Steric and electronic influence of Re(I) tricarbonyl complexes with various coordinated β-diketones

Supplementary Material

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Figure S1: Illustration (red dotted lines) of the short contacts observed in the structure of **6**. Hydrogen atoms and most of the atom labels are omitted for clarity. Ellipsoids are drawn at 50 % probability.

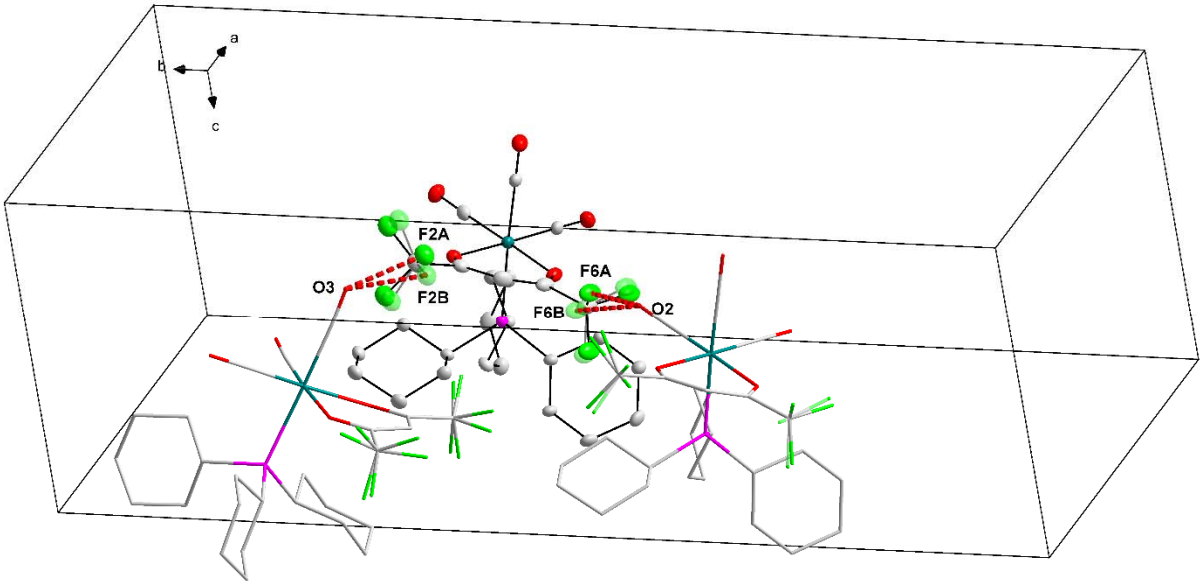

Table S1: Atomic charges (a.u.) from the Natural Population Analysis (NPA) for **6** and **8**.

Atom	Charge (a.u.)	
	6	**8**
Re	-0.81486	-0.80569
O_{OO}	-0.52647	-0.58365
O_{OO}	-0.53807	-0.58776
P	1.21196	1.21883
C_{COeq}	0.69788	-0.50184
C_{COeq}	0.70119	-0.49967
C_{COap}	0.72001	-0.45745

Table S2: The occupancies and hybridization of the calculated Natural Bond Orbitals (NBOs) between rhenium and its coordinated ligands for **6** and **8**.

Complex	BD	Occupancy	Composition of NBO	Energy (x 10^3 kJ.mol^{-1})
6	Re-O_{OO}	1.94418	(14.35%)Re($sp^{2.73}d^{3.97}$) + (85.65%)O($sp^{1.69}$)	-1.66725
	Re-O_{OO}	1.93958	(13.59%)Re($sp^{3.11}d^{3.70}$) + (86.41%)O($sp^{1.72}$)	-1.64590
	Re-P	1.88089	(30.59%)Re($sp^{2.13}d^{2.29}$) + (69.41%)P($sp^{2.08}$)	-0.93820
	Re-C_{COeq}	1.89871	(34.13%)Re($sp^{2.18}d^{2.37}$) + (65.87%)C($sp^{0.54}$)	-1.35006
	Re-C_{COeq}	1.90463	(34.95%)Re($sp^{1.99}d^{2.55}$) + (65.05%)C($sp^{0.54}$)	-1.35158
	Re-C_{COap}	1.93128	(33.76%)Re($sp^{1.61}d^{2.48}$) + (66.24%)C($sp^{0.54}$)	-1.36781
8	Re-O_{OO}	1.71128	(45.31%)Re($sp^{2.71}d^{3.99}$) + (54.69%)O($sp^{1.70}$)	-0.81984
	Re-O_{OO}	1.71001	(54.69%)Re($sp^{3.10}d^{3.74}$) + (45.31%)O($sp^{1.71}$)	-0.79965
	Re-P	1.88292	(31.59%)Re($sp^{2.68}d^{2.97}$) + (68.41%)P($sp^{2.18}$)	-0.97028
	Re-C_{COeq}	1.96187	(36.58%)Re($sp^{0.69}d^{2.53}$) + (63.42%)C($sp^{0.55}$)	-1.44318
	Re-C_{COeq}	1.96251	(37.17%)Re($sp^{0.66}d^{2.70}$) + (62.83%)C($sp^{0.55}$)	-1.44634
	Re-C_{COap}	1.94039	(33.95%)Re($sp^{2.11}d^{3.50}$) + (66.05%)C($sp^{0.55}$)	-1.44628

Table S3: Stabilization energies associated with delocalization from the lone pair orbitals of oxygen for **6** and **8**.

Complex	Donor orbital	Occupancy of donor orbital	Acceptor orbital	ΔE_{ij} (x 10^3 kJ.mol^{-1})
6	LP(1) O3	1.93	RY*(1) C44	12.16
			BD*(1) C32-C44	32.56
	LP(1) O4	1.93	RY*(1) C17	12.76
			BD*(1) C32-C44	32.90
8	LP(1) O3	1.92	RY*(1) C44	12.08
			BD*(1) C32-C44	33.42
	LP(1) O4	1.93	RY*(1) C17	12.23
			BD*(1) C32-C44	33.29

CheckCif of 4

checkCIF (full publication check) running

checkCIF/PLATON (full publication check)

Structure factors have been supplied for datablock(s) I

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No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: I

Bond precision: C-C = 0.0052 A Wavelength=0.71073

Cell: a=9.922(2) b=18.055(4) c=19.009(5)
alpha=62.485(8) beta=87.039(9) gamma=84.961(9)

Temperature: 106 K

	Calculated	Reported
Volume	3008.2(12)	3008.3(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C31 H42 O5 P Re	C31 H42 O5 P Re
Sum formula	C31 H42 O5 P Re	C31 H42 O5 P Re
Mr	711.83	711.83
Dx,g cm-3	1.572	1.574
Z	4	4
Mu (mm-1)	4.129	4.129
F000	1432.0	1432.0
F000'	1428.95	
h,k,lmax	13,23,25	13,23,25
Nref	14508	14506
Tmin,Tmax	0.631,0.758	0.631,0.758
Tmin'	0.454	

Correction method= # Reported T Limits: Tmin=0.631 Tmax=0.758 AbsCorr = NONE

Data completeness= 1.000 Theta(max)= 27.999

R(reflections)= 0.0248(12261) wR2(reflections)= 0.0612(14506)

S = 1.060 Npar= 695

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.20 Do !
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT411_ALERT_2_C Short Inter H...H Contact H13A ..H13A . 2.14 Ang.
2-x,-y,2-z = 2_757 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.326 Report

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.08 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 2 Note
PLAT230_ALERT_2_G Hirshfeld Test Diff for O1A --C1A . 5.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Re1A --C1A . 6.9 s.u.
And 3 other PLAT232 Alerts
More ...
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ..... Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 18 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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checkCIF publication errors

Alert level A

PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).

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1 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

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Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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Validation response form

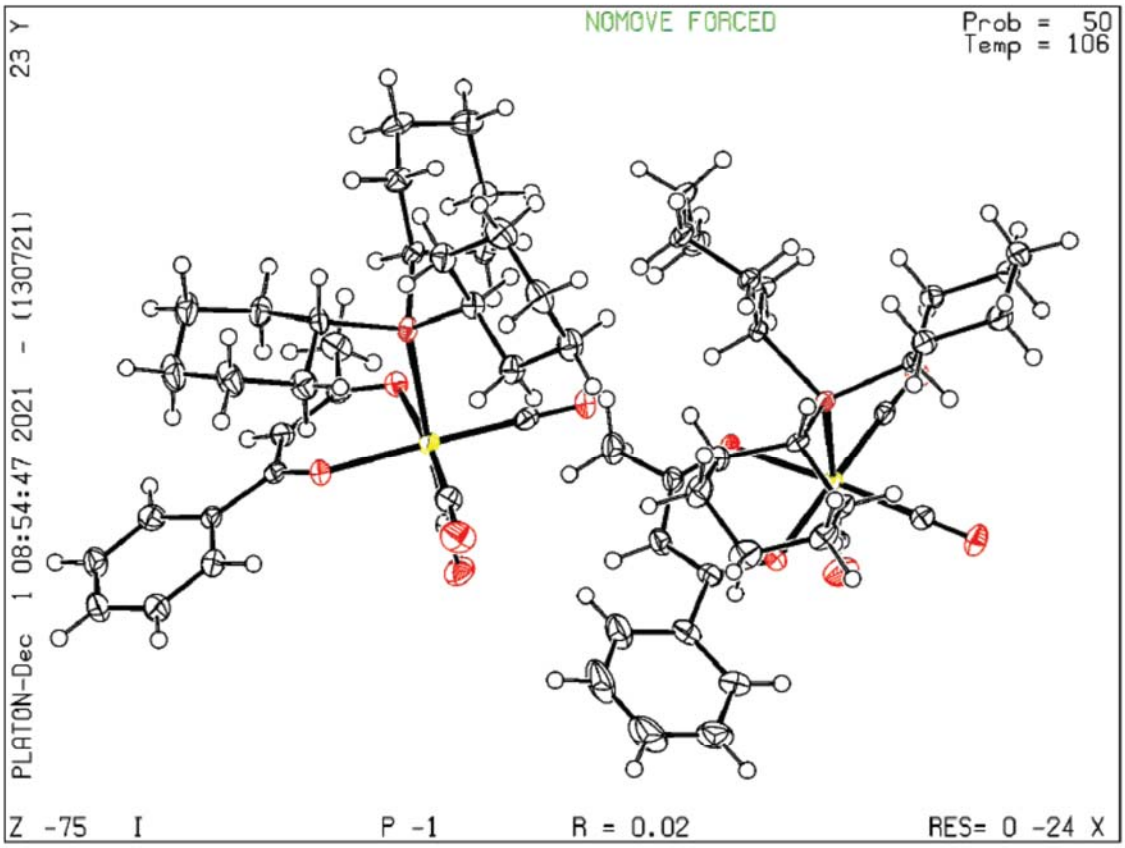
Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock I - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

CheckCif of 5

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Structure factors have been supplied for datablock(s) I

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No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: I

