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#==============================================================================
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#==============================================================================

_audit_creation_date               07-11-05
_audit_creation_method            SHELXL-97

# 1. Submission Details

_publ_contact_author_name          'Jun Okuda'
_publ_contact_author_address
;
        Institute of Inorganic Chemistry
        RWTH Aachen University
        Landoltweg 1
        D-52056 Aachen
        Germany
;
_publ_contact_author_phone         '0049-241-8094645'
_publ_contact_author_fax           '0049-241-8092644'
_publ_contact_author_email         'jun.okuda@ac.rwth-aachen.de'
_publ_requested_journal            'Inorganic Chemistry'



_publ_requested_coeditor_name      ?

_publ_contact_letter
;
March 4, 2005
This CIF file is part of a manuscript that is submitted for publication in the
journal 'Inorganic Chemistry'.
;
# 3. TITLE AND AUTHOR LIST

_publ_section_title
;
Rare-Earth Metal Complexes Supported by 1,\w-Dithia-alkanediyl-Bridged
Bis(phenolato) Ligands: Synthesis, Structure, and Heteroselective
Ring-Opening Polymerization of rac-Lactide
;

# The loop structure below should contain the names  and addresses of all
# authors, in the required order of publication. Repeat as necessary.

loop_
 _publ_author_name
 _publ_author_address


        'Ma, Haiyan'
;       Institute of Inorganic Chemistry
        RWTH Aachen University
        Landoltweg 1
        D-52056 Aachen
        Germany
;
```

```
        'Spaniol, Thomas P.'
;       Institute of Inorganic Chemistry
        RWTH Aachen University
        Landoltweg 1
        D-52056 Aachen
        Germany
;
        'Okuda, Jun'
;       Institute of Inorganic Chemistry
        RWTH Aachen University
        Landoltweg 1
        D-52056 Aachen
        Germany
;
#===============================================
_publ_section_abstract
;
;
_publ_section_references
;
Bruker (1999). SAINT. Version 6.02. Program for Reduction of Data
Collected on Bruker CCD Area Detector Diffractometer, Bruker AXS
Inc., Madison, Wisconson, USA.

Bruker (2001). SMART. Version 5.624. Program for Bruker CCD X-ray
Diffractometer Control. Bruker AXS Inc., Madison, Wisconson, USA.

Farrugia, L. J. (1999). J. Appl. Cryst. 32, 837.

Sheldrick, G. M. (1996). SADABS. Program for Empirical Absorption
Correction of Area Detector Data, University of G\"ottingen, Germany.

Sheldrick, G. M. (1986). SHELXS-86. A Program for Crystal Structure Solution,
University of G\"ottingen, Germany.

Sheldrick, G. M. (1997). SHELXL-97. A Program for Crystal Structure
Refinement, University of G\"ottingen, University of G\"ottingen, Germany.
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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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S2 S 0.46263(5) 0.02000(2) 0.79898(3) 0.01757(11) Uani 1 1 d . . .
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H1 H 0.795(2) 0.2220(10) 0.7949(13) 0.021 Uiso 1 1 d . . .
Si2 Si 1.06422(6) 0.09592(2) 0.78836(3) 0.01822(12) Uani 1 1 d . . .
H2 H 1.172(2) 0.1178(10) 0.8373(14) 0.022 Uiso 1 1 d . . .
O1 O 0.63436(14) 0.13010(6) 0.89443(8) 0.0166(3) Uani 1 1 d . . .
O2 O 0.70865(13) 0.01397(6) 0.72531(8) 0.0164(3) Uani 1 1 d . . .
O3 O 0.58770(15) 0.13489(7) 0.71379(8) 0.0225(3) Uani 1 1 d . . .
N N 0.91742(17) 0.12970(7) 0.80186(10) 0.0169(3) Uani 1 1 d . . .
C1 C 0.67293(19) 0.13711(8) 0.96907(11) 0.0135(4) Uani 1 1 d . . .
C2 C 0.77157(19) 0.10040(8) 1.00837(11) 0.0135(4) Uani 1 1 d . . .
C3 C 0.82388(19) 0.10796(8) 1.08551(11) 0.0144(4) Uani 1 1 d . . .
H3 H 0.8927 0.0830 1.1094 0.017 Uiso 1 1 calc R . .
C4 C 0.7759(2) 0.15159(8) 1.12743(11) 0.0154(4) Uani 1 1 d . . .
C5 C 0.67347(19) 0.18652(8) 1.08963(11) 0.0154(4) Uani 1 1 d . . .
H5 H 0.6382 0.2159 1.1185 0.019 Uiso 1 1 calc R . .
C6 C 0.62008(19) 0.18114(8) 1.01279(11) 0.0141(4) Uani 1 1 d . . .
C7 C 0.8288(2) 0.15983(10) 1.21134(12) 0.0228(4) Uani 1 1 d . . .
H7A H 0.9100 0.1363 1.2252 0.034 Uiso 1 1 calc R . .
H7B H 0.7592 0.1482 1.2423 0.034 Uiso 1 1 calc R . .
H7C H 0.8515 0.2003 1.2210 0.034 Uiso 1 1 calc R . .
C8 C 0.5087(2) 0.22163(8) 0.97476(11) 0.0168(4) Uani 1 1 d . . .
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C9 C 0.4597(2) 0.26270(10) 1.03304(13) 0.0279(5) Uani 1 1 d . . .
H9A H 0.3904 0.2883 1.0065 0.042 Uiso 1 1 calc R . .
H9B H 0.5363 0.2855 1.0578 0.042 Uiso 1 1 calc R . .
H9C H 0.4212 0.2406 1.0720 0.042 Uiso 1 1 calc R . .
C10 C 0.5651(2) 0.25809(9) 0.91398(12) 0.0228(4) Uani 1 1 d . . .
H10A H 0.6000 0.2329 0.8768 0.034 Uiso 1 1 calc R . .
H10B H 0.6385 0.2824 0.9390 0.034 Uiso 1 1 calc R . .
H10C H 0.4927 0.2822 0.8874 0.034 Uiso 1 1 calc R . .
C11 C 0.3861(2) 0.18700(10) 0.93806(13) 0.0237(4) Uani 1 1 d . . .
H11A H 0.3176 0.2131 0.9118 0.036 Uiso 1 1 calc R . .
H11B H 0.3478 0.1659 0.9780 0.036 Uiso 1 1 calc R . .
H11C H 0.4144 0.1599 0.9009 0.036 Uiso 1 1 calc R . .
C12 C 0.7137(2) -0.01477(9) 0.98141(12) 0.0195(4) Uani 1 1 d . . .
H12A H 0.7426 -0.0285 1.0345 0.023 Uiso 1 1 calc R . .
H12B H 0.6210 0.0010 0.9786 0.023 Uiso 1 1 calc R . .
C13 C 0.7136(2) -0.06385(8) 0.92605(11) 0.0176(4) Uani 1 1 d . . .
C14 C 0.6023(2) -0.07582(8) 0.86997(12) 0.0181(4) Uani 1 1 d . . .
C15 C 0.6114(2) -0.12162(9) 0.82006(12) 0.0223(4) Uani 1 1 d . . .
H15 H 0.5367 -0.1301 0.7819 0.027 Uiso 1 1 calc R . .
C16 C 0.7270(2) -0.15497(9) 0.82500(13) 0.0257(5) Uani 1 1 d . . .
H16 H 0.7317 -0.1856 0.7899 0.031 Uiso 1 1 calc R . .
C17 C 0.8350(2) -0.14364(9) 0.88078(14) 0.0255(5) Uani 1 1 d . . .
H17 H 0.9142 -0.1667 0.8848 0.031 Uiso 1 1 calc R . .
C18 C 0.8279(2) -0.09831(9) 0.93122(13) 0.0217(4) Uani 1 1 d . . .
H18 H 0.9025 -0.0908 0.9699 0.026 Uiso 1 1 calc R . .
C19 C 0.4724(2) -0.04256(9) 0.86271(12) 0.0212(4) Uani 1 1 d . . .
H19A H 0.4584 -0.0295 0.9145 0.025 Uiso 1 1 calc R . .
H19B H 0.3969 -0.0688 0.8438 0.025 Uiso 1 1 calc R . .
C20 C 0.4800(2) -0.01592(9) 0.71240(11) 0.0172(4) Uani 1 1 d . . .
C21 C 0.6078(2) -0.01611(8) 0.68709(11) 0.0161(4) Uani 1 1 d . . .
C22 C 0.6224(2) -0.05015(9) 0.62152(11) 0.0184(4) Uani 1 1 d . . .
C23 C 0.5109(2) -0.08157(9) 0.58821(12) 0.0226(4) Uani 1 1 d . . .
H23 H 0.5212 -0.1046 0.5449 0.027 Uiso 1 1 calc R . .
C24 C 0.3853(2) -0.08165(9) 0.61379(13) 0.0234(5) Uani 1 1 d . . .
C25 C 0.3703(2) -0.04742(9) 0.67606(12) 0.0214(4) Uani 1 1 d . . .
H25 H 0.2851 -0.0453 0.6942 0.026 Uiso 1 1 calc R . .
C26 C 0.2708(3) -0.11899(11) 0.57668(14) 0.0324(5) Uani 1 1 d . . .
H26A H 0.2835 -0.1582 0.5965 0.049 Uiso 1 1 calc R . .
H26B H 0.2700 -0.1192 0.5209 0.049 Uiso 1 1 calc R . .
H26C H 0.1845 -0.1038 0.5885 0.049 Uiso 1 1 calc R . .
C27 C 0.7591(2) -0.05456(10) 0.59176(12) 0.0223(4) Uani 1 1 d . . .
C28 C 0.8601(3) -0.08502(11) 0.65244(14) 0.0308(5) Uani 1 1 d . . .
H28A H 0.8635 -0.0651 0.7018 0.046 Uiso 1 1 calc R . .
H28B H 0.9502 -0.0847 0.6364 0.046 Uiso 1 1 calc R . .
H28C H 0.8310 -0.1247 0.6580 0.046 Uiso 1 1 calc R . .
C29 C 0.8110(3) 0.00527(11) 0.57394(15) 0.0328(6) Uani 1 1 d . . .
H29A H 0.7436 0.0244 0.5364 0.049 Uiso 1 1 calc R . .
H29B H 0.8963 0.0016 0.5528 0.049 Uiso 1 1 calc R . .
H29C H 0.8261 0.0280 0.6213 0.049 Uiso 1 1 calc R . .
C30 C 0.7493(3) -0.08935(11) 0.51677(14) 0.0317(5) Uani 1 1 d . . .
H30A H 0.7163 -0.1280 0.5255 0.048 Uiso 1 1 calc R . .
H30B H 0.8390 -0.0918 0.5004 0.048 Uiso 1 1 calc R . .
H30C H 0.6863 -0.0704 0.4767 0.048 Uiso 1 1 calc R . .
C31 C 0.9616(3) 0.22012(10) 0.92535(13) 0.0285(5) Uani 1 1 d . . .
H31A H 0.8978 0.2010 0.9545 0.043 Uiso 1 1 calc R . .
H31B H 0.9552 0.2617 0.9317 0.043 Uiso 1 1 calc R . .
H31C H 1.0540 0.2074 0.9444 0.043 Uiso 1 1 calc R . .
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C32 C 1.0399(2) 0.24320(10) 0.77087(14) 0.0266(5) Uani 1 1 d . . .
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H32B H 1.0384 0.2836 0.7861 0.040 Uiso 1 1 calc R . .
H32C H 1.0130 0.2400 0.7152 0.040 Uiso 1 1 calc R . .
C33 C 1.0537(2) 0.01807(9) 0.80966(14) 0.0259(5) Uani 1 1 d . . .
H33A H 1.0446 0.0128 0.8640 0.039 Uiso 1 1 calc R . .
H33B H 1.1361 -0.0011 0.7986 0.039 Uiso 1 1 calc R . .
H33C H 0.9747 0.0015 0.7776 0.039 Uiso 1 1 calc R . .
C34 C 1.1076(3) 0.10335(12) 0.68896(14) 0.0338(6) Uani 1 1 d . . .
H34A H 1.0313 0.0901 0.6518 0.051 Uiso 1 1 calc R . .
H34B H 1.1879 0.0802 0.6840 0.051 Uiso 1 1 calc R . .
H34C H 1.1265 0.1437 0.6790 0.051 Uiso 1 1 calc R . .
C35 C 0.4763(3) 0.17409(12) 0.71860(15) 0.0393(7) Uani 1 1 d . . .
H35A H 0.5069 0.2074 0.7513 0.047 Uiso 1 1 calc R . .
H35B H 0.4020 0.1546 0.7401 0.047 Uiso 1 1 calc R . .
C36 C 0.4304(3) 0.19270(14) 0.63662(16) 0.0512(9) Uani 1 1 d . . .
H36A H 0.3921 0.2319 0.6345 0.061 Uiso 1 1 calc R . .
H36B H 0.3620 0.1660 0.6101 0.061 Uiso 1 1 calc R . .
C37 C 0.5608(4) 0.19063(12) 0.60190(15) 0.0467(8) Uani 1 1 d . . .
H37A H 0.5425 0.1872 0.5453 0.056 Uiso 1 1 calc R . .
H37B H 0.6169 0.2251 0.6157 0.056 Uiso 1 1 calc R . .
C38 C 0.6282(3) 0.13772(11) 0.63760(13) 0.0321(5) Uani 1 1 d . . .
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H38B H 0.7279 0.1407 0.6411 0.039 Uiso 1 1 calc R . .

