

Supporting Information

for

Computational study of productive and non-productive cycles in fluoroalkene metathesis

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Table containing total electronic and free Gibbs energies in hartrees, total and relative electronic and free Gibbs energies in kJ/mol for all computed structures, as well as their coordinates in the pdb format.

Table S1. Total electronic and free Gibbs energies in hartrees, total and relative electronic and free Gibbs energies in kJ/mol for all computed structures.

Structure	Total electronic energy (hartree)	Total free Gibbs energy (hartree)	Total electronic energy (kJ/mol)	Relative electronic energy (kJ/mol)	Total free Gibbs energy (kJ/mol)	Relative free Gibbs energy (kJ/mol)
1a	-2482.573127	-2481.977548	-6517995.75	1.50	-6516432.05	0.00
1b	-2482.557065	-2481.958447	-6517953.57	43.67	-6516381.90	50.15
1c	-2482.559513	-2481.958603	-6517960.00	37.25	-6516382.31	49.74
1d	-2482.552073	-2481.948530	-6517940.47	56.78	-6516355.87	76.19
1I	-2482.571286	-2481.965937	-6517990.91	6.34	-6516401.57	30.48
1e	-2482.553076	-2481.948593	-6517943.10	54.15	-6516356.03	76.02
1f	-2482.559890	-2481.957404	-6517960.99	36.26	-6516379.16	52.89
s2a	-2680.988342	-2680.403412	-7038934.89	35.93	-7037399.16	33.32
s2b	-2680.968034	-2680.385592	-7038881.57	89.25	-7037352.37	80.11
s2c	-2680.968461	-2680.383870	-7038882.69	88.13	-7037347.85	84.63
s2d	-2680.955706	-2680.367753	-7038849.21	121.61	-7037305.54	126.95
s2I	-2680.986839	-2680.399458	-7038930.95	39.87	-7037388.78	43.70
s2e	-2680.985199	-2680.398466	-7038926.64	44.18	-7037386.17	46.31
s2f	-2681.002026	-2680.416104	-7038970.82	0.00	-7037432.48	0.00
a2a	-2680.986070	-2680.401973	-7038928.93	41.89	-7037395.38	37.10
a2b	-2680.965169	-2680.382171	-7038874.05	96.77	-7037343.39	89.09
a2c	-2680.968993	-2680.385796	-7038884.09	86.73	-7037352.91	79.57

a2d	-2680.948949	-2680.359077	-7038831.47	139.35	-7037282.76	149.72
a2I	-2680.963854	-2680.371511	-7038870.60	100.22	-7037315.40	117.08
a2e	-2680.942048	-2680.355736	-7038813.35	157.47	-7037273.98	158.50
a2f	-2680.960824	-2680.377057	-7038862.64	108.18	-7037329.96	102.52
sc3a	-2581.780048	-2581.190987	-6778463.51	0.00	-6776916.94	0.00
sc3b	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
sc3c	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
sc3d	-2581.750821	-2581.156613	-6778386.78	76.73	-6776826.69	90.25
sc3I	-2581.775253	-2581.178330	-6778450.93	12.59	-6776883.71	33.23
sc3e	-2581.761722	-2581.166154	-6778415.40	48.12	-6776851.74	65.20
sc3f	-2581.776091	-2581.182029	-6778453.13	10.39	-6776893.42	23.52
st3a	-2581.777829	-2581.187167	-6778457.69	5.83	-6776906.91	10.03
st3b	-2581.756024	-2581.159477	-6778400.44	63.07	-6776834.21	82.73
st3c	-2581.761868	-2581.167358	-6778415.78	47.73	-6776854.90	62.04
st3d	-2581.747896	-2581.155150	-6778379.10	84.41	-6776822.85	94.09
st3I	-2581.775970	-2581.178282	-6778452.81	10.71	-6776883.58	33.36
st3e	-2581.763141	-2581.167459	-6778419.13	44.39	-6776855.16	61.77
st3f	-2581.779831	-2581.188713	-6778462.95	0.57	-6776910.97	5.97
ac3a	-2581.771516	-2581.185848	-6778441.11	22.40	-6776903.44	13.49
ac3b	-2581.754684	-2581.162093	-6778396.92	66.59	-6776841.08	75.86
ac3c	-2581.761055	-2581.167999	-6778413.65	49.86	-6776856.58	60.35
ac3d	-2581.748141	-2581.152903	-6778379.75	83.77	-6776816.95	99.99
ac3I	-2581.760538	-2581.160331	-6778412.29	51.22	-6776836.45	80.49
ac3e	-2581.737046	-2581.141452	-6778350.61	112.90	-6776786.88	130.05
ac3f	-2581.747783	-2581.153042	-6778378.80	84.71	-6776817.31	99.62
at3a	-2581.773076	-2581.183512	-6778445.21	18.30	-6776897.31	19.63
at3b	-2581.756790	-2581.162633	-6778402.45	61.06	-6776842.49	74.44
at3c	-2581.758188	-2581.164675	-6778406.12	57.39	-6776847.85	69.08
at3d	-2581.746289	-2581.151835	-6778374.88	88.63	-6776814.14	102.79
at3I	-2581.761737	-2581.166037	-6778415.44	48.07	-6776851.43	65.51
at3e	-2581.738830	-2581.144079	-6778355.30	108.22	-6776793.78	123.16
at3f	-2581.760321	-2581.166387	-6778411.72	51.79	-6776852.35	64.59
s2g	-2455.278100	-2454.869732	-6446332.65	3.92	-6445260.48	13.48
s2h	-2455.260649	-2454.849518	-6446286.83	49.74	-6445207.41	66.55
s2NA	-2455.272139	-2454.864468	-6446317.00	19.57	-6445246.66	27.30
s2i	-2455.260649	-2454.849518	-6446286.83	49.74	-6445207.41	66.55
s2j	-2455.278100	-2454.869732	-6446332.65	3.92	-6445260.48	13.48
a2g	-2455.279592	-2454.874867	-6446336.57	0.00	-6445273.96	0.00
a2h	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
a2PA	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
a2i	-2455.207427	-2454.801310	-6446147.10	189.47	-6445080.84	193.12
a2j	-2455.215796	-2454.811428	-6446169.07	167.50	-6445107.40	166.56
s2k	-2256.835696	-2256.413633	-5925322.12	91.31	-5924213.99	84.68
s2l	-2256.822386	-2256.399978	-5925287.17	126.25	-5924178.14	120.53
s2PB	-2256.861741	-2256.438763	-5925390.50	22.93	-5924279.97	18.70
s2m	-2256.858350	-2256.433379	-5925381.60	31.83	-5924265.84	32.84
s2n	-2256.870473	-2256.445887	-5925413.43	0.00	-5924298.68	0.00
a2k	-2256.836828	-2256.415327	-5925325.09	88.34	-5924218.44	80.24
a2l	-2256.823518	-2256.399301	-5925290.15	123.28	-5924176.36	122.31
a2NB	-2256.841262	-2256.415358	-5925336.73	76.69	-5924218.52	80.15
a2m	-2256.823518	-2256.399301	-5925290.15	123.28	-5924176.36	122.31

a2n	-2256.836828	-2256.415327	-5925325.09	88.34	-5924218.44	80.24
sc3g	-2256.849388	-2256.427990	-5925358.07	19.30	-5924251.69	7.10
sc3h	-2256.838573	-2256.412564	-5925329.67	47.70	-5924211.19	47.60
sc3NA	-2256.853256	-2256.426577	-5925368.22	9.15	-5924247.98	10.81
sc3i	-2256.838573	-2256.412564	-5925329.67	47.70	-5924211.19	47.60
sc3j	-2256.849388	-2256.427990	-5925358.07	19.30	-5924251.69	7.10
st3g	-2256.850232	-2256.428577	-5925360.28	17.09	-5924253.23	5.56
st3h	-2256.841508	-2256.415519	-5925337.38	39.99	-5924218.95	39.84
st3NA	-2256.856740	-2256.430693	-5925377.37	0.00	-5924258.78	0.00
st3i	-2256.841508	-2256.415519	-5925337.38	39.99	-5924218.95	39.84
st3j	-2256.850232	-2256.428577	-5925360.28	17.09	-5924253.23	5.56
ac3g	-2256.850198	-2256.426778	-5925360.19	17.18	-5924248.51	10.28
ac3h	-2256.837399	-2256.412466	-5925326.59	50.78	-5924210.93	47.85
ac3PA	-2256.841934	-2256.415971	-5925338.50	38.87	-5924220.13	38.65
ac3i	-2256.814521	-2256.391862	-5925266.53	110.85	-5924156.83	101.95
ac3j	-2256.821547	-2256.402205	-5925284.97	92.40	-5924183.99	74.80
at3g	-2256.851405	-2256.428217	-5925363.36	14.01	-5924252.28	6.50
at3h	-2256.836260	-2256.411376	-5925323.60	53.77	-5924208.07	50.72
at3PA	-2256.842348	-2256.416065	-5925339.58	37.79	-5924220.38	38.41
at3i	-2256.810557	-2256.387829	-5925256.12	121.25	-5924146.25	112.54
at3j	-2256.817500	-2256.395121	-5925274.35	103.03	-5924165.39	93.39
s3k	-2157.627650	-2157.197385	-5664851.39	62.43	-5663721.73	55.44
s3l	-2157.622366	-2157.190129	-5664837.52	76.30	-5663702.68	74.49
s3PB	-2157.651429	-2157.218502	-5664913.83	0.00	-5663777.18	0.00
s3m	-2157.642241	-2157.209862	-5664889.70	24.12	-5663754.49	22.68
s3n	-2157.650156	-2157.217637	-5664910.48	3.34	-5663774.91	2.27
a3k	-2157.629594	-2157.198377	-5664856.50	57.33	-5663724.34	52.84
a3l	-2157.621859	-2157.189034	-5664836.19	77.64	-5663699.81	77.37
a3NB	-2157.640468	-2157.206005	-5664885.05	28.78	-5663744.37	32.81
a3m	-2157.621859	-2157.189034	-5664836.19	77.64	-5663699.81	77.37
a3n	-2157.629594	-2157.198377	-5664856.50	57.33	-5663724.34	52.84
4a	-2653.653700	-2653.263990	-6967167.79	0.00	-6966144.61	0.00
4b	-2653.644966	-2653.250541	-6967144.86	22.93	-6966109.30	35.31
4NA	-2653.651385	-2653.258662	-6967161.71	6.08	-6966130.62	13.99
s5a	-3014.014501	-3013.625279	-7913295.07	0.54	-7912273.17	8.57
s5b	-3014.001344	-3013.612325	-7913260.53	35.08	-7912239.16	42.58
s5PA	-3014.005400	-3013.616550	-7913271.18	24.44	-7912250.25	31.49
s5c	-3013.996461	-3013.608234	-7913247.71	47.90	-7912228.42	53.32
s5d	-3014.007883	-3013.620550	-7913277.70	17.92	-7912260.75	20.99
a5a	-3014.014707	-3013.628544	-7913295.61	0.00	-7912281.74	0.00
a5b	-3014.002632	-3013.614315	-7913263.91	31.70	-7912244.38	37.36
a5NA	-3014.007052	-3013.618624	-7913275.52	20.10	-7912255.70	26.04
a5c	-3014.002632	-3013.614315	-7913263.91	31.70	-7912244.38	37.36
a5d	-3014.014707	-3013.628544	-7913295.61	0.00	-7912281.74	0.00
sc5e	-3374.368689	-3373.983471	-8859404.99	13.22	-8858393.60	11.21
sc5f	-3374.355026	-3373.968736	-8859369.12	46.93	-8858354.92	49.89
sc5NB	-3374.359399	-3373.972199	-8859380.60	37.61	-8858364.01	40.80
sc5g	-3374.355026	-3373.968736	-8859369.12	46.93	-8858354.92	49.89
sc5h	-3374.368689	-3373.983471	-8859404.99	13.22	-8858393.60	11.21
st5e	-3374.369031	-3373.981034	-8859405.89	12.32	-8858387.20	17.60
st5f	-3374.354438	-3373.966917	-8859367.58	48.48	-8858350.14	54.67

st5NB	-3374.358728	-3373.972549	-8859378.84	39.37	-8858364.93	39.88
st5g	-3374.354438	-3373.966917	-8859367.58	48.48	-8858350.14	54.67
st5h	-3374.369031	-3373.981034	-8859405.89	12.32	-8858387.20	17.60
ac5e	-3374.368393	-3373.983597	-8859404.22	13.99	-8858393.93	10.87
ac5f	-3374.355166	-3373.968679	-8859369.49	46.57	-8858354.77	50.04
ac5NB	-3374.359740	-3373.973217	-8859381.50	36.71	-8858366.68	38.13
ac5g	-3374.358353	-3373.971373	-8859377.86	38.20	-8858361.84	42.97
ac5h	-3374.372902	-3373.987204	-8859416.05	2.15	-8858403.40	1.40
at5e	-3374.369568	-3373.987739	-8859407.30	10.91	-8858404.81	0.00
at5f	-3374.354242	-3373.965129	-8859367.06	48.99	-8858345.45	59.36
at5PB	-3374.360599	-3373.973985	-8859383.75	34.46	-8858368.70	36.11
at5g	-3374.358353	-3373.972653	-8859377.86	38.20	-8858365.20	39.61
at5h	-3374.373723	-3373.986934	-8859418.21	0.00	-8858402.70	2.11

List of all computed structures in the pdb format. For visualization, copy the corresponding part of the text into a separate file named „title“.pdb.

1a.pdb

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TITLE          1a
HETATM   1 Ru          0      -0.018   0.350   0.115                Ru
HETATM   2 C          0      -0.585  -3.913   0.231                C
HETATM   3 C          0       0.923  -3.775   0.385                C
HETATM   4 H          0      -1.067  -4.416   1.091                H
HETATM   5 H          0       1.298  -4.153   1.356                H
HETATM   6 C          0      -0.021  -1.613   0.146                C
HETATM   7 N          0       1.135  -2.335   0.288                N
HETATM   8 N          0      -1.037  -2.527   0.134                N
HETATM   9 Cl         0       0.909   0.625  -2.058               Cl
HETATM  10 Cl         0       0.215   0.528   2.471               Cl
HETATM  11 C          0      -1.804   0.744  -0.147                C
HETATM  12 H          0      -2.594  -0.004  -0.313                H
HETATM  13 C          0      -2.267   2.110  -0.150                C
HETATM  14 C          0      -1.326   3.157   0.023                C
HETATM  15 C          0      -3.628   2.436  -0.312                C
HETATM  16 C          0      -1.745   4.488   0.032                C
HETATM  17 C          0      -4.046   3.762  -0.300                C
HETATM  18 H          0      -4.349   1.619  -0.443                H
HETATM  19 C          0      -3.103   4.779  -0.129                C
HETATM  20 H          0      -1.036   5.307   0.163                H
HETATM  21 H          0      -5.106   4.010  -0.424                H
HETATM  22 H          0      -3.423   5.827  -0.119                H
HETATM  23 O          0      -0.062   2.700   0.167                O
HETATM  24 C          0       1.114   3.533   0.363                C
HETATM  25 H          0       1.894   2.756   0.436                H
HETATM  26 C          0       2.477  -1.864   0.167                C
HETATM  27 C          0       3.236  -1.582   1.320                C
HETATM  28 C          0       3.082  -1.870  -1.112                C
HETATM  29 C          0       4.583  -1.227   1.162                C
HETATM  30 C          0       4.426  -1.510  -1.218                C
HETATM  31 C          0       5.190  -1.175  -0.093                C

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HETATM	32	H	0	5.175	-0.997	2.059	H
HETATM	33	H	0	4.893	-1.493	-2.212	H
HETATM	34	C	0	-2.428	-2.283	-0.024	C
HETATM	35	C	0	-3.235	-2.123	1.115	C
HETATM	36	C	0	-2.968	-2.206	-1.321	C
HETATM	37	C	0	-4.603	-1.889	0.935	C
HETATM	38	C	0	-4.340	-1.975	-1.460	C
HETATM	39	C	0	-5.170	-1.812	-0.343	C
HETATM	40	H	0	-5.240	-1.755	1.819	H
HETATM	41	H	0	-4.768	-1.905	-2.468	H
HETATM	42	C	0	2.683	-1.740	2.704	C
HETATM	43	H	0	2.810	-0.817	3.296	H
HETATM	44	H	0	1.608	-1.969	2.711	H
HETATM	45	H	0	3.219	-2.545	3.243	H
HETATM	46	C	0	2.340	-2.336	-2.328	C
HETATM	47	H	0	1.253	-2.181	-2.252	H
HETATM	48	H	0	2.678	-1.796	-3.229	H
HETATM	49	H	0	2.523	-3.414	-2.510	H
HETATM	50	C	0	6.619	-0.751	-0.245	C
HETATM	51	H	0	6.681	0.291	-0.615	H
HETATM	52	H	0	7.168	-0.792	0.710	H
HETATM	53	H	0	7.160	-1.375	-0.978	H
HETATM	54	C	0	-2.622	-2.133	2.481	C
HETATM	55	H	0	-3.386	-2.009	3.265	H
HETATM	56	H	0	-2.077	-3.072	2.691	H
HETATM	57	H	0	-1.882	-1.316	2.594	H
HETATM	58	C	0	-2.064	-2.271	-2.514	C
HETATM	59	H	0	-1.428	-3.176	-2.517	H
HETATM	60	H	0	-2.637	-2.262	-3.456	H
HETATM	61	H	0	-1.372	-1.406	-2.531	H
HETATM	62	C	0	-6.632	-1.524	-0.517	C
HETATM	63	H	0	-6.812	-0.445	-0.687	H
HETATM	64	H	0	-7.056	-2.053	-1.389	H
HETATM	65	H	0	-7.218	-1.808	0.372	H
HETATM	66	C	0	1.073	4.266	1.687	C
HETATM	67	H	0	2.079	4.665	1.905	H
HETATM	68	H	0	0.373	5.118	1.707	H
HETATM	69	H	0	0.802	3.569	2.497	H
HETATM	70	C	0	1.415	4.369	-0.860	C
HETATM	71	H	0	0.718	5.212	-1.003	H
HETATM	72	H	0	2.431	4.789	-0.769	H
HETATM	73	H	0	1.393	3.736	-1.764	H
HETATM	74	H	0	1.487	-4.299	-0.409	H
HETATM	75	H	0	-0.880	-4.477	-0.676	H
HETATM	76	H	0	3.307	1.023	-0.310	H
HETATM	77	C	0	4.089	1.792	-0.406	C
HETATM	78	H	0	4.723	1.960	0.477	H
HETATM	79	C	0	4.258	2.466	-1.543	C
HETATM	80	H	0	5.040	3.230	-1.661	H
HETATM	81	H	0	3.612	2.280	-2.413	H

END

1b.pdb

TITLE	1b.pdb						
HETATM	1	Ru	0	-0.525	0.346	-0.407	Ru
HETATM	2	C	0	-0.272	-3.599	1.278	C
HETATM	3	C	0	-1.758	-3.261	1.342	C
HETATM	4	H	0	0.186	-3.712	2.280	H
HETATM	5	H	0	-2.166	-3.294	2.370	H
HETATM	6	C	0	-0.592	-1.454	0.358	C

HETATM	7	N	0	-1.800	-1.905	0.816	N
HETATM	8	N	0	0.313	-2.442	0.593	N
HETATM	9	Cl	0	-0.526	1.361	1.787	Cl
HETATM	10	Cl	0	-0.944	-0.534	-2.658	Cl
HETATM	11	C	0	1.282	0.307	-0.816	C
HETATM	12	H	0	1.620	-0.606	-1.342	H
HETATM	13	C	0	2.377	1.237	-0.643	C
HETATM	14	C	0	2.245	2.617	-0.303	C
HETATM	15	C	0	3.680	0.713	-0.815	C
HETATM	16	C	0	3.402	3.387	-0.106	C
HETATM	17	C	0	4.817	1.475	-0.587	C
HETATM	18	H	0	3.769	-0.338	-1.116	H
HETATM	19	C	0	4.668	2.817	-0.228	C
HETATM	20	H	0	3.322	4.452	0.121	H
HETATM	21	H	0	5.813	1.035	-0.704	H
HETATM	22	H	0	5.552	3.445	-0.062	H
HETATM	23	O	0	0.999	3.098	-0.286	O
HETATM	24	C	0	0.595	4.308	0.392	C
HETATM	25	H	0	-0.491	4.125	0.495	H
HETATM	26	C	0	-3.033	-1.240	0.545	C
HETATM	27	C	0	-3.696	-1.487	-0.679	C
HETATM	28	C	0	-3.603	-0.391	1.517	C
HETATM	29	C	0	-4.849	-0.752	-0.970	C
HETATM	30	C	0	-4.758	0.325	1.179	C
HETATM	31	C	0	-5.373	0.183	-0.069	C
HETATM	32	H	0	-5.352	-0.918	-1.932	H
HETATM	33	H	0	-5.190	1.009	1.921	H
HETATM	34	C	0	1.726	-2.435	0.408	C
HETATM	35	C	0	2.256	-3.069	-0.733	C
HETATM	36	C	0	2.564	-1.895	1.399	C
HETATM	37	C	0	3.645	-3.162	-0.860	C
HETATM	38	C	0	3.950	-2.013	1.234	C
HETATM	39	C	0	4.506	-2.642	0.116	C
HETATM	40	H	0	4.066	-3.648	-1.750	H
HETATM	41	H	0	4.612	-1.591	2.001	H
HETATM	42	C	0	-3.251	-2.571	-1.612	C
HETATM	43	H	0	-3.414	-2.289	-2.664	H
HETATM	44	H	0	-2.182	-2.816	-1.513	H
HETATM	45	H	0	-3.835	-3.495	-1.424	H
HETATM	46	C	0	-3.071	-0.323	2.915	C
HETATM	47	H	0	-3.122	0.701	3.320	H
HETATM	48	H	0	-3.682	-0.967	3.580	H
HETATM	49	H	0	-2.023	-0.647	2.989	H
HETATM	50	C	0	-6.562	1.017	-0.437	C
HETATM	51	H	0	-6.251	1.937	-0.968	H
HETATM	52	H	0	-7.249	0.481	-1.114	H
HETATM	53	H	0	-7.133	1.339	0.449	H
HETATM	54	C	0	1.341	-3.570	-1.807	C
HETATM	55	H	0	1.904	-4.051	-2.624	H
HETATM	56	H	0	0.607	-4.308	-1.430	H
HETATM	57	H	0	0.744	-2.744	-2.243	H
HETATM	58	C	0	1.993	-1.168	2.575	C
HETATM	59	H	0	1.137	-1.698	3.031	H
HETATM	60	H	0	2.753	-1.011	3.358	H
HETATM	61	H	0	1.597	-0.176	2.280	H
HETATM	62	C	0	5.992	-2.705	-0.067	C
HETATM	63	H	0	6.530	-2.692	0.897	H
HETATM	64	H	0	6.306	-3.605	-0.623	H
HETATM	65	H	0	6.360	-1.835	-0.645	H
HETATM	66	C	0	0.798	5.529	-0.486	C
HETATM	67	H	0	0.297	6.402	-0.031	H
HETATM	68	H	0	1.861	5.791	-0.618	H

HETATM	69	H	0	0.363	5.379	-1.489	H
HETATM	70	C	0	1.157	4.452	1.794	C
HETATM	71	H	0	2.180	4.861	1.826	H
HETATM	72	H	0	0.514	5.146	2.363	H
HETATM	73	H	0	1.139	3.482	2.317	H
HETATM	74	H	0	-2.379	-3.934	0.719	H
HETATM	75	H	0	-0.058	-4.528	0.717	H
HETATM	76	C	0	-1.559	2.624	-1.897	C
HETATM	77	H	0	-1.075	3.602	-1.786	H
HETATM	78	H	0	-1.385	2.081	-2.834	H
HETATM	79	C	0	-2.335	2.114	-0.926	C
HETATM	80	H	0	-2.879	1.163	-1.073	H
HETATM	81	H	0	-2.528	2.647	0.015	H

END

1c.pdb

TITLE	1c.pdb						
HETATM	1	Ru	0	-0.571	0.369	-0.649	Ru
HETATM	2	C	0	-0.670	-3.296	1.732	C
HETATM	3	C	0	-2.126	-2.850	1.691	C
HETATM	4	H	0	-0.232	-3.249	2.748	H
HETATM	5	H	0	-2.565	-2.700	2.695	H
HETATM	6	C	0	-0.816	-1.322	0.464	C
HETATM	7	N	0	-2.051	-1.583	0.968	N
HETATM	8	N	0	0.002	-2.324	0.859	N
HETATM	9	Cl	0	-0.568	1.553	1.501	Cl
HETATM	10	Cl	0	-1.033	-0.958	-2.658	Cl
HETATM	11	C	0	1.259	0.205	-0.935	C
HETATM	12	H	0	1.507	-0.791	-1.357	H
HETATM	13	C	0	2.465	0.995	-0.791	C
HETATM	14	C	0	2.571	2.359	-0.364	C
HETATM	15	C	0	3.670	0.302	-1.072	C
HETATM	16	C	0	3.846	2.931	-0.210	C
HETATM	17	C	0	4.921	0.876	-0.909	C
HETATM	18	H	0	3.586	-0.736	-1.419	H
HETATM	19	C	0	5.001	2.200	-0.470	C
HETATM	20	H	0	3.936	3.977	0.089	H
HETATM	21	H	0	5.829	0.304	-1.131	H
HETATM	22	H	0	5.978	2.683	-0.345	H
HETATM	23	O	0	1.436	3.041	-0.205	O
HETATM	24	C	0	1.282	4.194	0.655	C
HETATM	25	H	0	0.191	4.174	0.822	H
HETATM	26	C	0	-3.221	-0.839	0.621	C
HETATM	27	C	0	-3.919	-1.158	-0.566	C
HETATM	28	C	0	-3.712	0.148	1.500	C
HETATM	29	C	0	-5.006	-0.359	-0.935	C
HETATM	30	C	0	-4.801	0.924	1.087	C
HETATM	31	C	0	-5.438	0.708	-0.139	C
HETATM	32	H	0	-5.537	-0.589	-1.868	H
HETATM	33	H	0	-5.169	1.713	1.757	H
HETATM	34	C	0	1.402	-2.469	0.632	C
HETATM	35	C	0	1.832	-3.320	-0.406	C
HETATM	36	C	0	2.324	-1.843	1.489	C
HETATM	37	C	0	3.203	-3.535	-0.569	C
HETATM	38	C	0	3.689	-2.087	1.292	C
HETATM	39	C	0	4.145	-2.928	0.273	C
HETATM	40	H	0	3.545	-4.192	-1.379	H
HETATM	41	H	0	4.415	-1.595	1.953	H
HETATM	42	C	0	-3.613	-2.395	-1.357	C
HETATM	43	H	0	-3.743	-2.226	-2.437	H

HETATM	44	H	0	-2.584	-2.759	-1.217	H
HETATM	45	H	0	-4.310	-3.206	-1.064	H
HETATM	46	C	0	-3.178	0.316	2.890	C
HETATM	47	H	0	-3.065	1.380	3.152	H
HETATM	48	H	0	-3.886	-0.129	3.618	H
HETATM	49	H	0	-2.194	-0.154	3.030	H
HETATM	50	C	0	-6.562	1.591	-0.589	C
HETATM	51	H	0	-6.195	2.399	-1.250	H
HETATM	52	H	0	-7.320	1.034	-1.166	H
HETATM	53	H	0	-7.069	2.081	0.260	H
HETATM	54	C	0	0.836	-3.929	-1.344	C
HETATM	55	H	0	1.323	-4.614	-2.057	H
HETATM	56	H	0	0.050	-4.500	-0.815	H
HETATM	57	H	0	0.307	-3.146	-1.924	H
HETATM	58	C	0	1.866	-0.898	2.553	C
HETATM	59	H	0	1.006	-1.288	3.128	H
HETATM	60	H	0	2.676	-0.667	3.264	H
HETATM	61	H	0	1.510	0.055	2.116	H
HETATM	62	C	0	5.612	-3.137	0.048	C
HETATM	63	H	0	6.211	-2.852	0.929	H
HETATM	64	H	0	5.848	-4.187	-0.201	H
HETATM	65	H	0	5.978	-2.527	-0.801	H
HETATM	66	C	0	1.628	5.479	-0.072	C
HETATM	67	H	0	1.279	6.344	0.518	H
HETATM	68	H	0	2.711	5.612	-0.239	H
HETATM	69	H	0	1.126	5.521	-1.054	H
HETATM	70	C	0	1.933	4.025	2.013	C
HETATM	71	H	0	3.027	4.168	2.011	H
HETATM	72	H	0	1.508	4.771	2.706	H
HETATM	73	H	0	1.703	3.025	2.418	H
HETATM	74	H	0	-2.779	-3.560	1.146	H
HETATM	75	H	0	-0.513	-4.323	1.357	H
HETATM	76	C	0	-0.488	2.113	-2.355	C
HETATM	77	H	0	0.490	2.605	-2.330	H
HETATM	78	H	0	-0.723	1.516	-3.243	H
HETATM	79	C	0	-1.427	2.367	-1.395	C
HETATM	80	H	0	-2.464	2.011	-1.519	H
HETATM	81	H	0	-1.258	3.087	-0.587	H

END

1d.pdb

TITLE	1d.pdb						
HETATM	1	Ru	0	0.537	0.190	1.003	Ru
HETATM	2	C	0	0.815	-3.199	-1.687	C
HETATM	3	C	0	2.276	-2.910	-1.377	C
HETATM	4	H	0	0.559	-3.030	-2.753	H
HETATM	5	H	0	2.922	-2.885	-2.272	H
HETATM	6	C	0	0.945	-1.263	-0.381	C
HETATM	7	N	0	2.207	-1.587	-0.751	N
HETATM	8	N	0	0.111	-2.219	-0.851	N
HETATM	9	Cl	0	1.129	2.039	-0.463	Cl
HETATM	10	Cl	0	0.573	-1.709	2.585	Cl
HETATM	11	C	0	-1.297	0.289	1.497	C
HETATM	12	H	0	-1.521	-0.476	2.266	H
HETATM	13	C	0	-2.534	0.902	1.039	C
HETATM	14	C	0	-2.692	2.121	0.309	C
HETATM	15	C	0	-3.696	0.149	1.325	C
HETATM	16	C	0	-3.959	2.452	-0.203	C
HETATM	17	C	0	-4.949	0.502	0.844	C
HETATM	18	H	0	-3.579	-0.768	1.915	H

HETATM	19	C	0	-5.068	1.649	0.058	C
HETATM	20	H	0	-4.096	3.366	-0.783	H
HETATM	21	H	0	-5.825	-0.114	1.072	H
HETATM	22	H	0	-6.045	1.947	-0.342	H
HETATM	23	O	0	-1.614	2.899	0.244	O
HETATM	24	C	0	-1.474	4.073	-0.585	C
HETATM	25	H	0	-0.413	4.312	-0.397	H
HETATM	26	C	0	3.351	-0.736	-0.643	C
HETATM	27	C	0	4.214	-0.816	0.466	C
HETATM	28	C	0	3.619	0.146	-1.709	C
HETATM	29	C	0	5.305	0.062	0.521	C
HETATM	30	C	0	4.726	0.990	-1.621	C
HETATM	31	C	0	5.568	0.976	-0.502	C
HETATM	32	H	0	5.974	0.015	1.390	H
HETATM	33	H	0	4.929	1.689	-2.443	H
HETATM	34	C	0	-1.314	-2.208	-0.825	C
HETATM	35	C	0	-1.998	-3.215	-0.116	C
HETATM	36	C	0	-2.017	-1.257	-1.592	C
HETATM	37	C	0	-3.395	-3.252	-0.191	C
HETATM	38	C	0	-3.411	-1.344	-1.651	C
HETATM	39	C	0	-4.117	-2.335	-0.963	C
HETATM	40	H	0	-3.933	-4.026	0.372	H
HETATM	41	H	0	-3.963	-0.602	-2.244	H
HETATM	42	C	0	4.014	-1.840	1.541	C
HETATM	43	H	0	4.635	-1.613	2.424	H
HETATM	44	H	0	2.964	-1.917	1.875	H
HETATM	45	H	0	4.313	-2.848	1.192	H
HETATM	46	C	0	2.713	0.198	-2.900	C
HETATM	47	H	0	2.494	-0.803	-3.315	H
HETATM	48	H	0	1.748	0.659	-2.620	H
HETATM	49	H	0	3.151	0.807	-3.708	H
HETATM	50	C	0	6.718	1.932	-0.402	C
HETATM	51	H	0	7.202	2.099	-1.380	H
HETATM	52	H	0	6.383	2.924	-0.044	H
HETATM	53	H	0	7.489	1.579	0.304	H
HETATM	54	C	0	-1.257	-4.237	0.692	C
HETATM	55	H	0	-1.893	-4.636	1.499	H
HETATM	56	H	0	-0.953	-5.106	0.076	H
HETATM	57	H	0	-0.351	-3.811	1.156	H
HETATM	58	C	0	-1.297	-0.166	-2.321	C
HETATM	59	H	0	-0.458	-0.551	-2.930	H
HETATM	60	H	0	-1.980	0.384	-2.991	H
HETATM	61	H	0	-0.850	0.570	-1.621	H
HETATM	62	C	0	-5.611	-2.417	-1.051	C
HETATM	63	H	0	-6.050	-1.483	-1.441	H
HETATM	64	H	0	-5.937	-3.235	-1.723	H
HETATM	65	H	0	-6.070	-2.623	-0.068	H
HETATM	66	C	0	-2.306	5.244	-0.094	C
HETATM	67	H	0	-1.920	6.175	-0.546	H
HETATM	68	H	0	-3.377	5.181	-0.347	H
HETATM	69	H	0	-2.220	5.351	1.001	H
HETATM	70	C	0	-1.602	3.749	-2.059	C
HETATM	71	H	0	-2.615	3.425	-2.355	H
HETATM	72	H	0	-1.354	4.645	-2.655	H
HETATM	73	H	0	-0.884	2.956	-2.326	H
HETATM	74	H	0	2.712	-3.641	-0.667	H
HETATM	75	H	0	0.509	-4.226	-1.427	H
HETATM	76	C	0	-0.022	1.642	2.723	C
HETATM	77	H	0	-0.407	2.571	2.287	H
HETATM	78	H	0	-0.596	1.211	3.554	H
HETATM	79	C	0	1.351	1.336	2.625	C
HETATM	80	H	0	1.801	0.640	3.346	H

HETATM	81	H	0	2.021	2.059	2.140	H
END							

1I.pdb

TITLE	1I.pdb						
HETATM	1	Ru	0	0.524	-0.589	-0.370	Ru
HETATM	2	C	0	1.367	3.390	0.979	C
HETATM	3	C	0	2.770	2.791	1.078	C
HETATM	4	H	0	0.995	3.789	1.940	H
HETATM	5	H	0	3.158	2.762	2.115	H
HETATM	6	C	0	1.295	1.151	0.310	C
HETATM	7	N	0	2.587	1.426	0.573	N
HETATM	8	N	0	0.552	2.246	0.559	N
HETATM	9	Cl	0	-0.419	-1.121	1.787	Cl
HETATM	10	Cl	0	1.739	-0.055	-2.451	Cl
HETATM	11	C	0	-0.880	-1.270	-1.673	C
HETATM	12	H	0	-0.518	-0.990	-2.674	H
HETATM	13	C	0	-2.333	-1.049	-1.595	C
HETATM	14	C	0	-3.250	-1.595	-0.651	C
HETATM	15	C	0	-2.858	-0.215	-2.606	C
HETATM	16	C	0	-4.615	-1.280	-0.757	C
HETATM	17	C	0	-4.207	0.102	-2.695	C
HETATM	18	H	0	-2.154	0.198	-3.341	H
HETATM	19	C	0	-5.089	-0.437	-1.758	C
HETATM	20	H	0	-5.327	-1.730	-0.062	H
HETATM	21	H	0	-4.570	0.760	-3.493	H
HETATM	22	H	0	-6.162	-0.217	-1.811	H
HETATM	23	O	0	-2.760	-2.454	0.255	O
HETATM	24	C	0	-3.359	-2.697	1.547	C
HETATM	25	H	0	-2.481	-3.058	2.110	H
HETATM	26	C	0	3.673	0.509	0.429	C
HETATM	27	C	0	4.545	0.627	-0.669	C
HETATM	28	C	0	3.871	-0.479	1.412	C
HETATM	29	C	0	5.569	-0.315	-0.809	C
HETATM	30	C	0	4.906	-1.403	1.231	C
HETATM	31	C	0	5.751	-1.348	0.118	C
HETATM	32	H	0	6.238	-0.243	-1.677	H
HETATM	33	H	0	5.060	-2.180	1.991	H
HETATM	34	C	0	-0.875	2.292	0.509	C
HETATM	35	C	0	-1.516	2.501	-0.725	C
HETATM	36	C	0	-1.611	2.166	1.704	C
HETATM	37	C	0	-2.914	2.565	-0.746	C
HETATM	38	C	0	-3.005	2.217	1.631	C
HETATM	39	C	0	-3.673	2.409	0.416	C
HETATM	40	H	0	-3.421	2.730	-1.705	H
HETATM	41	H	0	-3.587	2.092	2.555	H
HETATM	42	C	0	4.419	1.746	-1.658	C
HETATM	43	H	0	4.714	1.416	-2.667	H
HETATM	44	H	0	3.385	2.119	-1.735	H
HETATM	45	H	0	5.079	2.596	-1.389	H
HETATM	46	C	0	3.014	-0.536	2.638	C
HETATM	47	H	0	2.880	0.462	3.096	H
HETATM	48	H	0	1.994	-0.912	2.428	H
HETATM	49	H	0	3.458	-1.197	3.400	H
HETATM	50	C	0	6.822	-2.376	-0.089	C
HETATM	51	H	0	6.491	-3.159	-0.798	H
HETATM	52	H	0	7.741	-1.937	-0.515	H
HETATM	53	H	0	7.091	-2.888	0.851	H
HETATM	54	C	0	-0.725	2.655	-1.988	C
HETATM	55	H	0	-1.375	2.944	-2.831	H

HETATM	56	H	0	0.065	3.424	-1.894	H
HETATM	57	H	0	-0.196	1.723	-2.273	H
HETATM	58	C	0	-0.931	2.004	3.029	C
HETATM	59	H	0	-0.761	2.982	3.522	H
HETATM	60	H	0	-1.548	1.401	3.717	H
HETATM	61	H	0	0.040	1.491	2.940	H
HETATM	62	C	0	-5.171	2.447	0.377	C
HETATM	63	H	0	-5.605	1.500	0.748	H
HETATM	64	H	0	-5.579	3.250	1.018	H
HETATM	65	H	0	-5.553	2.606	-0.646	H
HETATM	66	C	0	-4.376	-3.821	1.483	C
HETATM	67	H	0	-4.656	-4.129	2.506	H
HETATM	68	H	0	-5.306	-3.537	0.959	H
HETATM	69	H	0	-3.955	-4.703	0.971	H
HETATM	70	C	0	-3.847	-1.441	2.243	C
HETATM	71	H	0	-4.835	-1.090	1.900	H
HETATM	72	H	0	-3.931	-1.644	3.326	H
HETATM	73	H	0	-3.114	-0.627	2.113	H
HETATM	74	H	0	3.514	3.327	0.462	H
HETATM	75	H	0	1.294	4.203	0.232	H
HETATM	76	C	0	-0.146	-2.577	-1.200	C
HETATM	77	H	0	-0.802	-3.167	-0.549	H
HETATM	78	H	0	0.067	-3.084	-2.158	H
HETATM	79	C	0	1.267	-2.398	-0.547	C
HETATM	80	H	0	2.111	-2.518	-1.245	H
HETATM	81	H	0	1.373	-2.950	0.402	H

END

1e.pdb

TITLE	1e.pdb						
HETATM	1	Ru	0	-0.526	-0.716	0.318	Ru
HETATM	2	C	0	-1.222	3.427	-0.759	C
HETATM	3	C	0	-2.644	2.886	-0.875	C
HETATM	4	H	0	-0.848	3.874	-1.698	H
HETATM	5	H	0	-3.048	2.946	-1.904	H
HETATM	6	C	0	-1.214	1.140	-0.237	C
HETATM	7	N	0	-2.499	1.484	-0.470	N
HETATM	8	N	0	-0.444	2.230	-0.426	N
HETATM	9	Cl	0	0.443	-0.983	-1.905	Cl
HETATM	10	Cl	0	-1.596	-0.297	2.496	Cl
HETATM	11	C	0	0.756	-1.997	1.562	C
HETATM	12	H	0	0.287	-1.947	2.554	H
HETATM	13	C	0	2.107	-1.419	1.572	C
HETATM	14	C	0	3.138	-1.677	0.625	C
HETATM	15	C	0	2.409	-0.611	2.688	C
HETATM	16	C	0	4.416	-1.137	0.847	C
HETATM	17	C	0	3.674	-0.075	2.891	C
HETATM	18	H	0	1.603	-0.417	3.407	H
HETATM	19	C	0	4.679	-0.347	1.963	C
HETATM	20	H	0	5.229	-1.368	0.155	H
HETATM	21	H	0	3.877	0.548	3.770	H
HETATM	22	H	0	5.691	0.053	2.107	H
HETATM	23	O	0	2.831	-2.506	-0.382	O
HETATM	24	C	0	3.539	-2.570	-1.637	C
HETATM	25	H	0	2.754	-2.990	-2.290	H
HETATM	26	C	0	-3.628	0.615	-0.385	C
HETATM	27	C	0	-4.469	0.672	0.740	C
HETATM	28	C	0	-3.901	-0.260	-1.456	C
HETATM	29	C	0	-5.549	-0.217	0.808	C
HETATM	30	C	0	-4.987	-1.134	-1.344	C

HETATM	31	C	0	-5.811	-1.137	-0.212	C
HETATM	32	H	0	-6.197	-0.192	1.694	H
HETATM	33	H	0	-5.199	-1.824	-2.172	H
HETATM	34	C	0	0.983	2.265	-0.381	C
HETATM	35	C	0	1.632	2.392	0.862	C
HETATM	36	C	0	1.711	2.256	-1.586	C
HETATM	37	C	0	3.028	2.490	0.877	C
HETATM	38	C	0	3.106	2.339	-1.521	C
HETATM	39	C	0	3.780	2.448	-0.301	C
HETATM	40	H	0	3.538	2.602	1.841	H
HETATM	41	H	0	3.681	2.311	-2.457	H
HETATM	42	C	0	-4.261	1.679	1.830	C
HETATM	43	H	0	-4.543	1.264	2.811	H
HETATM	44	H	0	-3.211	2.000	1.908	H
HETATM	45	H	0	-4.889	2.577	1.665	H
HETATM	46	C	0	-3.060	-0.239	-2.695	C
HETATM	47	H	0	-3.057	0.760	-3.170	H
HETATM	48	H	0	-1.999	-0.489	-2.497	H
HETATM	49	H	0	-3.437	-0.956	-3.443	H
HETATM	50	C	0	-6.944	-2.111	-0.091	C
HETATM	51	H	0	-6.633	-3.023	0.455	H
HETATM	52	H	0	-7.795	-1.688	0.468	H
HETATM	53	H	0	-7.312	-2.441	-1.077	H
HETATM	54	C	0	0.850	2.455	2.138	C
HETATM	55	H	0	1.520	2.566	3.007	H
HETATM	56	H	0	0.145	3.309	2.149	H
HETATM	57	H	0	0.231	1.552	2.306	H
HETATM	58	C	0	1.030	2.195	-2.920	C
HETATM	59	H	0	0.930	3.203	-3.370	H
HETATM	60	H	0	1.612	1.582	-3.630	H
HETATM	61	H	0	0.027	1.742	-2.859	H
HETATM	62	C	0	5.277	2.492	-0.258	C
HETATM	63	H	0	5.707	1.478	-0.372	H
HETATM	64	H	0	5.699	3.106	-1.074	H
HETATM	65	H	0	5.652	2.892	0.700	H
HETATM	66	C	0	4.685	-3.561	-1.565	C
HETATM	67	H	0	5.098	-3.733	-2.575	H
HETATM	68	H	0	5.513	-3.209	-0.925	H
HETATM	69	H	0	4.343	-4.533	-1.171	H
HETATM	70	C	0	3.918	-1.217	-2.213	C
HETATM	71	H	0	4.874	-0.819	-1.831	H
HETATM	72	H	0	4.025	-1.315	-3.308	H
HETATM	73	H	0	3.118	-0.482	-2.024	H
HETATM	74	H	0	-3.360	3.401	-0.210	H
HETATM	75	H	0	-1.108	4.187	0.037	H
HETATM	76	C	0	0.127	-2.901	0.666	C
HETATM	77	H	0	0.614	-3.222	-0.260	H
HETATM	78	H	0	-0.569	-3.618	1.124	H
HETATM	79	C	0	-1.749	-2.053	-0.013	C
HETATM	80	H	0	-2.518	-2.347	0.731	H
HETATM	81	H	0	-1.796	-2.578	-0.990	H

END

1f.pdb

TITLE	1f.pdb						
HETATM	1	Ru	0	-0.520	-0.791	0.393	Ru
HETATM	2	C	0	-1.219	3.293	-0.766	C
HETATM	3	C	0	-2.665	2.836	-0.622	C
HETATM	4	H	0	-0.959	3.582	-1.803	H
HETATM	5	H	0	-3.269	3.004	-1.532	H

HETATM	6	C	0	-1.241	1.013	-0.191	C
HETATM	7	N	0	-2.531	1.401	-0.361	N
HETATM	8	N	0	-0.460	2.103	-0.378	N
HETATM	9	Cl	0	0.228	-1.322	-1.869	Cl
HETATM	10	Cl	0	-1.218	-0.123	2.657	Cl
HETATM	11	C	0	0.978	-2.156	1.706	C
HETATM	12	C	0	2.227	-1.387	1.656	C
HETATM	13	C	0	3.246	-1.555	0.672	C
HETATM	14	C	0	2.469	-0.508	2.731	C
HETATM	15	C	0	4.463	-0.871	0.831	C
HETATM	16	C	0	3.670	0.176	2.867	C
HETATM	17	H	0	1.668	-0.377	3.471	H
HETATM	18	C	0	4.669	-0.019	1.913	C
HETATM	19	H	0	5.272	-1.023	0.114	H
HETATM	20	H	0	3.828	0.856	3.712	H
HETATM	21	H	0	5.632	0.500	2.006	H
HETATM	22	O	0	2.988	-2.435	-0.304	O
HETATM	23	C	0	3.694	-2.517	-1.557	C
HETATM	24	H	0	2.982	-3.121	-2.148	H
HETATM	25	C	0	-3.693	0.578	-0.330	C
HETATM	26	C	0	-4.555	0.613	0.784	C
HETATM	27	C	0	-4.004	-0.197	-1.467	C
HETATM	28	C	0	-5.695	-0.199	0.765	C
HETATM	29	C	0	-5.152	-0.994	-1.440	C
HETATM	30	C	0	-6.001	-1.018	-0.327	C
HETATM	31	H	0	-6.361	-0.191	1.638	H
HETATM	32	H	0	-5.394	-1.605	-2.320	H
HETATM	33	C	0	0.966	2.129	-0.461	C
HETATM	34	C	0	1.716	2.445	0.691	C
HETATM	35	C	0	1.585	1.995	-1.719	C
HETATM	36	C	0	3.101	2.585	0.564	C
HETATM	37	C	0	2.977	2.121	-1.791	C
HETATM	38	C	0	3.749	2.407	-0.663	C
HETATM	39	H	0	3.690	2.837	1.455	H
HETATM	40	H	0	3.468	1.995	-2.766	H
HETATM	41	C	0	-4.284	1.505	1.955	C
HETATM	42	H	0	-4.711	1.086	2.881	H
HETATM	43	H	0	-3.203	1.642	2.126	H
HETATM	44	H	0	-4.745	2.504	1.816	H
HETATM	45	C	0	-3.126	-0.150	-2.678	C
HETATM	46	H	0	-2.977	0.888	-3.034	H
HETATM	47	H	0	-2.115	-0.556	-2.479	H
HETATM	48	H	0	-3.562	-0.728	-3.509	H
HETATM	49	C	0	-7.205	-1.911	-0.300	C
HETATM	50	H	0	-6.985	-2.866	0.214	H
HETATM	51	H	0	-8.049	-1.450	0.241	H
HETATM	52	H	0	-7.550	-2.169	-1.316	H
HETATM	53	C	0	1.046	2.654	2.013	C
HETATM	54	H	0	1.776	2.954	2.784	H
HETATM	55	H	0	0.268	3.440	1.964	H
HETATM	56	H	0	0.528	1.743	2.369	H
HETATM	57	C	0	0.796	1.792	-2.977	C
HETATM	58	H	0	0.663	2.750	-3.520	H
HETATM	59	H	0	1.319	1.105	-3.663	H
HETATM	60	H	0	-0.198	1.357	-2.793	H
HETATM	61	C	0	5.242	2.488	-0.756	C
HETATM	62	H	0	5.703	1.496	-0.581	H
HETATM	63	H	0	5.581	2.824	-1.752	H
HETATM	64	H	0	5.669	3.171	-0.000	H
HETATM	65	C	0	4.984	-3.306	-1.429	C
HETATM	66	H	0	5.372	-3.548	-2.434	H
HETATM	67	H	0	5.779	-2.759	-0.894	H

HETATM	68	H	0	4.811	-4.258	-0.899	H
HETATM	69	C	0	3.828	-1.181	-2.262	C
HETATM	70	H	0	4.607	-0.526	-1.838	H
HETATM	71	H	0	4.087	-1.357	-3.321	H
HETATM	72	H	0	2.862	-0.649	-2.231	H
HETATM	73	H	0	-3.188	3.328	0.220	H
HETATM	74	H	0	-0.962	4.145	-0.112	H
HETATM	75	C	0	0.429	-3.035	0.805	C
HETATM	76	H	0	0.870	-3.268	-0.165	H
HETATM	77	C	0	-2.069	-1.725	0.247	C
HETATM	78	H	0	-2.844	-1.736	1.043	H
HETATM	79	H	0	-2.259	-2.391	-0.625	H
HETATM	80	H	0	0.479	-2.084	2.681	H
HETATM	81	H	0	-0.418	-3.650	1.130	H

END

s2a.pdb

TITLE	s2a.pdb						
HETATM	1	Ru	0	0.125	0.317	-0.098	Ru
HETATM	2	C	0	0.794	-3.797	0.911	C
HETATM	3	C	0	-0.671	-3.814	0.528	C
HETATM	4	H	0	0.952	-3.917	2.001	H
HETATM	5	H	0	-1.327	-4.234	1.310	H
HETATM	6	C	0	0.170	-1.628	0.192	C
HETATM	7	N	0	-0.962	-2.400	0.312	N
HETATM	8	N	0	1.218	-2.465	0.482	N
HETATM	9	Cl	0	-0.358	0.715	2.199	Cl
HETATM	10	Cl	0	-0.617	0.403	-2.344	Cl
HETATM	11	C	0	1.921	0.678	-0.332	C
HETATM	12	H	0	2.704	-0.089	-0.409	H
HETATM	13	C	0	2.406	2.024	-0.517	C
HETATM	14	C	0	1.498	3.109	-0.455	C
HETATM	15	C	0	3.769	2.287	-0.763	C
HETATM	16	C	0	1.950	4.417	-0.638	C
HETATM	17	C	0	4.220	3.590	-0.938	C
HETATM	18	H	0	4.464	1.439	-0.809	H
HETATM	19	C	0	3.308	4.648	-0.875	C
HETATM	20	H	0	1.257	5.262	-0.614	H
HETATM	21	H	0	5.280	3.789	-1.128	H
HETATM	22	H	0	3.652	5.678	-1.021	H
HETATM	23	O	0	0.219	2.720	-0.246	O
HETATM	24	C	0	-0.831	3.600	0.246	C
HETATM	25	H	0	-1.581	2.849	0.531	H
HETATM	26	C	0	-2.294	-2.084	-0.097	C
HETATM	27	C	0	-2.658	-2.219	-1.452	C
HETATM	28	C	0	-3.271	-1.846	0.893	C
HETATM	29	C	0	-3.995	-2.005	-1.809	C
HETATM	30	C	0	-4.599	-1.669	0.493	C
HETATM	31	C	0	-4.976	-1.720	-0.854	C
HETATM	32	H	0	-4.277	-2.081	-2.867	H
HETATM	33	H	0	-5.358	-1.464	1.259	H
HETATM	34	C	0	2.615	-2.212	0.397	C
HETATM	35	C	0	3.251	-2.392	-0.846	C
HETATM	36	C	0	3.340	-1.826	1.537	C
HETATM	37	C	0	4.629	-2.174	-0.932	C
HETATM	38	C	0	4.717	-1.614	1.409	C
HETATM	39	C	0	5.377	-1.780	0.185	C
HETATM	40	H	0	5.130	-2.306	-1.900	H
HETATM	41	H	0	5.290	-1.303	2.293	H
HETATM	42	C	0	-1.683	-2.678	-2.493	C

