13D	S1D	129.2(5)	4_555	.	.	no
Rb4	O13D	S1D	94.0(4)	4_655	.	.	no
Rb2	O13D	Rb4	102.86(19)	4_555	.	4_655	no
Rb4	O1W	H12W	67.00	4_555	.	.	no

Rb4	O1W	H11W	119.00	.	.	.	no
Rb4	O1W	H12W	122.00	.	.	.	no
H11W	O1W	H12W	117.00	.	.	.	no
Rb3	N2A	C2A	107.5 (6)	1_655	.	.	no
Rb3	N2C	C2C	102.6 (6)	.	.	.	no
H21A	N2A	H22A	108.00	.	.	.	no
C2A	N2A	H22A	110.00	.	.	.	no
C2A	N2A	H21A	110.00	.	.	.	no
Rb3	N2A	H21A	110.00	1_655	.	.	no
Rb3	N2A	H22A	110.00	1_655	.	.	no
C2B	N2B	H21B	109.00	.	.	.	no
C2B	N2B	H22B	109.00	.	.	.	no
H21B	N2B	H22B	110.00	.	.	.	no
Rb3	N2C	H22C	111.00	.	.	.	no
Rb3	N2C	H21C	111.00	.	.	.	no
C2C	N2C	H22C	111.00	.	.	.	no
H21C	N2C	H22C	109.00	.	.	.	no
C2C	N2C	H21C	111.00	.	.	.	no
H21D	N2D	H22D	110.00	.	.	.	no
C2D	N2D	H21D	113.00	.	.	.	no
C2D	N2D	H22D	112.00	.	.	.	no
S1A	C1A	C6A	120.2 (7)	.	.	.	no
S1A	C1A	C2A	119.9 (7)	.	.	.	no
C2A	C1A	C6A	119.8 (9)	.	.	.	no
S1B	C1B	C6B	120.0 (7)	.	.	.	no
S1B	C1B	C2B	119.0 (7)	.	.	.	no
C2B	C1B	C6B	120.9 (9)	.	.	.	no
C2C	C1C	C6C	120.0 (9)	.	.	.	no
S1C	C1C	C2C	118.9 (7)	.	.	.	no
S1C	C1C	C6C	121.0 (7)	.	.	.	no
S1D	C1D	C2D	120.5 (8)	.	.	.	no
S1D	C1D	C6D	119.7 (8)	.	.	.	no
C2D	C1D	C6D	119.8 (9)	.	.	.	no
C1A	C2A	C3A	117.6 (9)	.	.	.	no
N2A	C2A	C3A	121.0 (9)	.	.	.	no
N2A	C2A	C1A	121.2 (9)	.	.	.	no
N2B	C2B	C3B	119.3 (10)	.	.	.	no
N2B	C2B	C1B	123.8 (9)	.	.	.	no
C1B	C2B	C3B	116.8 (10)	.	.	.	no
N2C	C2C	C1C	122.2 (9)	.	.	.	no
N2C	C2C	C3C	120.1 (9)	.	.	.	no
C1C	C2C	C3C	117.7 (9)	.	.	.	no
N2D	C2D	C3D	121.2 (12)	.	.	.	no
C1D	C2D	C3D	117.6 (12)	.	.	.	no
N2D	C2D	C1D	120.5 (9)	.	.	.	no
C2A	C3A	C4A	121.9 (10)	.	.	.	no
C2B	C3B	C4B	120.6 (10)	.	.	.	no
C2C	C3C	C4C	121.8 (10)	.	.	.	no
C2D	C3D	C4D	120.1 (14)	.	.	.	no
C3A	C4A	C5A	120.3 (10)	.	.	.	no
C3B	C4B	C5B	120.8 (9)	.	.	.	no
C3C	C4C	C5C	120.0 (9)	.	.	.	no
C3D	C4D	C5D	121.8 (13)	.	.	.	no
C4A	C5A	C6A	119.0 (11)	.	.	.	no
C4B	C5B	C6B	120.9 (10)	.	.	.	no
C4C	C5C	C6C	119.8 (10)	.	.	.	no
C4D	C5D	C6D	119.5 (15)	.	.	.	no
C1A	C6A	C5A	121.4 (10)	.	.	.	no

C1B	C6B	C5B	120.0 (9)	.	.	.	no
C1C	C6C	C5C	120.7 (9)	.	.	.	no
C1D	C6D	C5D	121.0 (12)	.	.	.	no
C2A	C3A	H3A	119.00	.	.	.	no
C4A	C3A	H3A	119.00	.	.	.	no
C2B	C3B	H3B	120.00	.	.	.	no
C4B	C3B	H3B	120.00	.	.	.	no
C2C	C3C	H3C	119.00	.	.	.	no
C4C	C3C	H3C	119.00	.	.	.	no
C2D	C3D	H3D	120.00	.	.	.	no
C4D	C3D	H3D	120.00	.	.	.	no
C3A	C4A	H4A	120.00	.	.	.	no
C5A	C4A	H4A	120.00	.	.	.	no
C3B	C4B	H4B	120.00	.	.	.	no
C5B	C4B	H4B	120.00	.	.	.	no
C3C	C4C	H4C	120.00	.	.	.	no
C5C	C4C	H4C	120.00	.	.	.	no
C3D	C4D	H4D	119.00	.	.	.	no
C5D	C4D	H4D	119.00	.	.	.	no
C4A	C5A	H5A	121.00	.	.	.	no
C6A	C5A	H5A	120.00	.	.	.	no
C4B	C5B	H5B	120.00	.	.	.	no
C6B	C5B	H5B	120.00	.	.	.	no
C4C	C5C	H5C	120.00	.	.	.	no
C6C	C5C	H5C	120.00	.	.	.	no
C4D	C5D	H5D	120.00	.	.	.	no
C6D	C5D	H5D	120.00	.	.	.	no
C1A	C6A	H6A	119.00	.	.	.	no
C5A	C6A	H6A	119.00	.	.	.	no
C1B	C6B	H6B	120.00	.	.	.	no
C5B	C6B	H6B	120.00	.	.	.	no
C1C	C6C	H6C	120.00	.	.	.	no
C5C	C6C	H6C	120.00	.	.	.	no
C1D	C6D	H6D	120.00	.	.	.	no
C5D	C6D	H6D	119.00	.	.	.	no

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O11C	Rb1	O11B	Rb2	-157.09 (16)	.	.	.	no
O11C	Rb1	O11B	S1B	54.2 (3)	.	.	.	no
O11D	Rb1	O11B	Rb2	-69.43 (19)	.	.	.	no
O11D	Rb1	O11B	S1B	141.8 (4)	.	.	.	no
O12B	Rb1	O11B	Rb2	158.9 (3)	.	.	.	no
O12B	Rb1	O11B	S1B	10.1 (3)	.	.	.	no
O13C	Rb1	O11B	Rb2	-109.90 (17)	.	.	.	no
O13C	Rb1	O11B	S1B	101.4 (3)	.	.	.	no
O12C	Rb1	O11B	Rb2	88.08 (17)	4_554	.	.	no
O12C	Rb1	O11B	S1B	-60.7 (3)	4_554	.	.	no
O13A	Rb1	O11B	Rb2	-4.9 (2)	4_555	.	.	no

O13A	Rb1	O11B	S1B	-153.6 (3)	4_555	.	.	.	no
O13B	Rb1	O11B	Rb2	125.0 (4)	4_555	.	.	.	no
O13B	Rb1	O11B	S1B	-23.7 (6)	4_555	.	.	.	no
O11B	Rb1	O11C	Rb3	-42.5 (2)	no
O11B	Rb1	O11C	S1C	112.7 (3)	no
O11B	Rb1	O11C	Rb4	-140.2 (2)	.	.	.	4_555	no
O11D	Rb1	O11C	Rb3	-101.5 (2)	no
O11D	Rb1	O11C	S1C	53.8 (3)	no
O11D	Rb1	O11C	Rb4	160.9 (2)	.	.	.	4_555	no
O12B	Rb1	O11C	Rb3	-11.19 (19)	no
O12B	Rb1	O11C	S1C	144.1 (4)	no
O12B	Rb1	O11C	Rb4	-108.8 (2)	.	.	.	4_555	no
O13C	Rb1	O11C	Rb3	-159.2 (3)	no
O13C	Rb1	O11C	S1C	-3.9 (3)	no
O13C	Rb1	O11C	Rb4	103.2 (3)	.	.	.	4_555	no
O12C	Rb1	O11C	Rb3	57.4 (2)	4_554	.	.	.	no
O12C	Rb1	O11C	S1C	-147.3 (3)	4_554	.	.	.	no
O12C	Rb1	O11C	Rb4	-40.2 (3)	4_554	.	.	4_555	no
O13A	Rb1	O11C	Rb3	-176.0 (2)	4_555	.	.	.	no
O13A	Rb1	O11C	S1C	-20.8 (5)	4_555	.	.	.	no
O13A	Rb1	O11C	Rb4	86.3 (3)	4_555	.	.	4_555	no
O13B	Rb1	O11C	Rb3	109.4 (2)	4_555	.	.	.	no
O13B	Rb1	O11C	S1C	-95.4 (3)	4_555	.	.	.	no
O13B	Rb1	O11C	Rb4	11.7 (2)	4_555	.	.	4_555	no
O11B	Rb1	O11D	S1D	138.0 (8)	no
O11C	Rb1	O11D	S1D	-118.8 (7)	no
O12B	Rb1	O11D	S1D	169.9 (7)	no
O13C	Rb1	O11D	S1D	-78.9 (7)	no
O12C	Rb1	O11D	S1D	96.4 (8)	4_554	.	.	.	no
O13A	Rb1	O11D	S1D	22.8 (7)	4_555	.	.	.	no
O13B	Rb1	O11D	S1D	-54.3 (9)	4_555	.	.	.	no
O11B	Rb1	O12B	Rb3	144.9 (3)	no
O11B	Rb1	O12B	Rb4	-121.7 (3)	no
O11B	Rb1	O12B	S1B	-10.3 (3)	no
O11C	Rb1	O12B	Rb3	10.38 (18)	no
O11C	Rb1	O12B	Rb4	103.7 (2)	no
O11C	Rb1	O12B	S1B	-144.8 (4)	no
O11D	Rb1	O12B	Rb3	105.3 (2)	no
O11D	Rb1	O12B	Rb4	-161.3 (2)	no
O11D	Rb1	O12B	S1B	-49.9 (3)	no
O13C	Rb1	O12B	Rb3	34.5 (2)	no
O13C	Rb1	O12B	Rb4	127.80 (18)	no
O13C	Rb1	O12B	S1B	-120.8 (3)	no
O12C	Rb1	O12B	Rb3	-108.9 (2)	4_554	.	.	.	no
O12C	Rb1	O12B	Rb4	-15.53 (19)	4_554	.	.	.	no
O12C	Rb1	O12B	S1B	95.9 (3)	4_554	.	.	.	no
O13A	Rb1	O12B	Rb3	173.7 (2)	4_555	.	.	.	no
O13A	Rb1	O12B	Rb4	-93.0 (3)	4_555	.	.	.	no
O13A	Rb1	O12B	S1B	18.4 (5)	4_555	.	.	.	no
O13B	Rb1	O12B	Rb3	-50.9 (2)	4_555	.	.	.	no
O13B	Rb1	O12B	Rb4	42.4 (2)	4_555	.	.	.	no
O13B	Rb1	O12B	S1B	153.9 (3)	4_555	.	.	.	no
O11B	Rb1	O13C	S1C	-77.8 (3)	no
O11B	Rb1	O13C	Rb2	110.94 (18)	.	.	.	4_555	no
O11C	Rb1	O13C	S1C	3.8 (2)	no
O11C	Rb1	O13C	Rb2	-167.5 (3)	.	.	.	4_555	no
O11D	Rb1	O13C	S1C	-113.6 (3)	no
O11D	Rb1	O13C	Rb2	75.18 (19)	.	.	.	4_555	no