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S2 0.0174(2) 0.0183(2) 0.0180(2) -0.00544(19) 0.00573(19) -0.00130(18)
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C5 0.0194(9) 0.0140(9) 0.0141(9) -0.0017(7) 0.0065(7) -0.0011(7)
C6 0.0167(9) 0.0117(9) 0.0143(9) -0.0012(7) 0.0037(7) -0.0018(7)
C7 0.0310(11) 0.0235(11) 0.0136(10) -0.0017(8) 0.0021(8) 0.0025(9)
C8 0.0224(10) 0.0141(9) 0.0140(9) -0.0017(7) 0.0034(8) 0.0038(8)
C9 0.0361(13) 0.0272(12) 0.0201(11) -0.0025(9) 0.0033(9) 0.0168(10)
C10 0.0320(12) 0.0161(10) 0.0203(11) 0.0023(8) 0.0037(9) 0.0011(8)
C11 0.0188(10) 0.0267(11) 0.0252(11) 0.0003(9) 0.0021(8) 0.0027(8)
C12 0.0278(11) 0.0163(10) 0.0163(10) -0.0006(8) 0.0091(8) -0.0054(8)
C13 0.0272(10) 0.0117(9) 0.0162(10) -0.0001(7) 0.0107(8) -0.0049(8)
C14 0.0240(10) 0.0147(10) 0.0177(10) 0.0003(8) 0.0106(8) -0.0048(8)
C15 0.0291(11) 0.0183(10) 0.0201(10) -0.0037(8) 0.0054(9) -0.0071(8)
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C17 0.0281(11) 0.0163(10) 0.0338(13) -0.0015(9) 0.0106(10) 0.0003(9)
C18 0.0256(11) 0.0181(10) 0.0212(11) 0.0000(8) 0.0027(9) -0.0032(8)
C19 0.0228(10) 0.0234(11) 0.0191(10) -0.0026(8) 0.0093(8) -0.0055(8)
C20 0.0210(10) 0.0174(10) 0.0133(9) -0.0037(8) 0.0028(8) 0.0001(8)
C21 0.0204(10) 0.0139(9) 0.0138(9) -0.0001(7) 0.0022(7) -0.0006(7)
C22 0.0255(10) 0.0169(10) 0.0131(9) -0.0019(8) 0.0034(8) 0.0007(8)
C23 0.0335(12) 0.0208(11) 0.0134(10) -0.0052(8) 0.0030(9) -0.0038(9)
C24 0.0301(12) 0.0214(11) 0.0176(10) -0.0025(8) -0.0011(9) -0.0055(9)
C25 0.0202(10) 0.0238(11) 0.0197(10) -0.0003(8) 0.0012(8) -0.0025(8)
C26 0.0375(13) 0.0344(14) 0.0242(12) -0.0070(10) 0.0011(10) -0.0156(11)
C27 0.0282(11) 0.0226(11) 0.0174(10) -0.0067(8) 0.0080(9) 0.0000(9)
C28 0.0309(12) 0.0345(14) 0.0273(12) -0.0095(10) 0.0053(10) 0.0088(10)
C29 0.0411(14) 0.0294(13) 0.0325(13) -0.0074(10) 0.0218(11) -0.0087(10)
C30 0.0413(14) 0.0350(14) 0.0206(12) -0.0127(10) 0.0104(10) 0.0003(11)
C31 0.0386(13) 0.0253(12) 0.0224(11) -0.0035(9) 0.0078(10) -0.0096(10)
C32 0.0313(12) 0.0204(11) 0.0287(12) 0.0081(9) 0.0061(10) -0.0058(9)
C33 0.0280(11) 0.0201(11) 0.0308(12) 0.0013(9) 0.0087(9) 0.0033(9)
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C35 0.0420(15) 0.0440(16) 0.0282(13) -0.0111(12) -0.0075(11) 0.0244(12)
C36 0.070(2) 0.0458(17) 0.0302(14) -0.0131(13) -0.0203(14) 0.0331(15)
C37 0.087(2) 0.0253(13) 0.0236(13) 0.0048(11) -0.0064(14) 0.0085(14)
C38 0.0460(14) 0.0349(13) 0.0155(11) 0.0052(10) 0.0049(10) 0.0072(11)

