

Table S1. Nilutamide docking score table

Conformers	Docking score (kcal/mol)
1	-9.1
2	-8.5
3	-8.5
4	-8.4
5	-7.9
6	-7.7
7	-7.6
8	-7.5
9	-7.3

Flutamide docking score table

Conformers	Docking score (kcal/mol)
1	-8.7
2	-8.3
3	-8.0
4	-7.7
5	-7.7
6	-6.9
7	-6.9
8	-6.8
9	-6.8

Table S2a. Intermolecular interactions between nilutamide and androgen receptor obtained from molecular docking

Types of interactions	Ligand atom identifier···Amino acid residue	Distance (Å)
Conventional Hydrogen Bond	O ···GLN711/HE21	1.88
Conventional Hydrogen Bond	O ···ARG752/HH21	2.72
Conventional Hydrogen Bond	O ···ARG752/HH21	6.38
Conventional Hydrogen Bond	H ···ASN705/OD1	2.85
Carbon Hydrogen Bond	O ···GLY708/CA	3.46
Halogen (Fluorine)	F ··· MET745/C	3.19
Pi-Sigma	LIG ···MET745/CE	3.95
Pi-Pi T-shaped	LIG ···PHE764	5.30
Alkyl	C ··· - VAL746	4.93
Alkyl	C ··· MET749	4.50
Alkyl	C ··· MET787	5.29
Pi-Alkyl	C ··· PHE764	5.03
Pi-Alkyl	LIG ···- LEU704	5.32

Table S2b. Intermolecular interactions between flutamide and androgen receptor obtained from molecular docking

Types of interactions	Ligand atom identifier···Amino acid residue	Distance (Å)
Conventional Hydrogen Bond	H ··· LEU704/O	3.04
Conventional Hydrogen Bond	O ··· GLN711/NE21	3.06
Conventional Hydrogen Bond	O ··· GLN711/HE12	2.43
Conventional Hydrogen Bond	O ··· ARG752/HH2	2.75
Halogen (Fluorine)	F ··· MET745/C	3.34
Pi-Sulfur	LIG··· MET745/SD	4.18
Pi-Pi T-shaped	LIG··· PHE764	5.22
Alkyl	C ··· LEU701	5.37
Alkyl	C ··· MET780	5.04
Alkyl	C ··· MET745	4.85
Alkyl	C ··· VAL746	5.05
Alkyl	C ··· MET787	5.37
Pi-Alkyl	LIG ··· LEU704	5.28
Pi-Alkyl	LIG··· A:LEU707	5.25
Pi-Alkyl	C··· PHE764	4.98
Pi-Alkyl	LIG··· PHE876	5.15

Table S3. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$) for (shelx)

Nilutamide

Atoms	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.26874 (2)	0.18084 (2)	0.59736 (3)	0.01983 (4)
F3	0.34537 (2)	0.05912 (2)	0.50336 (3)	0.02166 (4)
F2	0.23084 (2)	0.23001 (3)	0.41045 (3)	0.02532 (5)
O4	0.62103 (2)	0.25505 (3)	0.36308 (2)	0.01406 (3)
O3	0.89721 (2)	0.28715 (3)	0.77288 (2)	0.01522 (3)
O1	0.23868 (2)	0.46358 (3)	0.55936 (3)	0.02139 (5)
O2	0.35799 (3)	0.47314 (4)	0.75763 (3)	0.02560 (6)
N2	0.73373 (2)	0.27366 (2)	0.57651 (2)	0.01073 (3)
N3	0.82811 (2)	0.20386 (3)	0.46855 (2)	0.01266 (3)
N1	0.33750 (2)	0.44798 (3)	0.65169 (3)	0.01551 (4)
C5	0.43044 (2)	0.27691 (3)	0.56884 (2)	0.01121 (3)
C10	0.71809 (2)	0.24361 (3)	0.45563 (2)	0.01078 (3)
C8	0.85459 (2)	0.26485 (3)	0.66267 (2)	0.01075 (3)
C2	0.64207 (2)	0.43830 (3)	0.65843 (2)	0.01192 (3)
C9	0.92636 (2)	0.22151 (3)	0.59448 (2)	0.01120 (3)
C1	0.54358 (2)	0.47877 (3)	0.67719 (3)	0.01250 (3)
C4	0.53018 (2)	0.23563 (3)	0.55283 (2)	0.01165 (3)
C6	0.43968 (2)	0.39837 (3)	0.63192 (2)	0.01143 (3)
C3	0.63487 (2)	0.31659 (3)	0.59729 (2)	0.01043 (3)
C7	0.31848 (3)	0.18717 (3)	0.51961 (3)	0.01470 (4)
C11	1.01420 (3)	0.33485 (3)	0.60070 (3)	0.01564 (4)
C12	0.99417 (3)	0.08858 (3)	0.64891 (3)	0.01744 (5)
H4	0.5306 (8)	0.1520 (10)	0.5134 (8)	0.0262 (19)*
H1	0.5440 (8)	0.5628 (10)	0.7168 (9)	0.029 (2)*
H2	0.7140 (8)	0.4963 (10)	0.6874 (8)	0.0243 (18)*
H11A	0.9711 (8)	0.4188 (10)	0.5700 (8)	0.0247 (19)*
H3	0.8431 (8)	0.2053 (9)	0.4027 (8)	0.0231 (18)*
H11C	1.0518 (9)	0.3083 (10)	0.5502 (9)	0.031 (2)*
H12B	1.0417 (8)	0.0648 (9)	0.6070 (8)	0.0251 (19)*
H12C	0.9333 (8)	0.0141 (9)	0.6378 (8)	0.0254 (19)*

