Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Screened exchange hybrid density functional for accurate and efficient structures and interaction energies

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Supporting Information

A. HSE-3c definition

The HSE-3c energy can be expressed as

$$
\begin{aligned}
E^{\mathrm{HSE-3c}} =& E_{\mathrm{xc}}^{\mathrm{HSE-3c}} + E_{\mathrm{disp}}^{\mathrm{D3}} + E_{\mathrm{BSSE}}^{\mathrm{gCP}} \\
E_{\mathrm{xc}}^{\mathrm{HSE-3c}} =& a\, E_{\mathrm{x}}^{\mathrm{HF,SR}}(\omega) + (1-a)\, E_{\mathrm{x}}^{\mathrm{HSE,SR}}(\omega) + E_{\mathrm{x}}^{\mathrm{HSE,LR}}(\omega) + E_{\mathrm{c}}^{\mathrm{PBEh-3c}} .
\end{aligned} \tag{1}
$$

The semilocal exchange is described by the Henderson-Janesko-Scuseria (HJS) model.[1,2] Its exchange enhancement factor $F_x(s, \mathcal{H}(s))$ depends on the rational function

$$
\mathcal{H}(s) = \frac{\sum_{k=2}^{7} a_k s^k}{\sum_{k=1}^{9} b_k s^k} \tag{2}
$$

with parameter $\{a_i, b_i\}$ and reduced density gradient s. The free parameter $\{a_i, b_i\}$ are adjusted to reproduce closely the PBEh-3c exchange enhancement factor[3,4]

$$
F_x^{\mathrm{PBEh-3c}} = 1 + \kappa \frac{\mu s^2}{\kappa + \mu s^2} . \tag{3}
$$

with numerical values $\kappa = 1.0245$ and $\mu = 10/81$. The parametrization strategy closely follows the reference Ref.[5]

TABLE S1. Empirical parameters of the HSE-3c method.

E_{xc}	a_x	ω	β_{PBE}	
	0.42	0.11	0.03	
HJS$_x$	a_1	a_2	a_3	a_4
	†1.0000000000	0.0000008986	0.0822661747	-0.1405847975
	a_5	a_6	a_7	b_1
	0.1488803147	-0.1058446440	0.0497445704	8.2051102554
	b_2	b_3	b_4	b_5
	-13.1479358747	11.7388225392	-4.6420352940	1.5681751604
	b_6	b_7	b_8	b_9
	-0.6467545549	0.4096383705	-0.0591716296	0.0274713086
E_{disp}	s_6	s_8	a_1	a_2
	†1.00000	†0.00000	0.44110	4.51820
E_{gCP}	σ	η	α	β
	†1.00000	1.40858	0.29083	1.95260

† Constrained value.

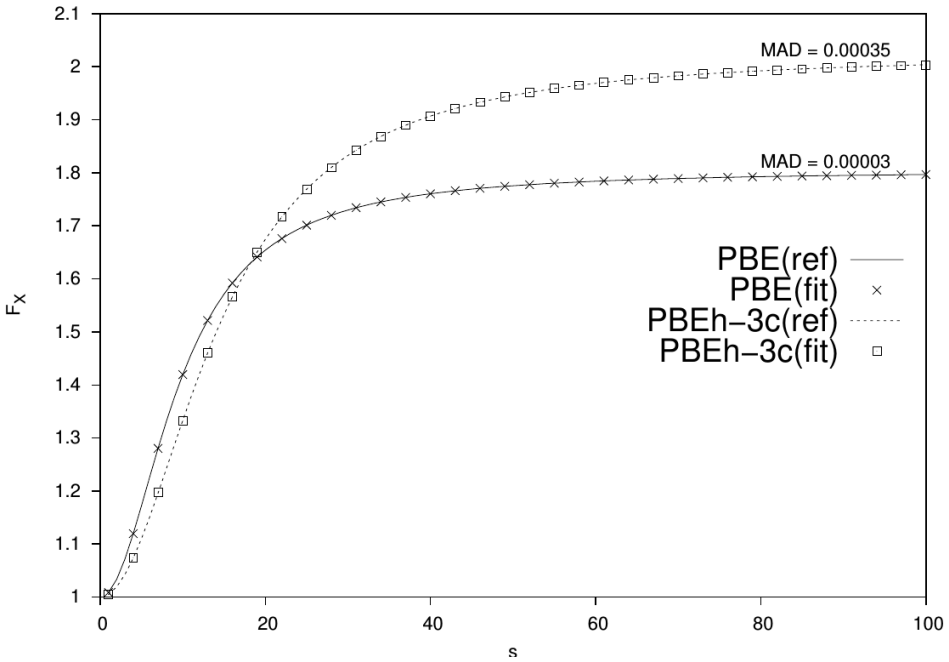

FIG. S1. Fitted HSJ enhancement factor as a function of the reduced density gradient for HSE06 and HSE-3c compared to the original PBE based reference.

In Fig. S1, we show the PBE based and fitted exchange enhancement factors. The fit has a small residual error compareable to the original HSE06 fit.

The HSE-3c exchange-correlation functional is evaluated in an unmodified small Gaussian orbital basis set of double-zeta quality. It is termed def2-mSVP as introduced in Ref. 4 and explicitly given in its ESI. Meanwhile it has been included in the TURBOMOMLE7.0 and ORCA3.1 program suites. The basis set in CRYTSAL format is provided in the tarball `def2msvp.tar.gz` and will be incuded in the next CRYSTAL version.

B. HSE-3c numerical example

CRYSTAL14 input examples for an HF-3c energy calculation of the benzene gas and solid phase are given below. They are intended for reproduction purposes, but also nicely show the usage of both point and space group symmetries. The calculation can be easily performed on a standard laptop and the resulting lattice energy is exceptionally close to the CCSD(T) reference of 13.2 kcal/mol.

```
!bz crystal
CRYSTAL
0 0 0
61
6.74427800429    7.30691991654    9.20995113206
6
6     0.36613211915     0.42927345151     0.40050928261
6     0.37153521385     0.36024420645     0.54092538074
6     0.49463808953     0.56843592353     0.35936193107
1     0.26045760036     0.37519728840     0.32328723077
1     0.49000991264     0.62141055688     0.24960361303
1     0.27174746575     0.25066643035     0.57135759632
BASISSET
def2-mSVP
DFT
HSE-3c
END
SHRINK
0 0
4 4 4
END
```

```
!bz gas
MOLECULE
40
2
6      1.201622903718     0.693757306926     0.000000000000
1      2.138625514345     1.234736016402     0.000000000000
BASISSET
def2-mSVP
DFT
HSE-3c
END
END
```

The different energy contributions are summarized in Table S2. Different numerical integration grids may lead to slightly different absolute energies. However, the relative energies should be less sensitive.

TABLE S2. Total and relative energies of HSE-3c for the gas and solid phase of benzene.

	gas [a.u.]	solid [a.u.]	relative [kcal/mol]
HSE/def2-mSVP	-231.7435401518	-927.0073324188	-5.20
D3	-0.0068628129	-0.0853526231	-9.08
gCP	0.0148400663	0.0668904983	1.18
HSE-3c	-231.7355628984	-927.0257945437	-13.11

C. Technical Details of Benchmark Calculations

All calculations were carried out with a development version of CRYSTAL14.[6] It is the ideal choice for cost effective DFT calculations in small basis sets as it can exploit full point and space group symmetry. The Brillouin zone is sampled with a Γ-centered k-mesh with grid density of approximately 0.025 $Å^{-1}$ (for details see references[7,8]). Standard integral thresholds and large DFT integration grids were used. The calculation of the D3(BJ)[9,10] dispersion correction and the gCP BSSE correction[11] were carried out with our own programs `dftd3` and `gcp`, respectively. These programs are freely available from our website[12]. The D3 energy calculations are all performed in the rational Becke-Johnson samping scheme and include the three-body Axilrog-Teller-Muto term. The basis sets and the compound DFT keyword HSE-3c have been implemented in CRYSTAL14 and will be available in the next release. The results for the estimated CBS were taken from previous work and were conducted with a projector-augmented plane-wave (PAW[13,14]) basis set with large energy cutoff of 1000 eV as implemented in VASP 5.3.[15,16] Note that the inclusion of the three-body term and the rational damping can lead to deviations from other errors reported in the literature, e.g. for TPSS-D3 and PBE0-D3 on the GMTKN subsets.

In some cases (e.g., for anions) it is necessary to add diffuse functions for specific atoms as usual. According to some test calculations for HSE-3c it seems to be the most robust

strategy to keep the gCP parameters in this case. The gCP program prints out a warning about this basis set mismatch and there are small inconsistencies in the treatment of BSSE. In particular, NCIs may be described less well for such choices because of the subtle balance of gCP and D3 correction terms (which are numerically of different sign).
For the computation of thermodynamic properties, we propose to use HSE-3c frequencies scaled by a factor of 0.95. The scaling was adjusted to reproduce the experimental heat capacities of ten small organic molecules (formic acid, butane, ethyne, ammonia, tetramethylsilane, benzene, acetone, and neopentane).[17]

D. Extended statistical measures

As statistical measure for a set $\{x_1, \ldots, x_n\}$ of data points with references $\{r_1, \ldots, r_n\}$ we use

- Mean deviation (MD): $MD = \frac{1}{n} \sum_i (x_i - r_i)$
- Mean absolute deviation (MAD): $MAD = \frac{1}{n} \sum_i |x_i - r_i|$
- Standard deviation (SD): $SD = \sqrt{\frac{1}{n-1} \sum_i (x_i - r_i - MD)^2}$
- Maximum absolute deviation (MAX): $MAX = \max \{|x_i - r_i|\}$

TABLE S3. MD, MAD, SD, and MAX of the methods HSE-3c, PBEh-3c, and HSE06/mSVP for the benchmark sets LMGB35, HMGB11, and TMC32. As perspective for converged basis sets, we give TPSS-D3/def2-QZVP and PBE0-D3/def2-QZVP results.

