

Tetrel bonds involving CF₃ group participate in protein-drug recognition: A combined crystallographic and computational study.

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Electronic Supporting Information

Index

Figure S1	2
Table S1	2
Cartesian coordinates of the PDB models	3
Cartesian coordinates of complexes 11 to 30	16

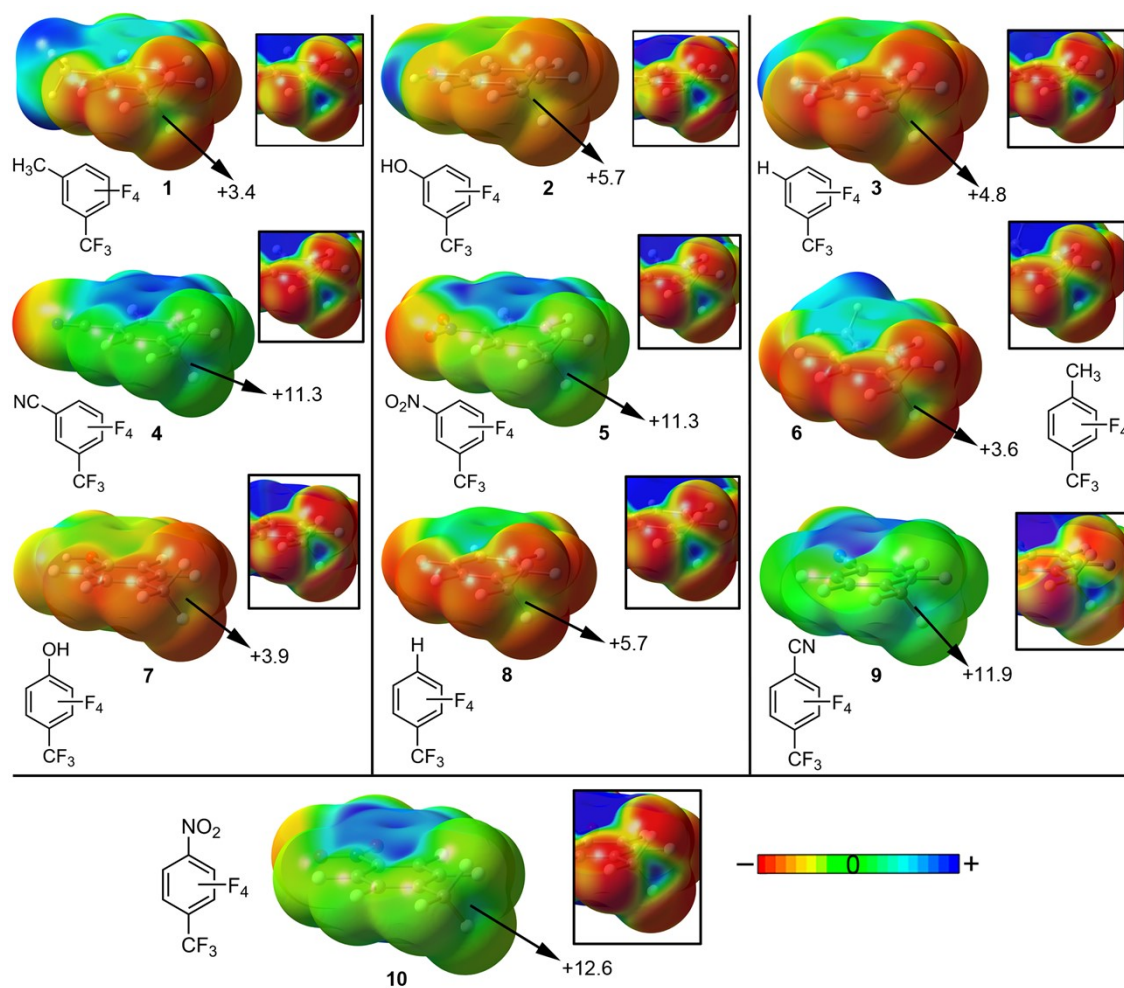


Figure S1. Molecular Electrostatic Potential (MEP) surfaces of compounds **1** to **10**. Energies at selected points in the surface are given in kJ/mol (0.001 a.u.).

Table S1. vdW radii values (in Å) used for C, N, O and S elements.

Element	C	N	O	S
vdW radii	1.77	1.66	1.50	1.89

Cartesian coordinates of the PDB models

PDBID 2PDL

C	5.3724970	1.5531333	-4.1467865
C	4.4234970	0.8921333	-5.1377865
O	4.4444970	1.2311333	-6.3307865
N	3.5724970	-0.0318667	-4.7007865
C	2.6644970	-0.6938667	-5.6467865
C	1.4904970	0.2001333	-5.9987865
O	0.6264970	-0.1468667	-6.8067865
C	2.1934970	-2.0198667	-5.0517865
O	1.4054970	-1.8058667	-3.8977865
N	1.4694970	1.3821333	-5.3817865
C	0.3264970	2.2811333	-5.5497865
C	-0.8415030	-0.9778667	-1.0507865
F	0.4764970	-0.9838667	-1.1357865
F	-1.3305030	-0.2648667	-2.0797865
F	-1.3525030	-2.2098667	-1.2687865
C	-1.3965030	-0.4358667	0.2942135
C	-2.1625030	0.7401333	0.3872135
O	-2.4275030	1.4511333	-0.7017865
C	-3.2095030	2.5931333	-0.4827865
C	-2.6345030	1.1471333	1.6432135
C	-2.3445030	0.3891333	2.7802135
C	-1.5845030	-0.7858667	2.6802135
C	-1.2875030	-1.5538667	3.8372135
C	-0.5385030	-2.7368667	3.7402135
C	-0.0535030	-3.1608667	2.4872135
C	-0.3455030	-2.3898667	1.3512135
C	-1.1065030	-1.2058667	1.4302135
C	-1.7895030	-1.1588667	5.1952135
S	-3.2305030	-1.9258667	5.7182135
N	-1.1775030	-0.2188667	5.9502135
C	0.2110172	-0.6677784	6.1273856
C	-1.6515030	0.1801333	7.2662135
C	-2.6785030	1.3361333	7.0812135
O	-3.2785030	1.8381333	8.0072135
O	-2.8745030	1.6031333	5.7992135
H	5.1798257	2.6438697	-4.1565231
H	3.0940763	-2.6495394	-4.8373621
H	1.6141630	-2.5241558	-5.8591959
H	0.8489938	-2.5877057	-3.7442755
H	3.2197945	-0.8821394	-6.5885716
H	-0.1732932	2.0174972	-6.4999150
H	-0.8124456	0.5625006	7.8724903
H	-2.1716501	-0.6454089	7.8014199
H	-4.2156247	2.3502912	-0.0749685
H	-2.7116476	3.3322626	0.1835967
H	-3.3492147	3.0666956	-1.4735795
H	-3.2341662	2.0525204	1.7682902
H	-2.7139236	0.7136495	3.7606089
H	-0.3453494	-3.3269126	4.6481992
H	0.5411891	-4.0812551	2.3950263
H	0.0513843	-2.7407126	0.3940790
H	0.8253138	0.1383254	6.5762036

