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Noncovalent Interactions within a Synthetic Receptor Can Reinforce Guest Binding

Rodriguez-Docampo, Zaida; Pascu, Sofia I.; Kubik, Stefan; Otto, Sijbren

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?
;

_chemical_melting_point      ?

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# _atom_sites_solution_secondary difmap
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# known chirality), ad (anomalous
# dispersion - ie. Flack param), rmad
# (both rm and ad), syn (known from
# synthetic pathway), unk (unknown)
# or . (not applicable).

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;
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_cell_measurement_theta_min 2.18
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CRYSTALS (Watkin et al 2001)
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CAMERON (Watkin et al 1996)
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Correction applied by SADABS - note that the transmission factors are not real since they include corrections for beam decay and possibly crystal decay (the two cannot be distinguished).

The numbers listed in the CIF are those calculated by CRYSTALS.

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# Number of reflections with Friedels Law is 8281
# Number of reflections without Friedels Law is 0
# Theoretical number of reflections is about 7972
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_reflns_number_gt                 5124
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_refine_ls_weighting_scheme        calc
_refine_ls_weighting_details
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Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982)
[weight] = 1.0/[A~0~*T~0~(x)+A~1~*T~1~(x) ... +A~n-1~*T~n-1~(x)]
where A~i~ are the Chebychev coefficients listed below and x= Fcalc/Fmax
Method = Robust Weighting (Prince, 1982)
W = [weight] * [1-(deltaF/6*sigmaF)^2]^2^
A~i~ are:
1.13 1.35 0.484
;

_exptl_special_details
;

Guest SO4(2-) disordered over two positions was modelled
with refined occupancies:
site (S100, O100, O200, O300, O400) occ 0.538 and
site (S101, O101, O201, O301, O401) occ 0.462

S-alkyl bridge also disordered over two postions was modelled with
refined occupancies:
site (S200, S300, C340, C350, C360, O500, S400, S500) 0.662
and site (S201, S301, C341, C351, C361, O501, S401, S501) 0.338

Butyl chains are disordered - restrained and isotropic refinement
A part of one of the butyl chains modeleled over two positions
with refined occupancies: (C871, C881, C891) occ 0.505
and c(870, C880, C890) occ 0.495
;

## -----REFERENCES -----##
## Insert your own references - in alphabetic order
_publ_section_references
;

Siemens Industrial Automation, Inc (1993)
SMART: Area-Detector Software Package; Madison, WI.

Siemens Industrial Automation, Inc (1995).
SAINT: Area-Detector Integration Software.; Madison, WI.

Betteridge, P.W., Carruthers, J.R., Cooper, R.I.,
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Sheldrick, G.M. (1986). SHELXS86. Program for the solution of crystal structures. Univ. of Gottingen, Federal Republic of Germany.

Watkin D.J. (1994),
Acta Cryst, A50, 411-437

Watkin, D.J., Prout, C.K. & Pearce, L.J. (1996) CAMERON, Chemical Crystallography Laboratory, OXFORD, UK.

;

Uequiv = arithmetic mean of Ui
i.e. Ueqiv = (U1+U2+U3)/3

Replace trailing . with the number of unfound
hydrogen atoms attaced to relavent atom

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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
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_atom_site_disorder_group
_atom_site_attached_hydrogens
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O16 O 0.2220(9) 0.4172(6) 0.8707(4) 0.0628 1.0000 Uani . . . . .
O17 O 0.2400(7) 0.6171(6) 0.6238(4) 0.0556 1.0000 Uani . . . . .
C1 C -0.2439(11) 0.4777(8) 0.8440(5) 0.0478 1.0000 Uani . . . . .
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C68 C -0.0120(12) 0.6169(10) 0.6177(5) 0.0594 1.0000 Uani
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O300 O -0.1644(1) 0.7520(1) 0.7545(1) 0.0470 0.5382 Uani D U . 6 1 .
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S101 S -0.0266(1) 0.7686(1) 0.7545(1) 0.0367 0.4618 Uani D U . 6 2 .
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O301 O 0.0825(1) 0.7590(1) 0.7505(1) 0.0521 0.4618 Uani D U . 6 2 .
O401 O -0.0763(1) 0.7118(1) 0.7197(1) 0.0456 0.4618 Uani D U . 6 2 .
S200 S 0.0573(7) 0.3528(6) 0.7463(4) 0.0853 0.651(18) Uani D U P 5 1 .
S300 S -0.0332(10) 0.2993(6) 0.6916(4) 0.0986 0.651(18) Uani D U P 5 1 .
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O500 O -0.170(3) 0.275(2) 0.5835(11) 0.1596 0.651(18) Uani D U P 5 1 0.651
S400 S -0.0418(12) 0.4405(8) 0.5471(5) 0.1156 0.651(18) Uani D U P 5 1 .
S500 S -0.1333(11) 0.5457(8) 0.5400(5) 0.1032 0.651(18) Uani D U P 5 1 .
S201 S 0.006(2) 0.3471(14) 0.7249(10) 0.1259 0.349(18) Uani D U P 5 2 .
S301 S -0.106(3) 0.3202(14) 0.6713(10) 0.1378 0.349(18) Uani D U P 5 2 .
C341 C -0.065(6) 0.376(4) 0.616(2) 0.1273 0.349(18) Uani D U P 5 2 .
C351 C -0.148(5) 0.428(4) 0.5852(17) 0.1176 0.349(18) Uani D U P 5 2 .
C361 C -0.249(5) 0.394(4) 0.596(3) 0.1218 0.349(18) Uani D U P 5 2 .
O501 O -0.290(3) 0.330(3) 0.5666(18) 0.1182 0.349(18) Uani D U P 5 2 0.349
S401 S -0.0942(16) 0.4699(11) 0.5287(8) 0.0922 0.349(18) Uani D U P 5 2 .
S501 S -0.1681(14) 0.5799(11) 0.5384(10) 0.0801 0.349(18) Uani D U P 5 2 .
N19 N 0.4518(6) 0.1563(6) 0.6036(4) 0.1092(19) 1.0000 Uiso D U
C70 C 0.4713(10) 0.1207(7) 0.5500(4) 0.112(2) 1.0000 Uiso D U
C71 C 0.4704(8) 0.0238(7) 0.5492(4) 0.115(2) 1.0000 Uiso D U
C72 C 0.4555(9) -0.0032(9) 0.4909(4) 0.118(3) 1.0000 Uiso D U
C73 C 0.4496(11) -0.1032(10) 0.4906(6) 0.120(3) 1.0000 Uiso D U
C74 C 0.3581(8) 0.1183(8) 0.6283(4) 0.106(2) 1.0000 Uiso D U
C75 C 0.2536(9) 0.1357(7) 0.5964(4) 0.106(2) 1.0000 Uiso D U
C76 C 0.1643(8) 0.0969(8) 0.6281(5) 0.106(2) 1.0000 Uiso D U
C77 C 0.0614(10) 0.1243(10) 0.6011(6) 0.106(3) 1.0000 Uiso D U
C78 C 0.4431(8) 0.2482(7) 0.5932(4) 0.113(2) 1.0000 Uiso D U
C79 C 0.4494(8) 0.3003(7) 0.6427(5) 0.118(2) 1.0000 Uiso D U
C80 C 0.3357(9) 0.3296(7) 0.6516(5) 0.122(3) 1.0000 Uiso D U
C81 C 0.3131(11) 0.4047(10) 0.6149(8) 0.124(3) 1.0000 Uiso D U
C82 C 0.5445(11) 0.1291(14) 0.6399(6) 0.109(2) 1.0000 Uiso D U
C83 C 0.6508(11) 0.1553(13) 0.6196(6) 0.109(3) 1.0000 Uiso D U
C84 C 0.7370(12) 0.1276(12) 0.6619(7) 0.110(3) 1.0000 Uiso D U
C85 C 0.7138(17) 0.1767(16) 0.7108(7) 0.111(3) 1.0000 Uiso D U
O103 O 0.3086(17) 0.6216(16) 0.5153(8) 0.160(7) 1.0000 Uiso 2
N20 N 0.4707(6) 0.2779(6) 0.9535(4) 0.1919(19) 1.0000 Uiso D U
C90 C 0.5673(10) 0.2532(7) 0.9865(4) 0.193(2) 1.0000 Uiso D U
C91 C 0.6654(8) 0.2982(7) 0.9699(4) 0.193(2) 1.0000 Uiso D U
C92 C 0.7562(9) 0.2706(9) 1.0081(4) 0.195(3) 1.0000 Uiso D U
C93 C 0.8621(11) 0.2870(10) 0.9794(6) 0.195(3) 1.0000 Uiso D U
C94 C 0.4684(8) 0.3766(8) 0.9487(4) 0.193(2) 1.0000 Uiso D U
C95 C 0.4357(9) 0.4204(7) 0.9996(4) 0.194(2) 1.0000 Uiso D U
C96 C 0.3854(8) 0.5079(8) 0.9830(5) 0.194(2) 1.0000 Uiso D U
C97 C 0.4253(10) 0.5730(10) 1.0243(6) 0.195(3) 1.0000 Uiso D U
C98 C 0.3658(8) 0.2465(7) 0.9729(4) 0.194(2) 1.0000 Uiso D U
C99 C 0.3717(8) 0.1520(7) 0.9909(5) 0.196(2) 1.0000 Uiso D U