Bond precision: C-C = 0.0073 A Wavelength=0.71073

Cell: a=9.1356(11) b=33.762(4) c=9.2315(12)
alpha=90 beta=106.007(4) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2736.9(6)	2737.0(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H37 F3 O5 P Re	C26 H37 F3 O5 P Re
Sum formula	C26 H37 F3 O5 P Re	C26 H37 F3 O5 P Re
Mr	703.74	703.72
Dx,g cm-3	1.708	1.708
Z	4	4
Mu (mm-1)	4.552	4.552
F000	1400.0	1400.0
F000'	1397.10	
h,k,lmax	12,44,12	12,44,12
Nref	6605	6605
Tmin,Tmax	0.238,0.579	0.238,0.579
Tmin'	0.136	

Correction method= # Reported T Limits: Tmin=0.238 Tmax=0.579 AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.999

R(reflections)= 0.0388(6549) wR2(reflections)= 0.0835(6571)

S = 1.246 Npar= 331

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.78Ang From Re1 4.96 eA-3

Author Response: see _publ_section_exptl_refinement

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as multi-scan
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.28 Report
PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio ..... 3.6 oblate
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.9 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.549 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 27 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.79Ang From C8 1.60 eA-3

Author Response: see _publ_section_exptl_refinement

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.65Ang From P1 1.56 eA-3

Author Response: see _publ_section_exptl_refinement

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.04Ang From C8 1.56 eA-3

Author Response: see _publ_section_exptl_refinement

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.24Ang From C3 -2.18 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.64Ang From Re1 -1.57 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H32A . -0.33 eA-3

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 22.52 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 1 Note
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ..... Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 24 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

1 **ALERT level A** = Most likely a serious problem - resolve or explain
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2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).