	def2-mSVP			**def2-QZVP**	
	HSE-3c	PBEh-3c	HSE06	TPSS-D3	PBE0-D3
			LMGB35 [pm]		
			Structures and reference from ref.[4]		
MD	-0.3	-0.6	0.7	0.7	-0.6
MAD	0.9	0.9	1.1	0.8	0.9
SD	1.6	1.5	1.3	0.6	1.3
MAX	6.9	5.3	6.3	3.0	4.5
			HMGB11 [pm]		
			Structures and reference from ref.[4]		
MD	0.3	-0.2	0.1	1.7	-0.3
MAD	0.9	0.8	0.9	1.8	1.0
SD	1.3	1.2	1.4	1.3	1.2
MAX	2.4	2.2	3.2	3.6	2.2
			TMC32 [pm]		
			Structures and reference from ref.[18]		
MD	-3.1	-2.7	-2.6	-0.3	-0.5
MAD	3.5	3.3	2.8	1.8	1.4
SD	2.6	2.7	1.9	3.0	1.9
MAX	7.5	10.5	6.5	12.6	7.0
			ROT34 [%]		
			Structures and reference from ref.[19,20]		
MD	-0.2	0.2	-0.4	1.2	-0.1
MAD	0.4	0.4	0.6	1.2	0.3
SD	0.5	0.5	0.6	0.5	0.3
MAX	1.3	1.2	1.6	3.2	0.9

TABLE S4. MD, MAD, SD, and MAX of the methods HSE-3c, PBEh-3c, and HSE06/mSVP for the benchmark sets S22, L7, IDISP, ADIM6, XCONF. As perspective for converged basis sets, we give TPSS-D3/def2-QZVP and PBE0-D3/def2-QZVP results. MD > 0 denotes underbound systems.

	def2-mSVP			**def2-QZVP**	
	HSE-3c	PBEh-3c	HSE06	TPSS-D3	PBE0-D3
	S22 [kcal/mol]				
	Structures from ref.[21] with reference energies from ref.[22]				
MD	-0.2	-0.1	0.2	0.0	-0.3
MAD	0.4	0.4	2.4	0.4	0.5
SD	0.5	0.6	3.1	0.6	0.7
MAX	1.4	1.4	6.0	1.5	1.8
	L7 [kcal/mol]				
	Structures from ref.[23] with reference energies from ref.[24]				
	because PBE0 data not available replaced by PW6B95				
MD	1.0	1.3	9.8	0.9	1.4
MAD	1.9	1.8	10.9	1.1	1.6
SD	2.4	2.2	8.7	1.2	1.2
MAX	4.4	4.5	21.9	2.8	3.0
	IDISP [kcal/mol]				
	Structures from ref.[25] with reference energies from ref.[26]				
MD	-2.1	-2.6	0.8	2.9	0.7
MAD	2.4	3.0	6.1	2.9	1.3
SD	2.3	2.9	7.1	3.4	1.8
MAX	4.5	7.0	8.6	9.3	3.4
	ADIM6 [kcal/mol]				
	Structures from ref.[25] with reference energies from ref.[27]				
MD	-0.2	0.0	-2.4	0.3	0.1
MAD	0.2	0.0	2.4	0.3	0.1
SD	0.1	0.0	1.1	0.2	0.1
MAX	0.4	0.1	3.9	0.6	0.1

TABLE S5. MD, MAD, SD, and MAX of the methods HSE-3c, PBEh-3c, and HSE06/mSVP for the benchmark sets PCONF, ACONF, SCONF, CYCONF, and XCONF. As perspective for converged basis sets, we give TPSS-D3/def2-QZVP and PBE0-D3/def2-QZVP results. MD > 0 denotes underbound systems.

	def2-mSVP			**def2-QZVP**	
	HSE-3c	PBEh-3c	HSE06	TPSS-D3	PBE0-D3
			PCONF [kcal/mol]		
			Structures and reference energies from ref.[25]		
MD	0.2	-0.0	-1.4	-1.6	-1.3
MAD	0.8	0.8	1.4	1.6	1.3
SD	1.0	0.9	0.6	0.8	0.5
MAX	1.6	1.5	2.2	2.6	1.9
			ACONF [kcal/mol]		
			Structures and reference energies from ref.[25]		
MD	-0.3	-0.3	0.1	-0.1	0.1
MAD	0.3	0.3	0.1	0.1	0.1
SD	0.1	0.2	0.2	0.1	0.1
MAX	0.6	0.8	0.5	0.2	0.2
			SCONF [kcal/mol]		
			Structures and reference energies from ref.[25]		
MD	-0.5	-0.4	1.3	0.1	-0.2
MAD	0.5	0.4	2.9	0.7	0.3
SD	0.5	0.4	3.0	1.1	0.3
MAX	1.4	1.4	6.5	3.0	1.1
			CYCONF [kcal/mol]		
			Structures and reference energies from ref.[25]		
MD	1.4	1.5	1.3	0.9	0.6
MAD	1.4	1.5	1.3	0.9	0.6
SD	0.9	0.9	0.6	0.8	0.5
MAX	2.6	2.8	2.6	1.6	1.1
			YMPJ [kcal/mol]		
			Structures and reference energies from ref.[28]		
MD	-0.7	-0.7	0.9	-0.0	0.2
MAD	1.1	1.1	1.0	0.5	0.4
SD	0.7	0.7	0.7	0.5	0.3
MAX	2.1	2.1	2.2	1.2	1.0

TABLE S6. M(R)D, M(R)AD, SD, and MAX of the methods HSE-3c, PBEh-3c, and HSE06/mSVP for the benchmark sets S66 and X23. As perspective for converged basis sets, we give TPSS-D3/def2-QZVP and TPSS-D3/PAW(1000eV) results.

	def2-mSVP			**PAW(1000eV)**
	HSE-3c	PBEh-3c	HSE06	TPSS-D3
	S66-CMA [%]			
	Structures from ref.[29] with reference energies from ref.[30]			
MD	0.6	0.8	0.7	1.4
MAD	1.5	1.5	5.2	1.7
SD	1.8	1.8	19.8	1.9
MAX	4.2	4.6	96.2	5.3
	S66-INT [kcal/mol]			
	Structures from ref.[29] with reference energies from ref.[30]			
MD	0.3	0.1	-0.3	0.0
MAD	0.5	0.5	2.2	0.3
SD	0.6	0.6	2.6	0.4
MAX	2.3	2.1	6.3	1.3
	X23-DENS [%]			
	Structures and references as listed in ref.[31]			
MD	-1.4	-1.8	-8.3	-3.8
MAD	2.6	2.7	8.4	3.8
SD	3.2	3.2	6.3	1.3
MAX	7.8	10.2	17.9	5.5
	X23-INT [kcal/mol]			
	Structures and references as listed in ref.[31]			
MD	0.3	0.1	-3.8	1.0
MAD	1.3	1.3	4.9	1.1
SD	1.6	1.7	5.9	0.7
MAX	3.8	3.7	19.9	2.3

E. X23 unit cell volumes

TABLE S7: Equilibrium volumes per molecule for the X23[8,32] test set of organic solids with various method combinations in Å^3. References as given in Ref. 4, TPSS values are taken from Refs. 33.

	ref	HSE-3c	PBEh-3c	HSE06/mSVP	TPSS-D3/'CBS'
X23: vdW bonded					
1 cyclohexanedione	136	145	144	160	138
2 CO_2	43	44	44	35	50
3 adamantane	191	192	190	231	191
4 hexamine	163	167	168	181	167
5 trioxane	100	109	110	103	103
6 anthracene	223	212	–	259	218
7 naphtalene	166	166	–	196	165
8 benzene	115	113	115	140	113
9 pyracine	99	98	98	118	97
10 triazine	96	90	92	103	92
X23: hydrogen bonded					
11 pyrazole	86	88	88	101	87
12 imidazole	85	85	86	102	86
13 acetic acid	72	75	76	76	76
14 ammonia	32	32	32	32	31
15 cyanamide	50	51	51	55	51
16 cytosine	116	115	114	129	113
17 ethylcarbanate	120	124	124	125	122
18 formamide	55	57	57	58	56
19 oxalic acid α	77	78	78	77	78
20 oxalic acid β	77	78	78	77	80

21 succinic acid	119	125	126	124	123
22 uracil	116	114	115	121	113
23 urea	71	76	70	72	71

F. X23 lattice energies

TABLE S8: Lattice energies for the X23[8,32] test sets of organic solids with various method combinations in kcal/mol. References as given in Ref. 31, TPSS values are taken from Refs. 33.

	ref	HSE-3c	PBEh-3c	HSE06/mSVP	TPSS-D3/'CBS'
X23: vdW bonded					
1 cyclohexanedione	21.2	19.6	19.8	15.6	19.7
2 CO_2	6.5	6.9	6.8	5.3	5.3
3 adamantane	16.6	14.4	15.9	2.7	14.9
4 hexamine	20.6	23.1	22.4	12.9	19.0
5 trioxane	15.9	14.9	14.1	12.7	13.2
6 anthracene	26.9	25.0	–	7.1	24.8
7 naphtalene	19.5	19.0	–	5.5	18.4
8 benzene	13.2	13.2	12.5	5.3	12.3
9 pyracine	14.7	16.0	16.0	9.6	14.9
10 triazine	14.8	15.5	14.4	8.4	13.7
X23: hydrogen bonded					
11 pyrazole	18.6	19.7	19.4	15.4	18.6
12 imidazole	20.8	22.8	22.5	18.2	21.1
13 acetic acid	17.4	17.5	15.7	17.5	15.8
14 ammonia	8.9	12.7	12.6	12.6	9.2
15 cyanamide	19.1	22.2	21.8	19.8	21.2
16 cytosine	38.6	38.6	36.5	34.3	36.7
17 ethylcarbanate	20.6	20.0	19.7	19.2	20.0
18 formamide	18.9	19.0	18.8	20.6	19.2
19 oxalic acid α	23.0	24.6	24.1	24.4	21.3
20 oxalic acid β	23.0	24.2	24.1	24.2	22.1

21 succinic acid	31.1	29.2	28.5	30.9	29.8
22 uracil	32.4	31.0	30.3	29.5	32.6
23 urea	24.5	24.9	25.2	28.3	26.0

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G. Adenine-thymine double helix structure

Geometry of Adenine-thymine double helix structure given in CRYSTAL14 format with explicit definition of eleven rotational translational symmetry operations.

```
  1    1    1
0.342098975469E+02 0.000000000000E+00 0.000000000000E+00
```

0.000000000000E+00 0.500000000000E+03 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.500000000000E+03
11
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
-0.233842846846E-16 0.841253532831E+00 -0.540640817456E+00
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0.233842846846E-16 -0.540640817456E+00 0.841253532831E+00
0.310999068607E+02 0.000000000000E+00 0.000000000000E+00
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
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0.155499534305E+02 0.000000000000E+00 0.000000000000E+00
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
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0.279899161747E+02 0.000000000000E+00 0.000000000000E+00
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0.621998137215E+01 0.000000000000E+00 0.000000000000E+00