H12A	1.0510 (8)	0.0982 (10)	0.7374 (9)	0.0269 (19)*
H11B	1.0776 (8)	0.3445 (9)	0.6814 (8)	0.0228 (17)*

Flutamide

Atoms	x	y	z	U _{iso} */U _{eq}
F1	0.57019 (3)	0.83040 (2)	1.03219 (7)	0.02006 (5)
F2	0.51358 (4)	0.86001 (2)	0.62733 (8)	0.02120 (5)
F3	0.68590 (3)	0.83205 (2)	0.69167 (9)	0.02213 (6)
O3	0.60776 (3)	0.51608 (2)	0.21835 (9)	0.02008 (6)
O1	0.34684 (4)	0.70790 (2)	1.19796 (8)	0.02180 (6)
O2	0.35183 (4)	0.79640 (2)	0.94725 (10)	0.02193 (6)
N2	0.67926 (2)	0.62003 (2)	0.25088 (7)	0.01276 (4)
N1	0.38384 (3)	0.74027 (2)	1.00491 (7)	0.01438 (4)
C3	0.60696 (2)	0.64713 (2)	0.44678 (7)	0.01095 (4)
C8	0.67751 (3)	0.55663 (2)	0.14836 (7)	0.01217 (4)
C9	0.77262 (3)	0.54092 (2)	-0.05146 (8)	0.01474 (5)
C4	0.52319 (3)	0.61134 (2)	0.58400 (8)	0.01309 (4)
C1	0.55296 (3)	0.74623 (2)	0.69648 (7)	0.01152 (4)
C2	0.62258 (3)	0.71408 (2)	0.51063 (7)	0.01180 (4)
C5	0.45457 (3)	0.64306 (2)	0.77376 (8)	0.01333 (4)
C6	0.46712 (3)	0.70989 (2)	0.82447 (7)	0.01190 (4)
C7	0.57944 (3)	0.81744 (2)	0.76202 (8)	0.01448 (4)
C11	0.74831 (6)	0.47591 (2)	-0.19814 (11)	0.02311 (8)
C10	0.88428 (4)	0.53767 (3)	0.10611 (12)	0.02246 (7)
H11C	0.7449 (14)	0.4395 (9)	-0.076 (4)	0.030 (4)*
H10B	0.9485 (18)	0.5291 (11)	-0.007 (5)	0.040 (5)*
H10C	0.882 (2)	0.5024 (14)	0.235 (6)	0.053 (6)*
H10A	0.9032 (18)	0.5807 (10)	0.206 (4)	0.038 (5)*
H11B	0.6768 (18)	0.4786 (10)	-0.305 (5)	0.036 (4)*
H11A	0.8035 (17)	0.4652 (9)	-0.330 (4)	0.032 (4)*
H4	0.5135 (14)	0.5661 (7)	0.550 (3)	0.021 (3)*
H9	0.7757 (16)	0.5764 (8)	-0.190 (4)	0.030 (4)*
H2A	0.7283 (14)	0.6468 (8)	0.183 (4)	0.026 (3)*
H5	0.3942 (13)	0.6203 (7)	0.877 (3)	0.020 (3)*
H2	0.6817 (13)	0.7371 (7)	0.422 (3)	0.020 (3)*