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Publication of your CIF

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Validation response form

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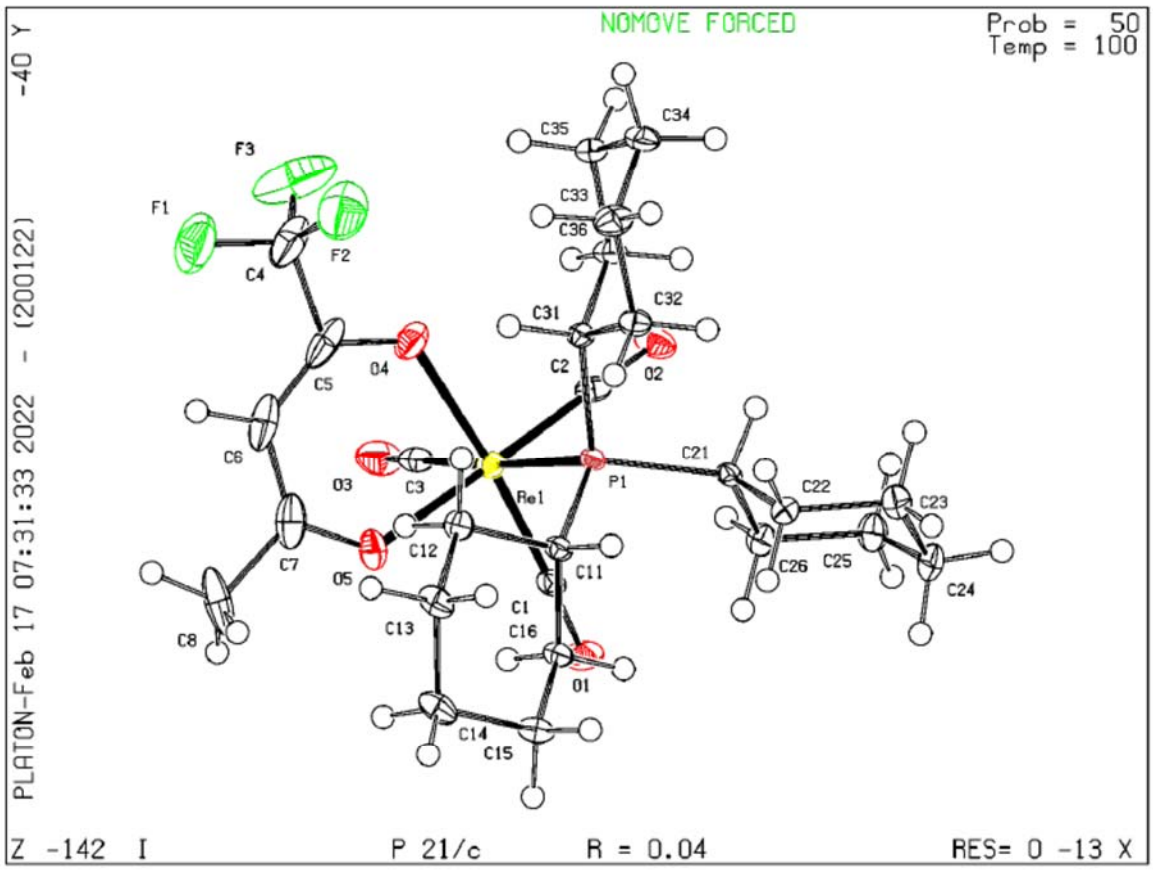
```
# start Validation Reply Form
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 20/01/2022; check.def file version of 19/01/2022

Datablock I - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC

CheckCif of 6

checkCIF (full publication check) running

checkCIF/PLATON (full publication check)

Structure factors have been supplied for datablock(s) I

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No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: I

Bond precision: C-C = 0.0084 A Wavelength=0.71073

Cell: a=9.2609(7) b=33.608(2) c=9.3712(7)
alpha=90 beta=106.717(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2793.4(3)	2793.4(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H34 F6 O5 P Re	C26 H34 F6 O5 P Re
Sum formula	C26 H34 F6 O5 P Re	C26 H34 F6 O5 P Re
Mr	757.71	757.70
Dx,g cm-3	1.802	1.802
Z	4	4
Mu (mm-1)	4.482	4.482
F000	1496.0	1496.0
F000'	1493.28	
h,k,lmax	12,44,12	12,44,12
Nref	6751	6747
Tmin,Tmax	0.626,0.878	0.626,0.878
Tmin'	0.364	

Correction method= # Reported T Limits: Tmin=0.626 Tmax=0.878 AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.999

R(reflections)= 0.0453(6293) wR2(reflections)= 0.0925(6747)

S = 1.352 Npar= 346

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.16Ang From C3 -3.28 eA-3

Author Response: see _publ_section_exptl_refinement

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as multi-scan
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00836 Ang.
PLAT350_ALERT_3_C Short C-H (X0.96,N1.08A) C6 - H6 . 0.76 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.868 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From Re1 2.08 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.56Ang From P1 1.66 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.76Ang From F4B -1.51 eA-3

Author Response: see _publ_section_exptl_refinement

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 20.97 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 1 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 15% Note
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ..... Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 1 Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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1 ALERT type 5 Informative message, check

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Alert level A

PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).

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Validation response form

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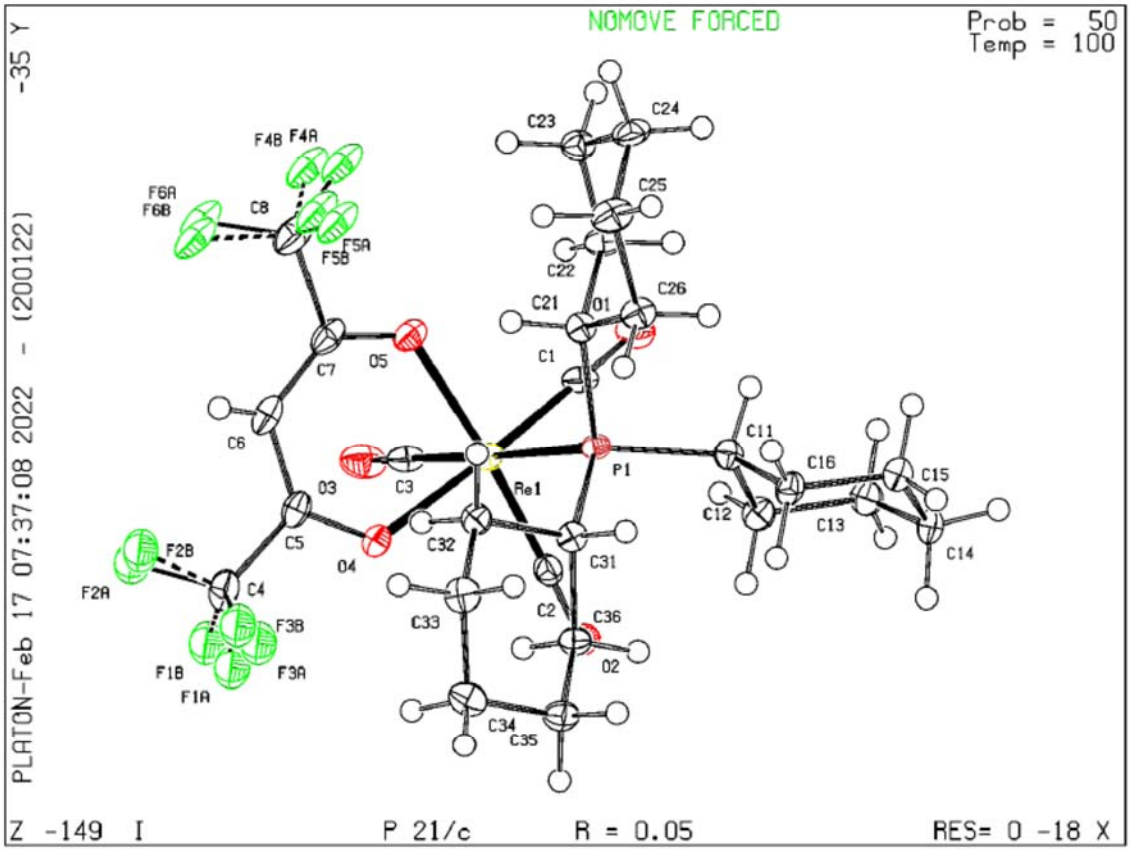
start Validation Reply Form
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 20/01/2022; check.def file version of 19/01/2022

Datablock I - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

Cif file of 4

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data_mo_v2_21dms1_0m

_audit_creation_date                2021-12-01T10:41:05-00:00
_audit_creation_method               'WinGX routine CIF_UPDATE'

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# CHEMICAL DATA

_chemical_formula_sum                'C31 H42 O5 P Re'
_chemical_formula_moiety             'C31 H42 O5 P Re'
_chemical_formula_weight              711.83

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

# CRYSTAL DATA

_symmetry_cell_setting               triclinic
_symmetry_space_group_name_H-M       'P -1'
_symmetry_space_group_name_Hall      '-P 1'

loop_
 _space_group_symop_operation_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                       9.922(2)
_cell_length_b                       18.055(4)
_cell_length_c                       19.009(5)
_cell_angle_alpha                    62.485(8)
_cell_angle_beta                     87.039(9)
_cell_angle_gamma                    84.961(9)
_cell_volume                         3008.3(13)
_cell_formula_units_Z                4
_cell_measurement_temperature        106(2)
_cell_measurement_reflns_used        9647
_cell_measurement_theta_min          2.27
_cell_measurement_theta_max          28.36

_exptl_crystal_description           'plate'
_exptl_crystal_colour          'yellow'
_exptl_crystal_size_max              0.189
_exptl_crystal_size_mid              0.095
_exptl_crystal_size_min              0.067
_exptl_crystal_density_diffrn        1.574
_exptl_crystal_F_000                 1432
_exptl_absorpt_coefficient_mu        4.129
_exptl_absorpt_correction_type       none
_exptl_absorpt_correction_T_min      0.631
_exptl_absorpt_correction_T_max      0.758

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# EXPERIMENTAL DATA

_diffrn_ambient_temperature          106(2)
_diffrn_radiation_type               MoK\a
_diffrn_radiation_wavelength         0.71073
_diffrn_reflns_number                122487
_diffrn_reflns_av_R_equivalents      0.0772
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_diffrn_reflns_theta_min         2.061
_diffrn_reflns_theta_max         27.999
_diffrn_reflns_theta_full        25.242
_diffrn_measurement_device_type   'Bruker APEX-II CCD'
_diffrn_measurement_method       '\f and \w scans'
_diffrn_measured_fraction_theta_max
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_diffrn_measured_fraction_theta_full
                                 1
_diffrn_reflns_Laue_measured_fraction_full
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_diffrn_reflns_Laue_measured_fraction_max
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_diffrn_reflns_point_group_measured_fraction_full
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_diffrn_reflns_point_group_measured_fraction_max
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# STRUCTURE SOLUTION

_atom_sites_solution_hydrogens     mixed

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

# REFINEMENT DATA

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_reflns_number_gt                12261
_reflns_threshold_expression      'I > 2\s(I)'
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_refine_ls_matrix_type           full
_refine_ls_R_factor_all          0.0352
_refine_ls_R_factor_gt           0.0248
_refine_ls_wR_factor_ref         0.0612
_refine_ls_goodness_of_fit_ref     1.06
_refine_ls_restrained_S_all      1.06
_refine_ls_number_reflns         14506
_refine_ls_number_parameters       695
_refine_ls_number_restraints     0
_refine_ls_hydrogen_treatment      mixed
_refine_ls_weighting_scheme        calc
_refine_ls_weighting_details
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_refine_ls_shift/su_max          0.002
_refine_ls_shift/su_mean         0
_refine_diff_density_max         1.678
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_refine_diff_density_rms         0.114
_refine_ls_extinction_method       none
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   _atom_type_scat_source
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H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.006 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Re Re -1.0185 7.231 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_computing_structure_refinement         'SHELXL-2018/3 (Sheldrick, 2018)'

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

# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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   _atom_site_fract_y
   _atom_site_fract_z
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   _atom_site_adp_type
   _atom_site_calc_flag
   _atom_site_occupancy
   _atom_site_disorder_assembly
   _atom_site_disorder_group
   _atom_site_type_symbol
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Re1B 0.20897(2) 0.64417(2) 0.70239(2) 0.01663(3) Uani d 1 . . Re
P1A 0.51815(8) 0.20805(5) 0.81917(4) 0.01402(14) Uani d 1 . . P
P1B 0.43363(8) 0.70124(5) 0.70051(5) 0.01723(15) Uani d 1 . . P
O5A 0.2933(2) 0.30981(13) 0.68112(13) 0.0187(4) Uani d 1 . . O
O4A 0.1860(2) 0.21556(13) 0.83742(13) 0.0178(4) Uani d 1 . . O
O4B 0.0963(2) 0.75729(13) 0.68464(13) 0.0201(5) Uani d 1 . . O
O5B 0.2289(2) 0.70601(14) 0.57660(13) 0.0208(5) Uani d 1 . . O
O1A 0.4913(2) 0.12522(14) 0.65671(14) 0.0235(5) Uani d 1 . . O
O2A 0.3312(3) -0.00507(14) 0.88635(14) 0.0289(5) Uani d 1 . . O
O1B 0.3628(2) 0.47971(14) 0.72887(15) 0.0289(5) Uani d 1 . . O
O3A 0.0755(2) 0.14969(17) 0.68475(15) 0.0336(6) Uani d 1 . . O
O3B -0.0550(3) 0.57377(16) 0.68800(17) 0.0346(6) Uani d 1 . . O
O2B 0.1521(3) 0.57227(18) 0.88058(15) 0.0384(6) Uani d 1 . . O
C2A 0.3262(3) 0.0648(2) 0.84037(18) 0.0196(6) Uani d 1 . . C
C31A 0.4883(3) 0.22070(18) 0.90999(17) 0.0164(6) Uani d 1 . . C
H31A 0.5794 0.218474 0.931356 0.02 Uiso calc 1 . . H
C1A 0.4274(3) 0.14740(19) 0.69698(19) 0.0187(6) Uani d 1 . . C
C1B 0.3053(3) 0.5420(2) 0.71861(19) 0.0208(6) Uani d 1 . . C
C21A 0.5896(3) 0.30802(18) 0.74990(17) 0.0157(6) Uani d 1 . . C
H21A 0.516804 0.35216 0.744644 0.019 Uiso calc 1 . . H
C11A 0.6515(3) 0.11988(19) 0.85002(18) 0.0178(6) Uani d 1 . . C
H11A 0.602425 0.067641 0.870464 0.021 Uiso calc 1 . . H
C3A 0.1601(3) 0.1617(2) 0.71559(19) 0.0207(6) Uani d 1 . . C
C16A 0.7403(3) 0.1222(2) 0.78064(19) 0.0200(6) Uani d 1 . . C
H16A 0.681879 0.127048 0.73783 0.024 Uiso calc 1 . . H
H16B 0.793704 0.172097 0.759141 0.024 Uiso calc 1 . . H
C26A 0.7122(3) 0.33042(19) 0.78018(19) 0.0192(6) Uani d 1 . . C
H26A 0.79247 0.293344 0.781079 0.023 Uiso calc 1 . . H
H26B 0.694086 0.322297 0.834902 0.023 Uiso calc 1 . . H
C21B 0.5241(3) 0.72336(19) 0.60589(18) 0.0178(6) Uani d 1 . . C
H21B 0.463885 0.765482 0.562861 0.021 Uiso calc 1 . . H
C23A 0.6453(4) 0.4116(2) 0.6102(2) 0.0272(7) Uani d 1 . . C
H23A 0.666529 0.418371 0.556206 0.033 Uiso calc 1 . . H
H23B 0.563748 0.448667 0.60714 0.033 Uiso calc 1 . . H
C32A 0.4154(3) 0.14703(19) 0.97409(18) 0.0201(6) Uani d 1 . . C
H32A 0.323963 0.14681 0.955701 0.024 Uiso calc 1 . . H
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H32B 0.46645 0.093645 0.983679 0.024 Uiso calc 1 . . H
C22A 0.6160(3) 0.3206(2) 0.66512(18) 0.0206(6) Uani d 1 . . C
H22A 0.694182 0.282823 0.664448 0.025 Uiso calc 1 . . H
H22B 0.535903 0.306355 0.646065 0.025 Uiso calc 1 . . H
C31B 0.4223(3) 0.80185(19) 0.7049(2) 0.0211(6) Uani d 1 . . C
H31B 0.516034 0.813797 0.711595 0.025 Uiso calc 1 . . H
C7A 0.2028(3) 0.36381(19) 0.68124(19) 0.0210(6) Uani d 1 . . C
C3B 0.0414(3) 0.6012(2) 0.6930(2) 0.0227(7) Uani d 1 . . C
C11B 0.5590(3) 0.6301(2) 0.77731(18) 0.0207(6) Uani d 1 . . C
H11B 0.613784 0.598787 0.75259 0.025 Uiso calc 1 . . H
C12A 0.7423(3) 0.1085(2) 0.91754(19) 0.0223(7) Uani d 1 . . C
H12A 0.795577 0.158076 0.899777 0.027 Uiso calc 1 . . H
H12B 0.685175 0.104411 0.963309 0.027 Uiso calc 1 . . H
C25B 0.7155(4) 0.7858(2) 0.5103(2) 0.0288(8) Uani d 1 . . C
H25C 0.803973 0.809907 0.503783 0.035 Uiso calc 1 . . H
H25D 0.652729 0.829066 0.470985 0.035 Uiso calc 1 . . H
C6B 0.0647(3) 0.8205(2) 0.54645(19) 0.0208(6) Uani d 1 . . C
C4B -0.0681(3) 0.86834(19) 0.6363(2) 0.0206(6) Uani d 1 . . C
C23B 0.6000(3) 0.6686(2) 0.50872(19) 0.0234(7) Uani d 1 . . C
H23C 0.615212 0.617337 0.501967 0.028 Uiso calc 1 . . H
H23D 0.533834 0.707321 0.468537 0.028 Uiso calc 1 . . H
C2B 0.1788(3) 0.5982(2) 0.8139(2) 0.0258(7) Uani d 1 . . C
C26B 0.6602(3) 0.7622(2) 0.5935(2) 0.0242(7) Uani d 1 . . C
H26C 0.648285 0.81277 0.601641 0.029 Uiso calc 1 . . H
H26D 0.725694 0.721698 0.632996 0.029 Uiso calc 1 . . H
C15A 0.8362(3) 0.0434(2) 0.8069(2) 0.0250(7) Uani d 1 . . C
H15A 0.782712 -0.006015 0.824276 0.03 Uiso calc 1 . . H
H15B 0.893935 0.047498 0.761353 0.03 Uiso calc 1 . . H
C8B 0.1893(4) 0.7929(2) 0.4421(2) 0.0291(8) Uani d 1 . . C
H8B1 0.286432 0.799056 0.431169 0.044 Uiso calc 1 . . H
H8B2 0.138608 0.845679 0.408012 0.044 Uiso calc 1 . . H
H8B3 0.161997 0.748302 0.431264 0.044 Uiso calc 1 . . H
C36A 0.4154(3) 0.30483(19) 0.89583(19) 0.0203(6) Uani d 1 . . C
H36A 0.468798 0.351001 0.857714 0.024 Uiso calc 1 . . H
H36B 0.325933 0.310852 0.872271 0.024 Uiso calc 1 . . H
C32B 0.3661(3) 0.8747(2) 0.6275(2) 0.0251(7) Uani d 1 . . C
H32C 0.428787 0.881512 0.583012 0.03 Uiso calc 1 . . H
H32D 0.277631 0.861356 0.616194 0.03 Uiso calc 1 . . H