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Y N 2.2345(17) . ?
Y O3 2.3069(16) . ?
Y S1 2.8831(10) . ?
Y S2 2.9736(9) . ?
Y Si1 3.3684(10) . ?
Y Si2 3.4809(12) . ?
S1 C2 1.7742(19) . ?
S1 C12 1.835(2) . ?
S2 C20 1.769(2) . ?
S2 C19 1.835(2) . ?
Si1 N 1.7098(18) . ?
Si1 C31 1.866(2) . ?
Si1 C32 1.869(2) . ?
Si1 H1 1.35(2) . ?
Si2 N 1.7092(18) . ?
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O3 C38 1.455(3) . ?
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C3 H3 0.9500 . ?
C4 C5 1.399(3) . ?
C4 C7 1.507(3) . ?
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C5 H5 0.9500 . ?
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C7 H7B 0.9800 . ?
C7 H7C 0.9800 . ?
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C8 C9 1.534(3) . ?
C8 C10 1.535(3) . ?
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C9 H9B 0.9800 . ?
C9 H9C 0.9800 . ?
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C11 H11B 0.9800 . ?
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C12 H12A 0.9900 . ?
C12 H12B 0.9900 . ?
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C13 C14 1.403(3) . ?
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C24 C26 1.508(3) . ?
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C28 H28C 0.9800 . ?
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C29 H29B 0.9800 . ?
C29 H29C 0.9800 . ?
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C30 H30B 0.9800 . ?
C30 H30C 0.9800 . ?
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C31 H31B 0.9800 . ?
C31 H31C 0.9800 . ?
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C32 H32B 0.9800 . ?
C32 H32C 0.9800 . ?
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C36 H36B 0.9900 . ?
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N Y O3 98.13(6) . . ?
O2 Y S1 109.82(5) . . ?
O1 Y S1 69.72(4) . . ?
N Y S1 89.67(5) . . ?
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N Y S2 174.73(4) . . ?
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S1 Y S2 94.619(19) . . ?
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O3 Y Si1 84.41(5) . . ?
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C32 Si1 Y 142.88(8) . . ?
N Si1 H1 107.2(10) . . ?
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Y Si1 H1 76.6(10) . . ?
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N Si2 C34 113.91(10) . . ?
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N Si2 H2 110.5(10) . . ?
C33 Si2 H2 107.3(10) . . ?
C34 Si2 H2 106.6(10) . . ?
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C35 O3 C38 109.92(17) . . ?
C35 O3 Y 131.32(13) . . ?
C38 O3 Y 117.96(13) . . ?
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Si2 N Y 123.38(9) . . ?
Si1 N Y 116.67(9) . . ?
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C1 C2 S1 118.67(15) . . ?
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C4 C3 H3 119.9 . . ?
C2 C3 H3 119.9 . . ?
C3 C4 C5 117.44(18) . . ?
C3 C4 C7 121.16(18) . . ?
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C6 C5 C4 124.30(18) . . ?
C6 C5 H5 117.9 . . ?
C4 C5 H5 117.9 . . ?
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C1 C6 C8 120.48(17) . . ?
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H7A C7 H7B 109.5 . . ?
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H7A C7 H7C 109.5 . . ?
H7B C7 H7C 109.5 . . ?
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C11 C8 C6 110.09(17) . . ?
C9 C8 C6 111.90(17) . . ?
C10 C8 C6 109.29(16) . . ?
C8 C9 H9A 109.5 . . ?
C8 C9 H9B 109.5 . . ?
H9A C9 H9B 109.5 . . ?
C8 C9 H9C 109.5 . . ?
H9A C9 H9C 109.5 . . ?
H9B C9 H9C 109.5 . . ?
C8 C10 H10A 109.5 . . ?
C8 C10 H10B 109.5 . . ?
H10A C10 H10B 109.5 . . ?
C8 C10 H10C 109.5 . . ?
H10A C10 H10C 109.5 . . ?
H10B C10 H10C 109.5 . . ?
C8 C11 H11A 109.5 . . ?
C8 C11 H11B 109.5 . . ?
H11A C11 H11B 109.5 . . ?
C8 C11 H11C 109.5 . . ?
H11A C11 H11C 109.5 . . ?
H11B C11 H11C 109.5 . . ?
C13 C12 S1 110.05(13) . . ?
C13 C12 H12A 109.7 . . ?
S1 C12 H12A 109.7 . . ?
C13 C12 H12B 109.7 . . ?
S1 C12 H12B 109.7 . . ?
H12A C12 H12B 108.2 . . ?
C18 C13 C14 119.38(19) . . ?
C18 C13 C12 118.3(2) . . ?
C14 C13 C12 122.30(19) . . ?
C15 C14 C13 118.6(2) . . ?
C15 C14 C19 118.4(2) . . ?
C13 C14 C19 122.92(18) . . ?
C16 C15 C14 121.4(2) . . ?
C16 C15 H15 119.3 . . ?
C14 C15 H15 119.3 . . ?
C17 C16 C15 119.8(2) . . ?
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C15 C16 H16 120.1 . . ?
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C13 C18 C17 121.1(2) . . ?
C13 C18 H18 119.5 . . ?
C17 C18 H18 119.5 . . ?
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S2 C19 H19A 108.4 . . ?
C14 C19 H19B 108.4 . . ?
S2 C19 H19B 108.4 . . ?
H19A C19 H19B 107.4 . . ?
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C25 C20 S2 118.48(15) . . ?
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C23 C22 C21 117.86(18) . . ?
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C21 C22 C27 120.84(18) . . ?
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C24 C23 H23 117.7 . . ?
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C23 C24 C26 121.5(2) . . ?
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C20 C25 H25 120.0 . . ?
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C24 C26 H26B 109.5 . . ?
H26A C26 H26B 109.5 . . ?
C24 C26 H26C 109.5 . . ?
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H26B C26 H26C 109.5 . . ?
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C22 C27 C30 112.15(19) . . ?
C29 C27 C30 106.64(18) . . ?
C27 C28 H28A 109.5 . . ?
C27 C28 H28B 109.5 . . ?
H28A C28 H28B 109.5 . . ?
C27 C28 H28C 109.5 . . ?
H28A C28 H28C 109.5 . . ?
H28B C28 H28C 109.5 . . ?
C27 C29 H29A 109.5 . . ?
C27 C29 H29B 109.5 . . ?
H29A C29 H29B 109.5 . . ?
C27 C29 H29C 109.5 . . ?
H29A C29 H29C 109.5 . . ?
H29B C29 H29C 109.5 . . ?
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C27 C30 H30B 109.5 . . ?
H30A C30 H30B 109.5 . . ?
C27 C30 H30C 109.5 . . ?
H30A C30 H30C 109.5 . . ?
H30B C30 H30C 109.5 . . ?
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Si2 C33 H33B 109.5 . . ?
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Si2 C33 H33C 109.5 . . ?
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H33B C33 H33C 109.5 . . ?
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Si2 C34 H34B 109.5 . . ?
H34A C34 H34B 109.5 . . ?
Si2 C34 H34C 109.5 . . ?
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H34B C34 H34C 109.5 . . ?
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O3 C35 H35B 110.8 . . ?
C36 C35 H35B 110.8 . . ?
H35A C35 H35B 108.9 . . ?
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C37 C36 H36A 111.3 . . ?
C35 C36 H36B 111.3 . . ?
C37 C36 H36B 111.3 . . ?
H36A C36 H36B 109.2 . . ?
C38 C37 C36 102.5(2) . . ?
C38 C37 H37A 111.3 . . ?
C36 C37 H37A 111.3 . . ?
C38 C37 H37B 111.3 . . ?
C36 C37 H37B 111.3 . . ?
H37A C37 H37B 109.2 . . ?
O3 C38 C37 104.8(2) . . ?
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N Y S1 C12 -167.62(8) . . . . ?
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O1 Y S2 C19 -91.29(9) . . . . ?
N Y S2 C19 121.6(5) . . . . ?
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S2 Y Si1 N -168.73(10) . . . . ?
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N Y O3 C35 -112.3(2) . . . . ?
S1 Y O3 C35 -1.6(3) . . . . ?
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N Y O3 C38 56.36(16) . . . . ?
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S2 Y O3 C38 -119.22(16) . . . . ?
Si1 Y O3 C38 79.65(16) . . . . ?
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C33 Si2 N Y -17.77(14) . . . . ?
C34 Si2 N Y 103.69(13) . . . . ?
C31 Si1 N Si2 -86.91(13) . . . . ?
C32 Si1 N Si2 35.43(15) . . . . ?
Y Si1 N Si2 -173.93(17) . . . . ?
C31 Si1 N Y 87.02(12) . . . . ?
C32 Si1 N Y -150.63(10) . . . . ?
O2 Y N Si2 -37.19(12) . . . . ?
O1 Y N Si2 142.62(10) . . . . ?
O3 Y N Si2 -126.15(10) . . . . ?
S1 Y N Si2 73.58(10) . . . . ?
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Y O1 C1 C2 -16.1(3) . . . . ?
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C12 S1 C2 C3 86.33(17) . . . . ?
Y S1 C2 C3 -165.52(14) . . . . ?
C12 S1 C2 C1 -92.71(16) . . . . ?
Y S1 C2 C1 15.44(15) . . . . ?
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S1 C2 C3 C4 -176.71(15) . . . . ?
C2 C3 C4 C5 0.8(3) . . . . ?
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C5 C6 C8 C11 -124.41(19) . . . . ?
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C1 C6 C8 C9 175.92(18) . . . . ?
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C2 S1 C12 C13 162.34(15) . . . . ?
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Y S1 C12 C13 63.44(16) . . . . ?