O12B	Rb1	O13C	S1C	-28.7 (3)	no
O12B	Rb1	O13C	Rb2	160.10 (16)	.	.	.	4_555	no
O12C	Rb1	O13C	S1C	71.0 (4)	4_554	.	.	.	no
O12C	Rb1	O13C	Rb2	-100.3 (3)	4_554	.	.	4_555	no
O13A	Rb1	O13C	S1C	173.3 (3)	4_555	.	.	.	no
O13A	Rb1	O13C	Rb2	2.05 (19)	4_555	.	.	4_555	no
O13B	Rb1	O13C	S1C	79.7 (3)	4_555	.	.	.	no
O13B	Rb1	O13C	Rb2	-91.56 (19)	4_555	.	.	4_555	no
O11B	Rb1	O12C	Rb4	57.47 (19)	.	.	4_554	.	no
O11B	Rb1	O12C	S1C	-43.4 (3)	.	.	4_554	4_554	no
O11C	Rb1	O12C	Rb4	-49.3 (2)	.	.	4_554	.	no
O11C	Rb1	O12C	S1C	-150.2 (3)	.	.	4_554	4_554	no
O11D	Rb1	O12C	Rb4	92.1 (3)	.	.	4_554	.	no
O11D	Rb1	O12C	S1C	-8.8 (5)	.	.	4_554	4_554	no
O12B	Rb1	O12C	Rb4	14.55 (17)	.	.	4_554	.	no
O12B	Rb1	O12C	S1C	-86.3 (3)	.	.	4_554	4_554	no
O13C	Rb1	O12C	Rb4	-95.5 (3)	.	.	4_554	.	no
O13C	Rb1	O12C	S1C	163.7 (3)	.	.	4_554	4_554	no
O13A	Rb1	O12C	Rb4	160.8 (2)	4_555	.	4_554	.	no
O13B	Rb1	O12C	Rb4	-104.9 (2)	4_555	.	4_554	.	no
O11B	Rb1	O13A	Rb2	4.53 (18)	.	.	4_555	.	no
O11C	Rb1	O13A	Rb2	138.2 (2)	.	.	4_555	.	no
O11D	Rb1	O13A	Rb2	57.06 (17)	.	.	4_555	.	no
O12B	Rb1	O13A	Rb2	-15.9 (4)	.	.	4_555	.	no
O13C	Rb1	O13A	Rb2	126.11 (15)	.	.	4_555	.	no
O12C	Rb1	O13A	Rb2	-89.43 (16)	4_554	.	4_555	.	no
O13B	Rb1	O13A	Rb2	-154.80 (16)	4_555	.	4_555	.	no
O11B	Rb1	O13B	Rb4	75.0 (4)	.	.	4_555	4_555	no
O11B	Rb1	O13B	S1B	-176.3 (3)	.	.	4_555	4_555	no
O11C	Rb1	O13B	Rb4	-10.83 (19)	.	.	4_555	4_555	no
O11C	Rb1	O13B	S1B	97.9 (5)	.	.	4_555	4_555	no
O11D	Rb1	O13B	Rb4	-81.8 (4)	.	.	4_555	4_555	no
O11D	Rb1	O13B	S1B	27.0 (7)	.	.	4_555	4_555	no
O12B	Rb1	O13B	Rb4	50.0 (2)	.	.	4_555	4_555	no
O12B	Rb1	O13B	S1B	158.7 (4)	.	.	4_555	4_555	no
O13C	Rb1	O13B	Rb4	-58.0 (2)	.	.	4_555	4_555	no
O13C	Rb1	O13B	S1B	50.7 (4)	.	.	4_555	4_555	no
O11B	Rb2	O11A	S1A	52.6 (3)	no
O11B	Rb2	O11A	Rb3	-105.5 (2)	.	.	.	1_655	no
O11B	Rb2	O11A	Rb4	158.56 (19)	.	.	.	1_655	no
O12D	Rb2	O11A	S1A	144.3 (4)	no
O12D	Rb2	O11A	Rb3	-13.8 (2)	.	.	.	1_655	no
O12D	Rb2	O11A	Rb4	-109.7 (2)	.	.	.	1_655	no
O13C	Rb2	O11A	S1A	-20.3 (5)	4_554	.	.	.	no
O13C	Rb2	O11A	Rb3	-178.4 (2)	4_554	.	.	1_655	no
O13C	Rb2	O11A	Rb4	85.7 (3)	4_554	.	.	1_655	no
O13D	Rb2	O11A	S1A	-90.4 (3)	4_554	.	.	.	no
O13D	Rb2	O11A	Rb3	111.5 (3)	4_554	.	.	1_655	no
O13D	Rb2	O11A	Rb4	15.6 (2)	4_554	.	.	1_655	no
O12A	Rb2	O11A	S1A	-145.0 (3)	4_555	.	.	.	no
O12A	Rb2	O11A	Rb3	56.9 (2)	4_555	.	.	1_655	no
O12A	Rb2	O11A	Rb4	-39.0 (2)	4_555	.	.	1_655	no
O13A	Rb2	O11A	S1A	178.2 (3)	4_555	.	.	.	no
O13A	Rb2	O11A	Rb3	20.1 (5)	4_555	.	.	1_655	no
O13A	Rb2	O11A	Rb4	-75.8 (4)	4_555	.	.	1_655	no
O11A	Rb2	O11B	Rb1	159.99 (14)	no
O11A	Rb2	O11B	S1B	-122.1 (8)	no
O12D	Rb2	O11B	Rb1	88.22 (17)	no

O12D	Rb2	O11B	S1B	166.1 (8)	no
O13C	Rb2	O11B	Rb1	-59.93 (16)	4_554	.	.	.	no
O13C	Rb2	O11B	S1B	18.0 (8)	4_554	.	.	.	no
O13D	Rb2	O11B	Rb1	-123.2 (3)	4_554	.	.	.	no
O13D	Rb2	O11B	S1B	-45.3 (9)	4_554	.	.	.	no
O12A	Rb2	O11B	Rb1	10.1 (4)	4_555	.	.	.	no
O12A	Rb2	O11B	S1B	88.0 (9)	4_555	.	.	.	no
O13A	Rb2	O11B	Rb1	4.29 (18)	4_555	.	.	.	no
O13A	Rb2	O11B	S1B	82.2 (8)	4_555	.	.	.	no
O11A	Rb2	O12D	S1D	-142.2 (4)	no
O11A	Rb2	O12D	Rb3	12.84 (18)	.	.	.	1_655	no
O11A	Rb2	O12D	Rb4	105.9 (2)	.	.	.	4_655	no
O11B	Rb2	O12D	S1D	-46.6 (4)	no
O11B	Rb2	O12D	Rb3	108.4 (2)	.	.	.	1_655	no
O11B	Rb2	O12D	Rb4	-158.6 (2)	.	.	.	4_655	no
O13C	Rb2	O12D	S1D	19.8 (6)	4_554	.	.	.	no
O13C	Rb2	O12D	Rb3	174.8 (2)	4_554	.	.	1_655	no
O13C	Rb2	O12D	Rb4	-92.2 (4)	4_554	.	.	4_655	no
O13D	Rb2	O12D	S1D	154.1 (3)	4_554	.	.	.	no
O13D	Rb2	O12D	Rb3	-50.8 (3)	4_554	.	.	1_655	no
O13D	Rb2	O12D	Rb4	42.2 (3)	4_554	.	.	4_655	no
O12A	Rb2	O12D	S1D	99.9 (4)	4_555	.	.	.	no
O12A	Rb2	O12D	Rb3	-105.0 (2)	4_555	.	.	1_655	no
O12A	Rb2	O12D	Rb4	-12.0 (2)	4_555	.	.	4_655	no
O13A	Rb2	O12D	S1D	54.0 (3)	4_555	.	.	.	no
O13A	Rb2	O12D	Rb3	-151.0 (2)	4_555	.	.	1_655	no
O13A	Rb2	O12D	Rb4	-58.0 (2)	4_555	.	.	4_655	no
O11A	Rb2	O13C	Rb1	12.9 (3)	.	.	4_554	4_554	no
O11B	Rb2	O13C	Rb1	-68.15 (18)	.	.	4_554	4_554	no
O12D	Rb2	O13C	Rb1	-140.1 (3)	.	.	4_554	4_554	no
O11A	Rb2	O13D	Rb4	-14.52 (18)	.	.	4_554	1_655	no
O11A	Rb2	O13D	S1D	91.6 (5)	.	.	4_554	4_554	no
O11B	Rb2	O13D	Rb4	-97.8 (3)	.	.	4_554	1_655	no
O11B	Rb2	O13D	S1D	8.3 (7)	.	.	4_554	4_554	no
O12D	Rb2	O13D	Rb4	46.2 (3)	.	.	4_554	1_655	no
O12D	Rb2	O13D	S1D	152.4 (5)	.	.	4_554	4_554	no
O11A	Rb2	O12A	S1A	-150.8 (3)	.	.	4_555	4_555	no
O11A	Rb2	O12A	Rb4	-54.3 (2)	.	.	4_555	4_655	no
O11B	Rb2	O12A	S1A	-3.5 (5)	.	.	4_555	4_555	no
O11B	Rb2	O12A	Rb4	92.9 (3)	.	.	4_555	4_655	no
O12D	Rb2	O12A	S1A	-85.6 (3)	.	.	4_555	4_555	no
O12D	Rb2	O12A	Rb4	10.87 (19)	.	.	4_555	4_655	no
O11A	Rb2	O13A	Rb1	-129.5 (3)	.	.	4_555	.	no
O11A	Rb2	O13A	S1A	46.3 (5)	.	.	4_555	4_555	no
O11B	Rb2	O13A	Rb1	-4.9 (2)	.	.	4_555	.	no
O11B	Rb2	O13A	S1A	170.9 (3)	.	.	4_555	4_555	no
O12D	Rb2	O13A	Rb1	-97.31 (19)	.	.	4_555	.	no
O12D	Rb2	O13A	S1A	78.4 (3)	.	.	4_555	4_555	no
O13C	Rb2	O13A	Rb1	63.21 (18)	4_554	.	4_555	.	no
O13D	Rb2	O13A	Rb1	145.9 (2)	4_554	.	4_555	.	no
O12A	Rb2	O13A	Rb1	179.7 (3)	4_555	.	4_555	.	no
O12B	Rb3	O11C	Rb1	11.28 (19)	no
O12B	Rb3	O11C	S1C	-132.6 (6)	no
O12B	Rb3	O11C	Rb4	124.08 (19)	.	.	.	4_555	no
N2C	Rb3	O11C	Rb1	157.9 (3)	no
N2C	Rb3	O11C	S1C	14.0 (5)	no
N2C	Rb3	O11C	Rb4	-89.3 (2)	.	.	.	4_555	no
O11A	Rb3	O11C	Rb1	-60.5 (3)	1_455	.	.	.	no