66

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8	-0.092020554507	1.034492630088	-10.343321875665
8	-0.682511976823	3.022484496213	-9.048144360747
6	-1.483348313453	4.093973977487	-8.557506672746
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8	-0.955803236054	3.571532310220	-6.290249725498
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8	0.591020768779	6.434296528477	-7.388121403182
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6	0.039687434617	3.835964802781	-5.326840704842
7	0.282672561686	2.643777039997	-4.580072841891
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6	0.265314288012	0.737780465114	-1.647610557282
7	0.376705616848	-0.538675144159	-1.284331779984
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6	-0.059685686252	2.963653555300	-1.093641029293
7	-0.038776354285	3.452769971790	-2.318794114288
6	0.172256592812	2.504767061754	-3.222937954772
1	0.173532176276	-0.816452146844	-0.332624103991
1	0.356288457582	-1.243366872300	-1.999344886779
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8	0.883863514648	2.849047784040	6.007598248003
6	-0.749451531989	3.759056024146	7.384340571243
8	-1.240846516189	4.940973007206	8.008914562458
6	-1.393160050932	3.380396381631	6.044108524926
6	-0.187666059689	3.124166238063	5.125623451089
7	-0.326964831978	2.040161248165	4.196317303335
6	-0.110581107591	2.279550923980	2.840927686152
8	0.074716888835	3.388144229570	2.395925505991
7	-0.141913641346	1.161178122608	2.055178921543
6	-0.388318583299	-0.132734309943	2.448722849610
8	-0.340646087880	-1.060044393206	1.658516396981
6	-0.699501142462	-0.300608423109	3.861032959924
6	-1.125721946203	-1.644581888884	4.342861264981
6	-0.633430603594	0.783056220445	4.646936586604
1	-0.006429304210	1.336813460783	1.030454262978

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1	-0.202021381287	3.668882511915	-0.285478276740
1	1.572190525141	4.169186190107	8.980457047229
1	2.708796957536	3.394886013936	7.871865768386
1	1.071116192481	4.771586523924	6.723159642754
1	-0.950557277729	2.981326086268	8.119922841186
1	-2.017246356621	2.493439110906	6.155754441229
1	-2.018801610766	4.166986965062	5.637620127634
1	0.025217017514	4.014963009564	4.531095325887
1	-1.291465435248	-1.644855420823	5.420468599016
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1	-0.384546027038	-2.408479634784	4.108420226760
1	-0.840395895035	0.708480473929	5.705565336879
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1	1.622466105948	1.552473583847	11.913208226523

Geometry of Adenine-thymine double helix structure given in cif format where the cell parameter of the non-periodic directions have been formally set to 50 Å.

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_cell_angle_gamma        90

_symmetry_space_group_name_H-M P 1
_symmetry_int_tables_number       1

loop_
   _symmetry_equiv_pos_as_xyz
   'x, y, z'

loop_
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   _atom_site_occupancy
    _atom_site_fract_x
    _atom_site_fract_y
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_atom_site_fract_z
_atom_site_thermal_displace_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol

H1	1.0000	0.00507	0.98367	0.99335	Biso	1.000	H
H2	1.0000	0.09598	0.98986	0.98558	Biso	1.000	H
H3	1.0000	0.91416	0.98267	0.00323	Biso	1.000	H
H4	1.0000	0.27780	0.00891	0.98478	Biso	1.000	H
H5	1.0000	0.73235	0.99574	0.01711	Biso	1.000	H
H6	1.0000	0.45962	0.01754	0.00178	Biso	1.000	H
H7	1.0000	0.55053	0.01379	0.01098	Biso	1.000	H
H8	1.0000	0.64144	0.00567	0.01670	Biso	1.000	H
H9	1.0000	0.36871	0.01572	0.99202	Biso	1.000	H
H10	1.0000	0.82325	0.98717	0.01209	Biso	1.000	H
H11	1.0000	0.18689	0.99927	0.98238	Biso	1.000	H
H12	1.0000	0.01041	0.97513	0.96001	Biso	1.000	H
H13	1.0000	0.10132	0.00070	0.95292	Biso	1.000	H
H14	1.0000	0.91951	0.95746	0.97981	Biso	1.000	H
H15	1.0000	0.28314	0.04312	0.98108	Biso	1.000	H
H16	1.0000	0.73769	0.96396	0.03030	Biso	1.000	H
H17	1.0000	0.46496	0.03513	0.03136	Biso	1.000	H
H18	1.0000	0.55587	0.01259	0.04537	Biso	1.000	H
H19	1.0000	0.64678	0.98606	0.04498	Biso	1.000	H
H20	1.0000	0.37405	0.04650	0.00739	Biso	1.000	H
H21	1.0000	0.82860	0.95330	0.00601	Biso	1.000	H
H22	1.0000	0.19223	0.02604	0.96077	Biso	1.000	H
H23	1.0000	0.99981	0.02674	0.02061	Biso	1.000	H
H24	1.0000	0.09072	0.01135	0.03179	Biso	1.000	H
H25	1.0000	0.90890	0.03363	0.00288	Biso	1.000	H
H26	1.0000	0.27254	0.97580	0.02353	Biso	1.000	H
H27	1.0000	0.72708	0.01659	0.97060	Biso	1.000	H
H28	1.0000	0.45436	0.96854	0.98776	Biso	1.000	H
H29	1.0000	0.54527	0.98015	0.97269	Biso	1.000	H
H30	1.0000	0.63618	0.99807	0.96630	Biso	1.000	H
H31	1.0000	0.36345	0.96692	0.00671	Biso	1.000	H
H32	1.0000	0.81799	0.02985	0.98424	Biso	1.000	H
H33	1.0000	0.18163	0.99236	0.03288	Biso	1.000	H
H34	1.0000	0.95620	0.09837	0.81450	Biso	1.000	H
H35	1.0000	0.04711	0.18305	0.89713	Biso	1.000	H
H36	1.0000	0.86529	0.98246	0.79076	Biso	1.000	H
H37	1.0000	0.22892	0.16962	0.12377	Biso	1.000	H
H38	1.0000	0.68347	0.80238	0.92903	Biso	1.000	H
H39	1.0000	0.41074	0.95788	0.20570	Biso	1.000	H
H40	1.0000	0.50165	0.85335	0.15028	Biso	1.000	H
H41	1.0000	0.59256	0.79539	0.04714	Biso	1.000	H
H42	1.0000	0.31983	0.07578	0.19582	Biso	1.000	H

H43	1.0000	0.77438	0.87212	0.83346	Biso	1.000	H
H44	1.0000	0.13802	0.20961	0.01242	Biso	1.000	H
H45	1.0000	0.92646	0.07542	0.83212	Biso	1.000	H
H46	1.0000	0.01737	0.15421	0.89955	Biso	1.000	H
H47	1.0000	0.83555	0.97269	0.81800	Biso	1.000	H
H48	1.0000	0.19919	0.15543	0.09855	Biso	1.000	H
H49	1.0000	0.65373	0.82310	0.94924	Biso	1.000	H
H50	1.0000	0.38100	0.97493	0.18232	Biso	1.000	H
H51	1.0000	0.47191	0.88034	0.13983	Biso	1.000	H
H52	1.0000	0.56282	0.82374	0.05293	Biso	1.000	H
H53	1.0000	0.29010	0.07748	0.16694	Biso	1.000	H
H54	1.0000	0.74464	0.87863	0.86166	Biso	1.000	H
H55	1.0000	0.10828	0.18404	0.99887	Biso	1.000	H
H56	1.0000	0.95689	0.10917	0.86106	Biso	1.000	H
H57	1.0000	0.04780	0.16696	0.94214	Biso	1.000	H
H58	1.0000	0.86598	0.01673	0.82410	Biso	1.000	H
H59	1.0000	0.22962	0.12198	0.12783	Biso	1.000	H
H60	1.0000	0.68416	0.84694	0.91171	Biso	1.000	H
H61	1.0000	0.41143	0.93439	0.16406	Biso	1.000	H
H62	1.0000	0.50234	0.85611	0.10255	Biso	1.000	H
H63	1.0000	0.59325	0.82351	0.00848	Biso	1.000	H
H64	1.0000	0.32052	0.03351	0.17349	Biso	1.000	H
H65	1.0000	0.77507	0.91897	0.84298	Biso	1.000	H
H66	1.0000	0.13871	0.17173	0.04159	Biso	1.000	H
H67	1.0000	0.03075	0.09291	0.83446	Biso	1.000	H
H68	1.0000	0.12166	0.16766	0.91097	Biso	1.000	H
H69	1.0000	0.93984	0.98867	0.81051	Biso	1.000	H
H70	1.0000	0.30347	0.15063	0.11553	Biso	1.000	H
H71	1.0000	0.75802	0.82292	0.93159	Biso	1.000	H
H72	1.0000	0.48529	0.95749	0.18501	Biso	1.000	H
H73	1.0000	0.57620	0.86421	0.13266	Biso	1.000	H
H74	1.0000	0.66711	0.81405	0.03819	Biso	1.000	H
H75	1.0000	0.39438	0.06426	0.17862	Biso	1.000	H
H76	1.0000	0.84893	0.88802	0.84672	Biso	1.000	H
H77	1.0000	0.21257	0.18918	0.01575	Biso	1.000	H
H78	1.0000	0.05421	0.07031	0.87082	Biso	1.000	H
H79	1.0000	0.14512	0.12899	0.92934	Biso	1.000	H
H80	1.0000	0.96330	0.98931	0.85331	Biso	1.000	H
H81	1.0000	0.32694	0.11786	0.08798	Biso	1.000	H
H82	1.0000	0.78148	0.86213	0.94878	Biso	1.000	H
H83	1.0000	0.50876	0.96893	0.14375	Biso	1.000	H
H84	1.0000	0.59967	0.89614	0.10413	Biso	1.000	H
H85	1.0000	0.69057	0.85633	0.03145	Biso	1.000	H
H86	1.0000	0.41785	0.05158	0.13773	Biso	1.000	H
H87	1.0000	0.87239	0.91171	0.88238	Biso	1.000	H
H88	1.0000	0.23603	0.14671	0.01030	Biso	1.000	H