C100 C 0.2564(9) 0.1251(7) 1.0012(5) 0.197(3) 1.0000 Uiso D U
C101 C 0.2563(11) 0.0256(10) 1.0041(8) 0.198(3) 1.0000 Uiso D U
C86 C 0.4889(15) 0.2463(13) 0.9004(8) 0.190(3) 1.0000 Uiso D U . 1 1 .
C870 C 0.392(4) 0.261(5) 0.8625(13) 0.189(3) 0.48(3) Uiso D U P 1 2 .
C880 C 0.408(5) 0.203(4) 0.8149(18) 0.188(4) 0.48(3) Uiso D U P 1 2 .
C890 C 0.325(6) 0.232(5) 0.7725(16) 0.187(4) 0.48(3) Uiso D U P 1 2 .
C871 C 0.536(5) 0.315(2) 0.8668(13) 0.189(3) 0.52(3) Uiso D U P 1 1 .
C881 C 0.569(4) 0.270(4) 0.8179(12) 0.187(4) 0.52(3) Uiso D U P 1 1 .
C891 C 0.689(4) 0.256(5) 0.825(3) 0.186(4) 0.52(3) Uiso D U P 1 1 .
C580 C 0.052(3) 0.5824(14) 0.9489(8) 0.0547 0.39(3) Uani D U P 2 2 .
C581 C -0.0098(14) 0.5590(11) 0.9216(9) 0.0566 0.61(3) Uani D U P 2 1 .
C110 C -0.0154(14) 0.9618(11) 0.9293(9) 0.0574 0.66(3) Uani D U P 3 1 .
C111 C -0.073(3) 0.9418(14) 0.9536(9) 0.0570 0.34(3) Uani D U P 3 2 .
C21 C -0.141(2) 0.9592(13) 0.5670(7) 0.0612 0.53(3) Uani D U P 4 1 .
C210 C -0.0751(16) 0.908(2) 0.5651(7) 0.0568 0.47(3) Uani D U P 4 2 .
H1 H -0.1712 0.7625 0.8400 0.0558 1.0000 Uiso
H2 H -0.1895 0.8842 0.7167 0.0505 1.0000 Uiso
H3 H -0.1971 0.6463 0.7111 0.0541 1.0000 Uiso
H4 H 0.0973 0.8887 0.7174 0.0556 1.0000 Uiso
H5 H 0.1179 0.7627 0.8383 0.0499 1.0000 Uiso
H6 H 0.1115 0.6525 0.7128 0.0499 1.0000 Uiso
H31 H -0.4375 0.5034 0.8647 0.0722 1.0000 Uiso
H41 H -0.5255 0.6370 0.8734 0.0936 1.0000 Uiso
H51 H -0.4308 0.7627 0.8712 0.0708 1.0000 Uiso
H81 H -0.1356 0.8947 0.8355 0.0495 1.0000 Uiso
H141 H -0.4427 1.0700 0.8339 0.0656 1.0000 Uiso
H151 H -0.5403 1.0148 0.7626 0.0609 1.0000 Uiso
H161 H -0.4559 0.9424 0.6988 0.0644 1.0000 Uiso
H191 H -0.1602 0.8063 0.6468 0.0402 1.0000 Uiso
H251 H -0.4858 0.7089 0.5541 0.0535 1.0000 Uiso
H261 H -0.5575 0.6129 0.6107 0.1077 1.0000 Uiso
H271 H -0.4532 0.5697 0.6849 0.0838 1.0000 Uiso
H301 H -0.1420 0.5908 0.7849 0.0589 1.0000 Uiso
H311 H -0.0197 0.5420 0.7336 0.0713 1.0000 Uiso
H312 H -0.1023 0.4776 0.7058 0.0713 1.0000 Uiso
H331 H -0.0905 0.3721 0.8337 0.0717 1.0000 Uiso
H332 H -0.1598 0.3554 0.7812 0.0717 1.0000 Uiso
H371 H -0.0065 0.7071 0.5102 0.0618 1.0000 Uiso
H372 H 0.0628 0.6231 0.5203 0.0618 1.0000 Uiso
H401 H 0.3611 0.8034 0.5679 0.0985 1.0000 Uiso
H411 H 0.4631 0.8660 0.6366 0.0882 1.0000 Uiso
H421 H 0.3633 0.9231 0.7079 0.0893 1.0000 Uiso
H451 H 0.0637 0.9449 0.7890 0.0465 1.0000 Uiso
H461 H 0.0347 1.0794 0.7180 0.0743 1.0000 Uiso
H462 H -0.0531 1.0140 0.7353 0.0743 1.0000 Uiso
H471 H -0.0831 1.0890 0.8079 0.0837 1.0000 Uiso
H472 H -0.0590 1.1650 0.7691 0.0837 1.0000 Uiso
H481 H 0.0435 1.1528 0.8514 0.0766 1.0000 Uiso
H482 H 0.1011 1.1794 0.8004 0.0766 1.0000 Uiso
H511 H 0.4054 1.0210 0.8730 0.0703 1.0000 Uiso
H521 H 0.4859 0.8848 0.8835 0.0625 1.0000 Uiso
H531 H 0.3900 0.7599 0.8709 0.0698 1.0000 Uiso
H561 H 0.0784 0.6292 0.8304 0.0508 1.0000 Uiso
H621 H 0.3824 0.4466 0.8208 0.0694 1.0000 Uiso
H631 H 0.4615 0.5068 0.7471 0.0985 1.0000 Uiso
H641 H 0.3729 0.5958 0.6948 0.0878 1.0000 Uiso
H671 H 0.0602 0.7282 0.6503 0.0437 1.0000 Uiso
H681 H -0.0635 0.6232 0.6443 0.0715 1.0000 Uiso
H682 H 0.0174 0.5593 0.6193 0.0715 1.0000 Uiso
H701 H 0.5401 0.1407 0.5397 0.1344 1.0000 Uiso
H702 H 0.4160 0.1416 0.5253 0.1344 1.0000 Uiso

H711	H	0.5372	0.0016	0.5644	0.1382	1.0000	Uiso	.	.	.	.	.	.	.
H712	H	0.4121	0.0021	0.5687	0.1382	1.0000	Uiso	.	.	.	.	.	.	.
H721	H	0.5153	0.0162	0.4718	0.1418	1.0000	Uiso	.	.	.	.	.	.	.
H722	H	0.3902	0.0210	0.4753	0.1418	1.0000	Uiso	.	.	.	.	.	.	.
H731	H	0.4402	-0.1234	0.4548	0.1441	1.0000	Uiso	.	.	.	.	.	.	.
H732	H	0.5150	-0.1265	0.5066	0.1441	1.0000	Uiso	.	.	.	.	.	.	.
H733	H	0.3899	-0.1218	0.5101	0.1441	1.0000	Uiso	.	.	.	.	.	.	.
H741	H	0.3534	0.1429	0.6628	0.1278	1.0000	Uiso	.	.	.	.	.	.	.
H742	H	0.3683	0.0567	0.6313	0.1278	1.0000	Uiso	.	.	.	.	.	.	.
H751	H	0.2429	0.1971	0.5919	0.1269	1.0000	Uiso	.	.	.	.	.	.	.
H752	H	0.2547	0.1084	0.5624	0.1269	1.0000	Uiso	.	.	.	.	.	.	.
H761	H	0.1693	0.1186	0.6636	0.1271	1.0000	Uiso	.	.	.	.	.	.	.
H762	H	0.1695	0.0347	0.6286	0.1271	1.0000	Uiso	.	.	.	.	.	.	.
H771	H	0.0025	0.1014	0.6196	0.1270	1.0000	Uiso	.	.	.	.	.	.	.
H772	H	0.0575	0.1865	0.6005	0.1270	1.0000	Uiso	.	.	.	.	.	.	.
H773	H	0.0576	0.1027	0.5655	0.1270	1.0000	Uiso	.	.	.	.	.	.	.
H781	H	0.5006	0.2653	0.5718	0.1361	1.0000	Uiso	.	.	.	.	.	.	.
H782	H	0.3754	0.2594	0.5745	0.1361	1.0000	Uiso	.	.	.	.	.	.	.
H791	H	0.4768	0.2655	0.6718	0.1419	1.0000	Uiso	.	.	.	.	.	.	.
H792	H	0.4953	0.3498	0.6389	0.1419	1.0000	Uiso	.	.	.	.	.	.	.
H801	H	0.3301	0.3477	0.6876	0.1470	1.0000	Uiso	.	.	.	.	.	.	.
H802	H	0.2858	0.2833	0.6438	0.1470	1.0000	Uiso	.	.	.	.	.	.	.
H811	H	0.2415	0.4257	0.6191	0.1483	1.0000	Uiso	.	.	.	.	.	.	.
H812	H	0.3638	0.4504	0.6229	0.1483	1.0000	Uiso	.	.	.	.	.	.	.
H813	H	0.3195	0.3859	0.5791	0.1483	1.0000	Uiso	.	.	.	.	.	.	.
H821	H	0.5372	0.1557	0.6737	0.1302	1.0000	Uiso	.	.	.	.	.	.	.
H822	H	0.5431	0.0671	0.6437	0.1302	1.0000	Uiso	.	.	.	.	.	.	.
H831	H	0.6531	0.2170	0.6144	0.1311	1.0000	Uiso	.	.	.	.	.	.	.
H832	H	0.6621	0.1263	0.5868	0.1311	1.0000	Uiso	.	.	.	.	.	.	.
H841	H	0.8074	0.1420	0.6509	0.1317	1.0000	Uiso	.	.	.	.	.	.	.
H842	H	0.7329	0.0662	0.6681	0.1317	1.0000	Uiso	.	.	.	.	.	.	.
H851	H	0.7659	0.1616	0.7386	0.1331	1.0000	Uiso	.	.	.	.	.	.	.
H852	H	0.7176	0.2379	0.7040	0.1331	1.0000	Uiso	.	.	.	.	.	.	.
H853	H	0.6431	0.1622	0.7212	0.1331	1.0000	Uiso	.	.	.	.	.	.	.
H901	H	0.5561	0.2680	1.0225	0.2311	1.0000	Uiso	.	.	.	.	.	.	.
H902	H	0.5778	0.1916	0.9837	0.2311	1.0000	Uiso	.	.	.	.	.	.	.
H911	H	0.6557	0.3600	0.9714	0.2321	1.0000	Uiso	.	.	.	.	.	.	.
H912	H	0.6804	0.2816	0.9346	0.2321	1.0000	Uiso	.	.	.	.	.	.	.
H921	H	0.7559	0.3046	1.0399	0.2336	1.0000	Uiso	.	.	.	.	.	.	.
H922	H	0.7496	0.2102	1.0167	0.2336	1.0000	Uiso	.	.	.	.	.	.	.
H931	H	0.9228	0.2704	1.0021	0.2344	1.0000	Uiso	.	.	.	.	.	.	.
H932	H	0.8675	0.3475	0.9707	0.2344	1.0000	Uiso	.	.	.	.	.	.	.
H933	H	0.8611	0.2531	0.9476	0.2344	1.0000	Uiso	.	.	.	.	.	.	.
H941	H	0.5388	0.3966	0.9408	0.2311	1.0000	Uiso	.	.	.	.	.	.	.
H942	H	0.4177	0.3925	0.9204	0.2311	1.0000	Uiso	.	.	.	.	.	.	.
H951	H	0.4977	0.4294	1.0232	0.2325	1.0000	Uiso	.	.	.	.	.	.	.
H952	H	0.3843	0.3852	1.0166	0.2325	1.0000	Uiso	.	.	.	.	.	.	.
H961	H	0.3083	0.5042	0.9820	0.2329	1.0000	Uiso	.	.	.	.	.	.	.
H962	H	0.4078	0.5246	0.9489	0.2329	1.0000	Uiso	.	.	.	.	.	.	.
H971	H	0.3959	0.6292	1.0157	0.2335	1.0000	Uiso	.	.	.	.	.	.	.
H972	H	0.4029	0.5554	1.0583	0.2335	1.0000	Uiso	.	.	.	.	.	.	.
H973	H	0.5024	0.5757	1.0251	0.2335	1.0000	Uiso	.	.	.	.	.	.	.
H981	H	0.3471	0.2821	1.0020	0.2325	1.0000	Uiso	.	.	.	.	.	.	.
H982	H	0.3113	0.2516	0.9448	0.2325	1.0000	Uiso	.	.	.	.	.	.	.
H991	H	0.4169	0.1469	1.0227	0.2350	1.0000	Uiso	.	.	.	.	.	.	.
H992	H	0.3996	0.1162	0.9639	0.2350	1.0000	Uiso	.	.	.	.	.	.	.
H1001	H	0.2354	0.1494	1.0340	0.2368	1.0000	Uiso	.	.	.	.	.	.	.
H1002	H	0.2078	0.1447	0.9730	0.2368	1.0000	Uiso	.	.	.	.	.	.	.
H1011	H	0.1852	0.0055	1.0105	0.2376	1.0000	Uiso	.	.	.	.	.	.	.
H1012	H	0.3056	0.0069	1.0323	0.2376	1.0000	Uiso	.	.	.	.	.	.	.
H1013	H	0.2780	0.0022	0.9713	0.2376	1.0000	Uiso	.	.	.	.	.	.	.