O11A	Rb3	O11C	S1C	155.6 (5)	1_455	.	.	.	no
O11A	Rb3	O11C	Rb4	52.3 (3)	1_455	.	.	4_555	no
O12D	Rb3	O11C	Rb1	-128.6 (2)	1_455	.	.	.	no
O12D	Rb3	O11C	S1C	87.5 (6)	1_455	.	.	.	no
O12D	Rb3	O11C	Rb4	-15.82 (18)	1_455	.	.	4_555	no
N2A	Rb3	O11C	Rb1	38.2 (5)	1_455	.	.	.	no
N2A	Rb3	O11C	S1C	-105.7 (6)	1_455	.	.	.	no
N2A	Rb3	O11C	Rb4	151.0 (3)	1_455	.	.	4_555	no
O11C	Rb3	O12B	Rb1	-10.67 (18)	no
O11C	Rb3	O12B	Rb4	-111.3 (2)	no
O11C	Rb3	O12B	S1B	127.9 (6)	no
N2C	Rb3	O12B	Rb1	-47.2 (3)	no
N2C	Rb3	O12B	Rb4	-147.9 (2)	no
N2C	Rb3	O12B	S1B	91.3 (6)	no
O11A	Rb3	O12B	Rb1	122.1 (2)	1_455	.	.	.	no
O11A	Rb3	O12B	Rb4	21.42 (18)	1_455	.	.	.	no
O11A	Rb3	O12B	S1B	-99.4 (6)	1_455	.	.	.	no
O12D	Rb3	O12B	Rb1	59.9 (3)	1_455	.	.	.	no
O12D	Rb3	O12B	Rb4	-40.8 (3)	1_455	.	.	.	no
O12D	Rb3	O12B	S1B	-161.6 (5)	1_455	.	.	.	no
N2A	Rb3	O12B	Rb1	-176.3 (2)	1_455	.	.	.	no
N2A	Rb3	O12B	Rb4	83.1 (2)	1_455	.	.	.	no
N2A	Rb3	O12B	S1B	-37.7 (6)	1_455	.	.	.	no
O11C	Rb3	N2C	C2C	-65.6 (6)	no
O12B	Rb3	N2C	C2C	-25.3 (7)	no
O11A	Rb3	N2C	C2C	174.3 (5)	1_455	.	.	.	no
O12D	Rb3	N2C	C2C	-162.8 (6)	1_455	.	.	.	no
N2A	Rb3	N2C	C2C	77.7 (6)	1_455	.	.	.	no
O11C	Rb3	O11A	Rb4	45.6 (3)	.	.	1_455	.	no
O11C	Rb3	O11A	Rb2	-61.2 (3)	.	.	1_455	1_455	no
O11C	Rb3	O11A	S1A	151.2 (5)	.	.	1_455	1_455	no
O12B	Rb3	O11A	Rb4	-20.42 (17)	.	.	1_455	.	no
O12B	Rb3	O11A	Rb2	-127.2 (2)	.	.	1_455	1_455	no
O12B	Rb3	O11A	S1A	85.2 (6)	.	.	1_455	1_455	no
N2C	Rb3	O11A	Rb4	143.7 (3)	.	.	1_455	.	no
N2C	Rb3	O11A	Rb2	36.9 (5)	.	.	1_455	1_455	no
N2C	Rb3	O11A	S1A	-110.7 (6)	.	.	1_455	1_455	no
O12D	Rb3	O11A	Rb4	120.62 (19)	1_455	.	1_455	.	no
N2A	Rb3	O11A	Rb4	-97.5 (2)	1_455	.	1_455	.	no
O11C	Rb3	O12D	Rb2	118.6 (2)	.	.	1_455	1_455	no
O11C	Rb3	O12D	S1D	-102.8 (7)	.	.	1_455	1_455	no
O11C	Rb3	O12D	Rb4	16.70 (19)	.	.	1_455	4_555	no
O12B	Rb3	O12D	Rb2	53.6 (4)	.	.	1_455	1_455	no
O12B	Rb3	O12D	S1D	-167.7 (6)	.	.	1_455	1_455	no
O12B	Rb3	O12D	Rb4	-48.2 (3)	.	.	1_455	4_555	no
N2C	Rb3	O12D	Rb2	179.8 (3)	.	.	1_455	1_455	no
N2C	Rb3	O12D	S1D	-41.5 (7)	.	.	1_455	1_455	no
N2C	Rb3	O12D	Rb4	77.9 (2)	.	.	1_455	4_555	no
O11C	Rb3	N2A	C2A	177.9 (5)	.	.	1_455	1_455	no
O12B	Rb3	N2A	C2A	-155.6 (6)	.	.	1_455	1_455	no
N2C	Rb3	N2A	C2A	79.1 (7)	.	.	1_455	1_455	no
O1W	Rb4	S1B	O11B	-66.2 (4)	no
O1W	Rb4	S1B	O12B	19.7 (4)	no
O1W	Rb4	S1B	O13B	-165.4 (4)	no
O1W	Rb4	S1B	C1B	102.6 (4)	no
O12B	Rb4	S1B	O11B	-85.8 (5)	no
O12B	Rb4	S1B	O13B	174.9 (5)	no
O12B	Rb4	S1B	C1B	82.9 (5)	no

O13B	Rb4	S1B	O11B	99.2 (5)	no
O13B	Rb4	S1B	O12B	-174.9 (5)	no
O13B	Rb4	S1B	C1B	-92.0 (5)	no
S1A	Rb4	S1B	O11B	-163.4 (4)	1_455	.	.	.	no
S1A	Rb4	S1B	O12B	-77.6 (3)	1_455	.	.	.	no
S1A	Rb4	S1B	O13B	97.3 (3)	1_455	.	.	.	no
S1A	Rb4	S1B	C1B	5.3 (4)	1_455	.	.	.	no
O11A	Rb4	S1B	O11B	-139.6 (4)	1_455	.	.	.	no
O11A	Rb4	S1B	O12B	-53.8 (4)	1_455	.	.	.	no
O11A	Rb4	S1B	O13B	121.1 (3)	1_455	.	.	.	no
O11A	Rb4	S1B	C1B	29.1 (4)	1_455	.	.	.	no
O12A	Rb4	S1B	O11B	174.4 (4)	1_455	.	.	.	no
O12A	Rb4	S1B	O12B	-99.8 (4)	1_455	.	.	.	no
O12A	Rb4	S1B	O13B	75.1 (3)	1_455	.	.	.	no
O12A	Rb4	S1B	C1B	-16.9 (4)	1_455	.	.	.	no
O12D	Rb4	S1B	O11B	99.4 (5)	4_454	.	.	.	no
O12D	Rb4	S1B	O12B	-174.7 (5)	4_454	.	.	.	no
O12D	Rb4	S1B	O13B	0.2 (5)	4_454	.	.	.	no
O12D	Rb4	S1B	C1B	-91.8 (5)	4_454	.	.	.	no
O13D	Rb4	S1B	O11B	-85.8 (6)	4_454	.	.	.	no
O13D	Rb4	S1B	O12B	0.1 (5)	4_454	.	.	.	no
O13D	Rb4	S1B	O13B	175.0 (5)	4_454	.	.	.	no
O13D	Rb4	S1B	C1B	83.0 (6)	4_454	.	.	.	no
S1C	Rb4	S1B	O11B	19.9 (4)	4_554	.	.	.	no
S1C	Rb4	S1B	O12B	105.7 (3)	4_554	.	.	.	no
S1C	Rb4	S1B	O13B	-79.4 (3)	4_554	.	.	.	no
S1C	Rb4	S1B	C1B	-171.4 (4)	4_554	.	.	.	no
O1W	Rb4	S1B	O11B	116.1 (4)	4_554	.	.	.	no
O1W	Rb4	S1B	O12B	-158.1 (4)	4_554	.	.	.	no
O1W	Rb4	S1B	O13B	16.9 (4)	4_554	.	.	.	no
O1W	Rb4	S1B	C1B	-75.1 (4)	4_554	.	.	.	no
O11C	Rb4	S1B	O11B	44.0 (4)	4_554	.	.	.	no
O11C	Rb4	S1B	O12B	129.9 (4)	4_554	.	.	.	no
O11C	Rb4	S1B	O13B	-55.2 (3)	4_554	.	.	.	no
O11C	Rb4	S1B	C1B	-147.2 (4)	4_554	.	.	.	no
O12C	Rb4	S1B	O11B	-3.0 (4)	4_554	.	.	.	no
O12C	Rb4	S1B	O12B	82.9 (4)	4_554	.	.	.	no
O12C	Rb4	S1B	O13B	-102.2 (3)	4_554	.	.	.	no
O12C	Rb4	S1B	C1B	165.8 (4)	4_554	.	.	.	no
S1B	Rb4	O1W	Rb4	-50.5 (9)	.	.	.	4_555	no
O12B	Rb4	O1W	Rb4	-42.9 (8)	.	.	.	4_555	no
O13B	Rb4	O1W	Rb4	-57.4 (9)	.	.	.	4_555	no
S1A	Rb4	O1W	Rb4	52.0 (9)	1_455	.	.	4_555	no
O11A	Rb4	O1W	Rb4	44.2 (8)	1_455	.	.	4_555	no
O12A	Rb4	O1W	Rb4	47.6 (9)	1_455	.	.	4_555	no
S1D	Rb4	O1W	Rb4	128.8 (9)	4_454	.	.	4_555	no
O12D	Rb4	O1W	Rb4	136.0 (8)	4_454	.	.	4_555	no
O13D	Rb4	O1W	Rb4	121.8 (9)	4_454	.	.	4_555	no
S1C	Rb4	O1W	Rb4	-125.3 (9)	4_554	.	.	4_555	no
O11C	Rb4	O1W	Rb4	-132.5 (8)	4_554	.	.	4_555	no
O12C	Rb4	O1W	Rb4	-127.4 (9)	4_554	.	.	4_555	no
S1B	Rb4	O12B	Rb1	109.3 (4)	no
S1B	Rb4	O12B	Rb3	-146.5 (4)	no
O1W	Rb4	O12B	Rb1	-51.1 (2)	no
O1W	Rb4	O12B	Rb3	53.0 (2)	no
O1W	Rb4	O12B	S1B	-160.4 (4)	no
O13B	Rb4	O12B	Rb1	112.1 (3)	no
O13B	Rb4	O12B	Rb3	-143.7 (3)	no