H89	1.0000	0.05402	0.10039	0.88904	Biso	1.000	H
H90	1.0000	0.14493	0.14444	0.96092	Biso	1.000	H
H91	1.0000	0.96311	0.02446	0.85238	Biso	1.000	H
H92	1.0000	0.32675	0.09555	0.11516	Biso	1.000	H
H93	1.0000	0.78130	0.87588	0.91643	Biso	1.000	H
H94	1.0000	0.50857	0.93494	0.13475	Biso	1.000	H
H95	1.0000	0.59948	0.87242	0.07819	Biso	1.000	H
H96	1.0000	0.69039	0.85040	0.99680	Biso	1.000	H
H97	1.0000	0.41766	0.01812	0.14853	Biso	1.000	H
H98	1.0000	0.87220	0.94077	0.86259	Biso	1.000	H
H99	1.0000	0.23584	0.14264	0.04522	Biso	1.000	H
H100	1.0000	0.99147	0.09178	0.90794	Biso	1.000	H
H101	1.0000	0.08238	0.12698	0.97217	Biso	1.000	H
H102	1.0000	0.90056	0.02744	0.87294	Biso	1.000	H
H103	1.0000	0.26419	0.07806	0.10394	Biso	1.000	H
H104	1.0000	0.71874	0.89582	0.92226	Biso	1.000	H
H105	1.0000	0.44601	0.93788	0.11418	Biso	1.000	H
H106	1.0000	0.53692	0.88601	0.06247	Biso	1.000	H
H107	1.0000	0.62783	0.87033	0.99093	Biso	1.000	H
H108	1.0000	0.35510	0.00947	0.12964	Biso	1.000	H
H109	1.0000	0.80965	0.95439	0.87828	Biso	1.000	H
H110	1.0000	0.17328	0.12186	0.04524	Biso	1.000	H
H111	1.0000	0.01998	0.02423	0.87748	Biso	1.000	H
H112	1.0000	0.11089	0.08662	0.91003	Biso	1.000	H
H113	1.0000	0.92907	0.95414	0.88383	Biso	1.000	H
H114	1.0000	0.29270	0.11783	0.04142	Biso	1.000	H
H115	1.0000	0.74725	0.87528	0.99346	Biso	1.000	H
H116	1.0000	0.47452	0.01127	0.12439	Biso	1.000	H
H117	1.0000	0.56543	0.94224	0.11073	Biso	1.000	H
H118	1.0000	0.65634	0.89154	0.06193	Biso	1.000	H
H119	1.0000	0.38361	0.07673	0.09854	Biso	1.000	H
H120	1.0000	0.83816	0.89861	0.92706	Biso	1.000	H
H121	1.0000	0.20180	0.12151	0.97114	Biso	1.000	H
H122	1.0000	0.99409	0.07338	0.99429	Biso	1.000	H
H123	1.0000	0.08500	0.06482	0.03487	Biso	1.000	H
H124	1.0000	0.90319	0.05864	0.95553	Biso	1.000	H
H125	1.0000	0.26682	0.99521	0.07344	Biso	1.000	H
H126	1.0000	0.72137	0.98391	0.92818	Biso	1.000	H
H127	1.0000	0.44864	0.93120	0.02615	Biso	1.000	H
H128	1.0000	0.53955	0.92799	0.98481	Biso	1.000	H
H129	1.0000	0.63046	0.94763	0.94828	Biso	1.000	H
H130	1.0000	0.35773	0.95626	0.05919	Biso	1.000	H
H131	1.0000	0.81228	0.02529	0.93088	Biso	1.000	H
H132	1.0000	0.17591	0.03568	0.06437	Biso	1.000	H
H133	1.0000	0.04596	0.08338	0.17961	Biso	1.000	H
H134	1.0000	0.13687	0.97304	0.19618	Biso	1.000	H

H135	1.0000	0.95505	0.16725	0.10602	Biso	1.000	H
H136	1.0000	0.31868	0.81035	0.05697	Biso	1.000	H
H137	1.0000	0.77323	0.16591	0.89190	Biso	1.000	H
H138	1.0000	0.50050	0.86939	0.85116	Biso	1.000	H
H139	1.0000	0.59141	0.97060	0.80417	Biso	1.000	H
H140	1.0000	0.68232	0.08113	0.81936	Biso	1.000	H
H141	1.0000	0.40959	0.80966	0.94540	Biso	1.000	H
H142	1.0000	0.86414	0.19802	0.99876	Biso	1.000	H
H143	1.0000	0.22778	0.87126	0.15046	Biso	1.000	H
H144	1.0000	0.07918	0.06790	0.15744	Biso	1.000	H
H145	1.0000	0.17009	0.97200	0.16915	Biso	1.000	H
H146	1.0000	0.98827	0.14224	0.09574	Biso	1.000	H
H147	1.0000	0.35191	0.83450	0.04480	Biso	1.000	H
H148	1.0000	0.80645	0.14617	0.91039	Biso	1.000	H
H149	1.0000	0.53373	0.89050	0.86807	Biso	1.000	H
H150	1.0000	0.62464	0.97921	0.82981	Biso	1.000	H
H151	1.0000	0.71555	0.07452	0.84559	Biso	1.000	H
H152	1.0000	0.44282	0.83655	0.94821	Biso	1.000	H
H153	1.0000	0.89736	0.17142	0.00364	Biso	1.000	H
H154	1.0000	0.26100	0.88500	0.12716	Biso	1.000	H
H155	1.0000	0.03131	0.09543	0.13446	Biso	1.000	H
H156	1.0000	0.12222	0.00759	0.16471	Biso	1.000	H
H157	1.0000	0.94040	0.15298	0.06152	Biso	1.000	H
H158	1.0000	0.30404	0.85332	0.07532	Biso	1.000	H
H159	1.0000	0.75858	0.11951	0.88640	Biso	1.000	H
H160	1.0000	0.48586	0.87055	0.89787	Biso	1.000	H
H161	1.0000	0.57676	0.94632	0.84410	Biso	1.000	H
H162	1.0000	0.66767	0.03913	0.83982	Biso	1.000	H
H163	1.0000	0.39495	0.83589	0.98407	Biso	1.000	H
H164	1.0000	0.84949	0.16196	0.96905	Biso	1.000	H
H165	1.0000	0.21313	0.91733	0.14267	Biso	1.000	H
H166	1.0000	0.97221	0.05963	0.16240	Biso	1.000	H
H167	1.0000	0.06312	0.96236	0.16885	Biso	1.000	H
H168	1.0000	0.88130	0.13796	0.10438	Biso	1.000	H
H169	1.0000	0.24494	0.83077	0.03591	Biso	1.000	H
H170	1.0000	0.69949	0.15226	0.91787	Biso	1.000	H
H171	1.0000	0.42676	0.89704	0.86098	Biso	1.000	H
H172	1.0000	0.51767	0.98854	0.82738	Biso	1.000	H
H173	1.0000	0.60858	0.08369	0.84859	Biso	1.000	H
H174	1.0000	0.33585	0.83822	0.93871	Biso	1.000	H
H175	1.0000	0.79040	0.17249	0.01322	Biso	1.000	H
H176	1.0000	0.15403	0.87705	0.12170	Biso	1.000	H
H177	1.0000	0.94103	0.04987	0.12312	Biso	1.000	H
H178	1.0000	0.03194	0.97539	0.13053	Biso	1.000	H
H179	1.0000	0.85012	0.10851	0.07661	Biso	1.000	H
H180	1.0000	0.21376	0.87104	0.03184	Biso	1.000	H

H181	1.0000	0.66831	0.11476	0.93312	Biso	1.000	H
H182	1.0000	0.39558	0.91747	0.89592	Biso	1.000	H
H183	1.0000	0.48649	0.98684	0.86782	Biso	1.000	H
H184	1.0000	0.57740	0.06039	0.88169	Biso	1.000	H
H185	1.0000	0.30467	0.87430	0.95707	Biso	1.000	H
H186	1.0000	0.75922	0.13271	0.00578	Biso	1.000	H
H187	1.0000	0.12285	0.90873	0.09651	Biso	1.000	H
H188	1.0000	0.94099	0.08334	0.11275	Biso	1.000	H
H189	1.0000	0.03190	0.00915	0.13991	Biso	1.000	H
H190	1.0000	0.85008	0.13107	0.04980	Biso	1.000	H
H191	1.0000	0.21372	0.87653	0.06645	Biso	1.000	H
H192	1.0000	0.66826	0.09974	0.90146	Biso	1.000	H
H193	1.0000	0.39553	0.88827	0.91529	Biso	1.000	H
H194	1.0000	0.48644	0.95180	0.86834	Biso	1.000	H
H195	1.0000	0.57735	0.03064	0.86318	Biso	1.000	H
H196	1.0000	0.30462	0.86021	0.98915	Biso	1.000	H
H197	1.0000	0.75917	0.13718	0.97103	Biso	1.000	H
H198	1.0000	0.12281	0.93206	0.12265	Biso	1.000	H
H199	1.0000	0.00074	0.08030	0.09062	Biso	1.000	H
H200	1.0000	0.09165	0.01856	0.11965	Biso	1.000	H
H201	1.0000	0.90983	0.11655	0.03282	Biso	1.000	H
H202	1.0000	0.27346	0.89887	0.06659	Biso	1.000	H
H203	1.0000	0.72801	0.07827	0.90762	Biso	1.000	H
H204	1.0000	0.45528	0.89742	0.93567	Biso	1.000	H
H205	1.0000	0.54619	0.94848	0.89043	Biso	1.000	H
H206	1.0000	0.63710	0.01590	0.87997	Biso	1.000	H
H207	1.0000	0.36437	0.87893	0.00134	Biso	1.000	H
H208	1.0000	0.81892	0.11579	0.96460	Biso	1.000	H
H209	1.0000	0.18256	0.95092	0.11069	Biso	1.000	H
H210	1.0000	0.96225	0.96710	0.10841	Biso	1.000	H
H211	1.0000	0.05316	0.91371	0.07341	Biso	1.000	H
H212	1.0000	0.87134	0.03094	0.10899	Biso	1.000	H
H213	1.0000	0.23498	0.89738	0.95201	Biso	1.000	H
H214	1.0000	0.68952	0.11199	0.01713	Biso	1.000	H
H215	1.0000	0.41679	0.00102	0.88671	Biso	1.000	H
H216	1.0000	0.50770	0.06211	0.90525	Biso	1.000	H
H217	1.0000	0.59861	0.10347	0.95387	Biso	1.000	H
H218	1.0000	0.32589	0.93961	0.90414	Biso	1.000	H
H219	1.0000	0.78043	0.08495	0.07496	Biso	1.000	H
H220	1.0000	0.14407	0.88772	0.01511	Biso	1.000	H
H221	1.0000	0.93989	0.96119	0.07713	Biso	1.000	H
H222	1.0000	0.03080	0.92565	0.04391	Biso	1.000	H
H223	1.0000	0.84898	0.00905	0.08587	Biso	1.000	H
H224	1.0000	0.21262	0.92918	0.95061	Biso	1.000	H
H225	1.0000	0.66716	0.08187	0.02744	Biso	1.000	H
H226	1.0000	0.39444	0.01551	0.91506	Biso	1.000	H