H	0.2531609	-1.5606233	6.7911979
H	0.6755878	-0.9312263	5.1607962
H	6.4072832	1.4048827	-4.5109994
H	5.2970404	1.1794183	-3.1051152
H	-0.4085476	2.1619854	-4.7239216
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H	-3.5886528	2.2789675	5.7611498

PDBID 3HQ5

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C	4.3920766	-0.0296978	-2.6667488
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C	2.6200806	1.8302981	-0.9127527
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C	2.5400808	-0.2276974	0.5402440
C	2.5670808	-1.7466939	0.7772434
C	2.2640814	-2.0486932	2.2542401
C	1.5940830	-2.4936923	-0.1417545
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H	5.7089355	-1.4629602	-3.6084164
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N	1.2312697	-3.3920942	-3.3639070
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H	-0.6828389	-0.6580773	4.1829227
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H	-1.7009848	0.8195060	1.7142627
H	0.8335744	0.3745243	2.3150168
H	-3.4926000	2.7986221	5.2499340
H	-4.9612820	2.5541570	4.2192302
H	-3.3445761	2.1154001	2.3410657
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H	1.7046183	-1.0371153	-6.3305586
H	2.8720634	-0.2452386	-5.2349777
H	-0.1789185	0.1430160	-5.3864680
H	1.0514597	1.4119387	-5.1425469
H	1.2525694	0.8443244	-2.7474018
H	-0.4524884	0.4020627	-3.0029913
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C	-1.3116284	-0.3176195	2.0309483
S	-1.1936284	-0.1046195	3.8389483
N	-3.2896284	-0.6156195	-0.3970517
C	-3.5576284	-0.5036195	-1.8210517
C	4.2903716	2.7363805	-2.3080517
C	1.9343716	1.3873805	-1.6300517
C	2.1523716	2.6883805	-1.1690517
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C	2.8983716	0.7753805	-2.4460517
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H	-0.9919739	-1.4255405	4.1058779
H	-3.2052066	-1.3397748	2.0601058
H	-2.6031006	-0.6186913	-2.3680227
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H	-1.7870248	-5.8473916	1.3903055
H	-2.3604575	-5.6664602	3.0684112
H	-3.9418405	-0.1745633	0.2529168
H	-0.6830991	-2.8758161	1.9946349
C	3.4322721	4.9227280	0.3441409
H	3.8816992	5.9209605	0.5026910
H	2.3671080	4.9610160	0.6670772
H	3.9669967	4.1738138	0.9697149

PDBID 4BVC

C	2.9308802	3.9516295	0.2307858
C	1.7538805	3.9726294	1.1887855
O	0.7438808	4.5516293	0.8897856
N	1.9138805	3.3386296	2.3477852
C	0.8498808	3.1566297	3.3327849
C	1.3308807	3.5126296	4.7497845
O	1.5608806	2.6256298	5.5737843
C	0.3428809	1.7116301	3.2457849
C	-0.2971189	1.4466302	1.9007853
C	-1.5851185	1.8926300	1.6367854
C	0.4048809	0.8216303	0.8717856

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O	-2.0641184	0.8586303	-1.8332136
N	1.4628806	4.8246292	5.0447844
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C	1.9778805	7.0736286	4.7447845
C	1.0178807	6.0146289	4.2997846
C	-2.9271181	-4.5583682	-6.6832123
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C	-0.9071187	-5.7383678	-6.2082124
C	-0.9451187	-5.2103680	-4.9362128
C	-1.9461184	-4.3593682	-4.5282129
C	-2.9571181	-4.0323683	-5.4082126
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F	-1.3361186	-2.1563688	-1.8892136
F	-3.1741181	-2.0093689	-3.1362133
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C	-1.2031186	-8.8373670	-1.8662136
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H	3.5076203	6.9484020	6.2795157
H	1.5335725	8.0880434	4.6941767
H	2.8380425	7.0877702	4.0395250
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H	1.0159177	5.8410216	3.2054921
H	3.0955410	4.5713483	6.3502827
H	-3.7328709	-4.2960811	-7.3863309
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H	-3.7623889	-3.3585605	-5.0860309
H	-1.0534575	-8.3856170	-0.8653258
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PDBID 4J8M

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N	1.4253263	0.2514440	-4.3432903
C	2.4203241	1.0554420	-3.6722919
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O	3.0973226	-0.8135536	-2.3402947
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H	3.2283414	1.3485683	-4.3873699
H	1.9368645	2.0157686	-3.3881521
N	3.7208118	1.2582477	-1.6402257
C	4.4123196	0.7424427	-0.4792990
H	3.5716401	2.2625370	-1.7388833
H	3.7467498	0.0766825	0.1081235
O	-0.4386695	-1.5675520	4.0856908
C	-1.5096671	-1.1525529	4.5206897
N	-2.4786649	-0.4315545	3.7366916
C	-2.4066649	-0.1065552	2.3256947
C	-3.5756624	0.2474440	1.6626961
C	-3.5396625	0.5434433	0.2906993
C	-2.3196652	0.4904435	-0.4062991
C	-1.1446679	0.1264443	0.2606993
C	0.1723292	0.0744443	-0.4832990
F	0.7823279	-1.0865532	-0.2572993
F	0.9393274	1.0544420	-0.0092999
F	-0.0266704	0.2464440	-1.7952959
C	-1.1836678	-0.1745550	1.6206963
N	-1.9146661	-1.3185525	5.9116866
H	-3.3477275	-0.1614783	4.1979710
H	-4.5359767	0.2786990	2.2054327
H	-4.4663201	0.8197177	-0.2340955
H	-2.2937971	0.7243317	-1.4780997
H	-0.2801341	-0.4893169	2.1567554
H	-2.8843522	-1.1087141	6.1484629
H	4.7375690	1.5825487	0.1620104
H	5.3048196	0.1491854	-0.7702384
H	-1.4362950	-0.1360514	-5.1675051
H	-0.1364975	-1.1360805	-5.9026526
C	-1.1122414	-1.9844823	6.9478073
H	-1.1994176	-1.4358130	7.9067350
H	-1.4088056	-3.0444577	7.1092281
H	-0.0548678	-1.9725238	6.6195283

PDBID 4UA7

C	-1.7201856	2.6847412	-5.9680821
C	-0.5581856	3.0117412	-5.0520821
O	0.1548144	3.9757412	-5.2220821
H	-2.5411835	2.1346634	-5.4653304
N	-0.2751856	2.1517412	-4.0800821
C	0.9298144	2.3387412	-3.2740821
C	2.1708144	2.0647412	-4.1270821
O	2.1748144	1.3337412	-5.1040821
C	0.9138144	1.4367412	-2.0670821
O	1.0538144	0.0897412	-2.4910821