O13B	Rb4	O12B	S1B	2.8 (3)	no
S1A	Rb4	O12B	Rb1	-144.95 (15)	1_455	.	.	.	no
S1A	Rb4	O12B	Rb3	-40.81 (14)	1_455	.	.	.	no
S1A	Rb4	O12B	S1B	105.7 (3)	1_455	.	.	.	no
O11A	Rb4	O12B	Rb1	-124.13 (19)	1_455	.	.	.	no
O11A	Rb4	O12B	Rb3	-19.99 (16)	1_455	.	.	.	no
O11A	Rb4	O12B	S1B	126.5 (3)	1_455	.	.	.	no
O12A	Rb4	O12B	Rb1	-169.11 (19)	1_455	.	.	.	no
O12A	Rb4	O12B	Rb3	-64.98 (19)	1_455	.	.	.	no
O12A	Rb4	O12B	S1B	81.5 (3)	1_455	.	.	.	no
O13D	Rb4	O12B	Rb1	-70.6 (3)	4_454	.	.	.	no
O13D	Rb4	O12B	Rb3	33.5 (3)	4_454	.	.	.	no
O13D	Rb4	O12B	S1B	-180.0 (3)	4_454	.	.	.	no
S1C	Rb4	O12B	Rb1	39.36 (15)	4_554	.	.	.	no
S1C	Rb4	O12B	Rb3	143.50 (15)	4_554	.	.	.	no
S1C	Rb4	O12B	S1B	-70.0 (3)	4_554	.	.	.	no
O1W	Rb4	O12B	Rb1	130.9 (2)	4_554	.	.	.	no
O1W	Rb4	O12B	Rb3	-125.0 (2)	4_554	.	.	.	no
O1W	Rb4	O12B	S1B	21.6 (4)	4_554	.	.	.	no
O11C	Rb4	O12B	Rb1	60.5 (2)	4_554	.	.	.	no
O11C	Rb4	O12B	Rb3	164.60 (17)	4_554	.	.	.	no
O11C	Rb4	O12B	S1B	-48.9 (3)	4_554	.	.	.	no
O12C	Rb4	O12B	Rb1	15.43 (18)	4_554	.	.	.	no
O12C	Rb4	O12B	Rb3	119.57 (19)	4_554	.	.	.	no
O12C	Rb4	O12B	S1B	-93.9 (3)	4_554	.	.	.	no
S1B	Rb4	O13B	Rb1	-129.2 (4)	.	.	.	4_554	no
O1W	Rb4	O13B	S1B	17.3 (4)	no
O1W	Rb4	O13B	Rb1	-111.9 (3)	.	.	.	4_554	no
O12B	Rb4	O13B	S1B	-2.7 (3)	no
O12B	Rb4	O13B	Rb1	-131.9 (3)	.	.	.	4_554	no
S1A	Rb4	O13B	S1B	-87.8 (3)	1_455	.	.	.	no
S1A	Rb4	O13B	Rb1	143.01 (17)	1_455	.	.	4_554	no
O11A	Rb4	O13B	S1B	-63.9 (3)	1_455	.	.	.	no
O11A	Rb4	O13B	Rb1	166.94 (18)	1_455	.	.	4_554	no
O12A	Rb4	O13B	S1B	-104.3 (3)	1_455	.	.	.	no
O12A	Rb4	O13B	Rb1	126.5 (2)	1_455	.	.	4_554	no
S1D	Rb4	O13B	S1B	-176.33 (15)	4_454	.	.	.	no
S1D	Rb4	O13B	Rb1	54.5 (4)	4_454	.	.	4_554	no
O12D	Rb4	O13B	S1B	-179.9 (3)	4_454	.	.	.	no
O12D	Rb4	O13B	Rb1	50.9 (3)	4_454	.	.	4_554	no
S1C	Rb4	O13B	S1B	93.8 (3)	4_554	.	.	.	no
S1C	Rb4	O13B	Rb1	-35.41 (16)	4_554	.	.	4_554	no
O1W	Rb4	O13B	S1B	-159.7 (4)	4_554	.	.	.	no
O1W	Rb4	O13B	Rb1	71.1 (3)	4_554	.	.	4_554	no
O11C	Rb4	O13B	S1B	118.3 (3)	4_554	.	.	.	no
O11C	Rb4	O13B	Rb1	-10.90 (19)	4_554	.	.	4_554	no
O12C	Rb4	O13B	S1B	76.1 (3)	4_554	.	.	.	no
O12C	Rb4	O13B	Rb1	-53.1 (2)	4_554	.	.	4_554	no
S1B	Rb4	S1A	O11A	83.8 (3)	.	.	1_455	1_455	no
S1B	Rb4	S1A	O12A	-67.8 (3)	.	.	1_455	1_455	no
S1B	Rb4	S1A	O13A	-172.6 (3)	.	.	1_455	1_455	no
S1B	Rb4	S1A	C1A	12.3 (5)	.	.	1_455	1_455	no
O1W	Rb4	S1A	O11A	-18.8 (4)	.	.	1_455	1_455	no
O1W	Rb4	S1A	O12A	-170.4 (4)	.	.	1_455	1_455	no
O1W	Rb4	S1A	O13A	84.8 (4)	.	.	1_455	1_455	no
O1W	Rb4	S1A	C1A	-90.3 (6)	.	.	1_455	1_455	no
O12B	Rb4	S1A	O11A	61.5 (3)	.	.	1_455	1_455	no
O12B	Rb4	S1A	O12A	-90.1 (3)	.	.	1_455	1_455	no

O12B	Rb4	S1A	O13A	165.1 (4)	.	.	1_455	1_455	no
O12B	Rb4	S1A	C1A	-10.0 (6)	.	.	1_455	1_455	no
O13B	Rb4	S1A	O11A	107.7 (3)	.	.	1_455	1_455	no
O13B	Rb4	S1A	O12A	-43.9 (3)	.	.	1_455	1_455	no
O13B	Rb4	S1A	O13A	-148.7 (4)	.	.	1_455	1_455	no
O13B	Rb4	S1A	C1A	36.3 (5)	.	.	1_455	1_455	no
S1B	Rb4	O11A	Rb3	39.20 (14)	.	.	1_455	.	no
S1B	Rb4	O11A	Rb2	148.46 (14)	.	.	1_455	1_455	no
S1B	Rb4	O11A	S1A	-100.2 (3)	.	.	1_455	1_455	no
O1W	Rb4	O11A	Rb3	-60.3 (2)	.	.	1_455	.	no
O1W	Rb4	O11A	Rb2	48.9 (2)	.	.	1_455	1_455	no
O1W	Rb4	O11A	S1A	160.3 (4)	.	.	1_455	1_455	no
O12B	Rb4	O11A	Rb3	20.92 (17)	.	.	1_455	.	no
O12B	Rb4	O11A	Rb2	130.2 (2)	.	.	1_455	1_455	no
O12B	Rb4	O11A	S1A	-118.5 (3)	.	.	1_455	1_455	no
O13B	Rb4	O11A	Rb3	60.35 (19)	.	.	1_455	.	no
O13B	Rb4	O11A	Rb2	169.62 (17)	.	.	1_455	1_455	no
O13B	Rb4	O11A	S1A	-79.0 (3)	.	.	1_455	1_455	no
S1A	Rb4	O11A	Rb3	139.4 (4)	1_455	.	1_455	.	no
O12A	Rb4	O11A	Rb3	123.8 (3)	1_455	.	1_455	.	no
S1D	Rb4	O11A	Rb3	-144.58 (14)	4_454	.	1_455	.	no
O12D	Rb4	O11A	Rb3	-163.10 (19)	4_454	.	1_455	.	no
O13D	Rb4	O11A	Rb3	-123.7 (2)	4_454	.	1_455	.	no
S1C	Rb4	O11A	Rb3	-30.1 (4)	4_554	.	1_455	.	no
O1W	Rb4	O11A	Rb3	117.6 (2)	4_554	.	1_455	.	no
O12C	Rb4	O11A	Rb3	-49.1 (3)	4_554	.	1_455	.	no
S1B	Rb4	O12A	S1A	114.7 (3)	.	.	1_455	1_455	no
S1B	Rb4	O12A	Rb2	-143.31 (15)	.	.	1_455	4_454	no
O1W	Rb4	O12A	S1A	10.9 (4)	.	.	1_455	1_455	no
O1W	Rb4	O12A	Rb2	112.9 (2)	.	.	1_455	4_454	no
O12B	Rb4	O12A	S1A	92.2 (3)	.	.	1_455	1_455	no
O12B	Rb4	O12A	Rb2	-165.81 (19)	.	.	1_455	4_454	no
O13B	Rb4	O12A	S1A	137.4 (3)	.	.	1_455	1_455	no
O13B	Rb4	O12A	Rb2	-120.60 (19)	.	.	1_455	4_454	no
O1W	Rb4	S1D	O11D	-114.1 (5)	.	.	4_454	4_454	no
O1W	Rb4	S1D	O12D	161.6 (4)	.	.	4_454	4_454	no
O1W	Rb4	S1D	O13D	-15.2 (4)	.	.	4_454	4_454	no
O1W	Rb4	S1D	C1D	78.0 (5)	.	.	4_454	4_454	no
O13B	Rb4	S1D	O11D	77.3 (5)	.	.	4_454	4_454	no
O13B	Rb4	S1D	O12D	-7.0 (5)	.	.	4_454	4_454	no
O13B	Rb4	S1D	O13D	176.2 (4)	.	.	4_454	4_454	no
O13B	Rb4	S1D	C1D	-90.6 (5)	.	.	4_454	4_454	no
S1B	Rb4	O12D	Rb2	65.2 (4)	.	.	4_454	4_454	no
S1B	Rb4	O12D	S1D	175.74 (15)	.	.	4_454	4_454	no
S1B	Rb4	O12D	Rb3	-38.4 (4)	.	.	4_454	4_554	no
O1W	Rb4	O12D	Rb2	-129.4 (2)	.	.	4_454	4_454	no
O1W	Rb4	O12D	S1D	-18.8 (4)	.	.	4_454	4_454	no
O1W	Rb4	O12D	Rb3	127.0 (2)	.	.	4_454	4_554	no
O13B	Rb4	O12D	Rb2	65.3 (3)	.	.	4_454	4_454	no
O13B	Rb4	O12D	S1D	175.9 (3)	.	.	4_454	4_454	no
O13B	Rb4	O12D	Rb3	-38.3 (3)	.	.	4_454	4_554	no
S1B	Rb4	O13D	Rb2	-43.4 (5)	.	.	4_454	1_455	no
S1B	Rb4	O13D	S1D	-175.11 (18)	.	.	4_454	4_454	no
O1W	Rb4	O13D	Rb2	-65.7 (3)	.	.	4_454	1_455	no
O1W	Rb4	O13D	S1D	162.5 (4)	.	.	4_454	4_454	no
O12B	Rb4	O13D	Rb2	-43.4 (4)	.	.	4_454	1_455	no
O12B	Rb4	O13D	S1D	-175.1 (3)	.	.	4_454	4_454	no
S1B	Rb4	S1C	O11C	94.6 (3)	.	.	4_554	4_554	no