H227	1.0000	0.48534	0.05897	0.93693	Biso	1.000	H
H228	1.0000	0.57625	0.08371	0.97882	Biso	1.000	H
H229	1.0000	0.30353	0.96712	0.92016	Biso	1.000	H
H230	1.0000	0.75807	0.05404	0.06734	Biso	1.000	H
H231	1.0000	0.12171	0.91372	0.99674	Biso	1.000	H
H232	1.0000	0.98876	0.95183	0.08217	Biso	1.000	H
H233	1.0000	0.07967	0.91505	0.04308	Biso	1.000	H
H234	1.0000	0.89785	0.00390	0.09517	Biso	1.000	H
H235	1.0000	0.26149	0.92552	0.94063	Biso	1.000	H
H236	1.0000	0.71603	0.08819	0.03599	Biso	1.000	H
H237	1.0000	0.44330	0.02307	0.90759	Biso	1.000	H
H238	1.0000	0.53421	0.06937	0.93473	Biso	1.000	H
H239	1.0000	0.62512	0.09364	0.98260	Biso	1.000	H
H240	1.0000	0.35240	0.96945	0.90979	Biso	1.000	H
H241	1.0000	0.80694	0.05473	0.07795	Biso	1.000	H
H242	1.0000	0.17058	0.90525	0.99032	Biso	1.000	H
H243	1.0000	0.97543	0.01417	0.11411	Biso	1.000	H
H244	1.0000	0.06634	0.95023	0.10366	Biso	1.000	H
H245	1.0000	0.88453	0.07361	0.08834	Biso	1.000	H
H246	1.0000	0.24816	0.88503	0.99779	Biso	1.000	H
H247	1.0000	0.70271	0.11093	0.96973	Biso	1.000	H
H248	1.0000	0.42998	0.95426	0.89450	Biso	1.000	H
H249	1.0000	0.52089	0.01855	0.88652	Biso	1.000	H
H250	1.0000	0.61180	0.07696	0.91456	Biso	1.000	H
H251	1.0000	0.33907	0.90448	0.93598	Biso	1.000	H
H252	1.0000	0.79362	0.10969	0.03451	Biso	1.000	H
H253	1.0000	0.15725	0.90209	0.06029	Biso	1.000	H
H254	1.0000	0.00810	0.01889	0.77544	Biso	1.000	H
H255	1.0000	0.09901	0.13729	0.82130	Biso	1.000	H
H256	1.0000	0.91719	0.89448	0.80088	Biso	1.000	H
H257	1.0000	0.28082	0.21959	0.05065	Biso	1.000	H
H258	1.0000	0.73537	0.77504	0.01327	Biso	1.000	H
H259	1.0000	0.46264	0.04515	0.22078	Biso	1.000	H
H260	1.0000	0.55355	0.91861	0.21014	Biso	1.000	H
H261	1.0000	0.64446	0.81792	0.13278	Biso	1.000	H
H262	1.0000	0.37173	0.15734	0.16133	Biso	1.000	H
H263	1.0000	0.82628	0.80358	0.88954	Biso	1.000	H
H264	1.0000	0.18991	0.21211	0.92389	Biso	1.000	H
H265	1.0000	0.04743	0.03105	0.23826	Biso	1.000	H
H266	1.0000	0.13834	0.89731	0.21723	Biso	1.000	H
H267	1.0000	0.95652	0.15494	0.18365	Biso	1.000	H
H268	1.0000	0.32015	0.75974	0.99682	Biso	1.000	H
H269	1.0000	0.77470	0.23142	0.93536	Biso	1.000	H
H270	1.0000	0.50197	0.90308	0.78013	Biso	1.000	H
H271	1.0000	0.59288	0.03734	0.76264	Biso	1.000	H
H272	1.0000	0.68379	0.15973	0.82050	Biso	1.000	H

H273	1.0000	0.41106	0.79960	0.86744	Biso	1.000	H
H274	1.0000	0.86561	0.22963	0.07073	Biso	1.000	H
H275	1.0000	0.22924	0.79617	0.12722	Biso	1.000	H
C1	1.0000	0.95664	0.08188	0.82885	Biso	1.000	C
C2	1.0000	0.04755	0.16141	0.90029	Biso	1.000	C
C3	1.0000	0.86573	0.97635	0.81175	Biso	1.000	C
C4	1.0000	0.22937	0.15776	0.10540	Biso	1.000	C
C5	1.0000	0.68391	0.81894	0.94331	Biso	1.000	C
C6	1.0000	0.41119	0.96966	0.18729	Biso	1.000	C
C7	1.0000	0.50209	0.87322	0.14115	Biso	1.000	C
C8	1.0000	0.59300	0.81703	0.05020	Biso	1.000	C
C9	1.0000	0.32028	0.07573	0.17396	Biso	1.000	C
C10	1.0000	0.77482	0.87833	0.85442	Biso	1.000	C
C11	1.0000	0.13846	0.18970	0.00338	Biso	1.000	C
C12	1.0000	0.97392	0.09161	0.85478	Biso	1.000	C
C13	1.0000	0.06483	0.15558	0.92736	Biso	1.000	C
C14	1.0000	0.88301	0.99856	0.82830	Biso	1.000	C
C15	1.0000	0.24665	0.13071	0.11135	Biso	1.000	C
C16	1.0000	0.70119	0.84322	0.92999	Biso	1.000	C
C17	1.0000	0.42846	0.95301	0.16515	Biso	1.000	C
C18	1.0000	0.51937	0.87118	0.11353	Biso	1.000	C
C19	1.0000	0.61028	0.83026	0.02586	Biso	1.000	C
C20	1.0000	0.33755	0.04976	0.16434	Biso	1.000	C
C21	1.0000	0.79210	0.90596	0.85634	Biso	1.000	C
C22	1.0000	0.15574	0.17016	0.02301	Biso	1.000	C
C23	1.0000	0.01722	0.10017	0.85282	Biso	1.000	C
C24	1.0000	0.10813	0.16384	0.93035	Biso	1.000	C
C25	1.0000	0.92631	0.00470	0.82203	Biso	1.000	C
C26	1.0000	0.28995	0.13142	0.12010	Biso	1.000	C
C27	1.0000	0.74449	0.84006	0.92179	Biso	1.000	C
C28	1.0000	0.47176	0.94535	0.16944	Biso	1.000	C
C29	1.0000	0.56267	0.86242	0.11299	Biso	1.000	C
C30	1.0000	0.65358	0.82317	0.02067	Biso	1.000	C
C31	1.0000	0.38085	0.04563	0.17209	Biso	1.000	C
C32	1.0000	0.83540	0.90774	0.84774	Biso	1.000	C
C33	1.0000	0.19904	0.17549	0.02998	Biso	1.000	C
C34	1.0000	0.03595	0.08701	0.87723	Biso	1.000	C
C35	1.0000	0.12686	0.13957	0.94376	Biso	1.000	C
C36	1.0000	0.94504	0.00682	0.84968	Biso	1.000	C
C37	1.0000	0.30867	0.10914	0.10359	Biso	1.000	C
C38	1.0000	0.76322	0.86609	0.93135	Biso	1.000	C
C39	1.0000	0.49049	0.95111	0.14231	Biso	1.000	C
C40	1.0000	0.58140	0.88193	0.09329	Biso	1.000	C
C41	1.0000	0.67231	0.85024	0.01464	Biso	1.000	C
C42	1.0000	0.39958	0.03581	0.14616	Biso	1.000	C
C43	1.0000	0.85413	0.92447	0.86985	Biso	1.000	C

C44	1.0000	0.21776	0.14782	0.02814	Biso	1.000	C
C45	1.0000	0.00116	0.07672	0.89346	Biso	1.000	C
C46	1.0000	0.09207	0.12214	0.95185	Biso	1.000	C
C47	1.0000	0.91025	0.00694	0.86890	Biso	1.000	C
C48	1.0000	0.27389	0.09453	0.09110	Biso	1.000	C
C49	1.0000	0.72843	0.88363	0.93922	Biso	1.000	C
C50	1.0000	0.45571	0.95640	0.12384	Biso	1.000	C
C51	1.0000	0.54661	0.89637	0.08061	Biso	1.000	C
C52	1.0000	0.63752	0.86924	0.01179	Biso	1.000	C
C53	1.0000	0.36480	0.03027	0.12775	Biso	1.000	C
C54	1.0000	0.81934	0.93496	0.88596	Biso	1.000	C
C55	1.0000	0.18298	0.12878	0.02553	Biso	1.000	C
C56	1.0000	0.01575	0.02773	0.89857	Biso	1.000	C
C57	1.0000	0.10665	0.07816	0.92966	Biso	1.000	C
C58	1.0000	0.92484	0.96849	0.89968	Biso	1.000	C
C59	1.0000	0.28847	0.09645	0.04188	Biso	1.000	C
C60	1.0000	0.74302	0.89566	0.98699	Biso	1.000	C
C61	1.0000	0.47029	0.00197	0.10513	Biso	1.000	C
C62	1.0000	0.56120	0.94482	0.08951	Biso	1.000	C
C63	1.0000	0.65211	0.90519	0.04547	Biso	1.000	C
C64	1.0000	0.37938	0.05850	0.08738	Biso	1.000	C
C65	1.0000	0.83393	0.91926	0.93264	Biso	1.000	C
C66	1.0000	0.19756	0.10378	0.98309	Biso	1.000	C
C67	1.0000	0.01043	0.02308	0.94028	Biso	1.000	C
C68	1.0000	0.10133	0.05170	0.96224	Biso	1.000	C
C69	1.0000	0.91952	0.98713	0.93728	Biso	1.000	C
C70	1.0000	0.28315	0.05583	0.03135	Biso	1.000	C
C71	1.0000	0.73770	0.93760	0.98565	Biso	1.000	C
C72	1.0000	0.46497	0.99468	0.06380	Biso	1.000	C
C73	1.0000	0.55588	0.96103	0.05080	Biso	1.000	C
C74	1.0000	0.64679	0.93975	0.02166	Biso	1.000	C
C75	1.0000	0.37406	0.03002	0.05655	Biso	1.000	C
C76	1.0000	0.82861	0.95527	0.95420	Biso	1.000	C
C77	1.0000	0.19224	0.06391	0.99619	Biso	1.000	C
C78	1.0000	0.00776	0.01476	0.96705	Biso	1.000	C
C79	1.0000	0.09866	0.03023	0.98026	Biso	1.000	C
C80	1.0000	0.91685	0.99460	0.96430	Biso	1.000	C
C81	1.0000	0.28048	0.03052	0.01930	Biso	1.000	C
C82	1.0000	0.73503	0.96528	0.99008	Biso	1.000	C
C83	1.0000	0.46230	0.99513	0.03577	Biso	1.000	C
C84	1.0000	0.55321	0.97656	0.02746	Biso	1.000	C
C85	1.0000	0.64412	0.96543	0.01043	Biso	1.000	C
C86	1.0000	0.37139	0.01524	0.03273	Biso	1.000	C
C87	1.0000	0.82594	0.97616	0.97289	Biso	1.000	C
C88	1.0000	0.18957	0.03610	0.99973	Biso	1.000	C
C89	1.0000	0.99826	0.05927	0.97813	Biso	1.000	C