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S1 C12 C13 C14 -109.22(19) . . . . ?
C18 C13 C14 C15 -1.2(3) . . . . ?
C12 C13 C14 C15 178.96(18) . . . . ?
C18 C13 C14 C19 177.04(18) . . . . ?
C12 C13 C14 C19 -2.8(3) . . . . ?
C13 C14 C15 C16 0.0(3) . . . . ?
C19 C14 C15 C16 -178.27(19) . . . . ?
C14 C15 C16 C17 1.0(3) . . . . ?
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C14 C13 C18 C17 1.4(3) . . . . ?
C12 C13 C18 C17 -178.75(19) . . . . ?
C16 C17 C18 C13 -0.4(3) . . . . ?
C15 C14 C19 S2 -91.6(2) . . . . ?
C13 C14 C19 S2 90.2(2) . . . . ?
C20 S2 C19 C14 61.53(17) . . . . ?
Y S2 C19 C14 -37.56(18) . . . . ?
C19 S2 C20 C25 74.03(18) . . . . ?
Y S2 C20 C25 -171.42(16) . . . . ?
C19 S2 C20 C21 -99.93(17) . . . . ?
Y S2 C20 C21 14.62(17) . . . . ?
Y O2 C21 C20 -18.0(3) . . . . ?
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C23 C22 C27 C29 127.2(2) . . . . ?
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C21 C22 C27 C30 -175.3(2) . . . . ?
C38 O3 C35 C36 11.2(3) . . . . ?
Y O3 C35 C36 -179.43(18) . . . . ?
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 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
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 factors based on ALL data will be even larger.
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C3 C 0.1562(2) -0.1561(5) 0.4422(4) 0.038(2) Uani 1 1 d . . .
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C5 C 0.1096(2) -0.1993(4) 0.4144(4) 0.038(2) Uani 1 1 d . . .
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C6 C 0.09867(17) -0.1451(4) 0.4392(4) 0.0270(18) Uani 1 1 d . . .
C7 C 0.1491(2) -0.2674(5) 0.3888(5) 0.059(3) Uani 1 1 d . . .
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H7B H 0.1447 -0.3063 0.4115 0.089 Uiso 1 1 calc R . .
H7C H 0.1697 -0.2641 0.3949 0.089 Uiso 1 1 calc R . .
C8 C 0.06708(18) -0.1412(4) 0.4378(4) 0.032(2) Uani 1 1 d . . .
C9 C 0.0505(2) -0.2017(5) 0.4041(5) 0.049(3) Uani 1 1 d . . .
H9A H 0.0537 -0.2066 0.3608 0.074 Uiso 1 1 calc R . .
H9B H 0.0302 -0.1955 0.4004 0.074 Uiso 1 1 calc R . .
H9C H 0.0572 -0.2414 0.4295 0.074 Uiso 1 1 calc R . .
C10 C 0.06368(19) -0.1399(5) 0.5076(4) 0.039(2) Uani 1 1 d . . .
H10A H 0.0741 -0.1771 0.5319 0.059 Uiso 1 1 calc R . .
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H10C H 0.0713 -0.0984 0.5284 0.059 Uiso 1 1 calc R . .
C11 C 0.05365(18) -0.0795(5) 0.4012(4) 0.041(2) Uani 1 1 d . . .
H11A H 0.0646 -0.0405 0.4198 0.061 Uiso 1 1 calc R . .
H11B H 0.0341 -0.0750 0.4048 0.061 Uiso 1 1 calc R . .
H11C H 0.0537 -0.0835 0.3556 0.061 Uiso 1 1 calc R . .
C12 C 0.16711(18) 0.0005(5) 0.4083(4) 0.038(2) Uani 1 1 d . . .
H12A H 0.1700 -0.0357 0.3796 0.046 Uiso 1 1 calc R . .
H12B H 0.1480 0.0197 0.3901 0.046 Uiso 1 1 calc R . .
C13 C 0.1894(2) 0.0526(6) 0.4114(4) 0.050(3) Uani 1 1 d . . .
C14 C 0.2174(2) 0.0330(7) 0.4275(4) 0.067(4) Uani 1 1 d . . .
H14 H 0.2219 -0.0122 0.4366 0.080 Uiso 1 1 calc R . .
C15 C 0.2393(3) 0.0782(10) 0.4308(6) 0.090(6) Uani 1 1 d . . .
H15 H 0.2585 0.0637 0.4401 0.108 Uiso 1 1 calc R . .
C16 C 0.2329(3) 0.1436(9) 0.4206(6) 0.089(6) Uani 1 1 d . . .
H16 H 0.2478 0.1748 0.4249 0.106 Uiso 1 1 calc R . .
C17 C 0.2045(3) 0.1654(7) 0.4038(5) 0.075(4) Uani 1 1 d . . .
H17 H 0.2001 0.2107 0.3955 0.090 Uiso 1 1 calc R . .
C18 C 0.1829(2) 0.1182(6) 0.3996(5) 0.055(3) Uani 1 1 d . . .
C19 C 0.1533(3) 0.1431(6) 0.3789(5) 0.061(3) Uani 1 1 d . . .
H19A H 0.1424 0.1161 0.3425 0.074 Uiso 1 1 calc R . .
H19B H 0.1534 0.1892 0.3637 0.074 Uiso 1 1 calc R . .
C20 C 0.09928(19) 0.1372(4) 0.4090(4) 0.032(2) Uani 1 1 d . . .
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C21 C 0.0820(2) 0.1291(4) 0.4534(4) 0.032(2) Uani 1 1 d . . .
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C23 C 0.0418(2) 0.1259(4) 0.3646(4) 0.039(2) Uani 1 1 d . . .
H23 H 0.0220 0.1196 0.3481 0.047 Uiso 1 1 calc R . .
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C25 C 0.0865(2) 0.1442(4) 0.3433(4) 0.040(2) Uani 1 1 d . . .
H25 H 0.0978 0.1519 0.3138 0.048 Uiso 1 1 calc R . .
C26 C 0.0434(3) 0.1536(6) 0.2509(5) 0.083(5) Uani 1 1 d . . .
H26A H 0.0547 0.1340 0.2238 0.124 Uiso 1 1 calc R . .
H26B H 0.0420 0.2013 0.2436 0.124 Uiso 1 1 calc R . .
H26C H 0.0243 0.1342 0.2398 0.124 Uiso 1 1 calc R . .
C27 C 0.03357(19) 0.1094(4) 0.4775(4) 0.0314(19) Uani 1 1 d . . .
C28 C 0.00449(19) 0.0808(5) 0.4409(5) 0.045(2) Uani 1 1 d . . .
H28A H 0.0074 0.0407 0.4179 0.067 Uiso 1 1 calc R . .
H28B H -0.0058 0.1134 0.4099 0.067 Uiso 1 1 calc R . .
H28C H -0.0066 0.0701 0.4719 0.067 Uiso 1 1 calc R . .
C29 C 0.0285(2) 0.1761(4) 0.5059(5) 0.044(2) Uani 1 1 d . . .
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H29B H 0.0195 0.2061 0.4708 0.066 Uiso 1 1 calc R . .
H29C H 0.0467 0.1946 0.5300 0.066 Uiso 1 1 calc R . .
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H30B H 0.0627 0.0826 0.5622 0.052 Uiso 1 1 calc R . .
H30C H 0.0531 0.0219 0.5137 0.052 Uiso 1 1 calc R . .
C31 C 0.1503(2) -0.0770(6) 0.6734(4) 0.053(3) Uani 1 1 d . . .
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C35A C 0.1723(5) -0.1685(11) 0.7297(10) 0.038(5) Uiso 0.50 1 d P A 1
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C36A C 0.1768(4) -0.1072(9) 0.7051(8) 0.027(4) Uiso 0.50 1 d P A 1
C37A C 0.1421(4) -0.2635(10) 0.7531(9) 0.044(5) Uiso 0.50 1 d P A 1
H37A H 0.1385 -0.2965 0.7185 0.066 Uiso 0.50 1 calc PR A 1
H37B H 0.1262 -0.2625 0.7733 0.066 Uiso 0.50 1 calc PR A 1
H37C H 0.1596 -0.2749 0.7857 0.066 Uiso 0.50 1 calc PR A 1
C38A C 0.2062(4) -0.0894(12) 0.7110(10) 0.038(5) Uiso 0.50 1 d P A 1
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H39B H 0.2311 -0.0688 0.6460 0.065 Uiso 0.50 1 calc PR A 1
H39C H 0.1999 -0.0381 0.6229 0.065 Uiso 0.50 1 calc PR A 1
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H41B H 0.2475 -0.1164 0.7486 0.090 Uiso 0.50 1 calc PR A 1
H41C H 0.2271 -0.1777 0.7225 0.090 Uiso 0.50 1 calc PR A 1
C33B C 0.1104(5) -0.1619(10) 0.6909(10) 0.038(5) Uiso 0.50 1 d P A 2
H33B H 0.0907 -0.1708 0.6852 0.046 Uiso 0.50 1 calc PR A 2
C34B C 0.1324(6) -0.2059(12) 0.7164(11) 0.052(7) Uiso 0.50 1 d P A 2
C35B C 0.1600(6) -0.1880(12) 0.7215(11) 0.050(6) Uiso 0.50 1 d P A 2
H35B H 0.1743 -0.2173 0.7442 0.060 Uiso 0.50 1 calc PR A 2
C36B C 0.1685(4) -0.1344(11) 0.6980(10) 0.040(5) Uiso 0.50 1 d P A 2
C37B C 0.1234(6) -0.2737(12) 0.7401(12) 0.074(7) Uiso 0.50 1 d P A 2
H37D H 0.1328 -0.2796 0.7860 0.110 Uiso 0.50 1 calc PR A 2
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H37E H 0.1290 -0.3094 0.7150 0.110 Uiso 0.50 1 calc PR A 2
H37F H 0.1028 -0.2745 0.7341 0.110 Uiso 0.50 1 calc PR A 2
C38B C 0.1993(6) -0.1222(15) 0.7041(13) 0.070(8) Uiso 0.50 1 d P A 2
C39B C 0.2044(5) -0.1128(12) 0.6343(11) 0.063(6) Uiso 0.50 1 d P A 2
H39D H 0.2036 -0.0658 0.6235 0.095 Uiso 0.50 1 calc PR A 2
H39E H 0.1896 -0.1364 0.6025 0.095 Uiso 0.50 1 calc PR A 2
H39F H 0.2231 -0.1305 0.6339 0.095 Uiso 0.50 1 calc PR A 2
C40B C 0.2095(6) -0.0623(16) 0.7397(15) 0.082(8) Uiso 0.50 1 d P A 2
H40D H 0.2053 -0.0639 0.7822 0.122 Uiso 0.50 1 calc PR A 2
H40E H 0.2001 -0.0240 0.7157 0.122 Uiso 0.50 1 calc PR A 2
H40F H 0.2301 -0.0586 0.7454 0.122 Uiso 0.50 1 calc PR A 2
C41B C 0.2172(7) -0.1843(17) 0.7335(16) 0.115(11) Uiso 0.50 1 d P A 2
H41D H 0.2368 -0.1788 0.7301 0.173 Uiso 0.50 1 calc PR A 2
H41E H 0.2089 -0.2238 0.7097 0.173 Uiso 0.50 1 calc PR A 2
H41F H 0.2171 -0.1889 0.7791 0.173 Uiso 0.50 1 calc PR A 2
C42 C 0.09608(17) -0.0018(4) 0.7257(4) 0.0272(18) Uani 1 1 d . . .
H42A H 0.0945 -0.0364 0.7573 0.033 Uiso 1 1 calc R . .
H42B H 0.1146 0.0207 0.7419 0.033 Uiso 1 1 calc R . .
C43 C 0.07218(17) 0.0477(4) 0.7198(4) 0.0270(18) Uani 1 1 d . . .
C44 C 0.04432(18) 0.0243(5) 0.7036(4) 0.036(2) Uani 1 1 d . . .
H44 H 0.0411 -0.0217 0.6974 0.043 Uiso 1 1 calc R . .
C45 C 0.0216(2) 0.0657(6) 0.6964(4) 0.052(3) Uani 1 1 d . . .
H45 H 0.0029 0.0486 0.6846 0.063 Uiso 1 1 calc R . .
C46 C 0.0261(2) 0.1324(6) 0.7064(5) 0.053(3) Uani 1 1 d . . .
H46 H 0.0104 0.1617 0.7015 0.064 Uiso 1 1 calc R . .
C47 C 0.0535(2) 0.1563(5) 0.7235(4) 0.044(3) Uani 1 1 d . . .
H47 H 0.0564 0.2023 0.7306 0.053 Uiso 1 1 calc R . .
C48 C 0.07762(19) 0.1147(4) 0.7311(4) 0.0295(19) Uani 1 1 d . . .
C49 C 0.10653(19) 0.1431(4) 0.7496(4) 0.033(2) Uani 1 1 d . . .
H49A H 0.1189 0.1163 0.7841 0.040 Uiso 1 1 calc R . .
H49B H 0.1059 0.1886 0.7658 0.040 Uiso 1 1 calc R . .
C50 C 0.15709(19) 0.1489(4) 0.7077(4) 0.034(2) Uani 1 1 d . . .
C51 C 0.1714(2) 0.1526(5) 0.6582(4) 0.041(2) Uani 1 1 d . . .
C52 C 0.2006(2) 0.1575(6) 0.6730(4) 0.054(3) Uani 1 1 d . . .
C53 C 0.2149(2) 0.1586(6) 0.7388(5) 0.064(4) Uani 1 1 d . . .
H53 H 0.2350 0.1624 0.7501 0.077 Uiso 1 1 calc R . .