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H861 H 0.5373 0.1978 0.9030 0.2280 1.0000 Uiso . . . . .
H862 H 0.4214 0.2279 0.8839 0.2280 1.0000 Uiso . . . . .
H8701 H 0.3271 0.2447 0.8788 0.2262 0.4821 Uiso . . . . .
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H8801 H 0.3977 0.1435 0.8238 0.2251 0.4821 Uiso . . . . .
H8802 H 0.4795 0.2110 0.8030 0.2251 0.4821 Uiso . . . . .
H8901 H 0.3324 0.1971 0.7414 0.2247 0.4821 Uiso . . . . .
H8902 H 0.2545 0.2242 0.7850 0.2247 0.4821 Uiso . . . . .
H8903 H 0.3363 0.2918 0.7642 0.2247 0.4821 Uiso . . . . .
H8711 H 0.5976 0.3405 0.8851 0.2264 0.5179 Uiso . . . . .
H8712 H 0.4836 0.3587 0.8580 0.2264 0.5179 Uiso . . . . .
H8811 H 0.5325 0.2148 0.8139 0.2248 0.5179 Uiso . . . . .
H8812 H 0.5517 0.3051 0.7874 0.2248 0.5179 Uiso . . . . .
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H8912 H 0.7048 0.2209 0.8556 0.2234 0.5179 Uiso . . . . .
H8913 H 0.7241 0.3112 0.8292 0.2234 0.5179 Uiso . . . . .
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H1905 H -0.2290 0.9005 0.5092 0.0810 1.0000 Uiso . . . 4 1 .
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H291 H -0.0453 0.9597 0.5506 0.0678 0.4707 Uiso . . . 4 2 .
H292 H -0.0237 0.8617 0.5642 0.0678 0.4707 Uiso . . . 4 2 .
H391 H 0.1098 0.6015 0.9726 0.0663 0.3920 Uiso . . . 2 2 .
H392 H -0.0114 0.5736 0.9683 0.0663 0.3920 Uiso . . . 2 2 .
H491 H 0.0682 0.6715 0.9359 0.0593 1.0000 Uiso . . . . .
H492 H -0.0251 0.6797 0.8921 0.0593 1.0000 Uiso . . . . .
H493 H -0.0362 0.5614 0.9564 0.0678 0.6080 Uiso . . . . .
H494 H -0.0664 0.5402 0.8970 0.0678 0.6080 Uiso . . . . .
H495 H 0.1281 0.5084 0.9515 0.0754 1.0000 Uiso . . . . .
H496 H 0.0595 0.4426 0.9166 0.0754 1.0000 Uiso . . . . .
H591 H -0.0890 0.8485 0.9401 0.0665 1.0000 Uiso . . . . .
H592 H -0.0088 0.8456 0.8946 0.0665 1.0000 Uiso . . . . .
H593 H 0.0141 0.9562 0.9649 0.0686 0.6598 Uiso . . . . .
H594 H 0.0400 0.9798 0.9068 0.0686 0.6598 Uiso . . . . .
H595 H -0.1392 1.0247 0.9591 0.0696 1.0000 Uiso . . . . .
H596 H -0.0774 1.0811 0.9192 0.0696 1.0000 Uiso . . . . .
H691 H -0.0069 0.9478 0.9743 0.0677 0.3402 Uiso . . . 3 2 .
H692 H -0.1290 0.9239 0.9759 0.0677 0.3402 Uiso . . . 3 2 .
H7901 H 0.0455 0.4124 0.6555 0.1496 0.6508 Uiso . . . 5 1 .
H7902 H 0.0458 0.3318 0.6177 0.1496 0.6508 Uiso . . . 5 1 .
H7903 H -0.2114 0.3499 0.6371 0.1727 0.6508 Uiso . . . 5 1 .
H7904 H -0.2342 0.3852 0.5796 0.1727 0.6508 Uiso . . . 5 1 .
H7905 H -0.1113 0.4539 0.6266 0.1556 0.6508 Uiso . . . 5 1 .
H7906 H 0.0313 0.4526 0.7912 0.0997 1.0000 Uiso . . . 5 1 .
H7907 H -0.1178 0.6732 0.5715 0.0999 1.0000 Uiso . . . 5 1 .
H8921 H -0.0086 0.4145 0.6280 0.1531 0.3492 Uiso . . . 5 2 .
H8922 H -0.0375 0.3333 0.5927 0.1531 0.3492 Uiso . . . 5 2 .
H8923 H -0.2432 0.3733 0.6321 0.1480 0.3492 Uiso . . . 5 2 .
H8924 H -0.2991 0.4412 0.5936 0.1480 0.3492 Uiso . . . 5 2 .
H8925 H -0.0923 0.4308 0.5606 0.1417 0.3492 Uiso . . . 5 2 .
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_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
N1 0.049(6) 0.031(6) 0.053(6) 0.010(5) 0.003(5) 0.003(5)

```

N3 0.050(6) 0.035(6) 0.052(6) -0.001(5) 0.019(5) 0.001(5)
 N4 0.046(6) 0.040(6) 0.044(6) -0.023(5) 0.005(5) -0.004(5)
 N6 0.042(6) 0.060(7) 0.025(5) 0.008(5) -0.007(4) -0.002(5)
 N7 0.064(7) 0.045(6) 0.022(5) 0.007(5) 0.003(5) -0.005(6)
 N9 0.047(6) 0.049(7) 0.039(6) 0.019(5) -0.012(5) -0.012(5)
 N10 0.049(6) 0.041(6) 0.032(5) -0.002(5) 0.005(5) -0.004(5)
 N12 0.030(6) 0.056(7) 0.051(6) -0.005(6) 0.002(5) -0.021(5)
 N13 0.048(6) 0.025(5) 0.063(7) -0.006(5) 0.003(5) -0.004(5)
 N15 0.040(6) 0.036(6) 0.046(6) 0.009(5) -0.012(5) -0.001(5)
 N16 0.056(7) 0.043(6) 0.038(6) 0.025(5) 0.017(5) 0.005(5)
 N18 0.045(6) 0.039(6) 0.042(6) 0.009(5) 0.001(5) 0.012(5)
 O5 0.041(5) 0.065(6) 0.041(5) -0.002(5) -0.012(4) 0.012(5)
 O6 0.077(8) 0.087(8) 0.092(8) 0.040(7) -0.013(6) -0.031(7)
 O7 0.072(7) 0.042(6) 0.077(7) 0.018(5) 0.020(5) 0.000(5)
 O8 0.058(6) 0.046(5) 0.054(5) -0.008(5) 0.012(5) 0.006(5)
 O10 0.096(7) 0.071(7) 0.033(5) -0.007(5) -0.013(5) -0.038(6)
 O11 0.082(7) 0.040(6) 0.054(6) -0.010(5) 0.001(5) 0.017(5)
 O12 0.079(7) 0.083(8) 0.043(6) 0.013(5) 0.009(5) -0.014(6)
 O13 0.043(5) 0.042(5) 0.066(6) -0.011(4) -0.002(4) -0.007(4)
 O14 0.131(10) 0.041(6) 0.053(6) -0.025(5) -0.025(6) 0.004(6)
 O15 0.046(6) 0.046(6) 0.068(6) 0.011(5) -0.008(5) 0.006(4)
 O16 0.095(8) 0.030(5) 0.064(6) 0.014(5) 0.008(5) 0.010(5)
 O17 0.060(6) 0.056(6) 0.053(5) -0.003(5) 0.011(5) 0.005(5)
 C1 0.058(9) 0.027(7) 0.059(9) -0.003(6) 0.008(7) 0.005(6)
 N2 0.062(4) 0.033(4) 0.036(4) 0.000(3) 0.012(3) 0.001(4)
 C2 0.040(5) 0.058(5) 0.040(5) 0.014(4) 0.011(4) -0.008(4)
 C3 0.064(7) 0.044(5) 0.073(6) -0.001(5) -0.006(5) 0.017(5)
 C4 0.032(5) 0.087(8) 0.115(7) -0.024(6) -0.002(5) 0.016(5)
 C5 0.056(6) 0.034(6) 0.087(7) -0.003(5) -0.010(5) -0.007(5)
 C6 0.054(6) 0.038(5) 0.032(5) -0.003(4) 0.005(4) 0.008(5)
 C7 0.050(8) 0.029(7) 0.038(7) 0.003(6) -0.002(6) 0.009(6)
 C8 0.038(7) 0.038(7) 0.048(7) 0.005(6) 0.008(6) 0.007(6)
 C9 0.042(7) 0.069(8) 0.055(7) -0.004(6) -0.014(6) -0.001(6)
 C11 0.054(8) 0.057(8) 0.063(8) -0.021(7) -0.008(7) -0.003(6)
 C12 0.043(8) 0.038(8) 0.044(7) 0.003(6) 0.010(6) 0.001(6)
 N5 0.047(4) 0.038(4) 0.029(4) -0.002(3) -0.001(3) 0.011(4)
 C13 0.036(5) 0.033(5) 0.055(5) 0.004(4) -0.005(4) 0.002(4)
 C14 0.074(7) 0.036(5) 0.055(6) 0.000(5) 0.016(5) 0.005(5)
 C15 0.020(5) 0.070(8) 0.062(7) -0.002(6) -0.001(5) 0.003(5)
 C16 0.027(6) 0.075(6) 0.059(7) -0.013(5) -0.009(5) 0.007(5)
 C17 0.051(6) 0.049(5) 0.037(5) -0.005(4) -0.002(4) -0.002(5)
 C18 0.045(8) 0.029(6) 0.032(6) 0.000(5) -0.001(6) 0.004(6)
 C19 0.038(7) 0.036(6) 0.027(6) -0.002(5) -0.007(5) -0.014(5)
 C20 0.036(7) 0.063(8) 0.040(6) 0.000(6) -0.009(5) -0.010(6)
 C22 0.068(8) 0.079(10) 0.056(8) 0.019(7) -0.001(7) -0.018(8)
 C23 0.051(8) 0.060(9) 0.040(8) 0.002(7) -0.006(6) -0.010(8)
 N8 0.046(4) 0.036(4) 0.033(4) 0.007(3) 0.000(3) -0.003(4)
 C24 0.056(5) 0.043(5) 0.029(5) -0.013(4) 0.008(4) -0.001(5)
 C25 0.031(6) 0.059(6) 0.044(6) 0.005(6) 0.010(5) 0.014(5)
 C26 0.055(6) 0.135(9) 0.079(8) -0.004(8) 0.011(6) -0.038(6)
 C27 0.047(6) 0.116(8) 0.046(7) 0.023(6) -0.010(5) -0.040(6)
 C28 0.037(5) 0.055(5) 0.054(5) -0.007(5) 0.007(4) -0.002(4)
 C29 0.070(10) 0.037(8) 0.054(8) -0.006(7) 0.007(7) -0.023(8)