C90	1.0000	0.08916	0.06169	0.01364	Biso	1.000	C
C91	1.0000	0.90735	0.03804	0.94955	Biso	1.000	C
C92	1.0000	0.27098	0.01321	0.06178	Biso	1.000	C
C93	1.0000	0.72553	0.96991	0.94444	Biso	1.000	C
C94	1.0000	0.45280	0.94929	0.03769	Biso	1.000	C
C95	1.0000	0.54371	0.93697	0.00429	Biso	1.000	C
C96	1.0000	0.63462	0.94465	0.96953	Biso	1.000	C
C97	1.0000	0.36189	0.97771	0.05912	Biso	1.000	C
C98	1.0000	0.81644	0.00473	0.93700	Biso	1.000	C
C99	1.0000	0.18007	0.04452	0.04483	Biso	1.000	C
C100	1.0000	0.00504	0.05010	0.93554	Biso	1.000	C
C101	1.0000	0.09594	0.07699	0.97286	Biso	1.000	C
C102	1.0000	0.91413	0.00729	0.91869	Biso	1.000	C
C103	1.0000	0.27776	0.05667	0.05876	Biso	1.000	C
C104	1.0000	0.73231	0.92907	0.95959	Biso	1.000	C
C105	1.0000	0.45958	0.97009	0.07596	Biso	1.000	C
C106	1.0000	0.55049	0.93377	0.04773	Biso	1.000	C
C107	1.0000	0.64140	0.91848	0.00435	Biso	1.000	C
C108	1.0000	0.36867	0.01591	0.08007	Biso	1.000	C
C109	1.0000	0.82322	0.96218	0.92765	Biso	1.000	C
C110	1.0000	0.18685	0.07944	0.01879	Biso	1.000	C
C111	1.0000	0.04877	0.06815	0.16405	Biso	1.000	C
C112	1.0000	0.13968	0.96864	0.17485	Biso	1.000	C
C113	1.0000	0.95786	0.14602	0.10116	Biso	1.000	C
C114	1.0000	0.32150	0.82792	0.04411	Biso	1.000	C
C115	1.0000	0.77604	0.15268	0.90920	Biso	1.000	C
C116	1.0000	0.50332	0.88839	0.86179	Biso	1.000	C
C117	1.0000	0.59423	0.98083	0.82339	Biso	1.000	C
C118	1.0000	0.68513	0.07935	0.84107	Biso	1.000	C
C119	1.0000	0.41241	0.83139	0.94407	Biso	1.000	C
C120	1.0000	0.86695	0.17754	0.00616	Biso	1.000	C
C121	1.0000	0.23059	0.87908	0.13014	Biso	1.000	C
C122	1.0000	0.02222	0.07545	0.14114	Biso	1.000	C
C123	1.0000	0.11313	0.98716	0.15953	Biso	1.000	C
C124	1.0000	0.93131	0.13978	0.07795	Biso	1.000	C
C125	1.0000	0.29495	0.84956	0.05459	Biso	1.000	C
C126	1.0000	0.74949	0.12897	0.90523	Biso	1.000	C
C127	1.0000	0.47677	0.88784	0.88583	Biso	1.000	C
C128	1.0000	0.56767	0.96737	0.84332	Biso	1.000	C
C129	1.0000	0.65858	0.05726	0.85055	Biso	1.000	C
C130	1.0000	0.38586	0.84392	0.96459	Biso	1.000	C
C131	1.0000	0.84040	0.15973	0.99000	Biso	1.000	C
C132	1.0000	0.20404	0.90295	0.12726	Biso	1.000	C
C133	1.0000	0.97809	0.07518	0.14769	Biso	1.000	C
C134	1.0000	0.06900	0.98340	0.16489	Biso	1.000	C
C135	1.0000	0.88718	0.14309	0.08360	Biso	1.000	C

C136	1.0000	0.25082	0.84312	0.05340	Biso	1.000	C
C137	1.0000	0.70537	0.13548	0.90457	Biso	1.000	C
C138	1.0000	0.43264	0.88626	0.87948	Biso	1.000	C
C139	1.0000	0.52355	0.96947	0.83711	Biso	1.000	C
C140	1.0000	0.61446	0.06238	0.84647	Biso	1.000	C
C141	1.0000	0.34173	0.83915	0.96010	Biso	1.000	C
C142	1.0000	0.79627	0.16557	0.99296	Biso	1.000	C
C143	1.0000	0.15991	0.89689	0.12974	Biso	1.000	C
C144	1.0000	0.95928	0.06761	0.12088	Biso	1.000	C
C145	1.0000	0.05019	0.99152	0.13824	Biso	1.000	C
C146	1.0000	0.86837	0.12223	0.06514	Biso	1.000	C
C147	1.0000	0.23200	0.87073	0.04972	Biso	1.000	C
C148	1.0000	0.68655	0.11003	0.91588	Biso	1.000	C
C149	1.0000	0.41382	0.90107	0.90306	Biso	1.000	C
C150	1.0000	0.50473	0.96919	0.86497	Biso	1.000	C
C151	1.0000	0.59564	0.04708	0.86974	Biso	1.000	C
C152	1.0000	0.32291	0.86437	0.97193	Biso	1.000	C
C153	1.0000	0.77746	0.13804	0.98872	Biso	1.000	C
C154	1.0000	0.14109	0.91813	0.11171	Biso	1.000	C
C155	1.0000	0.99451	0.06248	0.10251	Biso	1.000	C
C156	1.0000	0.08542	0.99714	0.12002	Biso	1.000	C
C157	1.0000	0.90361	0.10799	0.05246	Biso	1.000	C
C158	1.0000	0.26724	0.88964	0.04726	Biso	1.000	C
C159	1.0000	0.72179	0.09258	0.92356	Biso	1.000	C
C160	1.0000	0.44906	0.91117	0.91924	Biso	1.000	C
C161	1.0000	0.53997	0.96893	0.88404	Biso	1.000	C
C162	1.0000	0.63088	0.03656	0.88565	Biso	1.000	C
C163	1.0000	0.35815	0.88161	0.98009	Biso	1.000	C
C164	1.0000	0.81270	0.11921	0.98575	Biso	1.000	C
C165	1.0000	0.17633	0.93271	0.09942	Biso	1.000	C
C166	1.0000	0.99677	0.04559	0.05682	Biso	1.000	C
C167	1.0000	0.08768	0.00764	0.07245	Biso	1.000	C
C168	1.0000	0.90586	0.06907	0.02315	Biso	1.000	C
C169	1.0000	0.26949	0.93727	0.03704	Biso	1.000	C
C170	1.0000	0.72404	0.04975	0.94679	Biso	1.000	C
C171	1.0000	0.45131	0.94025	0.95833	Biso	1.000	C
C172	1.0000	0.54222	0.97226	0.93264	Biso	1.000	C
C173	1.0000	0.63313	0.01308	0.92834	Biso	1.000	C
C174	1.0000	0.36040	0.92720	0.99725	Biso	1.000	C
C175	1.0000	0.81495	0.07062	0.98213	Biso	1.000	C
C176	1.0000	0.17859	0.96726	0.06507	Biso	1.000	C
C177	1.0000	0.98865	0.99735	0.04897	Biso	1.000	C
C178	1.0000	0.07956	0.97129	0.03976	Biso	1.000	C
C179	1.0000	0.89774	0.02424	0.04264	Biso	1.000	C
C180	1.0000	0.26138	0.95190	0.99040	Biso	1.000	C
C181	1.0000	0.71592	0.04885	0.99566	Biso	1.000	C