C12B 0.4971(4) 0.5630(2) 0.85299(19) 0.0247(7) Uani d 1 . . C
H12C 0.442815 0.590203 0.880993 0.03 Uiso calc 1 . . H
H12D 0.435794 0.531673 0.838799 0.03 Uiso calc 1 . . H
C22B 0.5415(3) 0.64576(19) 0.59159(19) 0.0201(6) Uani d 1 . . C
H22C 0.60274 0.602349 0.631882 0.024 Uiso calc 1 . . H
H22D 0.452666 0.622371 0.597235 0.024 Uiso calc 1 . . H
C5A 0.1193(3) 0.2854(2) 0.81897(19) 0.0202(6) Uani d 1 . . C
C13A 0.8384(3) 0.0298(2) 0.9434(2) 0.0270(7) Uani d 1 . . C
H13A 0.897779 0.025341 0.985702 0.032 Uiso calc 1 . . H
H13B 0.785151 -0.020134 0.965558 0.032 Uiso calc 1 . . H
C41A -0.0015(3) 0.2174(2) 0.9492(2) 0.0287(8) Uani d 1 . . C
H41A 0.013942 0.165565 0.947477 0.034 Uiso calc 1 . . H
C16B 0.6610(3) 0.6758(2) 0.7984(2) 0.0260(7) Uani d 1 . . C
H16C 0.704083 0.716686 0.749122 0.031 Uiso calc 1 . . H
H16D 0.612734 0.706994 0.824459 0.031 Uiso calc 1 . . H
C7B 0.1602(3) 0.7708(2) 0.52756(19) 0.0199(6) Uani d 1 . . C
C45B -0.1324(3) 0.9390(2) 0.5750(2) 0.0269(7) Uani d 1 . . C
H45B -0.107713 0.954122 0.521395 0.032 Uiso calc 1 . . H
C4A 0.0430(3) 0.2899(2) 0.8869(2) 0.0258(7) Uani d 1 . . C
C6A 0.1163(3) 0.3551(2) 0.7443(2) 0.0240(7) Uani d 1 . . C
C5B 0.0369(3) 0.81156(19) 0.62231(19) 0.0196(6) Uani d 1 . . C
C42B -0.2054(4) 0.8964(2) 0.7305(2) 0.0316(8) Uani d 1 . . C
H42B -0.231008 0.881426 0.784023 0.038 Uiso calc 1 . . H
C33A 0.4037(4) 0.1544(2) 1.05118(19) 0.0266(7) Uani d 1 . . C

H33A 0.355066 0.107217 1.091751 0.032 Uiso calc 1 . . H
H33B 0.495285 0.151129 1.071208 0.032 Uiso calc 1 . . H
C8A 0.1936(4) 0.4448(2) 0.6052(2) 0.0305(8) Uani d 1 . . C
H8A1 0.282837 0.467424 0.591288 0.046 Uiso calc 1 . . H
H8A2 0.12897 0.485172 0.61223 0.046 Uiso calc 1 . . H
H8A3 0.163028 0.434402 0.562505 0.046 Uiso calc 1 . . H
C33B 0.3487(4) 0.9568(2) 0.6334(2) 0.0321(8) Uani d 1 . . C
H33C 0.439015 0.974887 0.635737 0.038 Uiso calc 1 . . H
H33D 0.303416 1.000706 0.585156 0.038 Uiso calc 1 . . H
C36B 0.3382(4) 0.7950(2) 0.7772(2) 0.0284(7) Uani d 1 . . C
H36C 0.380718 0.750355 0.826131 0.034 Uiso calc 1 . . H
H36D 0.246357 0.779313 0.774026 0.034 Uiso calc 1 . . H
C35B 0.3274(4) 0.8781(2) 0.7814(2) 0.0355(9) Uani d 1 . . C
H35C 0.270359 0.87265 0.827627 0.043 Uiso calc 1 . . H
H35D 0.41853 0.891681 0.788689 0.043 Uiso calc 1 . . H
C14B 0.7078(4) 0.5479(2) 0.9283(2) 0.0298(8) Uani d 1 . . C
H14D 0.661428 0.574466 0.959196 0.036 Uiso calc 1 . . H
H14C 0.780088 0.50714 0.961671 0.036 Uiso calc 1 . . H
C43B -0.2677(4) 0.9661(2) 0.6700(2) 0.0324(8) Uani d 1 . . C
H43B -0.335133 0.999686 0.681641 0.039 Uiso calc 1 . . H
C24B 0.7329(4) 0.7099(2) 0.4950(2) 0.0288(8) Uani d 1 . . C
H24C 0.802549 0.669025 0.530762 0.035 Uiso calc 1 . . H
H24D 0.764333 0.727505 0.439612 0.035 Uiso calc 1 . . H
C24A 0.7638(4) 0.4373(2) 0.6401(2) 0.0284(8) Uani d 1 . . C
H24A 0.847728 0.404865 0.637066 0.034 Uiso calc 1 . . H
H24B 0.776202 0.497419 0.605671 0.034 Uiso calc 1 . . H
C13B 0.6068(4) 0.5022(2) 0.9080(2) 0.0294(8) Uani d 1 . . C
H13C 0.56423 0.461213 0.957404 0.035 Uiso calc 1 . . H
H13D 0.655066 0.470884 0.881903 0.035 Uiso calc 1 . . H
C35A 0.3964(4) 0.3113(2) 0.9732(2) 0.0302(8) Uani d 1 . . C
H35A 0.485833 0.314528 0.991967 0.036 Uiso calc 1 . . H
H35B 0.340862 0.363437 0.962947 0.036 Uiso calc 1 . . H
C25A 0.7398(3) 0.4221(2) 0.7254(2) 0.0244(7) Uani d 1 . . C
H25A 0.661564 0.459058 0.727483 0.029 Uiso calc 1 . . H
H25B 0.820281 0.436294 0.744107 0.029 Uiso calc 1 . . H
C14A 0.9251(3) 0.0317(2) 0.8742(2) 0.0291(8) Uani d 1 . . C
H14A 0.985458 0.078256 0.855452 0.035 Uiso calc 1 . . H
H14B 0.982378 -0.021334 0.891945 0.035 Uiso calc 1 . . H
C44B -0.2321(4) 0.9872(2) 0.5923(2) 0.0316(8) Uani d 1 . . C
H44B -0.276136 1.034877 0.550443 0.038 Uiso calc 1 . . H
C34A 0.3281(4) 0.2368(2) 1.0377(2) 0.0314(8) Uani d 1 . . C
H34A 0.324758 0.241273 1.087778 0.038 Uiso calc 1 . . H
H34B 0.233926 0.237843 1.022228 0.038 Uiso calc 1 . . H
C41B -0.1060(4) 0.8479(2) 0.7141(2) 0.0273(7) Uani d 1 . . C
H41B -0.063138 0.800122 0.756448 0.033 Uiso calc 1 . . H
C15B 0.7703(4) 0.6144(2) 0.8536(2) 0.0315(8) Uani d 1 . . C
H15C 0.824643 0.587196 0.825639 0.038 Uiso calc 1 . . H
H15D 0.831623 0.645354 0.868234 0.038 Uiso calc 1 . . H
C34B 0.2660(4) 0.9484(2) 0.7060(3) 0.0380(9) Uani d 1 . . C
H34C 0.262408 1.001717 0.709172 0.046 Uiso calc 1 . . H
H34D 0.172285 0.936765 0.700957 0.046 Uiso calc 1 . . H
C42A -0.0683(4) 0.2201(3) 1.0139(2) 0.0420(10) Uani d 1 . . C
H42A -0.101398 0.170565 1.055369 0.05 Uiso calc 1 . . H
C45A 0.0243(4) 0.3651(3) 0.8919(2) 0.0387(9) Uani d 1 . . C
H45A 0.054669 0.415229 0.849924 0.046 Uiso calc 1 . . H
C43A -0.0870(5) 0.2943(3) 1.0185(3) 0.0546(13) Uani d 1 . . C
H43A -0.132907 0.296118 1.062849 0.065 Uiso calc 1 . . H
C44A -0.0383(5) 0.3663(3) 0.9578(3) 0.0535(13) Uani d 1 . . C
H44A -0.048188 0.417111 0.961726 0.064 Uiso calc 1 . . H
H6A 0.057(4) 0.403(2) 0.738(2) 0.021(9) Uiso d 1 . . H
H6B 0.015(4) 0.860(2) 0.506(2) 0.028(10) Uiso d 1 . . H

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   _atom_site_aniso_U_22
   _atom_site_aniso_U_33
   _atom_site_aniso_U_12
   _atom_site_aniso_U_13
   _atom_site_aniso_U_23
Re1A 0.01375(6) 0.01243(6) 0.01476(6) -0.00145(4) -0.00088(4) -0.00549(5)
Re1B 0.01738(6) 0.01386(6) 0.01788(6) -0.00077(4) -0.00082(5) -0.00666(5)
P1A 0.0145(3) 0.0127(3) 0.0138(4) -0.0021(3) 0.0002(3) -0.0050(3)
P1B 0.0202(4) 0.0139(4) 0.0183(4) -0.0009(3) -0.0029(3) -0.0078(3)
O5A 0.0197(11) 0.0131(10) 0.0182(11) 0.0012(8) -0.0020(8) -0.0032(9)
O4A 0.0167(10) 0.0173(10) 0.0199(11) 0.0000(8) 0.0017(8) -0.0093(9)
O4B 0.0211(11) 0.0163(11) 0.0217(11) 0.0019(9) -0.0017(9) -0.0081(9)
O5B 0.0214(11) 0.0195(11) 0.0211(11) 0.0004(9) -0.0021(9) -0.0091(9)
O1A 0.0240(12) 0.0264(12) 0.0235(12) 0.0024(10) 0.0008(9) -0.0152(10)
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MOLECULAR GEOMETRY

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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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C12B C11B P1B 114.8(2) . . ?
C16B C11B P1B 114.2(2) . . ?
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C16B C11B H11B 105.5 . . ?
P1B C11B H11B 105.5 . . ?
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C11A C12A H12A 109.4 . . ?
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C11A C12A H12B 109.4 . . ?
H12A C12A H12B 108 . . ?
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C26B C25B H25D 109.4 . . ?
C24B C25B H25D 109.4 . . ?
H25C C25B H25D 108 . . ?
C5B C6B C7B 125.3(3) . . ?
C5B C6B H6B 119(2) . . ?
C7B C6B H6B 116(2) . . ?
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C41B C4B C5B 118.0(3) . . ?
C45B C4B C5B 123.3(3) . . ?
C24B C23B C22B 111.8(3) . . ?
C24B C23B H23C 109.3 . . ?
C22B C23B H23C 109.3 . . ?
C24B C23B H23D 109.3 . . ?
C22B C23B H23D 109.3 . . ?
H23C C23B H23D 107.9 . . ?
O2B C2B Re1B 175.7(3) . . ?
C25B C26B C21B 110.6(3) . . ?
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C21B C26B H26C 109.5 . . ?
C25B C26B H26D 109.5 . . ?
C21B C26B H26D 109.5 . . ?
H26C C26B H26D 108.1 . . ?
C14A C15A C16A 111.4(3) . . ?

C14A C15A H15A 109.3 . . ?
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H8B1 C8B H8B3 109.5 . . ?
H8B2 C8B H8B3 109.5 . . ?
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C31A C36A H36B 109.4 . . ?
H36A C36A H36B 108 . . ?
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C31B C32B H32C 109.4 . . ?
C33B C32B H32D 109.4 . . ?
C31B C32B H32D 109.4 . . ?
H32C C32B H32D 108 . . ?
C13B C12B C11B 111.1(3) . . ?
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C11B C12B H12C 109.4 . . ?
C13B C12B H12D 109.4 . . ?
C11B C12B H12D 109.4 . . ?
H12C C12B H12D 108 . . ?
C23B C22B C21B 110.7(3) . . ?
C23B C22B H22C 109.5 . . ?
C21B C22B H22C 109.5 . . ?
C23B C22B H22D 109.5 . . ?
C21B C22B H22D 109.5 . . ?
H22C C22B H22D 108.1 . . ?
O4A C5A C6A 126.1(3) . . ?
O4A C5A C4A 113.9(3) . . ?
C6A C5A C4A 120.0(3) . . ?
C14A C13A C12A 111.4(3) . . ?
C14A C13A H13A 109.3 . . ?
C12A C13A H13A 109.3 . . ?
C14A C13A H13B 109.3 . . ?
C12A C13A H13B 109.3 . . ?
H13A C13A H13B 108 . . ?
C42A C41A C4A 120.4(4) . . ?
C42A C41A H41A 119.8 . . ?
C4A C41A H41A 119.8 . . ?
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C15B C16B H16C 109.3 . . ?
C11B C16B H16C 109.3 . . ?
C15B C16B H16D 109.3 . . ?
C11B C16B H16D 109.3 . . ?
H16C C16B H16D 108 . . ?
O5B C7B C6B 126.3(3) . . ?
O5B C7B C8B 114.2(3) . . ?
C6B C7B C8B 119.5(3) . . ?
C44B C45B C4B 120.1(3) . . ?
C44B C45B H45B 119.9 . . ?
C4B C45B H45B 119.9 . . ?
C41A C4A C45A 119.0(3) . . ?
C41A C4A C5A 119.8(3) . . ?
C45A C4A C5A 121.1(3) . . ?

C7A C6A C5A 124.7(3) . . ?
C7A C6A H6A 118(2) . . ?
C5A C6A H6A 117(2) . . ?
O4B C5B C6B 124.8(3) . . ?
O4B C5B C4B 114.1(3) . . ?
C6B C5B C4B 121.2(3) . . ?
C43B C42B C41B 120.4(4) . . ?
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C41B C42B H42B 119.8 . . ?
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C7A C8A H8A2 109.5 . . ?
H8A1 C8A H8A2 109.5 . . ?
C7A C8A H8A3 109.5 . . ?
H8A1 C8A H8A3 109.5 . . ?
H8A2 C8A H8A3 109.5 . . ?
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H33C C33B H33D 107.9 . . ?
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C35B C36B H36D 109.4 . . ?
H36C C36B H36D 108 . . ?
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H35C C35B H35D 108.1 . . ?
C15B C14B C13B 110.9(3) . . ?
C15B C14B H14D 109.5 . . ?
C13B C14B H14D 109.5 . . ?
C15B C14B H14C 109.5 . . ?
C13B C14B H14C 109.5 . . ?
H14D C14B H14C 108 . . ?
C42B C43B C44B 119.9(3) . . ?
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C44B C43B H43B 120.1 . . ?
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C23B C24B H24C 109.5 . . ?
C25B C24B H24D 109.5 . . ?
C23B C24B H24D 109.5 . . ?
H24C C24B H24D 108.1 . . ?
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C25A C24A H24A 109.4 . . ?
C23A C24A H24A 109.4 . . ?
C25A C24A H24B 109.4 . . ?
C23A C24A H24B 109.4 . . ?
H24A C24A H24B 108 . . ?
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H13C C13B H13D 108 . . ?
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C36A C35A H35A 109.2 . . ?
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C36A C35A H35B 109.2 . . ?
H35A C35A H35B 107.9 . . ?
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C26A C25A H25A 109.4 . . ?
C24A C25A H25B 109.4 . . ?
C26A C25A H25B 109.4 . . ?
H25A C25A H25B 108 . . ?
C15A C14A C13A 110.3(3) . . ?
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C13A C14A H14A 109.6 . . ?
C15A C14A H14B 109.6 . . ?
C13A C14A H14B 109.6 . . ?
H14A C14A H14B 108.1 . . ?
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C43B C44B H44B 119.9 . . ?
C45B C44B H44B 119.9 . . ?
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C33A C34A H34B 109.4 . . ?
C35A C34A H34B 109.4 . . ?
H34A C34A H34B 108 . . ?
C42B C41B C4B 120.6(3) . . ?
C42B C41B H41B 119.7 . . ?
C4B C41B H41B 119.7 . . ?
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C14B C15B H15C 109.4 . . ?
C16B C15B H15C 109.4 . . ?
C14B C15B H15D 109.4 . . ?
C16B C15B H15D 109.4 . . ?
H15C C15B H15D 108 . . ?
C35B C34B C33B 111.0(3) . . ?
C35B C34B H34C 109.4 . . ?
C33B C34B H34C 109.4 . . ?
C35B C34B H34D 109.4 . . ?
C33B C34B H34D 109.4 . . ?
H34C C34B H34D 108 . . ?
C43A C42A C41A 120.4(4) . . ?
C43A C42A H42A 119.8 . . ?
C41A C42A H42A 119.8 . . ?
C44A C45A C4A 119.9(4) . . ?
C44A C45A H45A 120 . . ?
C4A C45A H45A 120 . . ?
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C45A C44A H44A 119.6 . . ?
C43A C44A H44A 119.6 . . ?

loop_
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   _geom_hbond_atom_site_label_H
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   _geom_hbond_atom_site_label_A
   _geom_hbond_distance_DH
   _geom_hbond_distance_HA
   _geom_hbond_distance_DA
   _geom_hbond_angle_DHA
   _geom_hbond_site_symmetry_A
   _geom_hbond_publ_flag
C12A H12B O2A 0.99 2.58 3.383(4) 137.7 2_657 yes
C15A H15B O3A 0.99 2.57 3.290(4) 129.6 1_655 yes
C16A H16A O1A 0.99 2.51 3.481(4) 165.8 . yes
C21A H21A O1B 1 2.55 3.543(4) 170.6 . yes
C22A H22B O5A 0.99 2.47 3.215(4) 132 . yes
C22B H22D O5B 0.99 2.51 3.177(4) 124.2 . yes
C32A H32A O4A 0.99 2.43 3.257(4) 140.5 . yes
C32B H32D O4B 0.99 2.56 3.378(4) 139.9 . yes
C36B H36D O4B 0.99 2.5 3.339(4) 142.3 . yes
C41B H41B O4B 0.95 2.35 2.678(4) 100 . yes
C43B H43B O1A 0.95 2.59 3.496(4) 158.5 1_465 yes
```