HETATM	43	H	0	-1.873	-2.187	-3.462	H
HETATM	44	H	0	-0.638	-2.462	-2.225	H
HETATM	45	H	0	-1.778	-3.770	-2.658	H
HETATM	46	C	0	-2.906	-1.828	2.345	C
HETATM	47	H	0	-3.758	-1.502	2.964	H
HETATM	48	H	0	-2.611	-2.834	2.701	H
HETATM	49	H	0	-2.054	-1.156	2.549	H
HETATM	50	C	0	-6.390	-1.443	-1.263	C
HETATM	51	H	0	-6.556	-0.357	-1.403	H
HETATM	52	H	0	-6.648	-1.930	-2.219	H
HETATM	53	H	0	-7.115	-1.776	-0.500	H
HETATM	54	C	0	2.442	-2.729	-2.060	C
HETATM	55	H	0	3.086	-2.940	-2.930	H
HETATM	56	H	0	1.787	-3.606	-1.903	H
HETATM	57	H	0	1.772	-1.890	-2.335	H
HETATM	58	C	0	2.643	-1.597	2.842	C
HETATM	59	H	0	2.207	-2.527	3.253	H
HETATM	60	H	0	3.338	-1.201	3.601	H
HETATM	61	H	0	1.808	-0.879	2.738	H
HETATM	62	C	0	6.846	-1.507	0.067	C
HETATM	63	H	0	7.392	-1.777	0.986	H
HETATM	64	H	0	7.303	-2.055	-0.775	H
HETATM	65	H	0	7.042	-0.432	-0.110	H
HETATM	66	C	0	-1.405	4.451	-0.868	C
HETATM	67	H	0	-2.389	4.842	-0.554	H
HETATM	68	H	0	-0.776	5.318	-1.133	H
HETATM	69	H	0	-1.554	3.845	-1.778	H
HETATM	70	C	0	-0.434	4.339	1.504	C
HETATM	71	H	0	0.265	5.175	1.334	H
HETATM	72	H	0	-1.347	4.762	1.961	H
HETATM	73	H	0	0.012	3.640	2.230	H
HETATM	74	H	0	-0.861	-4.384	-0.406	H
HETATM	75	H	0	1.391	-4.575	0.403	H
HETATM	76	C	0	-3.491	1.467	-0.440	C
HETATM	77	H	0	-3.285	2.208	-1.216	H
HETATM	78	H	0	-3.332	0.408	-0.658	H
HETATM	79	C	0	-3.889	1.871	0.758	C
HETATM	80	F	0	-4.154	1.105	1.793	F
HETATM	81	F	0	-4.053	3.141	1.100	F

END

s2b.pdb

TITLE	s2b.pdb						
HETATM	1	Ru	0	-0.286	0.179	-0.354	Ru
HETATM	2	C	0	0.022	-3.747	1.298	C
HETATM	3	C	0	-1.478	-3.584	1.115	C
HETATM	4	H	0	0.327	-3.740	2.364	H
HETATM	5	H	0	-2.050	-3.726	2.049	H
HETATM	6	C	0	-0.392	-1.647	0.309	C
HETATM	7	N	0	-1.593	-2.208	0.647	N
HETATM	8	N	0	0.568	-2.570	0.620	N
HETATM	9	Cl	0	-0.730	1.048	1.823	Cl
HETATM	10	Cl	0	-0.785	-0.422	-2.631	Cl
HETATM	11	C	0	1.527	0.211	-0.723	C
HETATM	12	H	0	1.956	-0.730	-1.109	H
HETATM	13	C	0	2.522	1.260	-0.736	C
HETATM	14	C	0	2.286	2.603	-0.324	C
HETATM	15	C	0	3.835	0.901	-1.126	C
HETATM	16	C	0	3.355	3.511	-0.288	C
HETATM	17	C	0	4.885	1.806	-1.089	C

HETATM	18	H	0	4.007	-0.134	-1.448	H
HETATM	19	C	0	4.637	3.115	-0.663	C
HETATM	20	H	0	3.183	4.546	0.014	H
HETATM	21	H	0	5.893	1.502	-1.393	H
HETATM	22	H	0	5.452	3.848	-0.633	H
HETATM	23	O	0	1.016	2.918	-0.037	O
HETATM	24	C	0	0.649	3.927	0.944	C
HETATM	25	H	0	-0.374	3.604	1.190	H
HETATM	26	C	0	-2.878	-1.637	0.403	C
HETATM	27	C	0	-3.498	-1.827	-0.851	C
HETATM	28	C	0	-3.561	-0.990	1.454	C
HETATM	29	C	0	-4.739	-1.224	-1.078	C
HETATM	30	C	0	-4.804	-0.410	1.182	C
HETATM	31	C	0	-5.389	-0.485	-0.085	C
HETATM	32	H	0	-5.212	-1.343	-2.062	H
HETATM	33	H	0	-5.327	0.120	1.990	H
HETATM	34	C	0	1.981	-2.488	0.473	C
HETATM	35	C	0	2.564	-3.105	-0.651	C
HETATM	36	C	0	2.769	-1.843	1.441	C
HETATM	37	C	0	3.954	-3.069	-0.790	C
HETATM	38	C	0	4.158	-1.828	1.263	C
HETATM	39	C	0	4.766	-2.430	0.157	C
HETATM	40	H	0	4.414	-3.537	-1.671	H
HETATM	41	H	0	4.780	-1.316	2.009	H
HETATM	42	C	0	-2.922	-2.741	-1.890	C
HETATM	43	H	0	-3.092	-2.353	-2.908	H
HETATM	44	H	0	-1.837	-2.888	-1.783	H
HETATM	45	H	0	-3.411	-3.735	-1.833	H
HETATM	46	C	0	-3.041	-0.987	2.859	C
HETATM	47	H	0	-3.161	0.003	3.330	H
HETATM	48	H	0	-3.608	-1.712	3.477	H
HETATM	49	H	0	-1.973	-1.242	2.922	H
HETATM	50	C	0	-6.667	0.237	-0.381	C
HETATM	51	H	0	-6.460	1.269	-0.726	H
HETATM	52	H	0	-7.247	-0.254	-1.181	H
HETATM	53	H	0	-7.313	0.325	0.510	H
HETATM	54	C	0	1.691	-3.690	-1.719	C
HETATM	55	H	0	2.290	-4.159	-2.517	H
HETATM	56	H	0	0.993	-4.455	-1.331	H
HETATM	57	H	0	1.059	-2.908	-2.185	H
HETATM	58	C	0	2.144	-1.118	2.590	C
HETATM	59	H	0	1.219	-1.601	2.951	H
HETATM	60	H	0	2.844	-1.023	3.437	H
HETATM	61	H	0	1.839	-0.097	2.290	H
HETATM	62	C	0	6.249	-2.341	-0.042	C
HETATM	63	H	0	6.793	-2.290	0.916	H
HETATM	64	H	0	6.644	-3.196	-0.616	H
HETATM	65	H	0	6.518	-1.427	-0.607	H
HETATM	66	C	0	0.579	5.318	0.344	C
HETATM	67	H	0	0.085	5.996	1.062	H
HETATM	68	H	0	1.566	5.752	0.111	H
HETATM	69	H	0	-0.025	5.324	-0.578	H
HETATM	70	C	0	1.468	3.824	2.214	C
HETATM	71	H	0	2.497	4.209	2.116	H
HETATM	72	H	0	0.972	4.410	3.008	H
HETATM	73	H	0	1.509	2.776	2.554	H
HETATM	74	H	0	-1.898	-4.279	0.359	H
HETATM	75	H	0	0.422	-4.674	0.850	H
HETATM	76	C	0	-1.458	2.840	-1.885	C
HETATM	77	H	0	-0.748	3.663	-1.976	H
HETATM	78	H	0	-1.421	2.001	-2.585	H
HETATM	79	C	0	-2.361	2.858	-0.913	C

HETATM	80	F	0	-3.257	1.921	-0.692	F
HETATM	81	F	0	-2.503	3.827	-0.028	F
END							

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TITLE	s2c.pdb						
HETATM	1	Ru	0	-0.445	0.163	-0.477	Ru
HETATM	2	C	0	-0.248	-3.614	1.568	C
HETATM	3	C	0	-1.743	-3.336	1.483	C
HETATM	4	H	0	0.139	-3.565	2.605	H
HETATM	5	H	0	-2.244	-3.339	2.468	H
HETATM	6	C	0	-0.571	-1.579	0.428	C
HETATM	7	N	0	-1.785	-2.006	0.888	N
HETATM	8	N	0	0.338	-2.534	0.769	N
HETATM	9	Cl	0	-0.768	1.276	1.631	Cl
HETATM	10	Cl	0	-0.849	-0.857	-2.656	Cl
HETATM	11	C	0	1.382	0.145	-0.807	C
HETATM	12	H	0	1.730	-0.823	-1.212	H
HETATM	13	C	0	2.486	1.086	-0.792	C
HETATM	14	C	0	2.467	2.426	-0.289	C
HETATM	15	C	0	3.725	0.587	-1.271	C
HETATM	16	C	0	3.658	3.171	-0.266	C
HETATM	17	C	0	4.892	1.335	-1.250	C
HETATM	18	H	0	3.742	-0.441	-1.657	H
HETATM	19	C	0	4.852	2.634	-0.737	C
HETATM	20	H	0	3.646	4.199	0.101	H
HETATM	21	H	0	5.828	0.916	-1.634	H
HETATM	22	H	0	5.760	3.248	-0.714	H
HETATM	23	O	0	1.284	2.917	0.089	O
HETATM	24	C	0	1.111	3.958	1.081	C
HETATM	25	H	0	0.063	3.784	1.370	H
HETATM	26	C	0	-3.022	-1.357	0.589	C
HETATM	27	C	0	-3.664	-1.615	-0.641	C
HETATM	28	C	0	-3.619	-0.514	1.551	C
HETATM	29	C	0	-4.811	-0.881	-0.961	C
HETATM	30	C	0	-4.767	0.196	1.188	C
HETATM	31	C	0	-5.351	0.057	-0.075	C
HETATM	32	H	0	-5.295	-1.053	-1.931	H
HETATM	33	H	0	-5.216	0.881	1.920	H
HETATM	34	C	0	1.747	-2.526	0.563	C
HETATM	35	C	0	2.269	-3.250	-0.525	C
HETATM	36	C	0	2.590	-1.846	1.461	C
HETATM	37	C	0	3.656	-3.292	-0.695	C
HETATM	38	C	0	3.972	-1.910	1.252	C
HETATM	39	C	0	4.521	-2.628	0.183	C
HETATM	40	H	0	4.070	-3.850	-1.545	H
HETATM	41	H	0	4.637	-1.374	1.941	H
HETATM	42	C	0	-3.221	-2.725	-1.546	C
HETATM	43	H	0	-3.344	-2.456	-2.607	H
HETATM	44	H	0	-2.163	-2.999	-1.411	H
HETATM	45	H	0	-3.837	-3.628	-1.360	H
HETATM	46	C	0	-3.118	-0.441	2.960	C
HETATM	47	H	0	-3.188	0.584	3.361	H
HETATM	48	H	0	-3.734	-1.090	3.614	H
HETATM	49	H	0	-2.068	-0.754	3.055	H
HETATM	50	C	0	-6.518	0.906	-0.477	C
HETATM	51	H	0	-6.173	1.844	-0.953	H
HETATM	52	H	0	-7.168	0.400	-1.210	H
HETATM	53	H	0	-7.137	1.200	0.388	H
HETATM	54	C	0	1.345	-3.883	-1.519	C

HETATM	55	H	0	1.904	-4.429	-2.297	H
HETATM	56	H	0	0.639	-4.597	-1.053	H
HETATM	57	H	0	0.720	-3.117	-2.022	H
HETATM	58	C	0	2.015	-1.028	2.574	C
HETATM	59	H	0	1.282	-1.592	3.180	H
HETATM	60	H	0	2.803	-0.662	3.253	H
HETATM	61	H	0	1.462	-0.151	2.184	H
HETATM	62	C	0	6.002	-2.640	-0.046	C
HETATM	63	H	0	6.568	-2.587	0.900	H
HETATM	64	H	0	6.330	-3.541	-0.591	H
HETATM	65	H	0	6.319	-1.769	-0.651	H
HETATM	66	C	0	1.205	5.342	0.468	C
HETATM	67	H	0	0.822	6.089	1.185	H
HETATM	68	H	0	2.231	5.644	0.196	H
HETATM	69	H	0	0.577	5.403	-0.438	H
HETATM	70	C	0	1.950	3.732	2.321	C
HETATM	71	H	0	3.027	3.928	2.184	H
HETATM	72	H	0	1.593	4.401	3.123	H
HETATM	73	H	0	1.823	2.694	2.675	H
HETATM	74	H	0	-2.278	-4.060	0.835	H
HETATM	75	H	0	0.040	-4.599	1.159	H
HETATM	76	C	0	-0.778	2.357	-2.080	C
HETATM	77	H	0	0.155	2.919	-2.038	H
HETATM	78	H	0	-0.946	1.610	-2.860	H
HETATM	79	C	0	-1.767	2.674	-1.239	C
HETATM	80	F	0	-2.950	2.102	-1.224	F
HETATM	81	F	0	-1.724	3.634	-0.349	F

END

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TITLE	s2d.pdb						
HETATM	1	Ru	0	-0.302	0.021	-0.772	Ru
HETATM	2	C	0	-0.348	-3.423	1.921	C
HETATM	3	C	0	-1.834	-3.078	1.874	C
HETATM	4	H	0	0.092	-3.315	2.931	H
HETATM	5	H	0	-2.268	-2.884	2.871	H
HETATM	6	C	0	-0.650	-1.545	0.555	C
HETATM	7	N	0	-1.858	-1.860	1.061	N
HETATM	8	N	0	0.249	-2.440	1.009	N
HETATM	9	Cl	0	-0.722	1.354	1.251	Cl
HETATM	10	Cl	0	-0.058	-1.631	-2.548	Cl
HETATM	11	C	0	1.507	0.520	-1.052	C
HETATM	12	H	0	1.984	-0.265	-1.677	H
HETATM	13	C	0	2.490	1.467	-0.571	C
HETATM	14	C	0	2.254	2.778	-0.047	C
HETATM	15	C	0	3.823	0.990	-0.589	C
HETATM	16	C	0	3.329	3.489	0.515	C
HETATM	17	C	0	4.871	1.693	-0.016	C
HETATM	18	H	0	4.006	0.011	-1.049	H
HETATM	19	C	0	4.610	2.945	0.548	C
HETATM	20	H	0	3.174	4.498	0.900	H
HETATM	21	H	0	5.886	1.280	-0.020	H
HETATM	22	H	0	5.424	3.529	0.993	H
HETATM	23	O	0	1.035	3.278	-0.221	O
HETATM	24	C	0	0.476	4.393	0.520	C
HETATM	25	H	0	-0.599	4.190	0.397	H
HETATM	26	C	0	-3.072	-1.161	0.782	C
HETATM	27	C	0	-3.732	-1.364	-0.444	C
HETATM	28	C	0	-3.617	-0.311	1.768	C
HETATM	29	C	0	-4.896	-0.628	-0.705	C

HETATM	30	C	0	-4.779	0.399	1.464	C
HETATM	31	C	0	-5.420	0.270	0.225	C
HETATM	32	H	0	-5.407	-0.774	-1.666	H
HETATM	33	H	0	-5.193	1.082	2.218	H
HETATM	34	C	0	1.640	-2.491	0.695	C
HETATM	35	C	0	2.100	-3.434	-0.242	C
HETATM	36	C	0	2.540	-1.655	1.390	C
HETATM	37	C	0	3.475	-3.493	-0.509	C
HETATM	38	C	0	3.904	-1.771	1.114	C
HETATM	39	C	0	4.388	-2.671	0.155	C
HETATM	40	H	0	3.837	-4.210	-1.257	H
HETATM	41	H	0	4.608	-1.125	1.655	H
HETATM	42	C	0	-3.255	-2.357	-1.460	C
HETATM	43	H	0	-2.705	-1.878	-2.289	H
HETATM	44	H	0	-2.561	-3.104	-1.040	H
HETATM	45	H	0	-4.111	-2.894	-1.906	H
HETATM	46	C	0	-3.001	-0.190	3.128	C
HETATM	47	H	0	-3.154	0.821	3.542	H
HETATM	48	H	0	-3.460	-0.904	3.841	H
HETATM	49	H	0	-1.914	-0.367	3.111	H
HETATM	50	C	0	-6.639	1.084	-0.088	C
HETATM	51	H	0	-6.372	2.132	-0.320	H
HETATM	52	H	0	-7.185	0.689	-0.961	H
HETATM	53	H	0	-7.340	1.121	0.764	H
HETATM	54	C	0	1.169	-4.394	-0.916	C
HETATM	55	H	0	1.494	-4.603	-1.949	H
HETATM	56	H	0	1.143	-5.366	-0.384	H
HETATM	57	H	0	0.141	-4.004	-0.976	H
HETATM	58	C	0	2.050	-0.670	2.404	C
HETATM	59	H	0	1.469	-1.157	3.212	H
HETATM	60	H	0	2.891	-0.135	2.877	H
HETATM	61	H	0	1.369	0.084	1.963	H
HETATM	62	C	0	5.851	-2.716	-0.166	C
HETATM	63	H	0	6.475	-2.688	0.745	H
HETATM	64	H	0	6.124	-3.620	-0.736	H
HETATM	65	H	0	6.156	-1.845	-0.779	H
HETATM	66	C	0	0.807	5.704	-0.164	C
HETATM	67	H	0	0.231	6.522	0.304	H
HETATM	68	H	0	1.877	5.969	-0.089	H
HETATM	69	H	0	0.536	5.673	-1.233	H
HETATM	70	C	0	0.775	4.368	2.009	C
HETATM	71	H	0	1.716	4.870	2.290	H
HETATM	72	H	0	-0.040	4.892	2.539	H
HETATM	73	H	0	0.790	3.331	2.381	H
HETATM	74	H	0	-2.447	-3.864	1.393	H
HETATM	75	H	0	-0.128	-4.449	1.574	H
HETATM	76	C	0	0.047	1.485	-2.461	C
HETATM	77	H	0	0.673	2.373	-2.347	H
HETATM	78	H	0	0.169	0.873	-3.363	H
HETATM	79	C	0	-1.237	1.542	-1.858	C
HETATM	80	F	0	-2.283	0.947	-2.467	F
HETATM	81	F	0	-1.674	2.666	-1.293	F

END

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TITLE	S2I.pdb						
HETATM	1	Ru	0	0.490	-0.455	-0.334	Ru
HETATM	2	C	0	1.158	3.626	0.863	C
HETATM	3	C	0	2.573	3.069	1.021	C
HETATM	4	H	0	0.756	4.063	1.794	H

HETATM	5	H	0	2.932	3.085	2.068	H
HETATM	6	C	0	1.158	1.365	0.290	C
HETATM	7	N	0	2.436	1.682	0.560	N
HETATM	8	N	0	0.379	2.443	0.485	N
HETATM	9	Cl	0	-0.577	-0.846	1.794	Cl
HETATM	10	Cl	0	1.602	0.193	-2.431	Cl
HETATM	11	C	0	-0.863	-1.326	-1.637	C
HETATM	12	H	0	-0.479	-1.090	-2.640	H
HETATM	13	C	0	-2.312	-1.101	-1.587	C
HETATM	14	C	0	-3.240	-1.639	-0.648	C
HETATM	15	C	0	-2.821	-0.288	-2.624	C
HETATM	16	C	0	-4.605	-1.336	-0.785	C
HETATM	17	C	0	-4.170	0.016	-2.741	C
HETATM	18	H	0	-2.104	0.114	-3.351	H
HETATM	19	C	0	-5.064	-0.515	-1.810	C
HETATM	20	H	0	-5.329	-1.779	-0.098	H
HETATM	21	H	0	-4.524	0.656	-3.557	H
HETATM	22	H	0	-6.138	-0.306	-1.889	H
HETATM	23	O	0	-2.758	-2.480	0.276	O
HETATM	24	C	0	-3.384	-2.736	1.554	C
HETATM	25	H	0	-2.511	-3.069	2.142	H
HETATM	26	C	0	3.542	0.782	0.453	C
HETATM	27	C	0	4.425	0.888	-0.636	C
HETATM	28	C	0	3.736	-0.187	1.457	C
HETATM	29	C	0	5.457	-0.049	-0.747	C
HETATM	30	C	0	4.778	-1.106	1.304	C
HETATM	31	C	0	5.635	-1.064	0.198	C
HETATM	32	H	0	6.134	0.012	-1.610	H
HETATM	33	H	0	4.925	-1.872	2.076	H
HETATM	34	C	0	-1.051	2.433	0.452	C
HETATM	35	C	0	-1.719	2.575	-0.778	C
HETATM	36	C	0	-1.764	2.308	1.661	C
HETATM	37	C	0	-3.119	2.552	-0.780	C
HETATM	38	C	0	-3.159	2.277	1.609	C
HETATM	39	C	0	-3.853	2.387	0.397	C
HETATM	40	H	0	-3.647	2.664	-1.735	H
HETATM	41	H	0	-3.721	2.150	2.544	H
HETATM	42	C	0	4.302	1.986	-1.649	C
HETATM	43	H	0	4.602	1.635	-2.649	H
HETATM	44	H	0	3.269	2.357	-1.740	H
HETATM	45	H	0	4.960	2.842	-1.395	H
HETATM	46	C	0	2.863	-0.227	2.674	C
HETATM	47	H	0	2.754	0.772	3.135	H
HETATM	48	H	0	1.837	-0.579	2.456	H
HETATM	49	H	0	3.284	-0.902	3.438	H
HETATM	50	C	0	6.707	-2.095	0.021	C
HETATM	51	H	0	6.336	-2.955	-0.570	H
HETATM	52	H	0	7.582	-1.695	-0.520	H
HETATM	53	H	0	7.055	-2.500	0.986	H
HETATM	54	C	0	-0.957	2.770	-2.052	C
HETATM	55	H	0	-1.643	2.893	-2.907	H
HETATM	56	H	0	-0.313	3.669	-2.012	H
HETATM	57	H	0	-0.277	1.926	-2.281	H
HETATM	58	C	0	-1.062	2.237	2.983	C
HETATM	59	H	0	-0.939	3.244	3.432	H
HETATM	60	H	0	-1.638	1.632	3.702	H
HETATM	61	H	0	-0.065	1.773	2.903	H
HETATM	62	C	0	-5.351	2.344	0.375	C
HETATM	63	H	0	-5.735	1.414	0.832	H
HETATM	64	H	0	-5.794	3.179	0.950	H
HETATM	65	H	0	-5.748	2.398	-0.652	H
HETATM	66	C	0	-4.365	-3.889	1.462	C

HETATM	67	H	0	-4.674	-4.197	2.477	H
HETATM	68	H	0	-5.281	-3.634	0.902	H
HETATM	69	H	0	-3.901	-4.763	0.974	H
HETATM	70	C	0	-3.933	-1.495	2.234	C
HETATM	71	H	0	-4.938	-1.200	1.888	H
HETATM	72	H	0	-4.007	-1.689	3.319	H
HETATM	73	H	0	-3.239	-0.648	2.095	H
HETATM	74	H	0	3.320	3.601	0.407	H
HETATM	75	H	0	1.080	4.397	0.073	H
HETATM	76	C	0	-0.099	-2.508	-1.035	C
HETATM	77	H	0	-0.688	-3.082	-0.308	H
HETATM	78	H	0	0.238	-3.118	-1.890	H
HETATM	79	C	0	1.339	-2.179	-0.361	C
HETATM	80	F	0	2.364	-2.496	-1.163	F
HETATM	81	F	0	1.520	-2.900	0.758	F

END

s2e.pdb

TITLE	s2e.pdb						
HETATM	1	Ru	0	-0.474	-0.554	0.291	Ru
HETATM	2	Cl	0	-1.523	-0.005	2.450	Cl
HETATM	3	Cl	0	0.604	-0.763	-1.868	Cl
HETATM	4	C	0	-1.119	1.346	-0.215	C
HETATM	5	N	0	-2.397	1.701	-0.438	N
HETATM	6	C	0	-2.526	3.110	-0.829	C
HETATM	7	C	0	-1.103	3.640	-0.669	C
HETATM	8	N	0	-0.334	2.428	-0.372	N
HETATM	9	C	0	-3.526	0.828	-0.366	C
HETATM	10	C	0	-4.394	0.904	0.737	C
HETATM	11	C	0	-5.471	0.013	0.797	C
HETATM	12	C	0	-5.705	-0.927	-0.211	C
HETATM	13	C	0	-4.857	-0.941	-1.324	C
HETATM	14	C	0	-3.771	-0.066	-1.427	C
HETATM	15	C	0	-4.213	1.928	1.816	C
HETATM	16	C	0	-6.831	-1.909	-0.094	C
HETATM	17	C	0	-2.906	-0.067	-2.650	C
HETATM	18	C	0	1.095	2.416	-0.380	C
HETATM	19	C	0	1.771	2.383	-1.616	C
HETATM	20	C	0	3.168	2.367	-1.609	C
HETATM	21	C	0	3.897	2.397	-0.414	C
HETATM	22	C	0	3.200	2.463	0.794	C
HETATM	23	C	0	1.800	2.473	0.835	C
HETATM	24	C	0	1.030	2.387	-2.919	C
HETATM	25	C	0	5.396	2.363	-0.439	C
HETATM	26	C	0	1.075	2.572	2.142	C
HETATM	27	H	0	-3.256	3.621	-0.178	H
HETATM	28	H	0	-2.902	3.181	-1.868	H
HETATM	29	H	0	-0.999	4.366	0.160	H
HETATM	30	H	0	-0.713	4.124	-1.582	H
HETATM	31	H	0	-6.139	0.050	1.668	H
HETATM	32	H	0	-5.046	-1.649	-2.142	H
HETATM	33	H	0	-4.850	2.817	1.633	H
HETATM	34	H	0	-3.168	2.263	1.906	H
HETATM	35	H	0	-4.504	1.522	2.799	H
HETATM	36	H	0	-7.194	-2.241	-1.082	H
HETATM	37	H	0	-6.512	-2.819	0.450	H
HETATM	38	H	0	-7.687	-1.493	0.464	H
HETATM	39	H	0	-3.311	-0.746	-3.419	H
HETATM	40	H	0	-2.833	0.940	-3.102	H
HETATM	41	H	0	-1.868	-0.389	-2.445	H

HETATM	42	H	0	3.702	2.314	-2.568	H
HETATM	43	H	0	3.756	2.509	1.738	H
HETATM	44	H	0	0.915	3.415	-3.318	H
HETATM	45	H	0	1.574	1.806	-3.682	H
HETATM	46	H	0	0.027	1.939	-2.831	H
HETATM	47	H	0	5.816	3.170	-1.066	H
HETATM	48	H	0	5.772	1.413	-0.863	H
HETATM	49	H	0	5.826	2.465	0.572	H
HETATM	50	H	0	0.429	3.470	2.184	H
HETATM	51	H	0	1.784	2.633	2.985	H
HETATM	52	H	0	0.403	1.712	2.327	H
HETATM	53	C	0	0.791	-1.711	1.551	C
HETATM	54	C	0	2.195	-1.296	1.597	C
HETATM	55	C	0	3.218	-1.648	0.672	C
HETATM	56	C	0	4.532	-1.211	0.911	C
HETATM	57	C	0	4.841	-0.437	2.026	C
HETATM	58	C	0	3.847	-0.082	2.940	C
HETATM	59	C	0	2.548	-0.517	2.720	C
HETATM	60	O	0	2.860	-2.458	-0.333	O
HETATM	61	C	0	3.595	-2.623	-1.564	C
HETATM	62	C	0	4.068	-1.321	-2.184	C
HETATM	63	C	0	4.674	-3.681	-1.424	C
HETATM	64	H	0	0.328	-1.643	2.545	H
HETATM	65	H	0	5.336	-1.510	0.234	H
HETATM	66	H	0	5.879	-0.120	2.185	H
HETATM	67	H	0	4.088	0.525	3.820	H
HETATM	68	H	0	1.749	-0.255	3.426	H
HETATM	69	H	0	2.802	-3.024	-2.219	H
HETATM	70	H	0	3.287	-0.548	-2.090	H
HETATM	71	H	0	4.247	-1.487	-3.261	H
HETATM	72	H	0	5.011	-0.938	-1.757	H
HETATM	73	H	0	4.264	-4.606	-0.983	H
HETATM	74	H	0	5.079	-3.935	-2.419	H
HETATM	75	H	0	5.521	-3.353	-0.797	H
HETATM	76	C	0	0.111	-2.676	0.678	C
HETATM	77	C	0	-1.513	-2.088	0.042	C
HETATM	78	F	0	-2.484	-2.516	0.846	F
HETATM	79	F	0	-1.699	-2.722	-1.115	F
HETATM	80	H	0	-0.407	-3.449	1.267	H
HETATM	81	H	0	0.657	-3.061	-0.191	H

END

s2f.pdb

TITLE	s2f.pdb						
HETATM	1	Ru	0	-0.418	-0.699	0.418	Ru
HETATM	2	C	0	-1.010	3.444	-0.601	C
HETATM	3	C	0	-2.461	2.991	-0.680	C
HETATM	4	H	0	-0.637	3.879	-1.547	H
HETATM	5	H	0	-2.892	3.086	-1.696	H
HETATM	6	C	0	-1.119	1.140	-0.133	C
HETATM	7	N	0	-2.389	1.576	-0.302	N
HETATM	8	N	0	-0.293	2.201	-0.308	N
HETATM	9	Cl	0	0.341	-1.114	-1.858	Cl
HETATM	10	Cl	0	-0.940	-0.040	2.728	Cl
HETATM	11	C	0	1.074	-2.149	1.641	C
HETATM	12	C	0	2.341	-1.414	1.591	C
HETATM	13	C	0	3.334	-1.571	0.578	C
HETATM	14	C	0	2.634	-0.591	2.698	C
HETATM	15	C	0	4.571	-0.922	0.734	C
HETATM	16	C	0	3.856	0.055	2.833	C

HETATM	17	H	0	1.857	-0.474	3.464	H
HETATM	18	C	0	4.825	-0.123	1.844	C
HETATM	19	H	0	5.359	-1.066	-0.008	H
HETATM	20	H	0	4.055	0.689	3.704	H
HETATM	21	H	0	5.803	0.367	1.934	H
HETATM	22	O	0	3.033	-2.407	-0.422	O
HETATM	23	C	0	3.729	-2.486	-1.682	C
HETATM	24	H	0	2.994	-3.053	-2.280	H
HETATM	25	C	0	-3.586	0.798	-0.332	C
HETATM	26	C	0	-4.459	0.823	0.772	C
HETATM	27	C	0	-3.918	0.101	-1.510	C
HETATM	28	C	0	-5.654	0.102	0.688	C
HETATM	29	C	0	-5.119	-0.616	-1.545	C
HETATM	30	C	0	-5.994	-0.631	-0.454	C
HETATM	31	H	0	-6.335	0.108	1.549	H
HETATM	32	H	0	-5.377	-1.171	-2.457	H
HETATM	33	C	0	1.135	2.190	-0.397	C
HETATM	34	C	0	1.909	2.469	0.748	C
HETATM	35	C	0	1.734	2.079	-1.668	C
HETATM	36	C	0	3.297	2.565	0.605	C
HETATM	37	C	0	3.127	2.159	-1.757	C
HETATM	38	C	0	3.924	2.388	-0.632	C
HETATM	39	H	0	3.903	2.785	1.493	H
HETATM	40	H	0	3.600	2.049	-2.742	H
HETATM	41	C	0	-4.098	1.562	2.021	C
HETATM	42	H	0	-4.891	1.469	2.781	H
HETATM	43	H	0	-3.158	1.168	2.454	H
HETATM	44	H	0	-3.937	2.642	1.844	H
HETATM	45	C	0	-2.999	0.117	-2.691	C
HETATM	46	H	0	-2.768	1.148	-3.021	H
HETATM	47	H	0	-2.024	-0.360	-2.469	H
HETATM	48	H	0	-3.443	-0.413	-3.549	H
HETATM	49	C	0	-7.259	-1.433	-0.503	C
HETATM	50	H	0	-7.080	-2.484	-0.208	H
HETATM	51	H	0	-8.026	-1.037	0.184	H
HETATM	52	H	0	-7.691	-1.461	-1.518	H
HETATM	53	C	0	1.270	2.699	2.082	C
HETATM	54	H	0	2.026	2.958	2.842	H
HETATM	55	H	0	0.533	3.523	2.051	H
HETATM	56	H	0	0.717	1.811	2.441	H
HETATM	57	C	0	0.922	1.962	-2.923	C
HETATM	58	H	0	0.821	2.948	-3.419	H
HETATM	59	H	0	1.407	1.287	-3.647	H
HETATM	60	H	0	-0.088	1.560	-2.744	H
HETATM	61	C	0	5.417	2.419	-0.744	C
HETATM	62	H	0	5.842	1.402	-0.622	H
HETATM	63	H	0	5.755	2.787	-1.729	H
HETATM	64	H	0	5.880	3.049	0.035	H
HETATM	65	C	0	4.992	-3.322	-1.577	C
HETATM	66	H	0	5.366	-3.555	-2.590	H
HETATM	67	H	0	5.807	-2.814	-1.035	H
HETATM	68	H	0	4.789	-4.279	-1.068	H
HETATM	69	C	0	3.910	-1.142	-2.360	C
HETATM	70	H	0	4.722	-0.530	-1.931	H
HETATM	71	H	0	4.153	-1.308	-3.425	H
HETATM	72	H	0	2.971	-0.567	-2.310	H
HETATM	73	H	0	-3.127	3.539	0.009	H
HETATM	74	H	0	-0.827	4.186	0.198	H
HETATM	75	C	0	0.461	-2.958	0.714	C
HETATM	76	H	0	0.871	-3.169	-0.275	H
HETATM	77	C	0	-1.972	-1.643	0.281	C
HETATM	78	H	0	0.605	-2.110	2.632	H

HETATM	79	H	0	-0.383	-3.577	1.045	H
HETATM	80	F	0	-2.927	-1.778	1.175	F
HETATM	81	F	0	-2.290	-2.465	-0.703	F

END

a2a.pdb

TITLE	a2a.pdb						
HETATM	1	Ru	0	-0.001	0.264	0.226	Ru
HETATM	2	C	0	0.578	-3.925	-0.564	C
HETATM	3	C	0	-0.937	-3.796	-0.580	C
HETATM	4	H	0	0.947	-4.598	0.236	H
HETATM	5	H	0	-1.440	-4.463	0.144	H
HETATM	6	C	0	0.003	-1.678	-0.087	C
HETATM	7	N	0	-1.151	-2.400	-0.213	N
HETATM	8	N	0	1.025	-2.555	-0.317	N
HETATM	9	Cl	0	-0.675	0.098	2.514	Cl
HETATM	10	Cl	0	-0.283	0.772	-2.083	Cl
HETATM	11	C	0	1.810	0.597	0.319	C
HETATM	12	H	0	2.603	-0.120	0.586	H
HETATM	13	C	0	2.262	1.910	-0.088	C
HETATM	14	C	0	1.328	2.967	-0.111	C
HETATM	15	C	0	3.563	2.143	-0.571	C
HETATM	16	C	0	1.654	4.201	-0.663	C
HETATM	17	C	0	3.900	3.384	-1.106	C
HETATM	18	H	0	4.294	1.324	-0.544	H
HETATM	19	C	0	2.944	4.402	-1.165	C
HETATM	20	H	0	0.900	4.990	-0.725	H
HETATM	21	H	0	4.909	3.557	-1.497	H
HETATM	22	H	0	3.202	5.370	-1.610	H
HETATM	23	O	0	0.101	2.689	0.451	O
HETATM	24	C	0	-0.162	3.313	1.761	C
HETATM	25	H	0	-0.986	2.688	2.140	H
HETATM	26	C	0	-2.494	-1.933	-0.093	C
HETATM	27	C	0	-3.205	-1.551	-1.251	C
HETATM	28	C	0	-3.147	-2.035	1.154	C
HETATM	29	C	0	-4.548	-1.181	-1.117	C
HETATM	30	C	0	-4.485	-1.638	1.241	C
HETATM	31	C	0	-5.197	-1.194	0.120	C
HETATM	32	H	0	-5.097	-0.861	-2.013	H
HETATM	33	H	0	-4.990	-1.692	2.214	H
HETATM	34	C	0	2.422	-2.328	-0.188	C
HETATM	35	C	0	3.177	-1.990	-1.325	C
HETATM	36	C	0	3.024	-2.464	1.076	C
HETATM	37	C	0	4.554	-1.797	-1.176	C
HETATM	38	C	0	4.404	-2.261	1.184	C
HETATM	39	C	0	5.183	-1.926	0.070	C
HETATM	40	H	0	5.150	-1.527	-2.058	H
HETATM	41	H	0	4.880	-2.356	2.169	H
HETATM	42	C	0	-2.598	-1.613	-2.620	C
HETATM	43	H	0	-2.859	-0.719	-3.211	H
HETATM	44	H	0	-1.500	-1.671	-2.605	H
HETATM	45	H	0	-2.986	-2.491	-3.174	H
HETATM	46	C	0	-2.483	-2.647	2.350	C
HETATM	47	H	0	-2.746	-2.107	3.274	H
HETATM	48	H	0	-2.821	-3.695	2.479	H
HETATM	49	H	0	-1.386	-2.648	2.278	H
HETATM	50	C	0	-6.609	-0.711	0.249	C
HETATM	51	H	0	-6.636	0.376	0.463	H
HETATM	52	H	0	-7.185	-0.863	-0.680	H
HETATM	53	H	0	-7.146	-1.208	1.074	H

HETATM	54	C	0	2.502	-1.775	-2.644	C
HETATM	55	H	0	3.236	-1.600	-3.447	H
HETATM	56	H	0	1.876	-2.636	-2.942	H
HETATM	57	H	0	1.820	-0.903	-2.606	H
HETATM	58	C	0	2.180	-2.716	2.287	C
HETATM	59	H	0	1.509	-3.587	2.167	H
HETATM	60	H	0	2.798	-2.890	3.183	H
HETATM	61	H	0	1.519	-1.850	2.495	H
HETATM	62	C	0	6.655	-1.678	0.206	C
HETATM	63	H	0	7.050	-2.049	1.166	H
HETATM	64	H	0	7.230	-2.159	-0.605	H
HETATM	65	H	0	6.889	-0.598	0.155	H
HETATM	66	C	0	-0.630	4.741	1.596	C
HETATM	67	H	0	-1.065	5.097	2.547	H
HETATM	68	H	0	0.195	5.428	1.341	H
HETATM	69	H	0	-1.408	4.817	0.818	H
HETATM	70	C	0	1.017	3.156	2.693	C
HETATM	71	H	0	1.884	3.762	2.373	H
HETATM	72	H	0	0.729	3.487	3.706	H
HETATM	73	H	0	1.320	2.097	2.763	H
HETATM	74	H	0	-1.378	-3.999	-1.576	H
HETATM	75	H	0	0.996	-4.300	-1.517	H
HETATM	76	C	0	-3.057	2.269	-0.942	C
HETATM	77	C	0	-3.109	1.750	0.278	C
HETATM	78	H	0	-3.594	0.786	0.452	H
HETATM	79	H	0	-2.672	2.296	1.115	H
HETATM	80	F	0	-2.499	3.422	-1.247	F
HETATM	81	F	0	-3.569	1.725	-2.025	F

END

a2b.pdb

TITLE	a2b.pdb						
HETATM	1	Ru	0	0.594	-0.498	-0.271	Ru
HETATM	2	C	0	1.081	3.499	1.197	C
HETATM	3	C	0	2.513	2.987	1.190	C
HETATM	4	H	0	0.687	3.652	2.222	H
HETATM	5	H	0	3.003	3.044	2.180	H
HETATM	6	C	0	1.093	1.296	0.356	C
HETATM	7	N	0	2.359	1.597	0.774	N
HETATM	8	N	0	0.339	2.423	0.538	N
HETATM	9	Cl	0	0.755	-1.350	1.998	Cl
HETATM	10	Cl	0	1.494	-0.214	-2.494	Cl
HETATM	11	C	0	-1.060	0.036	-0.937	C
HETATM	12	H	0	-0.983	0.897	-1.627	H
HETATM	13	C	0	-2.417	-0.466	-0.932	C
HETATM	14	C	0	-2.950	-1.397	0.013	C
HETATM	15	C	0	-3.295	0.065	-1.907	C
HETATM	16	C	0	-4.306	-1.752	-0.060	C
HETATM	17	C	0	-4.630	-0.305	-1.982	C
HETATM	18	H	0	-2.884	0.790	-2.621	H
HETATM	19	C	0	-5.130	-1.215	-1.047	C
HETATM	20	H	0	-4.724	-2.475	0.641	H
HETATM	21	H	0	-5.281	0.114	-2.757	H
HETATM	22	H	0	-6.182	-1.522	-1.085	H
HETATM	23	O	0	-2.077	-1.865	0.907	O
HETATM	24	C	0	-2.425	-2.608	2.093	C
HETATM	25	H	0	-1.458	-2.575	2.625	H
HETATM	26	C	0	3.512	0.800	0.490	C
HETATM	27	C	0	4.140	0.925	-0.769	C
HETATM	28	C	0	4.054	-0.036	1.485	C

HETATM	29	C	0	5.229	0.101	-1.057	C
HETATM	30	C	0	5.144	-0.850	1.149	C
HETATM	31	C	0	5.725	-0.815	-0.121	C
HETATM	32	H	0	5.704	0.179	-2.044	H
HETATM	33	H	0	5.557	-1.520	1.915	H
HETATM	34	C	0	-1.072	2.568	0.391	C
HETATM	35	C	0	-1.567	3.226	-0.752	C
HETATM	36	C	0	-1.941	2.102	1.393	C
HETATM	37	C	0	-2.947	3.388	-0.886	C
HETATM	38	C	0	-3.320	2.279	1.216	C
HETATM	39	C	0	-3.840	2.914	0.087	C
HETATM	40	H	0	-3.340	3.877	-1.788	H
HETATM	41	H	0	-4.007	1.898	1.985	H
HETATM	42	C	0	3.729	1.980	-1.752	C
HETATM	43	H	0	3.913	1.653	-2.787	H
HETATM	44	H	0	2.660	2.236	-1.685	H
HETATM	45	H	0	4.317	2.907	-1.593	H
HETATM	46	C	0	3.576	-0.003	2.905	C
HETATM	47	H	0	3.419	-1.018	3.305	H
HETATM	48	H	0	4.336	0.486	3.547	H
HETATM	49	H	0	2.625	0.538	3.020	H
HETATM	50	C	0	6.858	-1.729	-0.477	C
HETATM	51	H	0	6.510	-2.574	-1.101	H
HETATM	52	H	0	7.639	-1.212	-1.061	H
HETATM	53	H	0	7.335	-2.165	0.418	H
HETATM	54	C	0	-0.627	3.656	-1.838	C
HETATM	55	H	0	-1.165	4.150	-2.663	H
HETATM	56	H	0	0.146	4.360	-1.477	H
HETATM	57	H	0	-0.077	2.792	-2.261	H
HETATM	58	C	0	-1.414	1.378	2.589	C
HETATM	59	H	0	-0.460	1.795	2.958	H
HETATM	60	H	0	-2.139	1.391	3.420	H
HETATM	61	H	0	-1.187	0.324	2.343	H
HETATM	62	C	0	-5.317	3.095	-0.090	C
HETATM	63	H	0	-5.643	2.799	-1.103	H
HETATM	64	H	0	-5.893	2.498	0.636	H
HETATM	65	H	0	-5.618	4.151	0.040	H
HETATM	66	C	0	-2.735	-4.059	1.783	C
HETATM	67	H	0	-2.816	-4.629	2.725	H
HETATM	68	H	0	-3.678	-4.201	1.228	H
HETATM	69	H	0	-1.923	-4.513	1.190	H
HETATM	70	C	0	-3.449	-1.907	2.969	C
HETATM	71	H	0	-4.492	-2.016	2.630	H
HETATM	72	H	0	-3.394	-2.329	3.988	H
HETATM	73	H	0	-3.224	-0.830	3.047	H
HETATM	74	H	0	3.157	3.531	0.471	H
HETATM	75	H	0	0.952	4.454	0.655	H
HETATM	76	C	0	-0.311	-3.125	-1.711	C
HETATM	77	C	0	0.693	-3.053	-0.826	C
HETATM	78	H	0	1.704	-2.860	-1.195	H
HETATM	79	H	0	0.523	-3.356	0.209	H
HETATM	80	F	0	-1.533	-3.501	-1.418	F
HETATM	81	F	0	-0.224	-2.865	-2.983	F

END

a2c.pdb

TITLE	a2c.pdb						
HETATM	1	Ru	0	0.699	-0.405	-0.483	Ru
HETATM	2	C	0	1.067	3.628	0.951	C
HETATM	3	C	0	2.454	3.048	1.211	C

HETATM	4	H	0	0.610	4.081	1.849	H
HETATM	5	H	0	2.702	2.996	2.291	H
HETATM	6	C	0	1.072	1.366	0.308	C
HETATM	7	N	0	2.346	1.706	0.650	N
HETATM	8	N	0	0.293	2.462	0.520	N
HETATM	9	Cl	0	0.659	-1.691	1.569	Cl
HETATM	10	Cl	0	1.419	0.483	-2.651	Cl
HETATM	11	C	0	-1.040	0.034	-1.004	C
HETATM	12	H	0	-1.023	0.893	-1.702	H
HETATM	13	C	0	-2.361	-0.567	-1.008	C
HETATM	14	C	0	-2.957	-1.330	0.043	C
HETATM	15	C	0	-3.112	-0.360	-2.189	C
HETATM	16	C	0	-4.211	-1.927	-0.174	C
HETATM	17	C	0	-4.350	-0.953	-2.393	C
HETATM	18	H	0	-2.665	0.265	-2.974	H
HETATM	19	C	0	-4.889	-1.748	-1.377	C
HETATM	20	H	0	-4.679	-2.525	0.609	H
HETATM	21	H	0	-4.894	-0.796	-3.330	H
HETATM	22	H	0	-5.867	-2.224	-1.512	H
HETATM	23	O	0	-2.290	-1.343	1.194	O
HETATM	24	C	0	-2.561	-2.213	2.312	C
HETATM	25	H	0	-1.707	-1.958	2.963	H
HETATM	26	C	0	3.447	0.802	0.561	C
HETATM	27	C	0	4.275	0.823	-0.581	C
HETATM	28	C	0	3.710	-0.082	1.630	C
HETATM	29	C	0	5.275	-0.150	-0.695	C
HETATM	30	C	0	4.718	-1.038	1.470	C
HETATM	31	C	0	5.488	-1.105	0.304	C
HETATM	32	H	0	5.907	-0.153	-1.593	H
HETATM	33	H	0	4.908	-1.746	2.288	H
HETATM	34	C	0	-1.128	2.516	0.454	C
HETATM	35	C	0	-1.761	3.120	-0.649	C
HETATM	36	C	0	-1.876	1.986	1.524	C
HETATM	37	C	0	-3.159	3.139	-0.686	C
HETATM	38	C	0	-3.271	2.028	1.447	C
HETATM	39	C	0	-3.929	2.582	0.342	C
HETATM	40	H	0	-3.661	3.580	-1.558	H
HETATM	41	H	0	-3.861	1.604	2.270	H
HETATM	42	C	0	4.172	1.907	-1.609	C
HETATM	43	H	0	4.383	1.525	-2.620	H
HETATM	44	H	0	3.174	2.369	-1.643	H
HETATM	45	H	0	4.916	2.702	-1.398	H
HETATM	46	C	0	3.007	0.051	2.946	C
HETATM	47	H	0	2.908	-0.924	3.450	H
HETATM	48	H	0	3.583	0.716	3.620	H
HETATM	49	H	0	1.991	0.464	2.849	H
HETATM	50	C	0	6.522	-2.177	0.133	C
HETATM	51	H	0	6.073	-3.108	-0.263	H
HETATM	52	H	0	7.313	-1.879	-0.577	H
HETATM	53	H	0	7.003	-2.444	1.090	H
HETATM	54	C	0	-0.955	3.666	-1.788	C
HETATM	55	H	0	-1.591	3.862	-2.667	H
HETATM	56	H	0	-0.462	4.623	-1.532	H
HETATM	57	H	0	-0.154	2.967	-2.098	H
HETATM	58	C	0	-1.179	1.366	2.693	C
HETATM	59	H	0	-0.390	2.027	3.101	H
HETATM	60	H	0	-1.885	1.144	3.512	H
HETATM	61	H	0	-0.681	0.418	2.407	H
HETATM	62	C	0	-5.423	2.532	0.245	C
HETATM	63	H	0	-5.761	1.543	-0.122	H
HETATM	64	H	0	-5.907	2.686	1.225	H
HETATM	65	H	0	-5.820	3.285	-0.456	H

HETATM	66	C	0	-2.427	-3.676	1.942	C
HETATM	67	H	0	-2.496	-4.295	2.854	H
HETATM	68	H	0	-3.209	-4.024	1.245	H
HETATM	69	H	0	-1.442	-3.856	1.481	H
HETATM	70	C	0	-3.835	-1.852	3.056	C
HETATM	71	H	0	-4.761	-2.204	2.572	H
HETATM	72	H	0	-3.805	-2.305	4.063	H
HETATM	73	H	0	-3.915	-0.760	3.189	H
HETATM	74	H	0	3.261	3.615	0.712	H
HETATM	75	H	0	1.072	4.401	0.158	H
HETATM	76	C	0	0.036	-2.745	-1.796	C
HETATM	77	C	0	1.327	-2.563	-1.451	C
HETATM	78	H	0	2.017	-2.162	-2.199	H
HETATM	79	H	0	1.691	-3.021	-0.527	H
HETATM	80	F	0	-0.851	-3.377	-1.067	F
HETATM	81	F	0	-0.484	-2.411	-2.947	F

END

a2d.pdb

TITLE	a2d.pdb						
HETATM	1	Ru	0	0.532	-0.668	-0.093	Ru
HETATM	2	C	0	1.169	3.616	0.211	C
HETATM	3	C	0	2.585	3.135	0.514	C
HETATM	4	H	0	0.748	4.259	1.002	H
HETATM	5	H	0	2.891	3.323	1.562	H
HETATM	6	C	0	1.224	1.279	0.116	C
HETATM	7	N	0	2.495	1.690	0.281	N
HETATM	8	N	0	0.419	2.358	0.120	N
HETATM	9	Cl	0	-0.133	-0.475	2.233	Cl
HETATM	10	Cl	0	1.883	-0.726	-2.151	Cl
HETATM	11	C	0	-0.844	-1.272	-1.281	C
HETATM	12	H	0	-0.433	-1.579	-2.259	H
HETATM	13	C	0	-2.284	-1.138	-1.350	C
HETATM	14	C	0	-3.189	-1.085	-0.246	C
HETATM	15	C	0	-2.820	-1.029	-2.656	C
HETATM	16	C	0	-4.560	-0.898	-0.491	C
HETATM	17	C	0	-4.174	-0.833	-2.884	C
HETATM	18	H	0	-2.124	-1.091	-3.502	H
HETATM	19	C	0	-5.042	-0.766	-1.789	C
HETATM	20	H	0	-5.259	-0.832	0.347	H
HETATM	21	H	0	-4.557	-0.741	-3.906	H
HETATM	22	H	0	-6.116	-0.612	-1.946	H
HETATM	23	O	0	-2.636	-1.217	0.949	O
HETATM	24	C	0	-3.303	-1.652	2.147	C
HETATM	25	H	0	-2.433	-1.946	2.760	H
HETATM	26	C	0	3.660	0.862	0.268	C
HETATM	27	C	0	4.478	0.869	-0.882	C
HETATM	28	C	0	4.004	0.094	1.394	C
HETATM	29	C	0	5.604	0.046	-0.906	C
HETATM	30	C	0	5.140	-0.725	1.322	C
HETATM	31	C	0	5.941	-0.772	0.180	C
HETATM	32	H	0	6.229	0.031	-1.809	H
HETATM	33	H	0	5.409	-1.330	2.198	H
HETATM	34	C	0	-1.004	2.337	0.005	C
HETATM	35	C	0	-1.597	2.166	-1.261	C
HETATM	36	C	0	-1.789	2.568	1.153	C
HETATM	37	C	0	-2.993	2.197	-1.352	C
HETATM	38	C	0	-3.179	2.587	1.015	C
HETATM	39	C	0	-3.798	2.404	-0.228	C
HETATM	40	H	0	-3.462	2.051	-2.333	H

HETATM	41	H	0	-3.797	2.752	1.908	H
HETATM	42	C	0	4.165	1.744	-2.058	C
HETATM	43	H	0	4.552	1.301	-2.991	H
HETATM	44	H	0	3.080	1.884	-2.194	H
HETATM	45	H	0	4.634	2.744	-1.961	H
HETATM	46	C	0	3.223	0.143	2.671	C
HETATM	47	H	0	2.532	1.001	2.723	H
HETATM	48	H	0	2.590	-0.751	2.807	H
HETATM	49	H	0	3.904	0.191	3.540	H
HETATM	50	C	0	7.127	-1.685	0.105	C
HETATM	51	H	0	6.893	-2.597	-0.477	H
HETATM	52	H	0	7.986	-1.207	-0.397	H
HETATM	53	H	0	7.457	-2.017	1.104	H
HETATM	54	C	0	-0.760	1.998	-2.494	C
HETATM	55	H	0	-1.395	1.923	-3.393	H
HETATM	56	H	0	-0.076	2.856	-2.644	H
HETATM	57	H	0	-0.111	1.101	-2.465	H
HETATM	58	C	0	-1.161	2.830	2.488	C
HETATM	59	H	0	-1.033	3.917	2.666	H
HETATM	60	H	0	-1.794	2.449	3.307	H
HETATM	61	H	0	-0.176	2.346	2.588	H
HETATM	62	C	0	-5.291	2.461	-0.349	C
HETATM	63	H	0	-5.788	1.809	0.393	H
HETATM	64	H	0	-5.674	3.483	-0.170	H
HETATM	65	H	0	-5.633	2.150	-1.350	H
HETATM	66	C	0	-4.161	-2.885	1.938	C
HETATM	67	H	0	-4.395	-3.330	2.921	H
HETATM	68	H	0	-5.121	-2.689	1.432	H
HETATM	69	H	0	-3.611	-3.645	1.356	H
HETATM	70	C	0	-3.981	-0.496	2.853	C
HETATM	71	H	0	-4.836	-0.080	2.290	H
HETATM	72	H	0	-4.356	-0.825	3.838	H
HETATM	73	H	0	-3.249	0.311	3.019	H
HETATM	74	H	0	3.349	3.586	-0.142	H
HETATM	75	H	0	1.095	4.170	-0.745	H
HETATM	76	C	0	0.088	-2.935	-0.237	C
HETATM	77	C	0	1.349	-2.544	0.306	C
HETATM	78	H	0	2.237	-2.739	-0.312	H
HETATM	79	H	0	1.455	-2.628	1.396	H
HETATM	80	F	0	0.084	-3.649	-1.369	F
HETATM	81	F	0	-0.865	-3.406	0.569	F