C54 C 0.2013(2) 0.1545(6) 0.7880(4) 0.055(3) Uani 1 1 d . . .
C55 C 0.1721(2) 0.1499(5) 0.7727(4) 0.043(2) Uani 1 1 d . . .
H55 H 0.1623 0.1474 0.8059 0.052 Uiso 1 1 calc R . .
C56 C 0.2185(2) 0.1577(7) 0.8585(4) 0.066(4) Uani 1 1 d . . .
H56A H 0.2387 0.1602 0.8602 0.099 Uiso 1 1 calc R . .
H56B H 0.2148 0.1181 0.8813 0.099 Uiso 1 1 calc R . .
H56C H 0.2129 0.1969 0.8792 0.099 Uiso 1 1 calc R . .
C57 C 0.2174(2) 0.1630(8) 0.6211(5) 0.077(5) Uani 1 1 d . . .
C58 C 0.2493(3) 0.1728(10) 0.6506(6) 0.134(8) Uani 1 1 d . . .
H58A H 0.2522 0.2114 0.6791 0.201 Uiso 1 1 calc R . .
H58B H 0.2589 0.1797 0.6160 0.201 Uiso 1 1 calc R . .
H58C H 0.2571 0.1336 0.6757 0.201 Uiso 1 1 calc R . .
C59 C 0.2135(2) 0.0982(7) 0.5824(5) 0.080(4) Uani 1 1 d . . .
H59A H 0.2202 0.0612 0.6117 0.120 Uiso 1 1 calc R . .
H59B H 0.2244 0.1001 0.5497 0.120 Uiso 1 1 calc R . .
H59C H 0.1933 0.0920 0.5611 0.120 Uiso 1 1 calc R . .
C60 C 0.2063(3) 0.2210(7) 0.5765(5) 0.090(5) Uani 1 1 d . . .
H60A H 0.1863 0.2132 0.5540 0.135 Uiso 1 1 calc R . .
H60B H 0.2175 0.2256 0.5447 0.135 Uiso 1 1 calc R . .
H60C H 0.2078 0.2616 0.6020 0.135 Uiso 1 1 calc R . .
C61 C 0.1266(2) 0.3307(5) 0.6871(4) 0.050(3) Uani 1 1 d . . .
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C62 C 0.0983(2) 0.3223(4) 0.6899(4) 0.045(3) Uani 1 1 d . . .
C63 C 0.0883(3) 0.3480(5) 0.7400(4) 0.053(3) Uani 1 1 d . . .
H63 H 0.0693 0.3393 0.7415 0.063 Uiso 1 1 calc R . .
C64 C 0.1057(3) 0.3862(5) 0.7881(5) 0.062(3) Uani 1 1 d . . .
C65 C 0.1334(3) 0.3968(5) 0.7839(4) 0.066(4) Uani 1 1 d . . .
H65 H 0.1454 0.4233 0.8162 0.079 Uiso 1 1 calc R . .
C66 C 0.1447(3) 0.3709(5) 0.7356(4) 0.054(3) Uani 1 1 d . . .
C67 C 0.0953(3) 0.4137(7) 0.8432(5) 0.092(5) Uani 1 1 d . . .
H67A H 0.1039 0.3889 0.8827 0.138 Uiso 1 1 calc R . .
H67B H 0.0746 0.4099 0.8333 0.138 Uiso 1 1 calc R . .
H67C H 0.1008 0.4602 0.8495 0.138 Uiso 1 1 calc R . .
C68 C 0.1754(3) 0.3837(6) 0.7353(5) 0.069(4) Uani 1 1 d . . .
C69 C 0.1774(3) 0.4151(7) 0.6715(5) 0.094(5) Uani 1 1 d . . .
H69A H 0.1974 0.4232 0.6726 0.142 Uiso 1 1 calc R . .
H69B H 0.1671 0.4570 0.6653 0.142 Uiso 1 1 calc R . .
H69C H 0.1691 0.3853 0.6356 0.142 Uiso 1 1 calc R . .
C70 C 0.1911(3) 0.4292(7) 0.7901(5) 0.091(5) Uani 1 1 d . . .
H70A H 0.1906 0.4099 0.8318 0.137 Uiso 1 1 calc R . .
H70B H 0.1819 0.4725 0.7855 0.137 Uiso 1 1 calc R . .
H70C H 0.2109 0.4342 0.7881 0.137 Uiso 1 1 calc R . .
C71 C 0.1911(3) 0.3194(7) 0.7434(6) 0.086(5) Uani 1 1 d . . .
H71A H 0.2097 0.3255 0.7344 0.129 Uiso 1 1 calc R . .
H71B H 0.1801 0.2868 0.7134 0.129 Uiso 1 1 calc R . .
H71C H 0.1937 0.3037 0.7879 0.129 Uiso 1 1 calc R . .
C72 C 0.0526(2) 0.3518(4) 0.5877(5) 0.047(3) Uani 1 1 d . . .
H72A H 0.0365 0.3346 0.5536 0.056 Uiso 1 1 calc R . .
H72B H 0.0446 0.3727 0.6212 0.056 Uiso 1 1 calc R . .
C73 C 0.0675(3) 0.4033(5) 0.5588(5) 0.055(3) Uani 1 1 d . . .
C74 C 0.0832(3) 0.4512(5) 0.5995(5) 0.069(4) Uani 1 1 d . . .
H74 H 0.0840 0.4502 0.6443 0.082 Uiso 1 1 calc R . .
C75 C 0.0976(3) 0.5000(6) 0.5762(6) 0.084(5) Uani 1 1 d . . .
H75 H 0.1079 0.5322 0.6050 0.101 Uiso 1 1 calc R . .
C76 C 0.0973(3) 0.5026(5) 0.5118(5) 0.087(5) Uani 1 1 d . . .
H76 H 0.1076 0.5359 0.4962 0.104 Uiso 1 1 calc R . .
C77 C 0.0818(3) 0.4563(5) 0.4703(5) 0.077(4) Uani 1 1 d . . .
H77 H 0.0810 0.4588 0.4254 0.093 Uiso 1 1 calc R . .
C78 C 0.0674(3) 0.4053(5) 0.4931(5) 0.060(3) Uani 1 1 d . . .
C79 C 0.0514(3) 0.3562(5) 0.4459(4) 0.053(3) Uani 1 1 d . . .
H79A H 0.0426 0.3793 0.4049 0.063 Uiso 1 1 calc R . .
H79B H 0.0358 0.3380 0.4628 0.063 Uiso 1 1 calc R . .
C80 C 0.0961(2) 0.3310(4) 0.3911(4) 0.047(3) Uani 1 1 d . . .
C81 C 0.1239(2) 0.3418(4) 0.4262(4) 0.046(3) Uani 1 1 d . . .
C82 C 0.1412(3) 0.3853(5) 0.3999(5) 0.063(4) Uani 1 1 d . . .
C83 C 0.1292(3) 0.4115(6) 0.3398(5) 0.078(4) Uani 1 1 d . . .
H83 H 0.1408 0.4394 0.3217 0.093 Uiso 1 1 calc R . .
C84 C 0.1025(3) 0.4008(5) 0.3046(5) 0.074(4) Uani 1 1 d . . .
C85 C 0.0855(3) 0.3595(5) 0.3307(4) 0.062(3) Uani 1 1 d . . .
H85 H 0.0666 0.3507 0.3071 0.074 Uiso 1 1 calc R . .
C86 C 0.0905(4) 0.4304(7) 0.2374(5) 0.115(7) Uani 1 1 d . . .
H86A H 0.0971 0.4760 0.2368 0.173 Uiso 1 1 calc R . .
H86B H 0.0697 0.4300 0.2272 0.173 Uiso 1 1 calc R . .
H86C H 0.0969 0.4044 0.2052 0.173 Uiso 1 1 calc R . .
C87 C 0.1711(3) 0.4010(6) 0.4376(5) 0.068(4) Uani 1 1 d . . .
C88 C 0.1859(3) 0.4502(7) 0.4017(6) 0.100(6) Uani 1 1 d . . .
H88A H 0.2064 0.4430 0.4148 0.151 Uiso 1 1 calc R . .
H88B H 0.1816 0.4954 0.4125 0.151 Uiso 1 1 calc R . .
H88C H 0.1790 0.4435 0.3550 0.151 Uiso 1 1 calc R . .
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C89 C 0.1715(3) 0.4305(6) 0.5034(5) 0.079(4) Uani 1 1 d . . .
H89A H 0.1609 0.4720 0.4975 0.118 Uiso 1 1 calc R . .
H89B H 0.1912 0.4388 0.5274 0.118 Uiso 1 1 calc R . .
H89C H 0.1627 0.3995 0.5278 0.118 Uiso 1 1 calc R . .
C90 C 0.1888(3) 0.3374(8) 0.4454(6) 0.093(5) Uani 1 1 d . . .
H90A H 0.1818 0.3063 0.4728 0.140 Uiso 1 1 calc R . .
H90B H 0.2087 0.3478 0.4655 0.140 Uiso 1 1 calc R . .
H90C H 0.1872 0.3175 0.4029 0.140 Uiso 1 1 calc R . .
C91 C 0.1249(5) 0.3064(12) 0.0587(12) 0.069(7) Uiso 0.50 1 d P . .
H91A H 0.1154 0.3187 0.0922 0.104 Uiso 0.50 1 calc PR . .
H91B H 0.1195 0.2613 0.0441 0.104 Uiso 0.50 1 calc PR . .
H91C H 0.1193 0.3367 0.0221 0.104 Uiso 0.50 1 calc PR . .
C92 C 0.1514(6) 0.3093(15) 0.0816(15) 0.094(9) Uiso 0.50 1 d P . .
H92A H 0.1603 0.2990 0.0459 0.113 Uiso 0.50 1 calc PR . .
H92B H 0.1567 0.2732 0.1135 0.113 Uiso 0.50 1 calc PR . .
C93 C 0.1632(5) 0.3613(11) 0.1086(11) 0.060(6) Uiso 0.50 1 d P . .
H93A H 0.1568 0.3958 0.0753 0.072 Uiso 0.50 1 calc PR . .
H93B H 0.1530 0.3706 0.1422 0.072 Uiso 0.50 1 calc PR . .
C94 C 0.1870(9) 0.376(2) 0.134(2) 0.144(15) Uiso 0.50 1 d P . .
H94A H 0.1936 0.3828 0.0939 0.172 Uiso 0.50 1 calc PR . .
H94B H 0.1942 0.3314 0.1482 0.172 Uiso 0.50 1 calc PR . .
C95 C 0.2062(6) 0.4100(14) 0.1729(14) 0.088(8) Uiso 0.50 1 d P . .
H95A H 0.2122 0.4467 0.1494 0.132 Uiso 0.50 1 calc PR . .
H95B H 0.2226 0.3819 0.1913 0.132 Uiso 0.50 1 calc PR . .
H95C H 0.1985 0.4275 0.2076 0.132 Uiso 0.50 1 calc PR . .
C96 C 0.2663(3) -0.1934(7) 0.5088(7) 0.086(4) Uiso 1 1 d . . .
H96 H 0.2776 -0.1559 0.5141 0.103 Uiso 1 1 d R . .
C97 C 0.2413(3) -0.1955(7) 0.5261(6) 0.081(4) Uiso 1 1 d . . .
H97 H 0.2350 -0.1575 0.5446 0.097 Uiso 1 1 calc R . .
C98 C 0.2252(3) -0.2500(7) 0.5177(6) 0.079(4) Uiso 1 1 d . . .
H98 H 0.2078 -0.2500 0.5300 0.095 Uiso 0.50 1 calc PR . .
C99 C 0.2829(7) -0.1279(16) 0.5143(16) 0.110(11) Uiso 0.50 1 d P . .
H99A H 0.2938 -0.1215 0.5591 0.165 Uiso 0.50 1 calc PR . .
H99B H 0.2695 -0.0912 0.5014 0.165 Uiso 0.50 1 calc PR . .
H99C H 0.2958 -0.1293 0.4859 0.165 Uiso 0.50 1 calc PR . .
C100 C 0.0283(4) 0.3474(11) 0.0971(9) 0.091(9) Uiso 0.50 1 d PG . .
C101 C 0.0225(5) 0.3031(9) 0.1416(12) 0.101(10) Uiso 0.50 1 d PG . .
H101 H 0.0248 0.2571 0.1362 0.121 Uiso 0.50 1 calc PR . .
C102 C 0.0133(5) 0.3262(14) 0.1941(11) 0.153(15) Uiso 0.50 1 d PG . .
H102 H 0.0093 0.2959 0.2246 0.184 Uiso 0.50 1 calc PR . .
C103 C 0.0100(6) 0.3935(15) 0.2020(11) 0.22(2) Uiso 0.50 1 d PG . .
H103 H 0.0037 0.4092 0.2379 0.266 Uiso 0.50 1 calc PR . .
C104 C 0.0158(6) 0.4377(10) 0.1574(14) 0.182(19) Uiso 0.50 1 d PG . .
H104 H 0.0135 0.4838 0.1628 0.218 Uiso 0.50 1 calc PR . .
C105 C 0.0250(4) 0.4147(10) 0.1050(11) 0.095(9) Uiso 0.50 1 d PG . .
H105 H 0.0289 0.4449 0.0745 0.114 Uiso 0.50 1 calc PR . .
C106 C 0.0383(6) 0.3331(15) 0.0584(14) 0.095(9) Uiso 0.50 1 d P . .
H10D H 0.0585 0.3242 0.0770 0.142 Uiso 0.50 1 calc PR . .
H10E H 0.0362 0.3691 0.0270 0.142 Uiso 0.50 1 calc PR . .
H10F H 0.0290 0.2934 0.0368 0.142 Uiso 0.50 1 calc PR . .
C107 C 0.0199(6) 0.6205(13) 0.3274(9) 0.136(14) Uiso 0.50 1 d PG . .
C108 C 0.0256(5) 0.5702(11) 0.2883(14) 0.19(2) Uiso 0.50 1 d PG . .
H108 H 0.0365 0.5331 0.3072 0.231 Uiso 0.50 1 calc PR . .
C109 C 0.0151(5) 0.5740(9) 0.2216(13) 0.109(10) Uiso 0.50 1 d PG . .
H109 H 0.0190 0.5396 0.1949 0.130 Uiso 0.50 1 calc PR . .
C110 C -0.0009(5) 0.6282(11) 0.1940(9) 0.122(12) Uiso 0.50 1 d PG . .
H110 H -0.0080 0.6308 0.1484 0.146 Uiso 0.50 1 calc PR . .
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C111 C -0.0065(5) 0.6785(8) 0.2331(10) 0.083(9) Uiso 0.50 1 d PG . .
H111 H -0.0175 0.7156 0.2142 0.100 Uiso 0.50 1 calc PR . .
C112 C 0.0039(6) 0.6747(10) 0.2998(9) 0.125(13) Uiso 0.50 1 d PG . .
H112 H 0.0000 0.7091 0.3265 0.150 Uiso 0.50 1 calc PR . .
C113 C 0.0192(11) 0.602(3) 0.394(2) 0.21(2) Uiso 0.50 1 d P . .
H11D H 0.0042 0.6274 0.4064 0.320 Uiso 0.50 1 calc PR . .
H11E H 0.0375 0.6123 0.4238 0.320 Uiso 0.50 1 calc PR . .
H11F H 0.0152 0.5550 0.3957 0.320 Uiso 0.50 1 calc PR . .