Cif file of 5

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data_q2_21cms1_0m
# start Validation Reply Form
_vrf_PLAT971_I
;
PROBLEM: Check Calcd Resid. Dens.  0.78Ang From Re1             4.96 eA-3
RESPONSE: see _publ_section_exptl_refinement
;
# end Validation Reply Form

_audit_creation_date                2021-12-03T09:09:25-00:00
_audit_creation_method               'WinGX routine CIF_UPDATE'

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

# CHEMICAL DATA

_chemical_formula_sum                'C26 H37 F3 O5 P Re'
_chemical_formula_moiety             'C26 H37 F3 O5 P Re'
_chemical_formula_weight              703.72

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

# CRYSTAL DATA

_symmetry_cell_setting               monoclinic
_symmetry_space_group_name_H-M       'P 21/c'
_symmetry_space_group_name_Hall      '-P 2ybc'

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y-1/2, z-1/2'

_cell_length_a                      9.1356(11)
_cell_length_b                      33.762(4)
_cell_length_c                      9.2315(12)
_cell_angle_alpha                    90
_cell_angle_beta                     106.007(4)
_cell_angle_gamma                    90
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_cell_volume                    2737.0(6)
_cell_formula_units_Z           4
_cell_measurement_temperature   100(2)
_cell_measurement_reflns_used   9548
_cell_measurement_theta_min     2.84
_cell_measurement_theta_max     28.31

_exptl_crystal_description      'Cuboid'
_exptl_crystal_colour           'yellow'
_exptl_crystal_size_max         0.43
_exptl_crystal_size_mid         0.27
_exptl_crystal_size_min         0.12
_exptl_crystal_density_diffrn   1.708
_exptl_crystal_F_000            1400
_exptl_absorpt_coefficient_mu   4.552
_exptl_absorpt_correction_type  'multi-scan'
_exptl_absorpt_correction_T_min 0.238
_exptl_absorpt_correction_T_max 0.579

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

# EXPERIMENTAL DATA

_diffrn_ambient_temperature     100(2)
_diffrn_radiation_type          MoK\a
_diffrn_radiation_wavelength    0.71073
_diffrn_measurement_device_type 'Bruker APEX-II CCD'
_diffrn_measurement_method      '\f and \w scans'
_diffrn_reflns_number           73558
_diffrn_reflns_av_R_equivalents 0.0433
_diffrn_reflns_theta_min        2.593
_diffrn_reflns_theta_max        27.999
_diffrn_reflns_theta_full       25.242
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_diffrn_measured_fraction_theta_full
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_diffrn_reflns_Laue_measured_fraction_full
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_diffrn_reflns_Laue_measured_fraction_max
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_diffrn_reflns_point_group_measured_fraction_full
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_diffrn_reflns_point_group_measured_fraction_max
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_diffrn_reflns_limit_h_min      -12
_diffrn_reflns_limit_h_max      12
_diffrn_reflns_limit_k_min      -44
_diffrn_reflns_limit_k_max      44
_diffrn_reflns_limit_l_min      -12
_diffrn_reflns_limit_l_max      12

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

# STRUCTURE SOLUTION

_atom_sites_solution_hydrogens  mixed

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

# REFINEMENT DATA
```

```
# There is residual electron density (4.96 eA^-3^ ) 0.78 \%A from the rhenium
# metal center likely caused by Fourier truncation ripples.