H	-0.6509271	1.2001692	-4.0941877
H	0.9430052	3.4067862	-2.9637977
H	1.7051087	1.7409643	-1.3437983
H	-0.0588093	1.5215053	-1.5377640
N	3.2658144	2.6807412	-3.6890821
C	4.5408144	2.6437412	-4.4290821
H	3.1681193	3.3993153	-2.9694426
H	4.4955325	1.7824931	-5.1202939
C	-2.9631856	-2.2192588	4.5279179
C	0.7748144	-2.9172588	4.2329179
C	1.1868144	-2.3372588	3.0519179
C	0.7418144	-4.0052588	6.0749179
C	0.5458144	-0.9692588	1.1079179
F	1.5648144	-0.0862588	1.3089179
F	1.0138144	-1.8162588	0.1809179
F	-0.3521856	-0.2722588	0.5959179
C	0.1908144	-1.6422588	2.3879179
N	1.5588144	-3.6552588	5.0939179
N	-0.6031856	-3.5832588	5.9019179
C	-0.5451856	-2.8822588	4.7379179
C	-1.1491856	-1.6202588	2.8319179
C	-1.5631856	-2.2052588	4.0259179
O	-3.3251856	-3.0472588	5.3699179
N	-3.8249208	-1.2497713	4.0100499
H	-1.3440786	2.0572960	-6.8026766
H	-2.1064927	3.6267537	-6.3968161
H	4.6867675	3.5680878	-5.0273904
H	5.3934043	2.5227943	-3.7313721
H	1.9860655	-0.1288323	-2.5598832
H	2.2174437	-2.3801821	2.6742553
H	-1.8827500	-1.1102770	2.1900270
H	-3.4133706	-0.5038415	3.4479247
H	2.5573232	-3.8402978	5.0019642
C	-5.2459165	-1.1016919	4.3677642
H	-5.8827184	-1.0890040	3.4591505
H	-5.5168609	-1.9723154	4.9953156
H	-5.4251316	-0.1737630	4.9514150
H	1.0587816	-4.6020674	6.9400219

PDBID 5HVE

C	-5.5009537	3.2402938	-2.1777907
C	-4.0719569	2.7912950	-2.2527905
O	-3.5239580	2.4562957	-3.3287881
N	-3.4709582	2.5882951	-1.0637931
C	-2.1289612	1.9702967	-0.9597934
C	-2.1069612	0.7052994	-0.0777955
O	-1.1689634	-0.0736986	-0.1597951
C	-0.9999636	2.9542943	-0.5447943
C	-1.2719631	3.5272933	0.8432026
C	-0.9879637	4.0682919	-1.6077919
C	-0.0489658	4.3352912	1.4382012
N	-3.1239589	0.4592999	0.7412027
C	-3.0599591	-0.7156974	1.5852009
F	0.3530332	-2.7516929	0.9892021
C	1.3070311	-2.0316945	1.4062013
F	0.8330322	-1.1866961	2.3531992

F	1.7980300	-1.3266961	0.3662036
O	2.3160288	-2.7816928	2.0321997
C	2.9500274	-3.8626904	1.4742011
C	4.1390247	-3.6196906	0.8072026
C	2.5040284	-5.2056873	1.5932009
C	3.2450268	-6.2486849	1.0752020
C	4.4740239	-5.9966856	0.4092035
C	4.8980230	-4.6396886	0.2382039
S	6.3890198	-4.3896889	-0.5637942
H	-6.1479040	2.3398387	-2.2201976
H	-5.7532531	3.8024885	-1.2551479
H	-0.0577543	2.3687389	-0.5504900
H	-0.1519063	4.7794563	-1.4523884
H	-0.9005426	3.6551210	-2.6312359
H	-1.9314601	4.6492002	-1.5688576
H	-1.5213584	2.7086653	1.5531193
H	-2.1598017	4.1983190	0.8074529
H	-0.2741003	4.7007477	2.4597903
H	0.8475148	3.6851168	1.4928298
H	0.1997750	5.2125775	0.8086832
H	-1.9158584	1.6090910	-1.9849483
H	-3.8418253	3.0658658	-0.2393759
H	-2.0690123	-0.7693516	2.0765042
H	-3.1785932	-1.6529704	0.9993870
H	-3.9826450	1.0058196	0.6777725
H	4.4672937	-2.5724355	0.7285102
H	1.5499176	-5.3936648	2.1090109
H	2.8871705	-7.2835766	1.1832290
H	5.0631227	-6.8171349	-0.0255720
H	-3.8548624	-0.6672369	2.3538335
H	-5.7430390	3.8607408	-3.0605266
C	6.1899055	-2.9209756	-1.5495078
H	5.2956666	-2.9823051	-2.2030145
H	6.1376472	-1.9871294	-0.9516336
H	7.0933633	-2.8648489	-2.1878387

PDBID 5LCK

C	0.0942801	-1.4472940	6.0496260
C	0.0002801	-2.4162940	4.8666260
O	-0.5277199	-3.5242940	5.0156260
N	0.5012801	-1.9832940	3.6876260
C	0.4102801	-2.7722940	2.4546260
C	1.7272801	-2.6882940	1.6726260
O	2.5332801	-1.7712940	1.8996260
C	-0.7787199	-2.2862940	1.5796260
C	-2.1517199	-2.4012940	2.2716260
C	-3.2877199	-1.7702940	1.4906260
O	-3.3657199	-0.5672940	1.3616260
N	-4.2347199	-2.5732940	1.0146260
N	1.9492801	-3.6492940	0.7516260
C	3.1332801	-3.6382940	-0.1283740
C	0.9912801	1.1107060	-2.3493740
C	-0.1987199	1.7527060	-2.0893740
C	-0.3697199	3.0537060	-2.6303740
C	-1.2407199	1.0117060	-1.2363740
N	-1.5047199	3.7757060	-2.4343740

N	0.6082801	3.6017060	-3.3593740
C	1.7292801	2.8917060	-3.5533740
N	2.7102801	3.4627060	-4.2953740
N	1.9672801	1.6557060	-3.0753740
F	-1.4047199	1.5907060	-0.0363740
F	-2.4547199	0.9747060	-1.7993740
F	-0.8897199	-0.2612940	-1.0133740
H	1.1760636	0.0995641	-1.9508285
H	-2.2370321	3.3098405	-1.8989910
H	3.5287009	2.8579665	-4.3810098
H	3.7270268	-4.5667806	-0.0042079
H	-2.3483742	-3.4611878	2.5415954
H	-2.1094514	-1.8410939	3.2267096
H	-4.2147653	-3.5874140	1.1124138
H	-5.0129379	-2.1464946	0.5095654
H	0.2158751	-3.8190780	2.7780494
H	-0.6068338	-1.2273746	1.2952191
H	-0.7878246	-2.8613911	0.6280774
H	1.0657081	-1.1316061	3.6171804
H	1.2564266	-4.3888390	0.6287285
H	0.7552718	-0.5747091	5.8760472
H	3.7476307	-2.7688008	0.1684111
H	-0.9264569	-1.0789264	6.2759839
H	0.4453862	-2.0123332	6.9333076
H	2.8391771	-3.5341121	-1.1932816
C	2.7457551	4.7450231	-5.0132212
H	1.8427054	4.8697617	-5.6465149
H	2.7872424	5.6104577	-4.3163099
H	3.6444283	4.7585709	-5.6561916
C	-1.7985358	5.1554990	-2.8475852
H	-1.7941171	5.2588904	-3.9533377
H	-2.7977394	5.4257177	-2.4616785
H	-1.0458914	5.8646718	-2.4433605