 C30 0.045(8) 0.057(9) 0.046(7) 0.016(7) 0.004(6) -0.005(7)
 C31 0.067(9) 0.050(9) 0.062(9) -0.006(7) 0.009(7) 0.009(8)
 C32 0.078(9) 0.058(8) 0.113(11) 0.004(8) 0.037(8) 0.002(7)
 C33 0.065(10) 0.050(9) 0.064(9) 0.016(7) 0.014(7) 0.013(8)
 C36 0.082(9) 0.106(10) 0.062(8) 0.015(8) -0.026(7) -0.031(8)
 C37 0.064(9) 0.056(8) 0.035(7) -0.003(6) 0.002(6) -0.006(7)
 C38 0.058(8) 0.037(7) 0.039(7) 0.004(6) 0.010(6) 0.004(7)
 N11 0.049(4) 0.042(4) 0.026(4) -0.001(3) 0.000(3) 0.003(4)

C39 0.040(5) 0.048(5) 0.046(5) 0.012(4) -0.004(4) 0.001(5)
C40 0.088(6) 0.064(6) 0.094(6) -0.029(6) 0.017(5) -0.009(5)
C41 0.048(6) 0.072(9) 0.100(8) -0.035(8) 0.005(6) 0.013(6)
C42 0.039(6) 0.063(8) 0.121(7) -0.029(6) 0.001(5) -0.011(6)
C43 0.040(5) 0.039(5) 0.046(5) 0.000(5) -0.002(4) -0.004(4)
C44 0.047(8) 0.051(9) 0.054(8) 0.000(7) 0.002(6) -0.013(7)
C45 0.040(7) 0.040(7) 0.036(6) 0.001(6) -0.002(5) 0.009(6)
C46 0.058(9) 0.072(10) 0.056(9) 0.013(8) 0.011(7) 0.019(8)
C47 0.063(10) 0.068(10) 0.079(11) 0.022(9) 0.015(9) 0.025(9)
C48 0.061(10) 0.048(9) 0.083(11) 0.007(8) 0.016(8) 0.013(8)
C49 0.063(9) 0.049(9) 0.035(7) -0.012(7) -0.008(7) 0.008(7)
N14 0.045(4) 0.035(4) 0.035(4) -0.002(3) -0.005(3) 0.005(3)
C50 0.061(5) 0.032(5) 0.036(5) 0.005(4) -0.029(4) 0.001(4)
C51 0.076(6) 0.062(7) 0.037(6) 0.017(5) -0.002(5) 0.022(5)
C52 0.042(6) 0.038(7) 0.076(7) 0.003(6) -0.013(5) 0.001(5)
C53 0.041(6) 0.063(8) 0.071(7) 0.016(6) 0.006(5) 0.009(6)
C54 0.054(6) 0.046(6) 0.041(5) 0.010(4) -0.010(4) 0.024(5)
C55 0.042(8) 0.055(9) 0.038(7) -0.005(7) 0.010(6) 0.008(7)
C56 0.053(8) 0.034(7) 0.040(7) -0.001(6) 0.004(6) -0.006(6)
C57 0.027(6) 0.068(8) 0.053(7) 0.011(6) 0.009(5) 0.002(6)
C59 0.078(9) 0.066(8) 0.045(7) 0.006(6) 0.015(7) -0.007(7)
C60 0.059(9) 0.040(8) 0.033(7) 0.009(6) -0.003(6) 0.007(7)
N17 0.048(4) 0.030(4) 0.053(4) -0.003(3) 0.021(3) -0.010(3)
C61 0.034(5) 0.039(5) 0.049(5) 0.010(4) 0.009(4) 0.010(4)
C62 0.037(6) 0.057(7) 0.079(6) 0.009(5) 0.006(5) 0.003(5)
C63 0.065(6) 0.098(7) 0.083(7) 0.015(6) 0.032(5) 0.020(5)
C64 0.039(6) 0.095(8) 0.085(7) 0.036(6) -0.003(5) 0.029(6)
C65 0.060(6) 0.048(6) 0.044(5) -0.004(4) 0.026(4) -0.001(5)
C66 0.051(8) 0.038(8) 0.044(8) -0.009(6) 0.016(7) -0.002(6)
C67 0.042(7) 0.040(7) 0.028(6) 0.004(5) 0.001(5) -0.007(6)
C68 0.073(10) 0.055(9) 0.051(8) -0.009(7) 0.010(7) -0.018(8)
S100 0.0313 0.0373 0.0350 0.0015 0.0028 0.0029
O100 0.0422 0.0425 0.0375 -0.0041 0.0011 -0.0012
O200 0.0274 0.0489 0.0411 0.0088 -0.0148 -0.0154
O300 0.0313 0.0446 0.0639 -0.0080 -0.0085 0.0012
O400 0.0402 0.0530 0.0592 -0.0044 0.0116 0.0168
S101 0.0343 0.0426 0.0327 0.0041 -0.0021 0.0015
O101 0.0473 0.0519 0.0408 0.0090 0.0089 -0.0012
O201 0.0293 0.0487 0.0410 0.0036 -0.0097 0.0109
O301 0.0401 0.0584 0.0587 -0.0069 0.0106 0.0130
O401 0.0375 0.0410 0.0575 0.0055 -0.0046 -0.0156
S200 0.073(5) 0.062(4) 0.122(7) 0.003(4) 0.026(4) 0.009(4)
S300 0.127(8) 0.073(5) 0.100(6) -0.014(5) 0.046(5) -0.017(5)
C340 0.164(15) 0.100(13) 0.110(12) 0.008(10) 0.034(11) -0.030(13)
C350 0.172(14) 0.111(13) 0.106(11) 0.022(11) 0.026(10) -0.043(12)
C360 0.190(18) 0.132(16) 0.110(15) 0.018(14) 0.019(15) -0.063(15)
O500 0.23(2) 0.131(16) 0.117(16) 0.008(15) -0.005(16) -0.075(18)
S400 0.151(9) 0.097(7) 0.101(7) 0.003(6) 0.031(6) -0.044(6)
S500 0.113(8) 0.116(8) 0.077(5) 0.010(7) -0.026(6) -0.048(6)
S201 0.152(15) 0.083(10) 0.146(13) -0.024(9) 0.045(11) 0.011(11)
S301 0.194(17) 0.080(10) 0.142(13) -0.024(10) 0.035(12) -0.019(12)
C341 0.163(19) 0.085(16) 0.136(16) -0.017(13) 0.015(15) -0.015(15)
C351 0.146(17) 0.087(15) 0.122(14) -0.029(12) 0.021(13) -0.015(14)
C361 0.14(2) 0.100(19) 0.13(2) -0.039(16) 0.047(18) -0.001(17)
O501 0.13(2) 0.11(2) 0.13(2) -0.048(17) 0.070(19) -0.010(18)
S401 0.120(11) 0.060(8) 0.094(10) -0.027(8) -0.019(8) -0.013(7)
S501 0.075(9) 0.070(9) 0.092(9) -0.007(8) -0.027(7) -0.009(6)
C580 0.051(13) 0.065(12) 0.050(12) 0.008(10) 0.019(11) -0.003(11)
C581 0.045(10) 0.081(11) 0.043(10) -0.002(9) 0.000(9) -0.015(9)
C110 0.041(10) 0.065(10) 0.065(11) -0.013(9) -0.003(9) -0.004(8)
C111 0.038(13) 0.067(12) 0.065(13) -0.011(10) -0.012(12) 0.005(12)

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C21 0.063(12) 0.066(12) 0.054(10) 0.019(9) 0.000(10) -0.002(11)
C210 0.052(12) 0.071(13) 0.047(10) 0.019(11) -0.004(9) -0.011(11)
_refine_ls_extinction_method
'None'
loop_
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  _geom_bond_site_symmetry_1
  _geom_bond_atom_site_label_2
  _geom_bond_site_symmetry_2
  _geom_bond_distance
  _geom_bond_publ_flag
N1 . C1 . 1.333(18) yes
N1 . C30 . 1.437(17) yes
N1 . C33 . 1.462(18) yes
N3 . C6 . 1.389(14) yes
N3 . C7 . 1.314(17) yes
N3 . H1 . 0.894 no
N4 . C8 . 1.442(17) yes
N4 . C11 . 1.522(17) yes
N4 . C12 . 1.359(17) yes
N6 . C17 . 1.401(14) yes
N6 . C18 . 1.423(15) yes
N6 . H2 . 0.909 no
N7 . C19 . 1.477(14) yes
N7 . C22 . 1.462(18) yes
N7 . C23 . 1.361(17) yes
N9 . C28 . 1.391(13) yes
N9 . C29 . 1.353(17) yes
N9 . H3 . 0.892 no
N10 . C37 . 1.437(17) yes
N10 . C38 . 1.346(17) yes
N10 . C67 . 1.492(15) yes
N12 . C43 . 1.409(14) yes
N12 . C44 . 1.306(18) yes
N12 . H4 . 0.901 no
N13 . C45 . 1.459(17) yes
N13 . C48 . 1.473(18) yes
N13 . C49 . 1.365(17) yes
N15 . C54 . 1.361(14) yes
N15 . C55 . 1.340(18) yes
N15 . H5 . 0.905 no
N16 . C56 . 1.451(17) yes
N16 . C59 . 1.457(17) yes
N16 . C60 . 1.361(17) yes
N18 . C65 . 1.345(13) yes
N18 . C66 . 1.347(17) yes
N18 . H6 . 0.896 no
O5 . C18 . 1.167(14) yes
O6 . C29 . 1.206(17) yes
O7 . C1 . 1.259(16) yes
O8 . C7 . 1.239(15) yes
O10 . C23 . 1.254(15) yes
O11 . C12 . 1.243(16) yes
O12 . C38 . 1.220(15) yes
O13 . C44 . 1.260(16) yes
O14 . C49 . 1.234(16) yes
O15 . C55 . 1.201(15) yes
O16 . C60 . 1.203(16) yes
O17 . C66 . 1.213(15) yes
C1 . C2 . 1.505(16) yes
N2 . C2 . 1.335(12) yes

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N2	.	C6	.	1.293(11)	yes
C2	.	C3	.	1.357(14)	yes
C3	.	C4	.	1.429(15)	yes
C3	.	H31	.	1.000	no
C4	.	C5	.	1.341(15)	yes
C4	.	H41	.	1.000	no
C5	.	C6	.	1.404(13)	yes
C5	.	H51	.	1.000	no
C7	.	C8	.	1.490(19)	yes
C8	.	C9	.	1.554(18)	yes
C8	.	H81	.	1.000	no
C9	.	C110	.	1.512(16)	yes
C9	.	H591	.	1.000	no
C9	.	H592	.	1.000	no
C11	.	C110	.	1.501(16)	yes
C11	.	H595	.	1.000	no
C11	.	H596	.	1.000	no
C12	.	C13	.	1.457(17)	yes
N5	.	C13	.	1.380(12)	yes
N5	.	C17	.	1.361(11)	yes