_refine_special_details
;
 Refined as a 2-component inversion twin.
;
_refln_number_total                  6605
_refln_number_gt                     6549
_refln_threshold_expression          'I > 2\s(I)'
_refine_ls_structure_factor_coef     Fsqd
_refine_ls_matrix_type               full
_refine_ls_R_factor_all              0.0389
_refine_ls_R_factor_gt               0.0388
_refine_ls_wR_factor_ref             0.0835
_refine_ls_goodness_of_fit_ref       1.246
_refine_ls_restrained_S_all          1.246
_refine_ls_number_refln              6571
_refine_ls_number_parameters         331
_refine_ls_number_restraints         0
_refine_ls_hydrogen_treatment        mixed
_refine_ls_weighting_scheme          calc
_refine_ls_weighting_details
                  'w=1/[\s^2^(Fo^2^)+22.5162P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_shift/su_max              0.001
_refine_ls_shift/su_mean             0
_refine_diff_density_max             5.108
_refine_diff_density_min             -2.242
_refine_diff_density_rms             0.147
_refine_ls_extinction_method         none
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   _atom_type_description
   _atom_type_scat_dispersion_real
   _atom_type_scat_dispersion_imag
   _atom_type_scat_source
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.006 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
F F 0.0171 0.0103 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Re Re -1.0185 7.231 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
V V 0.3005 0.5294 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_computing_structure_refinement      'SHELXL-2018/3 (Sheldrick, 2018)'

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

# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_U_iso_or_equiv
   _atom_site_adp_type
   _atom_site_calc_flag
   _atom_site_occupancy
   _atom_site_disorder_assembly
   _atom_site_disorder_group
   _atom_site_type_symbol
```

Re1 0.24245(2) 0.13805(2) 0.04519(2) 0.01435(6) Uani d 1 . . Re
P1 0.04235(13) 0.11852(3) 0.17467(12) 0.0115(2) Uani d 1 . . P
O1 0.0181(4) 0.15769(11) -0.2591(4) 0.0266(8) Uani d 1 . . O
O4 0.4056(4) 0.13104(12) 0.2611(4) 0.0251(8) Uani d 1 . . O
O5 0.2460(4) 0.19941(10) 0.1106(4) 0.0223(7) Uani d 1 . . O
C22 -0.2552(5) 0.08295(14) 0.1152(5) 0.0167(9) Uani d 1 . . C
H22A -0.23255 0.081693 0.226378 0.02 Uiso calc 1 . . H
H22B -0.310857 0.107903 0.080818 0.02 Uiso calc 1 . . H
C21 -0.1048(5) 0.08260(13) 0.0695(5) 0.0139(8) Uani d 1 . . C
H21 -0.059891 0.055704 0.096994 0.017 Uiso calc 1 . . H
F2 0.5057(5) 0.12592(15) 0.5780(5) 0.0572(12) Uani d 1 . . F
C12 0.0280(5) 0.18506(14) 0.3586(5) 0.0166(9) Uani d 1 . . C
H12B 0.069156 0.168268 0.448521 0.02 Uiso calc 1 . . H
H12A 0.115005 0.196964 0.329762 0.02 Uiso calc 1 . . H
C14 -0.1458(6) 0.24322(14) 0.2593(6) 0.0223(10) Uani d 1 . . C
H14B -0.214391 0.262718 0.28708 0.027 Uiso calc 1 . . H
H14A -0.066606 0.258026 0.227148 0.027 Uiso calc 1 . . H
C5 0.4688(6) 0.1591(2) 0.3500(6) 0.0331(14) Uani d 1 . . C
C31 0.1344(5) 0.09229(13) 0.3540(5) 0.0133(8) Uani d 1 . . C
H31 0.209465 0.111268 0.4171 0.016 Uiso calc 1 . . H
C3 0.4027(6) 0.14926(14) -0.0511(5) 0.0191(9) Uani d 1 . . C
C36 0.2265(5) 0.05630(14) 0.3274(5) 0.0174(9) Uani d 1 . . C
H36A 0.156621 0.036589 0.264924 0.021 Uiso calc 1 . . H
H36B 0.299393 0.064766 0.271627 0.021 Uiso calc 1 . . H
C16 -0.1381(5) 0.18514(13) 0.0890(5) 0.0149(8) Uani d 1 . . C
H16A -0.056677 0.197252 0.051771 0.018 Uiso calc 1 . . H
H16B -0.20146 0.168379 0.007537 0.018 Uiso calc 1 . . H
C13 -0.0704(6) 0.21782(14) 0.3964(5) 0.0191(9) Uani d 1 . . C
H13A -0.006368 0.234914 0.476194 0.023 Uiso calc 1 . . H
H13B -0.150182 0.205784 0.436273 0.023 Uiso calc 1 . . H
C15 -0.2370(6) 0.21784(14) 0.1288(5) 0.0184(9) Uani d 1 . . C
H15A -0.278084 0.234851 0.039419 0.022 Uiso calc 1 . . H
H15B -0.32407 0.205673 0.156495 0.022 Uiso calc 1 . . H
C34 0.2091(6) 0.02617(15) 0.5734(6) 0.0226(10) Uani d 1 . . C
H34A 0.138662 0.00489 0.523367 0.027 Uiso calc 1 . . H
H34B 0.270732 0.016039 0.672057 0.027 Uiso calc 1 . . H
C25 -0.2441(6) 0.05004(16) -0.1754(6) 0.0256(11) Uani d 1 . . C
H25B -0.270399 0.052577 -0.286444 0.031 Uiso calc 1 . . H
H25A -0.186296 0.025102 -0.146968 0.031 Uiso calc 1 . . H
C33 0.1179(6) 0.06193(16) 0.5980(6) 0.0239(10) Uani d 1 . . C
H33B 0.187977 0.082052 0.657603 0.029 Uiso calc 1 . . H
H33A 0.046723 0.053825 0.656287 0.029 Uiso calc 1 . . H
C26 -0.1440(6) 0.08490(14) -0.1035(5) 0.0182(9) Uani d 1 . . C
H26B -0.198062 0.110031 -0.138483 0.022 Uiso calc 1 . . H
H26A -0.048933 0.084649 -0.135195 0.022 Uiso calc 1 . . H
C11 -0.0663(5) 0.15932(13) 0.2277(5) 0.0136(8) Uani d 1 . . C
H11 -0.151414 0.147258 0.261428 0.016 Uiso calc 1 . . H
C35 0.3138(5) 0.03709(14) 0.4765(5) 0.0185(9) Uani d 1 . . C
H35A 0.365559 0.012922 0.455137 0.022 Uiso calc 1 . . H
H35B 0.39293 0.055666 0.533017 0.022 Uiso calc 1 . . H
C23 -0.3544(6) 0.04763(15) 0.0450(6) 0.0244(10) Uani d 1 . . C
H23A -0.300864 0.02273 0.084496 0.029 Uiso calc 1 . . H
H23B -0.450794 0.048411 0.074267 0.029 Uiso calc 1 . . H
F1 0.6561(6) 0.17380(15) 0.5818(5) 0.0648(14) Uani d 1 . . F
C24 -0.3900(6) 0.04802(16) -0.1263(6) 0.0268(11) Uani d 1 . . C
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H24B -0.45479 0.07118 -0.166868 0.032 Uiso calc 1 . . H
C4 0.5804(7) 0.1441(2) 0.4932(7) 0.0393(16) Uani d 1 . . C
O3 0.4914(5) 0.15396(12) -0.1170(5) 0.0315(9) Uani d 1 . . O
F3 0.6767(6) 0.1209(2) 0.4646(5) 0.0789(18) Uani d 1 . . F
O2 0.2440(4) 0.05115(11) -0.0456(4) 0.0254(8) Uani d 1 . . O
C1 0.0997(5) 0.14932(13) -0.1447(5) 0.0159(9) Uani d 1 . . C

C2 0.2444(5) 0.08388(14) -0.0122(5) 0.0172(9) Uani d 1 . . C
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H32B -0.028599 0.103712 0.468073 0.021 Uiso calc 1 . . H
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C8 0.3220(10) 0.2618(2) 0.2174(9) 0.053(2) Uani d 1 . . C
H8B 0.308176 0.272066 0.115213 0.079 Uiso calc 1 . . H
H8A 0.414156 0.27334 0.285085 0.079 Uiso calc 1 . . H
H8C 0.233562 0.268941 0.252599 0.079 Uiso calc 1 . . H
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C12 0.021(2) 0.016(2) 0.012(2) 0.0007(17) 0.0031(17) -0.0029(16)
C14 0.034(3) 0.013(2) 0.023(2) 0.0049(19) 0.013(2) -0.0001(18)
C5 0.016(2) 0.067(4) 0.016(2) -0.016(3) 0.0029(19) 0.002(2)
C31 0.016(2) 0.0121(19) 0.0096(18) 0.0007(16) 0.0005(15) -0.0005(15)
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C16 0.017(2) 0.0117(19) 0.016(2) 0.0024(16) 0.0040(17) 0.0020(16)
C13 0.030(3) 0.013(2) 0.016(2) 0.0035(18) 0.0102(19) -0.0043(17)
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C23 0.024(2) 0.020(2) 0.026(3) -0.0053(19) 0.001(2) 0.003(2)
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MOLECULAR GEOMETRY

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 are estimated using the full covariance matrix.  The cell esds are taken
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 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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P1 C31 C32 C33 -175.5(3) . . . . ?
Re1 O5 C7 C6 -10.8(8) . . . . ?
Re1 O5 C7 C8 170.9(4) . . . . ?
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Cif file of 6

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_symmetry_space_group_name_Hall      '-P 2ybc'

loop_
 _symmetry_equiv_pos_as_xyz
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'x, y, z'
'-x, y+1/2, -z+1/2'
'-x, -y, -z'
'x, -y-1/2, z-1/2'

_cell_length_a                    9.2609(7)
_cell_length_b                    33.608(2)
_cell_length_c                    9.3712(7)
_cell_angle_alpha                 90
_cell_angle_beta                  106.717(2)
_cell_angle_gamma                 90
_cell_volume                      2793.4(4)
_cell_formula_units_Z             4
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     9863
_cell_measurement_theta_min       2.42
_cell_measurement_theta_max       28.29

_exptl_crystal_description        'plate'
_exptl_crystal_colour             'Orange'
_exptl_crystal_size_max           0.223
_exptl_crystal_size_mid           0.089
_exptl_crystal_size_min           0.029
_exptl_crystal_density_diffrn     1.802
_exptl_crystal_F_000              1496
_exptl_absorpt_coefficient_mu     4.482
_exptl_absorpt_correction_type    'multi-scan'
_exptl_absorpt_correction_T_min   0.626
_exptl_absorpt_correction_T_max   0.878

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

# EXPERIMENTAL DATA

_diffrn_ambient_temperature       100(2)
_diffrn_radiation_type            MoK\a
_diffrn_radiation_wavelength      0.71073
_diffrn_measurement_device_type   'Bruker APEX-II CCD'
_diffrn_measurement_method        '\f and \w scans'
_diffrn_reflns_number             63361
_diffrn_reflns_av_R_equivalents   0.0561
_diffrn_reflns_theta_min          2.296
_diffrn_reflns_theta_max          27.999
_diffrn_reflns_theta_full         25.242
_diffrn_measured_fraction_theta_max
                                  0.999
_diffrn_measured_fraction_theta_full
                                  0.999
_diffrn_reflns_Laue_measured_fraction_full
                                  0.999
_diffrn_reflns_Laue_measured_fraction_max
                                  0.999
_diffrn_reflns_point_group_measured_fraction_full
                                  0.999
_diffrn_reflns_point_group_measured_fraction_max
                                  0.999
_diffrn_reflns_limit_h_min        -12
_diffrn_reflns_limit_h_max        10
_diffrn_reflns_limit_k_min        -44
_diffrn_reflns_limit_k_max        44
_diffrn_reflns_limit_l_min        -12
_diffrn_reflns_limit_l_max        12
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#==============================================================================

# STRUCTURE SOLUTION

_atom_sites_solution_hydrogens          mixed

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

# REFINEMENT DATA

_reflns_number_total                    6747
_reflns_number_gt                       6293
_reflns_threshold_expression            'I > 2\s(I)'
_refine_ls_structure_factor_coef        Fsqd
_refine_ls_matrix_type                  full
_refine_ls_R_factor_all                 0.0492
_refine_ls_R_factor_gt                  0.0453
_refine_ls_wR_factor_ref                0.0925
_refine_ls_goodness_of_fit_ref          1.352
_refine_ls_restrained_S_all             1.352
_refine_ls_number_reflns                6747
_refine_ls_number_parameters            346
_refine_ls_number_restraints            0
_refine_ls_hydrogen_treatment           mixed
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
                    'w=1/[\s^2^(Fo^2^)+20.9692P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_shift/su_max                 0.001
_refine_ls_shift/su_mean                0
_refine_diff_density_max                2.09
_refine_diff_density_min                -3.506
_refine_diff_density_rms                0.153
_refine_ls_extinction_method            none
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   _atom_type_scat_dispersion_real
   _atom_type_scat_dispersion_imag
   _atom_type_scat_source
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0 0 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
F F 0.0171 0.0103 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
O O 0.0106 0.006 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Re Re -1.0185 7.231 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_computing_structure_refinement         'SHELXL-2018/3 (Sheldrick, 2018)'

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

# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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   _atom_site_fract_z
   _atom_site_U_iso_or_equiv
   _atom_site_adp_type
   _atom_site_calc_flag
   _atom_site_occupancy
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   _atom_site_disorder_group
   _atom_site_type_symbol
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P1 0.54656(16) 0.61703(4) 0.67684(15) 0.0141(3) Uani d 1 . . P
O4 0.7644(4) 0.69496(11) 0.6165(4) 0.0177(8) Uani d 1 . . O
O5 0.9090(4) 0.62320(12) 0.7567(4) 0.0210(8) Uani d 1 . . O
O2 0.5166(5) 0.65553(13) 0.2487(5) 0.0268(9) Uani d 1 . . O
O1 0.7297(5) 0.54627(12) 0.4533(5) 0.0250(9) Uani d 1 . . O
O3 0.9819(5) 0.64871(14) 0.3821(5) 0.0314(10) Uani d 1 . . O
C2 0.5987(6) 0.64653(16) 0.3619(6) 0.0191(11) Uani d 1 . . C
C3 0.8971(7) 0.64374(16) 0.4472(6) 0.0194(8) Uani d 1 . . C
C1 0.7334(7) 0.57926(17) 0.4871(6) 0.0194(8) Uani d 1 . . C
C22 0.7190(7) 0.55276(17) 0.8323(6) 0.0197(11) Uani d 1 . . C
H22A 0.64436 0.533057 0.776677 0.024 Uiso calc 1 . . H
H22B 0.788304 0.558931 0.772192 0.024 Uiso calc 1 . . H
C21 0.6366(6) 0.59102(16) 0.8553(6) 0.0162(10) Uani d 1 . . C
H21 0.715627 0.60942 0.915677 0.019 Uiso calc 1 . . H
C36 0.3767(6) 0.68592(16) 0.5904(6) 0.0175(11) Uani d 1 . . C
H36A 0.457328 0.696724 0.55149 0.021 Uiso calc 1 . . H
H36B 0.309261 0.669405 0.511416 0.021 Uiso calc 1 . . H
C25 0.6223(7) 0.56376(19) 1.1014(6) 0.0252(13) Uani d 1 . . C
H25A 0.694775 0.583874 1.157423 0.03 Uiso calc 1 . . H
H25B 0.553034 0.556967 1.160875 0.03 Uiso calc 1 . . H
C32 0.5483(7) 0.68515(16) 0.8550(6) 0.0188(11) Uani d 1 . . C
H32A 0.588848 0.668253 0.944042 0.023 Uiso calc 1 . . H
H32B 0.634376 0.695792 0.824124 0.023 Uiso calc 1 . . H
C7 0.9862(6) 0.64886(19) 0.8409(6) 0.0228(12) Uani d 1 . . C
C8 1.0978(7) 0.6312(2) 0.9812(7) 0.0301(14) Uani d 1 . . C
C35 0.2873(7) 0.72002(17) 0.6297(6) 0.0209(11) Uani d 1 . . C
H35A 0.200179 0.709158 0.658231 0.025 Uiso calc 1 . . H
H35B 0.247788 0.737118 0.540953 0.025 Uiso calc 1 . . H
C16 0.2476(6) 0.58504(17) 0.6208(6) 0.0191(11) Uani d 1 . . C
H16A 0.271725 0.584413 0.730811 0.023 Uiso calc 1 . . H
H16B 0.196855 0.61061 0.585414 0.023 Uiso calc 1 . . H
C24 0.7076(7) 0.52667(18) 1.0797(7) 0.0238(12) Uani d 1 . . C
H24A 0.76972 0.516958 1.177906 0.029 Uiso calc 1 . . H
H24B 0.634616 0.505513 1.033782 0.029 Uiso calc 1 . . H
C11 0.3944(6) 0.58213(16) 0.5753(6) 0.0170(10) Uani d 1 . . C
H11 0.434592 0.554804 0.605127 0.02 Uiso calc 1 . . H
C13 0.2502(7) 0.54801(17) 0.3387(6) 0.0233(12) Uani d 1 . . C
H13A 0.223967 0.54911 0.228594 0.028 Uiso calc 1 . . H
H13B 0.304593 0.522764 0.371623 0.028 Uiso calc 1 . . H
C23 0.8084(7) 0.53499(17) 0.9814(6) 0.0205(11) Uani d 1 . . C
H23A 0.856665 0.509922 0.963684 0.025 Uiso calc 1 . . H
H23B 0.889044 0.553733 1.032843 0.025 Uiso calc 1 . . H
C12 0.3539(7) 0.58302(17) 0.4045(6) 0.0202(11) Uani d 1 . . C
H12A 0.302587 0.608381 0.36689 0.024 Uiso calc 1 . . H
H12B 0.447043 0.581385 0.37311 0.024 Uiso calc 1 . . H
C6 0.9819(7) 0.6900(2) 0.8260(7) 0.0235(12) Uani d 1 . . C
C14 0.1063(7) 0.54846(18) 0.3855(7) 0.0247(12) Uani d 1 . . C
H14A 0.047231 0.524095 0.348634 0.03 Uiso calc 1 . . H
H14B 0.044298 0.571725 0.340406 0.03 Uiso calc 1 . . H
C15 0.1418(7) 0.55052(17) 0.5542(7) 0.0231(12) Uani d 1 . . C
H15A 0.189096 0.525202 0.597872 0.028 Uiso calc 1 . . H
H15B 0.046636 0.553665 0.581203 0.028 Uiso calc 1 . . H
C31 0.4472(6) 0.65995(15) 0.7281(6) 0.0161(10) Uani d 1 . . C
H31 0.362956 0.64923 0.76366 0.019 Uiso calc 1 . . H
C34 0.3836(7) 0.74507(17) 0.7573(7) 0.0233(12) Uani d 1 . . C
H34A 0.319598 0.765477 0.785329 0.028 Uiso calc 1 . . H
H34B 0.462362 0.758992 0.723893 0.028 Uiso calc 1 . . H
C26 0.5314(7) 0.58136(17) 0.9510(6) 0.0190(11) Uani d 1 . . C
```