PDBID 5OCM

O	-0.3738053	-2.0429153	3.4435881
C	0.1671947	-2.5009153	2.1835881
O	-0.1988053	-3.8209153	1.8665881
C	1.6901947	-2.3979153	2.1455881
C	2.3721947	-1.8779153	3.2295881
C	3.7601947	-1.8989153	3.2605881
C	4.4731947	-2.4059153	2.2005881
C	3.7981947	-2.9029153	1.0965881
C	2.4091947	-2.9069153	1.0785881
C	-0.4168053	-1.5639153	1.1685881
F	-1.7568053	-1.5589153	1.2695881
F	-0.0458053	-1.8899153	-0.1004119
F	0.0531947	-0.3589153	1.4445881
O	-1.3608053	4.2700847	-0.8124119
C	-1.6178053	4.4440847	-2.2334119
C	-1.7138053	3.1630847	-2.9654119
O	-0.3808053	2.5960847	-3.0034119
C	-2.6098053	2.1420847	-2.2804119
O	-3.2028053	1.3740847	-3.3204119
C	-1.6628053	1.2350847	-1.4794119
O	-2.2368053	-0.0639153	-1.1614119

C	-0.4348053	1.2900847	-2.3584119
H	-0.3311645	-1.0681859	3.4399976
H	0.3833650	-4.3970260	2.3975354
H	1.8086132	-1.4988316	4.0932952
H	4.2875550	-1.5044329	4.1436728
H	5.5741651	-2.4188748	2.2265002
H	4.3556154	-3.3096292	0.2386565
H	1.8708698	-3.3323237	0.2199594
H	-0.8006261	5.0364096	-2.7081512
H	-2.5661592	5.0214408	-2.3851581
H	-2.0923221	3.3452430	-3.9961859
H	-3.3772059	2.6218649	-1.6348722
H	-4.0922694	1.1041453	-3.0310224
H	-1.4497306	1.7181006	-0.5053016
H	-2.6848940	-0.3409326	-1.9912752
H	-0.5040008	0.4836058	-3.1299497
H	-1.0578530	5.1310035	-0.4774689
H	0.5116527	1.1442459	-1.8004527

PDBID 5VBM

C	-1.6360475	-0.6063421	-6.4187441
C	-0.5940481	-0.7933419	-5.3207447
O	-0.1360483	-1.9193413	-5.0997449
H	-2.5304037	-1.1997343	-6.1440018
N	-0.2160483	0.2666575	-4.5987451
C	0.7649511	0.0636576	-3.5377457
C	0.1899515	-0.8253419	-2.4517463
O	0.8879511	-1.7003414	-1.9137467
H	-0.4763092	1.2110797	-4.8856797
H	1.6693612	-0.4507463	-3.9149666
N	-1.0930479	-0.6163420	-2.1297465
C	-1.7650475	-1.4223415	-1.1137471
H	-1.6449694	0.0113174	-2.7163610
H	-0.9856586	-1.8604825	-0.4643037
C	-1.3400477	-1.8013413	5.3592493
C	0.9129511	0.8496571	3.7822501
C	1.2539509	1.0076571	2.4382509
C	1.1279509	2.0796565	4.4112497
C	1.1809509	-0.0183423	1.3412515
C	0.4109513	-0.4213421	4.3752498
F	0.7209511	0.5486573	0.2372521
F	0.3719513	-1.0203417	1.6482513
F	2.3919503	-0.5413421	1.1072517
N	1.6489507	2.2736563	2.2882509
N	1.6019507	2.9446560	3.4732503
N	-0.9050479	-0.5063421	4.9192495
O	1.1039509	-1.4303415	4.3542498
H	-0.5350402	-2.2887965	5.9423973
H	-2.2388732	-1.7008840	5.9992106
H	0.9987353	2.3892001	5.4533263
H	-1.5640725	0.2597059	4.7784481
H	-2.4403558	-0.7888825	-0.5046348
H	-2.3525648	-2.2515160	-1.5642582
H	-1.2343574	-1.0388487	-7.3546828
H	-1.9457263	0.4429009	-6.6031566
H	1.0479542	1.0490586	-3.1155034

H	-1.5801108	-2.4841398	4.5121600
C	2.1387361	2.9449203	1.0756453
H	2.9429808	2.3414746	0.6137525
H	1.3148992	3.0780018	0.3492081
H	2.5309013	3.9260892	1.3932393

PDBID 6BU3

C	2.0567429	0.7737025	-6.1686327
C	0.7077429	0.1447025	-5.7776327
O	0.0337429	-0.4462975	-6.5466327
N	0.3427429	0.3507025	-4.5206327
C	-0.8972571	-0.2102975	-4.0036327
C	-2.0722571	0.4197025	-4.7106327
O	-2.0162571	1.5597025	-5.1686327
C	-1.0362571	0.0047025	-2.4926327
O	-1.1662571	1.3787025	-2.2446327
N	-3.1952571	-0.3092975	-4.7336327
C	-4.4232571	0.1337025	-5.3966327
C	2.8417429	-0.5732975	5.0283673
C	-0.9342571	0.1687025	5.2023673
C	-1.1952571	0.2927025	3.8293673
C	-0.9052571	0.0547025	7.3913673
C	-0.5642571	0.2867025	1.4583673
F	-1.4802571	-0.6042975	1.1113673
F	-1.0702571	1.4927025	1.2563673
F	0.4707429	0.1427025	0.5823673
C	-0.1812571	0.1327025	2.8973673
N	-1.7152571	0.2717025	6.3303673
N	0.3557429	-0.1762975	6.9663673
C	0.3717429	-0.1132975	5.6333673
C	1.1317429	-0.1492975	3.3053673
C	1.3887429	-0.2702975	4.6553673
O	3.1647429	-0.3882975	6.2003673
N	3.6957429	-1.0222975	4.0773673
H	2.6465380	1.1607834	-5.3145224
H	-0.1318068	-0.3495521	-1.9569588
H	-1.9019322	-0.5967471	-2.1177164
H	-0.8900894	-1.3029031	-4.2250952
H	-4.2955564	1.2040350	-5.6431014
H	-2.2133150	0.5187497	3.4732487
H	-1.2398696	0.0698155	8.4356480
H	-2.7151478	0.4773272	6.3409957
H	1.9185244	-0.2171220	2.5454470
H	3.2859553	-1.3018578	3.1857509
H	0.7819454	1.0750101	-3.9496912
H	-3.1457739	-1.2865016	-4.4397356
H	-5.3009545	0.0072015	-4.7305459
H	-4.5998075	-0.4275410	-6.3385774
H	1.8648554	1.6006041	-6.8814018
H	2.6518293	0.0103343	-6.7059237
H	-1.8918050	1.7181624	-2.8008956
C	5.1151544	-1.3711973	4.2336993
H	5.7333697	-0.8426980	3.4797081
H	5.4242851	-1.0553136	5.2487254
H	5.2759865	-2.4657650	4.1379294