S1B	Rb4	S1C	O12C	-106.8 (3)	.	.	4_554	4_554	no
S1B	Rb4	S1C	O13C	-5.4 (3)	.	.	4_554	4_554	no
S1B	Rb4	S1C	C1C	173.5 (4)	.	.	4_554	4_554	no
O1W	Rb4	S1C	O11C	-163.3 (4)	.	.	4_554	4_554	no
O1W	Rb4	S1C	O12C	-4.8 (4)	.	.	4_554	4_554	no
O1W	Rb4	S1C	O13C	96.6 (4)	.	.	4_554	4_554	no
O1W	Rb4	S1C	C1C	-84.5 (5)	.	.	4_554	4_554	no
O12B	Rb4	S1C	O11C	116.7 (3)	.	.	4_554	4_554	no
O12B	Rb4	S1C	O12C	-84.8 (3)	.	.	4_554	4_554	no
O12B	Rb4	S1C	O13C	16.7 (3)	.	.	4_554	4_554	no
O12B	Rb4	S1C	C1C	-164.4 (4)	.	.	4_554	4_554	no
O13B	Rb4	S1C	O11C	70.4 (3)	.	.	4_554	4_554	no
O13B	Rb4	S1C	O12C	-131.1 (3)	.	.	4_554	4_554	no
O13B	Rb4	S1C	O13C	-29.7 (3)	.	.	4_554	4_554	no
O13B	Rb4	S1C	C1C	149.3 (4)	.	.	4_554	4_554	no
S1B	Rb4	O1W	Rb4	-128.8 (9)	.	.	4_554	4_554	no
O12B	Rb4	O1W	Rb4	-137.2 (8)	.	.	4_554	4_554	no
O13B	Rb4	O1W	Rb4	-120.7 (9)	.	.	4_554	4_554	no
S1B	Rb4	O11C	Rb1	31.82 (17)	.	.	4_554	4_554	no
S1B	Rb4	O11C	Rb3	142.47 (15)	.	.	4_554	4_554	no
S1B	Rb4	O11C	S1C	-79.8 (3)	.	.	4_554	4_554	no
O1W	Rb4	O11C	Rb1	129.6 (3)	.	.	4_554	4_554	no
O1W	Rb4	O11C	Rb3	-119.8 (2)	.	.	4_554	4_554	no
O1W	Rb4	O11C	S1C	18.0 (4)	.	.	4_554	4_554	no
O12B	Rb4	O11C	Rb1	49.1 (2)	.	.	4_554	4_554	no
O12B	Rb4	O11C	Rb3	159.77 (18)	.	.	4_554	4_554	no
O12B	Rb4	O11C	S1C	-62.5 (3)	.	.	4_554	4_554	no
O13B	Rb4	O11C	Rb1	10.85 (19)	.	.	4_554	4_554	no
O13B	Rb4	O11C	Rb3	121.5 (2)	.	.	4_554	4_554	no
O13B	Rb4	O11C	S1C	-100.8 (3)	.	.	4_554	4_554	no
S1B	Rb4	O12C	Rb1	-37.96 (13)	.	.	4_554	.	no
S1B	Rb4	O12C	S1C	68.9 (3)	.	.	4_554	4_554	no
O1W	Rb4	O12C	Rb1	67.9 (2)	.	.	4_554	.	no
O1W	Rb4	O12C	S1C	174.7 (4)	.	.	4_554	4_554	no
O12B	Rb4	O12C	Rb1	-15.10 (18)	.	.	4_554	.	no
O12B	Rb4	O12C	S1C	91.7 (3)	.	.	4_554	4_554	no
O13B	Rb4	O12C	Rb1	-60.88 (18)	.	.	4_554	.	no
O13B	Rb4	O12C	S1C	45.9 (3)	.	.	4_554	4_554	no
O11A	Rb4	O12C	Rb1	56.1 (3)	1_455	.	4_554	.	no
S1D	Rb4	O12C	Rb1	145.03 (13)	4_454	.	4_554	.	no
O12D	Rb4	O12C	Rb1	168.1 (2)	4_454	.	4_554	.	no
O13D	Rb4	O12C	Rb1	121.98 (19)	4_454	.	4_554	.	no
S1C	Rb4	O12C	Rb1	-106.8 (4)	4_554	.	4_554	.	no
O1W	Rb4	O12C	Rb1	-109.6 (2)	4_554	.	4_554	.	no
O11C	Rb4	O12C	Rb1	-118.5 (3)	4_554	.	4_554	.	no
O12A	S1A	O11A	Rb2	136.4 (3)	no
O12A	S1A	O11A	Rb3	-75.8 (6)	.	.	.	1_655	no
O12A	S1A	O11A	Rb4	26.4 (4)	.	.	.	1_655	no
O13A	S1A	O11A	Rb2	8.4 (4)	no
O13A	S1A	O11A	Rb3	156.3 (5)	.	.	.	1_655	no
O13A	S1A	O11A	Rb4	-101.6 (4)	.	.	.	1_655	no
C1A	S1A	O11A	Rb2	-107.9 (4)	no
C1A	S1A	O11A	Rb3	40.0 (7)	.	.	.	1_655	no
C1A	S1A	O11A	Rb4	142.1 (4)	.	.	.	1_655	no
Rb4	S1A	O11A	Rb2	110.0 (3)	1_655	.	.	.	no
Rb4	S1A	O11A	Rb3	-102.1 (6)	1_655	.	.	1_655	no
O11A	S1A	O12A	Rb4	-25.2 (4)	.	.	.	1_655	no
O11A	S1A	O12A	Rb2	-120.2 (3)	.	.	.	4_554	no

O13A	S1A	O12A	Rb4	102.8 (4)	.	.	.	1_655	no
O13A	S1A	O12A	Rb2	7.7 (4)	.	.	.	4_554	no
C1A	S1A	O12A	Rb4	-139.9 (4)	.	.	.	1_655	no
C1A	S1A	O12A	Rb2	125.0 (4)	.	.	.	4_554	no
Rb4	S1A	O12A	Rb2	-95.0 (2)	1_655	.	.	4_554	no
O11A	S1A	O13A	Rb2	119.6 (3)	.	.	.	4_554	no
O12A	S1A	O13A	Rb2	-7.5 (4)	.	.	.	4_554	no
C1A	S1A	O13A	Rb2	-124.9 (4)	.	.	.	4_554	no
Rb4	S1A	O13A	Rb2	58.3 (3)	1_655	.	.	4_554	no
O11A	S1A	C1A	C2A	-65.9 (9)	no
O11A	S1A	C1A	C6A	114.3 (9)	no
O12A	S1A	C1A	C2A	52.8 (9)	no
O12A	S1A	C1A	C6A	-127.1 (9)	no
O13A	S1A	C1A	C2A	173.9 (8)	no
O13A	S1A	C1A	C6A	-5.9 (10)	no
Rb4	S1A	C1A	C2A	-10.8 (11)	1_655	.	.	.	no
Rb4	S1A	C1A	C6A	169.3 (6)	1_655	.	.	.	no
Rb4	S1B	O11B	Rb1	38.8 (4)	no
Rb4	S1B	O11B	Rb2	-33.6 (10)	no
O12B	S1B	O11B	Rb1	-16.0 (4)	no
O12B	S1B	O11B	Rb2	-88.3 (8)	no
O13B	S1B	O11B	Rb1	111.9 (4)	no
O13B	S1B	O11B	Rb2	39.5 (9)	no
C1B	S1B	O11B	Rb1	-131.3 (4)	no
C1B	S1B	O11B	Rb2	156.3 (7)	no
Rb4	S1B	O12B	Rb1	-106.0 (3)	no
Rb4	S1B	O12B	Rb3	115.7 (7)	no
O11B	S1B	O12B	Rb1	17.7 (4)	no
O11B	S1B	O12B	Rb3	-120.6 (6)	no
O11B	S1B	O12B	Rb4	123.7 (3)	no
O13B	S1B	O12B	Rb1	-110.9 (4)	no
O13B	S1B	O12B	Rb3	110.8 (6)	no
O13B	S1B	O12B	Rb4	-4.9 (5)	no
C1B	S1B	O12B	Rb1	134.4 (4)	no
C1B	S1B	O12B	Rb3	-3.9 (7)	no
C1B	S1B	O12B	Rb4	-119.6 (4)	no
Rb4	S1B	O13B	Rb1	115.8 (4)	.	.	.	4_554	no
O11B	S1B	O13B	Rb4	-123.2 (3)	no
O11B	S1B	O13B	Rb1	-7.5 (6)	.	.	.	4_554	no
O12B	S1B	O13B	Rb4	4.2 (4)	no
O12B	S1B	O13B	Rb1	119.9 (4)	.	.	.	4_554	no
C1B	S1B	O13B	Rb4	118.8 (4)	no
C1B	S1B	O13B	Rb1	-125.5 (5)	.	.	.	4_554	no
Rb4	S1B	C1B	C2B	-107.8 (8)	no
Rb4	S1B	C1B	C6B	70.8 (9)	no
O11B	S1B	C1B	C2B	63.1 (9)	no
O11B	S1B	C1B	C6B	-118.3 (8)	no
O12B	S1B	C1B	C2B	-56.0 (9)	no
O12B	S1B	C1B	C6B	122.6 (8)	no
O13B	S1B	C1B	C2B	-175.1 (8)	no
O13B	S1B	C1B	C6B	3.5 (9)	no
O12C	S1C	O11C	Rb1	135.1 (3)	no
O12C	S1C	O11C	Rb3	-80.3 (6)	no
O12C	S1C	O11C	Rb4	19.4 (4)	.	.	.	4_555	no
O13C	S1C	O11C	Rb1	6.8 (4)	no
O13C	S1C	O11C	Rb3	151.3 (5)	no
O13C	S1C	O11C	Rb4	-109.0 (3)	.	.	.	4_555	no
C1C	S1C	O11C	Rb1	-109.9 (4)	no