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La1 0.0336(3) 0.0356(3) 0.0212(2) -0.0052(2) 0.0119(2) -0.0134(2)
La2 0.0525(3) 0.0343(3) 0.0227(2) -0.0062(2) 0.0159(2) -0.0256(3)
S1 0.0284(12) 0.0765(18) 0.0233(11) -0.0043(11) 0.0115(9) -0.0132(12)
S2 0.0613(17) 0.0498(14) 0.0276(12) -0.0133(11) 0.0251(12) -0.0321(13)
S3 0.0390(12) 0.0276(11) 0.0253(10) -0.0015(9) 0.0167(9) -0.0011(9)
S4 0.0373(13) 0.0319(11) 0.0227(10) -0.0059(9) 0.0161(9) -0.0132(9)
S5 0.0655(17) 0.0281(12) 0.0289(11) -0.0003(9) 0.0175(11) -0.0110(11)
S6 0.0657(17) 0.0263(11) 0.0312(12) -0.0036(9) 0.0170(12) -0.0150(11)
O1 0.027(3) 0.028(3) 0.030(3) -0.007(2) 0.011(2) 0.003(2)
O2 0.032(3) 0.039(3) 0.023(3) -0.001(2) 0.011(3) -0.018(3)
O3 0.031(4) 0.090(6) 0.029(3) -0.001(4) 0.012(3) 0.008(4)
O4 0.037(3) 0.051(4) 0.022(3) -0.010(3) 0.016(3) -0.025(3)
O5 0.077(5) 0.045(4) 0.031(3) -0.012(3) 0.023(3) -0.035(4)
O6 0.071(5) 0.049(4) 0.029(3) 0.002(3) 0.020(3) -0.033(4)
C1 0.024(4) 0.037(5) 0.015(4) 0.004(3) 0.001(3) -0.001(4)
C2 0.030(5) 0.054(6) 0.020(4) 0.007(4) 0.009(4) -0.004(4)
C3 0.036(5) 0.058(6) 0.025(5) 0.010(4) 0.016(4) 0.019(5)
C4 0.060(7) 0.041(5) 0.028(5) 0.010(4) 0.025(5) 0.021(5)
C5 0.051(6) 0.036(5) 0.033(5) -0.002(4) 0.019(4) -0.001(4)
C6 0.032(5) 0.029(4) 0.022(4) 0.003(3) 0.012(4) 0.007(4)
C7 0.074(8) 0.049(7) 0.066(7) 0.011(5) 0.040(6) 0.033(6)
C8 0.028(5) 0.038(5) 0.032(5) -0.016(4) 0.010(4) -0.013(4)
C9 0.044(6) 0.056(6) 0.053(6) -0.028(5) 0.021(5) -0.024(5)
C10 0.037(5) 0.048(6) 0.041(5) -0.017(4) 0.025(4) -0.005(4)
C11 0.024(5) 0.052(6) 0.044(5) -0.008(5) 0.004(4) 0.008(4)
C12 0.033(5) 0.065(6) 0.020(4) -0.008(4) 0.013(4) -0.024(5)
C13 0.048(6) 0.084(9) 0.025(5) -0.022(5) 0.022(4) -0.039(6)
C14 0.046(7) 0.129(11) 0.031(5) -0.022(6) 0.023(5) -0.040(7)
C15 0.052(8) 0.182(16) 0.048(7) -0.049(10) 0.037(6) -0.066(10)
C16 0.088(11) 0.145(14) 0.044(7) -0.051(9) 0.038(7) -0.085(11)
C17 0.091(10) 0.103(10) 0.048(7) -0.030(7) 0.049(7) -0.061(8)
C18 0.047(7) 0.095(9) 0.033(5) -0.029(6) 0.031(5) -0.043(6)
C19 0.097(10) 0.065(7) 0.036(6) -0.020(5) 0.044(6) -0.048(7)
C20 0.052(6) 0.021(4) 0.026(4) 0.001(3) 0.013(4) -0.008(4)
C21 0.053(6) 0.022(4) 0.023(4) -0.003(3) 0.016(4) -0.012(4)
C22 0.045(5) 0.016(4) 0.023(4) 0.000(3) 0.005(4) -0.008(4)
C23 0.050(6) 0.027(5) 0.031(5) -0.007(4) -0.008(4) 0.017(4)
C24 0.076(8) 0.034(5) 0.022(5) -0.003(4) 0.008(5) 0.021(5)
C25 0.076(8) 0.026(5) 0.022(4) -0.001(4) 0.022(5) 0.006(5)
C26 0.125(12) 0.096(10) 0.021(5) -0.002(6) 0.010(6) 0.054(9)
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C28 0.033(5) 0.042(6) 0.053(6) -0.009(5) -0.001(5) -0.001(4)
C29 0.051(6) 0.034(5) 0.051(6) -0.010(4) 0.018(5) -0.003(4)
C30 0.026(5) 0.041(5) 0.039(5) 0.010(4) 0.013(4) 0.002(4)
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C32 0.074(7) 0.031(5) 0.025(4) 0.006(4) 0.024(5) 0.023(5)
C42 0.031(5) 0.032(5) 0.022(4) -0.002(3) 0.013(4) 0.003(4)
C43 0.029(4) 0.037(5) 0.020(4) 0.006(3) 0.014(3) 0.003(4)
C44 0.038(5) 0.043(5) 0.033(5) -0.008(4) 0.022(4) -0.012(4)
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C47 0.072(8) 0.037(5) 0.034(5) 0.015(4) 0.033(5) 0.020(5)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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S2 La2 S4 104.05(6) . . ?
O5 La2 La1 121.48(17) . . ?
O6 La2 La1 130.17(18) . . ?
O4 La2 La1 36.02(12) . . ?
O2 La2 La1 35.51(13) . . ?
S5 La2 La1 107.39(4) . . ?
S6 La2 La1 113.07(4) . . ?
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C12 S1 La1 114.6(3) . . ?
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La2 S2 La1 76.44(5) . . ?
C32 S3 C42 98.0(4) . . ?
C32 S3 La1 91.9(3) . . ?
C42 S3 La1 112.8(3) . . ?
C50 S4 C49 104.9(4) . . ?
C50 S4 La1 89.4(3) . . ?
C49 S4 La1 139.7(3) . . ?
C50 S4 La2 91.4(3) . . ?
C49 S4 La2 139.8(3) . . ?
La1 S4 La2 75.35(4) . . ?
C62 S5 C72 100.1(5) . . ?
C62 S5 La2 97.0(3) . . ?
C72 S5 La2 114.6(3) . . ?
C80 S6 C79 100.1(5) . . ?
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C31 O3 La1 134.5(6) . . ?
C51 O4 La2 120.8(5) . . ?
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C81 O6 La2 141.8(6) . . ?
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C2 C3 H3 119.8 . . ?
C3 C4 C5 118.7(8) . . ?
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C5 C4 C7 120.4(10) . . ?
C6 C5 C4 123.0(9) . . ?
C6 C5 H5 118.5 . . ?
C4 C5 H5 118.5 . . ?
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C5 C6 C8 121.0(8) . . ?
C1 C6 C8 120.3(7) . . ?
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C4 C7 H7B 109.5 . . ?
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C4 C7 H7C 109.5 . . ?
H7A C7 H7C 109.5 . . ?
H7B C7 H7C 109.5 . . ?
C11 C8 C6 110.4(7) . . ?
C11 C8 C10 110.1(7) . . ?
C6 C8 C10 109.6(7) . . ?
C11 C8 C9 107.8(7) . . ?
C6 C8 C9 111.8(7) . . ?
C10 C8 C9 107.1(7) . . ?
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C8 C9 H9B 109.5 . . ?
H9A C9 H9B 109.5 . . ?
C8 C9 H9C 109.5 . . ?
H9A C9 H9C 109.5 . . ?
H9B C9 H9C 109.5 . . ?
C8 C10 H10A 109.5 . . ?
C8 C10 H10B 109.5 . . ?
H10A C10 H10B 109.5 . . ?
C8 C10 H10C 109.5 . . ?
H10A C10 H10C 109.5 . . ?
H10B C10 H10C 109.5 . . ?
C8 C11 H11A 109.5 . . ?
C8 C11 H11B 109.5 . . ?
H11A C11 H11B 109.5 . . ?
C8 C11 H11C 109.5 . . ?
H11A C11 H11C 109.5 . . ?
H11B C11 H11C 109.5 . . ?
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C13 C12 H12A 109.6 . . ?
S1 C12 H12A 109.6 . . ?
C13 C12 H12B 109.6 . . ?
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C18 C13 C12 122.8(10) . . ?
C14 C13 C12 117.8(11) . . ?
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C13 C14 H14 119.4 . . ?
C15 C14 H14 119.4 . . ?
C16 C15 C14 119.3(14) . . ?
C16 C15 H15 120.3 . . ?
C14 C15 H15 120.3 . . ?
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C17 C16 H16 119.5 . . ?
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C18 C17 H17 120.9 . . ?
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C13 C18 C19 122.9(9) . . ?
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C18 C19 H19B 109.5 . . ?
S2 C19 H19B 109.5 . . ?
H19A C19 H19B 108.1 . . ?
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C25 C20 S2 126.4(7) . . ?
C21 C20 S2 113.9(6) . . ?
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O2 C21 C20 114.9(8) . . ?
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C21 C22 C23 116.2(8) . . ?
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C23 C22 C27 121.5(8) . . ?
C24 C23 C22 124.3(9) . . ?
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C22 C23 H23 117.8 . . ?
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C23 C24 C26 121.0(10) . . ?
C24 C25 C20 119.7(9) . . ?
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C20 C25 H25 120.1 . . ?
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C24 C26 H26C 109.5 . . ?
H26A C26 H26C 109.5 . . ?
H26B C26 H26C 109.5 . . ?
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C29 C27 C28 108.3(7) . . ?
C30 C27 C22 112.2(7) . . ?
C29 C27 C22 108.4(7) . . ?
C28 C27 C22 111.0(7) . . ?
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C27 C28 H28B 109.5 . . ?
H28A C28 H28B 109.5 . . ?
C27 C28 H28C 109.5 . . ?
H28A C28 H28C 109.5 . . ?
H28B C28 H28C 109.5 . . ?
C27 C29 H29A 109.5 . . ?
C27 C29 H29B 109.5 . . ?
H29A C29 H29B 109.5 . . ?
C27 C29 H29C 109.5 . . ?
H29A C29 H29C 109.5 . . ?
H29B C29 H29C 109.5 . . ?
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C27 C30 H30B 109.5 . . ?
H30A C30 H30B 109.5 . . ?
C27 C30 H30C 109.5 . . ?
H30A C30 H30C 109.5 . . ?
H30B C30 H30C 109.5 . . ?
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O3 C31 C36A 110.7(12) . . ?
C32 C31 C36A 128.8(12) . . ?
O3 C31 C36B 133.9(12) . . ?
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C36A C31 C36B 26.9(9) . . ?