PDBID 7OT2

C	-0.7551522	-3.1035650	-5.2261790
C	-0.1241522	-3.2805650	-3.8461790
O	-0.0011522	-4.4025650	-3.3401790
N	0.2668478	-2.1575650	-3.2321790
C	0.9328478	-2.1725650	-1.9271790
C	-0.0651522	-2.4305650	-0.8051790
O	-1.1381522	-1.8165650	-0.7591790
C	1.6638478	-0.8455650	-1.6731790
C	2.2688478	-0.7075650	-0.2621790
C	3.1558478	0.5274350	-0.1021790
O	4.3808478	0.4194350	-0.0581790
N	2.5358478	1.6994350	0.0058210
N	0.3038478	-3.3215650	0.1118210
C	-0.5861522	-3.7085650	1.1968210
C	-2.5681522	3.0274350	0.6288210
C	-1.7291522	3.3164350	1.8498210
C	-0.9751522	2.3054350	2.4658210
C	-0.2581522	2.5784350	3.6208210
C	-0.2561522	3.8544350	4.1568210
C	-0.9751522	4.8614350	3.5478210
C	-1.7091522	4.5954350	2.4038210
C	-0.8711522	0.9384350	1.8478210
F	-0.3711522	0.9714350	0.6088210
F	-0.0681522	0.1404350	2.5408210
F	-2.0411522	0.3004350	1.7848210
H	-0.7168900	-2.0697897	-5.6242756
H	0.9286261	-0.0230703	-1.8230697
H	2.4590215	-0.7200207	-2.4380393
H	1.4562548	-0.7008071	0.4929963
H	2.9277002	-1.5704347	-0.0445656
H	3.1074602	2.5342379	0.1426696
H	1.5214803	1.7800747	0.0768531
H	1.6717783	-3.0042330	-1.9603560
H	-0.4010936	-4.7616121	1.4811825
H	-1.6334205	-3.5892235	0.8577731
H	-3.3244071	2.2474823	0.8460772
H	-1.9565668	2.6363116	-0.2080541
H	0.3292032	1.7810978	4.0968601
H	0.3225860	4.0594156	5.0703959
H	-0.9689312	5.8784834	3.9701912
H	-2.2947874	5.3947462	1.9234372
H	-3.0943848	3.9349374	0.2772686
H	-1.8125542	-3.4308671	-5.1733387
H	-0.2390781	-3.7836866	-5.9308670
H	0.0025130	-1.2486183	-3.6127498
H	1.1479974	-3.8719552	-0.0493087
H	-0.4482034	-3.0618368	2.0900586

Cartesian coordinates of complexes 11 to 30

11.

O	-0.4630154	-4.7497062	0.0000000
C	-0.4106359	2.9834839	0.0000000
C	-1.6033372	2.2703849	0.0000000
C	-1.5583846	0.8861644	0.0000000
C	-0.3456037	0.1946606	0.0000000
C	-0.3917321	-1.3134567	0.0000000
F	-1.0453258	-1.7614687	-1.0819043
F	-1.0453258	-1.7614687	1.0819043
F	0.8187143	-1.8641914	0.0000000
C	0.8180203	0.9612772	0.0000000
C	0.8269274	2.3549584	0.0000000
C	-0.3965413	-5.9596027	0.0000000
H	0.5722831	-6.4872462	0.0000000
H	-1.3013934	-6.5904912	0.0000000
F	-2.7112324	0.2192269	0.0000000
F	2.0180868	0.3659652	0.0000000
F	-2.7714889	2.9073253	0.0000000
F	-0.4848051	4.3179625	0.0000000
C	2.1184741	3.1157427	0.0000000
H	2.7115114	2.8613215	0.8800155
H	2.7115114	2.8613215	-0.8800155
H	1.9332930	4.1878368	0.0000000

12.

O	-0.2104660	-4.3093633	0.0000000
C	-0.1679926	3.3519167	0.0000000
C	-1.3551004	2.6303046	0.0000000
C	-1.3176223	1.2439581	0.0000000
C	-0.1077934	0.5489994	0.0000000
C	-0.1502485	-0.9591699	0.0000000
F	-0.7995274	-1.4094715	-1.0817200
F	-0.7995274	-1.4094715	1.0817200
F	1.0665875	-1.4990297	0.0000000
C	1.0603573	1.3055027	0.0000000
C	1.0606857	2.6992296	0.0000000
C	-0.1782437	-5.5204769	0.0000000
H	0.7751248	-6.0749997	0.0000000
H	-1.1003960	-6.1251940	0.0000000
F	-2.4733552	0.5801835	0.0000000
F	2.2790297	0.7365084	0.0000000
F	-2.5197458	3.2720780	0.0000000
F	-0.2088824	4.6800818	0.0000000
H	2.9513756	2.8246635	0.0000000
O	2.1957406	3.4337503	0.0000000

13.

O	-0.4503029	-4.1514372	0.0000000
C	0.3056837	3.4982255	0.0000000
C	-0.9414566	2.8869659	0.0000000
C	-1.0046859	1.5011799	0.0000000
C	0.1425889	0.7047602	0.0000000

C	-0.0350682	-0.7939630	0.0000000
F	-0.7242103	-1.1819064	-1.0822796
F	-0.7242103	-1.1819064	1.0822796
F	1.1242725	-1.4444950	0.0000000
C	1.3697955	1.3672523	0.0000000
C	1.4682449	2.7503056	0.0000000
C	-0.5090959	-5.3617423	0.0000000
H	0.3999033	-5.9865432	0.0000000
H	-1.4743841	-5.8954395	0.0000000
F	-2.2090317	0.9346333	0.0000000
F	2.5158148	0.6793510	0.0000000
F	-2.0553456	3.6117280	0.0000000
F	0.3646144	4.8300756	0.0000000
H	2.4368736	3.2329558	0.0000000

14.