C1C	S1C	O11C	Rb3	34.7 (6)	no
C1C	S1C	O11C	Rb4	134.3 (3)	.	.	.	4_555	no
Rb4	S1C	O11C	Rb1	115.8 (3)	4_555	.	.	.	no
Rb4	S1C	O11C	Rb3	-99.7 (5)	4_555	.	.	.	no
O11C	S1C	O12C	Rb1	-118.0 (3)	.	.	.	4_555	no
O11C	S1C	O12C	Rb4	-19.3 (4)	.	.	.	4_555	no
O13C	S1C	O12C	Rb1	9.9 (4)	.	.	.	4_555	no
O13C	S1C	O12C	Rb4	108.6 (3)	.	.	.	4_555	no
C1C	S1C	O12C	Rb1	127.1 (3)	.	.	.	4_555	no
C1C	S1C	O12C	Rb4	-134.1 (3)	.	.	.	4_555	no
Rb4	S1C	O12C	Rb1	-98.7 (3)	4_555	.	.	4_555	no
O11C	S1C	O13C	Rb1	-6.0 (4)	no
O12C	S1C	O13C	Rb1	-133.4 (3)	no
C1C	S1C	O13C	Rb1	110.0 (3)	no
Rb4	S1C	O13C	Rb1	-69.3 (2)	4_555	.	.	.	no
O11C	S1C	C1C	C2C	-64.2 (8)	no
O11C	S1C	C1C	C6C	111.8 (8)	no
O12C	S1C	C1C	C2C	54.4 (8)	no
O12C	S1C	C1C	C6C	-129.6 (8)	no
O13C	S1C	C1C	C2C	175.7 (7)	no
O13C	S1C	C1C	C6C	-8.3 (9)	no
Rb4	S1C	C1C	C2C	-5.3 (10)	4_555	.	.	.	no
Rb4	S1C	C1C	C6C	170.7 (6)	4_555	.	.	.	no
O12D	S1D	O11D	Rb1	-89.1 (7)	no
O13D	S1D	O11D	Rb1	39.5 (8)	no
C1D	S1D	O11D	Rb1	156.6 (7)	no
Rb4	S1D	O11D	Rb1	-34.3 (9)	4_655	.	.	.	no
O11D	S1D	O12D	Rb2	18.7 (4)	no
O11D	S1D	O12D	Rb3	-119.5 (7)	.	.	.	1_655	no
O11D	S1D	O12D	Rb4	126.4 (4)	.	.	.	4_655	no
O13D	S1D	O12D	Rb2	-110.8 (4)	no
O13D	S1D	O12D	Rb3	111.1 (7)	.	.	.	1_655	no
O13D	S1D	O12D	Rb4	-3.1 (5)	.	.	.	4_655	no
C1D	S1D	O12D	Rb2	134.4 (4)	no
C1D	S1D	O12D	Rb3	-3.8 (8)	.	.	.	1_655	no
C1D	S1D	O12D	Rb4	-117.9 (4)	.	.	.	4_655	no
Rb4	S1D	O12D	Rb2	-107.7 (3)	4_655	.	.	.	no
Rb4	S1D	O12D	Rb3	114.1 (8)	4_655	.	.	1_655	no
O11D	S1D	O13D	Rb2	-15.4 (7)	.	.	.	4_555	no
O11D	S1D	O13D	Rb4	-125.5 (4)	.	.	.	4_655	no
O12D	S1D	O13D	Rb2	112.8 (5)	.	.	.	4_555	no
O12D	S1D	O13D	Rb4	2.7 (4)	.	.	.	4_655	no
C1D	S1D	O13D	Rb2	-133.1 (5)	.	.	.	4_555	no
C1D	S1D	O13D	Rb4	116.8 (4)	.	.	.	4_655	no
Rb4	S1D	O13D	Rb2	110.2 (5)	4_655	.	.	4_555	no
O11D	S1D	C1D	C2D	61.6 (10)	no
O11D	S1D	C1D	C6D	-119.3 (9)	no
O12D	S1D	C1D	C2D	-57.2 (10)	no
O12D	S1D	C1D	C6D	122.0 (9)	no
O13D	S1D	C1D	C2D	-176.2 (9)	no
O13D	S1D	C1D	C6D	3.0 (10)	no
Rb4	S1D	C1D	C2D	-108.9 (9)	4_655	.	.	.	no
Rb4	S1D	C1D	C6D	70.2 (9)	4_655	.	.	.	no
Rb3	N2A	C2A	C1A	67.8 (10)	1_655	.	.	.	no
Rb3	N2A	C2A	C3A	-106.4 (9)	1_655	.	.	.	no
Rb3	N2C	C2C	C1C	72.4 (9)	no
Rb3	N2C	C2C	C3C	-104.8 (9)	no
S1A	C1A	C2A	N2A	3.0 (13)	no

S1A	C1A	C2A	C3A	177.4 (8)	no
C6A	C1A	C2A	N2A	-177.1 (9)	no
C6A	C1A	C2A	C3A	-2.7 (15)	no
S1A	C1A	C6A	C5A	-178.0 (9)	no
C2A	C1A	C6A	C5A	2.2 (16)	no
S1B	C1B	C2B	N2B	1.1 (15)	no
S1B	C1B	C2B	C3B	177.3 (8)	no
C6B	C1B	C2B	N2B	-177.5 (10)	no
C6B	C1B	C2B	C3B	-1.3 (15)	no
S1B	C1B	C6B	C5B	-177.3 (8)	no
C2B	C1B	C6B	C5B	1.3 (15)	no
S1C	C1C	C2C	N2C	-1.2 (13)	no
S1C	C1C	C2C	C3C	176.1 (8)	no
C6C	C1C	C2C	N2C	-177.2 (9)	no
C6C	C1C	C2C	C3C	0.1 (14)	no
S1C	C1C	C6C	C5C	-174.9 (9)	no
C2C	C1C	C6C	C5C	1.0 (15)	no
S1D	C1D	C2D	N2D	2.5 (16)	no
S1D	C1D	C2D	C3D	173.5 (10)	no
C6D	C1D	C2D	N2D	-176.7 (11)	no
C6D	C1D	C2D	C3D	-5.7 (17)	no
S1D	C1D	C6D	C5D	-175.4 (9)	no
C2D	C1D	C6D	C5D	3.8 (16)	no
N2A	C2A	C3A	C4A	175.7 (10)	no
C1A	C2A	C3A	C4A	1.2 (16)	no
N2B	C2B	C3B	C4B	176.4 (11)	no
C1B	C2B	C3B	C4B	0.0 (16)	no
N2C	C2C	C3C	C4C	176.9 (11)	no
C1C	C2C	C3C	C4C	-0.5 (17)	no
N2D	C2D	C3D	C4D	175.4 (14)	no
C1D	C2D	C3D	C4D	5 (2)	no
C2A	C3A	C4A	C5A	0.9 (18)	no
C2B	C3B	C4B	C5B	1.3 (18)	no
C2C	C3C	C4C	C5C	0 (2)	no
C2D	C3D	C4D	C5D	-1 (2)	no
C3A	C4A	C5A	C6A	-1.5 (18)	no
C3B	C4B	C5B	C6B	-1.3 (17)	no
C3C	C4C	C5C	C6C	2 (2)	no
C3D	C4D	C5D	C6D	-1 (2)	no
C4A	C5A	C6A	C1A	-0.1 (17)	no
C4B	C5B	C6B	C1B	0.0 (15)	no
C4C	C5C	C6C	C1C	-1.8 (18)	no
C4D	C5D	C6D	C1D	-0.4 (18)	no

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 #D H A D - H H...A D...A D - H...A symm(A)

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N2B	H21B	O11B	0.89	2.53	3.189(12)	131	.	yes
N2B	H21B	O12B	0.89	2.38	3.020(12)	129	.	yes
N2C	H21C	O12C	0.90	2.30	2.950(11)	129	.	yes
N2D	H21D	O11D	0.90	2.48	3.129(14)	130	.	yes
O1W	H11W	O12A	0.91	2.65	3.026(11)	106	4_455	no
O1W	H12W	O13B	0.90	1.94	2.838(11)	180	4_555	yes
C6A	H6A	O13A	0.93	2.49	2.893(11)	106	.	no
C6B	H6B	O13B	0.93	2.48	2.867(11)	105	.	no
C6C	H6C	O13C	0.93	2.53	2.913(11)	105	.	no
C6D	H6D	O13D	0.93	2.46	2.854(14)	105	.	no

END of data for (1)

Compound 2: CCDC 858091 [ORTHCS]

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#-----
# Reference: Smith (2012). Aust. J. Chem.
# gs1lgs23 ORTHCS COMPOUND(2)
# CCDC reference: 858091
#-----
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data_(2)

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<i>O</i></i></i></i>^'^^caesium]
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loop_

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- 6 1/2-x, 1/2-y, 1/2+z
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- 8 1/2+x, 1/2-y, z

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_exptl_crystal_colour 'colourless'
_exptl_crystal_size_max 0.33
_exptl_crystal_size_mid 0.22
_exptl_crystal_size_min 0.08
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 2.244
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 1152
_exptl_absorpt_coefficient_mu 4.297
_exptl_absorpt_correction_type 'multi-scan'
_exptl_absorpt_correction_T_min 0.778
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_exptl_absorpt_process_details
'CrysAlis PRO (Oxford Diffraction, 2010)'

_exptl_special_details

;
?
;

_diffn_ambient_temperature 200 (2)
_diffn_radiation_wavelength 0.71073
_diffn_radiation_type MoK\alpha
_diffn_radiation_source 'Enhance (Mo) X-ray source'
_diffn_radiation_monochromator graphite
_diffn_measurement_device_type
'Oxford Diffraction Gemini-S CCD-detector diffractometer'
_diffn_measurement_method '\w scans'
_diffn_detector_area_resol_mean 16.077
_diffn_standards_number 0
_diffn_standards_interval_count .