Table S4. Atomic displacement parameters ($\text{\AA}^2$) for (shelx)**Nilutamide**

Atoms	U ¹¹	U ²²	U ³³	U ¹²	U ¹³	U ²³
F1	0.01711 (8)	0.01914 (8)	0.02977 (11)	-0.00146 (6)	0.01637 (8)	0.00201 (7)
F3	0.01884 (8)	0.01532 (8)	0.03379 (12)	-0.00477 (6)	0.01465 (9)	-0.00631 (8)
F2	0.01453 (8)	0.03042 (12)	0.02046 (10)	-0.00442 (8)	-0.00099 (7)	0.00258 (8)
O4	0.01201 (6)	0.01801 (8)	0.01002 (6)	0.00051 (6)	0.00325 (5)	-0.00169 (5)
O3	0.01243 (7)	0.02447 (10)	0.00910 (6)	-0.00094 (6)	0.00526 (5)	-0.00167 (6)
O1	0.01105 (7)	0.01818 (9)	0.03300 (13)	0.00267 (6)	0.00848 (8)	0.00329 (9)
O2	0.03104 (14)	0.02987 (14)	0.02645 (13)	0.00611 (11)	0.02229 (12)	0.00061 (10)
N2	0.00916 (6)	0.01467 (7)	0.00930 (6)	0.00000 (5)	0.00505 (5)	-0.00106 (5)
N3	0.01156 (7)	0.01802 (8)	0.00995 (6)	0.00104 (6)	0.00628 (6)	-0.00082 (6)
N1	0.01419 (8)	0.01450 (8)	0.02198 (10)	0.00275 (6)	0.01187 (8)	0.00259 (7)
C5	0.00931 (7)	0.01267 (8)	0.01190 (7)	-0.00038 (6)	0.00509 (6)	0.00048 (6)
C10	0.01093 (7)	0.01254 (7)	0.00942 (7)	-0.00013 (6)	0.00515 (6)	-0.00078 (6)
C8	0.00973 (7)	0.01412 (8)	0.00929 (7)	-0.00033 (6)	0.00515 (6)	-0.00002 (6)
C2	0.01074 (7)	0.01275 (8)	0.01292 (8)	-0.00090 (6)	0.00601 (6)	-0.00177 (6)
C9	0.01024 (7)	0.01399 (8)	0.01058 (7)	0.00089 (6)	0.00585 (6)	0.00073 (6)
C1	0.01190 (7)	0.01286 (8)	0.01356 (8)	0.00038 (6)	0.00657 (7)	-0.00151 (6)
C4	0.01046 (7)	0.01267 (8)	0.01285 (8)	-0.00103 (6)	0.00624 (6)	-0.00143 (6)
C6	0.01018 (7)	0.01283 (8)	0.01239 (8)	0.00159 (6)	0.00615 (6)	0.00126 (6)
C3	0.00946 (7)	0.01248 (7)	0.01037 (7)	-0.00022 (6)	0.00544 (6)	-0.00058 (6)
C7	0.01084 (8)	0.01529 (9)	0.01767 (10)	-0.00179 (7)	0.00631 (7)	0.00018 (7)
C11	0.01243 (8)	0.01899 (10)	0.01722 (10)	-0.00173 (7)	0.00830 (8)	0.00150 (8)
C12	0.01797 (10)	0.01626 (10)	0.01777 (11)	0.00490 (8)	0.00795 (9)	0.00276 (8)