END

a2I.pdb

TITLE	a2I.pdb						
HETATM	1	Ru	0	0.381	-0.503	0.132	Ru
HETATM	2	C	0	1.477	3.542	-0.045	C
HETATM	3	C	0	2.831	2.993	0.391	C
HETATM	4	H	0	1.078	4.310	0.639	H
HETATM	5	H	0	3.071	3.227	1.447	H
HETATM	6	C	0	1.370	1.219	0.086	C
HETATM	7	N	0	2.666	1.540	0.241	N
HETATM	8	N	0	0.635	2.344	-0.016	N
HETATM	9	Cl	0	-0.290	-0.256	2.383	Cl
HETATM	10	Cl	0	1.758	-0.649	-1.968	Cl
HETATM	11	C	0	-0.891	-1.604	-1.139	C
HETATM	12	H	0	-0.375	-1.712	-2.103	H
HETATM	13	C	0	-2.308	-1.292	-1.360	C
HETATM	14	C	0	-3.259	-1.078	-0.325	C
HETATM	15	C	0	-2.747	-1.172	-2.695	C

HETATM	16	C	0	-4.599	-0.815	-0.652	C
HETATM	17	C	0	-4.075	-0.911	-3.014	C
HETATM	18	H	0	-2.012	-1.321	-3.496	H
HETATM	19	C	0	-5.003	-0.739	-1.983	C
HETATM	20	H	0	-5.324	-0.632	0.145	H
HETATM	21	H	0	-4.388	-0.847	-4.062	H
HETATM	22	H	0	-6.054	-0.527	-2.214	H
HETATM	23	O	0	-2.765	-1.058	0.914	O
HETATM	24	C	0	-3.464	-1.484	2.097	C
HETATM	25	H	0	-2.619	-1.805	2.732	H
HETATM	26	C	0	3.793	0.661	0.216	C
HETATM	27	C	0	4.623	0.674	-0.923	C
HETATM	28	C	0	4.088	-0.157	1.318	C
HETATM	29	C	0	5.735	-0.169	-0.947	C
HETATM	30	C	0	5.211	-0.993	1.248	C
HETATM	31	C	0	6.039	-1.018	0.124	C
HETATM	32	H	0	6.375	-0.176	-1.840	H
HETATM	33	H	0	5.446	-1.634	2.108	H
HETATM	34	C	0	-0.794	2.367	-0.098	C
HETATM	35	C	0	-1.433	2.090	-1.324	C
HETATM	36	C	0	-1.538	2.726	1.047	C
HETATM	37	C	0	-2.832	2.138	-1.369	C
HETATM	38	C	0	-2.929	2.767	0.951	C
HETATM	39	C	0	-3.593	2.472	-0.247	C
HETATM	40	H	0	-3.338	1.912	-2.316	H
HETATM	41	H	0	-3.513	3.034	1.842	H
HETATM	42	C	0	4.342	1.564	-2.096	C
HETATM	43	H	0	4.657	1.082	-3.037	H
HETATM	44	H	0	3.267	1.791	-2.198	H
HETATM	45	H	0	4.895	2.522	-2.031	H
HETATM	46	C	0	3.240	-0.161	2.552	C
HETATM	47	H	0	2.723	0.799	2.720	H
HETATM	48	H	0	2.442	-0.923	2.499	H
HETATM	49	H	0	3.845	-0.390	3.446	H
HETATM	50	C	0	7.213	-1.947	0.052	C
HETATM	51	H	0	6.964	-2.860	-0.523	H
HETATM	52	H	0	8.077	-1.484	-0.455	H
HETATM	53	H	0	7.540	-2.278	1.052	H
HETATM	54	C	0	-0.662	1.790	-2.573	C
HETATM	55	H	0	-1.238	2.083	-3.467	H
HETATM	56	H	0	0.314	2.306	-2.601	H
HETATM	57	H	0	-0.422	0.716	-2.672	H
HETATM	58	C	0	-0.865	3.098	2.333	C
HETATM	59	H	0	-0.719	4.194	2.410	H
HETATM	60	H	0	-1.476	2.794	3.200	H
HETATM	61	H	0	0.119	2.615	2.449	H
HETATM	62	C	0	-5.087	2.550	-0.324	C
HETATM	63	H	0	-5.569	2.019	0.517	H
HETATM	64	H	0	-5.440	3.598	-0.272	H
HETATM	65	H	0	-5.472	2.116	-1.262	H
HETATM	66	C	0	-4.364	-2.684	1.876	C
HETATM	67	H	0	-4.617	-3.127	2.855	H
HETATM	68	H	0	-5.316	-2.444	1.373	H
HETATM	69	H	0	-3.845	-3.459	1.286	H
HETATM	70	C	0	-4.133	-0.307	2.778	C
HETATM	71	H	0	-4.965	0.110	2.182	H
HETATM	72	H	0	-4.544	-0.617	3.755	H
HETATM	73	H	0	-3.394	0.492	2.955	H
HETATM	74	H	0	3.669	3.351	-0.230	H
HETATM	75	H	0	1.491	3.973	-1.066	H
HETATM	76	C	0	-0.359	-2.800	-0.294	C
HETATM	77	C	0	0.973	-2.428	0.360	C

HETATM	78	H	0	1.826	-2.730	-0.265	H
HETATM	79	H	0	1.046	-2.749	1.412	H
HETATM	80	F	0	-0.179	-3.851	-1.162	F
HETATM	81	F	0	-1.256	-3.245	0.632	F

END

a2e.pdb

TITLE	a2e.pdb						
HETATM	1	Ru	0	0.592	-0.608	-0.225	Ru
HETATM	2	Cl	0	1.667	-0.349	-2.414	Cl
HETATM	3	Cl	0	-0.398	-0.715	1.982	Cl
HETATM	4	C	0	1.189	1.311	0.199	C
HETATM	5	N	0	2.461	1.688	0.436	N
HETATM	6	C	0	2.572	3.111	0.774	C
HETATM	7	C	0	1.142	3.617	0.604	C
HETATM	8	N	0	0.392	2.389	0.318	N
HETATM	9	C	0	3.616	0.848	0.390	C
HETATM	10	C	0	4.446	0.875	-0.744	C
HETATM	11	C	0	5.562	0.029	-0.770	C
HETATM	12	C	0	5.870	-0.815	0.300	C
HETATM	13	C	0	5.053	-0.783	1.437	C
HETATM	14	C	0	3.930	0.047	1.507	C
HETATM	15	C	0	4.186	1.805	-1.889	C
HETATM	16	C	0	7.041	-1.749	0.229	C
HETATM	17	C	0	3.090	0.093	2.746	C
HETATM	18	C	0	-1.033	2.409	0.221	C
HETATM	19	C	0	-1.804	2.478	1.398	C
HETATM	20	C	0	-3.194	2.556	1.276	C
HETATM	21	C	0	-3.823	2.598	0.027	C
HETATM	22	C	0	-3.028	2.563	-1.122	C
HETATM	23	C	0	-1.635	2.459	-1.050	C
HETATM	24	C	0	-1.171	2.507	2.756	C
HETATM	25	C	0	-5.316	2.676	-0.070	C
HETATM	26	C	0	-0.804	2.432	-2.296	C
HETATM	27	H	0	3.291	3.604	0.095	H
HETATM	28	H	0	2.956	3.228	1.805	H
HETATM	29	H	0	1.029	4.333	-0.232	H
HETATM	30	H	0	0.742	4.102	1.512	H
HETATM	31	H	0	6.203	0.029	-1.661	H
HETATM	32	H	0	5.300	-1.414	2.301	H
HETATM	33	H	0	4.743	2.756	-1.768	H
HETATM	34	H	0	3.115	2.041	-2.001	H
HETATM	35	H	0	4.514	1.360	-2.843	H
HETATM	36	H	0	7.830	-1.372	-0.444	H
HETATM	37	H	0	6.739	-2.740	-0.160	H
HETATM	38	H	0	7.491	-1.924	1.221	H
HETATM	39	H	0	2.054	-0.255	2.573	H
HETATM	40	H	0	3.004	1.121	3.148	H
HETATM	41	H	0	3.524	-0.535	3.542	H
HETATM	42	H	0	-3.804	2.583	2.190	H
HETATM	43	H	0	-3.503	2.610	-2.109	H
HETATM	44	H	0	-1.045	3.546	3.122	H
HETATM	45	H	0	-0.188	2.011	2.771	H
HETATM	46	H	0	-1.802	1.985	3.496	H
HETATM	47	H	0	-5.722	3.538	0.490	H
HETATM	48	H	0	-5.657	2.763	-1.115	H
HETATM	49	H	0	-5.794	1.774	0.359	H
HETATM	50	H	0	-1.439	2.487	-3.197	H
HETATM	51	H	0	-0.092	3.279	-2.338	H
HETATM	52	H	0	-0.185	1.517	-2.380	H

HETATM	53	C	0	-0.770	-1.850	-1.369	C
HETATM	54	C	0	-2.143	-1.329	-1.412	C
HETATM	55	C	0	-3.173	-1.511	-0.444	C
HETATM	56	C	0	-4.456	-1.002	-0.712	C
HETATM	57	C	0	-4.731	-0.328	-1.897	C
HETATM	58	C	0	-3.729	-0.132	-2.849	C
HETATM	59	C	0	-2.457	-0.625	-2.595	C
HETATM	60	O	0	-2.857	-2.243	0.623	O
HETATM	61	C	0	-3.554	-2.224	1.884	C
HETATM	62	C	0	-3.894	-0.829	2.373	C
HETATM	63	C	0	-4.717	-3.197	1.885	C
HETATM	64	H	0	-0.309	-1.821	-2.366	H
HETATM	65	H	0	-5.264	-1.174	0.002	H
HETATM	66	H	0	-5.748	0.041	-2.078	H
HETATM	67	H	0	-3.939	0.400	-3.784	H
HETATM	68	H	0	-1.655	-0.483	-3.331	H
HETATM	69	H	0	-2.769	-2.621	2.552	H
HETATM	70	H	0	-4.797	-0.397	1.910	H
HETATM	71	H	0	-3.041	-0.153	2.193	H
HETATM	72	H	0	-4.072	-0.865	3.463	H
HETATM	73	H	0	-5.561	-2.861	1.257	H
HETATM	74	H	0	-5.101	-3.320	2.913	H
HETATM	75	H	0	-4.400	-4.190	1.524	H
HETATM	76	C	0	-0.053	-2.836	-0.603	C
HETATM	77	C	0	1.715	-2.036	0.150	C
HETATM	78	F	0	0.631	-3.725	-1.355	F
HETATM	79	F	0	-0.538	-3.479	0.442	F
HETATM	80	H	0	2.472	-2.389	-0.576	H
HETATM	81	H	0	1.728	-2.510	1.152	H

END

a2f.pdb

TITLE	a2f.pdb						
HETATM	1	Ru	0	-0.496	-0.487	0.395	Ru
HETATM	2	C	0	-1.428	3.514	-0.637	C
HETATM	3	C	0	-2.847	2.996	-0.447	C
HETATM	4	H	0	-1.209	3.787	-1.689	H
HETATM	5	H	0	-3.506	3.198	-1.310	H
HETATM	6	C	0	-1.341	1.228	-0.113	C
HETATM	7	N	0	-2.650	1.553	-0.284	N
HETATM	8	N	0	-0.611	2.367	-0.241	N
HETATM	9	Cl	0	0.284	-1.097	-1.802	Cl
HETATM	10	Cl	0	-1.083	0.004	2.721	Cl
HETATM	11	C	0	1.115	-2.112	1.551	C
HETATM	12	C	0	2.340	-1.304	1.495	C
HETATM	13	C	0	3.373	-1.434	0.527	C
HETATM	14	C	0	2.523	-0.391	2.553	C
HETATM	15	C	0	4.546	-0.676	0.670	C
HETATM	16	C	0	3.684	0.362	2.677	C
HETATM	17	H	0	1.716	-0.287	3.289	H
HETATM	18	C	0	4.698	0.212	1.732	C
HETATM	19	H	0	5.363	-0.806	-0.044	H
HETATM	20	H	0	3.795	1.066	3.510	H
HETATM	21	H	0	5.627	0.789	1.818	H
HETATM	22	O	0	3.178	-2.360	-0.420	O
HETATM	23	C	0	3.770	-2.336	-1.733	C
HETATM	24	H	0	3.028	-2.925	-2.301	H
HETATM	25	C	0	-3.757	0.661	-0.344	C
HETATM	26	C	0	-4.639	0.544	0.748	C
HETATM	27	C	0	-3.994	-0.037	-1.548	C

HETATM	28	C	0	-5.732	-0.321	0.629	C
HETATM	29	C	0	-5.099	-0.890	-1.622	C
HETATM	30	C	0	-5.972	-1.052	-0.540	C
HETATM	31	H	0	-6.415	-0.428	1.482	H
HETATM	32	H	0	-5.285	-1.436	-2.556	H
HETATM	33	C	0	0.813	2.425	-0.352	C
HETATM	34	C	0	1.578	2.756	0.784	C
HETATM	35	C	0	1.418	2.270	-1.617	C
HETATM	36	C	0	2.962	2.892	0.638	C
HETATM	37	C	0	2.807	2.396	-1.709	C
HETATM	38	C	0	3.594	2.701	-0.594	C
HETATM	39	H	0	3.564	3.151	1.518	H
HETATM	40	H	0	3.285	2.261	-2.689	H
HETATM	41	C	0	-4.413	1.317	2.010	C
HETATM	42	H	0	-4.956	0.863	2.855	H
HETATM	43	H	0	-3.343	1.352	2.279	H
HETATM	44	H	0	-4.775	2.360	1.923	H
HETATM	45	C	0	-3.080	0.143	-2.719	C
HETATM	46	H	0	-2.936	1.212	-2.965	H
HETATM	47	H	0	-2.071	-0.271	-2.521	H
HETATM	48	H	0	-3.477	-0.358	-3.617	H
HETATM	49	C	0	-7.130	-2.000	-0.629	C
HETATM	50	H	0	-6.829	-3.028	-0.350	H
HETATM	51	H	0	-7.952	-1.714	0.049	H
HETATM	52	H	0	-7.536	-2.059	-1.654	H
HETATM	53	C	0	0.929	2.970	2.116	C
HETATM	54	H	0	1.660	3.325	2.861	H
HETATM	55	H	0	0.112	3.714	2.066	H
HETATM	56	H	0	0.467	2.042	2.505	H
HETATM	57	C	0	0.613	2.047	-2.862	C
HETATM	58	H	0	0.432	3.002	-3.394	H
HETATM	59	H	0	1.148	1.383	-3.562	H
HETATM	60	H	0	-0.361	1.575	-2.662	H
HETATM	61	C	0	5.082	2.813	-0.722	C
HETATM	62	H	0	5.550	1.816	-0.833	H
HETATM	63	H	0	5.378	3.398	-1.612	H
HETATM	64	H	0	5.539	3.288	0.163	H
HETATM	65	C	0	5.090	-3.082	-1.747	C
HETATM	66	H	0	5.436	-3.218	-2.787	H
HETATM	67	H	0	5.886	-2.545	-1.202	H
HETATM	68	H	0	4.984	-4.082	-1.294	H
HETATM	69	C	0	3.823	-0.954	-2.357	C
HETATM	70	H	0	4.689	-0.349	-2.036	H
HETATM	71	H	0	3.889	-1.058	-3.455	H
HETATM	72	H	0	2.897	-0.402	-2.128	H
HETATM	73	H	0	-3.334	3.418	0.453	H
HETATM	74	H	0	-1.195	4.392	-0.010	H
HETATM	75	C	0	0.588	-3.144	0.842	C
HETATM	76	C	0	-2.008	-1.477	0.240	C
HETATM	77	H	0	-2.184	-2.133	-0.642	H
HETATM	78	H	0	-2.769	-1.544	1.046	H
HETATM	79	H	0	0.552	-1.980	2.482	H
HETATM	80	F	0	-0.462	-3.792	1.318	F
HETATM	81	F	0	0.963	-3.710	-0.262	F

END

sc3a.pdb

TITLE	sc3a.pdb						
REMARK	1 File created by GaussView 5.0.8						
HETATM	1	Ru	0	0.073	0.277	0.091	Ru

HETATM	2	C	0	1.104	-3.893	0.274	C
HETATM	3	C	0	-0.413	-3.914	0.406	C
HETATM	4	H	0	1.622	-4.331	1.148	H
HETATM	5	H	0	-0.759	-4.312	1.380	H
HETATM	6	C	0	0.303	-1.669	0.151	C
HETATM	7	N	0	-0.773	-2.506	0.281	N
HETATM	8	N	0	1.410	-2.467	0.162	N
HETATM	9	Cl	0	-0.263	0.461	2.435	Cl
HETATM	10	Cl	0	-0.723	0.391	-2.150	Cl
HETATM	11	C	0	1.804	0.881	-0.108	C
HETATM	12	H	0	2.689	0.232	-0.199	H
HETATM	13	C	0	2.092	2.293	-0.167	C
HETATM	14	C	0	1.034	3.228	-0.027	C
HETATM	15	C	0	3.405	2.770	-0.351	C
HETATM	16	C	0	1.297	4.598	-0.068	C
HETATM	17	C	0	3.666	4.135	-0.391	C
HETATM	18	H	0	4.215	2.037	-0.460	H
HETATM	19	C	0	2.610	5.040	-0.248	C
HETATM	20	H	0	0.493	5.329	0.029	H
HETATM	21	H	0	4.689	4.500	-0.532	H
HETATM	22	H	0	2.805	6.118	-0.279	H
HETATM	23	O	0	-0.177	2.640	0.115	O
HETATM	24	C	0	-1.380	3.320	0.584	C
HETATM	25	H	0	-2.047	2.454	0.734	H
HETATM	26	C	0	-2.150	-2.143	0.183	C
HETATM	27	C	0	-2.777	-2.182	-1.081	C
HETATM	28	C	0	-2.901	-1.903	1.353	C
HETATM	29	C	0	-4.139	-1.879	-1.161	C
HETATM	30	C	0	-4.259	-1.588	1.221	C
HETATM	31	C	0	-4.892	-1.559	-0.025	C
HETATM	32	H	0	-4.626	-1.884	-2.145	H
HETATM	33	H	0	-4.842	-1.378	2.128	H
HETATM	34	C	0	2.766	-2.073	-0.000	C
HETATM	35	C	0	3.295	-1.950	-1.297	C
HETATM	36	C	0	3.551	-1.814	1.137	C
HETATM	37	C	0	4.635	-1.574	-1.439	C
HETATM	38	C	0	4.887	-1.438	0.954	C
HETATM	39	C	0	5.443	-1.313	-0.325	C
HETATM	40	H	0	5.055	-1.472	-2.448	H
HETATM	41	H	0	5.505	-1.227	1.836	H
HETATM	42	C	0	-2.044	-2.620	-2.313	C
HETATM	43	H	0	-2.401	-2.077	-3.203	H
HETATM	44	H	0	-0.958	-2.451	-2.248	H
HETATM	45	H	0	-2.213	-3.700	-2.503	H
HETATM	46	C	0	-2.321	-2.094	2.722	C
HETATM	47	H	0	-2.650	-1.301	3.414	H
HETATM	48	H	0	-2.665	-3.057	3.148	H
HETATM	49	H	0	-1.222	-2.087	2.725	H
HETATM	50	C	0	-6.335	-1.176	-0.142	C
HETATM	51	H	0	-6.452	-0.076	-0.133	H
HETATM	52	H	0	-6.786	-1.541	-1.080	H
HETATM	53	H	0	-6.934	-1.562	0.701	H
HETATM	54	C	0	2.412	-2.138	-2.492	C
HETATM	55	H	0	2.984	-2.063	-3.432	H
HETATM	56	H	0	1.899	-3.118	-2.491	H
HETATM	57	H	0	1.613	-1.371	-2.522	H
HETATM	58	C	0	2.942	-1.871	2.503	C
HETATM	59	H	0	2.472	-2.849	2.716	H
HETATM	60	H	0	3.696	-1.688	3.287	H
HETATM	61	H	0	2.142	-1.115	2.617	H
HETATM	62	C	0	6.866	-0.872	-0.500	C
HETATM	63	H	0	7.503	-1.187	0.344	H

HETATM	64	H	0	7.310	-1.266	-1.430	H
HETATM	65	H	0	6.941	0.231	-0.556	H
HETATM	66	C	0	-1.976	4.203	-0.492	C
HETATM	67	H	0	-3.022	4.436	-0.229	H
HETATM	68	H	0	-1.447	5.164	-0.614	H
HETATM	69	H	0	-1.985	3.681	-1.463	H
HETATM	70	C	0	-1.175	3.980	1.930	C
HETATM	71	H	0	-0.542	4.882	1.886	H
HETATM	72	H	0	-2.158	4.288	2.326	H
HETATM	73	H	0	-0.730	3.266	2.643	H
HETATM	74	H	0	-0.908	-4.509	-0.385	H
HETATM	75	H	0	1.469	-4.434	-0.620	H
HETATM	76	C	0	-4.342	1.725	-2.102	C
HETATM	77	H	0	-5.226	2.346	-2.290	H
HETATM	78	H	0	-3.749	1.362	-2.946	H
HETATM	79	C	0	-3.954	1.408	-0.872	C
HETATM	80	H	0	-3.080	0.791	-0.624	H
HETATM	81	F	0	-4.610	1.827	0.222	F

END

sc3d.pdb

TITLE	sc3d.pdb						
HETATM	1	Ru	0	-0.591	0.344	-0.578	Ru
HETATM	2	C	0	-1.081	-3.577	1.322	C
HETATM	3	C	0	-2.465	-2.944	1.467	C
HETATM	4	H	0	-0.637	-3.882	2.286	H
HETATM	5	H	0	-2.733	-2.727	2.520	H
HETATM	6	C	0	-1.046	-1.454	0.348	C
HETATM	7	N	0	-2.322	-1.696	0.717	N
HETATM	8	N	0	-0.289	-2.501	0.713	N
HETATM	9	Cl	0	0.517	0.726	1.583	Cl
HETATM	10	Cl	0	-1.747	-0.380	-2.614	Cl
HETATM	11	C	0	1.039	0.478	-1.507	C
HETATM	12	H	0	0.923	-0.023	-2.495	H
HETATM	13	C	0	2.415	0.861	-1.264	C
HETATM	14	C	0	2.892	1.920	-0.428	C
HETATM	15	C	0	3.369	0.066	-1.939	C
HETATM	16	C	0	4.275	2.041	-0.214	C
HETATM	17	C	0	4.733	0.196	-1.719	C
HETATM	18	H	0	2.997	-0.699	-2.632	H
HETATM	19	C	0	5.178	1.179	-0.834	C
HETATM	20	H	0	4.663	2.838	0.422	H
HETATM	21	H	0	5.443	-0.462	-2.233	H
HETATM	22	H	0	6.250	1.307	-0.644	H
HETATM	23	O	0	1.977	2.788	0.001	O
HETATM	24	C	0	2.200	3.835	0.969	C
HETATM	25	H	0	1.158	4.126	1.185	H
HETATM	26	C	0	-3.374	-0.745	0.539	C
HETATM	27	C	0	-4.307	-0.940	-0.506	C
HETATM	28	C	0	-3.478	0.363	1.403	C
HETATM	29	C	0	-5.281	0.034	-0.720	C
HETATM	30	C	0	-4.469	1.322	1.141	C
HETATM	31	C	0	-5.363	1.184	0.079	C
HETATM	32	H	0	-5.992	-0.102	-1.545	H
HETATM	33	H	0	-4.544	2.194	1.805	H
HETATM	34	C	0	1.125	-2.597	0.554	C
HETATM	35	C	0	1.657	-2.919	-0.707	C
HETATM	36	C	0	1.961	-2.396	1.669	C
HETATM	37	C	0	3.047	-3.014	-0.840	C
HETATM	38	C	0	3.344	-2.478	1.485	C

HETATM	39	C	0	3.904	-2.783	0.240	C
HETATM	40	H	0	3.471	-3.266	-1.822	H
HETATM	41	H	0	4.003	-2.299	2.345	H
HETATM	42	C	0	-4.277	-2.179	-1.347	C
HETATM	43	H	0	-4.747	-2.002	-2.329	H
HETATM	44	H	0	-3.248	-2.525	-1.535	H
HETATM	45	H	0	-4.836	-3.005	-0.863	H
HETATM	46	C	0	-2.626	0.534	2.623	C
HETATM	47	H	0	-1.981	-0.333	2.830	H
HETATM	48	H	0	-1.946	1.398	2.531	H
HETATM	49	H	0	-3.266	0.712	3.507	H
HETATM	50	C	0	-6.395	2.233	-0.207	C
HETATM	51	H	0	-6.149	2.798	-1.126	H
HETATM	52	H	0	-7.394	1.792	-0.374	H
HETATM	53	H	0	-6.479	2.965	0.613	H
HETATM	54	C	0	0.754	-3.173	-1.876	C
HETATM	55	H	0	1.332	-3.452	-2.773	H
HETATM	56	H	0	0.043	-3.997	-1.674	H
HETATM	57	H	0	0.129	-2.297	-2.138	H
HETATM	58	C	0	1.407	-2.144	3.038	C
HETATM	59	H	0	1.383	-3.076	3.637	H
HETATM	60	H	0	2.033	-1.423	3.590	H
HETATM	61	H	0	0.390	-1.721	3.008	H
HETATM	62	C	0	5.392	-2.844	0.075	C
HETATM	63	H	0	5.846	-1.840	0.174	H
HETATM	64	H	0	5.868	-3.480	0.844	H
HETATM	65	H	0	5.683	-3.237	-0.914	H
HETATM	66	C	0	2.899	5.027	0.341	C
HETATM	67	H	0	2.865	5.885	1.037	H
HETATM	68	H	0	3.960	4.836	0.106	H
HETATM	69	H	0	2.394	5.333	-0.591	H
HETATM	70	C	0	2.806	3.358	2.276	C
HETATM	71	H	0	3.901	3.236	2.249	H
HETATM	72	H	0	2.583	4.103	3.060	H
HETATM	73	H	0	2.346	2.402	2.577	H
HETATM	74	H	0	-3.273	-3.564	1.040	H
HETATM	75	H	0	-1.079	-4.464	0.660	H
HETATM	76	C	0	-0.437	2.318	-1.747	C
HETATM	77	H	0	0.458	2.943	-1.687	H
HETATM	78	H	0	-0.821	2.043	-2.736	H
HETATM	79	C	0	-1.322	2.322	-0.657	C
HETATM	80	F	0	-1.123	3.154	0.386	F
HETATM	81	H	0	-2.396	2.104	-0.795	H

END

sc3I.pdb

TITLE	sc3I.pdb						
HETATM	1	Ru	0	0.511	-0.487	-0.388	Ru
HETATM	2	C	0	1.300	3.477	1.074	C
HETATM	3	C	0	2.702	2.874	1.168	C
HETATM	4	H	0	0.926	3.864	2.039	H
HETATM	5	H	0	3.065	2.780	2.210	H
HETATM	6	C	0	1.235	1.266	0.328	C
HETATM	7	N	0	2.528	1.542	0.579	N
HETATM	8	N	0	0.485	2.340	0.636	N
HETATM	9	Cl	0	-0.551	-0.920	1.734	Cl
HETATM	10	Cl	0	1.739	0.067	-2.462	Cl
HETATM	11	C	0	-0.891	-1.195	-1.705	C
HETATM	12	H	0	-0.544	-0.876	-2.700	H
HETATM	13	C	0	-2.345	-1.010	-1.607	C

HETATM	14	C	0	-3.237	-1.622	-0.680	C
HETATM	15	C	0	-2.901	-0.154	-2.583	C
HETATM	16	C	0	-4.613	-1.349	-0.769	C
HETATM	17	C	0	-4.259	0.125	-2.650	C
HETATM	18	H	0	-2.215	0.307	-3.305	H
HETATM	19	C	0	-5.118	-0.480	-1.732	C
HETATM	20	H	0	-5.307	-1.851	-0.092	H
HETATM	21	H	0	-4.648	0.804	-3.418	H
HETATM	22	H	0	-6.197	-0.292	-1.772	H
HETATM	23	O	0	-2.713	-2.496	0.188	O
HETATM	24	C	0	-3.291	-2.815	1.475	C
HETATM	25	H	0	-2.389	-3.130	2.028	H
HETATM	26	C	0	3.611	0.623	0.425	C
HETATM	27	C	0	4.514	0.792	-0.643	C
HETATM	28	C	0	3.772	-0.419	1.357	C
HETATM	29	C	0	5.540	-0.144	-0.798	C
HETATM	30	C	0	4.811	-1.336	1.159	C
HETATM	31	C	0	5.692	-1.223	0.081	C
HETATM	32	H	0	6.233	-0.032	-1.642	H
HETATM	33	H	0	4.934	-2.156	1.878	H
HETATM	34	C	0	-0.940	2.395	0.551	C
HETATM	35	C	0	-1.551	2.596	-0.699	C
HETATM	36	C	0	-1.706	2.271	1.727	C
HETATM	37	C	0	-2.948	2.647	-0.758	C
HETATM	38	C	0	-3.098	2.308	1.618	C
HETATM	39	C	0	-3.736	2.488	0.385	C
HETATM	40	H	0	-3.431	2.804	-1.730	H
HETATM	41	H	0	-3.702	2.181	2.527	H
HETATM	42	C	0	4.400	1.950	-1.587	C
HETATM	43	H	0	4.765	1.678	-2.591	H
HETATM	44	H	0	3.356	2.283	-1.704	H
HETATM	45	H	0	5.006	2.814	-1.246	H
HETATM	46	C	0	2.867	-0.564	2.541	C
HETATM	47	H	0	2.531	0.410	2.939	H
HETATM	48	H	0	1.945	-1.122	2.298	H
HETATM	49	H	0	3.373	-1.108	3.356	H
HETATM	50	C	0	6.769	-2.241	-0.146	C
HETATM	51	H	0	6.464	-2.981	-0.910	H
HETATM	52	H	0	7.703	-1.781	-0.513	H
HETATM	53	H	0	7.003	-2.807	0.772	H
HETATM	54	C	0	-0.731	2.751	-1.944	C
HETATM	55	H	0	-1.358	3.070	-2.794	H
HETATM	56	H	0	0.076	3.498	-1.825	H
HETATM	57	H	0	-0.219	1.813	-2.238	H
HETATM	58	C	0	-1.062	2.124	3.072	C
HETATM	59	H	0	-0.924	3.107	3.567	H
HETATM	60	H	0	-1.687	1.512	3.743	H
HETATM	61	H	0	-0.080	1.628	3.009	H
HETATM	62	C	0	-5.233	2.507	0.305	C
HETATM	63	H	0	-5.665	1.560	0.680	H
HETATM	64	H	0	-5.668	3.314	0.923	H
HETATM	65	H	0	-5.590	2.644	-0.729	H
HETATM	66	C	0	-4.228	-4.003	1.367	C
HETATM	67	H	0	-4.504	-4.355	2.377	H
HETATM	68	H	0	-5.165	-3.765	0.833	H
HETATM	69	H	0	-3.742	-4.842	0.841	H
HETATM	70	C	0	-3.870	-1.621	2.212	C
HETATM	71	H	0	-4.899	-1.361	1.911	H
HETATM	72	H	0	-3.897	-1.854	3.292	H
HETATM	73	H	0	-3.220	-0.739	2.081	H
HETATM	74	H	0	3.459	3.445	0.603	H
HETATM	75	H	0	1.230	4.299	0.336	H

HETATM	76	C	0	-0.116	-2.463	-1.262	C
HETATM	77	H	0	-0.711	-3.109	-0.604	H
HETATM	78	H	0	0.148	-2.958	-2.213	H
HETATM	79	C	0	1.307	-2.245	-0.591	C
HETATM	80	F	0	1.496	-3.055	0.480	F
HETATM	81	H	0	2.161	-2.357	-1.281	H

END

sc3e.pdb

TITLE	sc3e.pdb						
HETATM	1	Ru	0	-0.497	-0.625	0.355	Ru
HETATM	2	Cl	0	-1.604	-0.155	2.505	Cl
HETATM	3	Cl	0	0.549	-0.858	-1.828	Cl
HETATM	4	C	0	-1.190	1.242	-0.222	C
HETATM	5	N	0	-2.473	1.583	-0.442	N
HETATM	6	C	0	-2.619	2.978	-0.875	C
HETATM	7	C	0	-1.202	3.528	-0.733	C
HETATM	8	N	0	-0.421	2.330	-0.411	N
HETATM	9	C	0	-3.598	0.706	-0.349	C
HETATM	10	C	0	-4.459	0.795	0.759	C
HETATM	11	C	0	-5.531	-0.101	0.838	C
HETATM	12	C	0	-5.765	-1.059	-0.154	C
HETATM	13	C	0	-4.917	-1.090	-1.267	C
HETATM	14	C	0	-3.839	-0.208	-1.394	C
HETATM	15	C	0	-4.268	1.832	1.823	C
HETATM	16	C	0	-6.891	-2.039	-0.018	C
HETATM	17	C	0	-2.972	-0.229	-2.614	C
HETATM	18	C	0	1.009	2.347	-0.418	C
HETATM	19	C	0	1.687	2.321	-1.653	C
HETATM	20	C	0	3.083	2.348	-1.641	C
HETATM	21	C	0	3.809	2.414	-0.446	C
HETATM	22	C	0	3.106	2.465	0.760	C
HETATM	23	C	0	1.708	2.431	0.799	C
HETATM	24	C	0	0.950	2.278	-2.957	C
HETATM	25	C	0	5.307	2.423	-0.468	C
HETATM	26	C	0	0.975	2.507	2.104	C
HETATM	27	H	0	-3.355	3.501	-0.239	H
HETATM	28	H	0	-2.998	3.015	-1.915	H
HETATM	29	H	0	-1.103	4.272	0.081	H
HETATM	30	H	0	-0.821	3.996	-1.657	H
HETATM	31	H	0	-6.197	-0.052	1.710	H
HETATM	32	H	0	-5.103	-1.816	-2.070	H
HETATM	33	H	0	-3.217	2.152	1.908	H
HETATM	34	H	0	-4.567	1.447	2.811	H
HETATM	35	H	0	-4.890	2.728	1.626	H
HETATM	36	H	0	-7.754	-1.605	0.516	H
HETATM	37	H	0	-7.243	-2.401	-0.999	H
HETATM	38	H	0	-6.581	-2.931	0.559	H
HETATM	39	H	0	-1.925	-0.510	-2.391	H
HETATM	40	H	0	-2.927	0.763	-3.102	H
HETATM	41	H	0	-3.353	-0.948	-3.358	H
HETATM	42	H	0	3.622	2.302	-2.598	H
HETATM	43	H	0	3.659	2.538	1.704	H
HETATM	44	H	0	1.495	1.665	-3.695	H
HETATM	45	H	0	-0.054	1.836	-2.858	H
HETATM	46	H	0	0.842	3.290	-3.397	H
HETATM	47	H	0	5.710	1.473	-0.867	H
HETATM	48	H	0	5.706	3.225	-1.116	H
HETATM	49	H	0	5.733	2.561	0.541	H
HETATM	50	H	0	1.678	2.603	2.948	H

HETATM	51	H	0	0.342	1.619	2.294	H
HETATM	52	H	0	0.288	3.374	2.139	H
HETATM	53	C	0	0.809	-1.798	1.633	C
HETATM	54	C	0	2.191	-1.304	1.634	C
HETATM	55	C	0	3.205	-1.627	0.688	C
HETATM	56	C	0	4.511	-1.153	0.899	C
HETATM	57	C	0	4.819	-0.364	2.006	C
HETATM	58	C	0	3.833	-0.031	2.934	C
HETATM	59	C	0	2.542	-0.504	2.742	C
HETATM	60	O	0	2.851	-2.450	-0.306	O
HETATM	61	C	0	3.551	-2.578	-1.562	C
HETATM	62	C	0	4.642	-3.628	-1.471	C
HETATM	63	C	0	4.000	-1.260	-2.167	C
HETATM	64	H	0	0.358	-1.713	2.631	H
HETATM	65	H	0	5.309	-1.436	0.210	H
HETATM	66	H	0	5.852	-0.019	2.144	H
HETATM	67	H	0	4.072	0.587	3.807	H
HETATM	68	H	0	1.752	-0.264	3.465	H
HETATM	69	H	0	5.037	-3.847	-2.479	H
HETATM	70	H	0	4.251	-4.570	-1.051	H
HETATM	71	H	0	5.493	-3.306	-0.846	H
HETATM	72	H	0	2.742	-2.970	-2.204	H
HETATM	73	H	0	4.119	-1.395	-3.257	H
HETATM	74	H	0	4.967	-0.896	-1.781	H
HETATM	75	H	0	3.232	-0.484	-2.010	H
HETATM	76	C	0	0.143	-2.748	0.783	C
HETATM	77	C	0	-1.636	-2.063	0.139	C
HETATM	78	H	0	-0.462	-3.489	1.328	H
HETATM	79	H	0	0.632	-3.123	-0.123	H
HETATM	80	F	0	-1.852	-2.760	-0.977	F
HETATM	81	H	0	-2.388	-2.364	0.899	H

END

sc3f.pdb

TITLE	sc3f.pdb						
HETATM	1	Ru	0	-0.486	-0.740	0.419	Ru
HETATM	2	Cl	0	-1.114	0.001	2.687	Cl
HETATM	3	Cl	0	0.317	-1.194	-1.831	Cl
HETATM	4	C	0	-1.187	1.090	-0.183	C
HETATM	5	N	0	-2.463	1.519	-0.331	N
HETATM	6	C	0	-2.560	2.953	-0.612	C
HETATM	7	C	0	-1.104	3.365	-0.773	C
HETATM	8	N	0	-0.377	2.155	-0.382	N
HETATM	9	C	0	-3.648	0.726	-0.312	C
HETATM	10	C	0	-4.507	0.770	0.803	C
HETATM	11	C	0	-5.655	-0.031	0.783	C
HETATM	12	C	0	-5.970	-0.844	-0.311	C
HETATM	13	C	0	-5.119	-0.829	-1.423	C
HETATM	14	C	0	-3.961	-0.047	-1.449	C
HETATM	15	C	0	-4.214	1.646	1.981	C
HETATM	16	C	0	-7.183	-1.724	-0.291	C
HETATM	17	C	0	-3.064	-0.039	-2.647	C
HETATM	18	C	0	1.053	2.159	-0.478	C
HETATM	19	C	0	1.656	2.026	-1.743	C
HETATM	20	C	0	3.050	2.124	-1.825	C
HETATM	21	C	0	3.838	2.389	-0.703	C
HETATM	22	C	0	3.204	2.576	0.530	C
HETATM	23	C	0	1.817	2.465	0.668	C
HETATM	24	C	0	0.857	1.848	-2.998	C
HETATM	25	C	0	5.332	2.441	-0.806	C

HETATM	26	C	0	1.163	2.708	1.992	C
HETATM	27	H	0	-3.063	3.469	0.228	H
HETATM	28	H	0	-3.169	3.125	-1.517	H
HETATM	29	H	0	-0.813	4.214	-0.130	H
HETATM	30	H	0	-0.844	3.638	-1.815	H
HETATM	31	H	0	-6.321	-0.020	1.656	H
HETATM	32	H	0	-5.363	-1.443	-2.300	H
HETATM	33	H	0	-3.130	1.756	2.151	H
HETATM	34	H	0	-4.651	1.230	2.904	H
HETATM	35	H	0	-4.649	2.657	1.852	H
HETATM	36	H	0	-6.928	-2.753	0.027	H
HETATM	37	H	0	-7.951	-1.355	0.410	H
HETATM	38	H	0	-7.645	-1.812	-1.290	H
HETATM	39	H	0	-2.083	-0.512	-2.439	H
HETATM	40	H	0	-2.840	0.991	-2.985	H
HETATM	41	H	0	-3.521	-0.578	-3.492	H
HETATM	42	H	0	3.530	1.996	-2.805	H
HETATM	43	H	0	3.804	2.820	1.415	H
HETATM	44	H	0	1.359	1.152	-3.690	H
HETATM	45	H	0	-0.147	1.436	-2.811	H
HETATM	46	H	0	0.745	2.811	-3.536	H
HETATM	47	H	0	5.777	1.449	-0.591	H
HETATM	48	H	0	5.670	2.730	-1.817	H
HETATM	49	H	0	5.773	3.147	-0.081	H
HETATM	50	H	0	1.908	2.984	2.757	H
HETATM	51	H	0	0.607	1.824	2.358	H
HETATM	52	H	0	0.419	3.526	1.940	H
HETATM	53	C	0	0.992	-2.144	1.708	C
HETATM	54	C	0	2.252	-1.393	1.674	C
HETATM	55	C	0	3.273	-1.563	0.691	C
HETATM	56	C	0	4.494	-0.889	0.855	C
HETATM	57	C	0	4.705	-0.044	1.940	C
HETATM	58	C	0	3.707	0.152	2.896	C
HETATM	59	C	0	2.501	-0.523	2.756	C
HETATM	60	O	0	3.014	-2.439	-0.288	O
HETATM	61	C	0	3.722	-2.518	-1.541	C
HETATM	62	C	0	4.996	-3.331	-1.418	C
HETATM	63	C	0	3.885	-1.176	-2.229	C
HETATM	64	H	0	0.491	-2.085	2.683	H
HETATM	65	H	0	5.303	-1.045	0.138	H
HETATM	66	H	0	5.671	0.468	2.037	H
HETATM	67	H	0	3.870	0.824	3.746	H
HETATM	68	H	0	1.702	-0.391	3.496	H
HETATM	69	H	0	5.390	-3.559	-2.424	H
HETATM	70	H	0	4.803	-4.291	-0.909	H
HETATM	71	H	0	5.794	-2.808	-0.864	H
HETATM	72	H	0	3.000	-3.101	-2.141	H
HETATM	73	H	0	4.709	-0.562	-1.825	H
HETATM	74	H	0	2.946	-0.603	-2.151	H
HETATM	75	H	0	4.096	-1.343	-3.300	H
HETATM	76	C	0	0.422	-2.977	0.777	C
HETATM	77	C	0	-2.063	-1.616	0.339	C
HETATM	78	H	0	-2.929	-1.467	1.020	H
HETATM	79	H	0	-0.439	-3.584	1.079	H
HETATM	80	F	0	-2.349	-2.620	-0.489	F
HETATM	81	H	0	0.871	-3.203	-0.191	H

END

st3a.pdb

TITLE st3a.pdb

HETATM	1	Ru	0	0.085	0.330	0.017	Ru
HETATM	2	C	0	0.845	-3.814	0.780	C
HETATM	3	C	0	-0.661	-3.801	0.581	C
HETATM	4	H	0	1.132	-3.993	1.834	H
HETATM	5	H	0	-1.221	-4.204	1.444	H
HETATM	6	C	0	0.172	-1.622	0.204	C
HETATM	7	N	0	-0.954	-2.383	0.392	N
HETATM	8	N	0	1.235	-2.466	0.370	N
HETATM	9	Cl	0	0.000	0.599	2.377	Cl
HETATM	10	Cl	0	-0.955	0.493	-2.122	Cl
HETATM	11	C	0	1.834	0.772	-0.377	C
HETATM	12	H	0	2.634	0.047	-0.593	H
HETATM	13	C	0	2.245	2.155	-0.425	C
HETATM	14	C	0	1.270	3.167	-0.225	C
HETATM	15	C	0	3.584	2.532	-0.643	C
HETATM	16	C	0	1.636	4.513	-0.235	C
HETATM	17	C	0	3.949	3.874	-0.655	C
HETATM	18	H	0	4.331	1.743	-0.797	H
HETATM	19	C	0	2.974	4.855	-0.450	C
HETATM	20	H	0	0.899	5.302	-0.074	H
HETATM	21	H	0	4.993	4.162	-0.822	H
HETATM	22	H	0	3.254	5.915	-0.454	H
HETATM	23	O	0	0.033	2.659	-0.033	O
HETATM	24	C	0	-1.190	3.428	0.129	C
HETATM	25	H	0	-1.919	2.606	0.204	H
HETATM	26	C	0	-2.294	-2.026	0.037	C
HETATM	27	C	0	-2.711	-2.177	-1.300	C
HETATM	28	C	0	-3.216	-1.681	1.047	C
HETATM	29	C	0	-4.048	-1.915	-1.619	C
HETATM	30	C	0	-4.543	-1.434	0.682	C
HETATM	31	C	0	-4.975	-1.538	-0.644	C
HETATM	32	H	0	-4.372	-2.018	-2.663	H
HETATM	33	H	0	-5.260	-1.151	1.464	H
HETATM	34	C	0	2.616	-2.170	0.203	C
HETATM	35	C	0	3.160	-2.215	-1.095	C
HETATM	36	C	0	3.417	-1.856	1.315	C
HETATM	37	C	0	4.518	-1.934	-1.266	C
HETATM	38	C	0	4.772	-1.575	1.101	C
HETATM	39	C	0	5.338	-1.607	-0.179	C
HETATM	40	H	0	4.945	-1.962	-2.278	H
HETATM	41	H	0	5.400	-1.316	1.963	H
HETATM	42	C	0	-1.785	-2.677	-2.367	C
HETATM	43	H	0	-2.009	-2.203	-3.337	H
HETATM	44	H	0	-0.727	-2.468	-2.145	H
HETATM	45	H	0	-1.894	-3.771	-2.508	H
HETATM	46	C	0	-2.811	-1.648	2.488	C
HETATM	47	H	0	-3.581	-1.157	3.106	H
HETATM	48	H	0	-2.679	-2.672	2.890	H
HETATM	49	H	0	-1.857	-1.118	2.645	H
HETATM	50	C	0	-6.397	-1.235	-1.005	C
HETATM	51	H	0	-6.574	-0.143	-1.041	H
HETATM	52	H	0	-6.670	-1.641	-1.994	H
HETATM	53	H	0	-7.107	-1.640	-0.262	H
HETATM	54	C	0	2.271	-2.481	-2.271	C
HETATM	55	H	0	2.852	-2.581	-3.203	H
HETATM	56	H	0	1.671	-3.402	-2.144	H
HETATM	57	H	0	1.544	-1.657	-2.415	H
HETATM	58	C	0	2.835	-1.799	2.693	C
HETATM	59	H	0	2.662	-2.810	3.111	H
HETATM	60	H	0	3.516	-1.281	3.389	H
HETATM	61	H	0	1.867	-1.267	2.711	H
HETATM	62	C	0	6.783	-1.265	-0.386	C

HETATM	63	H	0	7.401	-1.531	0.489	H
HETATM	64	H	0	7.206	-1.773	-1.270	H
HETATM	65	H	0	6.922	-0.179	-0.550	H
HETATM	66	C	0	-1.516	4.231	-1.110	C
HETATM	67	H	0	-2.545	4.620	-1.024	H
HETATM	68	H	0	-0.848	5.095	-1.265	H
HETATM	69	H	0	-1.469	3.585	-2.003	H
HETATM	70	C	0	-1.215	4.180	1.442	C
HETATM	71	H	0	-0.588	5.088	1.448	H
HETATM	72	H	0	-2.252	4.495	1.652	H
HETATM	73	H	0	-0.890	3.520	2.264	H
HETATM	74	H	0	-0.978	-4.376	-0.314	H
HETATM	75	H	0	1.363	-4.570	0.163	H
HETATM	76	C	0	-4.338	1.796	-0.627	C
HETATM	77	H	0	-5.086	2.171	-1.333	H
HETATM	78	H	0	-3.462	1.262	-1.021	H
HETATM	79	C	0	-4.527	1.994	0.674	C
HETATM	80	F	0	-3.657	1.578	1.603	F
HETATM	81	H	0	-5.383	2.509	1.129	H

END

st3b.pdb

TITLE	st3b.pdb						
HETATM	1	Ru	0	-0.332	0.323	-0.338	Ru
HETATM	2	Cl	0	-0.851	-0.244	-2.620	Cl
HETATM	3	Cl	0	-0.640	1.202	1.873	Cl
HETATM	4	C	0	-0.618	-1.484	0.334	C
HETATM	5	N	0	-1.867	-1.900	0.703	N
HETATM	6	C	0	-1.904	-3.282	1.164	C
HETATM	7	C	0	-0.430	-3.634	1.284	C
HETATM	8	N	0	0.234	-2.515	0.613	N
HETATM	9	C	0	-3.089	-1.214	0.421	C
HETATM	10	C	0	-3.698	-1.377	-0.842	C
HETATM	11	C	0	-4.877	-0.675	-1.108	C
HETATM	12	C	0	-5.480	0.140	-0.145	C
HETATM	13	C	0	-4.915	0.193	1.132	C
HETATM	14	C	0	-3.734	-0.488	1.443	C
HETATM	15	C	0	-3.187	-2.365	-1.847	C
HETATM	16	C	0	-6.694	0.951	-0.479	C
HETATM	17	C	0	-3.247	-0.508	2.861	C
HETATM	18	C	0	1.649	-2.577	0.471	C
HETATM	19	C	0	2.492	-2.038	1.459	C
HETATM	20	C	0	3.877	-2.164	1.292	C
HETATM	21	C	0	4.428	-2.805	0.179	C
HETATM	22	C	0	3.563	-3.334	-0.789	C
HETATM	23	C	0	2.175	-3.225	-0.663	C
HETATM	24	C	0	1.932	-1.280	2.621	C
HETATM	25	C	0	5.914	-2.879	-0.004	C
HETATM	26	C	0	1.258	-3.688	-1.753	C
HETATM	27	H	0	-2.438	-3.915	0.426	H
HETATM	28	H	0	-2.451	-3.357	2.121	H
HETATM	29	H	0	-0.165	-4.591	0.798	H
HETATM	30	H	0	-0.088	-3.696	2.336	H
HETATM	31	H	0	-5.340	-0.776	-2.099	H
HETATM	32	H	0	-5.407	0.782	1.918	H
HETATM	33	H	0	-2.110	-2.568	-1.746	H
HETATM	34	H	0	-3.349	-2.011	-2.877	H
HETATM	35	H	0	-3.729	-3.327	-1.743	H
HETATM	36	H	0	-6.406	1.946	-0.871	H
HETATM	37	H	0	-7.313	0.472	-1.258	H

HETATM	38	H	0	-7.331	1.131	0.404	H
HETATM	39	H	0	-2.200	-0.836	2.948	H
HETATM	40	H	0	-3.313	0.490	3.324	H
HETATM	41	H	0	-3.876	-1.188	3.470	H
HETATM	42	H	0	4.542	-1.741	2.056	H
HETATM	43	H	0	3.980	-3.829	-1.676	H
HETATM	44	H	0	1.686	-0.240	2.332	H
HETATM	45	H	0	2.649	-1.237	3.457	H
HETATM	46	H	0	0.985	-1.706	2.995	H
HETATM	47	H	0	6.291	-2.001	-0.566	H
HETATM	48	H	0	6.451	-2.889	0.960	H
HETATM	49	H	0	6.219	-3.772	-0.576	H
HETATM	50	H	0	1.813	-4.191	-2.561	H
HETATM	51	H	0	0.713	-2.831	-2.197	H
HETATM	52	H	0	0.482	-4.390	-1.393	H
HETATM	53	C	0	1.477	0.177	-0.695	C
HETATM	54	C	0	2.559	1.136	-0.742	C
HETATM	55	C	0	2.465	2.497	-0.330	C
HETATM	56	C	0	3.608	3.309	-0.363	C
HETATM	57	C	0	4.831	2.803	-0.799	C
HETATM	58	C	0	4.942	1.473	-1.216	C
HETATM	59	C	0	3.818	0.662	-1.188	C
HETATM	60	O	0	1.246	2.930	0.029	O
HETATM	61	C	0	1.036	3.946	1.043	C
HETATM	62	C	0	1.030	5.344	0.457	C
HETATM	63	C	0	1.929	3.761	2.251	C
HETATM	64	H	0	1.819	-0.803	-1.071	H
HETATM	65	H	0	3.540	4.359	-0.069	H
HETATM	66	H	0	5.705	3.464	-0.822	H
HETATM	67	H	0	5.903	1.079	-1.565	H
HETATM	68	H	0	3.885	-0.388	-1.503	H
HETATM	69	H	0	0.643	6.055	1.209	H
HETATM	70	H	0	2.028	5.702	0.154	H
HETATM	71	H	0	0.366	5.403	-0.423	H
HETATM	72	H	0	0.011	3.698	1.368	H
HETATM	73	H	0	2.977	4.062	2.083	H
HETATM	74	H	0	1.911	2.707	2.577	H
HETATM	75	H	0	1.540	4.373	3.083	H
HETATM	76	C	0	-1.164	3.022	-2.010	C
HETATM	77	C	0	-1.871	2.873	-0.891	C
HETATM	78	H	0	-1.394	2.449	-2.913	H
HETATM	79	H	0	-0.311	3.705	-2.019	H
HETATM	80	F	0	-2.917	2.040	-0.813	F
HETATM	81	H	0	-1.695	3.388	0.061	H

END

st3c.pdb

TITLE	st3c.pdb						
HETATM	1	Ru	0	-0.517	0.338	-0.628	Ru
HETATM	2	C	0	-0.514	-3.390	1.716	C
HETATM	3	C	0	-1.982	-2.982	1.700	C
HETATM	4	H	0	-0.065	-3.356	2.727	H
HETATM	5	H	0	-2.408	-2.844	2.711	H
HETATM	6	C	0	-0.733	-1.403	0.475	C
HETATM	7	N	0	-1.953	-1.712	0.978	N
HETATM	8	N	0	0.121	-2.379	0.859	N
HETATM	9	Cl	0	-0.505	1.433	1.580	Cl
HETATM	10	Cl	0	-0.984	-0.961	-2.643	Cl
HETATM	11	C	0	1.315	0.215	-0.901	C
HETATM	12	H	0	1.579	-0.782	-1.310	H