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_diffrn_reflns_number                 2985
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_diffrn_reflns_av_sigmaI/netI        0.0377
_diffrn_reflns_limit_h_min            -28
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_diffrn_reflns_limit_k_min            -13
_diffrn_reflns_limit_k_max            7
_diffrn_reflns_limit_l_min            -9
_diffrn_reflns_limit_l_max            9
_diffrn_reflns_theta_min               3.36
_diffrn_reflns_theta_max               28.70
_diffrn_measured_fraction_theta_max   0.877
_diffrn_reflns_theta_full              26.070
_diffrn_measured_fraction_theta_full  0.998

_reflns_number_total                  1815
_reflns_number_gt                     1673
_reflns_threshold_expression           'I>2\s(I) '

_computing_data_collection             'CrysAlis PRO'
_computing_cell_refinement             'CrysAlis PRO'
_computing_data_reduction              'CrysAlis PRO'
_computing_structure_solution          'SHELXS97 (Sheldrick, 2008) '
_computing_structure_refinement        'SHELXL97 (Sheldrick, 2008) within WinGX (Farrugia, 1999) '
_computing_molecular_graphics          'PLATON (Spek, 2009) '
_computing_publication_material        'PLATON'

_refine_special_details
;
Refinement on F2 for ALL reflections except those
flagged by the user for potential systematic errors.
Weighted R-factors wR and all goodnesses of fit S
are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The
observed criterion of F2 > 2sigma(F2) is used only
for calculating -R-factor-obs etc. and is not
relevant to the choice of reflections for refinement.
R-factors based on F2 are statistically about twice
as large as those based on F, and R-factors based on
ALL data will be even larger.
;
_refine_ls_structure_factor_coef       Fsqd
_refine_ls_matrix_type                 full
_refine_ls_weighting_scheme            calc
_refine_ls_weighting_details           'calc w=1/[\s^2^(Fo^2^)+(0.0431P)^2^] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary           direct
_atom_sites_solution_secondary         difmap
_atom_sites_solution_hydrogens         geom
_refine_ls_hydrogen_treatment          'noref'
_refine_ls_extinction_method           'SHELXL97'
_refine_ls_extinction_coef             0.00291(18)
_refine_ls_extinction_expression       'FC^*=KFC[1+0.001XFC^2^\L^3^\SIN(2\Q)]^-1/4^'
_refine_ls_abs_structure_details       'Flack (1983): 552 Friedel pairs'

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_refine_ls_abs_structure_Flack	0.03(3)
_refine_ls_number_reflns	1815
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_refine_ls_number_restraints	1
_refine_ls_number_constraints	?
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_refine_ls_R_factor_gt	0.0276
_refine_ls_wR_factor_ref	0.0696
_refine_ls_wR_factor_gt	0.0671
_refine_ls_goodness_of_fit_ref	0.956
_refine_ls_restrained_S_all	0.956
_refine_ls_shift/su_max	0.000
_refine_ls_shift/su_mean	0.000
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_refine_diff_density_min	-0.719
_refine_diff_density_rms	0.129

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_atom_site_fract_x										
_atom_site_fract_y										
_atom_site_fract_z										
_atom_site_occupancy										
_atom_site_U_iso_or_equiv										
_atom_site_calc_flag										
_atom_site_refinement_flags										
Cs1	Cs	Uani	0.31706(1)	1.17070(2)	0.94700(7)	1.000	0.0264(1)	.	.	
S1	S	Uani	0.33781(7)	0.81014(10)	0.97101(16)	1.000	0.0216(3)	.	.	
O11	O	Uani	0.3687(2)	0.9065(3)	1.0735(5)	1.000	0.0293(13)	.	.	
O12	O	Uani	0.28951(18)	0.8667(4)	0.8713(4)	1.000	0.0268(11)	.	.	
O13	O	Uani	0.31730(19)	0.6977(4)	1.0721(5)	1.000	0.0301(13)	.	.	
N2	N	Uani	0.3310(2)	0.5494(5)	0.7682(7)	1.000	0.0373(17)	.	.	
C1	C	Uani	0.3893(2)	0.7473(5)	0.8221(6)	1.000	0.0227(14)	.	.	
C2	C	Uani	0.3800(3)	0.6256(5)	0.7390(6)	1.000	0.0263(16)	.	.	
C3	C	Uani	0.4211(3)	0.5898(5)	0.6135(7)	1.000	0.0353(19)	.	.	
C4	C	Uani	0.4671(3)	0.6694(6)	0.5695(9)	1.000	0.041(2)	.	.	
C5	C	Uani	0.4757(3)	0.7897(7)	0.6497(8)	1.000	0.0390(19)	.	.	
C6	C	Uani	0.4366(3)	0.8277(5)	0.7769(8)	1.000	0.0290(17)	.	.	
H3	H	Uiso	0.41690	0.50940	0.55850	1.000	0.0420	calc	R	
H4	H	Uiso	0.49320	0.64260	0.48450	1.000	0.0490	calc	R	
H5	H	Uiso	0.50700	0.84370	0.61860	1.000	0.0470	calc	R	
H6	H	Uiso	0.44200	0.90750	0.83260	1.000	0.0350	calc	R	
H21	H	Uiso	0.32540	0.47920	0.70930	1.000	0.0450	calc	R	
H22	H	Uiso	0.30600	0.57190	0.84530	1.000	0.0450	calc	R	

loop_

_atom_site_aniso_label										
_atom_site_aniso_U_11										
_atom_site_aniso_U_22										
_atom_site_aniso_U_33										
_atom_site_aniso_U_23										
_atom_site_aniso_U_13										
_atom_site_aniso_U_12										
Cs1	0.0326(2)	0.0231(2)	0.0234(2)	-0.0004(2)	-0.0033(2)	0.0032(1)				
S1	0.0276(6)	0.0175(5)	0.0198(7)	0.0006(4)	0.0001(6)	-0.0002(4)				
O11	0.035(3)	0.0250(17)	0.0280(18)	-0.0063(14)	-0.0050(17)	0.0007(16)				

O12 0.023(2) 0.0251(17) 0.0323(19) 0.0018(15) -0.0025(16) 0.0025(17)
O13 0.040(3) 0.0203(17) 0.030(2) 0.0029(16) 0.0086(18) -0.0019(16)
N2 0.041(3) 0.032(3) 0.039(3) -0.014(2) 0.005(2) -0.009(2)
C1 0.022(3) 0.027(2) 0.019(2) 0.0005(18) -0.003(2) 0.005(2)
C2 0.032(3) 0.025(2) 0.022(3) -0.0024(19) -0.001(2) 0.005(2)
C3 0.039(4) 0.031(3) 0.036(3) -0.005(2) 0.003(3) 0.016(3)
C4 0.043(4) 0.044(4) 0.036(3) 0.002(2) 0.015(3) 0.017(3)
C5 0.031(4) 0.047(3) 0.039(3) 0.009(3) 0.007(3) 0.002(3)
C6 0.024(3) 0.032(3) 0.031(3) 0.006(2) -0.003(2) -0.001(2)

_geom_special_details

;

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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loop_

_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_1
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Cs1	O11	3.095(3)	.	.	yes
Cs1	O12	3.211(4)	.	.	yes
Cs1	O11	3.246(4)	.	4_574	yes
Cs1	O13	3.226(4)	.	4_574	yes
Cs1	O12	3.402(3)	.	4_575	yes
Cs1	O12	3.189(4)	.	7_555	yes
Cs1	O13	3.211(4)	.	7_555	yes
S1	O11	1.448(4)	.	.	no
S1	O12	1.463(4)	.	.	no
S1	O13	1.467(4)	.	.	no
S1	C1	1.769(5)	.	.	no
N2	C2	1.374(8)	.	.	no
N2	H22	0.8600	.	.	no
N2	H21	0.8600	.	.	no
C1	C6	1.395(8)	.	.	no
C1	C2	1.415(7)	.	.	no
C2	C3	1.402(8)	.	.	no
C3	C4	1.365(9)	.	.	no
C4	C5	1.390(9)	.	.	no
C5	C6	1.388(9)	.	.	no
C3	H3	0.9300	.	.	no
C4	H4	0.9300	.	.	no
C5	H5	0.9300	.	.	no
C6	H6	0.9300	.	.	no

loop_

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_geom_angle_site_symmetry_2

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

O11	Cs1	O12	45.23(10)	.	.	.	yes
O11	Cs1	O11	86.65(10)	.	.	4_574	yes
O11	Cs1	O13	130.62(10)	.	.	4_574	yes
O11	Cs1	O12	70.11(10)	.	.	4_575	yes
O11	Cs1	C2	98.96(12)	.	.	4_575	yes
O11	Cs1	O12	152.81(11)	.	.	7_555	yes
O11	Cs1	O13	109.60(11)	.	.	7_555	yes
O11	Cs1	O12	70.78(8)	4_574	.	.	yes
O12	Cs1	O13	103.44(9)	.	.	4_574	yes
O12	Cs1	O12	92.11(9)	.	.	4_575	yes
O12	Cs1	C2	142.48(11)	.	.	4_575	yes
O12	Cs1	O12	114.90(10)	.	.	7_555	yes
O12	Cs1	O13	87.38(10)	.	.	7_555	yes
O11	Cs1	O13	43.98(10)	4_574	.	4_574	yes
O11	Cs1	O12	156.76(9)	4_574	.	4_575	yes
O11	Cs1	C2	127.00(12)	4_574	.	4_575	yes
O11	Cs1	O12	104.91(9)	4_574	.	7_555	yes
O11	Cs1	O13	129.61(11)	4_574	.	7_555	yes
O12	Cs1	O13	159.27(10)	4_575	.	4_574	yes
O13	Cs1	C2	110.97(11)	4_574	.	4_575	yes
O12	Cs1	O13	64.69(10)	7_555	.	4_574	yes
O13	Cs1	O13	104.10(10)	4_574	.	7_555	yes
O12	Cs1	O12	96.45(9)	4_575	.	7_555	yes
O12	Cs1	O13	62.46(10)	4_575	.	7_555	yes
O12	Cs1	O13	44.31(10)	7_555	.	7_555	yes
Cs1	O11	S1	103.2(2)	.	.	.	yes
Cs1	O11	Cs1	111.23(12)	.	.	4_575	yes
Cs1	O11	S1	99.26(19)	4_575	.	.	yes
Cs1	O12	S1	97.76(18)	.	.	.	yes
Cs1	O12	Cs1	104.62(10)	.	.	4_574	yes
Cs1	O12	Cs1	135.70(13)	.	.	7_545	yes
Cs1	O12	S1	109.86(19)	4_574	.	.	yes
Cs1	O12	S1	102.82(19)	7_545	.	.	yes
Cs1	O12	Cs1	104.52(10)	4_574	.	7_545	yes
Cs1	O13	S1	99.65(19)	4_575	.	.	yes
Cs1	O13	S1	101.7(2)	7_545	.	.	yes
Cs1	O13	Cs1	108.14(12)	4_575	.	7_545	yes
H21	N2	H22	120.00	.	.	.	no
C2	N2	H22	120.00	.	.	.	no
C2	N2	H21	120.00	.	.	.	no
C2	C1	C6	120.8(5)	.	.	.	no
S1	C1	C6	117.6(4)	.	.	.	no
S1	C1	C2	121.4(4)	.	.	.	no
N2	C2	C1	122.6(5)	.	.	.	no
N2	C2	C3	120.5(5)	.	.	.	no
Cs1	C2	N2	96.7(4)	4_574	.	.	no
Cs1	C2	C3	88.1(3)	4_574	.	.	no
C1	C2	C3	116.8(5)	.	.	.	no
Cs1	C2	C1	80.7(3)	4_574	.	.	no
C2	C3	C4	122.0(5)	.	.	.	no
C3	C4	C5	121.1(6)	.	.	.	no
C4	C5	C6	118.7(6)	.	.	.	no
C1	C6	C5	120.6(5)	.	.	.	no
C2	C3	H3	119.00	.	.	.	no
C4	C3	H3	119.00	.	.	.	no
C3	C4	H4	119.00	.	.	.	no