Flutamide

Atoms	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.02549 (12)	0.01864 (10)	0.01604 (9)	-0.00124 (9)	0.00148 (8)	-0.00558 (8)
F2	0.02859 (14)	0.01240 (8)	0.02262 (11)	0.00485 (8)	0.00152 (10)	0.00226 (8)
F3	0.01923 (10)	0.01536 (9)	0.03181 (15)	-0.00637 (8)	0.00853 (10)	-0.00509 (9)
O3	0.01989 (11)	0.01441 (9)	0.02593 (14)	-0.00668 (8)	0.00721 (10)	-0.00596 (9)
O1	0.02123 (12)	0.02575 (14)	0.01842 (11)	0.00429 (10)	0.00987 (10)	0.00386 (10)
O2	0.02071 (12)	0.01616 (10)	0.02892 (15)	0.00668 (9)	0.00905 (12)	0.00070 (10)
N2	0.01199 (8)	0.01037 (7)	0.01593 (9)	-0.00101 (6)	0.00450 (7)	-0.00150 (7)
N1	0.01185 (8)	0.01592 (10)	0.01536 (10)	0.00218 (7)	0.00358 (7)	-0.00079 (8)
C3	0.00973 (7)	0.00980 (8)	0.01332 (9)	-0.00034 (6)	0.00222 (7)	-0.00008 (7)
C8	0.01213 (8)	0.01074 (8)	0.01362 (9)	-0.00017 (7)	0.00079 (7)	-0.00136 (7)
C9	0.01782 (11)	0.01277 (10)	0.01364 (10)	0.00325 (8)	0.00346 (9)	0.00041 (8)
C4	0.01139 (9)	0.01039 (8)	0.01749 (11)	-0.00102 (7)	0.00407 (8)	0.00026 (8)
C1	0.01126 (8)	0.01014 (8)	0.01316 (9)	0.00015 (6)	0.00210 (7)	-0.00028 (7)
C2	0.01122 (8)	0.01008 (8)	0.01410 (9)	-0.00102 (6)	0.00318 (7)	-0.00042 (7)
C5	0.01112 (8)	0.01213 (9)	0.01675 (11)	-0.00055 (7)	0.00420 (8)	0.00102 (8)
C6	0.01017 (8)	0.01199 (9)	0.01354 (9)	0.00094 (7)	0.00268 (7)	0.00032 (7)
C7	0.01628 (10)	0.01116 (9)	0.01599 (11)	-0.00051 (7)	0.00297 (9)	-0.00151 (8)
C11	0.0345 (2)	0.01594 (13)	0.01892 (14)	0.00326 (13)	0.00461 (14)	-0.00434 (11)
C10	0.01387 (11)	0.02728 (19)	0.02624 (18)	0.00390 (11)	0.00347 (12)	0.00161 (15)

Table S5. Geometric parameters (Å, °) for (shelx)**Nilutamide**

F1—C7	1.3464 (4)	C8—C9	1.5268 (3)
F3—C7	1.3396 (4)	C2—C3	1.3911 (4)
F2—C7	1.3385 (4)	C2—C1	1.3916 (4)
O4—C10	1.2136 (3)	C2—H2	0.973 (9)
O3—C8	1.2169 (3)	C9—C12	1.5283 (4)
O1—N1	1.2290 (4)	C9—C11	1.5302 (4)
O2—N1	1.2223 (4)	C1—C6	1.3841 (4)
N2—C8	1.3734 (3)	C1—H1	0.956 (10)
N2—C3	1.4169 (3)	C4—C3	1.3948 (3)
N2—C10	1.4272 (3)	C4—H4	0.954 (9)

N3—C10	1.3475 (3)	C11—H11A	0.959 (9)
N3—C9	1.4635 (3)	C11—H11C	0.961 (9)
N3—H3	0.903 (8)	C11—H11B	0.938 (9)
N1—C6	1.4691 (3)	C12—H12B	0.966 (9)
C5—C4	1.3898 (3)	C12—H12C	1.012 (9)
C5—C6	1.3966 (4)	C12—H12A	0.983 (9)
C5—C7	1.5090 (4)		
C8—N2—C3	126.81 (2)	C2—C1—H1	121.8 (5)
C8—N2—C10	111.15 (2)	C5—C4—C3	119.80 (2)
C3—N2—C10	121.87 (2)	C5—C4—H4	122.2 (5)
C10—N3—C9	112.90 (2)	C3—C4—H4	118.0 (5)
C10—N3—H3	119.9 (6)	C1—C6—C5	122.28 (2)
C9—N3—H3	121.5 (6)	C1—C6—N1	116.67 (2)
O2—N1—O1	125.37 (3)	C5—C6—N1	121.04 (2)
O2—N1—C6	117.72 (3)	C2—C3—C4	121.25 (2)
O1—N1—C6	116.89 (3)	C2—C3—N2	120.28 (2)
C4—C5—C6	118.29 (2)	C4—C3—N2	118.46 (2)
C4—C5—C7	118.54 (2)	F2—C7—F3	106.83 (3)
C6—C5—C7	123.16 (2)	F2—C7—F1	107.18 (3)
O4—C10—N3	129.95 (2)	F3—C7—F1	106.52 (3)
O4—C10—N2	123.26 (2)	F2—C7—C5	112.47 (3)
N3—C10—N2	106.79 (2)	F3—C7—C5	111.45 (2)
O3—C8—N2	126.74 (2)	F1—C7—C5	112.04 (3)
O3—C8—C9	126.06 (2)	C9—C11—H11A	110.8 (5)
N2—C8—C9	107.20 (2)	C9—C11—H11C	107.9 (6)
C3—C2—C1	119.27 (2)	H11A—C11—H11C	109.1 (8)
C3—C2—H2	121.5 (5)	C9—C11—H11B	110.7 (5)
C1—C2—H2	119.3 (5)	H11A—C11—H11B	111.5 (8)
N3—C9—C8	101.46 (2)	H11C—C11—H11B	106.6 (8)
N3—C9—C12	112.13 (2)	C9—C12—H12B	108.7 (5)
C8—C9—C12	109.85 (2)	C9—C12—H12C	109.8 (5)
N3—C9—C11	111.23 (2)	H12B—C12—H12C	110.2 (8)
C8—C9—C11	110.05 (2)	C9—C12—H12A	111.4 (6)
C12—C9—C11	111.66 (2)	H12B—C12—H12A	107.8 (7)