HETATM	13	C	0	2.504	1.030	-0.774	C
HETATM	14	C	0	2.587	2.390	-0.332	C
HETATM	15	C	0	3.720	0.367	-1.084	C
HETATM	16	C	0	3.850	2.990	-0.198	C
HETATM	17	C	0	4.960	0.969	-0.941	C
HETATM	18	H	0	3.654	-0.670	-1.436	H
HETATM	19	C	0	5.017	2.290	-0.489	C
HETATM	20	H	0	3.922	4.034	0.113	H
HETATM	21	H	0	5.877	0.421	-1.185	H
HETATM	22	H	0	5.984	2.795	-0.378	H
HETATM	23	O	0	1.439	3.042	-0.130	O
HETATM	24	C	0	1.283	4.160	0.776	C
HETATM	25	H	0	0.198	4.109	0.975	H
HETATM	26	C	0	-3.151	-0.999	0.664	C
HETATM	27	C	0	-3.852	-1.315	-0.521	C
HETATM	28	C	0	-3.660	-0.048	1.571	C
HETATM	29	C	0	-4.965	-0.541	-0.861	C
HETATM	30	C	0	-4.778	0.701	1.188	C
HETATM	31	C	0	-5.417	0.496	-0.038	C
HETATM	32	H	0	-5.495	-0.762	-1.797	H
HETATM	33	H	0	-5.161	1.466	1.877	H
HETATM	34	C	0	1.521	-2.491	0.607	C
HETATM	35	C	0	1.951	-3.301	-0.463	C
HETATM	36	C	0	2.444	-1.873	1.469	C
HETATM	37	C	0	3.324	-3.479	-0.655	C
HETATM	38	C	0	3.810	-2.078	1.241	C
HETATM	39	C	0	4.267	-2.875	0.188	C
HETATM	40	H	0	3.666	-4.104	-1.491	H
HETATM	41	H	0	4.536	-1.591	1.905	H
HETATM	42	C	0	-3.512	-2.520	-1.345	C
HETATM	43	H	0	-3.679	-2.335	-2.418	H
HETATM	44	H	0	-2.465	-2.841	-1.240	H
HETATM	45	H	0	-4.164	-3.370	-1.055	H
HETATM	46	C	0	-3.107	0.115	2.954	C
HETATM	47	H	0	-3.015	1.178	3.229	H
HETATM	48	H	0	-3.788	-0.356	3.690	H
HETATM	49	H	0	-2.108	-0.331	3.071	H
HETATM	50	C	0	-6.552	1.373	-0.470	C
HETATM	51	H	0	-6.186	2.207	-1.098	H
HETATM	52	H	0	-7.293	0.824	-1.076	H
HETATM	53	H	0	-7.077	1.826	0.389	H
HETATM	54	C	0	0.954	-3.903	-1.404	C
HETATM	55	H	0	1.442	-4.571	-2.133	H
HETATM	56	H	0	0.176	-4.488	-0.879	H
HETATM	57	H	0	0.415	-3.115	-1.967	H
HETATM	58	C	0	1.982	-0.973	2.570	C
HETATM	59	H	0	1.149	-1.406	3.154	H
HETATM	60	H	0	2.801	-0.737	3.269	H
HETATM	61	H	0	1.586	-0.021	2.168	H
HETATM	62	C	0	5.734	-3.042	-0.070	C
HETATM	63	H	0	6.343	-2.755	0.804	H
HETATM	64	H	0	5.992	-4.081	-0.340	H
HETATM	65	H	0	6.066	-2.410	-0.917	H
HETATM	66	C	0	1.576	5.478	0.085	C
HETATM	67	H	0	1.223	6.314	0.714	H
HETATM	68	H	0	2.650	5.644	-0.107	H
HETATM	69	H	0	1.045	5.540	-0.881	H
HETATM	70	C	0	1.976	3.958	2.107	C
HETATM	71	H	0	3.067	4.116	2.078	H
HETATM	72	H	0	1.561	4.677	2.836	H
HETATM	73	H	0	1.771	2.943	2.487	H
HETATM	74	H	0	-2.626	-3.707	1.164	H

HETATM	75	H	0	-0.333	-4.403	1.313	H
HETATM	76	C	0	-0.524	2.075	-2.237	C
HETATM	77	H	0	0.476	2.513	-2.268	H
HETATM	78	H	0	-0.908	1.587	-3.139	H
HETATM	79	C	0	-1.350	2.376	-1.190	C
HETATM	80	H	0	-1.130	3.055	-0.361	H
HETATM	81	F	0	-2.665	2.062	-1.261	F

END

st3d.pdb

TITLE	st3d.pdb						
HETATM	1	Ru	0	0.713	-0.557	-0.457	Ru
HETATM	2	C	0	0.735	3.532	1.092	C
HETATM	3	C	0	2.203	3.125	1.223	C
HETATM	4	H	0	0.293	3.887	2.041	H
HETATM	5	H	0	2.568	3.150	2.268	H
HETATM	6	C	0	0.964	1.304	0.403	C
HETATM	7	N	0	2.202	1.754	0.715	N
HETATM	8	N	0	0.084	2.290	0.658	N
HETATM	9	Cl	0	0.161	-1.618	1.682	Cl
HETATM	10	Cl	0	1.718	0.422	-2.474	Cl
HETATM	11	C	0	-0.844	-0.600	-1.542	C
HETATM	12	H	0	-0.555	-0.309	-2.572	H
HETATM	13	C	0	-2.281	-0.787	-1.488	C
HETATM	14	C	0	-3.049	-1.495	-0.509	C
HETATM	15	C	0	-2.986	-0.165	-2.550	C
HETATM	16	C	0	-4.453	-1.425	-0.559	C
HETATM	17	C	0	-4.371	-0.122	-2.602	C
HETATM	18	H	0	-2.395	0.327	-3.332	H
HETATM	19	C	0	-5.099	-0.741	-1.584	C
HETATM	20	H	0	-5.055	-1.940	0.191	H
HETATM	21	H	0	-4.881	0.390	-3.426	H
HETATM	22	H	0	-6.196	-0.718	-1.597	H
HETATM	23	O	0	-2.356	-2.261	0.325	O
HETATM	24	C	0	-2.877	-2.894	1.512	C
HETATM	25	H	0	-1.940	-3.284	1.945	H
HETATM	26	C	0	3.362	0.924	0.624	C
HETATM	27	C	0	4.243	1.049	-0.470	C
HETATM	28	C	0	3.613	-0.009	1.652	C
HETATM	29	C	0	5.259	0.101	-0.611	C
HETATM	30	C	0	4.639	-0.944	1.465	C
HETATM	31	C	0	5.438	-0.931	0.317	C
HETATM	32	H	0	5.920	0.163	-1.485	H
HETATM	33	H	0	4.825	-1.689	2.249	H
HETATM	34	C	0	-1.335	2.190	0.559	C
HETATM	35	C	0	-1.975	2.548	-0.639	C
HETATM	36	C	0	-2.069	1.785	1.690	C
HETATM	37	C	0	-3.373	2.500	-0.686	C
HETATM	38	C	0	-3.463	1.731	1.592	C
HETATM	39	C	0	-4.130	2.091	0.415	C
HETATM	40	H	0	-3.882	2.767	-1.621	H
HETATM	41	H	0	-4.043	1.408	2.467	H
HETATM	42	C	0	4.153	2.199	-1.425	C
HETATM	43	H	0	4.472	1.902	-2.438	H
HETATM	44	H	0	3.130	2.594	-1.515	H
HETATM	45	H	0	4.819	3.024	-1.099	H
HETATM	46	C	0	2.855	0.036	2.944	C
HETATM	47	H	0	2.658	1.074	3.268	H
HETATM	48	H	0	1.876	-0.473	2.871	H
HETATM	49	H	0	3.426	-0.463	3.746	H

HETATM	50	C	0	6.464	-1.996	0.079	C
HETATM	51	H	0	6.077	-2.763	-0.618	H
HETATM	52	H	0	7.383	-1.592	-0.380	H
HETATM	53	H	0	6.745	-2.519	1.009	H
HETATM	54	C	0	-1.172	2.946	-1.839	C
HETATM	55	H	0	-1.815	3.075	-2.726	H
HETATM	56	H	0	-0.639	3.904	-1.685	H
HETATM	57	H	0	-0.390	2.199	-2.084	H
HETATM	58	C	0	-1.370	1.407	2.959	C
HETATM	59	H	0	-0.677	2.197	3.309	H
HETATM	60	H	0	-2.091	1.219	3.772	H
HETATM	61	H	0	-0.763	0.491	2.822	H
HETATM	62	C	0	-5.628	2.061	0.353	C
HETATM	63	H	0	-6.042	1.187	0.886	H
HETATM	64	H	0	-6.074	2.957	0.826	H
HETATM	65	H	0	-5.995	2.029	-0.688	H
HETATM	66	C	0	-3.772	-4.081	1.204	C
HETATM	67	H	0	-3.880	-4.697	2.114	H
HETATM	68	H	0	-4.788	-3.812	0.871	H
HETATM	69	H	0	-3.316	-4.720	0.428	H
HETATM	70	C	0	-3.435	-1.885	2.493	C
HETATM	71	H	0	-4.389	-1.432	2.171	H
HETATM	72	H	0	-3.613	-2.376	3.466	H
HETATM	73	H	0	-2.699	-1.079	2.647	H
HETATM	74	H	0	2.882	3.758	0.623	H
HETATM	75	H	0	0.575	4.327	0.339	H
HETATM	76	C	0	0.474	-2.701	-1.349	C
HETATM	77	H	0	-0.215	-3.140	-0.621	H
HETATM	78	H	0	0.235	-2.783	-2.417	H
HETATM	79	C	0	1.781	-2.409	-0.984	C
HETATM	80	H	0	2.179	-2.607	0.023	H
HETATM	81	F	0	2.751	-2.339	-1.900	F

END

st3I.pdb

TITLE	st3I.pdb						
HETATM	1	Ru	0	0.516	-0.509	-0.352	Ru
HETATM	2	C	0	1.257	3.530	0.928	C
HETATM	3	C	0	2.661	2.944	1.080	C
HETATM	4	H	0	0.856	3.944	1.870	H
HETATM	5	H	0	3.022	2.942	2.126	H
HETATM	6	C	0	1.220	1.280	0.303	C
HETATM	7	N	0	2.499	1.566	0.600	N
HETATM	8	N	0	0.462	2.372	0.508	N
HETATM	9	Cl	0	-0.529	-0.911	1.807	Cl
HETATM	10	Cl	0	1.665	0.010	-2.454	Cl
HETATM	11	C	0	-0.887	-1.332	-1.590	C
HETATM	12	H	0	-0.524	-1.099	-2.602	H
HETATM	13	C	0	-2.341	-1.128	-1.518	C
HETATM	14	C	0	-3.257	-1.683	-0.578	C
HETATM	15	C	0	-2.869	-0.310	-2.540	C
HETATM	16	C	0	-4.627	-1.399	-0.706	C
HETATM	17	C	0	-4.222	-0.016	-2.643	C
HETATM	18	H	0	-2.164	0.109	-3.270	H
HETATM	19	C	0	-5.104	-0.569	-1.715	C
HETATM	20	H	0	-5.339	-1.863	-0.019	H
HETATM	21	H	0	-4.587	0.633	-3.447	H
HETATM	22	H	0	-6.181	-0.370	-1.783	H
HETATM	23	O	0	-2.766	-2.528	0.341	O
HETATM	24	C	0	-3.364	-2.748	1.639	C

HETATM	25	H	0	-2.480	-3.065	2.220	H
HETATM	26	C	0	3.592	0.652	0.483	C
HETATM	27	C	0	4.462	0.744	-0.618	C
HETATM	28	C	0	3.790	-0.312	1.490	C
HETATM	29	C	0	5.486	-0.200	-0.735	C
HETATM	30	C	0	4.827	-1.237	1.333	C
HETATM	31	C	0	5.670	-1.208	0.217	C
HETATM	32	H	0	6.152	-0.152	-1.607	H
HETATM	33	H	0	4.981	-1.997	2.110	H
HETATM	34	C	0	-0.965	2.403	0.428	C
HETATM	35	C	0	-1.583	2.560	-0.826	C
HETATM	36	C	0	-1.724	2.308	1.611	C
HETATM	37	C	0	-2.981	2.592	-0.879	C
HETATM	38	C	0	-3.116	2.325	1.508	C
HETATM	39	C	0	-3.762	2.458	0.272	C
HETATM	40	H	0	-3.471	2.716	-1.853	H
HETATM	41	H	0	-3.716	2.221	2.423	H
HETATM	42	C	0	4.332	1.838	-1.634	C
HETATM	43	H	0	4.634	1.485	-2.634	H
HETATM	44	H	0	3.296	2.202	-1.725	H
HETATM	45	H	0	4.984	2.698	-1.383	H
HETATM	46	C	0	2.919	-0.346	2.708	C
HETATM	47	H	0	2.798	0.657	3.160	H
HETATM	48	H	0	1.894	-0.703	2.490	H
HETATM	49	H	0	3.343	-1.009	3.480	H
HETATM	50	C	0	6.735	-2.246	0.032	C
HETATM	51	H	0	6.387	-3.056	-0.637	H
HETATM	52	H	0	7.646	-1.827	-0.430	H
HETATM	53	H	0	7.022	-2.720	0.986	H
HETATM	54	C	0	-0.770	2.689	-2.077	C
HETATM	55	H	0	-1.402	2.983	-2.932	H
HETATM	56	H	0	0.033	3.443	-1.978	H
HETATM	57	H	0	-0.253	1.747	-2.349	H
HETATM	58	C	0	-1.070	2.210	2.956	C
HETATM	59	H	0	-0.933	3.209	3.416	H
HETATM	60	H	0	-1.689	1.618	3.651	H
HETATM	61	H	0	-0.085	1.715	2.907	H
HETATM	62	C	0	-5.259	2.451	0.198	C
HETATM	63	H	0	-5.674	1.510	0.605	H
HETATM	64	H	0	-5.705	3.272	0.789	H
HETATM	65	H	0	-5.621	2.549	-0.840	H
HETATM	66	C	0	-4.348	-3.902	1.600	C
HETATM	67	H	0	-4.632	-4.186	2.628	H
HETATM	68	H	0	-5.277	-3.659	1.056	H
HETATM	69	H	0	-3.897	-4.787	1.120	H
HETATM	70	C	0	-3.897	-1.488	2.297	C
HETATM	71	H	0	-4.893	-1.178	1.936	H
HETATM	72	H	0	-3.986	-1.667	3.383	H
HETATM	73	H	0	-3.187	-0.657	2.152	H
HETATM	74	H	0	3.418	3.469	0.470	H
HETATM	75	H	0	1.199	4.327	0.164	H
HETATM	76	C	0	-0.118	-2.552	-1.019	C
HETATM	77	H	0	-0.772	-3.133	-0.355	H
HETATM	78	H	0	0.228	-3.120	-1.899	H
HETATM	79	C	0	1.254	-2.290	-0.257	C
HETATM	80	H	0	1.284	-2.762	0.741	H
HETATM	81	F	0	2.338	-2.688	-0.960	F

END

TITLE	st3e.pdb						
HETATM	1	Ru	0	-0.484	-0.655	0.289	Ru
HETATM	2	Cl	0	-1.508	-0.196	2.475	Cl
HETATM	3	Cl	0	0.496	-0.862	-1.938	Cl
HETATM	4	C	0	-1.163	1.235	-0.191	C
HETATM	5	N	0	-2.434	1.592	-0.444	N
HETATM	6	C	0	-2.564	3.013	-0.787	C
HETATM	7	C	0	-1.146	3.543	-0.589	C
HETATM	8	N	0	-0.384	2.328	-0.286	N
HETATM	9	C	0	-3.577	0.732	-0.394	C
HETATM	10	C	0	-4.419	0.760	0.730	C
HETATM	11	C	0	-5.516	-0.110	0.757	C
HETATM	12	C	0	-5.793	-0.979	-0.301	C
HETATM	13	C	0	-4.963	-0.947	-1.429	C
HETATM	14	C	0	-3.859	-0.094	-1.502	C
HETATM	15	C	0	-4.200	1.712	1.866	C
HETATM	16	C	0	-6.940	-1.940	-0.225	C
HETATM	17	C	0	-3.003	-0.051	-2.730	C
HETATM	18	C	0	1.048	2.322	-0.297	C
HETATM	19	C	0	1.723	2.321	-1.532	C
HETATM	20	C	0	3.121	2.332	-1.521	C
HETATM	21	C	0	3.849	2.362	-0.328	C
HETATM	22	C	0	3.148	2.403	0.882	C
HETATM	23	C	0	1.751	2.383	0.923	C
HETATM	24	C	0	0.989	2.331	-2.839	C
HETATM	25	C	0	5.347	2.316	-0.343	C
HETATM	26	C	0	1.020	2.456	2.227	C
HETATM	27	H	0	-3.306	3.497	-0.126	H
HETATM	28	H	0	-2.930	3.122	-1.826	H
HETATM	29	H	0	-1.061	4.262	0.248	H
HETATM	30	H	0	-0.736	4.036	-1.489	H
HETATM	31	H	0	-6.168	-0.109	1.640	H
HETATM	32	H	0	-5.187	-1.599	-2.284	H
HETATM	33	H	0	-4.395	1.223	2.834	H
HETATM	34	H	0	-4.887	2.579	1.795	H
HETATM	35	H	0	-3.166	2.089	1.909	H
HETATM	36	H	0	-6.612	-2.925	0.160	H
HETATM	37	H	0	-7.734	-1.584	0.453	H
HETATM	38	H	0	-7.392	-2.124	-1.215	H
HETATM	39	H	0	-1.957	-0.357	-2.535	H
HETATM	40	H	0	-2.945	0.970	-3.155	H
HETATM	41	H	0	-3.404	-0.711	-3.517	H
HETATM	42	H	0	3.658	2.306	-2.480	H
HETATM	43	H	0	3.703	2.451	1.827	H
HETATM	44	H	0	-0.039	1.943	-2.752	H
HETATM	45	H	0	1.503	1.697	-3.582	H
HETATM	46	H	0	0.938	3.352	-3.266	H
HETATM	47	H	0	5.771	2.841	-1.216	H
HETATM	48	H	0	5.709	1.270	-0.392	H
HETATM	49	H	0	5.783	2.758	0.570	H
HETATM	50	H	0	0.356	3.341	2.275	H
HETATM	51	H	0	1.724	2.521	3.074	H
HETATM	52	H	0	0.362	1.582	2.399	H
HETATM	53	C	0	0.809	-1.898	1.497	C
HETATM	54	C	0	2.186	-1.389	1.529	C
HETATM	55	C	0	3.209	-1.655	0.575	C
HETATM	56	C	0	4.508	-1.180	0.819	C
HETATM	57	C	0	4.802	-0.442	1.963	C
HETATM	58	C	0	3.805	-0.160	2.898	C
HETATM	59	C	0	2.520	-0.634	2.673	C
HETATM	60	O	0	2.872	-2.432	-0.463	O
HETATM	61	C	0	3.580	-2.480	-1.720	C

HETATM	62	C	0	3.987	-1.120	-2.258	C
HETATM	63	C	0	4.703	-3.499	-1.678	C
HETATM	64	H	0	5.314	-1.420	0.122	H
HETATM	65	H	0	5.829	-0.092	2.124	H
HETATM	66	H	0	4.031	0.422	3.799	H
HETATM	67	H	0	1.720	-0.432	3.397	H
HETATM	68	H	0	2.786	-2.865	-2.383	H
HETATM	69	H	0	3.182	-0.385	-2.091	H
HETATM	70	H	0	4.141	-1.203	-3.349	H
HETATM	71	H	0	4.926	-0.730	-1.830	H
HETATM	72	H	0	5.550	-3.180	-1.046	H
HETATM	73	H	0	5.097	-3.664	-2.696	H
HETATM	74	H	0	4.342	-4.469	-1.297	H
HETATM	75	H	0	0.348	-1.868	2.494	H
HETATM	76	C	0	0.161	-2.812	0.595	C
HETATM	77	C	0	-1.598	-2.071	-0.106	C
HETATM	78	F	0	-2.591	-2.556	0.635	F
HETATM	79	H	0	-0.475	-3.558	1.092	H
HETATM	80	H	0	0.683	-3.155	-0.304	H
HETATM	81	H	0	-1.629	-2.556	-1.106	H

END

st3f.pdb

TITLE	st3f.pdb						
HETATM	1	Ru	0	-0.471	-0.723	0.438	Ru
HETATM	2	C	0	-1.150	3.432	-0.456	C
HETATM	3	C	0	-2.602	2.991	-0.328	C
HETATM	4	H	0	-0.897	3.793	-1.472	H
HETATM	5	H	0	-3.216	3.239	-1.212	H
HETATM	6	C	0	-1.209	1.115	-0.060	C
HETATM	7	N	0	-2.492	1.537	-0.175	N
HETATM	8	N	0	-0.407	2.203	-0.172	N
HETATM	9	Cl	0	0.125	-1.187	-1.887	Cl
HETATM	10	Cl	0	-0.857	-0.039	2.763	Cl
HETATM	11	C	0	1.092	-2.160	1.628	C
HETATM	12	C	0	2.367	-1.442	1.527	C
HETATM	13	C	0	3.313	-1.604	0.474	C
HETATM	14	C	0	2.712	-0.619	2.619	C
HETATM	15	C	0	4.559	-0.963	0.574	C
HETATM	16	C	0	3.943	0.019	2.700	C
HETATM	17	H	0	1.967	-0.492	3.414	H
HETATM	18	C	0	4.867	-0.164	1.672	C
HETATM	19	H	0	5.314	-1.112	-0.202	H
HETATM	20	H	0	4.183	0.652	3.562	H
HETATM	21	H	0	5.851	0.320	1.719	H
HETATM	22	O	0	2.960	-2.439	-0.513	O
HETATM	23	C	0	3.583	-2.508	-1.810	C
HETATM	24	H	0	2.819	-3.078	-2.368	H
HETATM	25	C	0	-3.653	0.719	-0.309	C
HETATM	26	C	0	-4.499	0.485	0.792	C
HETATM	27	C	0	-3.959	0.204	-1.585	C
HETATM	28	C	0	-5.627	-0.322	0.601	C
HETATM	29	C	0	-5.098	-0.593	-1.731	C
HETATM	30	C	0	-5.936	-0.877	-0.646	C
HETATM	31	H	0	-6.282	-0.523	1.459	H
HETATM	32	H	0	-5.335	-1.003	-2.722	H
HETATM	33	C	0	1.016	2.198	-0.329	C
HETATM	34	C	0	1.838	2.493	0.780	C
HETATM	35	C	0	1.567	2.056	-1.620	C
HETATM	36	C	0	3.220	2.571	0.582	C

HETATM	37	C	0	2.956	2.122	-1.762	C
HETATM	38	C	0	3.799	2.364	-0.674	C
HETATM	39	H	0	3.862	2.800	1.443	H
HETATM	40	H	0	3.390	1.991	-2.763	H
HETATM	41	C	0	-4.204	1.079	2.132	C
HETATM	42	H	0	-4.883	0.679	2.903	H
HETATM	43	H	0	-3.165	0.874	2.451	H
HETATM	44	H	0	-4.330	2.179	2.128	H
HETATM	45	C	0	-3.053	0.469	-2.746	C
HETATM	46	H	0	-2.830	1.546	-2.865	H
HETATM	47	H	0	-2.075	-0.040	-2.620	H
HETATM	48	H	0	-3.496	0.112	-3.690	H
HETATM	49	C	0	-7.129	-1.770	-0.811	C
HETATM	50	H	0	-6.879	-2.821	-0.573	H
HETATM	51	H	0	-7.954	-1.483	-0.137	H
HETATM	52	H	0	-7.511	-1.761	-1.845	H
HETATM	53	C	0	1.251	2.770	2.128	C
HETATM	54	H	0	2.044	2.911	2.881	H
HETATM	55	H	0	0.635	3.690	2.125	H
HETATM	56	H	0	0.591	1.953	2.475	H
HETATM	57	C	0	0.708	1.932	-2.842	C
HETATM	58	H	0	0.581	2.917	-3.333	H
HETATM	59	H	0	1.168	1.260	-3.585	H
HETATM	60	H	0	-0.290	1.524	-2.624	H
HETATM	61	C	0	5.286	2.379	-0.847	C
HETATM	62	H	0	5.701	1.353	-0.782	H
HETATM	63	H	0	5.587	2.781	-1.831	H
HETATM	64	H	0	5.789	2.973	-0.065	H
HETATM	65	C	0	4.856	-3.334	-1.786	C
HETATM	66	H	0	5.165	-3.568	-2.820	H
HETATM	67	H	0	5.702	-2.819	-1.300	H
HETATM	68	H	0	4.694	-4.291	-1.261	H
HETATM	69	C	0	3.710	-1.158	-2.488	C
HETATM	70	H	0	4.533	-0.537	-2.094	H
HETATM	71	H	0	3.902	-1.312	-3.565	H
HETATM	72	H	0	2.765	-0.600	-2.385	H
HETATM	73	H	0	-3.106	3.426	0.556	H
HETATM	74	H	0	-0.870	4.227	0.257	H
HETATM	75	C	0	0.447	-2.985	0.740	C
HETATM	76	H	0	0.831	-3.221	-0.254	H
HETATM	77	C	0	-2.023	-1.630	0.308	C
HETATM	78	H	0	0.654	-2.096	2.631	H
HETATM	79	H	0	-0.401	-3.575	1.106	H
HETATM	80	F	0	-2.617	-2.296	1.294	F
HETATM	81	H	0	-2.594	-1.816	-0.628	H

END

ac3a.pdb

TITLE	ac3a.pdb						
HETATM	1	Ru	0	0.053	0.289	0.120	Ru
HETATM	2	C	0	1.012	-3.902	0.265	C
HETATM	3	C	0	-0.506	-3.916	0.241	C
HETATM	4	H	0	1.433	-4.280	1.218	H
HETATM	5	H	0	-0.956	-4.450	1.098	H
HETATM	6	C	0	0.234	-1.669	0.140	C
HETATM	7	N	0	-0.846	-2.498	0.293	N
HETATM	8	N	0	1.328	-2.484	0.100	N
HETATM	9	Cl	0	-0.424	0.397	2.440	Cl
HETATM	10	Cl	0	-0.710	0.492	-2.120	Cl
HETATM	11	C	0	1.814	0.823	-0.036	C

HETATM	12	H	0	2.666	0.132	-0.118	H
HETATM	13	C	0	2.179	2.216	-0.095	C
HETATM	14	C	0	1.174	3.206	0.041	C
HETATM	15	C	0	3.515	2.623	-0.282	C
HETATM	16	C	0	1.504	4.560	-0.018	C
HETATM	17	C	0	3.846	3.973	-0.332	C
HETATM	18	H	0	4.287	1.850	-0.387	H
HETATM	19	C	0	2.839	4.932	-0.200	C
HETATM	20	H	0	0.738	5.333	0.068	H
HETATM	21	H	0	4.887	4.282	-0.476	H
HETATM	22	H	0	3.089	5.999	-0.245	H
HETATM	23	O	0	-0.063	2.681	0.201	O
HETATM	24	C	0	-1.213	3.430	0.692	C
HETATM	25	H	0	-1.919	2.603	0.870	H
HETATM	26	C	0	-2.228	-2.150	0.180	C
HETATM	27	C	0	-2.829	-2.132	-1.099	C
HETATM	28	C	0	-3.011	-2.024	1.347	C
HETATM	29	C	0	-4.200	-1.877	-1.186	C
HETATM	30	C	0	-4.380	-1.768	1.207	C
HETATM	31	C	0	-4.988	-1.675	-0.048	C
HETATM	32	H	0	-4.669	-1.840	-2.179	H
HETATM	33	H	0	-4.990	-1.652	2.113	H
HETATM	34	C	0	2.698	-2.126	-0.050	C
HETATM	35	C	0	3.231	-2.017	-1.347	C
HETATM	36	C	0	3.488	-1.900	1.091	C
HETATM	37	C	0	4.584	-1.688	-1.484	C
HETATM	38	C	0	4.836	-1.573	0.910	C
HETATM	39	C	0	5.399	-1.462	-0.368	C
HETATM	40	H	0	5.009	-1.595	-2.492	H
HETATM	41	H	0	5.460	-1.385	1.793	H
HETATM	42	C	0	-2.067	-2.472	-2.344	C
HETATM	43	H	0	-2.377	-1.837	-3.190	H
HETATM	44	H	0	-0.979	-2.343	-2.236	H
HETATM	45	H	0	-2.262	-3.522	-2.641	H
HETATM	46	C	0	-2.438	-2.247	2.713	C
HETATM	47	H	0	-2.769	-1.470	3.422	H
HETATM	48	H	0	-2.783	-3.219	3.119	H
HETATM	49	H	0	-1.339	-2.239	2.716	H
HETATM	50	C	0	-6.442	-1.339	-0.174	C
HETATM	51	H	0	-6.582	-0.248	-0.299	H
HETATM	52	H	0	-6.904	-1.818	-1.055	H
HETATM	53	H	0	-7.016	-1.634	0.720	H
HETATM	54	C	0	2.342	-2.175	-2.541	C
HETATM	55	H	0	2.916	-2.137	-3.481	H
HETATM	56	H	0	1.781	-3.128	-2.528	H
HETATM	57	H	0	1.581	-1.370	-2.578	H
HETATM	58	C	0	2.872	-1.924	2.456	C
HETATM	59	H	0	2.363	-2.880	2.676	H
HETATM	60	H	0	3.629	-1.763	3.241	H
HETATM	61	H	0	2.100	-1.138	2.562	H
HETATM	62	C	0	6.836	-1.070	-0.539	C
HETATM	63	H	0	7.454	-1.374	0.323	H
HETATM	64	H	0	7.279	-1.509	-1.449	H
HETATM	65	H	0	6.945	0.028	-0.634	H
HETATM	66	C	0	-1.794	4.319	-0.387	C
HETATM	67	H	0	-2.831	4.588	-0.123	H
HETATM	68	H	0	-1.236	5.260	-0.535	H
HETATM	69	H	0	-1.829	3.782	-1.350	H
HETATM	70	C	0	-0.935	4.098	2.020	C
HETATM	71	H	0	-0.270	4.974	1.948	H
HETATM	72	H	0	-1.891	4.448	2.448	H
HETATM	73	H	0	-0.494	3.374	2.725	H

HETATM	74	H	0	-0.917	-4.372	-0.682	H
HETATM	75	H	0	1.472	-4.496	-0.547	H
HETATM	76	C	0	-3.928	1.933	-1.295	C
HETATM	77	C	0	-3.805	1.368	-0.099	C
HETATM	78	H	0	-3.080	0.556	0.034	H
HETATM	79	H	0	-4.407	1.685	0.762	H
HETATM	80	H	0	-3.346	1.656	-2.182	H
HETATM	81	F	0	-4.779	2.941	-1.532	F

END

ac3b.pdb

TITLE	ac3b.pdb						
HETATM	1	Ru	0	-0.561	0.333	-0.496	Ru
HETATM	2	C	0	-0.682	-3.449	1.587	C
HETATM	3	C	0	-2.145	-3.031	1.523	C
HETATM	4	H	0	-0.275	-3.430	2.618	H
HETATM	5	H	0	-2.635	-2.995	2.513	H
HETATM	6	C	0	-0.828	-1.401	0.447	C
HETATM	7	N	0	-2.064	-1.696	0.939	N
HETATM	8	N	0	-0.011	-2.431	0.772	N
HETATM	9	Cl	0	-0.703	1.401	1.693	Cl
HETATM	10	Cl	0	-1.013	-0.746	-2.662	Cl
HETATM	11	C	0	1.252	0.119	-0.851	C
HETATM	12	H	0	1.474	-0.827	-1.387	H
HETATM	13	C	0	2.466	0.891	-0.690	C
HETATM	14	C	0	2.572	2.203	-0.126	C
HETATM	15	C	0	3.664	0.249	-1.092	C
HETATM	16	C	0	3.844	2.781	0.035	C
HETATM	17	C	0	4.913	0.827	-0.924	C
HETATM	18	H	0	3.577	-0.749	-1.540	H
HETATM	19	C	0	4.994	2.098	-0.350	C
HETATM	20	H	0	3.939	3.787	0.446	H
HETATM	21	H	0	5.819	0.297	-1.239	H
HETATM	22	H	0	5.969	2.581	-0.215	H
HETATM	23	O	0	1.428	2.814	0.166	O
HETATM	24	C	0	1.293	3.951	1.043	C
HETATM	25	H	0	0.203	3.931	1.218	H
HETATM	26	C	0	-3.240	-0.950	0.602	C
HETATM	27	C	0	-3.882	-1.191	-0.634	C
HETATM	28	C	0	-3.780	-0.035	1.529	C
HETATM	29	C	0	-4.959	-0.375	-0.992	C
HETATM	30	C	0	-4.864	0.755	1.128	C
HETATM	31	C	0	-5.442	0.624	-0.138	C
HETATM	32	H	0	-5.447	-0.541	-1.962	H
HETATM	33	H	0	-5.273	1.487	1.837	H
HETATM	34	C	0	1.394	-2.557	0.554	C
HETATM	35	C	0	1.834	-3.344	-0.529	C
HETATM	36	C	0	2.303	-1.963	1.448	C
HETATM	37	C	0	3.208	-3.541	-0.692	C
HETATM	38	C	0	3.670	-2.184	1.242	C
HETATM	39	C	0	4.140	-2.970	0.187	C
HETATM	40	H	0	3.561	-4.149	-1.535	H
HETATM	41	H	0	4.390	-1.715	1.927	H
HETATM	42	C	0	-3.526	-2.366	-1.493	C
HETATM	43	H	0	-3.675	-2.144	-2.562	H
HETATM	44	H	0	-2.480	-2.688	-1.380	H
HETATM	45	H	0	-4.182	-3.224	-1.243	H
HETATM	46	C	0	-3.298	0.038	2.945	C
HETATM	47	H	0	-3.223	1.080	3.296	H
HETATM	48	H	0	-4.015	-0.481	3.613	H

HETATM	49	H	0	-2.306	-0.418	3.078	H
HETATM	50	C	0	-6.560	1.525	-0.569	C
HETATM	51	H	0	-6.173	2.411	-1.109	H
HETATM	52	H	0	-7.258	1.019	-1.258	H
HETATM	53	H	0	-7.139	1.905	0.289	H
HETATM	54	C	0	0.848	-3.884	-1.517	C
HETATM	55	H	0	1.336	-4.531	-2.264	H
HETATM	56	H	0	0.043	-4.472	-1.037	H
HETATM	57	H	0	0.340	-3.058	-2.056	H
HETATM	58	C	0	1.826	-1.072	2.550	C
HETATM	59	H	0	0.966	-1.496	3.099	H
HETATM	60	H	0	2.629	-0.864	3.277	H
HETATM	61	H	0	1.462	-0.104	2.153	H
HETATM	62	C	0	5.609	-3.155	-0.042	C
HETATM	63	H	0	6.204	-2.877	0.844	H
HETATM	64	H	0	5.859	-4.196	-0.309	H
HETATM	65	H	0	5.965	-2.525	-0.880	H
HETATM	66	C	0	1.637	5.255	0.348	C
HETATM	67	H	0	1.275	6.102	0.958	H
HETATM	68	H	0	2.720	5.404	0.194	H
HETATM	69	H	0	1.144	5.315	-0.636	H
HETATM	70	C	0	1.951	3.739	2.391	C
HETATM	71	H	0	3.050	3.831	2.376	H
HETATM	72	H	0	1.569	4.493	3.101	H
HETATM	73	H	0	1.684	2.744	2.786	H
HETATM	74	H	0	-2.753	-3.696	0.876	H
HETATM	75	H	0	-0.493	-4.459	1.182	H
HETATM	76	C	0	-0.570	2.374	-2.283	C
HETATM	77	C	0	-1.453	2.452	-1.262	C
HETATM	78	H	0	-2.407	1.914	-1.360	H
HETATM	79	H	0	-1.354	3.192	-0.461	H
HETATM	80	H	0	-0.664	1.699	-3.141	H
HETATM	81	F	0	0.489	3.171	-2.374	F

END

ac3c.pdb

TITLE	ac3c.pdb						
HETATM	1	Ru	0	-0.552	0.366	-0.494	Ru
HETATM	2	C	0	-0.787	-3.401	1.616	C
HETATM	3	C	0	-2.238	-2.942	1.553	C
HETATM	4	H	0	-0.378	-3.394	2.645	H
HETATM	5	H	0	-2.713	-2.861	2.548	H
HETATM	6	C	0	-0.880	-1.359	0.453	C
HETATM	7	N	0	-2.131	-1.628	0.926	N
HETATM	8	N	0	-0.088	-2.404	0.799	N
HETATM	9	Cl	0	-0.687	1.432	1.699	Cl
HETATM	10	Cl	0	-1.068	-0.688	-2.655	Cl
HETATM	11	C	0	1.251	0.078	-0.863	C
HETATM	12	H	0	1.429	-0.879	-1.395	H
HETATM	13	C	0	2.495	0.804	-0.723	C
HETATM	14	C	0	2.663	2.099	-0.134	C
HETATM	15	C	0	3.656	0.136	-1.187	C
HETATM	16	C	0	3.957	2.634	-0.011	C
HETATM	17	C	0	4.927	0.676	-1.064	C
HETATM	18	H	0	3.523	-0.851	-1.649	H
HETATM	19	C	0	5.069	1.931	-0.466	C
HETATM	20	H	0	4.100	3.625	0.423	H
HETATM	21	H	0	5.803	0.130	-1.432	H
HETATM	22	H	0	6.063	2.382	-0.362	H
HETATM	23	O	0	1.549	2.728	0.225	O

HETATM	24	C	0	1.478	3.871	1.100	C
HETATM	25	H	0	0.393	3.892	1.303	H
HETATM	26	C	0	-3.291	-0.869	0.578	C
HETATM	27	C	0	-3.940	-1.122	-0.651	C
HETATM	28	C	0	-3.820	0.065	1.492	C
HETATM	29	C	0	-5.016	-0.307	-1.017	C
HETATM	30	C	0	-4.899	0.859	1.081	C
HETATM	31	C	0	-5.486	0.711	-0.179	C
HETATM	32	H	0	-5.509	-0.486	-1.982	H
HETATM	33	H	0	-5.299	1.605	1.780	H
HETATM	34	C	0	1.312	-2.562	0.584	C
HETATM	35	C	0	1.737	-3.371	-0.488	C
HETATM	36	C	0	2.236	-1.976	1.467	C
HETATM	37	C	0	3.106	-3.595	-0.654	C
HETATM	38	C	0	3.599	-2.220	1.260	C
HETATM	39	C	0	4.050	-3.026	0.212	C
HETATM	40	H	0	3.444	-4.221	-1.491	H
HETATM	41	H	0	4.329	-1.755	1.936	H
HETATM	42	C	0	-3.594	-2.311	-1.496	C
HETATM	43	H	0	-3.746	-2.103	-2.567	H
HETATM	44	H	0	-2.549	-2.637	-1.381	H
HETATM	45	H	0	-4.253	-3.163	-1.231	H
HETATM	46	C	0	-3.345	0.150	2.910	C
HETATM	47	H	0	-3.260	1.196	3.247	H
HETATM	48	H	0	-4.074	-0.351	3.579	H
HETATM	49	H	0	-2.359	-0.314	3.058	H
HETATM	50	C	0	-6.600	1.610	-0.619	C
HETATM	51	H	0	-6.217	2.458	-1.219	H
HETATM	52	H	0	-7.331	1.082	-1.256	H
HETATM	53	H	0	-7.143	2.046	0.236	H
HETATM	54	C	0	0.738	-3.906	-1.467	C
HETATM	55	H	0	1.215	-4.564	-2.212	H
HETATM	56	H	0	-0.071	-4.481	-0.979	H
HETATM	57	H	0	0.238	-3.079	-2.011	H
HETATM	58	C	0	1.779	-1.065	2.561	C
HETATM	59	H	0	0.917	-1.471	3.121	H
HETATM	60	H	0	2.589	-0.859	3.280	H
HETATM	61	H	0	1.426	-0.097	2.153	H
HETATM	62	C	0	5.515	-3.241	-0.019	C
HETATM	63	H	0	6.120	-2.940	0.852	H
HETATM	64	H	0	5.749	-4.296	-0.249	H
HETATM	65	H	0	5.874	-2.648	-0.883	H
HETATM	66	C	0	1.851	5.162	0.394	C
HETATM	67	H	0	1.523	6.021	1.005	H
HETATM	68	H	0	2.934	5.280	0.220	H
HETATM	69	H	0	1.342	5.231	-0.582	H
HETATM	70	C	0	2.164	3.633	2.431	C
HETATM	71	H	0	3.265	3.647	2.378	H
HETATM	72	H	0	1.859	4.420	3.142	H
HETATM	73	H	0	1.844	2.663	2.848	H
HETATM	74	H	0	-2.873	-3.608	0.935	H
HETATM	75	H	0	-0.629	-4.416	1.210	H
HETATM	76	C	0	-0.438	2.388	-2.250	C
HETATM	77	C	0	-1.313	2.534	-1.229	C
HETATM	78	H	0	-2.308	2.078	-1.324	H
HETATM	79	H	0	-1.156	3.266	-0.429	H
HETATM	80	H	0	-0.584	1.725	-3.110	H
HETATM	81	F	0	0.677	3.106	-2.342	F

END

TITLE	ac3d.pdb						
HETATM	1	Ru	0	0.627	-0.692	-0.392	Ru
HETATM	2	C	0	1.046	3.335	1.187	C
HETATM	3	C	0	2.445	2.795	1.452	C
HETATM	4	H	0	0.564	3.767	2.081	H
HETATM	5	H	0	2.666	2.681	2.532	H
HETATM	6	C	0	1.155	1.116	0.457	C
HETATM	7	N	0	2.405	1.477	0.814	N
HETATM	8	N	0	0.322	2.139	0.735	N
HETATM	9	Cl	0	0.270	-1.522	1.867	Cl
HETATM	10	Cl	0	1.809	0.006	-2.440	Cl
HETATM	11	C	0	-0.882	-0.723	-1.569	C
HETATM	12	H	0	-0.572	-0.501	-2.609	H
HETATM	13	C	0	-2.333	-0.735	-1.487	C
HETATM	14	C	0	-3.133	-1.074	-0.354	C
HETATM	15	C	0	-2.998	-0.327	-2.668	C
HETATM	16	C	0	-4.533	-0.993	-0.457	C
HETATM	17	C	0	-4.380	-0.242	-2.756	C
HETATM	18	H	0	-2.381	-0.065	-3.537	H
HETATM	19	C	0	-5.145	-0.583	-1.637	C
HETATM	20	H	0	-5.153	-1.233	0.409	H
HETATM	21	H	0	-4.859	0.080	-3.686	H
HETATM	22	H	0	-6.240	-0.522	-1.677	H
HETATM	23	O	0	-2.478	-1.430	0.743	O
HETATM	24	C	0	-3.021	-2.239	1.807	C
HETATM	25	H	0	-2.086	-2.554	2.301	H
HETATM	26	C	0	3.589	0.725	0.538	C
HETATM	27	C	0	4.344	1.061	-0.606	C
HETATM	28	C	0	4.008	-0.301	1.405	C
HETATM	29	C	0	5.464	0.289	-0.918	C
HETATM	30	C	0	5.128	-1.062	1.042	C
HETATM	31	C	0	5.853	-0.796	-0.121	C
HETATM	32	H	0	6.039	0.531	-1.821	H
HETATM	33	H	0	5.448	-1.877	1.706	H
HETATM	34	C	0	-1.090	2.170	0.520	C
HETATM	35	C	0	-1.599	2.510	-0.746	C
HETATM	36	C	0	-1.946	1.932	1.612	C
HETATM	37	C	0	-2.988	2.592	-0.904	C
HETATM	38	C	0	-3.326	2.027	1.410	C
HETATM	39	C	0	-3.864	2.355	0.160	C
HETATM	40	H	0	-3.395	2.845	-1.892	H
HETATM	41	H	0	-4.001	1.837	2.256	H
HETATM	42	C	0	3.996	2.247	-1.454	C
HETATM	43	H	0	4.309	2.091	-2.499	H
HETATM	44	H	0	2.913	2.448	-1.471	H
HETATM	45	H	0	4.513	3.160	-1.094	H
HETATM	46	C	0	3.358	-0.552	2.732	C
HETATM	47	H	0	2.435	0.028	2.882	H
HETATM	48	H	0	3.081	-1.612	2.856	H
HETATM	49	H	0	4.061	-0.304	3.551	H
HETATM	50	C	0	7.017	-1.654	-0.516	C
HETATM	51	H	0	6.714	-2.422	-1.253	H
HETATM	52	H	0	7.822	-1.066	-0.991	H
HETATM	53	H	0	7.447	-2.190	0.346	H
HETATM	54	C	0	-0.681	2.772	-1.901	C
HETATM	55	H	0	-1.251	2.974	-2.823	H
HETATM	56	H	0	-0.030	3.649	-1.722	H
HETATM	57	H	0	0.001	1.923	-2.105	H
HETATM	58	C	0	-1.389	1.560	2.951	C
HETATM	59	H	0	-0.598	2.255	3.289	H
HETATM	60	H	0	-2.174	1.554	3.725	H
HETATM	61	H	0	-0.924	0.555	2.917	H

HETATM	62	C	0	-5.346	2.479	-0.021	C
HETATM	63	H	0	-5.890	1.672	0.503	H
HETATM	64	H	0	-5.728	3.434	0.388	H
HETATM	65	H	0	-5.635	2.442	-1.085	H
HETATM	66	C	0	-3.729	-3.485	1.310	C
HETATM	67	H	0	-3.858	-4.182	2.156	H
HETATM	68	H	0	-4.730	-3.298	0.887	H
HETATM	69	H	0	-3.121	-3.998	0.547	H
HETATM	70	C	0	-3.811	-1.415	2.806	C
HETATM	71	H	0	-4.789	-1.071	2.426	H
HETATM	72	H	0	-4.005	-2.021	3.709	H
HETATM	73	H	0	-3.231	-0.531	3.117	H
HETATM	74	H	0	3.244	3.415	1.010	H
HETATM	75	H	0	1.025	4.108	0.393	H
HETATM	76	C	0	-0.005	-2.643	-1.424	C
HETATM	77	C	0	1.317	-2.614	-0.895	C
HETATM	78	H	0	2.150	-2.512	-1.603	H
HETATM	79	H	0	1.492	-3.191	0.023	H
HETATM	80	F	0	-0.937	-3.382	-0.793	F
HETATM	81	H	0	-0.148	-2.667	-2.513	H

END

ac3I.pdb

TITLE	ac3I.pdb						
HETATM	1	Ru	0	-0.477	-0.672	0.063	Ru
HETATM	2	C	0	-1.340	3.474	-0.290	C
HETATM	3	C	0	-2.735	2.937	-0.592	C
HETATM	4	H	0	-0.945	4.134	-1.081	H
HETATM	5	H	0	-3.035	3.085	-1.648	H
HETATM	6	C	0	-1.314	1.144	-0.171	C
HETATM	7	N	0	-2.603	1.501	-0.318	N
HETATM	8	N	0	-0.542	2.248	-0.205	N
HETATM	9	Cl	0	0.258	-0.581	-2.226	Cl
HETATM	10	Cl	0	-1.847	-0.682	2.135	Cl
HETATM	11	C	0	0.854	-1.550	1.338	C
HETATM	12	H	0	0.380	-1.586	2.331	H
HETATM	13	C	0	2.285	-1.253	1.494	C
HETATM	14	C	0	3.236	-1.168	0.437	C
HETATM	15	C	0	2.735	-1.004	2.807	C
HETATM	16	C	0	4.582	-0.899	0.737	C
HETATM	17	C	0	4.067	-0.731	3.095	C
HETATM	18	H	0	2.000	-1.049	3.621	H
HETATM	19	C	0	4.993	-0.688	2.050	C
HETATM	20	H	0	5.309	-0.816	-0.075	H
HETATM	21	H	0	4.384	-0.555	4.129	H
HETATM	22	H	0	6.049	-0.471	2.253	H
HETATM	23	O	0	2.739	-1.271	-0.790	O
HETATM	24	C	0	3.439	-1.754	-1.948	C
HETATM	25	H	0	2.593	-2.104	-2.566	H
HETATM	26	C	0	-3.746	0.647	-0.252	C
HETATM	27	C	0	-4.580	0.723	0.881	C
HETATM	28	C	0	-4.052	-0.215	-1.319	C
HETATM	29	C	0	-5.698	-0.110	0.945	C
HETATM	30	C	0	-5.180	-1.039	-1.210	C
HETATM	31	C	0	-6.006	-1.008	-0.084	C
HETATM	32	H	0	-6.338	-0.070	1.836	H
HETATM	33	H	0	-5.421	-1.716	-2.041	H
HETATM	34	C	0	0.886	2.259	-0.118	C
HETATM	35	C	0	1.511	2.095	1.134	C
HETATM	36	C	0	1.642	2.504	-1.283	C

HETATM	37	C	0	2.909	2.137	1.190	C
HETATM	38	C	0	3.034	2.545	-1.177	C
HETATM	39	C	0	3.684	2.359	0.049	C
HETATM	40	H	0	3.403	1.989	2.159	H
HETATM	41	H	0	3.628	2.726	-2.083	H
HETATM	42	C	0	-4.292	1.672	2.005	C
HETATM	43	H	0	-4.646	1.263	2.965	H
HETATM	44	H	0	-3.211	1.864	2.116	H
HETATM	45	H	0	-4.804	2.646	1.865	H
HETATM	46	C	0	-3.212	-0.274	-2.557	C
HETATM	47	H	0	-2.701	0.679	-2.774	H
HETATM	48	H	0	-2.405	-1.024	-2.476	H
HETATM	49	H	0	-3.824	-0.546	-3.434	H
HETATM	50	C	0	-7.183	-1.928	0.033	C
HETATM	51	H	0	-6.932	-2.826	0.629	H
HETATM	52	H	0	-8.037	-1.445	0.540	H
HETATM	53	H	0	-7.529	-2.285	-0.952	H
HETATM	54	C	0	0.712	1.939	2.393	C
HETATM	55	H	0	1.371	1.946	3.277	H
HETATM	56	H	0	-0.022	2.758	2.517	H
HETATM	57	H	0	0.120	1.004	2.424	H
HETATM	58	C	0	0.983	2.754	-2.606	C
HETATM	59	H	0	0.845	3.838	-2.790	H
HETATM	60	H	0	1.600	2.366	-3.434	H
HETATM	61	H	0	-0.001	2.265	-2.681	H
HETATM	62	C	0	5.179	2.425	0.130	C
HETATM	63	H	0	5.658	1.662	-0.512	H
HETATM	64	H	0	5.562	3.404	-0.216	H
HETATM	65	H	0	5.543	2.268	1.160	H
HETATM	66	C	0	4.333	-2.946	-1.664	C
HETATM	67	H	0	4.583	-3.442	-2.618	H
HETATM	68	H	0	5.287	-2.687	-1.173	H
HETATM	69	H	0	3.809	-3.684	-1.034	H
HETATM	70	C	0	4.107	-0.615	-2.693	C
HETATM	71	H	0	4.942	-0.163	-2.128	H
HETATM	72	H	0	4.509	-0.977	-3.656	H
HETATM	73	H	0	3.365	0.173	-2.906	H
HETATM	74	H	0	-3.519	3.379	0.045	H
HETATM	75	H	0	-1.287	4.028	0.668	H
HETATM	76	C	0	0.283	-2.786	0.527	C
HETATM	77	C	0	-1.090	-2.546	-0.151	C
HETATM	78	H	0	-1.947	-2.859	0.465	H
HETATM	79	H	0	-1.104	-2.921	-1.187	H
HETATM	80	F	0	1.184	-3.370	-0.324	F
HETATM	81	H	0	0.080	-3.507	1.342	H

END

ac3e.pdb

TITLE	ac3e.pdb						
HETATM	1	Ru	0	-0.558	-0.621	0.344	Ru
HETATM	2	Cl	0	-1.606	-0.165	2.529	Cl
HETATM	3	Cl	0	0.423	-0.926	-1.850	Cl
HETATM	4	C	0	-1.243	1.216	-0.243	C
HETATM	5	N	0	-2.526	1.542	-0.498	N
HETATM	6	C	0	-2.679	2.938	-0.921	C
HETATM	7	C	0	-1.268	3.498	-0.770	C
HETATM	8	N	0	-0.482	2.312	-0.419	N
HETATM	9	C	0	-3.651	0.664	-0.408	C
HETATM	10	C	0	-4.495	0.728	0.714	C
HETATM	11	C	0	-5.565	-0.172	0.789	C