C182	1.0000	0.44319	0.98875	0.95226	Biso	1.000	C
C183	1.0000	0.53410	0.01634	0.95376	Biso	1.000	C
C184	1.0000	0.62501	0.03875	0.96993	Biso	1.000	C
C185	1.0000	0.35229	0.96473	0.96592	Biso	1.000	C
C186	1.0000	0.80683	0.04345	0.02276	Biso	1.000	C
C187	1.0000	0.17047	0.95435	0.01793	Biso	1.000	C
C188	1.0000	0.97955	0.99399	0.07722	Biso	1.000	C
C189	1.0000	0.07046	0.95319	0.06171	Biso	1.000	C
C190	1.0000	0.88864	0.03669	0.06821	Biso	1.000	C
C191	1.0000	0.25228	0.92442	0.98306	Biso	1.000	C
C192	1.0000	0.70683	0.07729	0.99496	Biso	1.000	C
C193	1.0000	0.43410	0.98401	0.92421	Biso	1.000	C
C194	1.0000	0.52501	0.02752	0.92760	Biso	1.000	C
C195	1.0000	0.61592	0.06230	0.95397	Biso	1.000	C
C196	1.0000	0.34319	0.94558	0.94489	Biso	1.000	C
C197	1.0000	0.79773	0.06774	0.03755	Biso	1.000	C
C198	1.0000	0.16137	0.92726	0.02661	Biso	1.000	C
C199	1.0000	0.96709	0.96711	0.08686	Biso	1.000	C
C200	1.0000	0.05800	0.92537	0.05529	Biso	1.000	C
C201	1.0000	0.87618	0.01929	0.09085	Biso	1.000	C
C202	1.0000	0.23982	0.91871	0.95508	Biso	1.000	C
C203	1.0000	0.69437	0.09065	0.02020	Biso	1.000	C
C204	1.0000	0.42164	0.00709	0.90739	Biso	1.000	C
C205	1.0000	0.51255	0.05603	0.92593	Biso	1.000	C
C206	1.0000	0.60346	0.08718	0.96798	Biso	1.000	C
C207	1.0000	0.33073	0.95590	0.91826	Biso	1.000	C
C208	1.0000	0.78528	0.06534	0.06600	Biso	1.000	C
C209	1.0000	0.14891	0.90733	0.00616	Biso	1.000	C
C210	1.0000	0.98148	0.01566	0.09294	Biso	1.000	C
C211	1.0000	0.07239	0.96293	0.08665	Biso	1.000	C
C212	1.0000	0.89057	0.06342	0.06972	Biso	1.000	C
C213	1.0000	0.25421	0.90578	0.00228	Biso	1.000	C
C214	1.0000	0.70876	0.08976	0.97127	Biso	1.000	C
C215	1.0000	0.43603	0.95879	0.91524	Biso	1.000	C
C216	1.0000	0.52694	0.01116	0.90641	Biso	1.000	C
C217	1.0000	0.61785	0.05998	0.92730	Biso	1.000	C
C218	1.0000	0.34512	0.91951	0.95097	Biso	1.000	C
C219	1.0000	0.79967	0.09105	0.02436	Biso	1.000	C
C220	1.0000	0.16330	0.92197	0.05285	Biso	1.000	C
N1	1.0000	0.00826	0.05288	0.90840	Biso	1.000	N
N2	1.0000	0.09917	0.09401	0.95153	Biso	1.000	N
N3	1.0000	0.91735	0.99496	0.89435	Biso	1.000	N
N4	1.0000	0.28099	0.08314	0.06537	Biso	1.000	N
N5	1.0000	0.73554	0.90181	0.96070	Biso	1.000	N
N6	1.0000	0.46281	0.97507	0.10279	Biso	1.000	N
N7	1.0000	0.55372	0.92346	0.07299	Biso	1.000	N

N8	1.0000	0.64463	0.89615	0.02003	Biso	1.000	N
N9	1.0000	0.37190	0.03460	0.09995	Biso	1.000	N
N10	1.0000	0.82644	0.93864	0.91385	Biso	1.000	N
N11	1.0000	0.19008	0.10529	0.01004	Biso	1.000	N
N12	1.0000	0.01707	0.00945	0.91691	Biso	1.000	N
N13	1.0000	0.10798	0.05287	0.93521	Biso	1.000	N
N14	1.0000	0.92616	0.96303	0.92500	Biso	1.000	N
N15	1.0000	0.28980	0.08090	0.02117	Biso	1.000	N
N16	1.0000	0.74435	0.91642	0.00247	Biso	1.000	N
N17	1.0000	0.47162	0.01434	0.08238	Biso	1.000	N
N18	1.0000	0.56253	0.96753	0.07706	Biso	1.000	N
N19	1.0000	0.65344	0.93102	0.04727	Biso	1.000	N
N20	1.0000	0.38071	0.05661	0.06155	Biso	1.000	N
N21	1.0000	0.83525	0.92835	0.95689	Biso	1.000	N
N22	1.0000	0.19889	0.07950	0.97408	Biso	1.000	N
N23	1.0000	0.01101	0.98923	0.97431	Biso	1.000	N
N24	1.0000	0.10192	0.00482	0.97257	Biso	1.000	N
N25	1.0000	0.92010	0.97705	0.98422	Biso	1.000	N
N26	1.0000	0.28374	0.02696	0.99299	Biso	1.000	N
N27	1.0000	0.73828	0.97611	0.01432	Biso	1.000	N
N28	1.0000	0.46556	0.01757	0.02161	Biso	1.000	N
N29	1.0000	0.55647	0.00310	0.02768	Biso	1.000	N
N30	1.0000	0.64738	0.98764	0.02496	Biso	1.000	N
N31	1.0000	0.37465	0.02647	0.00868	Biso	1.000	N
N32	1.0000	0.82919	0.97216	0.99913	Biso	1.000	N
N33	1.0000	0.19283	0.01889	0.97953	Biso	1.000	N
N34	1.0000	0.00227	0.03376	0.98555	Biso	1.000	N
N35	1.0000	0.09318	0.03622	0.00610	Biso	1.000	N
N36	1.0000	0.91136	0.02059	0.96959	Biso	1.000	N
N37	1.0000	0.27500	0.00950	0.03548	Biso	1.000	N
N38	1.0000	0.72954	0.98089	0.96864	Biso	1.000	N
N39	1.0000	0.45682	0.97168	0.02338	Biso	1.000	N
N40	1.0000	0.54773	0.96353	0.00435	Biso	1.000	N
N41	1.0000	0.63864	0.96697	0.98395	Biso	1.000	N
N42	1.0000	0.36591	0.98881	0.03498	Biso	1.000	N
N43	1.0000	0.82045	0.00088	0.96328	Biso	1.000	N
N44	1.0000	0.18409	0.02717	0.02471	Biso	1.000	N
N45	1.0000	0.99887	0.06906	0.95362	Biso	1.000	N
N46	1.0000	0.08978	0.08317	0.99832	Biso	1.000	N
N47	1.0000	0.90796	0.03302	0.92365	Biso	1.000	N
N48	1.0000	0.27159	0.03608	0.07495	Biso	1.000	N
N49	1.0000	0.72614	0.94427	0.93825	Biso	1.000	N
N50	1.0000	0.45341	0.94681	0.06395	Biso	1.000	N
N51	1.0000	0.54432	0.92068	0.02504	Biso	1.000	N
N52	1.0000	0.63523	0.91973	0.97818	Biso	1.000	N
N53	1.0000	0.36250	0.98983	0.08256	Biso	1.000	N

N54	1.0000	0.81705	0.98650	0.91792	Biso	1.000	N
N55	1.0000	0.18068	0.07087	0.04355	Biso	1.000	N
N56	1.0000	0.99044	0.04080	0.08393	Biso	1.000	N
N57	1.0000	0.08135	0.98895	0.09266	Biso	1.000	N
N58	1.0000	0.89953	0.07970	0.04854	Biso	1.000	N
N59	1.0000	0.26317	0.91112	0.02844	Biso	1.000	N
N60	1.0000	0.71772	0.07727	0.94767	Biso	1.000	N
N61	1.0000	0.44499	0.93720	0.93097	Biso	1.000	N
N62	1.0000	0.53590	0.98449	0.90798	Biso	1.000	N
N63	1.0000	0.62681	0.03671	0.91420	Biso	1.000	N
N64	1.0000	0.35408	0.90985	0.97588	Biso	1.000	N
N65	1.0000	0.80862	0.09329	0.99775	Biso	1.000	N
N66	1.0000	0.17226	0.94061	0.07198	Biso	1.000	N
N67	1.0000	0.99585	0.02322	0.04110	Biso	1.000	N
N68	1.0000	0.08676	0.99731	0.04713	Biso	1.000	N
N69	1.0000	0.90494	0.04176	0.02202	Biso	1.000	N
N70	1.0000	0.26858	0.95601	0.01714	Biso	1.000	N
N71	1.0000	0.72312	0.03738	0.97116	Biso	1.000	N
N72	1.0000	0.45040	0.96614	0.96710	Biso	1.000	N
N73	1.0000	0.54131	0.98930	0.95402	Biso	1.000	N
N74	1.0000	0.63222	0.01586	0.95553	Biso	1.000	N
N75	1.0000	0.35949	0.95373	0.99063	Biso	1.000	N
N76	1.0000	0.81403	0.04704	0.99595	Biso	1.000	N
N77	1.0000	0.17767	0.97226	0.03820	Biso	1.000	N
O1	1.0000	0.95582	0.05784	0.76961	Biso	1.000	O
O2	1.0000	0.04673	0.17322	0.83745	Biso	1.000	O
O3	1.0000	0.86491	0.92410	0.77491	Biso	1.000	O
O4	1.0000	0.22854	0.21981	0.09004	Biso	1.000	O
O5	1.0000	0.68309	0.76372	0.97554	Biso	1.000	O
O6	1.0000	0.41036	0.00941	0.23735	Biso	1.000	O
O7	1.0000	0.50127	0.87960	0.20476	Biso	1.000	O
O8	1.0000	0.59218	0.78801	0.10716	Biso	1.000	O
O9	1.0000	0.31945	0.13624	0.19459	Biso	1.000	O
O10	1.0000	0.77400	0.81446	0.85168	Biso	1.000	O
O11	1.0000	0.13763	0.23360	0.95690	Biso	1.000	O
O12	1.0000	0.99731	0.02069	0.79313	Biso	1.000	O
O13	1.0000	0.08822	0.12925	0.83716	Biso	1.000	O
O14	1.0000	0.90640	0.90556	0.81479	Biso	1.000	O
O15	1.0000	0.27004	0.20182	0.04992	Biso	1.000	O
O16	1.0000	0.72458	0.79229	0.00896	Biso	1.000	O
O17	1.0000	0.45186	0.03843	0.20432	Biso	1.000	O
O18	1.0000	0.54276	0.92187	0.19266	Biso	1.000	O
O19	1.0000	0.63367	0.83011	0.11983	Biso	1.000	O
O20	1.0000	0.36095	0.14279	0.15111	Biso	1.000	O
O21	1.0000	0.81549	0.82042	0.89524	Biso	1.000	O
O22	1.0000	0.17913	0.19677	0.93288	Biso	1.000	O