C33A C32 C31 112.8(12) . . ?
C33A C32 C33B 21.4(10) . . ?
C31 C32 C33B 132.8(12) . . ?
C33A C32 S3 128.2(11) . . ?
C31 C32 S3 118.5(7) . . ?
C33B C32 S3 108.7(10) . . ?
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C34A C33A H33A 116.3 . . ?
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C36A C35A C34A 126.4(19) . . ?
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C34A C35A H35A 116.8 . . ?
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H37A C37A H37B 109.5 . . ?
C34A C37A H37C 109.5 . . ?
H37A C37A H37C 109.5 . . ?
H37B C37A H37C 109.5 . . ?
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C41A C38A C40A 108.5(19) . . ?
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H39A C39A H39C 109.5 . . ?
H39B C39A H39C 109.5 . . ?
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C38A C40A H40B 109.5 . . ?
H40A C40A H40B 109.5 . . ?
C38A C40A H40C 109.5 . . ?
H40A C40A H40C 109.5 . . ?
H40B C40A H40C 109.5 . . ?
C38A C41A H41A 109.5 . . ?
C38A C41A H41B 109.5 . . ?
H41A C41A H41B 109.5 . . ?
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C32 C33B H33B 125.2 . . ?
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C36B C35B H35B 116.9 . . ?
C34B C35B H35B 116.9 . . ?
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C35B C36B C38B 121(2) . . ?
C31 C36B C38B 114(2) . . ?
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H37D C37B H37E 109.5 . . ?
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H37E C37B H37F 109.5 . . ?
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C41B C38B C39B 106(2) . . ?
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H39D C39B H39E 109.5 . . ?
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H39D C39B H39F 109.5 . . ?
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C38B C40B H40E 109.5 . . ?
H40D C40B H40E 109.5 . . ?
C38B C40B H40F 109.5 . . ?
H40D C40B H40F 109.5 . . ?
H40E C40B H40F 109.5 . . ?
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C38B C41B H41E 109.5 . . ?
H41D C41B H41E 109.5 . . ?
C38B C41B H41F 109.5 . . ?
H41D C41B H41F 109.5 . . ?
H41E C41B H41F 109.5 . . ?
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S3 C42 H42A 109.6 . . ?
C43 C42 H42B 109.6 . . ?
S3 C42 H42B 109.6 . . ?
H42A C42 H42B 108.1 . . ?
C48 C43 C44 120.3(8) . . ?
C48 C43 C42 121.5(7) . . ?
C44 C43 C42 118.2(8) . . ?
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C45 C44 H44 119.1 . . ?
C43 C44 H44 119.1 . . ?
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C46 C45 H45 120.1 . . ?
C45 C46 C47 119.2(9) . . ?
C45 C46 H46 120.4 . . ?
C47 C46 H46 120.4 . . ?
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C46 C47 H47 118.7 . . ?
C48 C47 H47 118.7 . . ?
C43 C48 C47 116.3(8) . . ?
C43 C48 C49 123.5(8) . . ?
C47 C48 C49 120.2(8) . . ?
C48 C49 S4 107.6(6) . . ?
C48 C49 H49A 110.2 . . ?
S4 C49 H49A 110.2 . . ?
C48 C49 H49B 110.2 . . ?
S4 C49 H49B 110.2 . . ?
H49A C49 H49B 108.5 . . ?
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C55 C50 S4 126.1(6) . . ?
C51 C50 S4 113.0(6) . . ?
O4 C51 C52 124.2(7) . . ?
O4 C51 C50 115.3(8) . . ?
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C51 C52 C53 117.0(8) . . ?
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C53 C52 C57 120.1(9) . . ?
C54 C53 C52 123.4(9) . . ?
C54 C53 H53 118.3 . . ?
C52 C53 H53 118.3 . . ?
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C55 C54 C56 120.7(8) . . ?
C53 C54 C56 120.0(9) . . ?
C54 C55 C50 119.0(8) . . ?
C54 C55 H55 120.5 . . ?
C50 C55 H55 120.5 . . ?
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C54 C56 H56B 109.5 . . ?
H56A C56 H56B 109.5 . . ?
C54 C56 H56C 109.5 . . ?
H56A C56 H56C 109.5 . . ?
H56B C56 H56C 109.5 . . ?
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C60 C57 C59 110.3(9) . . ?
C58 C57 C59 108.0(12) . . ?
C60 C57 C52 109.6(11) . . ?
C58 C57 C52 112.3(8) . . ?
C59 C57 C52 108.0(9) . . ?
C57 C58 H58A 109.5 . . ?
C57 C58 H58B 109.5 . . ?
H58A C58 H58B 109.5 . . ?
C57 C58 H58C 109.5 . . ?
H58A C58 H58C 109.5 . . ?
H58B C58 H58C 109.5 . . ?
C57 C59 H59A 109.5 . . ?
C57 C59 H59B 109.5 . . ?
H59A C59 H59B 109.5 . . ?
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H59A C59 H59C 109.5 . . ?
H59B C59 H59C 109.5 . . ?
C57 C60 H60A 109.5 . . ?
C57 C60 H60B 109.5 . . ?
H60A C60 H60B 109.5 . . ?
C57 C60 H60C 109.5 . . ?
H60A C60 H60C 109.5 . . ?
H60B C60 H60C 109.5 . . ?
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C63 C62 S5 120.5(8) . . ?
C61 C62 S5 117.5(7) . . ?
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C64 C65 H65 118.0 . . ?
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C61 C66 C68 121.2(9) . . ?
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H67A C67 H67B 109.5 . . ?
C64 C67 H67C 109.5 . . ?
H67A C67 H67C 109.5 . . ?
H67B C67 H67C 109.5 . . ?
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C66 C68 C69 111.1(11) . . ?
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C66 C68 C70 113.5(10) . . ?
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H69A C69 H69C 109.5 . . ?
H69B C69 H69C 109.5 . . ?
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C68 C70 H70B 109.5 . . ?
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C68 C70 H70C 109.5 . . ?
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H70B C70 H70C 109.5 . . ?
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C68 C71 H71B 109.5 . . ?
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C68 C71 H71C 109.5 . . ?
H71A C71 H71C 109.5 . . ?
H71B C71 H71C 109.5 . . ?
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S6 C79 H79B 108.6 . . ?
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C84 C86 H86B 109.5 . . ?
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C87 C90 H90B 109.5 . . ?
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S4 La2 O6 C81 -176.8(7) . . . . ?
La1 La2 O6 C81 92.6(10) . . . . ?
La1 O1 C1 C2 -20.1(11) . . . . ?
La1 O1 C1 C6 160.1(5) . . . . ?
O1 C1 C2 C3 176.0(7) . . . . ?
C6 C1 C2 C3 -4.2(11) . . . . ?
O1 C1 C2 S1 -8.6(10) . . . . ?
C6 C1 C2 S1 171.2(6) . . . . ?
C12 S1 C2 C1 -96.8(7) . . . . ?
La1 S1 C2 C1 18.7(6) . . . . ?
C12 S1 C2 C3 78.7(7) . . . . ?
La1 S1 C2 C3 -165.8(6) . . . . ?
C1 C2 C3 C4 4.0(12) . . . . ?
S1 C2 C3 C4 -171.5(7) . . . . ?
C2 C3 C4 C5 -1.6(13) . . . . ?
C2 C3 C4 C7 179.3(8) . . . . ?
C3 C4 C5 C6 -0.3(13) . . . . ?
C7 C4 C5 C6 178.8(8) . . . . ?
C4 C5 C6 C1 -0.1(12) . . . . ?
C4 C5 C6 C8 -178.8(8) . . . . ?
O1 C1 C6 C5 -178.0(7) . . . . ?
C2 C1 C6 C5 2.3(11) . . . . ?
O1 C1 C6 C8 0.8(11) . . . . ?
C2 C1 C6 C8 -179.0(7) . . . . ?
C5 C6 C8 C11 -122.3(8) . . . . ?
C1 C6 C8 C11 58.9(9) . . . . ?
C5 C6 C8 C10 116.2(8) . . . . ?
C1 C6 C8 C10 -62.5(10) . . . . ?
C5 C6 C8 C9 -2.4(11) . . . . ?
C1 C6 C8 C9 178.9(7) . . . . ?
C2 S1 C12 C13 -169.7(8) . . . . ?
La1 S1 C12 C13 92.4(7) . . . . ?
S1 C12 C13 C18 -111.7(9) . . . . ?
S1 C12 C13 C14 67.7(10) . . . . ?
C18 C13 C14 C15 -1.3(14) . . . . ?
C12 C13 C14 C15 179.4(8) . . . . ?
C13 C14 C15 C16 2.8(16) . . . . ?
C14 C15 C16 C17 -3.1(18) . . . . ?
C15 C16 C17 C18 1.8(16) . . . . ?
C14 C13 C18 C17 -0.1(14) . . . . ?
C12 C13 C18 C17 179.3(8) . . . . ?
C14 C13 C18 C19 176.9(8) . . . . ?
C12 C13 C18 C19 -3.7(14) . . . . ?
C16 C17 C18 C13 -0.2(14) . . . . ?
C16 C17 C18 C19 -177.4(9) . . . . ?
C13 C18 C19 S2 71.9(10) . . . . ?
C17 C18 C19 S2 -111.0(8) . . . . ?
C20 S2 C19 C18 -156.7(7) . . . . ?
La2 S2 C19 C18 100.3(9) . . . . ?
La1 S2 C19 C18 -43.3(10) . . . . ?
C19 S2 C20 C25 -6.7(9) . . . . ?
La2 S2 C20 C25 132.5(8) . . . . ?
La1 S2 C20 C25 -151.2(7) . . . . ?
C19 S2 C20 C21 175.3(6) . . . . ?
La2 S2 C20 C21 -45.4(6) . . . . ?
La1 S2 C20 C21 30.9(6) . . . . ?
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La1 O2 C21 C22 111.2(8) . . . . ?