C13	.	C14	.	1.375(14)	yes
C14	.	C15	.	1.370(15)	yes
C14	.	H141	.	1.000	no
C15	.	C16	.	1.362(15)	yes
C15	.	H151	.	1.000	no
C16	.	C17	.	1.368(13)	yes
C16	.	H161	.	1.000	no
C18	.	C19	.	1.541(17)	yes
C19	.	C20	.	1.555(17)	yes
C19	.	H191	.	1.000	no
C20	.	C21	.	1.517(17)	yes
C20	.	H1901	.	1.000	no
C20	.	H1902	.	1.000	no
C22	.	C21	.	1.508(17)	yes
C22	.	H1905	.	1.000	no
C22	.	H1906	.	1.000	no
C23	.	C24	.	1.435(17)	yes
N8	.	C24	.	1.331(11)	yes
N8	.	C28	.	1.333(12)	yes
C24	.	C25	.	1.431(14)	yes
C25	.	C26	.	1.357(18)	yes
C25	.	H251	.	1.000	no
C26	.	C27	.	1.402(18)	yes
C26	.	H261	.	1.000	no
C27	.	C28	.	1.415(13)	yes
C27	.	H271	.	1.000	no
C29	.	C30	.	1.50(2)	yes
C30	.	C31	.	1.53(2)	yes
C30	.	H301	.	1.000	no
C31	.	C32	.	1.49(2)	yes
C31	.	H311	.	1.000	no
C31	.	H312	.	1.000	no
C32	.	C33	.	1.53(2)	yes
C32	.	S200	.	1.786(14)	yes
C32	.	H7906	.	1.000	no
C33	.	H331	.	1.000	no
C33	.	H332	.	1.000	no
C36	.	C37	.	1.53(2)	yes
C36	.	C68	.	1.43(2)	yes
C36	.	S500	.	1.822(15)	yes
C36	.	H7907	.	1.000	no

C37	.	H371	.	1.000	no
C37	.	H372	.	1.000	no
C38	.	C39	.	1.522(16)	yes
N11	.	C39	.	1.317(11)	yes
N11	.	C43	.	1.308(11)	yes
C39	.	C40	.	1.404(13)	yes
C40	.	C41	.	1.364(16)	yes
C40	.	H401	.	1.000	no
C41	.	C42	.	1.469(17)	yes
C41	.	H411	.	1.000	no
C42	.	C43	.	1.416(13)	yes
C42	.	H421	.	1.000	no
C44	.	C45	.	1.496(19)	yes
C45	.	C46	.	1.527(19)	yes
C45	.	H451	.	1.000	no
C46	.	C47	.	1.54(2)	yes
C46	.	H461	.	1.000	no
C46	.	H462	.	1.000	no
C47	.	C48	.	1.43(2)	yes
C47	.	H471	.	1.000	no
C47	.	H472	.	1.000	no
C48	.	H481	.	1.000	no
C48	.	H482	.	1.000	no
C49	.	C50	.	1.477(17)	yes
N14	.	C50	.	1.369(12)	yes
N14	.	C54	.	1.342(12)	yes
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C51	.	C52	.	1.412(15)	yes
C51	.	H511	.	1.000	no
C52	.	C53	.	1.381(17)	yes
C52	.	H521	.	1.000	no
C53	.	C54	.	1.386(14)	yes
C53	.	H531	.	1.000	no
C55	.	C56	.	1.552(19)	yes
C56	.	C57	.	1.523(18)	yes
C56	.	H561	.	1.000	no
C57	.	C581	.	1.514(16)	yes
C57	.	H491	.	1.000	no
C57	.	H492	.	1.000	no
C59	.	C581	.	1.491(16)	yes
C59	.	H495	.	1.000	no
C59	.	H496	.	1.000	no
C60	.	C61	.	1.482(16)	yes
N17	.	C61	.	1.412(11)	yes
N17	.	C65	.	1.332(11)	yes
C61	.	C62	.	1.338(14)	yes
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C62	.	H621	.	1.000	no
C63	.	C64	.	1.274(15)	yes
C63	.	H631	.	1.000	no
C64	.	C65	.	1.444(14)	yes
C64	.	H641	.	1.000	no
C66	.	C67	.	1.489(19)	yes
C67	.	C68	.	1.558(19)	yes
C67	.	H671	.	1.000	no
C68	.	H681	.	1.000	no
C68	.	H682	.	1.000	no
S100	.	O100	.	1.45179(10)	yes
S100	.	O200	.	1.43345(14)	yes
S100	.	O300	.	1.42782(11)	yes
S100	.	O400	.	1.41719(13)	yes

S101	.	O101	.	1.44198(9)	yes
S101	.	O201	.	1.44275(12)	yes
S101	.	O301	.	1.43374(11)	yes
S101	.	O401	.	1.42264(15)	yes
S200	.	S300	.	2.005(12)	yes
S300	.	C340	.	1.802(17)	yes
C340	.	C350	.	1.555(19)	yes
C340	.	H7901	.	1.000	no
C340	.	H7902	.	1.000	no
C340	.	H8921	.	0.860	no
C350	.	C360	.	1.471(19)	yes
C350	.	S400	.	1.826(18)	yes
C350	.	H7905	.	1.000	no
C360	.	O500	.	1.397(19)	yes
C360	.	H7903	.	1.000	no
C360	.	H7904	.	1.000	no
S400	.	S500	.	2.066(14)	yes
S201	.	S301	.	2.021(18)	yes
S301	.	C341	.	1.807(19)	yes
C341	.	C351	.	1.558(19)	yes
C341	.	H8921	.	1.000	no
C341	.	H8922	.	1.000	no
C351	.	C361	.	1.462(19)	yes
C351	.	S401	.	1.814(19)	yes
C351	.	H8925	.	1.000	no
C361	.	O501	.	1.384(19)	yes
C361	.	H8923	.	1.000	no
C361	.	H8924	.	1.000	no
S401	.	S501	.	2.031(15)	yes
S401	.	H8925	.	1.050	no
N19	.	C70	.	1.559(12)	yes
N19	.	C74	.	1.538(10)	yes
N19	.	C78	.	1.501(8)	yes
N19	.	C82	.	1.560(14)	yes
C70	.	C71	.	1.555(12)	yes
C70	.	H701	.	1.000	no
C70	.	H702	.	1.000	no
C71	.	C72	.	1.602(12)	yes
C71	.	H711	.	1.000	no
C71	.	H712	.	1.000	no
C72	.	C73	.	1.605(16)	yes
C72	.	H721	.	1.000	no
C72	.	H722	.	1.000	no
C73	.	H731	.	1.000	no
C73	.	H732	.	1.000	no
C73	.	H733	.	1.000	no
C74	.	C75	.	1.581(13)	yes
C74	.	H741	.	1.000	no
C74	.	H742	.	1.000	no
C75	.	C76	.	1.594(13)	yes
C75	.	H751	.	1.000	no
C75	.	H752	.	1.000	no
C76	.	C77	.	1.542(10)	yes
C76	.	H761	.	1.000	no
C76	.	H762	.	1.000	no
C77	.	H771	.	1.000	no
C77	.	H772	.	1.000	no
C77	.	H773	.	1.000	no
C78	.	C79	.	1.551(13)	yes
C78	.	H781	.	1.000	no
C78	.	H782	.	1.000	no

C79	.	C80	.	1.579(10)	yes
C79	.	H791	.	1.000	no
C79	.	H792	.	1.000	no
C80	.	C81	.	1.564(14)	yes
C80	.	H801	.	1.000	no
C80	.	H802	.	1.000	no
C81	.	H811	.	1.000	no
C81	.	H812	.	1.000	no
C81	.	H813	.	1.000	no
C82	.	C83	.	1.565(16)	yes
C82	.	H821	.	1.000	no
C82	.	H822	.	1.000	no
C83	.	C84	.	1.600(16)	yes
C83	.	H831	.	1.000	no
C83	.	H832	.	1.000	no
C84	.	C85	.	1.557(17)	yes
C84	.	H841	.	1.000	no
C84	.	H842	.	1.000	no
C85	.	H851	.	1.000	no
C85	.	H852	.	1.000	no
C85	.	H853	.	1.000	no
N20	.	C90	.	1.538(13)	yes
N20	.	C94	.	1.589(13)	yes
N20	.	C98	.	1.564(12)	yes
N20	.	C86	.	1.523(17)	yes
C90	.	C91	.	1.548(13)	yes
C90	.	H901	.	1.000	no
C90	.	H902	.	1.000	no
C91	.	C92	.	1.572(11)	yes
C91	.	H911	.	1.000	no
C91	.	H912	.	1.000	no
C92	.	C93	.	1.628(15)	yes
C92	.	H921	.	1.000	no
C92	.	H922	.	1.000	no
C93	.	H931	.	1.000	no
C93	.	H932	.	1.000	no
C93	.	H933	.	1.000	no
C94	.	C95	.	1.596(13)	yes
C94	.	H941	.	1.000	no
C94	.	H942	.	1.000	no
C95	.	C96	.	1.599(11)	yes
C95	.	H951	.	1.000	no
C95	.	H952	.	1.000	no
C96	.	C97	.	1.576(16)	yes
C96	.	H961	.	1.000	no
C96	.	H962	.	1.000	no
C97	.	H971	.	1.000	no
C97	.	H972	.	1.000	no
C97	.	H973	.	1.000	no
C98	.	C99	.	1.589(11)	yes
C98	.	H981	.	1.000	no
C98	.	H982	.	1.000	no
C99	.	C100	.	1.594(10)	yes
C99	.	H991	.	1.000	no
C99	.	H992	.	1.000	no
C100	.	C101	.	1.598(15)	yes
C100	.	H1001	.	1.000	no
C100	.	H1002	.	1.000	no
C101	.	H1011	.	1.000	no
C101	.	H1012	.	1.000	no
C101	.	H1013	.	1.000	no

C86	.	C871	.	1.556(19)	yes
C86	.	H861	.	1.000	no
C86	.	H862	.	1.000	no
C870	.	C880	.	1.582(19)	yes
C870	.	H8701	.	1.000	no
C870	.	H8702	.	1.000	no
C880	.	C890	.	1.578(19)	yes
C880	.	H8801	.	1.000	no
C880	.	H8802	.	1.000	no
C890	.	H8901	.	1.000	no
C890	.	H8902	.	1.000	no
C890	.	H8903	.	1.000	no
C871	.	C881	.	1.560(19)	yes
C871	.	H8711	.	1.000	no
C871	.	H8712	.	1.000	no
C881	.	C891	.	1.574(19)	yes
C881	.	H8811	.	1.000	no
C881	.	H8812	.	1.000	no
C891	.	H8911	.	1.000	no
C891	.	H8912	.	1.000	no
C891	.	H8913	.	1.000	no
C580	.	H391	.	1.000	no
C580	.	H392	.	1.000	no
C581	.	H493	.	1.000	no
C581	.	H494	.	1.000	no
C110	.	H593	.	1.000	no
C110	.	H594	.	1.000	no
C111	.	H691	.	1.000	no
C111	.	H692	.	1.000	no
C21	.	H1903	.	1.000	no
C21	.	H1904	.	1.000	no
C210	.	H291	.	1.000	no