O23	1.0000	0.98005	0.06045	0.81904	Biso	1.000	O
O24	1.0000	0.07096	0.14869	0.88045	Biso	1.000	O
O25	1.0000	0.88914	0.95302	0.81508	Biso	1.000	O
O26	1.0000	0.25278	0.17052	0.08559	Biso	1.000	O
O27	1.0000	0.70732	0.81228	0.96592	Biso	1.000	O
O28	1.0000	0.43459	0.99298	0.19066	Biso	1.000	O
O29	1.0000	0.52550	0.89102	0.15660	Biso	1.000	O
O30	1.0000	0.61641	0.82365	0.07282	Biso	1.000	O
O31	1.0000	0.34369	0.09718	0.16419	Biso	1.000	O
O32	1.0000	0.79823	0.86050	0.86984	Biso	1.000	O
O33	1.0000	0.16187	0.18972	0.97981	Biso	1.000	O
O34	1.0000	0.97206	0.07143	0.87420	Biso	1.000	O
O35	1.0000	0.06297	0.12811	0.93278	Biso	1.000	O
O36	1.0000	0.88115	0.99208	0.85555	Biso	1.000	O
O37	1.0000	0.24479	0.11436	0.08861	Biso	1.000	O
O38	1.0000	0.69933	0.86531	0.94720	Biso	1.000	O
O39	1.0000	0.42661	0.96691	0.14083	Biso	1.000	O
O40	1.0000	0.51752	0.89602	0.10058	Biso	1.000	O
O41	1.0000	0.60842	0.85815	0.02840	Biso	1.000	O
O42	1.0000	0.33570	0.04830	0.13637	Biso	1.000	O
O43	1.0000	0.79024	0.91524	0.88276	Biso	1.000	O
O44	1.0000	0.15388	0.14411	0.01271	Biso	1.000	O
O45	1.0000	0.01728	0.12869	0.85224	Biso	1.000	O
O46	1.0000	0.10819	0.18814	0.94527	Biso	1.000	O
O47	1.0000	0.92637	0.02837	0.80612	Biso	1.000	O
O48	1.0000	0.29000	0.12794	0.14840	Biso	1.000	O
O49	1.0000	0.74455	0.83543	0.89365	Biso	1.000	O
O50	1.0000	0.47182	0.91816	0.17803	Biso	1.000	O
O51	1.0000	0.56273	0.83490	0.10552	Biso	1.000	O
O52	1.0000	0.65364	0.80406	0.99951	Biso	1.000	O
O53	1.0000	0.38091	0.02740	0.19402	Biso	1.000	O
O54	1.0000	0.83546	0.91905	0.82156	Biso	1.000	O
O55	1.0000	0.19909	0.18787	0.05567	Biso	1.000	O
O56	1.0000	0.10174	0.03609	0.20099	Biso	1.000	O
O57	1.0000	0.19265	0.92169	0.18859	Biso	1.000	O
O58	1.0000	0.01083	0.13902	0.14957	Biso	1.000	O
O59	1.0000	0.37446	0.79592	0.00711	Biso	1.000	O
O60	1.0000	0.82901	0.19381	0.93568	Biso	1.000	O
O61	1.0000	0.55628	0.90875	0.81732	Biso	1.000	O
O62	1.0000	0.64719	0.02200	0.79698	Biso	1.000	O
O63	1.0000	0.73810	0.12827	0.84111	Biso	1.000	O
O64	1.0000	0.46537	0.82447	0.89565	Biso	1.000	O
O65	1.0000	0.91992	0.19782	0.05067	Biso	1.000	O
O66	1.0000	0.28356	0.83216	0.11632	Biso	1.000	O
O67	1.0000	0.03309	0.02895	0.22183	Biso	1.000	O
O68	1.0000	0.12400	0.90442	0.20227	Biso	1.000	O

O69	1.0000	0.94218	0.14429	0.17097	Biso	1.000	O
O70	1.0000	0.30582	0.77631	0.99709	Biso	1.000	O
O71	1.0000	0.76036	0.21545	0.93977	Biso	1.000	O
O72	1.0000	0.48764	0.90973	0.79531	Biso	1.000	O
O73	1.0000	0.57855	0.03472	0.77900	Biso	1.000	O
O74	1.0000	0.66945	0.14869	0.83285	Biso	1.000	O
O75	1.0000	0.39673	0.81339	0.87661	Biso	1.000	O
O76	1.0000	0.85127	0.21381	0.06582	Biso	1.000	O
O77	1.0000	0.21491	0.81024	0.11849	Biso	1.000	O
O78	1.0000	0.03750	0.04251	0.17381	Biso	1.000	O
O79	1.0000	0.12841	0.94179	0.16920	Biso	1.000	O
O80	1.0000	0.94659	0.12973	0.12324	Biso	1.000	O
O81	1.0000	0.31023	0.82191	0.01734	Biso	1.000	O
O82	1.0000	0.76477	0.16600	0.93319	Biso	1.000	O
O83	1.0000	0.49205	0.91025	0.84520	Biso	1.000	O
O84	1.0000	0.58296	0.00818	0.82125	Biso	1.000	O
O85	1.0000	0.67386	0.10352	0.85405	Biso	1.000	O
O86	1.0000	0.40114	0.84080	0.91830	Biso	1.000	O
O87	1.0000	0.85568	0.17577	0.03354	Biso	1.000	O
O88	1.0000	0.21932	0.85955	0.11087	Biso	1.000	O
O89	1.0000	0.02584	0.05698	0.12015	Biso	1.000	O
O90	1.0000	0.11675	0.98298	0.13188	Biso	1.000	O
O91	1.0000	0.93493	0.11289	0.07027	Biso	1.000	O
O92	1.0000	0.29856	0.87296	0.03930	Biso	1.000	O
O93	1.0000	0.75311	0.11082	0.92650	Biso	1.000	O
O94	1.0000	0.48038	0.91148	0.90077	Biso	1.000	O
O95	1.0000	0.57129	0.97918	0.86866	Biso	1.000	O
O96	1.0000	0.66220	0.05349	0.87825	Biso	1.000	O
O97	1.0000	0.38947	0.87188	0.96438	Biso	1.000	O
O98	1.0000	0.84402	0.13296	0.99808	Biso	1.000	O
O99	1.0000	0.20765	0.91438	0.10174	Biso	1.000	O
O100	1.0000	0.96373	0.09882	0.16018	Biso	1.000	O
O101	1.0000	0.05464	0.99653	0.18818	Biso	1.000	O
O102	1.0000	0.87282	0.16973	0.08132	Biso	1.000	O
O103	1.0000	0.23646	0.82739	0.07502	Biso	1.000	O
O104	1.0000	0.69100	0.14448	0.87939	Biso	1.000	O
O105	1.0000	0.41827	0.86006	0.87415	Biso	1.000	O
O106	1.0000	0.50918	0.95031	0.81847	Biso	1.000	O
O107	1.0000	0.60009	0.05634	0.82042	Biso	1.000	O
O108	1.0000	0.32736	0.81423	0.96979	Biso	1.000	O
O109	1.0000	0.78191	0.18675	0.97665	Biso	1.000	O
O110	1.0000	0.14555	0.89535	0.15643	Biso	1.000	O
O111	1.0000	0.00218	0.06776	0.04792	Biso	1.000	O
O112	1.0000	0.09309	0.03110	0.07695	Biso	1.000	O
O113	1.0000	0.91127	0.08291	0.00368	Biso	1.000	O
O114	1.0000	0.27491	0.94293	0.06025	Biso	1.000	O

O115	1.0000	0.72946	0.03779	0.92611	Biso	1.000	O
O116	1.0000	0.45673	0.92148	0.97311	Biso	1.000	O
O117	1.0000	0.54764	0.94848	0.93493	Biso	1.000	O
O118	1.0000	0.63855	0.99184	0.91741	Biso	1.000	O
O119	1.0000	0.36582	0.91941	0.01983	Biso	1.000	O
O120	1.0000	0.82037	0.07174	0.95827	Biso	1.000	O
O121	1.0000	0.18400	0.98456	0.08155	Biso	1.000	O
O122	1.0000	0.99004	0.97880	0.03317	Biso	1.000	O
O123	1.0000	0.08095	0.96423	0.01644	Biso	1.000	O
O124	1.0000	0.89913	0.00010	0.03937	Biso	1.000	O
O125	1.0000	0.26277	0.97018	0.97429	Biso	1.000	O
O126	1.0000	0.71732	0.03585	0.01626	Biso	1.000	O
O127	1.0000	0.44459	0.01100	0.96220	Biso	1.000	O
O128	1.0000	0.53550	0.02969	0.97415	Biso	1.000	O
O129	1.0000	0.62641	0.03895	0.99430	Biso	1.000	O
O130	1.0000	0.35368	0.98882	0.96226	Biso	1.000	O
O131	1.0000	0.80822	0.02137	0.03306	Biso	1.000	O
O132	1.0000	0.17186	0.96102	0.99449	Biso	1.000	O
P1	1.0000	0.96398	0.04319	0.79436	Biso	1.000	P
P2	1.0000	0.05489	0.14751	0.85035	Biso	1.000	P
P3	1.0000	0.87307	0.92515	0.80366	Biso	1.000	P
P4	1.0000	0.23671	0.19740	0.07201	Biso	1.000	P
P5	1.0000	0.69125	0.79031	0.98652	Biso	1.000	P
P6	1.0000	0.41853	0.01650	0.20948	Biso	1.000	P
P7	1.0000	0.50944	0.90063	0.18514	Biso	1.000	P
P8	1.0000	0.60034	0.81631	0.10203	Biso	1.000	P
P9	1.0000	0.32762	0.12713	0.16730	Biso	1.000	P
P10	1.0000	0.78216	0.83088	0.87529	Biso	1.000	P
P11	1.0000	0.14580	0.20500	0.95386	Biso	1.000	P
P12	1.0000	0.06135	0.02698	0.19644	Biso	1.000	P
P13	1.0000	0.15225	0.91649	0.17985	Biso	1.000	P
P14	1.0000	0.97044	0.12890	0.15067	Biso	1.000	P
P15	1.0000	0.33407	0.80172	0.99875	Biso	1.000	P
P16	1.0000	0.78862	0.19060	0.94534	Biso	1.000	P
P17	1.0000	0.51589	0.91877	0.81912	Biso	1.000	P
P18	1.0000	0.60680	0.02945	0.80391	Biso	1.000	P
P19	1.0000	0.69771	0.13079	0.85097	Biso	1.000	P
P20	1.0000	0.42498	0.83387	0.89175	Biso	1.000	P
P21	1.0000	0.87953	0.18990	0.05706	Biso	1.000	P
P22	1.0000	0.24316	0.83252	0.10615	Biso	1.000	P