H26A 0.453738 0.562065 0.897935 0.023 Uiso calc 1 . . H
H26B 0.479671 0.605914 0.968083 0.023 Uiso calc 1 . . H
C5 0.8721(6) 0.70951(17) 0.7170(6) 0.0192(11) Uani d 1 . . C
C4 0.8758(7) 0.75507(19) 0.7171(7) 0.0256(13) Uani d 1 . . C
C33 0.4586(7) 0.71949(17) 0.8935(6) 0.0219(12) Uani d 1 . . C
H33A 0.526813 0.736337 0.970626 0.026 Uiso calc 1 . . H
H33B 0.380027 0.708681 0.935449 0.026 Uiso calc 1 . . H
F1A 0.8324(12) 0.7697(2) 0.5727(10) 0.0322(8) Uani d 0.559(13) A 1 F
F3A 0.7502(11) 0.7695(3) 0.7440(11) 0.0322(8) Uani d 0.559(13) A 1 F
F2A 1.0104(10) 0.7707(2) 0.7784(12) 0.0322(8) Uani d 0.559(13) A 1 F
F2B 0.9909(13) 0.7686(3) 0.8308(15) 0.0322(8) Uani d 0.441(13) A 2 F
F1B 0.8899(15) 0.7678(3) 0.5900(14) 0.0322(8) Uani d 0.441(13) A 2 F
F3B 0.7844(14) 0.7707(4) 0.7822(15) 0.0322(8) Uani d 0.441(13) A 2 F
F5A 1.0445(10) 0.6267(4) 1.0920(13) 0.0323(8) Uani d 0.582(11) B 3 F
F4A 1.1288(10) 0.5914(3) 0.9534(10) 0.0323(8) Uani d 0.582(11) B 3 F
F6A 1.2268(9) 0.6495(3) 1.0213(8) 0.0323(8) Uani d 0.582(11) B 3 F
F5B 1.0084(13) 0.6250(5) 1.0798(19) 0.0323(8) Uani d 0.418(11) B 4 F
F6B 1.1960(12) 0.6607(4) 1.0611(12) 0.0323(8) Uani d 0.418(11) B 4 F
F4B 1.1698(13) 0.6011(4) 0.9591(14) 0.0323(8) Uani d 0.418(11) B 4 F
H6 1.032(10) 0.703(2) 0.886(9) 0.04(2) Uiso d 1 . . H