HETATM	12	C	0	-5.815	-1.106	-0.221	C
HETATM	13	C	0	-4.986	-1.109	-1.350	C
HETATM	14	C	0	-3.907	-0.227	-1.470	C
HETATM	15	C	0	-4.298	1.750	1.791	C
HETATM	16	C	0	-6.941	-2.088	-0.094	C
HETATM	17	C	0	-3.051	-0.227	-2.697	C
HETATM	18	C	0	0.948	2.354	-0.392	C
HETATM	19	C	0	1.658	2.336	-1.608	C
HETATM	20	C	0	3.052	2.425	-1.562	C
HETATM	21	C	0	3.743	2.548	-0.352	C
HETATM	22	C	0	3.007	2.594	0.836	C
HETATM	23	C	0	1.612	2.495	0.842	C
HETATM	24	C	0	0.958	2.246	-2.930	C
HETATM	25	C	0	5.240	2.604	-0.330	C
HETATM	26	C	0	0.846	2.568	2.127	C
HETATM	27	H	0	-3.421	3.450	-0.283	H
HETATM	28	H	0	-3.056	2.981	-1.961	H
HETATM	29	H	0	-1.183	4.258	0.031	H
HETATM	30	H	0	-0.877	3.953	-1.698	H
HETATM	31	H	0	-6.218	-0.142	1.671	H
HETATM	32	H	0	-5.190	-1.811	-2.169	H
HETATM	33	H	0	-3.250	2.078	1.869	H
HETATM	34	H	0	-4.581	1.347	2.778	H
HETATM	35	H	0	-4.932	2.642	1.614	H
HETATM	36	H	0	-6.624	-2.993	0.458	H
HETATM	37	H	0	-7.796	-1.666	0.461	H
HETATM	38	H	0	-7.305	-2.427	-1.078	H
HETATM	39	H	0	-2.023	-0.589	-2.498	H
HETATM	40	H	0	-2.936	0.789	-3.120	H
HETATM	41	H	0	-3.483	-0.867	-3.484	H
HETATM	42	H	0	3.616	2.390	-2.504	H
HETATM	43	H	0	3.532	2.714	1.792	H
HETATM	44	H	0	1.540	1.636	-3.641	H
HETATM	45	H	0	0.833	3.246	-3.392	H
HETATM	46	H	0	-0.036	1.775	-2.848	H
HETATM	47	H	0	5.678	1.593	-0.445	H
HETATM	48	H	0	5.645	3.218	-1.155	H
HETATM	49	H	0	5.625	3.012	0.620	H
HETATM	50	H	0	1.527	2.688	2.987	H
HETATM	51	H	0	0.230	1.667	2.311	H
HETATM	52	H	0	0.139	3.420	2.138	H
HETATM	53	C	0	0.788	-1.834	1.576	C
HETATM	54	C	0	2.160	-1.307	1.581	C
HETATM	55	C	0	3.188	-1.567	0.630	C
HETATM	56	C	0	4.463	-1.014	0.837	C
HETATM	57	C	0	4.733	-0.221	1.949	C
HETATM	58	C	0	3.733	0.050	2.883	C
HETATM	59	C	0	2.468	-0.488	2.689	C
HETATM	60	O	0	2.878	-2.401	-0.362	O
HETATM	61	C	0	3.544	-2.469	-1.637	C
HETATM	62	C	0	4.696	-3.455	-1.593	C
HETATM	63	C	0	3.902	-1.116	-2.226	C
HETATM	64	H	0	0.311	-1.693	2.556	H
HETATM	65	H	0	5.270	-1.244	0.137	H
HETATM	66	H	0	5.744	0.184	2.085	H
HETATM	67	H	0	3.938	0.676	3.759	H
HETATM	68	H	0	1.666	-0.283	3.410	H
HETATM	69	H	0	5.078	-3.633	-2.614	H
HETATM	70	H	0	4.370	-4.425	-1.182	H
HETATM	71	H	0	5.542	-3.093	-0.982	H
HETATM	72	H	0	2.739	-2.897	-2.261	H
HETATM	73	H	0	4.863	-0.712	-1.865	H

HETATM	74	H	0	3.101	-0.387	-2.019	H
HETATM	75	H	0	3.985	-1.216	-3.323	H
HETATM	76	C	0	0.056	-2.830	0.858	C
HETATM	77	C	0	-1.759	-2.006	0.102	C
HETATM	78	F	0	0.527	-3.548	-0.158	F
HETATM	79	H	0	-0.631	-3.434	1.470	H
HETATM	80	H	0	-1.782	-2.604	-0.833	H
HETATM	81	H	0	-2.546	-2.238	0.849	H

END

ac3f.pdb

TITLE	ac3f.pdb						
HETATM	1	Ru	0	-0.539	-0.605	0.434	Ru
HETATM	2	Cl	0	-1.201	0.013	2.715	Cl
HETATM	3	Cl	0	0.284	-1.243	-1.742	Cl
HETATM	4	C	0	-1.348	1.102	-0.192	C
HETATM	5	N	0	-2.647	1.426	-0.407	N
HETATM	6	C	0	-2.834	2.849	-0.697	C
HETATM	7	C	0	-1.406	3.352	-0.858	C
HETATM	8	N	0	-0.608	2.223	-0.382	N
HETATM	9	C	0	-3.772	0.551	-0.359	C
HETATM	10	C	0	-4.628	0.565	0.759	C
HETATM	11	C	0	-5.733	-0.294	0.756	C
HETATM	12	C	0	-6.006	-1.142	-0.322	C
HETATM	13	C	0	-5.157	-1.106	-1.435	C
HETATM	14	C	0	-4.043	-0.263	-1.480	C
HETATM	15	C	0	-4.374	1.473	1.921	C
HETATM	16	C	0	-7.172	-2.083	-0.283	C
HETATM	17	C	0	-3.159	-0.211	-2.686	C
HETATM	18	C	0	0.819	2.273	-0.486	C
HETATM	19	C	0	1.427	2.095	-1.745	C
HETATM	20	C	0	2.817	2.225	-1.834	C
HETATM	21	C	0	3.600	2.553	-0.723	C
HETATM	22	C	0	2.963	2.766	0.504	C
HETATM	23	C	0	1.579	2.629	0.647	C
HETATM	24	C	0	0.633	1.828	-2.987	C
HETATM	25	C	0	5.090	2.648	-0.838	C
HETATM	26	C	0	0.920	2.878	1.969	C
HETATM	27	H	0	-3.367	3.339	0.140	H
HETATM	28	H	0	-3.451	2.978	-1.604	H
HETATM	29	H	0	-1.189	4.258	-0.263	H
HETATM	30	H	0	-1.147	3.579	-1.912	H
HETATM	31	H	0	-6.397	-0.302	1.631	H
HETATM	32	H	0	-5.372	-1.747	-2.301	H
HETATM	33	H	0	-3.295	1.623	2.096	H
HETATM	34	H	0	-4.803	1.060	2.849	H
HETATM	35	H	0	-4.841	2.467	1.771	H
HETATM	36	H	0	-6.867	-3.086	0.074	H
HETATM	37	H	0	-7.964	-1.731	0.399	H
HETATM	38	H	0	-7.619	-2.228	-1.281	H
HETATM	39	H	0	-2.130	-0.560	-2.466	H
HETATM	40	H	0	-3.058	0.820	-3.075	H
HETATM	41	H	0	-3.557	-0.838	-3.501	H
HETATM	42	H	0	3.300	2.070	-2.808	H
HETATM	43	H	0	3.559	3.050	1.380	H
HETATM	44	H	0	1.159	1.115	-3.644	H
HETATM	45	H	0	-0.355	1.388	-2.778	H
HETATM	46	H	0	0.483	2.757	-3.573	H
HETATM	47	H	0	5.561	1.656	-0.692	H
HETATM	48	H	0	5.409	3.008	-1.832	H

HETATM	49	H	0	5.522	3.319	-0.075	H
HETATM	50	H	0	1.649	3.236	2.714	H
HETATM	51	H	0	0.437	1.968	2.374	H
HETATM	52	H	0	0.114	3.632	1.894	H
HETATM	53	C	0	1.120	-2.011	1.717	C
HETATM	54	C	0	2.371	-1.252	1.647	C
HETATM	55	C	0	3.395	-1.435	0.677	C
HETATM	56	C	0	4.581	-0.690	0.786	C
HETATM	57	C	0	4.755	0.228	1.819	C
HETATM	58	C	0	3.751	0.430	2.766	C
HETATM	59	C	0	2.575	-0.304	2.671	C
HETATM	60	O	0	3.172	-2.383	-0.236	O
HETATM	61	C	0	3.778	-2.445	-1.540	C
HETATM	62	C	0	5.088	-3.209	-1.499	C
HETATM	63	C	0	3.852	-1.104	-2.243	C
HETATM	64	H	0	0.548	-1.786	2.626	H
HETATM	65	H	0	5.391	-0.856	0.073	H
HETATM	66	H	0	5.695	0.791	1.880	H
HETATM	67	H	0	3.882	1.161	3.573	H
HETATM	68	H	0	1.771	-0.155	3.403	H
HETATM	69	H	0	5.434	-3.420	-2.526	H
HETATM	70	H	0	4.964	-4.176	-0.981	H
HETATM	71	H	0	5.891	-2.650	-0.988	H
HETATM	72	H	0	3.032	-3.057	-2.079	H
HETATM	73	H	0	4.707	-0.479	-1.931	H
HETATM	74	H	0	2.918	-0.542	-2.074	H
HETATM	75	H	0	3.952	-1.272	-3.330	H
HETATM	76	C	0	0.517	-3.039	1.049	C
HETATM	77	C	0	-2.041	-1.614	0.297	C
HETATM	78	H	0	-2.823	-1.644	1.086	H
HETATM	79	H	0	-2.190	-2.312	-0.558	H
HETATM	80	H	0	-0.398	-3.481	1.461	H
HETATM	81	F	0	0.933	-3.704	-0.007	F

END

at3a.pdb

TITLE	at3a.pdb						
HETATM	1	Ru	0	-0.019	0.361	0.139	Ru
HETATM	2	C	0	0.268	-3.886	-0.482	C
HETATM	3	C	0	-1.236	-3.660	-0.448	C
HETATM	4	H	0	0.620	-4.600	0.286	H
HETATM	5	H	0	-1.739	-4.210	0.371	H
HETATM	6	C	0	-0.148	-1.589	-0.081	C
HETATM	7	N	0	-1.349	-2.221	-0.228	N
HETATM	8	N	0	0.810	-2.553	-0.219	N
HETATM	9	Cl	0	-0.726	0.360	2.424	Cl
HETATM	10	Cl	0	-0.189	0.748	-2.207	Cl
HETATM	11	C	0	1.804	0.569	0.288	C
HETATM	12	H	0	2.531	-0.198	0.600	H
HETATM	13	C	0	2.375	1.838	-0.109	C
HETATM	14	C	0	1.530	2.965	-0.206	C
HETATM	15	C	0	3.723	1.965	-0.493	C
HETATM	16	C	0	2.001	4.169	-0.721	C
HETATM	17	C	0	4.201	3.173	-0.994	C
HETATM	18	H	0	4.380	1.089	-0.412	H
HETATM	19	C	0	3.339	4.266	-1.117	C
HETATM	20	H	0	1.326	5.022	-0.833	H
HETATM	21	H	0	5.248	3.264	-1.304	H
HETATM	22	H	0	3.709	5.212	-1.529	H
HETATM	23	O	0	0.243	2.782	0.249	O

HETATM	24	C	0	-0.144	3.518	1.468	C
HETATM	25	H	0	-0.978	2.903	1.836	H
HETATM	26	C	0	-2.660	-1.669	-0.102	C
HETATM	27	C	0	-3.369	-1.283	-1.258	C
HETATM	28	C	0	-3.299	-1.707	1.157	C
HETATM	29	C	0	-4.697	-0.861	-1.117	C
HETATM	30	C	0	-4.622	-1.264	1.249	C
HETATM	31	C	0	-5.334	-0.832	0.125	C
HETATM	32	H	0	-5.245	-0.544	-2.014	H
HETATM	33	H	0	-5.116	-1.280	2.230	H
HETATM	34	C	0	2.220	-2.421	-0.090	C
HETATM	35	C	0	3.006	-2.177	-1.230	C
HETATM	36	C	0	2.801	-2.554	1.183	C
HETATM	37	C	0	4.392	-2.070	-1.072	C
HETATM	38	C	0	4.191	-2.441	1.300	C
HETATM	39	C	0	5.000	-2.196	0.184	C
HETATM	40	H	0	5.012	-1.872	-1.956	H
HETATM	41	H	0	4.651	-2.535	2.292	H
HETATM	42	C	0	-2.784	-1.377	-2.634	C
HETATM	43	H	0	-2.844	-0.407	-3.155	H
HETATM	44	H	0	-1.723	-1.669	-2.632	H
HETATM	45	H	0	-3.349	-2.109	-3.244	H
HETATM	46	C	0	-2.643	-2.301	2.367	C
HETATM	47	H	0	-2.831	-1.689	3.265	H
HETATM	48	H	0	-3.052	-3.311	2.570	H
HETATM	49	H	0	-1.551	-2.388	2.267	H
HETATM	50	C	0	-6.737	-0.321	0.256	C
HETATM	51	H	0	-6.747	0.761	0.493	H
HETATM	52	H	0	-7.311	-0.445	-0.678	H
HETATM	53	H	0	-7.288	-0.825	1.068	H
HETATM	54	C	0	2.363	-1.974	-2.566	C
HETATM	55	H	0	3.117	-1.832	-3.357	H
HETATM	56	H	0	1.727	-2.829	-2.862	H
HETATM	57	H	0	1.699	-1.088	-2.562	H
HETATM	58	C	0	1.931	-2.712	2.392	C
HETATM	59	H	0	1.218	-3.552	2.295	H
HETATM	60	H	0	2.529	-2.883	3.302	H
HETATM	61	H	0	1.314	-1.806	2.556	H
HETATM	62	C	0	6.484	-2.038	0.329	C
HETATM	63	H	0	6.851	-2.443	1.287	H
HETATM	64	H	0	7.034	-2.539	-0.486	H
HETATM	65	H	0	6.781	-0.972	0.296	H
HETATM	66	C	0	-0.645	4.906	1.135	C
HETATM	67	H	0	-1.176	5.322	2.009	H
HETATM	68	H	0	0.172	5.607	0.890	H
HETATM	69	H	0	-1.357	4.884	0.292	H
HETATM	70	C	0	0.948	3.483	2.510	C
HETATM	71	H	0	1.827	4.089	2.223	H
HETATM	72	H	0	0.556	3.891	3.458	H
HETATM	73	H	0	1.268	2.446	2.704	H
HETATM	74	H	0	-1.742	-3.942	-1.391	H
HETATM	75	H	0	0.629	-4.259	-1.460	H
HETATM	76	C	0	-2.867	2.362	-1.069	C
HETATM	77	C	0	-3.259	2.065	0.168	C
HETATM	78	H	0	-4.152	1.464	0.365	H
HETATM	79	H	0	-2.662	2.400	1.019	H
HETATM	80	F	0	-3.549	1.968	-2.149	F
HETATM	81	H	0	-1.966	2.926	-1.335	H

END

TITLE	at3b.pdb						
HETATM	1	Ru	0	-0.421	0.246	-0.235	Ru
HETATM	2	C	0	-0.256	-3.791	1.187	C
HETATM	3	C	0	-1.745	-3.461	1.184	C
HETATM	4	H	0	0.148	-3.940	2.207	H
HETATM	5	H	0	-2.218	-3.581	2.176	H
HETATM	6	C	0	-0.536	-1.597	0.379	C
HETATM	7	N	0	-1.762	-2.065	0.770	N
HETATM	8	N	0	0.355	-2.607	0.578	N
HETATM	9	Cl	0	-0.553	1.035	2.048	Cl
HETATM	10	Cl	0	-0.868	-0.341	-2.536	Cl
HETATM	11	C	0	1.386	0.262	-0.630	C
HETATM	12	H	0	1.787	-0.658	-1.092	H
HETATM	13	C	0	2.405	1.291	-0.592	C
HETATM	14	C	0	2.209	2.641	-0.175	C
HETATM	15	C	0	3.708	0.903	-0.992	C
HETATM	16	C	0	3.301	3.521	-0.161	C
HETATM	17	C	0	4.783	1.777	-0.956	C
HETATM	18	H	0	3.848	-0.133	-1.328	H
HETATM	19	C	0	4.572	3.094	-0.537	C
HETATM	20	H	0	3.153	4.565	0.125	H
HETATM	21	H	0	5.780	1.445	-1.266	H
HETATM	22	H	0	5.403	3.808	-0.518	H
HETATM	23	O	0	0.952	3.014	0.122	O
HETATM	24	C	0	0.650	4.012	1.136	C
HETATM	25	H	0	-0.361	3.694	1.445	H
HETATM	26	C	0	-2.983	-1.367	0.516	C
HETATM	27	C	0	-3.599	-1.489	-0.750	C
HETATM	28	C	0	-3.597	-0.623	1.546	C
HETATM	29	C	0	-4.738	-0.722	-1.014	C
HETATM	30	C	0	-4.738	0.127	1.236	C
HETATM	31	C	0	-5.300	0.118	-0.045	C
HETATM	32	H	0	-5.201	-0.790	-2.007	H
HETATM	33	H	0	-5.204	0.729	2.027	H
HETATM	34	C	0	1.764	-2.588	0.372	C
HETATM	35	C	0	2.272	-3.111	-0.831	C
HETATM	36	C	0	2.618	-2.072	1.364	C
HETATM	37	C	0	3.657	-3.108	-1.029	C
HETATM	38	C	0	3.997	-2.084	1.124	C
HETATM	39	C	0	4.532	-2.592	-0.065	C
HETATM	40	H	0	4.060	-3.503	-1.971	H
HETATM	41	H	0	4.671	-1.673	1.887	H
HETATM	42	C	0	-3.133	-2.493	-1.759	C
HETATM	43	H	0	-3.322	-2.147	-2.787	H
HETATM	44	H	0	-2.056	-2.708	-1.688	H
HETATM	45	H	0	-3.684	-3.446	-1.625	H
HETATM	46	C	0	-3.127	-0.699	2.966	C
HETATM	47	H	0	-3.164	0.286	3.459	H
HETATM	48	H	0	-3.786	-1.377	3.545	H
HETATM	49	H	0	-2.093	-1.065	3.054	H
HETATM	50	C	0	-6.473	0.990	-0.374	C
HETATM	51	H	0	-6.140	1.966	-0.777	H
HETATM	52	H	0	-7.123	0.538	-1.143	H
HETATM	53	H	0	-7.090	1.208	0.514	H
HETATM	54	C	0	1.335	-3.559	-1.909	C
HETATM	55	H	0	1.880	-3.999	-2.761	H
HETATM	56	H	0	0.603	-4.308	-1.555	H
HETATM	57	H	0	0.740	-2.705	-2.290	H
HETATM	58	C	0	2.066	-1.463	2.613	C
HETATM	59	H	0	1.245	-2.060	3.050	H
HETATM	60	H	0	2.847	-1.343	3.382	H
HETATM	61	H	0	1.629	-0.465	2.414	H

HETATM	62	C	0	6.007	-2.529	-0.321	C
HETATM	63	H	0	6.596	-2.758	0.585	H
HETATM	64	H	0	6.321	-3.224	-1.118	H
HETATM	65	H	0	6.310	-1.512	-0.641	H
HETATM	66	C	0	0.555	5.403	0.540	C
HETATM	67	H	0	0.124	6.093	1.286	H
HETATM	68	H	0	1.531	5.817	0.236	H
HETATM	69	H	0	-0.109	5.415	-0.341	H
HETATM	70	C	0	1.532	3.902	2.362	C
HETATM	71	H	0	2.546	4.312	2.222	H
HETATM	72	H	0	1.061	4.461	3.189	H
HETATM	73	H	0	1.612	2.848	2.676	H
HETATM	74	H	0	-2.319	-4.081	0.466	H
HETATM	75	H	0	-0.007	-4.697	0.604	H
HETATM	76	C	0	-1.472	2.849	-1.844	C
HETATM	77	H	0	-0.556	3.453	-1.828	H
HETATM	78	C	0	-2.096	2.371	-0.760	C
HETATM	79	H	0	-3.008	1.767	-0.857	H
HETATM	80	F	0	-1.902	2.624	-3.076	F
HETATM	81	H	0	-1.752	2.648	0.241	H

END

at3c.pdb

TITLE	at3c.pdb						
HETATM	1	Ru	0	0.583	0.318	0.459	Ru
HETATM	2	C	0	0.495	-3.521	-1.524	C
HETATM	3	C	0	1.963	-3.113	-1.570	C
HETATM	4	H	0	0.031	-3.572	-2.528	H
HETATM	5	H	0	2.373	-3.076	-2.596	H
HETATM	6	C	0	0.727	-1.435	-0.465	C
HETATM	7	N	0	1.943	-1.781	-0.976	N
HETATM	8	N	0	-0.130	-2.448	-0.742	N
HETATM	9	Cl	0	0.557	1.390	-1.741	Cl
HETATM	10	Cl	0	1.067	-0.725	2.596	Cl
HETATM	11	C	0	-1.233	0.226	0.844	C
HETATM	12	H	0	-1.496	-0.707	1.383	H
HETATM	13	C	0	-2.424	1.036	0.660	C
HETATM	14	C	0	-2.500	2.374	0.160	C
HETATM	15	C	0	-3.645	0.390	0.981	C
HETATM	16	C	0	-3.758	2.967	-0.033	C
HETATM	17	C	0	-4.882	0.980	0.773	C
HETATM	18	H	0	-3.586	-0.629	1.386	H
HETATM	19	C	0	-4.932	2.276	0.256	C
HETATM	20	H	0	-3.824	3.998	-0.384	H
HETATM	21	H	0	-5.804	0.440	1.019	H
HETATM	22	H	0	-5.897	2.772	0.096	H
HETATM	23	O	0	-1.345	3.026	-0.018	O
HETATM	24	C	0	-1.163	4.137	-0.927	C
HETATM	25	H	0	-0.075	4.078	-1.103	H
HETATM	26	C	0	3.142	-1.056	-0.692	C
HETATM	27	C	0	3.832	-1.311	0.514	C
HETATM	28	C	0	3.658	-0.147	-1.639	C
HETATM	29	C	0	4.944	-0.523	0.825	C
HETATM	30	C	0	4.775	0.619	-1.284	C
HETATM	31	C	0	5.408	0.469	-0.047	C
HETATM	32	H	0	5.469	-0.701	1.773	H
HETATM	33	H	0	5.166	1.347	-2.008	H
HETATM	34	C	0	-1.532	-2.520	-0.496	C
HETATM	35	C	0	-1.983	-3.242	0.627	C
HETATM	36	C	0	-2.435	-1.953	-1.411	C

HETATM	37	C	0	-3.360	-3.400	0.807	C
HETATM	38	C	0	-3.807	-2.137	-1.193	C
HETATM	39	C	0	-4.285	-2.859	-0.096	C
HETATM	40	H	0	-3.720	-3.957	1.683	H
HETATM	41	H	0	-4.519	-1.692	-1.900	H
HETATM	42	C	0	3.482	-2.473	1.394	C
HETATM	43	H	0	3.660	-2.242	2.456	H
HETATM	44	H	0	2.429	-2.780	1.310	H
HETATM	45	H	0	4.118	-3.344	1.134	H
HETATM	46	C	0	3.117	-0.061	-3.033	C
HETATM	47	H	0	3.047	0.984	-3.377	H
HETATM	48	H	0	3.796	-0.591	-3.731	H
HETATM	49	H	0	2.112	-0.498	-3.128	H
HETATM	50	C	0	6.563	1.344	0.337	C
HETATM	51	H	0	6.225	2.207	0.942	H
HETATM	52	H	0	7.305	0.804	0.950	H
HETATM	53	H	0	7.081	1.758	-0.545	H
HETATM	54	C	0	-1.002	-3.764	1.630	C
HETATM	55	H	0	-1.511	-4.310	2.442	H
HETATM	56	H	0	-0.260	-4.451	1.181	H
HETATM	57	H	0	-0.420	-2.937	2.084	H
HETATM	58	C	0	-1.945	-1.130	-2.560	C
HETATM	59	H	0	-1.112	-1.613	-3.104	H
HETATM	60	H	0	-2.751	-0.926	-3.284	H
HETATM	61	H	0	-1.539	-0.160	-2.214	H
HETATM	62	C	0	-5.756	-3.014	0.145	C
HETATM	63	H	0	-6.355	-2.686	-0.721	H
HETATM	64	H	0	-6.031	-4.060	0.371	H
HETATM	65	H	0	-6.086	-2.414	1.015	H
HETATM	66	C	0	-1.464	5.459	-0.246	C
HETATM	67	H	0	-1.107	6.292	-0.876	H
HETATM	68	H	0	-2.540	5.622	-0.065	H
HETATM	69	H	0	-0.942	5.528	0.725	H
HETATM	70	C	0	-1.830	3.941	-2.274	C
HETATM	71	H	0	-2.914	4.145	-2.276	H
HETATM	72	H	0	-1.368	4.631	-3.001	H
HETATM	73	H	0	-1.657	2.914	-2.635	H
HETATM	74	H	0	2.614	-3.786	-0.977	H
HETATM	75	H	0	0.327	-4.500	-1.038	H
HETATM	76	C	0	0.661	2.492	2.159	C
HETATM	77	H	0	-0.362	2.865	2.047	H
HETATM	78	C	0	1.576	2.435	1.166	C
HETATM	79	H	0	2.610	2.138	1.389	H
HETATM	80	F	0	0.948	2.158	3.404	F
HETATM	81	H	0	1.352	2.882	0.193	H

END

at3d.pdb

TITLE	at3d.pdb						
HETATM	1	Ru	0	0.648	-0.715	-0.192	Ru
HETATM	2	C	0	1.079	3.582	0.459	C
HETATM	3	C	0	2.503	3.098	0.721	C
HETATM	4	H	0	0.634	4.110	1.321	H
HETATM	5	H	0	2.829	3.251	1.767	H
HETATM	6	C	0	1.163	1.262	0.145	C
HETATM	7	N	0	2.420	1.665	0.423	N
HETATM	8	N	0	0.351	2.335	0.199	N
HETATM	9	Cl	0	-0.275	-0.691	2.068	Cl
HETATM	10	Cl	0	1.947	-0.709	-2.265	Cl
HETATM	11	C	0	-0.823	-1.182	-1.294	C

HETATM	12	H	0	-0.438	-1.352	-2.319	H
HETATM	13	C	0	-2.278	-1.161	-1.307	C
HETATM	14	C	0	-3.177	-1.458	-0.240	C
HETATM	15	C	0	-2.833	-0.794	-2.556	C
HETATM	16	C	0	-4.557	-1.277	-0.437	C
HETATM	17	C	0	-4.196	-0.616	-2.739	C
HETATM	18	H	0	-2.141	-0.620	-3.390	H
HETATM	19	C	0	-5.056	-0.848	-1.664	C
HETATM	20	H	0	-5.258	-1.514	0.366	H
HETATM	21	H	0	-4.589	-0.306	-3.714	H
HETATM	22	H	0	-6.139	-0.723	-1.784	H
HETATM	23	O	0	-2.637	-2.008	0.849	O
HETATM	24	C	0	-3.262	-2.047	2.151	C
HETATM	25	H	0	-2.387	-2.282	2.779	H
HETATM	26	C	0	3.583	0.832	0.379	C
HETATM	27	C	0	4.399	0.855	-0.768	C
HETATM	28	C	0	3.914	0.035	1.492	C
HETATM	29	C	0	5.509	0.009	-0.812	C
HETATM	30	C	0	5.030	-0.805	1.400	C
HETATM	31	C	0	5.828	-0.843	0.251	C
HETATM	32	H	0	6.134	0.003	-1.715	H
HETATM	33	H	0	5.291	-1.434	2.261	H
HETATM	34	C	0	-1.069	2.320	0.071	C
HETATM	35	C	0	-1.646	2.243	-1.209	C
HETATM	36	C	0	-1.866	2.446	1.225	C
HETATM	37	C	0	-3.041	2.276	-1.313	C
HETATM	38	C	0	-3.255	2.462	1.074	C
HETATM	39	C	0	-3.860	2.371	-0.185	C
HETATM	40	H	0	-3.499	2.217	-2.309	H
HETATM	41	H	0	-3.884	2.537	1.972	H
HETATM	42	C	0	4.112	1.775	-1.915	C
HETATM	43	H	0	4.451	1.335	-2.867	H
HETATM	44	H	0	3.034	1.979	-2.024	H
HETATM	45	H	0	4.638	2.743	-1.798	H
HETATM	46	C	0	3.128	0.109	2.765	C
HETATM	47	H	0	3.054	1.147	3.142	H
HETATM	48	H	0	2.086	-0.246	2.653	H
HETATM	49	H	0	3.603	-0.494	3.557	H
HETATM	50	C	0	6.992	-1.782	0.154	C
HETATM	51	H	0	6.722	-2.694	-0.411	H
HETATM	52	H	0	7.846	-1.327	-0.378	H
HETATM	53	H	0	7.342	-2.110	1.147	H
HETATM	54	C	0	-0.786	2.147	-2.433	C
HETATM	55	H	0	-1.395	2.168	-3.351	H
HETATM	56	H	0	-0.062	2.982	-2.493	H
HETATM	57	H	0	-0.173	1.223	-2.455	H
HETATM	58	C	0	-1.257	2.595	2.587	C
HETATM	59	H	0	-1.129	3.662	2.861	H
HETATM	60	H	0	-1.901	2.146	3.361	H
HETATM	61	H	0	-0.274	2.101	2.659	H
HETATM	62	C	0	-5.354	2.385	-0.310	C
HETATM	63	H	0	-5.815	1.566	0.274	H
HETATM	64	H	0	-5.791	3.326	0.073	H
HETATM	65	H	0	-5.679	2.266	-1.358	H
HETATM	66	C	0	-4.255	-3.188	2.275	C
HETATM	67	H	0	-4.504	-3.343	3.339	H
HETATM	68	H	0	-5.204	-3.013	1.740	H
HETATM	69	H	0	-3.820	-4.129	1.897	H
HETATM	70	C	0	-3.776	-0.692	2.594	C
HETATM	71	H	0	-4.720	-0.388	2.108	H
HETATM	72	H	0	-3.958	-0.711	3.683	H
HETATM	73	H	0	-3.014	0.078	2.388	H

HETATM	74	H	0	3.251	3.579	0.067	H
HETATM	75	H	0	1.002	4.253	-0.417	H
HETATM	76	C	0	0.132	-2.995	-0.431	C
HETATM	77	H	0	-0.759	-3.239	0.162	H
HETATM	78	C	0	1.375	-2.676	0.154	C
HETATM	79	H	0	2.279	-2.897	-0.432	H
HETATM	80	H	0	1.449	-2.719	1.249	H
HETATM	81	F	0	0.140	-3.604	-1.630	F

END

at3I.pdb

TITLE	at3I.pdb						
HETATM	1	Ru	0	0.585	-0.498	-0.348	Ru
HETATM	2	C	0	1.380	3.574	0.740	C
HETATM	3	C	0	2.712	2.920	1.098	C
HETATM	4	H	0	0.922	4.122	1.581	H
HETATM	5	H	0	2.917	2.921	2.187	H
HETATM	6	C	0	1.266	1.298	0.253	C
HETATM	7	N	0	2.537	1.544	0.622	N
HETATM	8	N	0	0.544	2.428	0.367	N
HETATM	9	Cl	0	-0.605	-0.491	1.796	Cl
HETATM	10	Cl	0	1.897	-0.436	-2.371	Cl
HETATM	11	C	0	-0.914	-1.347	-1.418	C
HETATM	12	H	0	-0.589	-1.209	-2.465	H
HETATM	13	C	0	-2.371	-1.176	-1.322	C
HETATM	14	C	0	-3.231	-1.703	-0.318	C
HETATM	15	C	0	-2.965	-0.466	-2.386	C
HETATM	16	C	0	-4.617	-1.507	-0.427	C
HETATM	17	C	0	-4.333	-0.246	-2.468	C
HETATM	18	H	0	-2.302	-0.072	-3.168	H
HETATM	19	C	0	-5.162	-0.777	-1.480	C
HETATM	20	H	0	-5.286	-1.962	0.307	H
HETATM	21	H	0	-4.754	0.321	-3.306	H
HETATM	22	H	0	-6.249	-0.643	-1.534	H
HETATM	23	O	0	-2.666	-2.445	0.648	O
HETATM	24	C	0	-3.208	-2.584	1.983	C
HETATM	25	H	0	-2.285	-2.765	2.561	H
HETATM	26	C	0	3.616	0.612	0.522	C
HETATM	27	C	0	4.496	0.698	-0.573	C
HETATM	28	C	0	3.786	-0.365	1.521	C
HETATM	29	C	0	5.519	-0.248	-0.679	C
HETATM	30	C	0	4.820	-1.296	1.371	C
HETATM	31	C	0	5.685	-1.261	0.272	C
HETATM	32	H	0	6.193	-0.203	-1.544	H
HETATM	33	H	0	4.954	-2.066	2.142	H
HETATM	34	C	0	-0.872	2.528	0.214	C
HETATM	35	C	0	-1.434	2.524	-1.074	C
HETATM	36	C	0	-1.680	2.632	1.364	C
HETATM	37	C	0	-2.827	2.598	-1.194	C
HETATM	38	C	0	-3.065	2.682	1.198	C
HETATM	39	C	0	-3.657	2.653	-0.071	C
HETATM	40	H	0	-3.273	2.590	-2.196	H
HETATM	41	H	0	-3.703	2.727	2.091	H
HETATM	42	C	0	4.360	1.776	-1.604	C
HETATM	43	H	0	4.724	1.429	-2.585	H
HETATM	44	H	0	3.312	2.090	-1.745	H
HETATM	45	H	0	4.954	2.673	-1.337	H
HETATM	46	C	0	2.901	-0.395	2.730	C
HETATM	47	H	0	2.929	0.565	3.281	H
HETATM	48	H	0	1.837	-0.570	2.482	H

HETATM	49	H	0	3.217	-1.184	3.432	H
HETATM	50	C	0	6.755	-2.296	0.103	C
HETATM	51	H	0	6.433	-3.090	-0.598	H
HETATM	52	H	0	7.683	-1.869	-0.314	H
HETATM	53	H	0	7.004	-2.793	1.056	H
HETATM	54	C	0	-0.563	2.443	-2.291	C
HETATM	55	H	0	-1.141	2.638	-3.210	H
HETATM	56	H	0	0.268	3.172	-2.254	H
HETATM	57	H	0	-0.077	1.453	-2.414	H
HETATM	58	C	0	-1.086	2.691	2.739	C
HETATM	59	H	0	-0.912	3.736	3.066	H
HETATM	60	H	0	-1.765	2.235	3.479	H
HETATM	61	H	0	-0.131	2.144	2.801	H
HETATM	62	C	0	-5.149	2.669	-0.210	C
HETATM	63	H	0	-5.599	1.760	0.234	H
HETATM	64	H	0	-5.605	3.531	0.311	H
HETATM	65	H	0	-5.464	2.706	-1.266	H
HETATM	66	C	0	-4.089	-3.815	2.080	C
HETATM	67	H	0	-4.328	-4.023	3.138	H
HETATM	68	H	0	-5.046	-3.699	1.541	H
HETATM	69	H	0	-3.575	-4.702	1.671	H
HETATM	70	C	0	-3.843	-1.322	2.539	C
HETATM	71	H	0	-4.891	-1.172	2.226	H
HETATM	72	H	0	-3.842	-1.385	3.642	H
HETATM	73	H	0	-3.253	-0.435	2.257	H
HETATM	74	H	0	3.575	3.390	0.596	H
HETATM	75	H	0	1.457	4.276	-0.114	H
HETATM	76	C	0	-0.134	-2.605	-0.887	C
HETATM	77	H	0	-0.875	-3.216	-0.345	H
HETATM	78	C	0	1.058	-2.366	0.079	C
HETATM	79	H	0	1.995	-2.743	-0.365	H
HETATM	80	H	0	0.868	-2.682	1.117	H
HETATM	81	F	0	0.318	-3.301	-1.986	F

END

at3e.pdb

TITLE	at3e.pdb						
HETATM	1	Ru	0	0.552	-0.651	-0.240	Ru
HETATM	2	Cl	0	1.644	-0.418	-2.413	Cl
HETATM	3	Cl	0	-0.452	-0.783	1.976	Cl
HETATM	4	C	0	1.198	1.257	0.191	C
HETATM	5	N	0	2.471	1.614	0.446	N
HETATM	6	C	0	2.603	3.038	0.771	C
HETATM	7	C	0	1.185	3.568	0.573	C
HETATM	8	N	0	0.421	2.350	0.284	N
HETATM	9	C	0	3.616	0.757	0.395	C
HETATM	10	C	0	4.439	0.771	-0.745	C
HETATM	11	C	0	5.536	-0.098	-0.777	C
HETATM	12	C	0	5.832	-0.952	0.290	C
HETATM	13	C	0	5.019	-0.908	1.428	C
HETATM	14	C	0	3.914	-0.054	1.508	C
HETATM	15	C	0	4.187	1.704	-1.889	C
HETATM	16	C	0	6.985	-1.906	0.207	C
HETATM	17	C	0	3.077	0.007	2.748	C
HETATM	18	C	0	-1.008	2.372	0.219	C
HETATM	19	C	0	-1.752	2.420	1.415	C
HETATM	20	C	0	-3.145	2.474	1.323	C
HETATM	21	C	0	-3.802	2.515	0.088	C
HETATM	22	C	0	-3.033	2.501	-1.078	C
HETATM	23	C	0	-1.637	2.422	-1.039	C

HETATM	24	C	0	-1.089	2.441	2.758	C
HETATM	25	C	0	-5.298	2.563	0.026	C
HETATM	26	C	0	-0.832	2.415	-2.303	C
HETATM	27	H	0	3.342	3.512	0.101	H
HETATM	28	H	0	2.974	3.159	1.807	H
HETATM	29	H	0	1.099	4.279	-0.270	H
HETATM	30	H	0	0.778	4.069	1.469	H
HETATM	31	H	0	6.173	-0.110	-1.671	H
HETATM	32	H	0	5.255	-1.550	2.287	H
HETATM	33	H	0	3.118	1.953	-1.997	H
HETATM	34	H	0	4.506	1.256	-2.843	H
HETATM	35	H	0	4.756	2.648	-1.769	H
HETATM	36	H	0	7.838	-1.477	-0.347	H
HETATM	37	H	0	7.342	-2.210	1.205	H
HETATM	38	H	0	6.700	-2.833	-0.327	H
HETATM	39	H	0	2.022	-0.272	2.565	H
HETATM	40	H	0	3.054	1.027	3.177	H
HETATM	41	H	0	3.471	-0.667	3.527	H
HETATM	42	H	0	-3.735	2.485	2.250	H
HETATM	43	H	0	-3.532	2.548	-2.053	H
HETATM	44	H	0	-1.681	1.876	3.498	H
HETATM	45	H	0	-0.086	1.984	2.740	H
HETATM	46	H	0	-0.993	3.475	3.146	H
HETATM	47	H	0	-5.747	1.646	0.452	H
HETATM	48	H	0	-5.709	3.409	0.609	H
HETATM	49	H	0	-5.664	2.658	-1.010	H
HETATM	50	H	0	-1.487	2.459	-3.189	H
HETATM	51	H	0	-0.194	1.514	-2.401	H
HETATM	52	H	0	-0.140	3.278	-2.356	H
HETATM	53	C	0	-0.788	-1.912	-1.384	C
HETATM	54	C	0	-2.151	-1.367	-1.415	C
HETATM	55	C	0	-3.169	-1.608	-0.451	C
HETATM	56	C	0	-4.468	-1.136	-0.700	C
HETATM	57	C	0	-4.763	-0.426	-1.862	C
HETATM	58	C	0	-3.770	-0.170	-2.807	C
HETATM	59	C	0	-2.483	-0.638	-2.575	C
HETATM	60	O	0	-2.825	-2.369	0.597	O
HETATM	61	C	0	-3.516	-2.377	1.865	C
HETATM	62	C	0	-4.637	-3.399	1.868	C
HETATM	63	C	0	-3.920	-1.001	2.362	C
HETATM	64	H	0	-0.345	-1.970	-2.389	H
HETATM	65	H	0	-5.272	-1.360	0.004	H
HETATM	66	H	0	-5.791	-0.081	-2.029	H
HETATM	67	H	0	-3.999	0.387	-3.723	H
HETATM	68	H	0	-1.688	-0.465	-3.311	H
HETATM	69	H	0	-5.023	-3.529	2.895	H
HETATM	70	H	0	-4.278	-4.381	1.518	H
HETATM	71	H	0	-5.488	-3.102	1.231	H
HETATM	72	H	0	-2.712	-2.738	2.531	H
HETATM	73	H	0	-4.870	-0.632	1.937	H
HETATM	74	H	0	-3.123	-0.270	2.149	H
HETATM	75	H	0	-4.052	-1.044	3.458	H
HETATM	76	C	0	-0.158	-2.850	-0.507	C
HETATM	77	C	0	1.644	-2.069	0.219	C
HETATM	78	F	0	0.517	-3.846	-1.144	F
HETATM	79	H	0	-0.616	-3.195	0.427	H
HETATM	80	H	0	2.383	-2.490	-0.490	H
HETATM	81	H	0	1.651	-2.494	1.244	H

END

TITLE	at3f.pdb						
HETATM	1	Ru	0	-0.495	-0.716	0.249	Ru
HETATM	2	C	0	-1.180	3.478	-0.398	C
HETATM	3	C	0	-2.628	3.017	-0.292	C
HETATM	4	H	0	-0.929	3.887	-1.396	H
HETATM	5	H	0	-3.243	3.300	-1.165	H
HETATM	6	C	0	-1.217	1.145	-0.101	C
HETATM	7	N	0	-2.504	1.560	-0.209	N
HETATM	8	N	0	-0.428	2.243	-0.167	N
HETATM	9	Cl	0	0.289	-0.960	-2.052	Cl
HETATM	10	Cl	0	-1.223	-0.378	2.575	Cl
HETATM	11	C	0	0.910	-2.339	1.352	C
HETATM	12	C	0	2.123	-1.522	1.466	C
HETATM	13	C	0	3.187	-1.535	0.518	C
HETATM	14	C	0	2.292	-0.793	2.660	C
HETATM	15	C	0	4.374	-0.847	0.816	C
HETATM	16	C	0	3.469	-0.109	2.939	C
HETATM	17	H	0	1.458	-0.781	3.372	H
HETATM	18	C	0	4.511	-0.146	2.013	C
HETATM	19	H	0	5.213	-0.878	0.119	H
HETATM	20	H	0	3.574	0.448	3.877	H
HETATM	21	H	0	5.451	0.381	2.216	H
HETATM	22	O	0	2.985	-2.293	-0.570	O
HETATM	23	C	0	3.782	-2.257	-1.769	C
HETATM	24	H	0	3.133	-2.827	-2.458	H
HETATM	25	C	0	-3.669	0.745	-0.270	C
HETATM	26	C	0	-4.517	0.637	0.847	C
HETATM	27	C	0	-3.984	0.110	-1.491	C
HETATM	28	C	0	-5.654	-0.172	0.740	C
HETATM	29	C	0	-5.131	-0.689	-1.552	C
HETATM	30	C	0	-5.968	-0.852	-0.442	C
HETATM	31	H	0	-6.311	-0.275	1.614	H
HETATM	32	H	0	-5.378	-1.190	-2.496	H
HETATM	33	C	0	0.998	2.266	-0.245	C
HETATM	34	C	0	1.746	2.421	0.941	C
HETATM	35	C	0	1.620	2.283	-1.507	C
HETATM	36	C	0	3.133	2.552	0.839	C
HETATM	37	C	0	3.015	2.396	-1.557	C
HETATM	38	C	0	3.785	2.522	-0.399	C
HETATM	39	H	0	3.720	2.676	1.758	H
HETATM	40	H	0	3.510	2.385	-2.538	H
HETATM	41	C	0	-4.232	1.375	2.118	C
HETATM	42	H	0	-4.667	0.852	2.986	H
HETATM	43	H	0	-3.149	1.470	2.303	H
HETATM	44	H	0	-4.675	2.391	2.104	H
HETATM	45	C	0	-3.114	0.304	-2.693	C
HETATM	46	H	0	-2.948	1.378	-2.908	H
HETATM	47	H	0	-2.107	-0.141	-2.562	H
HETATM	48	H	0	-3.566	-0.150	-3.590	H
HETATM	49	C	0	-7.169	-1.746	-0.516	C
HETATM	50	H	0	-6.902	-2.797	-0.296	H
HETATM	51	H	0	-7.946	-1.457	0.212	H
HETATM	52	H	0	-7.624	-1.742	-1.522	H
HETATM	53	C	0	1.066	2.486	2.273	C
HETATM	54	H	0	1.803	2.562	3.090	H
HETATM	55	H	0	0.398	3.366	2.349	H
HETATM	56	H	0	0.430	1.602	2.468	H
HETATM	57	C	0	0.836	2.244	-2.784	C
HETATM	58	H	0	0.730	3.259	-3.217	H
HETATM	59	H	0	1.345	1.622	-3.539	H
HETATM	60	H	0	-0.171	1.817	-2.653	H
HETATM	61	C	0	5.280	2.593	-0.471	C

HETATM	62	H	0	5.734	1.606	-0.252	H
HETATM	63	H	0	5.635	2.895	-1.471	H
HETATM	64	H	0	5.699	3.298	0.269	H
HETATM	65	C	0	5.081	-3.027	-1.613	C
HETATM	66	H	0	5.544	-3.173	-2.605	H
HETATM	67	H	0	5.821	-2.511	-0.979	H
HETATM	68	H	0	4.898	-4.025	-1.180	H
HETATM	69	C	0	3.926	-0.864	-2.347	C
HETATM	70	H	0	4.648	-0.229	-1.806	H
HETATM	71	H	0	4.275	-0.940	-3.393	H
HETATM	72	H	0	2.943	-0.363	-2.347	H
HETATM	73	H	0	-3.136	3.406	0.611	H
HETATM	74	H	0	-0.907	4.242	0.351	H
HETATM	75	C	0	0.459	-3.089	0.301	C
HETATM	76	C	0	-2.051	-1.599	-0.052	C
HETATM	77	H	0	-2.196	-2.201	-0.976	H
HETATM	78	H	0	-2.869	-1.656	0.695	H
HETATM	79	H	0	0.373	-2.497	2.296	H
HETATM	80	F	0	-0.517	-3.980	0.527	F
HETATM	81	H	0	0.875	-3.160	-0.705	H

END

s2g.pdb

TITLE	s2g.pdb						
HETATM	1	Ru	0	-0.299	-0.773	-0.087	Ru
HETATM	2	C	0	0.035	3.385	0.099	C
HETATM	3	C	0	1.536	3.101	0.176	C
HETATM	4	H	0	-0.344	3.942	0.976	H
HETATM	5	H	0	1.984	3.415	1.138	H
HETATM	6	C	0	0.399	1.061	0.011	C
HETATM	7	N	0	1.618	1.642	0.042	N
HETATM	8	N	0	-0.538	2.046	0.054	N
HETATM	9	Cl	0	-0.698	-1.100	2.268	Cl
HETATM	10	Cl	0	-0.388	-0.744	-2.496	Cl
HETATM	11	C	0	-2.683	-2.553	-0.271	C
HETATM	12	C	0	2.878	0.979	0.077	C
HETATM	13	C	0	3.616	0.854	-1.116	C
HETATM	14	C	0	3.376	0.497	1.300	C
HETATM	15	C	0	4.871	0.243	-1.062	C
HETATM	16	C	0	4.630	-0.128	1.306	C
HETATM	17	C	0	5.389	-0.259	0.139	C
HETATM	18	H	0	5.450	0.137	-1.988	H
HETATM	19	H	0	5.025	-0.513	2.256	H
HETATM	20	C	0	-1.931	1.735	0.087	C
HETATM	21	C	0	-2.654	1.614	-1.121	C
HETATM	22	C	0	-2.566	1.545	1.335	C
HETATM	23	C	0	-3.975	1.156	-1.059	C
HETATM	24	C	0	-3.888	1.093	1.346	C
HETATM	25	C	0	-4.593	0.859	0.159	C
HETATM	26	H	0	-4.531	1.023	-1.996	H
HETATM	27	H	0	-4.374	0.907	2.312	H
HETATM	28	C	0	3.019	1.285	-2.419	C
HETATM	29	H	0	3.740	1.181	-3.246	H
HETATM	30	H	0	2.131	0.669	-2.663	H
HETATM	31	H	0	2.674	2.335	-2.406	H
HETATM	32	C	0	2.577	0.626	2.560	C
HETATM	33	H	0	2.179	1.648	2.698	H
HETATM	34	H	0	1.697	-0.047	2.566	H
HETATM	35	H	0	3.186	0.381	3.445	H
HETATM	36	C	0	6.720	-0.949	0.161	C

HETATM	37	H	0	6.647	-1.975	-0.247	H
HETATM	38	H	0	7.467	-0.421	-0.457	H
HETATM	39	H	0	7.123	-1.037	1.183	H
HETATM	40	C	0	-2.075	2.046	-2.433	C
HETATM	41	H	0	-2.405	1.392	-3.255	H
HETATM	42	H	0	-2.413	3.075	-2.672	H
HETATM	43	H	0	-0.975	2.040	-2.439	H
HETATM	44	C	0	-1.877	1.885	2.620	C
HETATM	45	H	0	-2.082	2.939	2.897	H
HETATM	46	H	0	-2.232	1.250	3.446	H
HETATM	47	H	0	-0.784	1.757	2.563	H
HETATM	48	C	0	-5.970	0.272	0.193	C
HETATM	49	H	0	-5.923	-0.834	0.184	H
HETATM	50	H	0	-6.521	0.556	1.106	H
HETATM	51	H	0	-6.572	0.572	-0.681	H
HETATM	52	H	0	2.112	3.594	-0.627	H
HETATM	53	H	0	-0.249	3.959	-0.805	H
HETATM	54	C	0	-1.462	-3.106	-0.331	C
HETATM	55	H	0	-1.027	-3.521	0.581	H
HETATM	56	C	0	1.281	-1.675	-0.067	C
HETATM	57	H	0	-1.021	-3.295	-1.312	H
HETATM	58	F	0	-3.380	-2.390	0.820	F
HETATM	59	F	0	-3.357	-2.122	-1.304	F
HETATM	60	F	0	2.227	-1.690	-0.980	F
HETATM	61	F	0	1.641	-2.574	0.833	F

END

s2h.pdb

TITLE	s2h.pdb						
HETATM	1	Ru	0	0.202	-0.802	0.007	Ru
HETATM	2	Cl	0	1.033	-0.673	-2.277	Cl
HETATM	3	Cl	0	-0.621	-0.865	2.288	Cl
HETATM	4	C	0	-0.145	1.220	0.009	C
HETATM	5	N	0	0.880	2.086	0.078	N
HETATM	6	C	0	0.433	3.473	0.215	C
HETATM	7	C	0	-1.089	3.348	0.062	C
HETATM	8	N	0	-1.302	1.896	0.020	N
HETATM	9	C	0	2.225	1.605	0.121	C
HETATM	10	C	0	3.005	1.652	-1.055	C
HETATM	11	C	0	4.245	1.018	-1.054	C
HETATM	12	C	0	4.723	0.336	0.075	C
HETATM	13	C	0	3.963	0.365	1.244	C
HETATM	14	C	0	2.719	1.011	1.301	C
HETATM	15	C	0	-2.587	1.277	-0.047	C
HETATM	16	C	0	-3.361	1.157	1.120	C
HETATM	17	C	0	-4.587	0.488	1.036	C
HETATM	18	C	0	-5.051	-0.049	-0.170	C
HETATM	19	C	0	-4.275	0.121	-1.323	C
HETATM	20	C	0	-3.046	0.787	-1.286	C
HETATM	21	C	0	2.501	2.353	-2.278	C
HETATM	22	C	0	6.001	-0.441	0.010	C
HETATM	23	C	0	2.023	1.125	2.624	C
HETATM	24	C	0	-2.910	1.739	2.425	C
HETATM	25	C	0	-6.339	-0.813	-0.222	C
HETATM	26	C	0	-2.240	0.975	-2.535	C
HETATM	27	H	0	0.894	4.111	-0.560	H
HETATM	28	H	0	0.736	3.872	1.202	H
HETATM	29	H	0	-1.468	3.812	-0.868	H
HETATM	30	H	0	-1.647	3.792	0.906	H
HETATM	31	H	0	4.840	1.018	-1.976	H

HETATM	32	H	0	4.338	-0.130	2.150	H
HETATM	33	H	0	-5.189	0.372	1.946	H
HETATM	34	H	0	-4.637	-0.270	-2.283	H
HETATM	35	H	0	1.430	2.147	-2.447	H
HETATM	36	H	0	3.043	2.021	-3.178	H
HETATM	37	H	0	2.631	3.451	-2.203	H
HETATM	38	H	0	5.816	-1.458	-0.387	H
HETATM	39	H	0	6.464	-0.565	1.003	H
HETATM	40	H	0	6.740	0.029	-0.661	H
HETATM	41	H	0	2.641	1.725	3.319	H
HETATM	42	H	0	1.869	0.138	3.093	H
HETATM	43	H	0	1.030	1.595	2.560	H
HETATM	44	H	0	-1.812	1.763	2.510	H
HETATM	45	H	0	-3.285	1.145	3.274	H
HETATM	46	H	0	-3.291	2.772	2.559	H
HETATM	47	H	0	-6.169	-1.893	-0.048	H
HETATM	48	H	0	-6.832	-0.726	-1.205	H
HETATM	49	H	0	-7.051	-0.478	0.550	H
HETATM	50	H	0	-2.823	0.697	-3.428	H
HETATM	51	H	0	-1.313	0.369	-2.542	H
HETATM	52	H	0	-1.915	2.025	-2.661	H
HETATM	53	C	0	-1.217	-1.903	-0.524	C
HETATM	54	F	0	-1.511	-2.248	-1.758	F
HETATM	55	F	0	-2.190	-2.363	0.225	F
HETATM	56	C	0	1.620	-2.325	0.385	C
HETATM	57	C	0	0.450	-3.051	0.009	C
HETATM	58	F	0	2.693	-2.324	-0.399	F
HETATM	59	F	0	2.035	-2.336	1.653	F
HETATM	60	H	0	0.499	-3.540	-0.972	H
HETATM	61	H	0	-0.070	-3.572	0.823	H

END

s2NA.pdb

TITLE	s2NA.pdb						
HETATM	1	Ru	0	-0.002	-0.799	-0.005	Ru
HETATM	2	C	0	-0.761	3.425	-0.033	C
HETATM	3	C	0	0.768	3.419	0.089	C
HETATM	4	H	0	-1.262	3.915	0.821	H
HETATM	5	H	0	1.131	3.884	1.025	H
HETATM	6	C	0	-0.002	1.229	0.004	C
HETATM	7	N	0	1.097	1.989	0.078	N
HETATM	8	N	0	-1.097	1.995	-0.057	N
HETATM	9	Cl	0	-0.815	-0.764	2.278	Cl
HETATM	10	Cl	0	0.814	-0.755	-2.287	Cl
HETATM	11	C	0	-1.281	-2.221	-0.428	C
HETATM	12	C	0	2.422	1.447	0.101	C
HETATM	13	C	0	3.174	1.410	-1.090	C
HETATM	14	C	0	2.938	0.940	1.309	C
HETATM	15	C	0	4.422	0.783	-1.066	C
HETATM	16	C	0	4.195	0.323	1.286	C
HETATM	17	C	0	4.937	0.216	0.106	C
HETATM	18	H	0	5.002	0.726	-1.996	H
HETATM	19	H	0	4.600	-0.083	2.221	H
HETATM	20	C	0	-2.423	1.456	-0.086	C
HETATM	21	C	0	-2.940	0.974	-1.306	C
HETATM	22	C	0	-3.173	1.394	1.104	C
HETATM	23	C	0	-4.191	0.347	-1.293	C
HETATM	24	C	0	-4.418	0.761	1.068	C
HETATM	25	C	0	-4.930	0.212	-0.113	C
HETATM	26	H	0	-4.596	-0.041	-2.236	H