O	0.1120041	-4.3549694	0.0000000
C	-0.4775403	3.2568663	0.0000000
C	-1.5960387	2.4378597	0.0000000
C	-1.4220162	1.0605093	0.0000000
C	-0.1571732	0.4697811	0.0000000
C	-0.0797659	-1.0417383	0.0000000
F	-0.6951543	-1.5322336	-1.0826414
F	-0.6951543	-1.5322336	1.0826414
F	1.1719843	-1.4831004	0.0000000
C	0.9437390	1.3201383	0.0000000
C	0.8048732	2.7112899	0.0000000
C	0.2880360	-5.5539627	0.0000000
H	1.3004136	-5.9910310	0.0000000
H	-0.5561472	-6.2632689	0.0000000
F	-2.5101569	0.3007599	0.0000000
F	2.1833564	0.8422452	0.0000000
F	-2.8139097	2.9606183	0.0000000
F	-0.6387017	4.5722929	0.0000000
C	1.9495312	3.5584554	0.0000000
N	2.8878206	4.2617216	0.0000000

15.

O	0.3021630	-4.5601019	0.0000000
C	-0.7744158	3.0552008	0.0000000
C	-1.8258766	2.1472049	0.0000000
C	-1.5680282	0.7881986	0.0000000
C	-0.2657371	0.2967280	0.0000000
C	-0.0935070	-1.2108375	0.0000000
F	-0.6832597	-1.7329459	-1.0828977
F	-0.6832597	-1.7329459	1.0828977
F	1.1759453	-1.5916733	0.0000000
C	0.7845328	1.2142067	0.0000000
C	0.5527733	2.6021506	0.0000000
C	0.5796416	-5.7399702	0.0000000
H	1.6258825	-6.0888122	0.0000000
H	-0.2016672	-6.5183057	0.0000000
F	-2.6013241	-0.0427900	0.0000000
F	2.0229911	0.7519022	0.0000000
F	-3.0743678	2.5904938	0.0000000
F	-1.1122860	4.3316669	0.0000000

N	1.6652416	3.5653057	0.0000000
O	1.3675157	4.7556581	0.0000000
O	2.8070423	3.1196663	0.0000000

16.

C	-0.4163037	3.9338109	0.0000000
C	-1.5847625	3.1815281	0.0000000
C	-1.4935072	1.7996407	0.0000000
C	-0.2587062	1.1482021	0.0000000
C	-0.2605698	-0.3610659	0.0000000
F	-0.9006382	-0.8256411	-1.0821733
F	-0.9006382	-0.8256411	1.0821733
F	0.9668955	-0.8771623	0.0000000
C	0.8788116	1.9530091	0.0000000
C	0.8414984	3.3464198	0.0000000
F	-2.6238506	1.0948644	0.0000000
F	2.0978405	1.3970523	0.0000000
F	-2.7735615	3.7786069	0.0000000
F	-0.5349368	5.2649002	0.0000000
C	2.1066925	4.1504680	0.0000000
H	2.7079438	3.9165265	0.8801760
H	2.7079438	3.9165265	-0.8801760
H	1.8852567	5.2157270	0.0000000
O	-0.3005855	-3.7344097	0.0000000
C	0.8891046	-4.4928323	0.0000000
H	1.7208585	-3.7903720	0.0000000
H	0.9541719	-5.1305637	0.8908621
H	0.9541719	-5.1305637	-0.8908621
C	-1.4356052	-4.5726975	0.0000000
H	-2.3140271	-3.9294793	0.0000000
H	-1.4567485	-5.2134270	-0.8907885
H	-1.4567485	-5.2134270	0.8907885

17.

C	-0.2296684	4.2971903	0.0000000
C	-1.3940439	3.5395969	0.0000000
C	-1.3142594	2.1551896	0.0000000
C	-0.0839404	1.4971226	0.0000000
C	-0.0842927	-0.0120024	0.0000000
F	-0.7208310	-0.4775844	-1.0820254
F	-0.7208310	-0.4775844	1.0820254
F	1.1486222	-0.5185301	0.0000000
C	1.0603047	2.2889919	0.0000000
C	1.0183769	3.6821915	0.0000000
F	-2.4496870	1.4566854	0.0000000
F	2.2957451	1.7570193	0.0000000
F	-2.5777826	4.1451470	0.0000000
F	-0.3113150	5.6232699	0.0000000
O	-0.0958563	-3.2989748	0.0000000
C	1.0875788	-4.0664510	0.0000000
H	1.9248136	-3.3702037	0.0000000
H	1.1479825	-4.7043064	0.8909465
H	1.1479825	-4.7043064	-0.8909465
C	-1.2392306	-4.1259933	0.0000000
H	-2.1110489	-3.4736953	0.0000000
H	-1.2666460	-4.7660139	-0.8910552

H	-1.2666460	-4.7660139	0.8910552
O	2.1298864	4.4516890	0.0000000
H	2.9047864	3.8675664	0.0000000

18.

C	-0.1355512	4.4716074	0.0000000
C	-1.2839776	3.6981232	0.0000000
C	-1.2066340	2.3131943	0.0000000
C	0.0277503	1.6606791	0.0000000
C	0.0226704	0.1487777	0.0000000
F	-0.6173754	-0.3100917	-1.0827204
F	-0.6173754	-0.3100917	1.0827204
F	1.2509918	-0.3630618	0.0000000
C	1.1833960	2.4414774	0.0000000
C	1.0896452	3.8303508	0.0000000
F	-2.3356246	1.6056583	0.0000000
F	2.4009811	1.9040895	0.0000000
F	-2.4840725	4.2818179	0.0000000
O	0.0433844	-3.0996247	0.0000000
C	1.2373346	-3.8508165	0.0000000
H	2.0646862	-3.1429799	0.0000000
H	1.3064198	-4.4875585	0.8910638
H	1.3064198	-4.4875585	-0.8910638
C	-1.0888915	-3.9412007	0.0000000
H	-1.9691821	-3.3001786	0.0000000
H	-1.1081895	-4.5814814	-0.8909558
H	-1.1081895	-4.5814814	0.8909558
H	-0.1944004	5.5529110	0.0000000
F	2.2157841	4.5474389	0.0000000

19.

C	-0.5256806	4.2559288	0.0000000
C	-1.6352269	3.4244019	0.0000000
C	-1.4465948	2.0488623	0.0000000
C	-0.1754657	1.4711013	0.0000000
C	-0.0849532	-0.0401448	0.0000000
F	-0.6960247	-0.5342449	-1.0827799
F	-0.6960247	-0.5342449	1.0827799
F	1.1719359	-0.4723698	0.0000000
C	0.9158734	2.3337098	0.0000000
C	0.7624715	3.7237487	0.0000000
F	-2.5269240	1.2774895	0.0000000
F	2.1604659	1.8688287	0.0000000
F	-2.8586213	3.9340999	0.0000000
F	-0.7013077	5.5693878	0.0000000
O	0.0922765	-3.4019209	0.0000000
C	1.3302256	-4.0805315	0.0000000
H	2.1147660	-3.3258031	0.0000000
H	1.4367561	-4.7123745	0.8907611
H	1.4367561	-4.7123745	-0.8907611
C	-0.9841396	-4.3155071	0.0000000
H	-1.9042652	-3.7333308	0.0000000
H	-0.9615575	-4.9555782	-0.8910783
H	-0.9615575	-4.9555782	0.8910783
C	1.9002805	4.5802125	0.0000000
N	2.8365358	5.2862320	0.0000000

20.