C210	.	H292	.	1.000	no

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C1	.	N1	.	C30	126.2(11) yes
C1	.	N1	.	C33	120.7(11) yes
C30	.	N1	.	C33	112.2(11) yes
C6	.	N3	.	C7	129.9(10) yes
C6	.	N3	.	H1	114.221 no
C7	.	N3	.	H1	115.890 no
C8	.	N4	.	C11	114.6(10) yes
C8	.	N4	.	C12	125.7(10) yes
C11	.	N4	.	C12	119.6(10) yes
C17	.	N6	.	C18	123.9(10) yes
C17	.	N6	.	H2	115.526 no
C18	.	N6	.	H2	120.165 no
C19	.	N7	.	C22	110.8(10) yes
C19	.	N7	.	C23	127.5(10) yes
C22	.	N7	.	C23	121.1(10) yes
C28	.	N9	.	C29	129.2(11) yes
C28	.	N9	.	H3	115.330 no
C29	.	N9	.	H3	114.968 no

C37 . N10 . C38 . 123.1(10)	yes
C37 . N10 . C67 . 112.2(10)	yes
C38 . N10 . C67 . 124.1(10)	yes
C43 . N12 . C44 . 128.7(10)	yes
C43 . N12 . H4 . 114.891	no
C44 . N12 . H4 . 116.369	no
C45 . N13 . C48 . 111.9(11)	yes
C45 . N13 . C49 . 128.0(10)	yes
C48 . N13 . C49 . 119.6(12)	yes
C54 . N15 . C55 . 124.8(10)	yes
C54 . N15 . H5 . 121.035	no
C55 . N15 . H5 . 114.019	no
C56 . N16 . C59 . 112.5(10)	yes
C56 . N16 . C60 . 127.8(10)	yes
C59 . N16 . C60 . 118.6(10)	yes
C65 . N18 . C66 . 128.7(10)	yes
C65 . N18 . H6 . 114.573	no
C66 . N18 . H6 . 114.583	no
N1 . C1 . O7 . 121.8(12)	yes
N1 . C1 . C2 . 117.4(11)	yes
O7 . C1 . C2 . 120.7(12)	yes
C2 . N2 . C6 . 119.5(8)	yes
C1 . C2 . N2 . 119.4(9)	yes
C1 . C2 . C3 . 118.2(9)	yes
N2 . C2 . C3 . 122.0(9)	yes
C2 . C3 . C4 . 117.1(9)	yes
C2 . C3 . H31 . 121.473	no
C4 . C3 . H31 . 121.473	no
C3 . C4 . C5 . 121.0(8)	yes
C3 . C4 . H41 . 119.520	no
C5 . C4 . H41 . 119.520	no
C4 . C5 . C6 . 116.0(9)	yes
C4 . C5 . H51 . 121.980	no
C6 . C5 . H51 . 121.981	no
C5 . C6 . N3 . 121.3(9)	yes
C5 . C6 . N2 . 124.2(9)	yes
N3 . C6 . N2 . 114.5(8)	yes
N3 . C7 . O8 . 124.3(12)	yes
N3 . C7 . C8 . 115.0(11)	yes
O8 . C7 . C8 . 120.7(11)	yes
C7 . C8 . N4 . 115.9(10)	yes
C7 . C8 . C9 . 112.0(10)	yes
N4 . C8 . C9 . 102.1(10)	yes
C7 . C8 . H81 . 101.172	no
N4 . C8 . H81 . 111.176	no
C9 . C8 . H81 . 115.143	no
C8 . C9 . C110 . 106.6(12)	yes
C8 . C9 . H591 . 110.191	no
C110 . C9 . H591 . 110.192	no
C8 . C9 . H592 . 110.191	no
C110 . C9 . H592 . 110.192	no
H591 . C9 . H592 . 109.467	no
N4 . C11 . C110 . 101.0(11)	yes
N4 . C11 . H595 . 111.557	no
C110 . C11 . H595 . 111.557	no
N4 . C11 . H596 . 111.558	no
C110 . C11 . H596 . 111.557	no
H595 . C11 . H596 . 109.467	no
N4 . C12 . O11 . 120.9(12)	yes
N4 . C12 . C13 . 121.2(11)	yes
O11 . C12 . C13 . 117.9(11)	yes

C13 . N5 . C17 . 116.3(7)	yes
C12 . C13 . N5 . 115.9(8)	yes
C12 . C13 . C14 . 120.7(10)	yes
N5 . C13 . C14 . 122.5(9)	yes
C13 . C14 . C15 . 117.9(9)	yes
C13 . C14 . H141 . 121.025	no
C15 . C14 . H141 . 121.025	no
C14 . C15 . C16 . 120.8(8)	yes
C14 . C15 . H151 . 119.604	no
C16 . C15 . H151 . 119.603	no
C15 . C16 . C17 . 119.0(9)	yes
C15 . C16 . H161 . 120.524	no
C17 . C16 . H161 . 120.524	no
N6 . C17 . C16 . 125.8(8)	yes
N6 . C17 . N5 . 111.2(8)	yes
C16 . C17 . N5 . 122.8(8)	yes
N6 . C18 . O5 . 125.6(11)	yes
N6 . C18 . C19 . 108.1(10)	yes
O5 . C18 . C19 . 126.0(10)	yes
C18 . C19 . N7 . 108.3(9)	yes
C18 . C19 . C20 . 110.0(10)	yes
N7 . C19 . C20 . 103.9(8)	yes
C18 . C19 . H191 . 108.183	no
N7 . C19 . H191 . 113.938	no
C20 . C19 . H191 . 112.347	no
C19 . C20 . C21 . 102.9(12)	yes
C19 . C20 . H1901 . 111.091	no
C21 . C20 . H1901 . 111.093	no
C19 . C20 . H1902 . 111.090	no
C21 . C20 . H1902 . 111.092	no
H1901 . C20 . H1902 . 109.467	no
N7 . C22 . C21 . 104.4(13)	yes
N7 . C22 . H1905 . 110.726	no
C21 . C22 . H1905 . 110.725	no
N7 . C22 . H1906 . 110.726	no
C21 . C22 . H1906 . 110.726	no
H1905 . C22 . H1906 . 109.467	no
N7 . C23 . O10 . 119.2(12)	yes
N7 . C23 . C24 . 120.4(10)	yes
O10 . C23 . C24 . 120.4(12)	yes
C24 . N8 . C28 . 119.6(7)	yes
C23 . C24 . N8 . 119.3(9)	yes
C23 . C24 . C25 . 118.6(9)	yes
N8 . C24 . C25 . 121.6(8)	yes
C24 . C25 . C26 . 119.8(10)	yes
C24 . C25 . H251 . 120.107	no
C26 . C25 . H251 . 120.106	no
C25 . C26 . C27 . 118.1(10)	yes
C25 . C26 . H261 . 120.970	no
C27 . C26 . H261 . 120.970	no
C26 . C27 . C28 . 119.5(10)	yes
C26 . C27 . H271 . 120.241	no
C28 . C27 . H271 . 120.241	no
C27 . C28 . N9 . 124.3(9)	yes
C27 . C28 . N8 . 121.4(9)	yes
N9 . C28 . N8 . 114.3(8)	yes
N9 . C29 . O6 . 122.9(14)	yes
N9 . C29 . C30 . 113.9(11)	yes
O6 . C29 . C30 . 123.2(13)	yes
C29 . C30 . N1 . 111.5(11)	yes
C29 . C30 . C31 . 109.7(12)	yes

N1 . C30 . C31 . 104.6(11)	yes
C29 . C30 . H301 . 106.487	no
N1 . C30 . H301 . 111.436	no
C31 . C30 . H301 . 113.146	no
C30 . C31 . C32 . 105.6(12)	yes
C30 . C31 . H311 . 110.434	no
C32 . C31 . H311 . 110.434	no
C30 . C31 . H312 . 110.433	no
C32 . C31 . H312 . 110.434	no
H311 . C31 . H312 . 109.467	no
C31 . C32 . C33 . 104.8(12)	yes
C31 . C32 . S200 . 123.4(13)	yes
C33 . C32 . S200 . 117.5(11)	yes
C31 . C32 . H7906 . 106.516	no
C33 . C32 . H7906 . 114.514	no
S200 . C32 . H7906 . 88.896	no
C32 . C33 . N1 . 101.8(11)	yes
C32 . C33 . H331 . 111.363	no
N1 . C33 . H331 . 111.363	no
C32 . C33 . H332 . 111.363	no
N1 . C33 . H332 . 111.363	no
H331 . C33 . H332 . 109.467	no
C37 . C36 . C68 . 106.0(12)	yes
C37 . C36 . S500 . 115.4(13)	yes
C68 . C36 . S500 . 116.0(13)	yes
C37 . C36 . H7907 . 110.440	no
C68 . C36 . H7907 . 109.746	no
S500 . C36 . H7907 . 99.073	no
C36 . C37 . N10 . 102.9(10)	yes
C36 . C37 . H371 . 111.082	no
N10 . C37 . H371 . 111.082	no
C36 . C37 . H372 . 111.082	no
N10 . C37 . H372 . 111.082	no
H371 . C37 . H372 . 109.467	no
N10 . C38 . O12 . 120.3(12)	yes
N10 . C38 . C39 . 117.0(10)	yes
O12 . C38 . C39 . 122.6(12)	yes
C39 . N11 . C43 . 117.3(8)	yes
C38 . C39 . N11 . 117.2(8)	yes
C38 . C39 . C40 . 117.0(9)	yes
N11 . C39 . C40 . 125.4(8)	yes
C39 . C40 . C41 . 119.8(9)	yes
C39 . C40 . H401 . 120.102	no
C41 . C40 . H401 . 120.103	no
C40 . C41 . C42 . 114.8(9)	yes
C40 . C41 . H411 . 122.610	no
C42 . C41 . H411 . 122.610	no
C41 . C42 . C43 . 119.2(9)	yes
C41 . C42 . H421 . 120.411	no
C43 . C42 . H421 . 120.411	no
C42 . C43 . N12 . 122.0(9)	yes
C42 . C43 . N11 . 123.0(9)	yes
N12 . C43 . N11 . 114.9(8)	yes
N12 . C44 . O13 . 123.6(13)	yes
N12 . C44 . C45 . 114.4(11)	yes
O13 . C44 . C45 . 121.9(12)	yes
C44 . C45 . N13 . 112.8(10)	yes
C44 . C45 . C46 . 111.6(11)	yes
N13 . C45 . C46 . 102.8(11)	yes
C44 . C45 . H451 . 103.810	no
N13 . C45 . H451 . 112.450	no

C46 . C45 . H451 . 113.643	no
C45 . C46 . C47 . 103.7(12)	yes
C45 . C46 . H461 . 110.901	no
C47 . C46 . H461 . 110.902	no
C45 . C46 . H462 . 110.901	no