HETATM	27	H	0	-4.997	0.682	1.997	H
HETATM	28	C	0	2.675	2.046	-2.351	C
HETATM	29	H	0	3.089	1.542	-3.239	H
HETATM	30	H	0	1.578	1.999	-2.439	H
HETATM	31	H	0	2.980	3.111	-2.412	H
HETATM	32	C	0	2.185	1.052	2.598	C
HETATM	33	H	0	1.577	1.972	2.654	H
HETATM	34	H	0	1.473	0.217	2.742	H
HETATM	35	H	0	2.876	1.047	3.457	H
HETATM	36	C	0	6.247	-0.511	0.090	C
HETATM	37	H	0	6.101	-1.580	-0.155	H
HETATM	38	H	0	6.938	-0.105	-0.669	H
HETATM	39	H	0	6.752	-0.476	1.069	H
HETATM	40	C	0	-2.189	1.140	-2.591	C
HETATM	41	H	0	-2.845	0.948	-3.455	H
HETATM	42	H	0	-1.779	2.161	-2.701	H
HETATM	43	H	0	-1.325	0.452	-2.673	H
HETATM	44	C	0	-2.679	2.011	2.376	C
HETATM	45	H	0	-3.001	3.069	2.457	H
HETATM	46	H	0	-3.082	1.483	3.255	H
HETATM	47	H	0	-1.581	1.980	2.459	H
HETATM	48	C	0	-6.233	-0.527	-0.110	C
HETATM	49	H	0	-6.075	-1.603	0.096	H
HETATM	50	H	0	-6.920	-0.154	0.669	H
HETATM	51	H	0	-6.748	-0.463	-1.083	H
HETATM	52	H	0	1.271	3.929	-0.752	H
HETATM	53	H	0	-1.121	3.915	-0.956	H
HETATM	54	C	0	-0.002	-3.040	-0.008	C
HETATM	55	H	0	-0.292	-3.639	0.870	H
HETATM	56	H	0	0.286	-3.638	-0.888	H
HETATM	57	C	0	1.277	-2.223	0.412	C
HETATM	58	F	0	2.341	-2.465	-0.355	F
HETATM	59	F	0	1.665	-2.457	1.670	F
HETATM	60	F	0	-1.666	-2.450	-1.687	F
HETATM	61	F	0	-2.346	-2.464	0.336	F

END

s2i.pdb

TITLE	s2i.pdb						
HETATM	1	Ru	0	0.202	-0.802	0.007	Ru
HETATM	2	Cl	0	1.033	-0.673	-2.277	Cl
HETATM	3	Cl	0	-0.621	-0.865	2.288	Cl
HETATM	4	C	0	-0.145	1.220	0.009	C
HETATM	5	N	0	0.880	2.086	0.078	N
HETATM	6	C	0	0.433	3.473	0.215	C
HETATM	7	C	0	-1.089	3.348	0.062	C
HETATM	8	N	0	-1.302	1.896	0.020	N
HETATM	9	C	0	2.225	1.605	0.121	C
HETATM	10	C	0	3.005	1.652	-1.055	C
HETATM	11	C	0	4.245	1.018	-1.054	C
HETATM	12	C	0	4.723	0.336	0.075	C
HETATM	13	C	0	3.963	0.365	1.244	C
HETATM	14	C	0	2.719	1.011	1.301	C
HETATM	15	C	0	-2.587	1.277	-0.047	C
HETATM	16	C	0	-3.361	1.157	1.120	C
HETATM	17	C	0	-4.587	0.488	1.036	C
HETATM	18	C	0	-5.051	-0.049	-0.170	C
HETATM	19	C	0	-4.275	0.121	-1.323	C
HETATM	20	C	0	-3.046	0.787	-1.286	C
HETATM	21	C	0	2.501	2.353	-2.278	C
HETATM	22	C	0	6.001	-0.441	0.010	C

HETATM	23	C	0	2.023	1.125	2.624	C
HETATM	24	C	0	-2.910	1.739	2.425	C
HETATM	25	C	0	-6.339	-0.813	-0.222	C
HETATM	26	C	0	-2.240	0.975	-2.535	C
HETATM	27	H	0	0.894	4.111	-0.560	H
HETATM	28	H	0	0.736	3.872	1.202	H
HETATM	29	H	0	-1.468	3.812	-0.868	H
HETATM	30	H	0	-1.647	3.792	0.906	H
HETATM	31	H	0	4.840	1.018	-1.976	H
HETATM	32	H	0	4.338	-0.130	2.150	H
HETATM	33	H	0	-5.189	0.372	1.946	H
HETATM	34	H	0	-4.637	-0.270	-2.283	H
HETATM	35	H	0	1.430	2.147	-2.447	H
HETATM	36	H	0	3.043	2.021	-3.178	H
HETATM	37	H	0	2.631	3.451	-2.203	H
HETATM	38	H	0	5.816	-1.458	-0.387	H
HETATM	39	H	0	6.464	-0.565	1.003	H
HETATM	40	H	0	6.740	0.029	-0.661	H
HETATM	41	H	0	2.641	1.725	3.319	H
HETATM	42	H	0	1.869	0.138	3.093	H
HETATM	43	H	0	1.030	1.595	2.560	H
HETATM	44	H	0	-1.812	1.763	2.510	H
HETATM	45	H	0	-3.285	1.145	3.274	H
HETATM	46	H	0	-3.291	2.772	2.559	H
HETATM	47	H	0	-6.169	-1.893	-0.048	H
HETATM	48	H	0	-6.832	-0.726	-1.205	H
HETATM	49	H	0	-7.051	-0.478	0.550	H
HETATM	50	H	0	-2.823	0.697	-3.428	H
HETATM	51	H	0	-1.313	0.369	-2.542	H
HETATM	52	H	0	-1.915	2.025	-2.661	H
HETATM	53	C	0	-1.217	-1.903	-0.524	C
HETATM	54	F	0	-1.511	-2.248	-1.758	F
HETATM	55	F	0	-2.190	-2.363	0.225	F
HETATM	56	C	0	1.620	-2.325	0.385	C
HETATM	57	C	0	0.450	-3.051	0.009	C
HETATM	58	F	0	2.693	-2.324	-0.399	F
HETATM	59	F	0	2.035	-2.336	1.653	F
HETATM	60	H	0	0.499	-3.540	-0.972	H
HETATM	61	H	0	-0.070	-3.572	0.823	H

END

s2j.pdb

TITLE	s2j.pdb						
HETATM	1	Ru	0	-0.299	-0.773	-0.087	Ru
HETATM	2	C	0	0.035	3.385	0.099	C
HETATM	3	C	0	1.536	3.101	0.176	C
HETATM	4	H	0	-0.344	3.942	0.976	H
HETATM	5	H	0	1.984	3.415	1.138	H
HETATM	6	C	0	0.399	1.061	0.011	C
HETATM	7	N	0	1.618	1.642	0.042	N
HETATM	8	N	0	-0.538	2.046	0.054	N
HETATM	9	Cl	0	-0.698	-1.100	2.268	Cl
HETATM	10	Cl	0	-0.388	-0.744	-2.496	Cl
HETATM	11	C	0	-2.683	-2.553	-0.271	C
HETATM	12	C	0	2.878	0.979	0.077	C
HETATM	13	C	0	3.616	0.854	-1.116	C
HETATM	14	C	0	3.376	0.497	1.300	C
HETATM	15	C	0	4.871	0.243	-1.062	C
HETATM	16	C	0	4.630	-0.128	1.306	C
HETATM	17	C	0	5.389	-0.259	0.139	C
HETATM	18	H	0	5.450	0.137	-1.988	H

HETATM	19	H	0	5.025	-0.513	2.256	H
HETATM	20	C	0	-1.931	1.735	0.087	C
HETATM	21	C	0	-2.654	1.614	-1.121	C
HETATM	22	C	0	-2.566	1.545	1.335	C
HETATM	23	C	0	-3.975	1.156	-1.059	C
HETATM	24	C	0	-3.888	1.093	1.346	C
HETATM	25	C	0	-4.593	0.859	0.159	C
HETATM	26	H	0	-4.531	1.023	-1.996	H
HETATM	27	H	0	-4.374	0.907	2.312	H
HETATM	28	C	0	3.019	1.285	-2.419	C
HETATM	29	H	0	3.740	1.181	-3.246	H
HETATM	30	H	0	2.131	0.669	-2.663	H
HETATM	31	H	0	2.674	2.335	-2.406	H
HETATM	32	C	0	2.577	0.626	2.560	C
HETATM	33	H	0	2.179	1.648	2.698	H
HETATM	34	H	0	1.697	-0.047	2.566	H
HETATM	35	H	0	3.186	0.381	3.445	H
HETATM	36	C	0	6.720	-0.949	0.161	C
HETATM	37	H	0	6.647	-1.975	-0.247	H
HETATM	38	H	0	7.467	-0.421	-0.457	H
HETATM	39	H	0	7.123	-1.037	1.183	H
HETATM	40	C	0	-2.075	2.046	-2.433	C
HETATM	41	H	0	-2.405	1.392	-3.255	H
HETATM	42	H	0	-2.413	3.075	-2.672	H
HETATM	43	H	0	-0.975	2.040	-2.439	H
HETATM	44	C	0	-1.877	1.885	2.620	C
HETATM	45	H	0	-2.082	2.939	2.897	H
HETATM	46	H	0	-2.232	1.250	3.446	H
HETATM	47	H	0	-0.784	1.757	2.563	H
HETATM	48	C	0	-5.970	0.272	0.193	C
HETATM	49	H	0	-5.923	-0.834	0.184	H
HETATM	50	H	0	-6.521	0.556	1.106	H
HETATM	51	H	0	-6.572	0.572	-0.681	H
HETATM	52	H	0	2.112	3.594	-0.627	H
HETATM	53	H	0	-0.249	3.959	-0.805	H
HETATM	54	C	0	-1.462	-3.106	-0.331	C
HETATM	55	H	0	-1.027	-3.521	0.581	H
HETATM	56	C	0	1.281	-1.675	-0.067	C
HETATM	57	H	0	-1.021	-3.295	-1.312	H
HETATM	58	F	0	-3.380	-2.390	0.820	F
HETATM	59	F	0	-3.357	-2.122	-1.304	F
HETATM	60	F	0	2.227	-1.690	-0.980	F
HETATM	61	F	0	1.641	-2.574	0.833	F

END

a2g.pdb

TITLE	a2g.pdb						
HETATM	1	Ru	0	-0.383	0.750	0.013	Ru
HETATM	2	C	0	-0.545	-3.446	0.043	C
HETATM	3	C	0	0.980	-3.330	0.112	C
HETATM	4	H	0	-0.897	-3.944	-0.881	H
HETATM	5	H	0	1.493	-3.844	-0.721	H
HETATM	6	C	0	0.068	-1.176	0.028	C
HETATM	7	N	0	1.215	-1.885	0.038	N
HETATM	8	N	0	-0.970	-2.050	0.062	N
HETATM	9	Cl	0	-0.573	0.926	-2.399	Cl
HETATM	10	Cl	0	-0.615	0.840	2.424	Cl
HETATM	11	C	0	-1.899	2.641	0.024	C
HETATM	12	H	0	-2.394	2.428	0.976	H
HETATM	13	C	0	2.535	-1.348	0.003	C
HETATM	14	C	0	3.209	-1.086	1.212	C

HETATM	15	C	0	3.148	-1.123	-1.243	C
HETATM	16	C	0	4.511	-0.585	1.150	C
HETATM	17	C	0	4.454	-0.622	-1.260	C
HETATM	18	C	0	5.147	-0.346	-0.076	C
HETATM	19	H	0	5.040	-0.364	2.086	H
HETATM	20	H	0	4.937	-0.433	-2.227	H
HETATM	21	C	0	-2.322	-1.593	0.008	C
HETATM	22	C	0	-3.033	-1.378	1.209	C
HETATM	23	C	0	-2.931	-1.368	-1.247	C
HETATM	24	C	0	-4.307	-0.808	1.132	C
HETATM	25	C	0	-4.206	-0.795	-1.273	C
HETATM	26	C	0	-4.895	-0.483	-0.096	C
HETATM	27	H	0	-4.857	-0.616	2.063	H
HETATM	28	H	0	-4.675	-0.595	-2.246	H
HETATM	29	C	0	2.516	-1.283	2.524	C
HETATM	30	H	0	3.190	-1.069	3.369	H
HETATM	31	H	0	1.635	-0.619	2.619	H
HETATM	32	H	0	2.141	-2.316	2.653	H
HETATM	33	C	0	2.391	-1.353	-2.512	C
HETATM	34	H	0	1.573	-0.613	-2.627	H
HETATM	35	H	0	3.047	-1.268	-3.394	H
HETATM	36	H	0	1.911	-2.349	-2.544	H
HETATM	37	C	0	6.539	0.209	-0.108	C
HETATM	38	H	0	6.576	1.230	0.315	H
HETATM	39	H	0	7.236	-0.401	0.494	H
HETATM	40	H	0	6.939	0.263	-1.134	H
HETATM	41	C	0	-2.495	-1.828	2.532	C
HETATM	42	H	0	-2.780	-1.134	3.339	H
HETATM	43	H	0	-2.907	-2.824	2.790	H
HETATM	44	H	0	-1.397	-1.898	2.544	H
HETATM	45	C	0	-2.285	-1.821	-2.520	C
HETATM	46	H	0	-2.622	-2.847	-2.771	H
HETATM	47	H	0	-2.558	-1.168	-3.364	H
HETATM	48	H	0	-1.185	-1.828	-2.464	H
HETATM	49	C	0	-6.232	0.192	-0.148	C
HETATM	50	H	0	-6.120	1.294	-0.157	H
HETATM	51	H	0	-6.795	-0.074	-1.059	H
HETATM	52	H	0	-6.856	-0.055	0.727	H
HETATM	53	H	0	1.398	-3.736	1.053	H
HETATM	54	H	0	-0.977	-3.994	0.901	H
HETATM	55	C	0	-0.813	3.446	0.034	C
HETATM	56	C	0	1.326	1.403	0.035	C
HETATM	57	H	0	-2.385	2.439	-0.935	H
HETATM	58	F	0	2.026	1.753	1.095	F
HETATM	59	F	0	2.058	1.745	-1.004	F
HETATM	60	F	0	-0.247	3.918	1.111	F
HETATM	61	F	0	-0.233	3.930	-1.030	F

END

a2i.pdb

TITLE	a2i.pdb						
HETATM	1	Ru	0	0.057	0.902	0.236	Ru
HETATM	2	Cl	0	-0.844	0.611	2.429	Cl
HETATM	3	Cl	0	1.031	0.978	-2.027	Cl
HETATM	4	C	0	0.227	-1.184	-0.024	C
HETATM	5	N	0	1.376	-1.880	-0.050	N
HETATM	6	C	0	1.152	-3.325	-0.185	C
HETATM	7	C	0	-0.369	-3.428	-0.305	C
HETATM	8	N	0	-0.803	-2.033	-0.157	N
HETATM	9	C	0	2.685	-1.314	0.028	C
HETATM	10	C	0	3.186	-0.905	1.279	C

HETATM	11	C	0	4.447	-0.301	1.329	C
HETATM	12	C	0	5.216	-0.117	0.174	C
HETATM	13	C	0	4.714	-0.584	-1.046	C
HETATM	14	C	0	3.456	-1.189	-1.142	C
HETATM	15	C	0	-2.180	-1.649	-0.174	C
HETATM	16	C	0	-2.738	-1.141	-1.364	C
HETATM	17	C	0	-4.083	-0.756	-1.354	C
HETATM	18	C	0	-4.870	-0.872	-0.204	C
HETATM	19	C	0	-4.297	-1.418	0.950	C
HETATM	20	C	0	-2.960	-1.821	0.985	C
HETATM	21	C	0	2.398	-1.127	2.534	C
HETATM	22	C	0	6.543	0.576	0.238	C
HETATM	23	C	0	2.978	-1.707	-2.464	C
HETATM	24	C	0	-1.922	-1.023	-2.614	C
HETATM	25	C	0	-6.292	-0.399	-0.197	C
HETATM	26	C	0	-2.392	-2.443	2.225	C
HETATM	27	H	0	1.555	-3.852	0.700	H
HETATM	28	H	0	1.686	-3.713	-1.071	H
HETATM	29	H	0	-0.826	-4.053	0.483	H
HETATM	30	H	0	-0.705	-3.826	-1.280	H
HETATM	31	H	0	4.842	0.022	2.301	H
HETATM	32	H	0	5.312	-0.463	-1.958	H
HETATM	33	H	0	-4.524	-0.353	-2.275	H
HETATM	34	H	0	-4.906	-1.527	1.857	H
HETATM	35	H	0	1.490	-0.496	2.593	H
HETATM	36	H	0	3.006	-0.909	3.427	H
HETATM	37	H	0	2.042	-2.171	2.620	H
HETATM	38	H	0	7.015	0.475	1.230	H
HETATM	39	H	0	6.437	1.661	0.045	H
HETATM	40	H	0	7.248	0.191	-0.517	H
HETATM	41	H	0	3.334	-1.069	-3.290	H
HETATM	42	H	0	1.879	-1.734	-2.532	H
HETATM	43	H	0	3.363	-2.729	-2.656	H
HETATM	44	H	0	-1.140	-0.243	-2.537	H
HETATM	45	H	0	-2.557	-0.768	-3.478	H
HETATM	46	H	0	-1.390	-1.963	-2.854	H
HETATM	47	H	0	-6.369	0.621	0.225	H
HETATM	48	H	0	-6.939	-1.044	0.423	H
HETATM	49	H	0	-6.720	-0.359	-1.212	H
HETATM	50	H	0	-2.880	-2.041	3.128	H
HETATM	51	H	0	-1.312	-2.253	2.331	H
HETATM	52	H	0	-2.551	-3.540	2.234	H
HETATM	53	C	0	-1.417	2.131	-0.514	C
HETATM	54	F	0	-2.584	1.830	0.067	F
HETATM	55	F	0	-1.609	2.302	-1.818	F
HETATM	56	C	0	1.447	2.071	0.614	C
HETATM	57	C	0	-0.558	3.055	0.191	C
HETATM	58	F	0	-0.995	3.605	1.315	F
HETATM	59	F	0	0.062	3.963	-0.565	F
HETATM	60	H	0	1.931	2.788	-0.071	H
HETATM	61	H	0	1.908	1.942	1.617	H

END

a2j.pdb

TITLE	a2j.pdb						
HETATM	1	Ru	0	0.066	0.660	0.012	Ru
HETATM	2	C	0	-0.554	-3.469	0.201	C
HETATM	3	C	0	-2.027	-3.055	0.161	C
HETATM	4	H	0	-0.291	-4.041	1.111	H
HETATM	5	H	0	-2.584	-3.356	1.068	H
HETATM	6	C	0	-0.697	-1.118	0.082	C

HETATM	7	N	0	-1.966	-1.596	0.066	N
HETATM	8	N	0	0.143	-2.190	0.182	N
HETATM	9	Cl	0	0.590	0.758	2.315	Cl
HETATM	10	Cl	0	0.650	0.684	-2.279	Cl
HETATM	11	C	0	2.842	2.428	0.004	C
HETATM	12	C	0	-3.158	-0.821	0.012	C
HETATM	13	C	0	-3.704	-0.490	-1.241	C
HETATM	14	C	0	-3.757	-0.391	1.209	C
HETATM	15	C	0	-4.880	0.266	-1.276	C
HETATM	16	C	0	-4.933	0.362	1.132	C
HETATM	17	C	0	-5.507	0.699	-0.100	C
HETATM	18	H	0	-5.312	0.531	-2.250	H
HETATM	19	H	0	-5.407	0.705	2.061	H
HETATM	20	C	0	1.562	-2.057	0.078	C
HETATM	21	C	0	2.160	-2.048	-1.200	C
HETATM	22	C	0	2.345	-1.929	1.244	C
HETATM	23	C	0	3.519	-1.741	-1.297	C
HETATM	24	C	0	3.702	-1.618	1.099	C
HETATM	25	C	0	4.292	-1.477	-0.161	C
HETATM	26	H	0	3.980	-1.689	-2.292	H
HETATM	27	H	0	4.309	-1.472	2.002	H
HETATM	28	C	0	-2.993	-0.884	-2.499	C
HETATM	29	H	0	-3.583	-0.625	-3.393	H
HETATM	30	H	0	-2.014	-0.371	-2.580	H
HETATM	31	H	0	-2.778	-1.968	-2.541	H
HETATM	32	C	0	-3.102	-0.678	2.525	C
HETATM	33	H	0	-2.926	-1.758	2.685	H
HETATM	34	H	0	-2.110	-0.190	2.591	H
HETATM	35	H	0	-3.713	-0.313	3.367	H
HETATM	36	C	0	-6.749	1.536	-0.165	C
HETATM	37	H	0	-6.506	2.605	-0.316	H
HETATM	38	H	0	-7.402	1.242	-1.005	H
HETATM	39	H	0	-7.339	1.472	0.765	H
HETATM	40	C	0	1.386	-2.433	-2.424	C
HETATM	41	H	0	1.797	-1.955	-3.327	H
HETATM	42	H	0	1.435	-3.529	-2.582	H
HETATM	43	H	0	0.322	-2.150	-2.365	H
HETATM	44	C	0	1.783	-2.205	2.604	C
HETATM	45	H	0	2.013	-3.247	2.903	H
HETATM	46	H	0	2.223	-1.542	3.367	H
HETATM	47	H	0	0.692	-2.073	2.650	H
HETATM	48	C	0	5.717	-1.033	-0.291	C
HETATM	49	H	0	5.778	0.071	-0.360	H
HETATM	50	H	0	6.327	-1.330	0.579	H
HETATM	51	H	0	6.195	-1.433	-1.202	H
HETATM	52	H	0	-2.572	-3.472	-0.707	H
HETATM	53	H	0	-0.259	-4.084	-0.671	H
HETATM	54	C	0	1.865	3.342	-0.021	C
HETATM	55	C	0	-1.363	1.763	-0.025	C
HETATM	56	H	0	-2.445	1.536	-0.027	H
HETATM	57	H	0	-1.111	2.851	-0.047	H
HETATM	58	F	0	1.378	3.851	-1.129	F
HETATM	59	F	0	1.357	3.884	1.063	F
HETATM	60	F	0	3.397	1.938	-1.076	F
HETATM	61	F	0	3.374	1.975	1.110	F

END

s2k.pdb

TITLE	s2k.pdb						
HETATM	1	Ru	0	0.113	-0.961	-0.252	Ru
HETATM	2	C	0	-0.078	2.977	1.153	C

HETATM	3	C	0	-1.578	2.693	1.189	C
HETATM	4	H	0	0.191	3.737	0.392	H
HETATM	5	H	0	-2.175	3.428	0.621	H
HETATM	6	C	0	-0.468	0.799	0.377	C
HETATM	7	N	0	-1.682	1.369	0.571	N
HETATM	8	N	0	0.485	1.678	0.791	N
HETATM	9	Cl	0	0.552	-0.462	-2.574	Cl
HETATM	10	Cl	0	-0.088	-1.873	1.991	Cl
HETATM	11	C	0	2.682	-2.473	-0.325	C
HETATM	12	C	0	-2.944	0.794	0.245	C
HETATM	13	C	0	-3.716	0.177	1.248	C
HETATM	14	C	0	-3.413	0.892	-1.082	C
HETATM	15	C	0	-4.962	-0.353	0.896	C
HETATM	16	C	0	-4.663	0.344	-1.390	C
HETATM	17	C	0	-5.447	-0.285	-0.416	C
HETATM	18	H	0	-5.566	-0.844	1.670	H
HETATM	19	H	0	-5.033	0.416	-2.421	H
HETATM	20	C	0	1.870	1.486	0.484	C
HETATM	21	C	0	2.732	0.953	1.467	C
HETATM	22	C	0	2.361	1.879	-0.779	C
HETATM	23	C	0	4.075	0.748	1.129	C
HETATM	24	C	0	3.709	1.653	-1.071	C
HETATM	25	C	0	4.574	1.074	-0.137	C
HETATM	26	H	0	4.749	0.322	1.883	H
HETATM	27	H	0	4.089	1.934	-2.061	H
HETATM	28	C	0	-3.197	0.052	2.646	C
HETATM	29	H	0	-3.863	-0.574	3.262	H
HETATM	30	H	0	-2.191	-0.408	2.661	H
HETATM	31	H	0	-3.116	1.032	3.154	H
HETATM	32	C	0	-2.578	1.549	-2.136	C
HETATM	33	H	0	-2.221	2.547	-1.819	H
HETATM	34	H	0	-1.673	0.953	-2.372	H
HETATM	35	H	0	-3.145	1.676	-3.073	H
HETATM	36	C	0	-6.767	-0.894	-0.779	C
HETATM	37	H	0	-6.639	-1.916	-1.185	H
HETATM	38	H	0	-7.437	-0.980	0.093	H
HETATM	39	H	0	-7.290	-0.312	-1.556	H
HETATM	40	C	0	2.237	0.639	2.843	C
HETATM	41	H	0	3.071	0.357	3.508	H
HETATM	42	H	0	1.722	1.503	3.301	H
HETATM	43	H	0	1.507	-0.193	2.837	H
HETATM	44	C	0	1.489	2.577	-1.778	C
HETATM	45	H	0	1.551	3.677	-1.656	H
HETATM	46	H	0	1.802	2.341	-2.807	H
HETATM	47	H	0	0.431	2.282	-1.696	H
HETATM	48	C	0	5.998	0.777	-0.495	C
HETATM	49	H	0	6.087	-0.224	-0.958	H
HETATM	50	H	0	6.401	1.499	-1.225	H
HETATM	51	H	0	6.657	0.777	0.390	H
HETATM	52	H	0	-1.978	2.668	2.221	H
HETATM	53	H	0	0.322	3.322	2.122	H
HETATM	54	C	0	1.536	-3.068	-0.693	C
HETATM	55	H	0	1.269	-3.082	-1.753	H
HETATM	56	C	0	-1.550	-1.563	-0.647	C
HETATM	57	H	0	-2.238	-1.975	0.121	H
HETATM	58	H	0	-1.920	-1.586	-1.696	H
HETATM	59	H	0	0.995	-3.667	0.043	H
HETATM	60	F	0	3.470	-1.819	-1.133	F
HETATM	61	F	0	3.167	-2.473	0.885	F

END

TITLE	s21.pdb						
HETATM	1	Ru	0	0.154	-0.908	-0.130	Ru
HETATM	2	Cl	0	-0.620	-1.389	2.134	Cl
HETATM	3	Cl	0	0.861	-0.602	-2.440	Cl
HETATM	4	C	0	-0.302	1.027	0.188	C
HETATM	5	N	0	-1.491	1.655	0.259	N
HETATM	6	C	0	-1.346	3.070	0.621	C
HETATM	7	C	0	0.174	3.257	0.715	C
HETATM	8	N	0	0.679	1.905	0.475	N
HETATM	9	C	0	-2.751	1.021	0.054	C
HETATM	10	C	0	-3.546	0.654	1.155	C
HETATM	11	C	0	-4.749	-0.018	0.910	C
HETATM	12	C	0	-5.172	-0.325	-0.387	C
HETATM	13	C	0	-4.377	0.084	-1.465	C
HETATM	14	C	0	-3.171	0.763	-1.268	C
HETATM	15	C	0	2.053	1.535	0.327	C
HETATM	16	C	0	2.695	1.746	-0.911	C
HETATM	17	C	0	3.996	1.267	-1.075	C
HETATM	18	C	0	4.666	0.595	-0.047	C
HETATM	19	C	0	4.028	0.452	1.189	C
HETATM	20	C	0	2.727	0.921	1.404	C
HETATM	21	C	0	-3.142	0.988	2.558	C
HETATM	22	C	0	-6.440	-1.090	-0.618	C
HETATM	23	C	0	-2.342	1.213	-2.431	C
HETATM	24	C	0	2.019	2.485	-2.024	C
HETATM	25	C	0	6.029	0.016	-0.275	C
HETATM	26	C	0	2.090	0.785	2.754	C
HETATM	27	H	0	-1.860	3.273	1.578	H
HETATM	28	H	0	-1.815	3.710	-0.149	H
HETATM	29	H	0	0.505	3.627	1.702	H
HETATM	30	H	0	0.568	3.954	-0.049	H
HETATM	31	H	0	-5.367	-0.319	1.766	H
HETATM	32	H	0	-4.708	-0.121	-2.492	H
HETATM	33	H	0	4.489	1.399	-2.047	H
HETATM	34	H	0	4.556	-0.038	2.018	H
HETATM	35	H	0	-3.544	1.972	2.870	H
HETATM	36	H	0	-2.048	1.006	2.681	H
HETATM	37	H	0	-3.532	0.242	3.270	H
HETATM	38	H	0	-7.177	-0.923	0.186	H
HETATM	39	H	0	-6.915	-0.822	-1.578	H
HETATM	40	H	0	-6.251	-2.180	-0.653	H
HETATM	41	H	0	-2.877	1.062	-3.383	H
HETATM	42	H	0	-1.379	0.668	-2.499	H
HETATM	43	H	0	-2.085	2.286	-2.358	H
HETATM	44	H	0	0.928	2.326	-2.033	H
HETATM	45	H	0	2.396	2.152	-3.004	H
HETATM	46	H	0	2.203	3.576	-1.953	H
HETATM	47	H	0	5.956	-1.020	-0.660	H
HETATM	48	H	0	6.604	0.590	-1.022	H
HETATM	49	H	0	6.621	-0.032	0.654	H
HETATM	50	H	0	2.854	0.620	3.531	H
HETATM	51	H	0	1.376	-0.060	2.800	H
HETATM	52	H	0	1.512	1.685	3.033	H
HETATM	53	C	0	-1.332	-1.812	-0.736	C
HETATM	54	H	0	-2.094	-2.229	-0.043	H
HETATM	55	H	0	-1.505	-1.977	-1.821	H
HETATM	56	C	0	1.666	-2.583	0.040	C
HETATM	57	C	0	0.525	-3.227	-0.425	C
HETATM	58	F	0	2.066	-2.677	1.299	F
HETATM	59	F	0	2.715	-2.351	-0.730	F
HETATM	60	H	0	-0.073	-3.792	0.296	H

HETATM	61	H	0	0.484	-3.478	-1.489	H
END							

s2PB.pdb

TITLE	s2PB.pdb						
HETATM	1	Ru	0	-0.033	-0.964	0.195	Ru
HETATM	2	C	0	1.145	3.165	-0.193	C
HETATM	3	C	0	-0.373	3.267	-0.374	C
HETATM	4	H	0	1.711	3.551	-1.059	H
HETATM	5	H	0	-0.668	3.635	-1.375	H
HETATM	6	C	0	0.213	1.038	-0.035	C
HETATM	7	N	0	-0.817	1.881	-0.197	N
HETATM	8	N	0	1.368	1.722	-0.047	N
HETATM	9	Cl	0	1.025	-1.351	-1.957	Cl
HETATM	10	Cl	0	-0.843	-0.624	2.455	Cl
HETATM	11	C	0	1.059	-2.499	0.854	C
HETATM	12	H	0	1.259	-2.474	1.936	H
HETATM	13	C	0	-2.179	1.450	-0.246	C
HETATM	14	C	0	-3.002	1.627	0.883	C
HETATM	15	C	0	-2.666	0.847	-1.423	C
HETATM	16	C	0	-4.306	1.126	0.836	C
HETATM	17	C	0	-3.979	0.362	-1.423	C
HETATM	18	C	0	-4.803	0.475	-0.299	C
HETATM	19	H	0	-4.946	1.235	1.721	H
HETATM	20	H	0	-4.364	-0.117	-2.333	H
HETATM	21	C	0	2.665	1.124	0.019	C
HETATM	22	C	0	3.175	0.713	1.264	C
HETATM	23	C	0	3.405	0.958	-1.167	C
HETATM	24	C	0	4.424	0.082	1.296	C
HETATM	25	C	0	4.651	0.329	-1.088	C
HETATM	26	C	0	5.167	-0.129	0.129	C
HETATM	27	H	0	4.828	-0.244	2.263	H
HETATM	28	H	0	5.225	0.176	-2.011	H
HETATM	29	C	0	-2.511	2.346	2.101	C
HETATM	30	H	0	-3.031	1.993	3.006	H
HETATM	31	H	0	-1.433	2.189	2.268	H
HETATM	32	H	0	-2.692	3.437	2.027	H
HETATM	33	C	0	-1.817	0.730	-2.651	C
HETATM	34	H	0	-1.209	1.636	-2.826	H
HETATM	35	H	0	-1.100	-0.112	-2.594	H
HETATM	36	H	0	-2.441	0.566	-3.545	H
HETATM	37	C	0	-6.182	-0.110	-0.298	C
HETATM	38	H	0	-6.176	-1.133	0.124	H
HETATM	39	H	0	-6.882	0.481	0.317	H
HETATM	40	H	0	-6.599	-0.188	-1.316	H
HETATM	41	C	0	2.410	0.954	2.529	C
HETATM	42	H	0	3.030	0.738	3.414	H
HETATM	43	H	0	2.065	2.002	2.609	H
HETATM	44	H	0	1.496	0.331	2.604	H
HETATM	45	C	0	2.886	1.444	-2.485	C
HETATM	46	H	0	3.153	2.505	-2.665	H
HETATM	47	H	0	3.313	0.861	-3.317	H
HETATM	48	H	0	1.789	1.348	-2.555	H
HETATM	49	C	0	6.481	-0.849	0.178	C
HETATM	50	H	0	6.350	-1.931	-0.015	H
HETATM	51	H	0	7.186	-0.477	-0.585	H
HETATM	52	H	0	6.966	-0.759	1.165	H
HETATM	53	H	0	-0.855	3.920	0.375	H
HETATM	54	H	0	1.510	3.695	0.706	H
HETATM	55	C	0	-0.257	-3.170	0.460	C

HETATM	56	H	0	-0.077	-3.890	-0.355	H
HETATM	57	H	0	-0.731	-3.613	1.351	H
HETATM	58	C	0	-1.439	-2.234	-0.143	C
HETATM	59	H	0	1.920	-2.757	0.220	H
HETATM	60	F	0	-2.557	-2.312	0.583	F
HETATM	61	F	0	-1.787	-2.586	-1.389	F

END

s2m.pdb

TITLE	s2m.pdb						
HETATM	1	Ru	0	0.114	-1.017	0.206	Ru
HETATM	2	Cl	0	1.115	-1.361	-1.977	Cl
HETATM	3	Cl	0	-0.651	-0.704	2.490	Cl
HETATM	4	C	0	0.135	1.030	-0.017	C
HETATM	5	N	0	1.252	1.779	0.000	N
HETATM	6	C	0	0.968	3.212	-0.120	C
HETATM	7	C	0	-0.558	3.249	-0.246	C
HETATM	8	N	0	-0.933	1.833	-0.141	N
HETATM	9	C	0	2.569	1.222	0.016	C
HETATM	10	C	0	3.268	1.070	-1.197	C
HETATM	11	C	0	4.521	0.454	-1.169	C
HETATM	12	C	0	5.090	-0.001	0.026	C
HETATM	13	C	0	4.394	0.208	1.222	C
HETATM	14	C	0	3.139	0.826	1.243	C
HETATM	15	C	0	-2.282	1.370	-0.205	C
HETATM	16	C	0	-3.112	1.479	0.925	C
HETATM	17	C	0	-4.417	0.980	0.840	C
HETATM	18	C	0	-4.905	0.394	-0.332	C
HETATM	19	C	0	-4.066	0.330	-1.451	C
HETATM	20	C	0	-2.756	0.815	-1.411	C
HETATM	21	C	0	2.698	1.558	-2.494	C
HETATM	22	C	0	6.409	-0.711	0.020	C
HETATM	23	C	0	2.438	1.080	2.542	C
HETATM	24	C	0	-2.635	2.130	2.187	C
HETATM	25	C	0	-6.288	-0.181	-0.382	C
HETATM	26	C	0	-1.879	0.745	-2.625	C
HETATM	27	H	0	1.485	3.630	-1.002	H
HETATM	28	H	0	1.342	3.752	0.770	H
HETATM	29	H	0	-0.905	3.662	-1.211	H
HETATM	30	H	0	-1.045	3.831	0.557	H
HETATM	31	H	0	5.059	0.308	-2.114	H
HETATM	32	H	0	4.843	-0.109	2.173	H
HETATM	33	H	0	-5.065	1.043	1.724	H
HETATM	34	H	0	-4.440	-0.108	-2.385	H
HETATM	35	H	0	3.016	2.598	-2.709	H
HETATM	36	H	0	1.596	1.532	-2.501	H
HETATM	37	H	0	3.039	0.934	-3.335	H
HETATM	38	H	0	7.090	-0.313	-0.751	H
HETATM	39	H	0	6.280	-1.788	-0.201	H
HETATM	40	H	0	6.920	-0.645	0.996	H
HETATM	41	H	0	3.105	0.874	3.395	H
HETATM	42	H	0	1.532	0.456	2.670	H
HETATM	43	H	0	2.099	2.129	2.629	H
HETATM	44	H	0	-1.548	2.016	2.327	H
HETATM	45	H	0	-3.119	1.681	3.070	H
HETATM	46	H	0	-2.875	3.212	2.201	H
HETATM	47	H	0	-6.278	-1.265	-0.158	H
HETATM	48	H	0	-6.746	-0.070	-1.379	H
HETATM	49	H	0	-6.958	0.289	0.358	H
HETATM	50	H	0	-2.462	0.466	-3.517	H

HETATM	51	H	0	-1.064	0.002	-2.518	H
HETATM	52	H	0	-1.387	1.713	-2.836	H
HETATM	53	C	0	1.264	-2.624	0.860	C
HETATM	54	H	0	2.138	-2.730	0.201	H
HETATM	55	H	0	1.466	-2.507	1.935	H
HETATM	56	C	0	-1.389	-2.046	-0.183	C
HETATM	57	C	0	0.029	-3.253	0.464	C
HETATM	58	F	0	-1.738	-2.472	-1.387	F
HETATM	59	F	0	-2.434	-2.257	0.597	F
HETATM	60	H	0	0.062	-3.851	-0.458	H
HETATM	61	H	0	-0.594	-3.651	1.278	H

END

s2n.pdb

TITLE	s2n.pdb						
HETATM	1	Ru	0	0.390	-0.978	0.190	Ru
HETATM	2	C	0	0.591	3.216	-0.114	C
HETATM	3	C	0	-0.936	3.126	-0.065	C
HETATM	4	H	0	0.965	3.594	-1.086	H
HETATM	5	H	0	-1.428	3.587	-0.940	H
HETATM	6	C	0	-0.052	0.962	0.041	C
HETATM	7	N	0	-1.188	1.682	-0.045	N
HETATM	8	N	0	0.997	1.825	0.078	N
HETATM	9	Cl	0	0.857	-1.384	-2.161	Cl
HETATM	10	Cl	0	0.250	-0.856	2.611	Cl
HETATM	11	C	0	1.996	-2.711	0.535	C
HETATM	12	C	0	-2.510	1.151	-0.123	C
HETATM	13	C	0	-3.304	1.088	1.037	C
HETATM	14	C	0	-3.000	0.722	-1.371	C
HETATM	15	C	0	-4.602	0.584	0.926	C
HETATM	16	C	0	-4.300	0.208	-1.434	C
HETATM	17	C	0	-5.113	0.133	-0.297	C
HETATM	18	H	0	-5.227	0.526	1.827	H
HETATM	19	H	0	-4.688	-0.135	-2.402	H
HETATM	20	C	0	2.339	1.341	-0.036	C
HETATM	21	C	0	3.111	1.144	1.131	C
HETATM	22	C	0	2.882	1.091	-1.316	C
HETATM	23	C	0	4.375	0.557	0.997	C
HETATM	24	C	0	4.150	0.508	-1.399	C
HETATM	25	C	0	4.894	0.204	-0.254	C
HETATM	26	H	0	4.975	0.385	1.900	H
HETATM	27	H	0	4.562	0.282	-2.391	H
HETATM	28	C	0	-2.742	1.477	2.369	C
HETATM	29	H	0	-3.487	1.344	3.170	H
HETATM	30	H	0	-1.857	0.862	2.623	H
HETATM	31	H	0	-2.413	2.533	2.401	H
HETATM	32	C	0	-2.139	0.787	-2.594	C
HETATM	33	H	0	-1.658	1.776	-2.712	H
HETATM	34	H	0	-1.315	0.046	-2.560	H
HETATM	35	H	0	-2.725	0.588	-3.506	H
HETATM	36	C	0	-6.493	-0.447	-0.380	C
HETATM	37	H	0	-6.482	-1.537	-0.188	H
HETATM	38	H	0	-7.173	-0.002	0.366	H
HETATM	39	H	0	-6.941	-0.307	-1.379	H
HETATM	40	C	0	2.625	1.608	2.468	C
HETATM	41	H	0	3.378	1.416	3.249	H
HETATM	42	H	0	2.421	2.695	2.464	H
HETATM	43	H	0	1.692	1.098	2.767	H
HETATM	44	C	0	2.164	1.507	-2.563	C
HETATM	45	H	0	2.432	2.549	-2.833	H
HETATM	46	H	0	2.439	0.864	-3.414	H

HETATM	47	H	0	1.069	1.451	-2.465	H
HETATM	48	C	0	6.218	-0.488	-0.366	C
HETATM	49	H	0	6.089	-1.588	-0.380	H
HETATM	50	H	0	6.748	-0.223	-1.297	H
HETATM	51	H	0	6.880	-0.257	0.485	H
HETATM	52	H	0	-1.361	3.601	0.839	H
HETATM	53	H	0	1.012	3.863	0.676	H
HETATM	54	C	0	0.831	-3.410	0.473	C
HETATM	55	H	0	0.475	-3.829	-0.477	H
HETATM	56	C	0	-1.306	-1.665	0.057	C
HETATM	57	H	0	2.409	-2.394	1.502	H
HETATM	58	H	0	0.279	-3.671	1.386	H
HETATM	59	H	0	2.610	-2.560	-0.363	H
HETATM	60	F	0	-1.805	-2.337	-0.960	F
HETATM	61	F	0	-2.237	-1.680	0.983	F

END

a2k.pdb

TITLE	a2k.pdb						
HETATM	1	Ru	0	-0.264	0.867	0.062	Ru
HETATM	2	C	0	-0.350	-3.333	0.224	C
HETATM	3	C	0	1.169	-3.180	0.310	C
HETATM	4	H	0	-0.676	-3.814	-0.719	H
HETATM	5	H	0	1.708	-3.735	-0.478	H
HETATM	6	C	0	0.203	-1.053	0.140	C
HETATM	7	N	0	1.370	-1.737	0.143	N
HETATM	8	N	0	-0.812	-1.949	0.272	N
HETATM	9	Cl	0	-0.679	1.061	-2.320	Cl
HETATM	10	Cl	0	-0.141	0.978	2.489	Cl
HETATM	11	C	0	-1.852	2.709	0.180	C
HETATM	12	C	0	2.673	-1.181	-0.006	C
HETATM	13	C	0	3.462	-0.932	1.133	C
HETATM	14	C	0	3.152	-0.903	-1.302	C
HETATM	15	C	0	4.741	-0.395	0.951	C
HETATM	16	C	0	4.436	-0.364	-1.437	C
HETATM	17	C	0	5.241	-0.101	-0.323	C
HETATM	18	H	0	5.359	-0.189	1.835	H
HETATM	19	H	0	4.815	-0.145	-2.444	H
HETATM	20	C	0	-2.178	-1.561	0.095	C
HETATM	21	C	0	-2.983	-1.314	1.230	C
HETATM	22	C	0	-2.712	-1.470	-1.208	C
HETATM	23	C	0	-4.291	-0.861	1.029	C
HETATM	24	C	0	-4.027	-1.017	-1.359	C
HETATM	25	C	0	-4.821	-0.686	-0.256	C
HETATM	26	H	0	-4.919	-0.657	1.905	H
HETATM	27	H	0	-4.441	-0.925	-2.371	H
HETATM	28	C	0	2.918	-1.178	2.506	C
HETATM	29	H	0	3.621	-0.830	3.280	H
HETATM	30	H	0	1.958	-0.646	2.655	H
HETATM	31	H	0	2.725	-2.250	2.700	H
HETATM	32	C	0	2.290	-1.155	-2.499	C
HETATM	33	H	0	1.878	-2.182	-2.507	H
HETATM	34	H	0	1.419	-0.469	-2.523	H
HETATM	35	H	0	2.853	-1.012	-3.435	H
HETATM	36	C	0	6.599	0.512	-0.491	C
HETATM	37	H	0	6.536	1.616	-0.542	H
HETATM	38	H	0	7.269	0.270	0.350	H
HETATM	39	H	0	7.087	0.182	-1.424	H
HETATM	40	C	0	-2.475	-1.589	2.609	C
HETATM	41	H	0	-3.237	-1.345	3.367	H
HETATM	42	H	0	-2.214	-2.656	2.737	H

HETATM	43	H	0	-1.570	-0.999	2.837	H
HETATM	44	C	0	-1.937	-1.922	-2.408	C
HETATM	45	H	0	-2.142	-2.991	-2.620	H
HETATM	46	H	0	-2.219	-1.347	-3.303	H
HETATM	47	H	0	-0.849	-1.801	-2.286	H
HETATM	48	C	0	-6.210	-0.156	-0.444	C
HETATM	49	H	0	-6.208	0.946	-0.544	H
HETATM	50	H	0	-6.683	-0.553	-1.358	H
HETATM	51	H	0	-6.863	-0.395	0.413	H
HETATM	52	H	0	1.574	-3.514	1.284	H
HETATM	53	H	0	-0.774	-3.919	1.058	H
HETATM	54	C	0	-0.834	3.595	0.114	C
HETATM	55	C	0	1.422	1.520	-0.107	C
HETATM	56	H	0	2.195	1.427	0.684	H
HETATM	57	H	0	1.717	2.104	-1.008	H
HETATM	58	H	0	-2.265	2.471	1.164	H
HETATM	59	H	0	-2.394	2.472	-0.739	H
HETATM	60	F	0	-0.368	4.112	-0.988	F
HETATM	61	F	0	-0.230	4.111	1.149	F

END

a2l.pdb

TITLE	a2l.pdb						
HETATM	1	Ru	0	-0.119	0.897	0.039	Ru
HETATM	2	Cl	0	-0.993	0.983	-2.224	Cl
HETATM	3	Cl	0	0.667	0.910	2.338	Cl
HETATM	4	C	0	0.065	-1.129	0.026	C
HETATM	5	N	0	-0.997	-1.945	0.162	N
HETATM	6	C	0	-0.617	-3.361	0.158	C
HETATM	7	C	0	0.908	-3.304	0.026	C
HETATM	8	N	0	1.186	-1.865	-0.047	N
HETATM	9	C	0	-2.342	-1.461	0.140	C
HETATM	10	C	0	-3.047	-1.427	-1.080	C
HETATM	11	C	0	-4.329	-0.872	-1.091	C
HETATM	12	C	0	-4.922	-0.367	0.073	C
HETATM	13	C	0	-4.220	-0.464	1.279	C
HETATM	14	C	0	-2.935	-1.016	1.339	C
HETATM	15	C	0	2.505	-1.327	-0.137	C
HETATM	16	C	0	3.312	-1.262	1.012	C
HETATM	17	C	0	4.582	-0.686	0.898	C
HETATM	18	C	0	5.058	-0.188	-0.319	C
HETATM	19	C	0	4.243	-0.296	-1.453	C
HETATM	20	C	0	2.968	-0.865	-1.385	C
HETATM	21	C	0	-2.462	-1.996	-2.337	C
HETATM	22	C	0	-6.278	0.269	0.019	C
HETATM	23	C	0	-2.229	-1.152	2.653	C
HETATM	24	C	0	2.852	-1.813	2.327	C
HETATM	25	C	0	6.404	0.467	-0.405	C
HETATM	26	C	0	2.111	-0.975	-2.608	C
HETATM	27	H	0	-1.105	-3.881	-0.688	H
HETATM	28	H	0	-0.956	-3.854	1.088	H
HETATM	29	H	0	1.285	-3.810	-0.882	H
HETATM	30	H	0	1.430	-3.748	0.894	H
HETATM	31	H	0	-4.873	-0.819	-2.043	H
HETATM	32	H	0	-4.687	-0.109	2.207	H
HETATM	33	H	0	5.213	-0.617	1.794	H
HETATM	34	H	0	4.611	0.067	-2.422	H
HETATM	35	H	0	-2.738	-3.063	-2.458	H
HETATM	36	H	0	-1.363	-1.923	-2.359	H
HETATM	37	H	0	-2.834	-1.459	-3.224	H
HETATM	38	H	0	-6.969	-0.289	-0.636	H

HETATM	39	H	0	-6.221	1.295	-0.389	H
HETATM	40	H	0	-6.739	0.344	1.018	H
HETATM	41	H	0	-2.914	-0.940	3.491	H
HETATM	42	H	0	-1.365	-0.465	2.745	H
HETATM	43	H	0	-1.827	-2.171	2.801	H
HETATM	44	H	0	1.760	-1.729	2.455	H
HETATM	45	H	0	3.315	-1.269	3.167	H
HETATM	46	H	0	3.134	-2.879	2.440	H
HETATM	47	H	0	7.104	0.074	0.351	H
HETATM	48	H	0	6.329	1.557	-0.230	H
HETATM	49	H	0	6.864	0.338	-1.399	H
HETATM	50	H	0	2.692	-0.766	-3.521	H
HETATM	51	H	0	1.256	-0.269	-2.590	H
HETATM	52	H	0	1.669	-1.984	-2.715	H
HETATM	53	C	0	1.325	1.953	-0.430	C
HETATM	54	H	0	1.482	2.256	-1.484	H
HETATM	55	H	0	2.095	2.249	0.309	H
HETATM	56	C	0	-1.435	2.495	0.499	C
HETATM	57	H	0	-2.261	2.462	-0.223	H
HETATM	58	H	0	-1.657	2.438	1.572	H
HETATM	59	C	0	-0.306	3.269	0.130	C
HETATM	60	F	0	-0.321	3.960	-1.000	F
HETATM	61	F	0	0.370	3.933	1.055	F

END

a2NB.pdb

TITLE	a2NB.pdb						
HETATM	1	Ru	0	0.223	0.833	0.151	Ru
HETATM	2	C	0	0.384	-3.334	-0.401	C
HETATM	3	C	0	-1.067	-3.229	0.067	C
HETATM	4	H	0	0.988	-4.031	0.204	H
HETATM	5	H	0	-1.220	-3.631	1.089	H
HETATM	6	C	0	-0.153	-1.105	-0.033	C
HETATM	7	N	0	-1.311	-1.781	0.066	N
HETATM	8	N	0	0.863	-1.960	-0.238	N
HETATM	9	Cl	0	1.322	1.215	2.197	Cl
HETATM	10	Cl	0	-0.927	0.610	-2.058	Cl
HETATM	11	C	0	1.387	2.118	-0.911	C
HETATM	12	H	0	1.401	1.979	-2.001	H
HETATM	13	C	0	-2.608	-1.201	0.203	C
HETATM	14	C	0	-3.532	-1.324	-0.852	C
HETATM	15	C	0	-2.943	-0.520	1.386	C
HETATM	16	C	0	-4.789	-0.731	-0.706	C
HETATM	17	C	0	-4.209	0.069	1.486	C
HETATM	18	C	0	-5.140	-0.021	0.448	C
HETATM	19	H	0	-5.508	-0.809	-1.531	H
HETATM	20	H	0	-4.473	0.602	2.408	H
HETATM	21	C	0	2.231	-1.541	-0.178	C
HETATM	22	C	0	2.883	-1.099	-1.347	C
HETATM	23	C	0	2.890	-1.567	1.066	C
HETATM	24	C	0	4.198	-0.635	-1.232	C
HETATM	25	C	0	4.203	-1.098	1.133	C
HETATM	26	C	0	4.865	-0.614	-0.002	C
HETATM	27	H	0	4.714	-0.280	-2.133	H
HETATM	28	H	0	4.715	-1.092	2.103	H
HETATM	29	C	0	-3.190	-2.054	-2.115	C
HETATM	30	H	0	-3.745	-1.638	-2.972	H
HETATM	31	H	0	-2.116	-1.974	-2.352	H
HETATM	32	H	0	-3.455	-3.129	-2.059	H
HETATM	33	C	0	-1.977	-0.424	2.528	C
HETATM	34	H	0	-1.410	-1.360	2.680	H

HETATM	35	H	0	-1.219	0.373	2.390	H
HETATM	36	H	0	-2.499	-0.187	3.470	H
HETATM	37	C	0	-6.479	0.644	0.555	C
HETATM	38	H	0	-6.497	1.598	-0.005	H
HETATM	39	H	0	-7.286	0.019	0.134	H
HETATM	40	H	0	-6.741	0.881	1.600	H
HETATM	41	C	0	2.197	-1.142	-2.676	C
HETATM	42	H	0	2.828	-0.699	-3.463	H
HETATM	43	H	0	1.971	-2.181	-2.983	H
HETATM	44	H	0	1.232	-0.600	-2.667	H
HETATM	45	C	0	2.197	-2.083	2.290	C
HETATM	46	H	0	2.067	-3.183	2.260	H
HETATM	47	H	0	2.772	-1.846	3.199	H
HETATM	48	H	0	1.198	-1.632	2.416	H
HETATM	49	C	0	6.253	-0.059	0.105	C
HETATM	50	H	0	6.229	1.014	0.374	H
HETATM	51	H	0	6.842	-0.566	0.888	H
HETATM	52	H	0	6.805	-0.137	-0.846	H
HETATM	53	H	0	-1.776	-3.742	-0.603	H
HETATM	54	H	0	0.470	-3.643	-1.461	H
HETATM	55	C	0	0.364	3.193	-0.493	C
HETATM	56	C	0	-0.863	2.551	0.188	C
HETATM	57	H	0	-1.748	2.577	-0.462	H
HETATM	58	H	0	-1.031	2.912	1.215	H
HETATM	59	H	0	2.378	2.247	-0.447	H
HETATM	60	F	0	-0.046	3.885	-1.598	F
HETATM	61	F	0	0.949	4.104	0.341	F