C6—C1—C2	119.10 (2)	H12C—C12—H12A	109.0 (7)
C6—C1—H1	119.0 (5)		
C9—N3—C10—O4	172.10 (3)	C2—C1—C6—N1	-178.47 (2)
C9—N3—C10—N2	-7.49 (3)	C4—C5—C6—C1	0.77 (4)
C8—N2—C10—O4	-174.08 (3)	C7—C5—C6—C1	179.50 (3)
C3—N2—C10—O4	1.48 (4)	C4—C5—C6—N1	179.82 (2)
C8—N2—C10—N3	5.54 (3)	C7—C5—C6—N1	-1.45 (4)
C3—N2—C10—N3	-178.89 (2)	O2—N1—C6—C1	-55.41 (4)
C3—N2—C8—O3	3.18 (5)	O1—N1—C6—C1	123.03 (3)
C10—N2—C8—O3	178.48 (3)	O2—N1—C6—C5	125.49 (3)
C3—N2—C8—C9	-176.86 (2)	O1—N1—C6—C5	-56.07 (4)
C10—N2—C8—C9	-1.56 (3)	C1—C2—C3—C4	1.03 (4)
C10—N3—C9—C8	6.34 (3)	C1—C2—C3—N2	179.64 (2)
C10—N3—C9—C12	123.50 (3)	C5—C4—C3—C2	0.38 (4)
C10—N3—C9—C11	-110.67 (3)	C5—C4—C3—N2	-178.26 (2)
O3—C8—C9—N3	177.33 (3)	C8—N2—C3—C2	50.78 (4)
N2—C8—C9—N3	-2.63 (3)	C10—N2—C3—C2	-124.05 (3)
O3—C8—C9—C12	58.52 (4)	C8—N2—C3—C4	-130.56 (3)
N2—C8—C9—C12	-121.44 (3)	C10—N2—C3—C4	54.60 (3)
O3—C8—C9—C11	-64.80 (4)	C4—C5—C7—F2	-99.17 (3)
N2—C8—C9—C11	115.23 (2)	C6—C5—C7—F2	82.11 (4)
C3—C2—C1—C6	-1.51 (4)	C4—C5—C7—F3	20.77 (4)
C6—C5—C4—C3	-1.26 (4)	C6—C5—C7—F3	-157.95 (3)
C7—C5—C4—C3	179.95 (2)	C4—C5—C7—F1	140.02 (3)
C2—C1—C6—C5	0.62 (4)	C6—C5—C7—F1	-38.70 (4)

Flutamide

F1—C7	1.3458 (5)	C9—H9	0.989 (18)
F2—C7	1.3387 (5)	C4—C5	1.3912 (5)
F3—C7	1.3458 (5)	C4—H4	0.940 (15)
O3—C8	1.2181 (5)	C1—C2	1.3898 (4)
O1—N1	1.2286 (5)	C1—C6	1.4060 (5)
O2—N1	1.2344 (5)	C1—C7	1.5142 (5)