C47 . C46 . H462 . 110.902	no
H461 . C46 . H462 . 109.467	no
C46 . C47 . C48 . 105.0(12)	yes
C46 . C47 . H471 . 110.574	no
C48 . C47 . H471 . 110.574	no
C46 . C47 . H472 . 110.574	no
C48 . C47 . H472 . 110.574	no
H471 . C47 . H472 . 109.467	no
N13 . C48 . C47 . 103.5(13)	yes
N13 . C48 . H481 . 110.944	no
C47 . C48 . H481 . 110.943	no
N13 . C48 . H482 . 110.944	no
C47 . C48 . H482 . 110.943	no
H481 . C48 . H482 . 109.466	no
N13 . C49 . O14 . 120.7(12)	yes
N13 . C49 . C50 . 118.8(11)	yes
O14 . C49 . C50 . 120.0(12)	yes
C50 . N14 . C54 . 119.9(8)	yes
C49 . C50 . N14 . 117.1(9)	yes
C49 . C50 . C51 . 119.3(9)	yes
N14 . C50 . C51 . 122.8(8)	yes
C50 . C51 . C52 . 114.4(9)	yes
C50 . C51 . H511 . 122.816	no
C52 . C51 . H511 . 122.816	no
C51 . C52 . C53 . 123.1(9)	yes
C51 . C52 . H521 . 118.434	no
C53 . C52 . H521 . 118.433	no
C52 . C53 . C54 . 118.0(10)	yes
C52 . C53 . H531 . 121.018	no
C54 . C53 . H531 . 121.018	no
C53 . C54 . N15 . 125.7(10)	yes
C53 . C54 . N14 . 121.7(10)	yes
N15 . C54 . N14 . 112.5(8)	yes
N15 . C55 . O15 . 127.9(13)	yes
N15 . C55 . C56 . 113.3(11)	yes
O15 . C55 . C56 . 118.5(12)	yes
C55 . C56 . N16 . 114.9(11)	yes
C55 . C56 . C57 . 110.9(10)	yes
N16 . C56 . C57 . 103.5(10)	yes
C55 . C56 . H561 . 102.948	no
N16 . C56 . H561 . 110.430	no
C57 . C56 . H561 . 114.492	no
C56 . C57 . C581 . 103.1(12)	yes
C56 . C57 . H491 . 111.035	no
C581 . C57 . H491 . 111.035	no
C56 . C57 . H492 . 111.036	no
C581 . C57 . H492 . 111.035	no
H491 . C57 . H492 . 109.467	no
N16 . C59 . C581 . 100.2(12)	yes
N16 . C59 . H495 . 111.737	no
C581 . C59 . H495 . 111.737	no
N16 . C59 . H496 . 111.737	no
C581 . C59 . H496 . 111.737	no
H495 . C59 . H496 . 109.467	no
N16 . C60 . O16 . 120.7(12)	yes
N16 . C60 . C61 . 119.1(10)	yes

O16	.	C60	.	C61	.	120.1(12)	yes
C61	.	N17	.	C65	.	118.6(7)	yes
C60	.	C61	.	N17	.	116.1(8)	yes
C60	.	C61	.	C62	.	120.4(9)	yes
N17	.	C61	.	C62	.	122.2(8)	yes
C61	.	C62	.	C63	.	116.5(9)	yes
C61	.	C62	.	H621	.	121.737	no
C63	.	C62	.	H621	.	121.737	no
C62	.	C63	.	C64	.	121.9(10)	yes
C62	.	C63	.	H631	.	119.069	no
C64	.	C63	.	H631	.	119.069	no
C63	.	C64	.	C65	.	120.4(10)	yes
C63	.	C64	.	H641	.	119.776	no
C65	.	C64	.	H641	.	119.776	no
C64	.	C65	.	N18	.	124.7(9)	yes
C64	.	C65	.	N17	.	119.0(8)	yes
N18	.	C65	.	N17	.	115.9(8)	yes
N18	.	C66	.	O17	.	124.3(13)	yes
N18	.	C66	.	C67	.	112.6(11)	yes
O17	.	C66	.	C67	.	122.9(12)	yes
N10	.	C67	.	C66	.	112.4(10)	yes
N10	.	C67	.	C68	.	101.8(9)	yes
C66	.	C67	.	C68	.	111.1(11)	yes
N10	.	C67	.	H671	.	113.201	no
C66	.	C67	.	H671	.	104.234	no
C68	.	C67	.	H671	.	114.408	no
C67	.	C68	.	C36	.	107.1(12)	yes
C67	.	C68	.	H681	.	110.066	no
C36	.	C68	.	H681	.	110.066	no
C67	.	C68	.	H682	.	110.066	no
C36	.	C68	.	H682	.	110.067	no
H681	.	C68	.	H682	.	109.466	no
O100	.	S100	.	O200	.	112.164(11)	yes
O100	.	S100	.	O300	.	108.860(9)	yes
O200	.	S100	.	O300	.	109.850(10)	yes
O100	.	S100	.	O400	.	108.706(11)	yes
O200	.	S100	.	O400	.	110.646(8)	yes
O300	.	S100	.	O400	.	106.431(12)	yes
O101	.	S101	.	O201	.	110.660(10)	yes
O101	.	S101	.	O301	.	109.212(9)	yes
O201	.	S101	.	O301	.	110.421(9)	yes
O101	.	S101	.	O401	.	108.878(11)	yes
O201	.	S101	.	O401	.	110.346(11)	yes
O301	.	S101	.	O401	.	107.243(12)	yes
C32	.	S200	.	S300	.	101.4(8)	yes
S200	.	S300	.	C340	.	97.0(14)	yes
S300	.	C340	.	C350	.	116(2)	yes
S300	.	C340	.	H7901	.	107.855	no
C350	.	C340	.	H7901	.	107.859	no
S300	.	C340	.	H7902	.	107.854	no
C350	.	C340	.	H7902	.	107.858	no
H7901	.	C340	.	H7902	.	109.465	no
S300	.	C340	.	H8921	.	140.990	no
C350	.	C340	.	H8921	.	46.363	no
H7901	.	C340	.	H8921	.	63.233	no
H7902	.	C340	.	H8921	.	110.849	no
C340	.	C350	.	C360	.	116(3)	yes
C340	.	C350	.	S400	.	110.1(18)	yes
C360	.	C350	.	S400	.	114(2)	yes
C340	.	C350	.	H7905	.	106.025	no
C360	.	C350	.	H7905	.	100.924	no

S400 . C350 . H7905 . 108.259	no
C360 . C350 . H8921 . 147.654	no
S400 . C350 . H8921 . 92.480	no
H7905 . C350 . H8921 . 86.428	no
C340 . C350 . H8925 . 130.926	no
C360 . C350 . H8925 . 95.791	no
H7905 . C350 . H8925 . 102.891	no
H8921 . C350 . H8925 . 113.382	no
C350 . C360 . O500 . 114(4)	yes
C350 . C360 . H7903 . 108.372	no
O500 . C360 . H7903 . 108.373	no
C350 . C360 . H7904 . 108.371	no
O500 . C360 . H7904 . 108.372	no
H7903 . C360 . H7904 . 109.463	no
C350 . C360 . H8923 . 113.487	no
O500 . C360 . H8923 . 125.144	no
C350 . S400 . S500 . 97.2(16)	yes
C36 . S500 . S400 . 107.6(9)	yes
S201 . S301 . C341 . 103(3)	yes
S201 . S301 . H7903 . 149.010	no
S301 . C341 . C351 . 118(3)	yes
S301 . C341 . H8921 . 107.388	no
C351 . C341 . H8921 . 107.392	no
S301 . C341 . H8922 . 107.391	no
C351 . C341 . H8922 . 107.393	no
H8921 . C341 . H8922 . 109.467	no
C341 . C351 . C361 . 107(5)	yes
C341 . C351 . S401 . 110(3)	yes
C361 . C351 . S401 . 134(5)	yes
C341 . C351 . H7904 . 109.691	no
C361 . C351 . H7905 . 104.551	no
H7905 . C351 . H8925 . 107.785	no
C351 . C361 . H8923 . 107.095	no
O501 . C361 . H8923 . 107.093	no
C351 . C361 . H8924 . 107.094	no
O501 . C361 . H8924 . 107.089	no
H8923 . C361 . H8924 . 109.465	no
S501 . S401 . H8925 . 114.116	no
C70 . N19 . C74 . 114.4(7)	yes
C70 . N19 . C78 . 102.1(5)	yes
C74 . N19 . C78 . 114.4(6)	yes
C70 . N19 . C82 . 107.3(10)	yes
C74 . N19 . C82 . 103.1(6)	yes
C78 . N19 . C82 . 115.8(10)	yes
N19 . C70 . C71 . 112.1(8)	yes
N19 . C70 . H701 . 108.796	no
C71 . C70 . H701 . 108.794	no
N19 . C70 . H702 . 108.799	no
C71 . C70 . H702 . 108.795	no
H701 . C70 . H702 . 109.466	no
C70 . C71 . C72 . 106.5(9)	yes
C70 . C71 . H711 . 110.212	no
C72 . C71 . H711 . 110.208	no
C70 . C71 . H712 . 110.212	no
C72 . C71 . H712 . 110.213	no
H711 . C71 . H712 . 109.467	no
C71 . C72 . C73 . 106.1(10)	yes
C71 . C72 . H721 . 110.290	no
C73 . C72 . H721 . 110.292	no
C71 . C72 . H722 . 110.284	no
C73 . C72 . H722 . 110.290	no

H721 . C72 . H722 . 109.466	no
C72 . C73 . H731 . 109.465	no
C72 . C73 . H732 . 109.465	no
H731 . C73 . H732 . 109.482	no
C72 . C73 . H733 . 109.463	no
H731 . C73 . H733 . 109.475	no
H732 . C73 . H733 . 109.476	no
N19 . C74 . C75 . 112.2(9)	yes
N19 . C74 . H741 . 108.790	no
C75 . C74 . H741 . 108.786	no
N19 . C74 . H742 . 108.792	no
C75 . C74 . H742 . 108.788	no
H741 . C74 . H742 . 109.468	no
C74 . C75 . C76 . 106.1(9)	yes
C74 . C75 . H751 . 110.305	no
C76 . C75 . H751 . 110.304	no
C74 . C75 . H752 . 110.306	no
C76 . C75 . H752 . 110.308	no
H751 . C75 . H752 . 109.466	no