C	-0.8192031	3.9967042	0.0000000
C	-1.8691797	3.0871146	0.0000000
C	-1.6085112	1.7288034	0.0000000
C	-0.3052494	1.2400907	0.0000000
C	-0.1351832	-0.2676405	0.0000000
F	-0.7261074	-0.7852261	-1.0835226
F	-0.7261074	-0.7852261	1.0835226
F	1.1355140	-0.6500193	0.0000000
C	0.7433873	2.1589728	0.0000000
C	0.5086296	3.5463313	0.0000000
F	-2.6403610	0.8954626	0.0000000
F	1.9829763	1.6986013	0.0000000
F	-3.1182805	3.5282540	0.0000000
F	-1.1595669	5.2724132	0.0000000
O	0.2031095	-3.4945886	0.0000000
C	1.4796780	-4.0966083	0.0000000
H	2.2161088	-3.2946232	0.0000000
H	1.6242377	-4.7202726	0.8911261
H	1.6242377	-4.7202726	-0.8911261
C	-0.8181369	-4.4687370	0.0000000
H	-1.7707199	-3.9410765	0.0000000
H	-0.7585656	-5.1066332	-0.8907605
H	-0.7585656	-5.1066332	0.8907605
N	1.6181216	4.5126081	0.0000000
O	1.3166445	5.7019919	0.0000000
O	2.7610929	4.0702089	0.0000000

21.

O	-0.1319541	-4.9629781	0.0000000
C	0.0241859	2.8095039	0.0000000
C	-1.1449124	2.0559625	0.0000000
C	-1.1285381	0.6710195	0.0000000
C	0.0754013	-0.0350396	0.0000000
C	0.0153317	-1.5436059	0.0000000
F	-0.6410897	-1.9840125	-1.0821093
F	-0.6410897	-1.9840125	1.0821093
F	1.2222964	-2.1021737	0.0000000
C	1.2553619	0.7055798	0.0000000
C	1.2159369	2.0971438	0.0000000
C	-0.0766951	-6.1734689	0.0000000
H	0.8871048	-6.7101416	0.0000000
H	-0.9875492	-6.7957058	0.0000000
F	-2.2890005	0.0139536	0.0000000
F	2.4546620	0.1254667	0.0000000
F	-2.3243857	2.6872823	0.0000000
F	2.3822164	2.7536425	0.0000000
C	-0.0258945	4.3066960	0.0000000
H	-0.5597867	4.6698084	-0.8800588
H	-0.5597867	4.6698084	0.8800588
H	0.9781851	4.7252713	0.0000000

22.

O	-0.1548214	-4.4778076	0.0000000
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C	-0.0537130	3.2782824	0.0000000
C	-1.2303346	2.5325392	0.0000000
C	-1.1780535	1.1479824	0.0000000
C	0.0307340	0.4489427	0.0000000
C	-0.0177143	-1.0586107	0.0000000
F	-0.6694627	-1.5068749	-1.0816235
F	-0.6694627	-1.5068749	1.0816235
F	1.1959407	-1.6043859	0.0000000
C	1.2050228	1.1994001	0.0000000
C	1.1514615	2.5855186	0.0000000
C	-0.0947776	-5.6880525	0.0000000
H	0.8711550	-6.2208833	0.0000000
H	-1.0030983	-6.3139543	0.0000000
F	-2.3312835	0.4794722	0.0000000
F	2.4127665	0.6378651	0.0000000
F	-2.4050105	3.1563873	0.0000000
F	2.2853048	3.3048190	0.0000000
H	0.7793940	4.9807530	0.0000000
O	-0.1240471	4.6254821	0.0000000

23.

O	-0.0954752	-4.1525152	0.0000000
C	-0.0187273	3.5356654	0.0000000
C	-1.1887161	2.7952722	0.0000000
C	-1.1511553	1.4085760	0.0000000
C	0.0642753	0.7207667	0.0000000
C	0.0203248	-0.7903748	0.0000000
F	-0.6309947	-1.2351516	-1.0825913
F	-0.6309947	-1.2351516	1.0825913
F	1.2331699	-1.3347266	0.0000000
C	1.2414543	1.4686536	0.0000000
C	1.1874637	2.8596278	0.0000000
H	-0.0458700	4.6181216	0.0000000
C	-0.0460230	-5.3632013	0.0000000
H	0.9149458	-5.9047176	0.0000000
H	-0.9596636	-5.9811544	0.0000000
F	-2.3002497	0.7347096	0.0000000
F	2.4436628	0.8982228	0.0000000
F	-2.3714285	3.4137887	0.0000000
F	2.3340016	3.5435888	0.0000000

24.

O	-0.1105380	-4.4507675	0.0000000
C	0.0031481	3.2082298	0.0000000
C	-1.1812271	2.4695347	0.0000000
C	-1.1418306	1.0842359	0.0000000
C	0.0700635	0.3903302	0.0000000
C	0.0142707	-1.1232778	0.0000000
F	-0.6410097	-1.5567047	-1.0829263
F	-0.6410097	-1.5567047	1.0829263
F	1.2227100	-1.6732538	0.0000000
C	1.2524789	1.1304869	0.0000000
C	1.2159462	2.5205856	0.0000000
C	-0.0652921	-5.6619598	0.0000000
H	0.8939569	-6.2058715	0.0000000
H	-0.9812202	-6.2758340	0.0000000

F	-2.2913168	0.4188482	0.0000000
F	2.4473465	0.5534323	0.0000000
F	-2.3513743	3.0946596	0.0000000
F	2.3572650	3.1979487	0.0000000
C	-0.0249370	4.6317836	0.0000000
N	-0.0474301	5.8042984	0.0000000

25.

O	-0.0958062	-4.6870384	0.0000000
C	-0.0022460	3.0025490	0.0000000
C	-1.1909482	2.2566073	0.0000000
C	-1.1354590	0.8684368	0.0000000
C	0.0682451	0.1693714	0.0000000
C	0.0174307	-1.3436764	0.0000000
F	-0.6359030	-1.7790193	-1.0829987
F	-0.6359030	-1.7790193	1.0829987
F	1.2278843	-1.8890913	0.0000000
C	1.2405105	0.9169252	0.0000000
C	1.2167551	2.3107873	0.0000000
C	-0.0472014	-5.8978957	0.0000000
H	0.9138176	-6.4390153	0.0000000
H	-0.9617147	-6.5141770	0.0000000
F	-2.2857892	0.2055340	0.0000000
F	2.4369269	0.3447948	0.0000000
F	-2.3939758	2.8046737	0.0000000
F	2.3922249	2.9162274	0.0000000
N	-0.0344757	4.4709405	0.0000000
O	1.0439408	5.0556029	0.0000000
O	-1.1383137	5.0064826	0.0000000

26.