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_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
Re1 0.01510(11) 0.01749(10) 0.01393(10) 0.00242(8) 0.00423(7) 0.00093(8)
P1 0.0149(6) 0.0153(6) 0.0120(6) 0.0019(5) 0.0035(5) 0.0004(5)
O4 0.0143(19) 0.0212(19) 0.0175(19) -0.0006(15) 0.0043(15) -0.0018(15)
O5 0.0149(19) 0.029(2) 0.0184(19) 0.0010(16) 0.0041(16) 0.0049(16)
O2 0.026(2) 0.030(2) 0.020(2) 0.0014(18) -0.0004(18) 0.0047(17)
O1 0.029(2) 0.023(2) 0.024(2) 0.0042(17) 0.0083(19) -0.0016(17)
O3 0.031(3) 0.032(2) 0.036(3) 0.0087(19) 0.016(2) 0.010(2)
C2 0.018(3) 0.015(2) 0.024(3) -0.001(2) 0.007(2) -0.002(2)
C3 0.021(2) 0.0211(19) 0.0171(18) 0.0063(15) 0.0063(16) 0.0050(14)
C1 0.021(2) 0.0211(19) 0.0171(18) 0.0063(15) 0.0063(16) 0.0050(14)
C22 0.022(3) 0.021(3) 0.017(3) 0.007(2) 0.007(2) 0.002(2)
C21 0.017(3) 0.019(3) 0.014(2) 0.000(2) 0.007(2) 0.0012(19)
C36 0.019(3) 0.018(3) 0.016(3) 0.002(2) 0.005(2) 0.001(2)
C25 0.027(3) 0.036(3) 0.014(3) 0.004(3) 0.008(2) 0.006(2)
C32 0.021(3) 0.019(3) 0.015(2) -0.001(2) 0.004(2) -0.001(2)
C7 0.012(3) 0.038(3) 0.019(3) 0.000(2) 0.005(2) 0.004(2)
C8 0.019(3) 0.049(4) 0.021(3) -0.002(3) 0.003(2) 0.009(3)
C35 0.020(3) 0.021(3) 0.023(3) 0.006(2) 0.009(2) 0.002(2)
C16 0.013(3) 0.022(3) 0.023(3) 0.000(2) 0.007(2) -0.003(2)
C24 0.021(3) 0.029(3) 0.019(3) 0.004(2) 0.002(2) 0.010(2)
C11 0.017(3) 0.018(3) 0.018(3) 0.000(2) 0.007(2) 0.001(2)
C13 0.028(3) 0.021(3) 0.017(3) -0.002(2) 0.001(2) -0.004(2)
C23 0.021(3) 0.022(3) 0.019(3) 0.002(2) 0.007(2) 0.004(2)
C12 0.023(3) 0.022(3) 0.015(3) -0.001(2) 0.004(2) -0.002(2)
C6 0.015(3) 0.035(3) 0.018(3) -0.003(2) 0.001(2) -0.005(2)
C14 0.021(3) 0.021(3) 0.026(3) -0.006(2) -0.003(2) -0.003(2)
C15 0.020(3) 0.022(3) 0.024(3) -0.002(2) 0.002(2) 0.000(2)
C31 0.016(3) 0.018(2) 0.015(2) 0.001(2) 0.007(2) -0.0008(19)
C34 0.028(3) 0.020(3) 0.024(3) 0.004(2) 0.012(3) -0.002(2)
C26 0.020(3) 0.025(3) 0.014(2) 0.002(2) 0.008(2) 0.004(2)
C5 0.013(3) 0.027(3) 0.019(3) -0.002(2) 0.006(2) -0.004(2)
C4 0.020(3) 0.028(3) 0.028(3) -0.004(2) 0.004(2) -0.007(2)
C33 0.026(3) 0.023(3) 0.018(3) 0.002(2) 0.007(2) -0.004(2)

F1A 0.026(2) 0.0305(13) 0.039(3) -0.0038(15) 0.008(2) -0.0044(15)
F3A 0.026(2) 0.0305(13) 0.039(3) -0.0038(15) 0.008(2) -0.0044(15)
F2A 0.026(2) 0.0305(13) 0.039(3) -0.0038(15) 0.008(2) -0.0044(15)
F2B 0.026(2) 0.0305(13) 0.039(3) -0.0038(15) 0.008(2) -0.0044(15)
F1B 0.026(2) 0.0305(13) 0.039(3) -0.0038(15) 0.008(2) -0.0044(15)
F3B 0.026(2) 0.0305(13) 0.039(3) -0.0038(15) 0.008(2) -0.0044(15)
F5A 0.014(3) 0.056(2) 0.0246(15) 0.0011(17) 0.0006(18) 0.0058(16)
F4A 0.014(3) 0.056(2) 0.0246(15) 0.0011(17) 0.0006(18) 0.0058(16)
F6A 0.014(3) 0.056(2) 0.0246(15) 0.0011(17) 0.0006(18) 0.0058(16)
F5B 0.014(3) 0.056(2) 0.0246(15) 0.0011(17) 0.0006(18) 0.0058(16)
F6B 0.014(3) 0.056(2) 0.0246(15) 0.0011(17) 0.0006(18) 0.0058(16)
F4B 0.014(3) 0.056(2) 0.0246(15) 0.0011(17) 0.0006(18) 0.0058(16)

#===

MOLECULAR GEOMETRY

_geom_special_details
;
 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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   _geom_bond_atom_site_label_2
   _geom_bond_site_symmetry_2
   _geom_bond_distance
   _geom_bond_publ_flag
Re1 C1 . 1.897(6) ?
Re1 C2 . 1.906(6) ?
Re1 C3 . 1.956(6) ?
Re1 O5 . 2.153(4) ?
Re1 O4 . 2.164(4) ?
Re1 P1 . 2.5172(14) ?
P1 C31 . 1.847(5) ?
P1 C21 . 1.859(5) ?
P1 C11 . 1.870(6) ?
O4 C5 . 1.257(7) ?
O5 C7 . 1.246(7) ?
O2 C2 . 1.154(7) ?
O1 C1 . 1.151(7) ?
O3 C3 . 1.136(7) ?
C22 C23 . 1.526(8) ?
C22 C21 . 1.542(7) ?
C22 H22A . 0.99 ?
C22 H22B . 0.99 ?
C21 C26 . 1.537(7) ?
C21 H21 . 1 ?
C36 C35 . 1.520(7) ?
C36 C31 . 1.538(7) ?
C36 H36A . 0.99 ?
C36 H36B . 0.99 ?
C25 C24 . 1.520(9) ?
C25 C26 . 1.537(8) ?
C25 H25A . 0.99 ?
C25 H25B . 0.99 ?
C32 C33 . 1.525(8) ?

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C32 C31 . 1.538(7) ?
C32 H32A . 0.99 ?
C32 H32B . 0.99 ?
C7 C6 . 1.391(9) ?
C7 C8 . 1.538(8) ?
C8 F4B . 1.262(16) ?
C8 F5A . 1.281(14) ?
C8 F6A . 1.299(10) ?
C8 F6B . 1.406(14) ?
C8 F4A . 1.407(13) ?
C8 F5B . 1.423(18) ?
C35 C34 . 1.524(8) ?
C35 H35A . 0.99 ?
C35 H35B . 0.99 ?
C16 C15 . 1.531(8) ?
C16 C11 . 1.540(7) ?
C16 H16A . 0.99 ?
C16 H16B . 0.99 ?
C24 C23 . 1.514(8) ?
C24 H24A . 0.99 ?
C24 H24B . 0.99 ?
C11 C12 . 1.536(7) ?
C11 H11 . 1 ?
C13 C14 . 1.518(9) ?
C13 C12 . 1.532(8) ?
C13 H13A . 0.99 ?
C13 H13B . 0.99 ?
C23 H23A . 0.99 ?
C23 H23B . 0.99 ?
C12 H12A . 0.99 ?
C12 H12B . 0.99 ?
C6 C5 . 1.382(8) ?
C6 H6 . 0.76(8) ?
C14 C15 . 1.521(8) ?
C14 H14A . 0.99 ?
C14 H14B . 0.99 ?
C15 H15A . 0.99 ?
C15 H15B . 0.99 ?
C31 H31 . 1 ?
C34 C33 . 1.530(8) ?
C34 H34A . 0.99 ?
C34 H34B . 0.99 ?
C26 H26A . 0.99 ?
C26 H26B . 0.99 ?
C5 C4 . 1.532(8) ?
C4 F3B . 1.290(15) ?
C4 F1B . 1.307(14) ?
C4 F2A . 1.322(10) ?
C4 F3A . 1.349(12) ?
C4 F2B . 1.351(13) ?
C4 F1A . 1.386(11) ?
C33 H33A . 0.99 ?
C33 H33B . 0.99 ?

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   _geom_angle_atom_site_label_3
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   _geom_angle_site_symmetry_1
   _geom_angle_site_symmetry_3
   _geom_angle_publ_flag
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C1 Re1 C2 89.8(2) . . ?
C1 Re1 C3 90.3(2) . . ?
C2 Re1 C3 86.6(2) . . ?
C1 Re1 O5 94.3(2) . . ?
C2 Re1 O5 175.6(2) . . ?
C3 Re1 O5 91.7(2) . . ?
C1 Re1 O4 177.0(2) . . ?
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O5 Re1 O4 83.89(15) . . ?
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C3 Re1 P1 177.56(16) . . ?
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O4 Re1 P1 94.67(11) . . ?
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C31 P1 C11 105.3(3) . . ?
C21 P1 C11 103.9(2) . . ?
C31 P1 Re1 115.91(18) . . ?
C21 P1 Re1 109.87(18) . . ?
C11 P1 Re1 115.58(17) . . ?
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C7 O5 Re1 126.9(4) . . ?
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O3 C3 Re1 175.9(6) . . ?
O1 C1 Re1 178.9(5) . . ?
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P1 C21 H21 106.5 . . ?
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C24 C25 C26 111.2(5) . . ?
C24 C25 H25A 109.4 . . ?
C26 C25 H25A 109.4 . . ?
C24 C25 H25B 109.4 . . ?
C26 C25 H25B 109.4 . . ?
H25A C25 H25B 108 . . ?
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F5A C8 F4A 100.7(9) . . ?

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F4B C8 F5B 114.9(11) . . ?
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F5A C8 C7 114.6(6) . . ?
F6A C8 C7 113.6(6) . . ?
F6B C8 C7 110.8(7) . . ?
F4A C8 C7 109.4(6) . . ?
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C36 C35 C34 111.7(5) . . ?
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C34 C35 H35B 109.3 . . ?
H35A C35 H35B 107.9 . . ?
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C11 C16 H16A 109.5 . . ?
C15 C16 H16B 109.5 . . ?
C11 C16 H16B 109.5 . . ?
H16A C16 H16B 108.1 . . ?
C23 C24 C25 111.4(5) . . ?
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C25 C24 H24A 109.3 . . ?
C23 C24 H24B 109.3 . . ?
C25 C24 H24B 109.3 . . ?
H24A C24 H24B 108 . . ?
C12 C11 C16 108.5(5) . . ?
C12 C11 P1 116.1(4) . . ?
C16 C11 P1 114.5(4) . . ?
C12 C11 H11 105.6 . . ?
C16 C11 H11 105.6 . . ?
P1 C11 H11 105.6 . . ?
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C14 C13 H13B 109.2 . . ?
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C22 C23 H23B 109.4 . . ?
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C15 C14 H14B 109.5 . . ?
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C26 C25 C24 C23 55.6(7) . . . . ?
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C6 C5 C4 F3A -116.1(7) . . . . ?
O4 C5 C4 F2B 177.8(8) . . . . ?

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C6 C5 C4 F1A 144.0(7) . . . . ?
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C22 H22B O5 0.99 2.46 3.150(7) 126.8 . yes
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