END

a2m.pdb

TITLE	a2m.pdb						
HETATM	1	Ru	0	-0.119	0.897	0.039	Ru
HETATM	2	Cl	0	-0.993	0.983	-2.224	Cl
HETATM	3	Cl	0	0.667	0.910	2.338	Cl
HETATM	4	C	0	0.065	-1.129	0.026	C
HETATM	5	N	0	-0.997	-1.945	0.162	N
HETATM	6	C	0	-0.617	-3.361	0.158	C
HETATM	7	C	0	0.908	-3.304	0.026	C
HETATM	8	N	0	1.186	-1.865	-0.047	N
HETATM	9	C	0	-2.342	-1.461	0.140	C
HETATM	10	C	0	-3.047	-1.427	-1.080	C
HETATM	11	C	0	-4.329	-0.872	-1.091	C
HETATM	12	C	0	-4.922	-0.367	0.073	C
HETATM	13	C	0	-4.220	-0.464	1.279	C
HETATM	14	C	0	-2.935	-1.016	1.339	C
HETATM	15	C	0	2.505	-1.327	-0.137	C
HETATM	16	C	0	3.312	-1.262	1.012	C
HETATM	17	C	0	4.582	-0.686	0.898	C
HETATM	18	C	0	5.058	-0.188	-0.319	C
HETATM	19	C	0	4.243	-0.296	-1.453	C
HETATM	20	C	0	2.968	-0.865	-1.385	C
HETATM	21	C	0	-2.462	-1.996	-2.337	C
HETATM	22	C	0	-6.278	0.269	0.019	C
HETATM	23	C	0	-2.229	-1.152	2.653	C
HETATM	24	C	0	2.852	-1.813	2.327	C
HETATM	25	C	0	6.404	0.467	-0.405	C
HETATM	26	C	0	2.111	-0.975	-2.608	C
HETATM	27	H	0	-1.105	-3.881	-0.688	H
HETATM	28	H	0	-0.956	-3.854	1.088	H
HETATM	29	H	0	1.285	-3.810	-0.882	H
HETATM	30	H	0	1.430	-3.748	0.894	H

HETATM	31	H	0	-4.873	-0.819	-2.043	H
HETATM	32	H	0	-4.687	-0.109	2.207	H
HETATM	33	H	0	5.213	-0.617	1.794	H
HETATM	34	H	0	4.611	0.067	-2.422	H
HETATM	35	H	0	-2.738	-3.063	-2.458	H
HETATM	36	H	0	-1.363	-1.923	-2.359	H
HETATM	37	H	0	-2.834	-1.459	-3.224	H
HETATM	38	H	0	-6.969	-0.289	-0.636	H
HETATM	39	H	0	-6.221	1.295	-0.389	H
HETATM	40	H	0	-6.739	0.344	1.018	H
HETATM	41	H	0	-2.914	-0.940	3.491	H
HETATM	42	H	0	-1.365	-0.465	2.745	H
HETATM	43	H	0	-1.827	-2.171	2.801	H
HETATM	44	H	0	1.760	-1.729	2.455	H
HETATM	45	H	0	3.315	-1.269	3.167	H
HETATM	46	H	0	3.134	-2.879	2.440	H
HETATM	47	H	0	7.104	0.074	0.351	H
HETATM	48	H	0	6.329	1.557	-0.230	H
HETATM	49	H	0	6.864	0.338	-1.399	H
HETATM	50	H	0	2.692	-0.766	-3.521	H
HETATM	51	H	0	1.256	-0.269	-2.590	H
HETATM	52	H	0	1.669	-1.984	-2.715	H
HETATM	53	C	0	1.325	1.953	-0.430	C
HETATM	54	H	0	1.482	2.256	-1.484	H
HETATM	55	H	0	2.095	2.249	0.309	H
HETATM	56	C	0	-1.435	2.495	0.499	C
HETATM	57	H	0	-2.261	2.462	-0.223	H
HETATM	58	H	0	-1.657	2.438	1.572	H
HETATM	59	C	0	-0.306	3.269	0.130	C
HETATM	60	F	0	-0.321	3.960	-1.000	F
HETATM	61	F	0	0.370	3.933	1.055	F

END

a2n.pdb

TITLE	a2n.pdb						
HETATM	1	Ru	0	-0.264	0.867	0.062	Ru
HETATM	2	C	0	-0.350	-3.333	0.224	C
HETATM	3	C	0	1.169	-3.180	0.310	C
HETATM	4	H	0	-0.676	-3.814	-0.719	H
HETATM	5	H	0	1.708	-3.735	-0.478	H
HETATM	6	C	0	0.203	-1.053	0.140	C
HETATM	7	N	0	1.370	-1.737	0.143	N
HETATM	8	N	0	-0.812	-1.949	0.272	N
HETATM	9	Cl	0	-0.679	1.061	-2.320	Cl
HETATM	10	Cl	0	-0.141	0.978	2.489	Cl
HETATM	11	C	0	-1.852	2.709	0.180	C
HETATM	12	C	0	2.673	-1.181	-0.006	C
HETATM	13	C	0	3.462	-0.932	1.133	C
HETATM	14	C	0	3.152	-0.903	-1.302	C
HETATM	15	C	0	4.741	-0.395	0.951	C
HETATM	16	C	0	4.436	-0.364	-1.437	C
HETATM	17	C	0	5.241	-0.101	-0.323	C
HETATM	18	H	0	5.359	-0.189	1.835	H
HETATM	19	H	0	4.815	-0.145	-2.444	H
HETATM	20	C	0	-2.178	-1.561	0.095	C
HETATM	21	C	0	-2.983	-1.314	1.230	C
HETATM	22	C	0	-2.712	-1.470	-1.208	C
HETATM	23	C	0	-4.291	-0.861	1.029	C
HETATM	24	C	0	-4.027	-1.017	-1.359	C
HETATM	25	C	0	-4.821	-0.686	-0.256	C
HETATM	26	H	0	-4.919	-0.657	1.905	H

HETATM	27	H	0	-4.441	-0.925	-2.371	H
HETATM	28	C	0	2.918	-1.178	2.506	C
HETATM	29	H	0	3.621	-0.830	3.280	H
HETATM	30	H	0	1.958	-0.646	2.655	H
HETATM	31	H	0	2.725	-2.250	2.700	H
HETATM	32	C	0	2.290	-1.155	-2.499	C
HETATM	33	H	0	1.878	-2.182	-2.507	H
HETATM	34	H	0	1.419	-0.469	-2.523	H
HETATM	35	H	0	2.853	-1.012	-3.435	H
HETATM	36	C	0	6.599	0.512	-0.491	C
HETATM	37	H	0	6.536	1.616	-0.542	H
HETATM	38	H	0	7.269	0.270	0.350	H
HETATM	39	H	0	7.087	0.182	-1.424	H
HETATM	40	C	0	-2.475	-1.589	2.609	C
HETATM	41	H	0	-3.237	-1.345	3.367	H
HETATM	42	H	0	-2.214	-2.656	2.737	H
HETATM	43	H	0	-1.570	-0.999	2.837	H
HETATM	44	C	0	-1.937	-1.922	-2.408	C
HETATM	45	H	0	-2.142	-2.991	-2.620	H
HETATM	46	H	0	-2.219	-1.347	-3.303	H
HETATM	47	H	0	-0.849	-1.801	-2.286	H
HETATM	48	C	0	-6.210	-0.156	-0.444	C
HETATM	49	H	0	-6.208	0.946	-0.544	H
HETATM	50	H	0	-6.683	-0.553	-1.358	H
HETATM	51	H	0	-6.863	-0.395	0.413	H
HETATM	52	H	0	1.574	-3.514	1.284	H
HETATM	53	H	0	-0.774	-3.919	1.058	H
HETATM	54	C	0	-0.834	3.595	0.114	C
HETATM	55	C	0	1.422	1.520	-0.107	C
HETATM	56	H	0	2.195	1.427	0.684	H
HETATM	57	H	0	1.717	2.104	-1.008	H
HETATM	58	H	0	-2.265	2.471	1.164	H
HETATM	59	H	0	-2.394	2.472	-0.739	H
HETATM	60	F	0	-0.368	4.112	-0.988	F
HETATM	61	F	0	-0.230	4.111	1.149	F

END

sc3g.pdb

TITLE	sc3g.pdb						
HETATM	1	Ru	0	-0.262	0.936	-0.279	Ru
HETATM	2	C	0	-0.244	-2.860	1.519	C
HETATM	3	C	0	1.276	-2.689	1.492	C
HETATM	4	H	0	-0.587	-3.747	0.953	H
HETATM	5	H	0	1.796	-3.495	0.942	H
HETATM	6	C	0	0.288	-0.824	0.460	C
HETATM	7	N	0	1.460	-1.407	0.803	N
HETATM	8	N	0	-0.718	-1.636	0.883	N
HETATM	9	Cl	0	-0.825	0.126	-2.500	Cl
HETATM	10	Cl	0	-0.236	1.907	1.918	Cl
HETATM	11	C	0	-2.202	2.550	-0.778	C
HETATM	12	C	0	2.753	-0.970	0.396	C
HETATM	13	C	0	3.539	-0.186	1.260	C
HETATM	14	C	0	3.214	-1.332	-0.883	C
HETATM	15	C	0	4.797	0.237	0.815	C
HETATM	16	C	0	4.479	-0.895	-1.288	C
HETATM	17	C	0	5.280	-0.106	-0.453	C
HETATM	18	H	0	5.413	0.855	1.480	H
HETATM	19	H	0	4.843	-1.171	-2.286	H
HETATM	20	C	0	-2.084	-1.399	0.532	C
HETATM	21	C	0	-2.923	-0.654	1.386	C
HETATM	22	C	0	-2.578	-1.930	-0.682	C

HETATM	23	C	0	-4.217	-0.345	0.943	C
HETATM	24	C	0	-3.877	-1.610	-1.073	C
HETATM	25	C	0	-4.702	-0.793	-0.286	C
HETATM	26	H	0	-4.863	0.261	1.593	H
HETATM	27	H	0	-4.252	-1.997	-2.029	H
HETATM	28	C	0	3.016	0.218	2.603	C
HETATM	29	H	0	3.754	0.822	3.156	H
HETATM	30	H	0	2.085	0.811	2.514	H
HETATM	31	H	0	2.766	-0.657	3.232	H
HETATM	32	C	0	2.329	-2.098	-1.818	C
HETATM	33	H	0	1.899	-3.003	-1.349	H
HETATM	34	H	0	1.468	-1.482	-2.151	H
HETATM	35	H	0	2.877	-2.416	-2.720	H
HETATM	36	C	0	6.615	0.392	-0.921	C
HETATM	37	H	0	6.528	1.390	-1.391	H
HETATM	38	H	0	7.331	0.498	-0.088	H
HETATM	39	H	0	7.064	-0.276	-1.675	H
HETATM	40	C	0	-2.523	-0.270	2.777	C
HETATM	41	H	0	-2.723	0.796	2.975	H
HETATM	42	H	0	-3.113	-0.855	3.509	H
HETATM	43	H	0	-1.455	-0.436	2.981	H
HETATM	44	C	0	-1.749	-2.853	-1.521	C
HETATM	45	H	0	-1.878	-3.906	-1.200	H
HETATM	46	H	0	-2.043	-2.797	-2.581	H
HETATM	47	H	0	-0.674	-2.617	-1.474	H
HETATM	48	C	0	-6.067	-0.405	-0.765	C
HETATM	49	H	0	-6.015	0.445	-1.472	H
HETATM	50	H	0	-6.566	-1.229	-1.305	H
HETATM	51	H	0	-6.723	-0.092	0.064	H
HETATM	52	H	0	1.722	-2.645	2.503	H
HETATM	53	H	0	-0.650	-2.945	2.544	H
HETATM	54	C	0	-1.067	3.230	-1.043	C
HETATM	55	H	0	-0.615	3.131	-2.033	H
HETATM	56	C	0	1.377	1.535	-0.735	C
HETATM	57	H	0	2.210	0.948	-1.177	H
HETATM	58	H	0	-0.666	3.961	-0.334	H
HETATM	59	H	0	-2.687	1.849	-1.471	H
HETATM	60	F	0	1.769	2.806	-0.660	F
HETATM	61	F	0	-2.907	2.742	0.332	F

END

sc3h.pdb

TITLE	sc3h.pdb						
HETATM	1	Ru	0	0.221	-0.949	-0.134	Ru
HETATM	2	Cl	0	0.935	-0.741	-2.470	Cl
HETATM	3	Cl	0	-0.425	-1.262	2.189	Cl
HETATM	4	C	0	-0.119	1.031	0.216	C
HETATM	5	N	0	0.921	1.836	0.508	N
HETATM	6	C	0	0.506	3.211	0.790	C
HETATM	7	C	0	-1.024	3.120	0.725	C
HETATM	8	N	0	-1.262	1.728	0.323	N
HETATM	9	C	0	2.266	1.393	0.290	C
HETATM	10	C	0	2.843	1.553	-0.988	C
HETATM	11	C	0	4.112	1.017	-1.216	C
HETATM	12	C	0	4.817	0.345	-0.210	C
HETATM	13	C	0	4.246	0.252	1.063	C
HETATM	14	C	0	2.979	0.781	1.343	C
HETATM	15	C	0	-2.559	1.186	0.082	C
HETATM	16	C	0	-3.402	0.857	1.159	C
HETATM	17	C	0	-4.644	0.277	0.877	C
HETATM	18	C	0	-5.058	0.026	-0.434	C

HETATM	19	C	0	-4.214	0.398	-1.488	C
HETATM	20	C	0	-2.967	0.984	-1.252	C
HETATM	21	C	0	2.136	2.308	-2.071	C
HETATM	22	C	0	6.150	-0.274	-0.502	C
HETATM	23	C	0	2.424	0.728	2.731	C
HETATM	24	C	0	-3.002	1.130	2.577	C
HETATM	25	C	0	-6.369	-0.648	-0.708	C
HETATM	26	C	0	-2.082	1.388	-2.391	C
HETATM	27	H	0	0.927	3.900	0.033	H
HETATM	28	H	0	0.878	3.537	1.778	H
HETATM	29	H	0	-1.469	3.810	-0.015	H
HETATM	30	H	0	-1.506	3.322	1.699	H
HETATM	31	H	0	4.554	1.114	-2.216	H
HETATM	32	H	0	4.801	-0.239	1.872	H
HETATM	33	H	0	-5.299	0.002	1.714	H
HETATM	34	H	0	-4.536	0.237	-2.525	H
HETATM	35	H	0	1.043	2.168	-2.035	H
HETATM	36	H	0	2.468	1.978	-3.067	H
HETATM	37	H	0	2.340	3.395	-1.997	H
HETATM	38	H	0	6.034	-1.247	-1.016	H
HETATM	39	H	0	6.728	-0.464	0.418	H
HETATM	40	H	0	6.763	0.358	-1.168	H
HETATM	41	H	0	3.167	0.322	3.437	H
HETATM	42	H	0	1.517	0.097	2.798	H
HETATM	43	H	0	2.137	1.733	3.092	H
HETATM	44	H	0	-1.913	1.046	2.721	H
HETATM	45	H	0	-3.474	0.411	3.266	H
HETATM	46	H	0	-3.320	2.141	2.900	H
HETATM	47	H	0	-6.247	-1.745	-0.785	H
HETATM	48	H	0	-7.103	-0.467	0.095	H
HETATM	49	H	0	-6.815	-0.312	-1.661	H
HETATM	50	H	0	-2.627	1.352	-3.349	H
HETATM	51	H	0	-1.197	0.729	-2.488	H
HETATM	52	H	0	-1.690	2.415	-2.265	H
HETATM	53	C	0	-1.254	-1.909	-0.690	C
HETATM	54	F	0	-2.206	-2.454	0.043	F
HETATM	55	H	0	-1.504	-2.046	-1.765	H
HETATM	56	C	0	1.645	-2.548	-0.013	C
HETATM	57	C	0	0.500	-3.193	-0.530	C
HETATM	58	F	0	2.076	-2.845	1.221	F
HETATM	59	H	0	2.466	-2.214	-0.665	H
HETATM	60	H	0	0.482	-3.385	-1.610	H
HETATM	61	H	0	-0.022	-3.895	0.133	H

END

sc3NA.pdb

TITLE	sc3NA.pdb						
HETATM	1	Ru	0	0.042	-0.963	-0.133	Ru
HETATM	2	C	0	0.734	3.199	0.607	C
HETATM	3	C	0	-0.777	3.233	0.360	C
HETATM	4	H	0	1.299	3.865	-0.068	H
HETATM	5	H	0	-1.056	3.811	-0.542	H
HETATM	6	C	0	-0.013	1.046	0.131	C
HETATM	7	N	0	-1.111	1.816	0.169	N
HETATM	8	N	0	1.079	1.798	0.343	N
HETATM	9	Cl	0	1.029	-0.787	-2.370	Cl
HETATM	10	Cl	0	-0.945	-1.171	2.066	Cl
HETATM	11	C	0	1.365	-2.368	0.169	C
HETATM	12	C	0	-2.441	1.319	0.003	C
HETATM	13	C	0	-3.277	1.192	1.128	C
HETATM	14	C	0	-2.885	0.961	-1.284	C

HETATM	15	C	0	-4.550	0.643	0.947	C
HETATM	16	C	0	-4.164	0.408	-1.416	C
HETATM	17	C	0	-5.001	0.228	-0.310	C
HETATM	18	H	0	-5.200	0.519	1.823	H
HETATM	19	H	0	-4.517	0.122	-2.416	H
HETATM	20	C	0	2.416	1.297	0.254	C
HETATM	21	C	0	2.979	0.616	1.352	C
HETATM	22	C	0	3.134	1.484	-0.941	C
HETATM	23	C	0	4.263	0.077	1.208	C
HETATM	24	C	0	4.416	0.936	-1.037	C
HETATM	25	C	0	4.989	0.218	0.020	C
HETATM	26	H	0	4.708	-0.461	2.054	H
HETATM	27	H	0	4.975	1.059	-1.973	H
HETATM	28	C	0	-2.834	1.641	2.486	C
HETATM	29	H	0	-3.357	1.080	3.278	H
HETATM	30	H	0	-1.753	1.481	2.639	H
HETATM	31	H	0	-3.055	2.714	2.653	H
HETATM	32	C	0	-2.026	1.189	-2.491	C
HETATM	33	H	0	-1.601	2.211	-2.508	H
HETATM	34	H	0	-1.161	0.501	-2.545	H
HETATM	35	H	0	-2.606	1.057	-3.419	H
HETATM	36	C	0	-6.346	-0.414	-0.465	C
HETATM	37	H	0	-6.289	-1.504	-0.285	H
HETATM	38	H	0	-7.081	-0.014	0.254	H
HETATM	39	H	0	-6.754	-0.281	-1.482	H
HETATM	40	C	0	2.231	0.475	2.642	C
HETATM	41	H	0	2.871	0.033	3.422	H
HETATM	42	H	0	1.871	1.451	3.017	H
HETATM	43	H	0	1.333	-0.166	2.548	H
HETATM	44	C	0	2.556	2.255	-2.088	C
HETATM	45	H	0	2.761	3.341	-1.995	H
HETATM	46	H	0	2.992	1.925	-3.044	H
HETATM	47	H	0	1.464	2.121	-2.170	H
HETATM	48	C	0	6.344	-0.405	-0.126	C
HETATM	49	H	0	6.273	-1.411	-0.583	H
HETATM	50	H	0	7.006	0.190	-0.778	H
HETATM	51	H	0	6.846	-0.534	0.848	H
HETATM	52	H	0	-1.344	3.649	1.209	H
HETATM	53	H	0	1.008	3.467	1.645	H
HETATM	54	C	0	0.170	-3.153	-0.474	C
HETATM	55	H	0	0.560	-3.578	-1.415	H
HETATM	56	H	0	-0.143	-3.912	0.262	H
HETATM	57	C	0	-1.123	-2.353	-0.867	C
HETATM	58	H	0	-1.313	-2.305	-1.954	H
HETATM	59	H	0	2.279	-2.335	-0.447	H
HETATM	60	F	0	1.677	-2.782	1.415	F
HETATM	61	F	0	-2.234	-2.778	-0.240	F

END

sc3i.pdb

TITLE	sc3i.pdb						
HETATM	1	Ru	0	0.221	-0.949	-0.134	Ru
HETATM	2	Cl	0	0.935	-0.741	-2.470	Cl
HETATM	3	Cl	0	-0.425	-1.262	2.189	Cl
HETATM	4	C	0	-0.119	1.031	0.216	C
HETATM	5	N	0	0.921	1.836	0.508	N
HETATM	6	C	0	0.506	3.211	0.790	C
HETATM	7	C	0	-1.024	3.120	0.725	C
HETATM	8	N	0	-1.262	1.728	0.323	N
HETATM	9	C	0	2.266	1.393	0.290	C

HETATM	10	C	0	2.843	1.553	-0.988	C
HETATM	11	C	0	4.112	1.017	-1.216	C
HETATM	12	C	0	4.817	0.345	-0.210	C
HETATM	13	C	0	4.246	0.252	1.063	C
HETATM	14	C	0	2.979	0.781	1.343	C
HETATM	15	C	0	-2.559	1.186	0.082	C
HETATM	16	C	0	-3.402	0.857	1.159	C
HETATM	17	C	0	-4.644	0.277	0.877	C
HETATM	18	C	0	-5.058	0.026	-0.434	C
HETATM	19	C	0	-4.214	0.398	-1.488	C
HETATM	20	C	0	-2.967	0.984	-1.252	C
HETATM	21	C	0	2.136	2.308	-2.071	C
HETATM	22	C	0	6.150	-0.274	-0.502	C
HETATM	23	C	0	2.424	0.728	2.731	C
HETATM	24	C	0	-3.002	1.130	2.577	C
HETATM	25	C	0	-6.369	-0.648	-0.708	C
HETATM	26	C	0	-2.082	1.388	-2.391	C
HETATM	27	H	0	0.927	3.900	0.033	H
HETATM	28	H	0	0.878	3.537	1.778	H
HETATM	29	H	0	-1.469	3.810	-0.015	H
HETATM	30	H	0	-1.506	3.322	1.699	H
HETATM	31	H	0	4.554	1.114	-2.216	H
HETATM	32	H	0	4.801	-0.239	1.872	H
HETATM	33	H	0	-5.299	0.002	1.714	H
HETATM	34	H	0	-4.536	0.237	-2.525	H
HETATM	35	H	0	1.043	2.168	-2.035	H
HETATM	36	H	0	2.468	1.978	-3.067	H
HETATM	37	H	0	2.340	3.395	-1.997	H
HETATM	38	H	0	6.034	-1.247	-1.016	H
HETATM	39	H	0	6.728	-0.464	0.418	H
HETATM	40	H	0	6.763	0.358	-1.168	H
HETATM	41	H	0	3.167	0.322	3.437	H
HETATM	42	H	0	1.517	0.097	2.798	H
HETATM	43	H	0	2.137	1.733	3.092	H
HETATM	44	H	0	-1.913	1.046	2.721	H
HETATM	45	H	0	-3.474	0.411	3.266	H
HETATM	46	H	0	-3.320	2.141	2.900	H
HETATM	47	H	0	-6.247	-1.745	-0.785	H
HETATM	48	H	0	-7.103	-0.467	0.095	H
HETATM	49	H	0	-6.815	-0.312	-1.661	H
HETATM	50	H	0	-2.627	1.352	-3.349	H
HETATM	51	H	0	-1.197	0.729	-2.488	H
HETATM	52	H	0	-1.690	2.415	-2.265	H
HETATM	53	C	0	-1.254	-1.909	-0.690	C
HETATM	54	F	0	-2.206	-2.454	0.043	F
HETATM	55	H	0	-1.504	-2.046	-1.765	H
HETATM	56	C	0	1.645	-2.548	-0.013	C
HETATM	57	C	0	0.500	-3.193	-0.530	C
HETATM	58	F	0	2.076	-2.845	1.221	F
HETATM	59	H	0	2.466	-2.214	-0.665	H
HETATM	60	H	0	0.482	-3.385	-1.610	H
HETATM	61	H	0	-0.022	-3.895	0.133	H

END

sc3j.pdb

TITLE	sc3j.pdb						
HETATM	1	Ru	0	-0.262	0.936	-0.279	Ru
HETATM	2	C	0	-0.244	-2.860	1.519	C
HETATM	3	C	0	1.276	-2.689	1.492	C
HETATM	4	H	0	-0.587	-3.747	0.953	H

HETATM	5	H	0	1.796	-3.495	0.942	H
HETATM	6	C	0	0.288	-0.824	0.460	C
HETATM	7	N	0	1.460	-1.407	0.803	N
HETATM	8	N	0	-0.718	-1.636	0.883	N
HETATM	9	Cl	0	-0.825	0.126	-2.500	Cl
HETATM	10	Cl	0	-0.236	1.907	1.918	Cl
HETATM	11	C	0	-2.202	2.550	-0.778	C
HETATM	12	C	0	2.753	-0.970	0.396	C
HETATM	13	C	0	3.539	-0.186	1.260	C
HETATM	14	C	0	3.214	-1.332	-0.883	C
HETATM	15	C	0	4.797	0.237	0.815	C
HETATM	16	C	0	4.479	-0.895	-1.288	C
HETATM	17	C	0	5.280	-0.106	-0.453	C
HETATM	18	H	0	5.413	0.855	1.480	H
HETATM	19	H	0	4.843	-1.171	-2.286	H
HETATM	20	C	0	-2.084	-1.399	0.532	C
HETATM	21	C	0	-2.923	-0.654	1.386	C
HETATM	22	C	0	-2.578	-1.930	-0.682	C
HETATM	23	C	0	-4.217	-0.345	0.943	C
HETATM	24	C	0	-3.877	-1.610	-1.073	C
HETATM	25	C	0	-4.702	-0.793	-0.286	C
HETATM	26	H	0	-4.863	0.261	1.593	H
HETATM	27	H	0	-4.252	-1.997	-2.029	H
HETATM	28	C	0	3.016	0.218	2.603	C
HETATM	29	H	0	3.754	0.822	3.156	H
HETATM	30	H	0	2.085	0.811	2.514	H
HETATM	31	H	0	2.766	-0.657	3.232	H
HETATM	32	C	0	2.329	-2.098	-1.818	C
HETATM	33	H	0	1.899	-3.003	-1.349	H
HETATM	34	H	0	1.468	-1.482	-2.151	H
HETATM	35	H	0	2.877	-2.416	-2.720	H
HETATM	36	C	0	6.615	0.392	-0.921	C
HETATM	37	H	0	6.528	1.390	-1.391	H
HETATM	38	H	0	7.331	0.498	-0.088	H
HETATM	39	H	0	7.064	-0.276	-1.675	H
HETATM	40	C	0	-2.523	-0.270	2.777	C
HETATM	41	H	0	-2.723	0.796	2.975	H
HETATM	42	H	0	-3.113	-0.855	3.509	H
HETATM	43	H	0	-1.455	-0.436	2.981	H
HETATM	44	C	0	-1.749	-2.853	-1.521	C
HETATM	45	H	0	-1.878	-3.906	-1.200	H
HETATM	46	H	0	-2.043	-2.797	-2.581	H
HETATM	47	H	0	-0.674	-2.617	-1.474	H
HETATM	48	C	0	-6.067	-0.405	-0.765	C
HETATM	49	H	0	-6.015	0.445	-1.472	H
HETATM	50	H	0	-6.566	-1.229	-1.305	H
HETATM	51	H	0	-6.723	-0.092	0.064	H
HETATM	52	H	0	1.722	-2.645	2.503	H
HETATM	53	H	0	-0.650	-2.945	2.544	H
HETATM	54	C	0	-1.067	3.230	-1.043	C
HETATM	55	H	0	-0.615	3.131	-2.033	H
HETATM	56	C	0	1.377	1.535	-0.735	C
HETATM	57	H	0	2.210	0.948	-1.177	H
HETATM	58	H	0	-0.666	3.961	-0.334	H
HETATM	59	H	0	-2.687	1.849	-1.471	H
HETATM	60	F	0	1.769	2.806	-0.660	F
HETATM	61	F	0	-2.907	2.742	0.332	F

END

st3g.pdb

TITLE st3g.pdb

HETATM	1	Ru	0	0.238	-0.976	0.076	Ru
HETATM	2	C	0	0.326	3.236	0.200	C
HETATM	3	C	0	-1.196	3.094	0.269	C
HETATM	4	H	0	0.666	3.742	-0.724	H
HETATM	5	H	0	-1.720	3.622	-0.548	H
HETATM	6	C	0	-0.242	0.956	0.123	C
HETATM	7	N	0	-1.403	1.648	0.149	N
HETATM	8	N	0	0.779	1.848	0.213	N
HETATM	9	Cl	0	0.756	-1.132	-2.297	Cl
HETATM	10	Cl	0	0.054	-1.049	2.495	Cl
HETATM	11	C	0	2.089	-2.697	0.130	C
HETATM	12	C	0	-2.706	1.085	0.029	C
HETATM	13	C	0	-3.482	0.869	1.183	C
HETATM	14	C	0	-3.184	0.737	-1.250	C
HETATM	15	C	0	-4.748	0.289	1.033	C
HETATM	16	C	0	-4.453	0.157	-1.353	C
HETATM	17	C	0	-5.245	-0.078	-0.223	C
HETATM	18	H	0	-5.356	0.108	1.929	H
HETATM	19	H	0	-4.829	-0.121	-2.346	H
HETATM	20	C	0	2.143	1.454	0.030	C
HETATM	21	C	0	2.950	1.184	1.157	C
HETATM	22	C	0	2.672	1.383	-1.276	C
HETATM	23	C	0	4.253	0.722	0.944	C
HETATM	24	C	0	3.981	0.919	-1.439	C
HETATM	25	C	0	4.774	0.557	-0.345	C
HETATM	26	H	0	4.879	0.490	1.815	H
HETATM	27	H	0	4.389	0.836	-2.455	H
HETATM	28	C	0	-2.943	1.192	2.541	C
HETATM	29	H	0	-3.641	0.874	3.332	H
HETATM	30	H	0	-1.975	0.683	2.719	H
HETATM	31	H	0	-2.768	2.276	2.681	H
HETATM	32	C	0	-2.332	0.946	-2.463	C
HETATM	33	H	0	-1.911	1.968	-2.505	H
HETATM	34	H	0	-1.466	0.253	-2.483	H
HETATM	35	H	0	-2.908	0.782	-3.389	H
HETATM	36	C	0	-6.585	-0.737	-0.355	C
HETATM	37	H	0	-6.488	-1.839	-0.385	H
HETATM	38	H	0	-7.248	-0.499	0.494	H
HETATM	39	H	0	-7.100	-0.442	-1.285	H
HETATM	40	C	0	2.457	1.450	2.544	C
HETATM	41	H	0	3.206	1.148	3.294	H
HETATM	42	H	0	2.257	2.528	2.696	H
HETATM	43	H	0	1.523	0.907	2.767	H
HETATM	44	C	0	1.897	1.865	-2.464	C
HETATM	45	H	0	2.102	2.939	-2.652	H
HETATM	46	H	0	2.180	1.311	-3.374	H
HETATM	47	H	0	0.809	1.741	-2.345	H
HETATM	48	C	0	6.150	0.000	-0.546	C
HETATM	49	H	0	6.126	-1.105	-0.605	H
HETATM	50	H	0	6.608	0.357	-1.483	H
HETATM	51	H	0	6.826	0.256	0.288	H
HETATM	52	H	0	-1.615	3.466	1.223	H
HETATM	53	H	0	0.747	3.793	1.056	H
HETATM	54	C	0	0.931	-3.390	0.210	C
HETATM	55	H	0	0.432	-3.681	-0.718	H
HETATM	56	C	0	-1.432	-1.639	-0.119	C
HETATM	57	H	0	-2.291	-1.442	0.557	H
HETATM	58	H	0	0.569	-3.776	1.169	H
HETATM	59	H	0	2.560	-2.361	-0.803	H
HETATM	60	F	0	2.832	-2.441	1.204	F
HETATM	61	F	0	-1.820	-2.512	-1.042	F

END

st3h.pdb

TITLE	st3h.pdb						
HETATM	1	Ru	0	0.221	-0.949	-0.134	Ru
HETATM	2	Cl	0	0.935	-0.741	-2.470	Cl
HETATM	3	Cl	0	-0.425	-1.262	2.189	Cl
HETATM	4	C	0	-0.119	1.031	0.216	C
HETATM	5	N	0	0.921	1.836	0.508	N
HETATM	6	C	0	0.506	3.211	0.790	C
HETATM	7	C	0	-1.024	3.120	0.725	C
HETATM	8	N	0	-1.262	1.728	0.323	N
HETATM	9	C	0	2.266	1.393	0.290	C
HETATM	10	C	0	2.843	1.553	-0.988	C
HETATM	11	C	0	4.112	1.017	-1.216	C
HETATM	12	C	0	4.817	0.345	-0.210	C
HETATM	13	C	0	4.246	0.252	1.063	C
HETATM	14	C	0	2.979	0.781	1.343	C
HETATM	15	C	0	-2.559	1.186	0.082	C
HETATM	16	C	0	-3.402	0.857	1.159	C
HETATM	17	C	0	-4.644	0.277	0.877	C
HETATM	18	C	0	-5.058	0.026	-0.434	C
HETATM	19	C	0	-4.214	0.398	-1.488	C
HETATM	20	C	0	-2.967	0.984	-1.252	C
HETATM	21	C	0	2.136	2.308	-2.071	C
HETATM	22	C	0	6.150	-0.274	-0.502	C
HETATM	23	C	0	2.424	0.728	2.731	C
HETATM	24	C	0	-3.002	1.130	2.577	C
HETATM	25	C	0	-6.369	-0.648	-0.708	C
HETATM	26	C	0	-2.082	1.388	-2.391	C
HETATM	27	H	0	0.927	3.900	0.033	H
HETATM	28	H	0	0.878	3.537	1.778	H
HETATM	29	H	0	-1.469	3.810	-0.015	H
HETATM	30	H	0	-1.506	3.322	1.699	H
HETATM	31	H	0	4.554	1.114	-2.216	H
HETATM	32	H	0	4.801	-0.239	1.872	H
HETATM	33	H	0	-5.299	0.002	1.714	H
HETATM	34	H	0	-4.536	0.237	-2.525	H
HETATM	35	H	0	1.043	2.168	-2.035	H
HETATM	36	H	0	2.468	1.978	-3.067	H
HETATM	37	H	0	2.340	3.395	-1.997	H
HETATM	38	H	0	6.034	-1.247	-1.016	H
HETATM	39	H	0	6.728	-0.464	0.418	H
HETATM	40	H	0	6.763	0.358	-1.168	H
HETATM	41	H	0	3.167	0.322	3.437	H
HETATM	42	H	0	1.517	0.097	2.798	H
HETATM	43	H	0	2.137	1.733	3.092	H
HETATM	44	H	0	-1.913	1.046	2.721	H
HETATM	45	H	0	-3.474	0.411	3.266	H
HETATM	46	H	0	-3.320	2.141	2.900	H
HETATM	47	H	0	-6.247	-1.745	-0.785	H
HETATM	48	H	0	-7.103	-0.467	0.095	H
HETATM	49	H	0	-6.815	-0.312	-1.661	H
HETATM	50	H	0	-2.627	1.352	-3.349	H
HETATM	51	H	0	-1.197	0.729	-2.488	H
HETATM	52	H	0	-1.690	2.415	-2.265	H
HETATM	53	C	0	-1.254	-1.909	-0.690	C
HETATM	54	F	0	-2.206	-2.454	0.043	F
HETATM	55	H	0	-1.504	-2.046	-1.765	H
HETATM	56	C	0	1.645	-2.548	-0.013	C
HETATM	57	C	0	0.500	-3.193	-0.530	C
HETATM	58	F	0	2.076	-2.845	1.221	F

HETATM	59	H	0	2.466	-2.214	-0.665	H
HETATM	60	H	0	0.482	-3.385	-1.610	H
HETATM	61	H	0	-0.022	-3.895	0.133	H

END

st3NA.pdb

TITLE	st3NA						
HETATM	1	Ru	0	0.004	-0.965	0.007	Ru
HETATM	2	C	0	0.755	3.262	0.085	C
HETATM	3	C	0	-0.772	3.258	-0.044	C
HETATM	4	H	0	1.258	3.798	-0.739	H
HETATM	5	H	0	-1.128	3.707	-0.990	H
HETATM	6	C	0	-0.003	1.061	0.010	C
HETATM	7	N	0	-1.103	1.829	-0.013	N
HETATM	8	N	0	1.093	1.835	0.041	N
HETATM	9	Cl	0	0.935	-1.001	-2.242	Cl
HETATM	10	Cl	0	-0.921	-0.984	2.259	Cl
HETATM	11	C	0	1.304	-2.377	0.370	C
HETATM	12	C	0	-2.433	1.310	-0.070	C
HETATM	13	C	0	-3.225	1.308	1.096	C
HETATM	14	C	0	-2.921	0.798	-1.287	C
HETATM	15	C	0	-4.494	0.729	1.033	C
HETATM	16	C	0	-4.199	0.226	-1.302	C
HETATM	17	C	0	-4.990	0.170	-0.151	C
HETATM	18	H	0	-5.108	0.704	1.943	H
HETATM	19	H	0	-4.584	-0.181	-2.246	H
HETATM	20	C	0	2.426	1.319	0.071	C
HETATM	21	C	0	2.939	0.805	1.277	C
HETATM	22	C	0	3.193	1.321	-1.111	C
HETATM	23	C	0	4.218	0.235	1.264	C
HETATM	24	C	0	4.464	0.744	-1.076	C
HETATM	25	C	0	4.986	0.183	0.097	C
HETATM	26	H	0	4.622	-0.175	2.198	H
HETATM	27	H	0	5.059	0.721	-1.998	H
HETATM	28	C	0	-2.734	1.920	2.372	C
HETATM	29	H	0	-3.209	1.446	3.246	H
HETATM	30	H	0	-1.644	1.803	2.493	H
HETATM	31	H	0	-2.972	3.002	2.422	H
HETATM	32	C	0	-2.108	0.857	-2.544	C
HETATM	33	H	0	-1.524	1.791	-2.624	H
HETATM	34	H	0	-1.369	0.035	-2.608	H
HETATM	35	H	0	-2.755	0.784	-3.434	H
HETATM	36	C	0	-6.337	-0.487	-0.174	C
HETATM	37	H	0	-6.288	-1.512	0.241	H
HETATM	38	H	0	-7.075	0.061	0.437	H
HETATM	39	H	0	-6.737	-0.575	-1.197	H
HETATM	40	C	0	2.151	0.860	2.550	C
HETATM	41	H	0	2.811	0.740	3.425	H
HETATM	42	H	0	1.606	1.814	2.665	H
HETATM	43	H	0	1.382	0.065	2.607	H
HETATM	44	C	0	2.670	1.931	-2.375	C
HETATM	45	H	0	2.879	3.019	-2.420	H
HETATM	46	H	0	3.146	1.476	-3.260	H
HETATM	47	H	0	1.582	1.785	-2.484	H
HETATM	48	C	0	6.333	-0.472	0.090	C
HETATM	49	H	0	6.278	-1.494	-0.330	H
HETATM	50	H	0	7.059	0.082	-0.531	H
HETATM	51	H	0	6.753	-0.565	1.106	H
HETATM	52	H	0	-1.278	3.785	0.785	H
HETATM	53	H	0	1.108	3.704	1.035	H
HETATM	54	C	0	0.008	-3.184	0.015	C

HETATM	55	H	0	0.230	-3.790	-0.879	H
HETATM	56	H	0	-0.212	-3.786	0.913	H
HETATM	57	C	0	-1.291	-2.383	-0.342	C
HETATM	58	H	0	-2.117	-2.497	0.379	H
HETATM	59	H	0	2.132	-2.493	-0.349	H
HETATM	60	F	0	1.754	-2.606	1.622	F
HETATM	61	F	0	-1.743	-2.622	-1.592	F

END

st3i.pdb

TITLE	st3i.pdb						
HETATM	1	Ru	0	0.221	-0.949	-0.134	Ru
HETATM	2	Cl	0	0.935	-0.741	-2.470	Cl
HETATM	3	Cl	0	-0.425	-1.262	2.189	Cl
HETATM	4	C	0	-0.119	1.031	0.216	C
HETATM	5	N	0	0.921	1.836	0.508	N
HETATM	6	C	0	0.506	3.211	0.790	C
HETATM	7	C	0	-1.024	3.120	0.725	C
HETATM	8	N	0	-1.262	1.728	0.323	N
HETATM	9	C	0	2.266	1.393	0.290	C
HETATM	10	C	0	2.843	1.553	-0.988	C
HETATM	11	C	0	4.112	1.017	-1.216	C
HETATM	12	C	0	4.817	0.345	-0.210	C
HETATM	13	C	0	4.246	0.252	1.063	C
HETATM	14	C	0	2.979	0.781	1.343	C
HETATM	15	C	0	-2.559	1.186	0.082	C
HETATM	16	C	0	-3.402	0.857	1.159	C
HETATM	17	C	0	-4.644	0.277	0.877	C
HETATM	18	C	0	-5.058	0.026	-0.434	C
HETATM	19	C	0	-4.214	0.398	-1.488	C
HETATM	20	C	0	-2.967	0.984	-1.252	C
HETATM	21	C	0	2.136	2.308	-2.071	C
HETATM	22	C	0	6.150	-0.274	-0.502	C
HETATM	23	C	0	2.424	0.728	2.731	C
HETATM	24	C	0	-3.002	1.130	2.577	C
HETATM	25	C	0	-6.369	-0.648	-0.708	C
HETATM	26	C	0	-2.082	1.388	-2.391	C
HETATM	27	H	0	0.927	3.900	0.033	H
HETATM	28	H	0	0.878	3.537	1.778	H
HETATM	29	H	0	-1.469	3.810	-0.015	H
HETATM	30	H	0	-1.506	3.322	1.699	H
HETATM	31	H	0	4.554	1.114	-2.216	H
HETATM	32	H	0	4.801	-0.239	1.872	H
HETATM	33	H	0	-5.299	0.002	1.714	H
HETATM	34	H	0	-4.536	0.237	-2.525	H
HETATM	35	H	0	1.043	2.168	-2.035	H
HETATM	36	H	0	2.468	1.978	-3.067	H
HETATM	37	H	0	2.340	3.395	-1.997	H
HETATM	38	H	0	6.034	-1.247	-1.016	H
HETATM	39	H	0	6.728	-0.464	0.418	H
HETATM	40	H	0	6.763	0.358	-1.168	H
HETATM	41	H	0	3.167	0.322	3.437	H
HETATM	42	H	0	1.517	0.097	2.798	H
HETATM	43	H	0	2.137	1.733	3.092	H
HETATM	44	H	0	-1.913	1.046	2.721	H
HETATM	45	H	0	-3.474	0.411	3.266	H
HETATM	46	H	0	-3.320	2.141	2.900	H
HETATM	47	H	0	-6.247	-1.745	-0.785	H
HETATM	48	H	0	-7.103	-0.467	0.095	H
HETATM	49	H	0	-6.815	-0.312	-1.661	H
HETATM	50	H	0	-2.627	1.352	-3.349	H

HETATM	51	H	0	-1.197	0.729	-2.488	H
HETATM	52	H	0	-1.690	2.415	-2.265	H
HETATM	53	C	0	-1.254	-1.909	-0.690	C
HETATM	54	F	0	-2.206	-2.454	0.043	F
HETATM	55	H	0	-1.504	-2.046	-1.765	H
HETATM	56	C	0	1.645	-2.548	-0.013	C
HETATM	57	C	0	0.500	-3.193	-0.530	C
HETATM	58	F	0	2.076	-2.845	1.221	F
HETATM	59	H	0	2.466	-2.214	-0.665	H
HETATM	60	H	0	0.482	-3.385	-1.610	H
HETATM	61	H	0	-0.022	-3.895	0.133	H

END

st3j.pdb

TITLE	st3j.pdb						
HETATM	1	Ru	0	0.238	-0.976	0.076	Ru
HETATM	2	C	0	0.326	3.236	0.200	C
HETATM	3	C	0	-1.196	3.094	0.269	C
HETATM	4	H	0	0.666	3.742	-0.724	H
HETATM	5	H	0	-1.720	3.622	-0.548	H
HETATM	6	C	0	-0.242	0.956	0.123	C
HETATM	7	N	0	-1.403	1.648	0.149	N
HETATM	8	N	0	0.779	1.848	0.213	N
HETATM	9	Cl	0	0.756	-1.132	-2.297	Cl
HETATM	10	Cl	0	0.054	-1.049	2.495	Cl
HETATM	11	C	0	2.089	-2.697	0.130	C
HETATM	12	C	0	-2.706	1.085	0.029	C
HETATM	13	C	0	-3.482	0.869	1.183	C
HETATM	14	C	0	-3.184	0.737	-1.250	C
HETATM	15	C	0	-4.748	0.289	1.033	C
HETATM	16	C	0	-4.453	0.157	-1.353	C
HETATM	17	C	0	-5.245	-0.078	-0.223	C
HETATM	18	H	0	-5.356	0.108	1.929	H
HETATM	19	H	0	-4.829	-0.121	-2.346	H
HETATM	20	C	0	2.143	1.454	0.030	C
HETATM	21	C	0	2.950	1.184	1.157	C
HETATM	22	C	0	2.672	1.383	-1.276	C
HETATM	23	C	0	4.253	0.722	0.944	C
HETATM	24	C	0	3.981	0.919	-1.439	C
HETATM	25	C	0	4.774	0.557	-0.345	C
HETATM	26	H	0	4.879	0.490	1.815	H
HETATM	27	H	0	4.389	0.836	-2.455	H
HETATM	28	C	0	-2.943	1.192	2.541	C
HETATM	29	H	0	-3.641	0.874	3.332	H
HETATM	30	H	0	-1.975	0.683	2.719	H
HETATM	31	H	0	-2.768	2.276	2.681	H
HETATM	32	C	0	-2.332	0.946	-2.463	C
HETATM	33	H	0	-1.911	1.968	-2.505	H
HETATM	34	H	0	-1.466	0.253	-2.483	H
HETATM	35	H	0	-2.908	0.782	-3.389	H
HETATM	36	C	0	-6.585	-0.737	-0.355	C
HETATM	37	H	0	-6.488	-1.839	-0.385	H
HETATM	38	H	0	-7.248	-0.499	0.494	H
HETATM	39	H	0	-7.100	-0.442	-1.285	H
HETATM	40	C	0	2.457	1.450	2.544	C
HETATM	41	H	0	3.206	1.148	3.294	H
HETATM	42	H	0	2.257	2.528	2.696	H
HETATM	43	H	0	1.523	0.907	2.767	H
HETATM	44	C	0	1.897	1.865	-2.464	C
HETATM	45	H	0	2.102	2.939	-2.652	H
HETATM	46	H	0	2.180	1.311	-3.374	H

HETATM	47	H	0	0.809	1.741	-2.345	H
HETATM	48	C	0	6.150	0.000	-0.546	C
HETATM	49	H	0	6.126	-1.105	-0.605	H
HETATM	50	H	0	6.608	0.357	-1.483	H
HETATM	51	H	0	6.826	0.256	0.288	H
HETATM	52	H	0	-1.615	3.466	1.223	H
HETATM	53	H	0	0.747	3.793	1.056	H
HETATM	54	C	0	0.931	-3.390	0.210	C
HETATM	55	H	0	0.432	-3.681	-0.718	H
HETATM	56	C	0	-1.432	-1.639	-0.119	C
HETATM	57	H	0	-2.291	-1.442	0.557	H
HETATM	58	H	0	0.569	-3.776	1.169	H
HETATM	59	H	0	2.560	-2.361	-0.803	H
HETATM	60	F	0	2.832	-2.441	1.204	F
HETATM	61	F	0	-1.820	-2.512	-1.042	F

END

ac3g.pdb

TITLE	ac3g.pdb						
HETATM	1	Ru	0	-0.286	0.907	0.257	Ru
HETATM	2	C	0	-0.525	-3.285	-0.211	C
HETATM	3	C	0	0.999	-3.198	-0.113	C
HETATM	4	H	0	-0.869	-3.633	-1.204	H
HETATM	5	H	0	1.518	-3.650	-0.976	H
HETATM	6	C	0	0.108	-1.034	0.020	C
HETATM	7	N	0	1.248	-1.755	-0.071	N
HETATM	8	N	0	-0.938	-1.902	0.011	N
HETATM	9	Cl	0	-0.866	1.359	-2.048	Cl
HETATM	10	Cl	0	0.017	0.694	2.677	Cl
HETATM	11	C	0	-1.837	2.665	0.680	C
HETATM	12	C	0	2.565	-1.218	-0.137	C
HETATM	13	C	0	3.370	-1.187	1.018	C
HETATM	14	C	0	3.034	-0.720	-1.369	C
HETATM	15	C	0	4.649	-0.626	0.921	C
HETATM	16	C	0	4.318	-0.166	-1.420	C
HETATM	17	C	0	5.134	-0.104	-0.285	C
HETATM	18	H	0	5.279	-0.589	1.819	H
HETATM	19	H	0	4.686	0.228	-2.376	H
HETATM	20	C	0	-2.291	-1.444	-0.080	C
HETATM	21	C	0	-3.043	-1.264	1.101	C
HETATM	22	C	0	-2.859	-1.196	-1.347	C
HETATM	23	C	0	-4.324	-0.712	0.994	C
HETATM	24	C	0	-4.144	-0.649	-1.405	C
HETATM	25	C	0	-4.878	-0.374	-0.247	C
HETATM	26	H	0	-4.911	-0.558	1.909	H
HETATM	27	H	0	-4.578	-0.426	-2.388	H
HETATM	28	C	0	2.856	-1.700	2.327	C
HETATM	29	H	0	3.541	-1.442	3.152	H
HETATM	30	H	0	1.865	-1.270	2.567	H
HETATM	31	H	0	2.747	-2.802	2.334	H
HETATM	32	C	0	2.163	-0.753	-2.585	C
HETATM	33	H	0	1.677	-1.736	-2.722	H
HETATM	34	H	0	1.343	-0.008	-2.523	H
HETATM	35	H	0	2.741	-0.531	-3.497	H
HETATM	36	C	0	6.490	0.531	-0.352	C
HETATM	37	H	0	6.429	1.623	-0.178	H
HETATM	38	H	0	7.175	0.126	0.411	H
HETATM	39	H	0	6.960	0.398	-1.341	H
HETATM	40	C	0	-2.510	-1.700	2.431	C
HETATM	41	H	0	-3.259	-1.549	3.224	H

HETATM	42	H	0	-2.246	-2.774	2.426	H
HETATM	43	H	0	-1.598	-1.144	2.718	H
HETATM	44	C	0	-2.141	-1.559	-2.611	C
HETATM	45	H	0	-2.378	-2.601	-2.909	H
HETATM	46	H	0	-2.442	-0.903	-3.443	H
HETATM	47	H	0	-1.047	-1.471	-2.518	H
HETATM	48	C	0	-6.226	0.273	-0.333	C
HETATM	49	H	0	-6.137	1.376	-0.365	H
HETATM	50	H	0	-6.769	-0.023	-1.247	H
HETATM	51	H	0	-6.860	0.030	0.536	H
HETATM	52	H	0	1.393	-3.681	0.801	H
HETATM	53	H	0	-0.969	-3.955	0.547	H
HETATM	54	C	0	-0.701	3.382	0.865	C
HETATM	55	C	0	1.413	1.513	0.090	C
HETATM	56	H	0	2.252	1.280	0.783	H
HETATM	57	H	0	-2.261	2.136	1.542	H
HETATM	58	H	0	-0.122	3.408	1.796	H
HETATM	59	H	0	-2.427	2.777	-0.236	H
HETATM	60	F	0	1.847	2.368	-0.823	F
HETATM	61	F	0	-0.247	4.218	-0.055	F

END

ac3h.pdb

TITLE	ac3h.pdb						
HETATM	1	Ru	0	-0.038	0.956	0.255	Ru
HETATM	2	Cl	0	0.843	0.654	2.523	Cl
HETATM	3	Cl	0	-1.100	1.326	-1.883	Cl
HETATM	4	C	0	-0.094	-1.076	-0.043	C
HETATM	5	N	0	0.982	-1.871	-0.176	N
HETATM	6	C	0	0.616	-3.281	-0.356	C
HETATM	7	C	0	-0.908	-3.260	-0.217	C
HETATM	8	N	0	-1.206	-1.831	-0.079	N
HETATM	9	C	0	2.329	-1.400	-0.224	C
HETATM	10	C	0	3.157	-1.538	0.905	C
HETATM	11	C	0	4.453	-1.015	0.844	C
HETATM	12	C	0	4.935	-0.377	-0.305	C
HETATM	13	C	0	4.099	-0.287	-1.424	C
HETATM	14	C	0	2.797	-0.796	-1.407	C
HETATM	15	C	0	-2.532	-1.300	-0.019	C
HETATM	16	C	0	-3.270	-1.159	-1.209	C
HETATM	17	C	0	-4.540	-0.581	-1.138	C
HETATM	18	C	0	-5.081	-0.143	0.076	C
HETATM	19	C	0	-4.339	-0.328	1.247	C
HETATM	20	C	0	-3.067	-0.913	1.224	C
HETATM	21	C	0	2.683	-2.243	2.140	C
HETATM	22	C	0	6.311	0.217	-0.326	C
HETATM	23	C	0	1.919	-0.689	-2.616	C
HETATM	24	C	0	-2.713	-1.605	-2.526	C
HETATM	25	C	0	-6.420	0.529	0.114	C
HETATM	26	C	0	-2.306	-1.132	2.496	C
HETATM	27	H	0	1.112	-3.903	0.410	H
HETATM	28	H	0	0.957	-3.639	-1.345	H
HETATM	29	H	0	-1.270	-3.811	0.671	H
HETATM	30	H	0	-1.429	-3.676	-1.098	H
HETATM	31	H	0	5.099	-1.101	1.727	H
HETATM	32	H	0	4.469	0.191	-2.341	H
HETATM	33	H	0	-5.111	-0.445	-2.066	H
HETATM	34	H	0	-4.762	-0.018	2.212	H
HETATM	35	H	0	1.597	-2.131	2.288	H
HETATM	36	H	0	3.174	-1.837	3.040	H
HETATM	37	H	0	2.917	-3.325	2.102	H