C	-0.0682650	3.7749912	0.0000000
C	-1.2131989	2.9853731	0.0000000
C	-1.1525790	1.6019540	0.0000000
C	0.0726895	0.9340930	0.0000000
C	0.0542155	-0.5754881	0.0000000
F	-0.5904265	-1.0305520	-1.0825089
F	-0.5904265	-1.0305520	1.0825089
F	1.2779065	-1.0993298	0.0000000
C	1.2288672	1.7108804	0.0000000
C	1.1453114	3.1004924	0.0000000
F	-2.2915370	0.9077869	0.0000000
F	2.4458121	1.1682922	0.0000000
F	-2.4123145	3.5781675	0.0000000
O	0.0442715	-3.8295066	0.0000000
C	1.2250058	-4.6007187	0.0000000
H	2.0641401	-3.9065498	0.0000000
H	1.2826363	-5.2386380	0.8912389
H	1.2826363	-5.2386380	-0.8912389
C	-1.1024432	-4.6510634	0.0000000
H	-1.9714469	-3.9946941	0.0000000
H	-1.1328414	-5.2908817	-0.8911355
H	-1.1328414	-5.2908817	0.8911355
F	2.2899506	3.7938081	0.0000000
C	-0.1641412	5.2697168	0.0000000
H	-0.7088115	5.6166841	-0.8798099

H	-0.7088115	5.6166841	0.8798099
H	0.8266415	5.7185700	0.0000000

27.

C	-0.1520933	4.3094634	0.0000000
C	-1.2904046	3.5067592	0.0000000
C	-1.1690759	2.1264857	0.0000000
C	0.0724891	1.4872319	0.0000000
C	0.0925868	-0.0214199	0.0000000
F	-0.5369254	-0.4977628	-1.0817605
F	-0.5369254	-0.4977628	1.0817605
F	1.3312609	-0.5143443	0.0000000
C	1.2082432	2.2947310	0.0000000
C	1.0858117	3.6767246	0.0000000
F	-2.2879932	1.4017156	0.0000000
F	2.4422024	1.7927907	0.0000000
F	-2.4947685	4.0709100	0.0000000
O	-0.0727973	-3.5206330	0.0000000
C	1.1302895	-4.2572739	0.0000000
H	1.9498122	-3.5403085	0.0000000
H	1.2064990	-4.8940197	0.8908790
H	1.2064990	-4.8940197	-0.8908790
C	-1.1915029	-4.3815114	0.0000000
H	-2.0829979	-3.7565413	0.0000000
H	-1.1995507	-5.0229420	-0.8905303
H	-1.1995507	-5.0229420	0.8905303
F	2.1820134	4.4517643	0.0000000
O	-0.2887902	5.6513273	0.0000000
H	0.5956688	6.0515776	0.0000000

28.

C	-0.1355512	4.4716074	0.0000000
C	-1.2839776	3.6981232	0.0000000
C	-1.2066340	2.3131943	0.0000000
C	0.0277503	1.6606791	0.0000000
C	0.0226704	0.1487777	0.0000000
F	-0.6173754	-0.3100917	-1.0827204
F	-0.6173754	-0.3100917	1.0827204
F	1.2509918	-0.3630618	0.0000000
C	1.1833960	2.4414774	0.0000000
C	1.0896452	3.8303508	0.0000000
F	-2.3356246	1.6056583	0.0000000
F	2.4009811	1.9040895	0.0000000
F	-2.4840725	4.2818179	0.0000000
O	0.0433844	-3.0996247	0.0000000
C	1.2373346	-3.8508165	0.0000000
H	2.0646862	-3.1429799	0.0000000
H	1.3064198	-4.4875585	0.8910638
H	1.3064198	-4.4875585	-0.8910638
C	-1.0888915	-3.9412007	0.0000000
H	-1.9691821	-3.3001786	0.0000000
H	-1.1081895	-4.5814814	-0.8909558
H	-1.1081895	-4.5814814	0.8909558
H	-0.1944004	5.5529110	0.0000000
F	2.2157841	4.5474389	0.0000000

29.

C	-0.0505972	4.1991190	0.0000000
C	-1.2154680	3.4301147	0.0000000
C	-1.1406152	2.0466814	0.0000000
C	0.0886545	1.3835665	0.0000000
C	0.0670903	-0.1311901	0.0000000
F	-0.5782376	-0.5767665	-1.0831450
F	-0.5782376	-0.5767665	1.0831450
F	1.2888571	-0.6553867	0.0000000
C	1.2517017	2.1537923	0.0000000
C	1.1795663	3.5427772	0.0000000
F	-2.2726932	1.3515909	0.0000000
F	2.4607191	1.6067504	0.0000000
F	-2.4018241	4.0240051	0.0000000
O	-0.0244844	-3.4279646	0.0000000
C	1.1511762	-4.2089330	0.0000000
H	1.9966512	-3.5228561	0.0000000
H	1.2034481	-4.8472293	0.8909523
H	1.2034481	-4.8472293	-0.8909523
C	-1.1748328	-4.2463436	0.0000000
H	-2.0423515	-3.5882996	0.0000000
H	-1.2067057	-4.8860979	-0.8908405
H	-1.2067057	-4.8860979	0.8908405
F	2.3030732	4.2490465	0.0000000
C	-0.1193784	5.6212424	0.0000000
N	-0.1822545	6.7924749	0.0000000

30.

C	-0.0225024	3.9741785	0.0000000
C	-1.1993860	3.2098119	0.0000000
C	-1.1229943	1.8228193	0.0000000
C	0.0906858	1.1410600	0.0000000
C	0.0572582	-0.3731232	0.0000000
F	-0.5915123	-0.8128452	-1.0832750
F	-0.5915123	-0.8128452	1.0832750
F	1.2758397	-0.9039588	0.0000000
C	1.2513908	1.9067633	0.0000000
C	1.2068849	3.3004871	0.0000000
F	-2.2641856	1.1438041	0.0000000
F	2.4562566	1.3520508	0.0000000
F	-2.4108264	3.7389458	0.0000000
O	-0.0264655	-3.6074112	0.0000000
C	1.1388404	-4.4034710	0.0000000
H	1.9929537	-3.7280731	0.0000000
H	1.1830372	-5.0421240	0.8910677
H	1.1830372	-5.0421240	-0.8910677
C	-1.1892512	-4.4075479	0.0000000
H	-2.0457452	-3.7350185	0.0000000
H	-1.2312349	-5.0463938	-0.8911360
H	-1.2312349	-5.0463938	0.8911360
F	2.3727256	3.9244510	0.0000000
N	-0.0791708	5.4423725	0.0000000
O	0.9890348	6.0454094	0.0000000
O	-1.1919230	5.9591759	0.0000000