La2 O2 C21 C22 -118.0(7) . . . . ?
La1 O2 C21 C20 -69.7(7) . . . . ?
La2 O2 C21 C20 61.1(8) . . . . ?
C25 C20 C21 O2 -171.3(7) . . . . ?
S2 C20 C21 O2 6.8(9) . . . . ?
C25 C20 C21 C22 7.8(12) . . . . ?
S2 C20 C21 C22 -174.1(6) . . . . ?
O2 C21 C22 C23 173.3(7) . . . . ?
C20 C21 C22 C23 -5.7(11) . . . . ?
O2 C21 C22 C27 -2.7(12) . . . . ?
C20 C21 C22 C27 178.3(7) . . . . ?
C21 C22 C23 C24 -0.7(12) . . . . ?
C27 C22 C23 C24 175.4(8) . . . . ?
C22 C23 C24 C25 5.1(13) . . . . ?
C22 C23 C24 C26 -172.4(9) . . . . ?
C23 C24 C25 C20 -2.9(13) . . . . ?
C26 C24 C25 C20 174.6(9) . . . . ?
C21 C20 C25 C24 -3.3(12) . . . . ?
S2 C20 C25 C24 178.9(7) . . . . ?
C21 C22 C27 C30 -43.2(10) . . . . ?
C23 C22 C27 C30 141.0(8) . . . . ?
C21 C22 C27 C29 78.1(10) . . . . ?
C23 C22 C27 C29 -97.7(9) . . . . ?
C21 C22 C27 C28 -163.1(8) . . . . ?
C23 C22 C27 C28 21.1(10) . . . . ?
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La1 O3 C31 C36A 155.7(9) . . . . ?
La1 O3 C31 C36B 139.3(14) . . . . ?
O3 C31 C32 C33A 179.2(11) . . . . ?
C36A C31 C32 C33A -7.9(18) . . . . ?
C36B C31 C32 C33A 7.0(15) . . . . ?
O3 C31 C32 C33B 170.2(13) . . . . ?
C36A C31 C32 C33B -17(2) . . . . ?
C36B C31 C32 C33B -2.0(18) . . . . ?
O3 C31 C32 S3 -8.6(12) . . . . ?
C36A C31 C32 S3 164.4(11) . . . . ?
C36B C31 C32 S3 179.3(9) . . . . ?
C42 S3 C32 C33A 81.1(12) . . . . ?
La1 S3 C32 C33A -165.5(12) . . . . ?
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C42 S3 C32 C33B 91.2(9) . . . . ?
La1 S3 C32 C33B -155.4(9) . . . . ?
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C33B C32 C33A C34A 158(5) . . . . ?
S3 C32 C33A C34A -174.9(13) . . . . ?
C32 C33A C34A C35A 11(2) . . . . ?
C32 C33A C34A C37A -177.1(16) . . . . ?
C33A C34A C35A C36A -8(3) . . . . ?
C37A C34A C35A C36A 180.0(18) . . . . ?
C34A C35A C36A C31 -1(3) . . . . ?
C34A C35A C36A C38A -176.0(19) . . . . ?
O3 C31 C36A C35A -176.6(13) . . . . ?
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C36B C31 C36A C35A -23(2) . . . . ?
O3 C31 C36A C38A -3(3) . . . . ?
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C35A C36A C38A C40A -126.4(18) . . . . ?
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S3 C32 C33B C34B -175.3(14) . . . . ?
C32 C33B C34B C35B -1(3) . . . . ?
C32 C33B C34B C37B 177.0(17) . . . . ?
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C35B C36B C38B C39B 122(2) . . . . ?
C31 C36B C38B C39B -67(3) . . . . ?
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S3 C42 C43 C48 -115.9(7) . . . . ?
S3 C42 C43 C44 65.2(8) . . . . ?
C48 C43 C44 C45 2.0(12) . . . . ?
C42 C43 C44 C45 -179.1(7) . . . . ?
C43 C44 C45 C46 -1.1(14) . . . . ?
C44 C45 C46 C47 -0.1(14) . . . . ?
C45 C46 C47 C48 0.4(14) . . . . ?
C44 C43 C48 C47 -1.6(11) . . . . ?
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C44 C43 C48 C49 178.9(7) . . . . ?
C42 C43 C48 C49 0.1(11) . . . . ?
C46 C47 C48 C43 0.5(12) . . . . ?
C46 C47 C48 C49 179.9(8) . . . . ?
C43 C48 C49 S4 73.9(9) . . . . ?
C47 C48 C49 S4 -105.5(7) . . . . ?
C50 S4 C49 C48 -160.0(6) . . . . ?
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La2 S4 C49 C48 89.3(6) . . . . ?
C49 S4 C50 C55 3.0(9) . . . . ?
La1 S4 C50 C55 -138.9(8) . . . . ?
La2 S4 C50 C55 145.8(8) . . . . ?
C49 S4 C50 C51 -177.4(7) . . . . ?
La1 S4 C50 C51 40.8(7) . . . . ?
La2 S4 C50 C51 -34.6(7) . . . . ?
La2 O4 C51 C52 -113.2(10) . . . . ?
La1 O4 C51 C52 112.4(10) . . . . ?
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La2 O4 C51 C50 68.2(9) . . . . ?
La1 O4 C51 C50 -66.2(9) . . . . ?
C55 C50 C51 O4 178.3(8) . . . . ?
S4 C50 C51 O4 -1.4(11) . . . . ?
C55 C50 C51 C52 -0.4(15) . . . . ?
S4 C50 C51 C52 179.9(8) . . . . ?
O4 C51 C52 C53 -178.5(10) . . . . ?
C50 C51 C52 C53 0.0(16) . . . . ?
O4 C51 C52 C57 2.7(18) . . . . ?
C50 C51 C52 C57 -178.8(11) . . . . ?
C51 C52 C53 C54 0.6(19) . . . . ?
C57 C52 C53 C54 179.5(12) . . . . ?
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C53 C54 C55 C50 0.5(16) . . . . ?
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C51 C50 C55 C54 0.1(15) . . . . ?
S4 C50 C55 C54 179.8(8) . . . . ?
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C53 C52 C57 C60 -123.8(12) . . . . ?
C51 C52 C57 C58 175.9(13) . . . . ?
C53 C52 C57 C58 -3(2) . . . . ?
C51 C52 C57 C59 -65.2(16) . . . . ?
C53 C52 C57 C59 116.0(12) . . . . ?
La2 O5 C61 C62 -6.0(16) . . . . ?
La2 O5 C61 C66 178.2(7) . . . . ?
O5 C61 C62 C63 179.7(9) . . . . ?
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O5 C61 C62 S5 -4.1(13) . . . . ?
C66 C61 C62 S5 171.8(7) . . . . ?
C72 S5 C62 C63 66.7(9) . . . . ?
La2 S5 C62 C63 -176.6(8) . . . . ?
C72 S5 C62 C61 -109.5(8) . . . . ?
La2 S5 C62 C61 7.1(8) . . . . ?
C61 C62 C63 C64 3.3(15) . . . . ?
S5 C62 C63 C64 -172.8(8) . . . . ?
C62 C63 C64 C65 -0.6(16) . . . . ?
C62 C63 C64 C67 -179.2(11) . . . . ?
C63 C64 C65 C66 -0.9(17) . . . . ?
C67 C64 C65 C66 177.7(11) . . . . ?
C64 C65 C66 C61 -0.3(17) . . . . ?
C64 C65 C66 C68 -178.7(11) . . . . ?
O5 C61 C66 C65 178.7(10) . . . . ?
C62 C61 C66 C65 2.8(15) . . . . ?
O5 C61 C66 C68 -2.8(16) . . . . ?
C62 C61 C66 C68 -178.7(10) . . . . ?
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C61 C66 C68 C71 -62.1(13) . . . . ?
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C65 C66 C68 C70 -2.8(17) . . . . ?
C61 C66 C68 C70 178.7(11) . . . . ?
C62 S5 C72 C73 67.0(8) . . . . ?
La2 S5 C72 C73 -35.6(8) . . . . ?
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C78 C73 C74 C75 2(2) . . . . ?
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C74 C75 C76 C77 1(2) . . . . ?
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C74 C73 C78 C79 179.7(11) . . . . ?
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C73 C78 C79 S6 -97.8(12) . . . . ?
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La2 S6 C79 C78 36.0(8) . . . . ?
C79 S6 C80 C85 -69.0(9) . . . . ?
La2 S6 C80 C85 176.2(8) . . . . ?
C79 S6 C80 C81 104.1(9) . . . . ?
La2 S6 C80 C81 -10.7(8) . . . . ?
La2 O6 C81 C80 -0.1(16) . . . . ?
La2 O6 C81 C82 -179.5(7) . . . . ?
C85 C80 C81 O6 -176.9(9) . . . . ?
S6 C80 C81 O6 10.2(13) . . . . ?
C85 C80 C81 C82 2.5(15) . . . . ?
S6 C80 C81 C82 -170.4(8) . . . . ?
O6 C81 C82 C83 176.8(10) . . . . ?
C80 C81 C82 C83 -2.6(16) . . . . ?
O6 C81 C82 C87 -3.4(16) . . . . ?
C80 C81 C82 C87 177.2(10) . . . . ?
C81 C82 C83 C84 2(2) . . . . ?
C87 C82 C83 C84 -178.1(13) . . . . ?
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C82 C83 C84 C86 -179.0(13) . . . . ?
C83 C84 C85 C80 0.3(18) . . . . ?
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C81 C82 C87 C88 -178.5(11) . . . . ?
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C92 C93 C94 C95 -156(8) . . . . ?
C98 C96 C97 C98 0(2) 7_546 . . . ?
C99 C96 C97 C98 175.1(18) . . . . ?
C96 C97 C98 C96 0(2) . . . 7_546 ?
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C103 C104 C105 C100 0.0 . . . . ?
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C110 C107 C108 C109 41.2(16) 2 . . . ?
C112 C107 C108 C109 0.0 . . . . ?
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C109 C107 C108 C109 63.3(15) 2 . . . ?
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C107 C108 C109 C107 -28.4(16) . . . 2 ?
C108 C109 C110 C111 0.0 . . . . ?
C107 C109 C110 C111 115(2) 2 . . . ?
C109 C110 C111 C112 0.0 . . . . ?
C109 C110 C111 C107 -126(3) . . . 2 ?
C110 C111 C112 C107 0.0 . . . . ?
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C110 C107 C112 C111 -70(3) 2 . . . ?
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C113 C107 C112 C111 -152(3) . . . . ?
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_refine_diff_density_max    1.546
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