N2—C8	1.3812 (5)	C2—H2	0.949 (16)
N2—C3	1.3975 (4)	C5—C6	1.3878 (5)
N2—H2A	0.863 (17)	C5—H5	0.990 (16)
N1—C6	1.4612 (5)	C11—H11C	0.949 (19)
C3—C4	1.4032 (4)	C11—H11B	1.00 (2)
C3—C2	1.4073 (5)	C11—H11A	0.95 (2)
C8—C9	1.5263 (5)	C10—H10B	0.96 (2)
C9—C11	1.5288 (7)	C10—H10C	0.95 (3)
C9—C10	1.5360 (7)	C10—H10A	1.03 (2)
C8—N2—C3	127.19 (3)	C3—C2—H2	118.2 (9)
C8—N2—H2A	117.3 (11)	C6—C5—C4	120.52 (3)
C3—N2—H2A	115.4 (11)	C6—C5—H5	116.4 (9)
O1—N1—O2	123.88 (4)	C4—C5—H5	123.0 (9)
O1—N1—C6	118.49 (4)	C5—C6—C1	120.86 (3)
O2—N1—C6	117.57 (3)	C5—C6—N1	116.55 (3)
N2—C3—C4	123.94 (3)	C1—C6—N1	122.52 (3)
N2—C3—C2	116.74 (3)	F2—C7—F1	107.73 (3)
C4—C3—C2	119.30 (3)	F2—C7—F3	106.52 (4)
O3—C8—N2	122.67 (3)	F1—C7—F3	106.41 (4)
O3—C8—C9	122.84 (3)	F2—C7—C1	113.07 (4)
N2—C8—C9	114.46 (3)	F1—C7—C1	112.07 (3)
C8—C9—C11	109.75 (4)	F3—C7—C1	110.67 (3)
C8—C9—C10	109.42 (4)	C9—C11—H11C	112.9 (11)
C11—C9—C10	111.09 (4)	C9—C11—H11B	110.9 (12)
C8—C9—H9	108.1 (11)	H11C—C11— H11B	109.3 (16)
C11—C9—H9	108.5 (10)	C9—C11—H11A	112.6 (11)
C10—C9—H9	109.9 (11)	H11C—C11— H11A	106.1 (16)
C5—C4—C3	119.56 (3)	H11B—C11— H11A	104.6 (18)
C5—C4—H4	119.7 (10)	C9—C10—H10B	114.2 (14)
C3—C4—H4	120.7 (10)	C9—C10—H10C	109.7 (15)
C2—C1—C6	118.36 (3)	H10B—C10— H10C	105 (2)

C2—C1—C7	117.51 (3)	C9—C10—H10A	113.0 (12)
C6—C1—C7	124.01 (3)	H10B—C10— H10A	104.7 (18)
C1—C2—C3	121.27 (3)	H10C—C10— H10A	110 (2)
C1—C2—H2	120.6 (9)		
C8—N2—C3—C4	3.98 (6)	C4—C5—C6—N1	173.75 (3)
C8—N2—C3—C2	-177.45 (3)	C2—C1—C6—C5	2.17 (5)
C3—N2—C8—O3	1.44 (6)	C7—C1—C6—C5	-173.67 (3)
C3—N2—C8—C9	-176.42 (3)	C2—C1—C6—N1	-174.75 (3)
O3—C8—C9— C11	14.46 (6)	C7—C1—C6—N1	9.41 (5)
N2—C8—C9— C11	-167.68 (4)	O1—N1—C6—C5	35.60 (5)
O3—C8—C9— C10	-107.67 (5)	O2—N1—C6—C5	-141.76 (4)
N2—C8—C9— C10	70.18 (4)	O1—N1—C6—C1	-147.35 (4)
N2—C3—C4—C5	-179.31 (3)	O2—N1—C6—C1	35.29 (6)
C2—C3—C4—C5	2.16 (5)	C2—C1—C7—F2	100.79 (4)
C6—C1—C2—C3	1.17 (5)	C6—C1—C7—F2	-83.33 (5)
C7—C1—C2—C3	177.29 (3)	C2—C1—C7—F1	-137.22 (4)
N2—C3—C2—C1	178.03 (3)	C6—C1—C7—F1	38.66 (5)
C4—C3—C2—C1	-3.33 (5)	C2—C1—C7—F3	-18.61 (5)
C3—C4—C5—C6	1.13 (6)	C6—C1—C7—F3	157.26 (4)
C4—C5—C6—C1	-3.35 (6)		