C5	C4	H4	119.00	.	.	.	no
C4	C5	H5	121.00	.	.	.	no
C6	C5	H5	121.00	.	.	.	no
C1	C6	H6	120.00	.	.	.	no
C5	C6	H6	120.00	.	.	.	no

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 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
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O12	Cs1	O11	S1	5.30 (16)	no
O12	Cs1	O11	Cs1	-100.26 (17)	.	.	.	4_575	no
O11	Cs1	O11	Cs1	-166.28 (13)	4_574	.	.	4_575	no
O13	Cs1	O11	S1	-59.9 (3)	4_574	.	.	.	no
O13	Cs1	O11	Cs1	-165.45 (11)	4_574	.	.	4_575	no
O12	Cs1	O11	S1	119.8 (2)	4_575	.	.	.	no
O12	Cs1	O11	Cs1	14.19 (11)	4_575	.	.	4_575	no
O12	Cs1	O11	S1	56.0 (3)	7_555	.	.	.	no
O12	Cs1	O11	Cs1	-49.5 (3)	7_555	.	.	4_575	no
O13	Cs1	O11	S1	70.4 (2)	7_555	.	.	.	no
O13	Cs1	O11	Cs1	-35.20 (15)	7_555	.	.	4_575	no
O11	Cs1	O12	S1	-5.15 (15)	no
O11	Cs1	O12	Cs1	-118.10 (18)	.	.	.	4_574	no
O11	Cs1	O12	Cs1	112.3 (2)	.	.	.	7_545	no
O11	Cs1	O12	S1	99.85 (19)	4_574	.	.	.	no
O11	Cs1	O12	Cs1	-13.10 (10)	4_574	.	.	4_574	no
O11	Cs1	O12	Cs1	-142.75 (19)	4_574	.	.	7_545	no
O13	Cs1	O12	S1	129.75 (17)	4_574	.	.	.	no
O13	Cs1	O12	Cs1	16.80 (13)	4_574	.	.	4_574	no
O13	Cs1	O12	Cs1	-112.85 (16)	4_574	.	.	7_545	no
O12	Cs1	O12	S1	-64.09 (17)	4_575	.	.	.	no
O12	Cs1	O12	Cs1	-177.03 (11)	4_575	.	.	4_574	no
O12	Cs1	O12	Cs1	53.32 (17)	4_575	.	.	7_545	no
O12	Cs1	O12	S1	-162.20 (15)	7_555	.	.	.	no
O12	Cs1	O12	Cs1	84.86 (12)	7_555	.	.	4_574	no
O12	Cs1	O12	Cs1	-44.79 (18)	7_555	.	.	7_545	no
O13	Cs1	O12	S1	-126.38 (17)	7_555	.	.	.	no
O13	Cs1	O12	Cs1	120.67 (12)	7_555	.	.	4_574	no
O13	Cs1	O12	Cs1	-8.98 (16)	7_555	.	.	7_545	no
O11	Cs1	S1	Cs1	33.56 (9)	.	.	4_574	4_574	no
O11	Cs1	S1	O11	-14.2 (2)	.	.	4_574	4_574	no
O11	Cs1	S1	O12	88.8 (2)	.	.	4_574	4_574	no
O11	Cs1	S1	O13	-171.0 (2)	.	.	4_574	4_574	no
O11	Cs1	S1	C1	-93.5 (3)	.	.	4_574	4_574	no
O12	Cs1	S1	Cs1	-4.95 (8)	.	.	4_574	4_574	no
O12	Cs1	S1	O11	-52.7 (2)	.	.	4_574	4_574	no
O12	Cs1	S1	O12	50.3 (2)	.	.	4_574	4_574	no
O12	Cs1	S1	O13	150.5 (2)	.	.	4_574	4_574	no
O12	Cs1	S1	C1	-132.0 (3)	.	.	4_574	4_574	no
O11	Cs1	O11	Cs1	58.37 (13)	.	.	4_574	4_574	no

O11	Cs1	O11	S1	166.5(2)	.	.	4_574	4_574	no
O12	Cs1	O11	Cs1	14.98(11)	.	.	4_574	4_574	no
O12	Cs1	O11	S1	123.1(2)	.	.	4_574	4_574	no
O11	Cs1	O13	S1	11.3(3)	.	.	4_574	4_574	no
O12	Cs1	O13	S1	-30.3(2)	.	.	4_574	4_574	no
O11	Cs1	O12	Cs1	-13.81(11)	.	.	4_575	4_575	no
O11	Cs1	O12	S1	90.2(2)	.	.	4_575	4_575	no
O11	Cs1	O12	Cs1	-160.07(14)	.	.	4_575	6_575	no
O12	Cs1	O12	Cs1	26.49(12)	.	.	4_575	4_575	no
O12	Cs1	O12	S1	130.5(2)	.	.	4_575	4_575	no
O12	Cs1	O12	Cs1	-119.77(12)	.	.	4_575	6_575	no
O11	Cs1	C2	N2	-137.6(3)	.	.	4_575	4_575	no
O11	Cs1	C2	C1	-15.6(3)	.	.	4_575	4_575	no
O11	Cs1	C2	C3	101.9(3)	.	.	4_575	4_575	no
O12	Cs1	C2	N2	-122.5(3)	.	.	4_575	4_575	no
O12	Cs1	C2	C1	-0.5(4)	.	.	4_575	4_575	no
O12	Cs1	C2	C3	117.1(3)	.	.	4_575	4_575	no
O11	Cs1	S1	Cs1	67.44(10)	.	.	7_555	6_575	no
O11	Cs1	S1	Cs1	155.73(10)	.	.	7_555	7_555	no
O11	Cs1	S1	O11	102.7(2)	.	.	7_555	7_555	no
O11	Cs1	S1	O12	-169.9(2)	.	.	7_555	7_555	no
O11	Cs1	S1	O13	15.2(2)	.	.	7_555	7_555	no
O11	Cs1	S1	C1	-77.5(2)	.	.	7_555	7_555	no
O12	Cs1	S1	Cs1	105.74(6)	.	.	7_555	6_575	no
O12	Cs1	S1	Cs1	-165.97(6)	.	.	7_555	7_555	no
O12	Cs1	S1	O11	141.0(2)	.	.	7_555	7_555	no
O12	Cs1	S1	O12	-131.62(18)	.	.	7_555	7_555	no
O12	Cs1	S1	O13	53.5(2)	.	.	7_555	7_555	no
O12	Cs1	S1	C1	-39.21(19)	.	.	7_555	7_555	no
O11	Cs1	O12	Cs1	132.3(2)	.	.	7_555	7_555	no
O11	Cs1	O12	S1	16.7(3)	.	.	7_555	7_555	no
O12	Cs1	O12	Cs1	169.58(14)	.	.	7_555	7_555	no
O12	Cs1	O12	S1	54.02(19)	.	.	7_555	7_555	no
O11	Cs1	O13	Cs1	87.72(13)	.	.	7_555	6_575	no
O11	Cs1	O13	S1	-167.92(17)	.	.	7_555	7_555	no
O12	Cs1	O13	Cs1	127.84(12)	.	.	7_555	6_575	no
O12	Cs1	O13	S1	-127.80(19)	.	.	7_555	7_555	no
O12	S1	O11	Cs1	-9.0(3)	no
O12	S1	O11	Cs1	105.52(19)	.	.	.	4_575	no
O13	S1	O11	Cs1	-135.6(2)	no
O13	S1	O11	Cs1	-21.1(3)	.	.	.	4_575	no
C1	S1	O11	Cs1	107.9(2)	no
C1	S1	O11	Cs1	-137.59(19)	.	.	.	4_575	no
O11	S1	O12	Cs1	8.5(2)	no
O11	S1	O12	Cs1	117.2(2)	.	.	.	4_574	no
O11	S1	O12	Cs1	-132.0(2)	.	.	.	7_545	no
O13	S1	O12	Cs1	135.97(19)	no
O13	S1	O12	Cs1	-115.4(2)	.	.	.	4_574	no
O13	S1	O12	Cs1	-4.6(2)	.	.	.	7_545	no
C1	S1	O12	Cs1	-108.61(19)	no
C1	S1	O12	Cs1	0.1(2)	.	.	.	4_574	no
C1	S1	O12	Cs1	110.9(2)	.	.	.	7_545	no
O11	S1	O13	Cs1	21.3(3)	.	.	.	4_575	no
O11	S1	O13	Cs1	132.2(2)	.	.	.	7_545	no
O12	S1	O13	Cs1	-106.47(19)	.	.	.	4_575	no
O12	S1	O13	Cs1	4.5(2)	.	.	.	7_545	no
C1	S1	O13	Cs1	138.04(18)	.	.	.	4_575	no
C1	S1	O13	Cs1	-111.0(2)	.	.	.	7_545	no

O11	S1	C1	C2	160.2(4)	no
O11	S1	C1	C6	-25.9(5)	no
O12	S1	C1	C2	-78.7(5)	no
O12	S1	C1	C6	95.3(5)	no
O13	S1	C1	C2	39.8(5)	no
O13	S1	C1	C6	-146.3(4)	no
S1	C1	C2	N2	0.0(7)	no
S1	C1	C2	C3	175.1(4)	no
S1	C1	C2	Cs1	92.1(3)	.	.	.	4_574	no
C6	C1	C2	N2	-173.7(5)	no
C6	C1	C2	C3	1.4(8)	no
C6	C1	C2	Cs1	-81.7(5)	.	.	.	4_574	no
S1	C1	C6	C5	-174.2(5)	no
C2	C1	C6	C5	-0.2(9)	no
N2	C2	C3	C4	173.5(6)	no
C1	C2	C3	C4	-1.7(9)	no
C2	C3	C4	C5	0.9(10)	no
C3	C4	C5	C6	0.3(10)	no
C4	C5	C6	C1	-0.6(9)	no

loop_

_geom_hbond_atom_site_label_D
 _geom_hbond_atom_site_label_H
 _geom_hbond_atom_site_label_A
 _geom_hbond_distance_DH
 _geom_hbond_distance_HA
 _geom_hbond_distance_DA
 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A
 _geom_hbond_publ_flag

#	D	H	A	D - H	H...A	D...A	D - H...A	symm(A)	
#									
N2		H21	O13	0.86	2.10	2.963(7)	176	4_564	yes
N2		H22	O13	0.86	2.20	2.835(7)	130	.	yes
C6		H6	O11	0.93	2.51	2.899(8)	105	.	no
#	END of data for (2)								