C75 . C76 . C77 . 106.4(10)	yes
C75 . C76 . H761 . 110.260	no
C77 . C76 . H761 . 110.260	no
C75 . C76 . H762 . 110.255	no
C77 . C76 . H762 . 110.259	no
H761 . C76 . H762 . 109.466	no
C76 . C77 . H771 . 109.465	no
C76 . C77 . H772 . 109.464	no
H771 . C77 . H772 . 109.482	no
C76 . C77 . H773 . 109.463	no
H771 . C77 . H773 . 109.476	no
H772 . C77 . H773 . 109.477	no
N19 . C78 . C79 . 112.0(9)	yes
N19 . C78 . H781 . 108.806	no
C79 . C78 . H781 . 108.808	no
N19 . C78 . H782 . 108.805	no
C79 . C78 . H782 . 108.806	no
H781 . C78 . H782 . 109.468	no
C78 . C79 . C80 . 106.3(9)	yes
C78 . C79 . H791 . 110.253	no
C80 . C79 . H791 . 110.254	no
C78 . C79 . H792 . 110.253	no
C80 . C79 . H792 . 110.254	no
H791 . C79 . H792 . 109.465	no
C79 . C80 . C81 . 106.3(10)	yes
C79 . C80 . H801 . 110.268	no
C81 . C80 . H801 . 110.268	no
C79 . C80 . H802 . 110.267	no
C81 . C80 . H802 . 110.267	no
H801 . C80 . H802 . 109.466	no
C80 . C81 . H811 . 109.469	no
C80 . C81 . H812 . 109.465	no
H811 . C81 . H812 . 109.478	no
C80 . C81 . H813 . 109.465	no
H811 . C81 . H813 . 109.478	no
H812 . C81 . H813 . 109.473	no
N19 . C82 . C83 . 112.2(13)	yes
N19 . C82 . H821 . 108.798	no
C83 . C82 . H821 . 108.795	no
N19 . C82 . H822 . 108.798	no
C83 . C82 . H822 . 108.795	no
H821 . C82 . H822 . 109.467	no

C82 . C83 . C84 . 106.3(13)	yes
C82 . C83 . H831 . 110.262	no
C84 . C83 . H831 . 110.260	no
C82 . C83 . H832 . 110.263	no
C84 . C83 . H832 . 110.263	no
H831 . C83 . H832 . 109.465	no
C83 . C84 . C85 . 106.2(14)	yes
C83 . C84 . H841 . 110.274	no
C85 . C84 . H841 . 110.272	no
C83 . C84 . H842 . 110.270	no
C85 . C84 . H842 . 110.271	no
H841 . C84 . H842 . 109.466	no
C84 . C85 . H851 . 109.468	no
C84 . C85 . H852 . 109.465	no
H851 . C85 . H852 . 109.477	no
C84 . C85 . H853 . 109.466	no
H851 . C85 . H853 . 109.477	no
H852 . C85 . H853 . 109.475	no
C90 . N20 . C94 . 108.3(6)	yes
C90 . N20 . C98 . 115.3(5)	yes
C94 . N20 . C98 . 109.5(4)	yes
C90 . N20 . C86 . 105.9(9)	yes
C94 . N20 . C86 . 105.2(9)	yes
C98 . N20 . C86 . 112.1(9)	yes
N20 . C90 . C91 . 112.1(8)	yes
N20 . C90 . H901 . 108.831	no
C91 . C90 . H901 . 108.827	no
N20 . C90 . H902 . 108.828	no
C91 . C90 . H902 . 108.826	no
H901 . C90 . H902 . 109.466	no
C90 . C91 . C92 . 106.6(9)	yes
C90 . C91 . H911 . 110.183	no
C92 . C91 . H911 . 110.185	no
C90 . C91 . H912 . 110.183	no
C92 . C91 . H912 . 110.180	no
H911 . C91 . H912 . 109.466	no
C91 . C92 . C93 . 106.1(9)	yes
C91 . C92 . H921 . 110.305	no
C93 . C92 . H921 . 110.312	no
C91 . C92 . H922 . 110.310	no
C93 . C92 . H922 . 110.313	no
H921 . C92 . H922 . 109.466	no
C92 . C93 . H931 . 109.464	no
C92 . C93 . H932 . 109.463	no
H931 . C93 . H932 . 109.476	no
C92 . C93 . H933 . 109.465	no
H931 . C93 . H933 . 109.482	no
H932 . C93 . H933 . 109.478	no
N20 . C94 . C95 . 112.1(9)	yes
N20 . C94 . H941 . 108.807	no
C95 . C94 . H941 . 108.806	no
N20 . C94 . H942 . 108.805	no
C95 . C94 . H942 . 108.803	no
H941 . C94 . H942 . 109.466	no
C94 . C95 . C96 . 106.2(9)	yes
C94 . C95 . H951 . 110.277	no
C96 . C95 . H951 . 110.276	no
C94 . C95 . H952 . 110.279	no
C96 . C95 . H952 . 110.276	no
H951 . C95 . H952 . 109.468	no
C95 . C96 . C97 . 106.2(10)	yes

C95 . C96 . H961 . 110.292	no
C97 . C96 . H961 . 110.294	no
C95 . C96 . H962 . 110.290	no
C97 . C96 . H962 . 110.295	no
H961 . C96 . H962 . 109.467	no
C96 . C97 . H971 . 109.467	no
C96 . C97 . H972 . 109.466	no
H971 . C97 . H972 . 109.482	no
C96 . C97 . H973 . 109.463	no
H971 . C97 . H973 . 109.475	no
H972 . C97 . H973 . 109.474	no
N20 . C98 . C99 . 112.2(8)	yes
N20 . C98 . H981 . 108.794	no
C99 . C98 . H981 . 108.790	no
N20 . C98 . H982 . 108.793	no
C99 . C98 . H982 . 108.789	no
H981 . C98 . H982 . 109.467	no
C98 . C99 . C100 . 106.2(8)	yes
C98 . C99 . H991 . 110.275	no
C100 . C99 . H991 . 110.275	no
C98 . C99 . H992 . 110.276	no
C100 . C99 . H992 . 110.276	no
H991 . C99 . H992 . 109.464	no
C99 . C100 . C101 . 106.4(9)	yes
C99 . C100 . H1001 . 110.244	no
C101 . C100 . H1001 . 110.242	no
C99 . C100 . H1002 . 110.244	no
C101 . C100 . H1002 . 110.243	no
H1001 . C100 . H1002 . 109.467	no
C100 . C101 . H1011 . 109.470	no
C100 . C101 . H1012 . 109.466	no
H1011 . C101 . H1012 . 109.477	no
C100 . C101 . H1013 . 109.465	no
H1011 . C101 . H1013 . 109.476	no
H1012 . C101 . H1013 . 109.472	no
N20 . C86 . C871 . 112.1(2)	yes
N20 . C86 . H861 . 108.822	no
C871 . C86 . H861 . 108.819	no
N20 . C86 . H862 . 108.818	no
C871 . C86 . H862 . 108.814	no
H861 . C86 . H862 . 109.468	no
C880 . C870 . H8701 . 110.254	no
C880 . C870 . H8702 . 110.274	no
H862 . C870 . H8702 . 142.854	no
H8701 . C870 . H8702 . 109.466	no
C870 . C880 . C890 . 106.3(2)	yes
C870 . C880 . H8801 . 110.271	no
C890 . C880 . H8801 . 110.265	no
C870 . C880 . H8802 . 110.257	no
C890 . C880 . H8802 . 110.266	no
H8801 . C880 . H8802 . 109.462	no
C880 . C890 . H8901 . 109.464	no
C880 . C890 . H8902 . 109.465	no
H8901 . C890 . H8902 . 109.479	no
C880 . C890 . H8903 . 109.463	no
H8901 . C890 . H8903 . 109.475	no
H8902 . C890 . H8903 . 109.481	no
C86 . C871 . C881 . 106.3(2)	yes
C86 . C871 . H8711 . 110.265	no
C881 . C871 . H8711 . 110.264	no
C86 . C871 . H8712 . 110.270	no

C881 . C871 . H8712 . 110.266	no
H8711 . C871 . H8712 . 109.465	no
C871 . C881 . C891 . 106.2(2)	yes
C871 . C881 . H8811 . 110.272	no
C891 . C881 . H8811 . 110.265	no
C871 . C881 . H8812 . 110.276	no
C891 . C881 . H8812 . 110.285	no
H8811 . C881 . H8812 . 109.467	no
C881 . C891 . H8911 . 109.469	no
C881 . C891 . H8912 . 109.480	no
H8911 . C891 . H8912 . 109.496	no
C881 . C891 . H8913 . 109.451	no
H8911 . C891 . H8913 . 109.459	no
H8912 . C891 . H8913 . 109.472	no
H391 . C580 . H392 . 109.467	no
C57 . C581 . C59 . 104.2(13)	yes
C59 . C581 . H392 . 100.951	no
C57 . C581 . H493 . 110.772	no
C59 . C581 . H493 . 110.771	no
C57 . C581 . H494 . 110.772	no
C59 . C581 . H494 . 110.771	no
H493 . C581 . H494 . 109.467	no
C9 . C110 . C11 . 106.0(13)	yes
C9 . C110 . H593 . 110.340	no
C11 . C110 . H593 . 110.341	no
C9 . C110 . H594 . 110.340	no
C11 . C110 . H594 . 110.341	no
H593 . C110 . H594 . 109.467	no
C11 . C110 . H691 . 101.086	no
H691 . C111 . H692 . 109.467	no
C20 . C21 . C22 . 103.6(14)	yes
C20 . C21 . H1903 . 110.928	no
C22 . C21 . H1903 . 110.927	no
C20 . C21 . H1904 . 110.928	no
C22 . C21 . H1904 . 110.927	no
H1903 . C21 . H1904 . 109.467	no
H291 . C210 . H292 . 109.467	no