HETATM	38	H	0	7.022	-0.365	0.287	H
HETATM	39	H	0	6.311	1.245	0.085	H
HETATM	40	H	0	6.717	0.284	-1.349	H
HETATM	41	H	0	2.497	-0.371	-3.499	H
HETATM	42	H	0	1.098	0.041	-2.479	H
HETATM	43	H	0	1.433	-1.652	-2.863	H
HETATM	44	H	0	-1.622	-1.451	-2.580	H
HETATM	45	H	0	-3.161	-1.036	-3.357	H
HETATM	46	H	0	-2.921	-2.677	-2.719	H
HETATM	47	H	0	-7.115	0.108	-0.633	H
HETATM	48	H	0	-6.331	1.608	-0.114	H
HETATM	49	H	0	-6.895	0.450	1.106	H
HETATM	50	H	0	-2.945	-0.945	3.375	H
HETATM	51	H	0	-1.419	-0.476	2.589	H
HETATM	52	H	0	-1.923	-2.167	2.575	H
HETATM	53	C	0	-1.108	2.588	0.977	C
HETATM	54	H	0	-1.343	2.380	2.030	H
HETATM	55	H	0	-1.936	2.859	0.307	H
HETATM	56	C	0	1.517	1.908	-0.072	C
HETATM	57	C	0	0.160	3.198	0.689	C
HETATM	58	F	0	1.880	2.422	-1.237	F
HETATM	59	F	0	0.192	4.106	-0.300	F
HETATM	60	H	0	2.366	1.952	0.641	H
HETATM	61	H	0	0.817	3.473	1.528	H

END

ac3PA.pdb

TITLE	ac3PA.pdb						
HETATM	1	Ru	0	0.039	0.905	0.204	Ru
HETATM	2	Cl	0	0.937	0.439	2.452	Cl
HETATM	3	Cl	0	-1.011	1.413	-1.888	Cl
HETATM	4	C	0	-0.128	-1.086	-0.080	C
HETATM	5	N	0	0.935	-1.889	-0.250	N
HETATM	6	C	0	0.534	-3.275	-0.511	C
HETATM	7	C	0	-0.977	-3.242	-0.270	C
HETATM	8	N	0	-1.257	-1.809	-0.121	N
HETATM	9	C	0	2.283	-1.417	-0.289	C
HETATM	10	C	0	3.130	-1.661	0.811	C
HETATM	11	C	0	4.422	-1.132	0.782	C
HETATM	12	C	0	4.886	-0.380	-0.306	C
HETATM	13	C	0	4.039	-0.191	-1.400	C
HETATM	14	C	0	2.737	-0.709	-1.420	C
HETATM	15	C	0	-2.574	-1.258	-0.033	C
HETATM	16	C	0	-3.320	-1.076	-1.213	C
HETATM	17	C	0	-4.583	-0.488	-1.116	C
HETATM	18	C	0	-5.112	-0.082	0.114	C
HETATM	19	C	0	-4.361	-0.306	1.274	C
HETATM	20	C	0	-3.095	-0.899	1.224	C
HETATM	21	C	0	2.673	-2.478	1.980	C
HETATM	22	C	0	6.261	0.215	-0.286	C
HETATM	23	C	0	1.876	-0.515	-2.630	C
HETATM	24	C	0	-2.778	-1.494	-2.545	C
HETATM	25	C	0	-6.444	0.600	0.183	C
HETATM	26	C	0	-2.321	-1.154	2.481	C
HETATM	27	H	0	1.066	-3.964	0.169	H
HETATM	28	H	0	0.801	-3.556	-1.548	H
HETATM	29	H	0	-1.280	-3.782	0.647	H
HETATM	30	H	0	-1.559	-3.660	-1.110	H
HETATM	31	H	0	5.081	-1.300	1.644	H
HETATM	32	H	0	4.396	0.369	-2.273	H
HETATM	33	H	0	-5.161	-0.322	-2.035	H

HETATM	34	H	0	-4.773	-0.017	2.250	H
HETATM	35	H	0	1.599	-2.336	2.185	H
HETATM	36	H	0	3.218	-2.198	2.896	H
HETATM	37	H	0	2.852	-3.559	1.816	H
HETATM	38	H	0	7.003	-0.472	0.158	H
HETATM	39	H	0	6.289	1.139	0.323	H
HETATM	40	H	0	6.608	0.487	-1.297	H
HETATM	41	H	0	2.495	-0.410	-3.537	H
HETATM	42	H	0	1.243	0.391	-2.562	H
HETATM	43	H	0	1.178	-1.356	-2.790	H
HETATM	44	H	0	-1.697	-1.288	-2.627	H
HETATM	45	H	0	-3.274	-0.946	-3.363	H
HETATM	46	H	0	-2.938	-2.574	-2.737	H
HETATM	47	H	0	-7.151	0.203	-0.565	H
HETATM	48	H	0	-6.348	1.683	-0.020	H
HETATM	49	H	0	-6.909	0.502	1.179	H
HETATM	50	H	0	-2.924	-0.917	3.373	H
HETATM	51	H	0	-1.391	-0.556	2.540	H
HETATM	52	H	0	-2.007	-2.211	2.565	H
HETATM	53	C	0	-1.027	2.329	1.092	C
HETATM	54	H	0	-1.228	2.175	2.164	H
HETATM	55	H	0	-1.870	2.721	0.501	H
HETATM	56	C	0	1.493	2.190	0.176	C
HETATM	57	C	0	0.282	3.072	0.787	C
HETATM	58	F	0	1.928	2.704	-0.989	F
HETATM	59	F	0	0.078	4.126	-0.053	F
HETATM	60	H	0	2.339	2.057	0.870	H
HETATM	61	H	0	0.700	3.424	1.748	H

END

ac3i.pdb

TITLE	ac3i.pdb						
HETATM	1	Ru	0	-0.201	0.866	-0.170	Ru
HETATM	2	Cl	0	-0.909	0.547	-2.500	Cl
HETATM	3	Cl	0	0.494	1.365	2.102	Cl
HETATM	4	C	0	0.234	-1.072	0.237	C
HETATM	5	N	0	-0.772	-1.909	0.555	N
HETATM	6	C	0	-0.303	-3.256	0.878	C
HETATM	7	C	0	1.222	-3.107	0.801	C
HETATM	8	N	0	1.405	-1.718	0.363	N
HETATM	9	C	0	-2.133	-1.518	0.348	C
HETATM	10	C	0	-2.732	-1.758	-0.909	C
HETATM	11	C	0	-4.020	-1.272	-1.135	C
HETATM	12	C	0	-4.725	-0.572	-0.147	C
HETATM	13	C	0	-4.129	-0.394	1.104	C
HETATM	14	C	0	-2.838	-0.866	1.381	C
HETATM	15	C	0	2.681	-1.132	0.114	C
HETATM	16	C	0	3.496	-0.730	1.187	C
HETATM	17	C	0	4.716	-0.108	0.896	C
HETATM	18	C	0	5.137	0.109	-0.420	C
HETATM	19	C	0	4.318	-0.332	-1.468	C
HETATM	20	C	0	3.092	-0.957	-1.222	C
HETATM	21	C	0	-2.017	-2.533	-1.972	C
HETATM	22	C	0	-6.089	-0.022	-0.438	C
HETATM	23	C	0	-2.252	-0.683	2.746	C
HETATM	24	C	0	3.090	-0.968	2.609	C
HETATM	25	C	0	6.425	0.820	-0.705	C
HETATM	26	C	0	2.225	-1.420	-2.352	C
HETATM	27	H	0	-0.701	-3.984	0.147	H
HETATM	28	H	0	-0.657	-3.564	1.878	H
HETATM	29	H	0	1.690	-3.798	0.076	H

HETATM	30	H	0	1.717	-3.266	1.777	H
HETATM	31	H	0	-4.479	-1.431	-2.120	H
HETATM	32	H	0	-4.681	0.123	1.899	H
HETATM	33	H	0	5.350	0.224	1.728	H
HETATM	34	H	0	4.644	-0.192	-2.507	H
HETATM	35	H	0	-0.930	-2.346	-1.966	H
HETATM	36	H	0	-2.382	-2.259	-2.974	H
HETATM	37	H	0	-2.175	-3.624	-1.849	H
HETATM	38	H	0	-6.716	-0.745	-0.988	H
HETATM	39	H	0	-6.029	0.882	-1.073	H
HETATM	40	H	0	-6.625	0.263	0.483	H
HETATM	41	H	0	-3.047	-0.553	3.498	H
HETATM	42	H	0	-1.590	0.203	2.797	H
HETATM	43	H	0	-1.629	-1.542	3.052	H
HETATM	44	H	0	1.996	-0.943	2.734	H
HETATM	45	H	0	3.508	-0.195	3.275	H
HETATM	46	H	0	3.461	-1.945	2.977	H
HETATM	47	H	0	7.162	0.681	0.104	H
HETATM	48	H	0	6.268	1.911	-0.805	H
HETATM	49	H	0	6.885	0.479	-1.649	H
HETATM	50	H	0	2.767	-1.383	-3.312	H
HETATM	51	H	0	1.314	-0.798	-2.461	H
HETATM	52	H	0	1.874	-2.459	-2.205	H
HETATM	53	C	0	1.242	1.848	-0.755	C
HETATM	54	H	0	1.521	1.868	-1.830	H
HETATM	55	H	0	1.858	2.454	-0.062	H
HETATM	56	C	0	-1.731	2.387	-0.117	C
HETATM	57	C	0	-0.679	3.128	-0.691	C
HETATM	58	F	0	-2.189	2.764	1.082	F
HETATM	59	F	0	-0.170	4.130	0.019	F
HETATM	60	H	0	-2.494	1.913	-0.752	H
HETATM	61	H	0	-0.580	3.229	-1.778	H

END

ac3j.pdb

TITLE	ac3j.pdb						
HETATM	1	Ru	0	-0.252	0.834	-0.151	Ru
HETATM	2	C	0	0.071	-3.225	0.807	C
HETATM	3	C	0	1.562	-2.899	0.906	C
HETATM	4	H	0	-0.163	-3.882	-0.055	H
HETATM	5	H	0	2.193	-3.545	0.270	H
HETATM	6	C	0	0.402	-0.956	0.319	C
HETATM	7	N	0	1.629	-1.507	0.448	N
HETATM	8	N	0	-0.528	-1.906	0.617	N
HETATM	9	Cl	0	-0.358	0.558	-2.579	Cl
HETATM	10	Cl	0	-0.377	1.561	2.145	Cl
HETATM	11	C	0	-2.434	2.163	-0.520	C
HETATM	12	C	0	2.872	-0.850	0.217	C
HETATM	13	C	0	3.536	-0.207	1.280	C
HETATM	14	C	0	3.432	-0.897	-1.075	C
HETATM	15	C	0	4.769	0.401	1.022	C
HETATM	16	C	0	4.669	-0.280	-1.287	C
HETATM	17	C	0	5.347	0.376	-0.253	C
HETATM	18	H	0	5.290	0.909	1.844	H
HETATM	19	H	0	5.112	-0.312	-2.291	H
HETATM	20	C	0	-1.908	-1.656	0.328	C
HETATM	21	C	0	-2.770	-1.249	1.371	C
HETATM	22	C	0	-2.379	-1.795	-0.994	C
HETATM	23	C	0	-4.074	-0.870	1.041	C
HETATM	24	C	0	-3.691	-1.394	-1.279	C
HETATM	25	C	0	-4.537	-0.900	-0.281	C

HETATM	26	H	0	-4.742	-0.525	1.840	H
HETATM	27	H	0	-4.053	-1.469	-2.312	H
HETATM	28	C	0	2.913	-0.146	2.639	C
HETATM	29	H	0	3.555	0.403	3.348	H
HETATM	30	H	0	1.928	0.360	2.614	H
HETATM	31	H	0	2.739	-1.152	3.065	H
HETATM	32	C	0	2.693	-1.554	-2.198	C
HETATM	33	H	0	2.335	-2.566	-1.931	H
HETATM	34	H	0	1.793	-0.968	-2.477	H
HETATM	35	H	0	3.325	-1.644	-3.096	H
HETATM	36	C	0	6.654	1.064	-0.511	C
HETATM	37	H	0	6.502	2.132	-0.759	H
HETATM	38	H	0	7.315	1.038	0.372	H
HETATM	39	H	0	7.196	0.615	-1.360	H
HETATM	40	C	0	-2.305	-1.245	2.792	C
HETATM	41	H	0	-3.132	-1.000	3.478	H
HETATM	42	H	0	-1.900	-2.229	3.092	H
HETATM	43	H	0	-1.505	-0.498	2.948	H
HETATM	44	C	0	-1.540	-2.424	-2.063	C
HETATM	45	H	0	-1.697	-3.521	-2.080	H
HETATM	46	H	0	-1.805	-2.036	-3.059	H
HETATM	47	H	0	-0.463	-2.238	-1.927	H
HETATM	48	C	0	-5.907	-0.391	-0.611	C
HETATM	49	H	0	-5.931	0.716	-0.585	H
HETATM	50	H	0	-6.235	-0.700	-1.617	H
HETATM	51	H	0	-6.663	-0.732	0.118	H
HETATM	52	H	0	1.945	-2.979	1.941	H
HETATM	53	H	0	-0.326	-3.713	1.714	H
HETATM	54	C	0	-1.492	3.081	-0.838	C
HETATM	55	H	0	-0.910	3.025	-1.764	H
HETATM	56	C	0	1.390	1.599	-0.300	C
HETATM	57	H	0	1.905	2.069	0.566	H
HETATM	58	H	0	1.918	1.661	-1.276	H
HETATM	59	H	0	-2.688	1.321	-1.179	H
HETATM	60	F	0	-3.217	2.311	0.536	F
HETATM	61	F	0	-1.292	4.148	-0.087	F

END

at3g.pdb

TITLE	at3g.pdb						
HETATM	1	Ru	0	-0.302	0.913	0.061	Ru
HETATM	2	C	0	-0.492	-3.301	0.074	C
HETATM	3	C	0	1.029	-3.198	-0.050	C
HETATM	4	H	0	-0.955	-3.873	-0.751	H
HETATM	5	H	0	1.410	-3.592	-1.013	H
HETATM	6	C	0	0.133	-1.032	0.028	C
HETATM	7	N	0	1.275	-1.755	0.030	N
HETATM	8	N	0	-0.909	-1.903	0.029	N
HETATM	9	Cl	0	-0.822	1.096	-2.306	Cl
HETATM	10	Cl	0	-0.211	0.932	2.484	Cl
HETATM	11	C	0	-1.880	2.729	0.319	C
HETATM	12	C	0	2.593	-1.222	-0.028	C
HETATM	13	C	0	3.329	-1.088	1.164	C
HETATM	14	C	0	3.124	-0.819	-1.268	C
HETATM	15	C	0	4.613	-0.540	1.094	C
HETATM	16	C	0	4.411	-0.272	-1.293	C
HETATM	17	C	0	5.166	-0.121	-0.124	C
HETATM	18	H	0	5.192	-0.424	2.019	H
HETATM	19	H	0	4.831	0.052	-2.255	H
HETATM	20	C	0	-2.264	-1.452	0.010	C
HETATM	21	C	0	-2.929	-1.165	1.221	C

HETATM	22	C	0	-2.920	-1.303	-1.233	C
HETATM	23	C	0	-4.210	-0.600	1.156	C
HETATM	24	C	0	-4.200	-0.747	-1.247	C
HETATM	25	C	0	-4.847	-0.361	-0.065	C
HETATM	26	H	0	-4.725	-0.355	2.094	H
HETATM	27	H	0	-4.704	-0.605	-2.212	H
HETATM	28	C	0	2.710	-1.452	2.478	C
HETATM	29	H	0	3.431	-1.344	3.305	H
HETATM	30	H	0	1.841	-0.799	2.696	H
HETATM	31	H	0	2.333	-2.491	2.496	H
HETATM	32	C	0	2.305	-0.921	-2.517	C
HETATM	33	H	0	1.822	-1.910	-2.623	H
HETATM	34	H	0	1.483	-0.177	-2.529	H
HETATM	35	H	0	2.921	-0.750	-3.415	H
HETATM	36	C	0	6.528	0.504	-0.167	C
HETATM	37	H	0	6.476	1.591	0.030	H
HETATM	38	H	0	7.202	0.078	0.596	H
HETATM	39	H	0	7.007	0.383	-1.153	H
HETATM	40	C	0	-2.358	-1.544	2.553	C
HETATM	41	H	0	-2.520	-0.754	3.303	H
HETATM	42	H	0	-2.856	-2.461	2.926	H
HETATM	43	H	0	-1.274	-1.732	2.521	H
HETATM	44	C	0	-2.296	-1.795	-2.502	C
HETATM	45	H	0	-2.549	-2.861	-2.672	H
HETATM	46	H	0	-2.661	-1.229	-3.373	H
HETATM	47	H	0	-1.198	-1.703	-2.493	H
HETATM	48	C	0	-6.192	0.297	-0.115	C
HETATM	49	H	0	-6.098	1.378	-0.334	H
HETATM	50	H	0	-6.831	-0.128	-0.908	H
HETATM	51	H	0	-6.731	0.211	0.843	H
HETATM	52	H	0	1.567	-3.728	0.755	H
HETATM	53	H	0	-0.816	-3.768	1.024	H
HETATM	54	C	0	-0.802	3.447	-0.074	C
HETATM	55	H	0	-0.486	3.590	-1.114	H
HETATM	56	C	0	1.398	1.517	-0.063	C
HETATM	57	H	0	2.228	1.296	0.642	H
HETATM	58	H	0	-2.188	2.713	1.370	H
HETATM	59	H	0	-2.545	2.324	-0.452	H
HETATM	60	F	0	1.846	2.385	-0.968	F
HETATM	61	F	0	-0.067	4.132	0.795	F

END

at3h.pdb

TITLE	at3h.pdb						
HETATM	1	Ru	0	-0.090	0.967	0.066	Ru
HETATM	2	Cl	0	0.719	0.980	2.348	Cl
HETATM	3	Cl	0	-1.072	1.016	-2.167	Cl
HETATM	4	C	0	-0.067	-1.083	0.083	C
HETATM	5	N	0	1.013	-1.880	0.035	N
HETATM	6	C	0	0.657	-3.302	0.112	C
HETATM	7	C	0	-0.868	-3.272	0.249	C
HETATM	8	N	0	-1.172	-1.838	0.209	N
HETATM	9	C	0	2.355	-1.405	-0.070	C
HETATM	10	C	0	3.171	-1.364	1.076	C
HETATM	11	C	0	4.457	-0.830	0.953	C
HETATM	12	C	0	4.941	-0.349	-0.269	C
HETATM	13	C	0	4.118	-0.434	-1.397	C
HETATM	14	C	0	2.826	-0.965	-1.322	C
HETATM	15	C	0	-2.495	-1.296	0.161	C
HETATM	16	C	0	-3.192	-1.289	-1.063	C
HETATM	17	C	0	-4.449	-0.682	-1.107	C

HETATM	18	C	0	-5.022	-0.094	0.027	C
HETATM	19	C	0	-4.327	-0.156	1.239	C
HETATM	20	C	0	-3.068	-0.762	1.332	C
HETATM	21	C	0	2.693	-1.888	2.395	C
HETATM	22	C	0	6.307	0.264	-0.357	C
HETATM	23	C	0	1.962	-1.056	-2.542	C
HETATM	24	C	0	-2.621	-1.926	-2.293	C
HETATM	25	C	0	-6.348	0.599	-0.064	C
HETATM	26	C	0	-2.368	-0.856	2.654	C
HETATM	27	H	0	1.158	-3.773	0.977	H
HETATM	28	H	0	1.002	-3.829	-0.797	H
HETATM	29	H	0	-1.229	-3.713	1.196	H
HETATM	30	H	0	-1.387	-3.793	-0.577	H
HETATM	31	H	0	5.095	-0.777	1.846	H
HETATM	32	H	0	4.489	-0.080	-2.368	H
HETATM	33	H	0	-4.988	-0.652	-2.063	H
HETATM	34	H	0	-4.778	0.267	2.145	H
HETATM	35	H	0	1.610	-1.734	2.533	H
HETATM	36	H	0	3.198	-1.376	3.231	H
HETATM	37	H	0	2.906	-2.970	2.504	H
HETATM	38	H	0	7.044	-0.281	0.258	H
HETATM	39	H	0	6.302	1.307	0.012	H
HETATM	40	H	0	6.681	0.291	-1.394	H
HETATM	41	H	0	2.546	-0.859	-3.456	H
HETATM	42	H	0	1.125	-0.329	-2.525	H
HETATM	43	H	0	1.500	-2.055	-2.647	H
HETATM	44	H	0	-1.519	-1.909	-2.300	H
HETATM	45	H	0	-2.952	-1.396	-3.200	H
HETATM	46	H	0	-2.949	-2.980	-2.390	H
HETATM	47	H	0	-7.047	0.067	-0.733	H
HETATM	48	H	0	-6.237	1.620	-0.475	H
HETATM	49	H	0	-6.830	0.701	0.923	H
HETATM	50	H	0	-3.055	-0.608	3.480	H
HETATM	51	H	0	-1.499	-0.175	2.730	H
HETATM	52	H	0	-1.974	-1.872	2.840	H
HETATM	53	C	0	-1.276	2.660	0.410	C
HETATM	54	H	0	-1.549	2.739	1.472	H
HETATM	55	H	0	-2.086	2.650	-0.331	H
HETATM	56	C	0	1.399	1.923	-0.472	C
HETATM	57	C	0	-0.035	3.269	0.039	C
HETATM	58	F	0	1.785	2.154	-1.724	F
HETATM	59	H	0	2.200	2.245	0.227	H
HETATM	60	H	0	0.059	3.751	-0.946	H
HETATM	61	F	0	0.628	3.942	0.997	F

END

at3PA.pdb

TITLE	at3PA.pdb						
HETATM	1	Ru	0	0.064	0.916	0.047	Ru
HETATM	2	Cl	0	0.928	0.983	2.294	Cl
HETATM	3	Cl	0	-0.909	0.897	-2.192	Cl
HETATM	4	C	0	-0.160	-1.086	0.046	C
HETATM	5	N	0	0.878	-1.935	-0.007	N
HETATM	6	C	0	0.442	-3.334	-0.037	C
HETATM	7	C	0	-1.078	-3.221	0.124	C
HETATM	8	N	0	-1.311	-1.773	0.096	N
HETATM	9	C	0	2.238	-1.495	-0.068	C
HETATM	10	C	0	3.015	-1.496	1.108	C
HETATM	11	C	0	4.308	-0.974	1.047	C
HETATM	12	C	0	4.842	-0.469	-0.147	C
HETATM	13	C	0	4.065	-0.528	-1.307	C

HETATM	14	C	0	2.762	-1.043	-1.294	C
HETATM	15	C	0	-2.609	-1.175	0.140	C
HETATM	16	C	0	-3.401	-1.158	-1.024	C
HETATM	17	C	0	-4.644	-0.522	-0.970	C
HETATM	18	C	0	-5.113	0.080	0.204	C
HETATM	19	C	0	-4.321	0.011	1.354	C
HETATM	20	C	0	-3.071	-0.618	1.348	C
HETATM	21	C	0	2.479	-2.049	2.392	C
HETATM	22	C	0	6.214	0.132	-0.168	C
HETATM	23	C	0	1.969	-1.101	-2.562	C
HETATM	24	C	0	-2.947	-1.818	-2.289	C
HETATM	25	C	0	-6.429	0.796	0.218	C
HETATM	26	C	0	-2.262	-0.704	2.606	C
HETATM	27	H	0	0.923	-3.900	0.781	H
HETATM	28	H	0	0.743	-3.806	-0.991	H
HETATM	29	H	0	-1.445	-3.642	1.079	H
HETATM	30	H	0	-1.638	-3.712	-0.692	H
HETATM	31	H	0	4.912	-0.947	1.963	H
HETATM	32	H	0	4.479	-0.165	-2.256	H
HETATM	33	H	0	-5.259	-0.489	-1.878	H
HETATM	34	H	0	-4.689	0.448	2.292	H
HETATM	35	H	0	1.403	-1.843	2.512	H
HETATM	36	H	0	2.990	-1.603	3.260	H
HETATM	37	H	0	2.628	-3.146	2.456	H
HETATM	38	H	0	6.928	-0.446	0.444	H
HETATM	39	H	0	6.206	1.158	0.246	H
HETATM	40	H	0	6.619	0.202	-1.192	H
HETATM	41	H	0	2.635	-1.194	-3.437	H
HETATM	42	H	0	1.354	-0.193	-2.711	H
HETATM	43	H	0	1.260	-1.947	-2.579	H
HETATM	44	H	0	-1.851	-1.793	-2.399	H
HETATM	45	H	0	-3.370	-1.312	-3.172	H
HETATM	46	H	0	-3.277	-2.876	-2.336	H
HETATM	47	H	0	-7.182	0.289	-0.410	H
HETATM	48	H	0	-6.330	1.824	-0.180	H
HETATM	49	H	0	-6.839	0.886	1.238	H
HETATM	50	H	0	-2.890	-0.512	3.492	H
HETATM	51	H	0	-1.430	0.027	2.632	H
HETATM	52	H	0	-1.792	-1.696	2.734	H
HETATM	53	C	0	-1.058	2.546	0.291	C
HETATM	54	H	0	-1.330	2.764	1.337	H
HETATM	55	H	0	-1.856	2.691	-0.452	H
HETATM	56	C	0	1.455	2.145	-0.517	C
HETATM	57	C	0	0.296	3.162	-0.085	C
HETATM	58	F	0	1.835	2.294	-1.805	F
HETATM	59	H	0	2.335	2.248	0.144	H
HETATM	60	H	0	0.168	3.773	-0.997	H
HETATM	61	F	0	0.779	3.939	0.935	F

END

at3i.pdb

TITLE	at3i.pdb						
HETATM	1	Ru	0	-0.188	0.908	-0.009	Ru
HETATM	2	Cl	0	-1.062	0.842	-2.279	Cl
HETATM	3	Cl	0	0.667	1.087	2.268	Cl
HETATM	4	C	0	0.216	-1.076	0.067	C
HETATM	5	N	0	-0.790	-1.960	0.212	N
HETATM	6	C	0	-0.312	-3.311	0.499	C
HETATM	7	C	0	1.194	-3.184	0.255	C
HETATM	8	N	0	1.388	-1.735	0.125	N
HETATM	9	C	0	-2.155	-1.540	0.162	C

HETATM	10	C	0	-2.865	-1.712	-1.047	C
HETATM	11	C	0	-4.159	-1.205	-1.136	C
HETATM	12	C	0	-4.758	-0.524	-0.065	C
HETATM	13	C	0	-4.047	-0.396	1.127	C
HETATM	14	C	0	-2.749	-0.914	1.274	C
HETATM	15	C	0	2.669	-1.131	-0.043	C
HETATM	16	C	0	3.504	-0.951	1.073	C
HETATM	17	C	0	4.736	-0.312	0.883	C
HETATM	18	C	0	5.147	0.138	-0.375	C
HETATM	19	C	0	4.306	-0.083	-1.473	C
HETATM	20	C	0	3.068	-0.718	-1.331	C
HETATM	21	C	0	-2.234	-2.406	-2.213	C
HETATM	22	C	0	-6.131	0.057	-0.215	C
HETATM	23	C	0	-2.086	-0.852	2.617	C
HETATM	24	C	0	3.110	-1.440	2.432	C
HETATM	25	C	0	6.449	0.860	-0.546	C
HETATM	26	C	0	2.188	-0.954	-2.520	C
HETATM	27	H	0	-0.798	-4.051	-0.160	H
HETATM	28	H	0	-0.555	-3.584	1.545	H
HETATM	29	H	0	1.523	-3.693	-0.672	H
HETATM	30	H	0	1.803	-3.582	1.085	H
HETATM	31	H	0	-4.707	-1.314	-2.081	H
HETATM	32	H	0	-4.508	0.112	1.985	H
HETATM	33	H	0	5.388	-0.154	1.753	H
HETATM	34	H	0	4.624	0.241	-2.473	H
HETATM	35	H	0	-1.192	-2.075	-2.363	H
HETATM	36	H	0	-2.782	-2.192	-3.145	H
HETATM	37	H	0	-2.225	-3.507	-2.085	H
HETATM	38	H	0	-6.845	-0.678	-0.627	H
HETATM	39	H	0	-6.130	0.914	-0.915	H
HETATM	40	H	0	-6.535	0.419	0.745	H
HETATM	41	H	0	-2.658	-1.451	3.351	H
HETATM	42	H	0	-2.045	0.181	3.003	H
HETATM	43	H	0	-1.047	-1.215	2.608	H
HETATM	44	H	0	2.018	-1.423	2.574	H
HETATM	45	H	0	3.548	-0.807	3.222	H
HETATM	46	H	0	3.470	-2.473	2.611	H
HETATM	47	H	0	7.158	0.634	0.268	H
HETATM	48	H	0	6.302	1.957	-0.546	H
HETATM	49	H	0	6.938	0.611	-1.504	H
HETATM	50	H	0	2.728	-0.754	-3.460	H
HETATM	51	H	0	1.284	-0.312	-2.515	H
HETATM	52	H	0	1.820	-1.996	-2.562	H
HETATM	53	C	0	1.307	1.858	-0.517	C
HETATM	54	H	0	1.432	2.223	-1.558	H
HETATM	55	H	0	2.115	2.103	0.203	H
HETATM	56	C	0	-1.638	2.503	0.321	C
HETATM	57	C	0	-0.497	3.265	0.030	C
HETATM	58	F	0	-2.081	2.453	1.592	F
HETATM	59	H	0	-2.435	2.375	-0.425	H
HETATM	60	H	0	0.101	3.728	0.825	H
HETATM	61	F	0	-0.429	3.882	-1.151	F

END

at3j.pdb

TITLE	at3j.pdb						
HETATM	1	Ru	0	-0.201	0.982	0.087	Ru
HETATM	2	C	0	-0.244	-3.260	0.062	C
HETATM	3	C	0	1.270	-3.097	0.178	C
HETATM	4	H	0	-0.555	-3.710	-0.901	H
HETATM	5	H	0	1.828	-3.605	-0.629	H

HETATM	6	C	0	0.284	-0.973	0.083	C
HETATM	7	N	0	1.456	-1.644	0.084	N
HETATM	8	N	0	-0.721	-1.881	0.147	N
HETATM	9	Cl	0	-0.542	1.201	-2.325	Cl
HETATM	10	Cl	0	-0.070	0.944	2.518	Cl
HETATM	11	C	0	-1.908	2.637	0.011	C
HETATM	12	C	0	2.757	-1.072	-0.022	C
HETATM	13	C	0	3.529	-0.873	1.138	C
HETATM	14	C	0	3.250	-0.732	-1.297	C
HETATM	15	C	0	4.802	-0.309	0.999	C
HETATM	16	C	0	4.527	-0.168	-1.389	C
HETATM	17	C	0	5.313	0.056	-0.253	C
HETATM	18	H	0	5.407	-0.140	1.899	H
HETATM	19	H	0	4.917	0.102	-2.379	H
HETATM	20	C	0	-2.097	-1.519	-0.003	C
HETATM	21	C	0	-2.907	-1.382	1.145	C
HETATM	22	C	0	-2.638	-1.371	-1.297	C
HETATM	23	C	0	-4.234	-0.981	0.976	C
HETATM	24	C	0	-3.967	-0.950	-1.416	C
HETATM	25	C	0	-4.770	-0.728	-0.293	C
HETATM	26	H	0	-4.867	-0.859	1.864	H
HETATM	27	H	0	-4.387	-0.805	-2.420	H
HETATM	28	C	0	2.978	-1.201	2.490	C
HETATM	29	H	0	3.672	-0.892	3.288	H
HETATM	30	H	0	2.011	-0.688	2.663	H
HETATM	31	H	0	2.795	-2.284	2.621	H
HETATM	32	C	0	2.413	-0.950	-2.518	C
HETATM	33	H	0	2.000	-1.975	-2.561	H
HETATM	34	H	0	1.543	-0.263	-2.545	H
HETATM	35	H	0	2.996	-0.784	-3.438	H
HETATM	36	C	0	6.663	0.696	-0.372	C
HETATM	37	H	0	6.583	1.800	-0.388	H
HETATM	38	H	0	7.320	0.437	0.475	H
HETATM	39	H	0	7.176	0.406	-1.305	H
HETATM	40	C	0	-2.371	-1.692	2.507	C
HETATM	41	H	0	-3.152	-1.574	3.275	H
HETATM	42	H	0	-1.997	-2.732	2.571	H
HETATM	43	H	0	-1.529	-1.028	2.772	H
HETATM	44	C	0	-1.863	-1.745	-2.524	C
HETATM	45	H	0	-2.068	-2.799	-2.798	H
HETATM	46	H	0	-2.149	-1.119	-3.384	H
HETATM	47	H	0	-0.774	-1.630	-2.400	H
HETATM	48	C	0	-6.174	-0.225	-0.439	C
HETATM	49	H	0	-6.217	0.873	-0.311	H
HETATM	50	H	0	-6.592	-0.446	-1.436	H
HETATM	51	H	0	-6.849	-0.655	0.321	H
HETATM	52	H	0	1.666	-3.473	1.140	H
HETATM	53	H	0	-0.679	-3.875	0.870	H
HETATM	54	C	0	-0.863	3.356	0.515	C
HETATM	55	C	0	1.472	1.671	-0.080	C
HETATM	56	H	0	2.284	1.458	0.645	H
HETATM	57	H	0	1.717	2.389	-0.892	H
HETATM	58	H	0	-0.617	3.450	1.578	H
HETATM	59	H	0	-2.244	2.676	-1.030	H
HETATM	60	F	0	-2.748	2.009	0.847	F
HETATM	61	F	0	-0.193	4.172	-0.300	F
END							

s3k.pdb

TITLE	s3k.pdb						
HETATM	1	Ru	0	0.220	-1.025	0.003	Ru

HETATM	2	C	0	0.114	3.159	0.278	C
HETATM	3	C	0	-1.396	2.933	0.348	C
HETATM	4	H	0	0.424	3.664	-0.659	H
HETATM	5	H	0	-1.955	3.473	-0.437	H
HETATM	6	C	0	-0.327	0.857	0.170	C
HETATM	7	N	0	-1.527	1.484	0.162	N
HETATM	8	N	0	0.642	1.799	0.320	N
HETATM	9	Cl	0	0.416	-1.010	-2.404	Cl
HETATM	10	Cl	0	0.236	-1.476	2.402	Cl
HETATM	11	C	0	2.349	-2.605	0.114	C
HETATM	12	C	0	-2.803	0.863	0.048	C
HETATM	13	C	0	-3.490	0.455	1.209	C
HETATM	14	C	0	-3.376	0.712	-1.230	C
HETATM	15	C	0	-4.761	-0.111	1.066	C
HETATM	16	C	0	-4.648	0.138	-1.328	C
HETATM	17	C	0	-5.352	-0.280	-0.193	C
HETATM	18	H	0	-5.303	-0.431	1.965	H
HETATM	19	H	0	-5.099	0.016	-2.321	H
HETATM	20	C	0	2.025	1.462	0.184	C
HETATM	21	C	0	2.781	1.181	1.343	C
HETATM	22	C	0	2.618	1.441	-1.096	C
HETATM	23	C	0	4.107	0.764	1.184	C
HETATM	24	C	0	3.948	1.022	-1.204	C
HETATM	25	C	0	4.694	0.651	-0.082	C
HETATM	26	H	0	4.698	0.529	2.078	H
HETATM	27	H	0	4.406	0.972	-2.201	H
HETATM	28	C	0	-2.847	0.577	2.555	C
HETATM	29	H	0	-3.559	0.340	3.362	H
HETATM	30	H	0	-1.985	-0.115	2.650	H
HETATM	31	H	0	-2.448	1.590	2.744	H
HETATM	32	C	0	-2.611	1.114	-2.452	C
HETATM	33	H	0	-2.231	2.151	-2.389	H
HETATM	34	H	0	-1.723	0.466	-2.593	H
HETATM	35	H	0	-3.234	1.039	-3.359	H
HETATM	36	C	0	-6.701	-0.920	-0.322	C
HETATM	37	H	0	-6.618	-2.023	-0.361	H
HETATM	38	H	0	-7.353	-0.684	0.536	H
HETATM	39	H	0	-7.220	-0.607	-1.243	H
HETATM	40	C	0	2.194	1.371	2.707	C
HETATM	41	H	0	2.947	1.184	3.490	H
HETATM	42	H	0	1.818	2.402	2.846	H
HETATM	43	H	0	1.346	0.685	2.887	H
HETATM	44	C	0	1.885	1.924	-2.309	C
HETATM	45	H	0	2.071	3.005	-2.469	H
HETATM	46	H	0	2.223	1.396	-3.215	H
HETATM	47	H	0	0.797	1.769	-2.240	H
HETATM	48	C	0	6.085	0.118	-0.235	C
HETATM	49	H	0	6.065	-0.970	-0.439	H
HETATM	50	H	0	6.620	0.586	-1.079	H
HETATM	51	H	0	6.689	0.262	0.678	H
HETATM	52	H	0	-1.828	3.233	1.323	H
HETATM	53	H	0	0.501	3.759	1.120	H
HETATM	54	C	0	1.294	-3.390	-0.172	C
HETATM	55	H	0	1.119	-3.760	-1.188	H
HETATM	56	C	0	-1.464	-1.693	-0.112	C
HETATM	57	H	0	-2.036	-2.020	0.785	H
HETATM	58	H	0	-1.969	-1.841	-1.091	H
HETATM	59	H	0	2.602	-2.232	1.116	H
HETATM	60	H	0	0.660	-3.729	0.652	H
HETATM	61	F	0	3.233	-2.244	-0.807	F

END

s3l.pdb

TITLE	s3l.pdb						
REMARK	1 File created by GaussView 5.0.8						
HETATM	1	Ru	0	0.242	-0.972	0.083	Ru
HETATM	2	Cl	0	-0.283	-1.097	2.475	Cl
HETATM	3	Cl	0	0.779	-1.104	-2.285	Cl
HETATM	4	C	0	-0.255	0.983	0.001	C
HETATM	5	N	0	-1.443	1.611	-0.085	N
HETATM	6	C	0	-1.296	3.070	-0.006	C
HETATM	7	C	0	0.220	3.273	-0.088	C
HETATM	8	N	0	0.724	1.911	0.074	N
HETATM	9	H	0	-1.721	3.443	0.946	H
HETATM	10	H	0	-1.847	3.557	-0.830	H
HETATM	11	H	0	0.612	3.938	0.701	H
HETATM	12	H	0	0.542	3.687	-1.064	H
HETATM	13	C	0	-2.709	0.957	-0.119	C
HETATM	14	C	0	-3.444	0.783	1.069	C
HETATM	15	C	0	-4.672	0.115	0.998	C
HETATM	16	C	0	-5.175	-0.372	-0.213	C
HETATM	17	C	0	-4.431	-0.166	-1.381	C
HETATM	18	C	0	-3.199	0.496	-1.356	C
HETATM	19	C	0	2.093	1.496	0.067	C
HETATM	20	C	0	2.780	1.351	-1.156	C
HETATM	21	C	0	4.052	0.775	-1.136	C
HETATM	22	C	0	4.654	0.366	0.060	C
HETATM	23	C	0	3.990	0.613	1.267	C
HETATM	24	C	0	2.714	1.188	1.297	C
HETATM	25	C	0	-2.938	1.307	2.378	C
HETATM	26	C	0	-6.473	-1.121	-0.256	C
HETATM	27	C	0	-2.411	0.706	-2.611	C
HETATM	28	C	0	2.183	1.833	-2.442	C
HETATM	29	C	0	5.971	-0.346	0.043	C
HETATM	30	C	0	2.045	1.502	2.599	C
HETATM	31	H	0	-5.246	-0.034	1.922	H
HETATM	32	H	0	-4.820	-0.526	-2.343	H
HETATM	33	H	0	4.575	0.618	-2.087	H
HETATM	34	H	0	4.478	0.357	2.217	H
HETATM	35	H	0	-3.162	2.386	2.500	H
HETATM	36	H	0	-1.849	1.168	2.483	H
HETATM	37	H	0	-3.415	0.786	3.224	H
HETATM	38	H	0	-7.172	-0.782	0.528	H
HETATM	39	H	0	-6.318	-2.205	-0.093	H
HETATM	40	H	0	-6.978	-1.017	-1.231	H
HETATM	41	H	0	-3.004	0.443	-3.503	H
HETATM	42	H	0	-1.488	0.091	-2.627	H
HETATM	43	H	0	-2.081	1.756	-2.722	H
HETATM	44	H	0	1.090	1.698	-2.471	H
HETATM	45	H	0	2.596	1.282	-3.302	H
HETATM	46	H	0	2.403	2.908	-2.599	H
HETATM	47	H	0	6.634	0.023	-0.759	H
HETATM	48	H	0	5.825	-1.427	-0.142	H
HETATM	49	H	0	6.507	-0.254	1.003	H
HETATM	50	H	0	2.755	1.411	3.437	H
HETATM	51	H	0	1.198	0.819	2.804	H
HETATM	52	H	0	1.640	2.531	2.611	H
HETATM	53	C	0	-1.232	-2.015	-0.265	C
HETATM	54	H	0	-1.428	-2.411	-1.283	H
HETATM	55	H	0	-1.955	-2.293	0.530	H
HETATM	56	C	0	1.805	-2.499	0.466	C
HETATM	57	C	0	0.670	-3.289	0.322	C
HETATM	58	F	0	2.790	-2.541	-0.438	F

HETATM	59	H	0	2.151	-2.135	1.444	H
HETATM	60	H	0	0.565	-3.898	-0.584	H
HETATM	61	H	0	0.113	-3.568	1.222	H

END

s3PB.pdb

TITLE	s3PB.pdb						
HETATM	1	Ru	0	0.012	-1.031	-0.083	Ru
HETATM	2	C	0	-0.967	3.145	-0.150	C
HETATM	3	C	0	0.535	3.219	0.133	C
HETATM	4	H	0	-1.577	3.708	0.578	H
HETATM	5	H	0	0.769	3.667	1.119	H
HETATM	6	C	0	-0.119	0.986	0.035	C
HETATM	7	N	0	0.939	1.810	0.111	N
HETATM	8	N	0	-1.248	1.708	-0.054	N
HETATM	9	Cl	0	-0.861	-1.471	2.149	Cl
HETATM	10	Cl	0	0.775	-0.753	-2.370	Cl
HETATM	11	C	0	-1.136	-2.514	-0.717	C
HETATM	12	H	0	-1.311	-2.524	-1.804	H
HETATM	13	C	0	2.284	1.340	0.220	C
HETATM	14	C	0	3.128	1.380	-0.907	C
HETATM	15	C	0	2.731	0.819	1.450	C
HETATM	16	C	0	4.401	0.815	-0.800	C
HETATM	17	C	0	4.017	0.271	1.512	C
HETATM	18	C	0	4.854	0.239	0.392	C
HETATM	19	H	0	5.054	0.814	-1.683	H
HETATM	20	H	0	4.372	-0.141	2.466	H
HETATM	21	C	0	-2.560	1.136	-0.067	C
HETATM	22	C	0	-3.129	0.709	-1.281	C
HETATM	23	C	0	-3.258	1.018	1.151	C
HETATM	24	C	0	-4.391	0.104	-1.245	C
HETATM	25	C	0	-4.515	0.409	1.141	C
HETATM	26	C	0	-5.088	-0.068	-0.044	C
HETATM	27	H	0	-4.841	-0.235	-2.187	H
HETATM	28	H	0	-5.058	0.301	2.088	H
HETATM	29	C	0	2.695	2.025	-2.188	C
HETATM	30	H	0	3.183	1.550	-3.054	H
HETATM	31	H	0	1.608	1.942	-2.348	H
HETATM	32	H	0	2.968	3.099	-2.209	H
HETATM	33	C	0	1.860	0.841	2.670	C
HETATM	34	H	0	1.265	1.770	2.745	H
HETATM	35	H	0	1.128	0.009	2.679	H
HETATM	36	H	0	2.465	0.754	3.587	H
HETATM	37	C	0	6.197	-0.420	0.456	C
HETATM	38	H	0	6.144	-1.461	0.083	H
HETATM	39	H	0	6.945	0.099	-0.168	H
HETATM	40	H	0	6.586	-0.470	1.487	H
HETATM	41	C	0	-2.410	0.893	-2.582	C
HETATM	42	H	0	-3.071	0.666	-3.435	H
HETATM	43	H	0	-2.042	1.927	-2.711	H
HETATM	44	H	0	-1.517	0.243	-2.666	H
HETATM	45	C	0	-2.652	1.516	2.427	C
HETATM	46	H	0	-2.391	2.590	2.377	H
HETATM	47	H	0	-3.345	1.384	3.274	H
HETATM	48	H	0	-1.729	0.958	2.665	H
HETATM	49	C	0	-6.417	-0.760	-0.022	C
HETATM	50	H	0	-6.302	-1.836	0.210	H
HETATM	51	H	0	-7.087	-0.343	0.749	H
HETATM	52	H	0	-6.933	-0.697	-0.995	H
HETATM	53	H	0	1.093	3.788	-0.631	H
HETATM	54	H	0	-1.232	3.515	-1.159	H

HETATM	55	C	0	0.154	-3.246	-0.277	C
HETATM	56	H	0	-0.108	-3.924	0.552	H
HETATM	57	H	0	0.590	-3.757	-1.152	H
HETATM	58	C	0	1.366	-2.371	0.274	C
HETATM	59	H	0	1.603	-2.565	1.335	H
HETATM	60	H	0	-2.016	-2.735	-0.093	H
HETATM	61	F	0	2.488	-2.496	-0.462	F

END

s3m.pdb

TITLE	s3m.pdb						
HETATM	1	Ru	0	0.219	-1.089	-0.013	Ru
HETATM	2	Cl	0	0.931	-0.973	-2.345	Cl
HETATM	3	Cl	0	-0.281	-1.382	2.350	Cl
HETATM	4	C	0	-0.007	0.926	0.232	C
HETATM	5	N	0	1.061	1.721	0.441	N
HETATM	6	C	0	0.692	3.128	0.615	C
HETATM	7	C	0	-0.832	3.097	0.481	C
HETATM	8	N	0	-1.126	1.671	0.287	N
HETATM	9	C	0	2.399	1.246	0.254	C
HETATM	10	C	0	2.985	1.335	-1.024	C
HETATM	11	C	0	4.254	0.782	-1.214	C
HETATM	12	C	0	4.948	0.160	-0.170	C
HETATM	13	C	0	4.368	0.141	1.103	C
HETATM	14	C	0	3.103	0.690	1.344	C
HETATM	15	C	0	-2.447	1.185	0.045	C
HETATM	16	C	0	-3.312	0.939	1.127	C
HETATM	17	C	0	-4.598	0.461	0.854	C
HETATM	18	C	0	-5.032	0.223	-0.456	C
HETATM	19	C	0	-4.158	0.499	-1.512	C
HETATM	20	C	0	-2.866	0.989	-1.285	C
HETATM	21	C	0	2.297	2.038	-2.154	C
HETATM	22	C	0	6.279	-0.482	-0.415	C
HETATM	23	C	0	2.533	0.714	2.728	C
HETATM	24	C	0	-2.862	1.164	2.537	C
HETATM	25	C	0	-6.400	-0.331	-0.716	C
HETATM	26	C	0	-1.951	1.294	-2.430	C
HETATM	27	H	0	1.181	3.749	-0.158	H
HETATM	28	H	0	1.032	3.498	1.600	H
HETATM	29	H	0	-1.204	3.681	-0.383	H
HETATM	30	H	0	-1.351	3.477	1.379	H
HETATM	31	H	0	4.706	0.826	-2.214	H
HETATM	32	H	0	4.919	-0.302	1.943	H
HETATM	33	H	0	-5.276	0.260	1.693	H
HETATM	34	H	0	-4.490	0.342	-2.547	H
HETATM	35	H	0	2.573	3.112	-2.180	H
HETATM	36	H	0	1.199	1.975	-2.086	H
HETATM	37	H	0	2.583	1.603	-3.125	H
HETATM	38	H	0	6.871	0.066	-1.168	H
HETATM	39	H	0	6.160	-1.513	-0.799	H
HETATM	40	H	0	6.881	-0.553	0.507	H
HETATM	41	H	0	2.219	1.732	3.023	H
HETATM	42	H	0	3.277	0.369	3.465	H
HETATM	43	H	0	1.639	0.068	2.826	H
HETATM	44	H	0	-2.608	2.223	2.732	H
HETATM	45	H	0	-1.964	0.562	2.766	H
HETATM	46	H	0	-3.650	0.883	3.255	H
HETATM	47	H	0	-7.151	0.079	-0.019	H
HETATM	48	H	0	-6.740	-0.126	-1.745	H
HETATM	49	H	0	-6.419	-1.430	-0.585	H
HETATM	50	H	0	-1.520	2.311	-2.357	H

HETATM	51	H	0	-2.483	1.228	-3.393	H
HETATM	52	H	0	-1.092	0.596	-2.477	H
HETATM	53	C	0	-1.302	-1.982	-0.553	C
HETATM	54	F	0	-2.314	-2.390	0.199	F
HETATM	55	H	0	-1.552	-2.153	-1.622	H
HETATM	56	C	0	1.482	-2.795	0.146	C
HETATM	57	C	0	0.254	-3.367	-0.283	C
HETATM	58	H	0	2.293	-2.676	-0.586	H
HETATM	59	H	0	1.760	-2.881	1.205	H
HETATM	60	H	0	0.189	-3.705	-1.326	H
HETATM	61	H	0	-0.351	-3.912	0.454	H

END

s3n.pdb

TITLE	s3n.pdb						
HETATM	1	Ru	0	-0.325	1.016	0.272	Ru
HETATM	2	C	0	-0.465	-3.175	-0.206	C
HETATM	3	C	0	1.057	-3.058	-0.292	C
HETATM	4	H	0	-0.913	-3.653	-1.098	H
HETATM	5	H	0	1.459	-3.366	-1.277	H
HETATM	6	C	0	0.153	-0.911	-0.016	C
HETATM	7	N	0	1.297	-1.627	-0.080	N
HETATM	8	N	0	-0.885	-1.781	-0.105	N
HETATM	9	Cl	0	-0.790	1.541	-2.049	Cl
HETATM	10	Cl	0	-0.277	0.641	2.673	Cl
HETATM	11	C	0	-2.011	2.645	0.703	C
HETATM	12	C	0	2.611	-1.082	-0.141	C
HETATM	13	C	0	3.399	-1.047	1.024	C
HETATM	14	C	0	3.088	-0.570	-1.363	C
HETATM	15	C	0	4.677	-0.481	0.947	C
HETATM	16	C	0	4.369	-0.010	-1.396	C
HETATM	17	C	0	5.173	0.048	-0.252	C
HETATM	18	H	0	5.296	-0.443	1.853	H
HETATM	19	H	0	4.746	0.395	-2.344	H
HETATM	20	C	0	-2.239	-1.329	-0.156	C
HETATM	21	C	0	-2.988	-1.195	1.032	C
HETATM	22	C	0	-2.810	-1.023	-1.412	C
HETATM	23	C	0	-4.264	-0.623	0.951	C
HETATM	24	C	0	-4.088	-0.463	-1.444	C
HETATM	25	C	0	-4.816	-0.226	-0.271	C
HETATM	26	H	0	-4.844	-0.495	1.875	H
HETATM	27	H	0	-4.524	-0.195	-2.415	H
HETATM	28	C	0	2.847	-1.535	2.328	C
HETATM	29	H	0	3.592	-1.448	3.135	H
HETATM	30	H	0	1.953	-0.951	2.625	H
HETATM	31	H	0	2.528	-2.593	2.284	H
HETATM	32	C	0	2.223	-0.584	-2.586	C
HETATM	33	H	0	1.745	-1.567	-2.749	H
HETATM	34	H	0	1.397	0.152	-2.512	H
HETATM	35	H	0	2.804	-0.339	-3.490	H
HETATM	36	C	0	6.527	0.689	-0.301	C
HETATM	37	H	0	6.460	1.780	-0.126	H
HETATM	38	H	0	7.205	0.286	0.470	H
HETATM	39	H	0	7.011	0.558	-1.284	H
HETATM	40	C	0	-2.503	-1.739	2.341	C
HETATM	41	H	0	-2.778	-1.079	3.180	H
HETATM	42	H	0	-2.967	-2.727	2.533	H
HETATM	43	H	0	-1.411	-1.857	2.379	H
HETATM	44	C	0	-2.101	-1.353	-2.690	C
HETATM	45	H	0	-2.338	-2.389	-3.007	H
HETATM	46	H	0	-2.412	-0.680	-3.505	H

HETATM	47	H	0	-1.007	-1.268	-2.604	H
HETATM	48	C	0	-6.152	0.449	-0.327	C
HETATM	49	H	0	-6.039	1.550	-0.342	H
HETATM	50	H	0	-6.714	0.180	-1.238	H
HETATM	51	H	0	-6.778	0.204	0.548	H
HETATM	52	H	0	1.581	-3.656	0.474	H
HETATM	53	H	0	-0.804	-3.745	0.681	H
HETATM	54	C	0	-0.878	3.397	0.700	C
HETATM	55	H	0	-0.537	3.900	-0.212	H
HETATM	56	C	0	1.362	1.670	0.239	C
HETATM	57	H	0	2.227	1.241	0.787	H
HETATM	58	H	0	-2.413	2.235	1.640	H
HETATM	59	H	0	-0.331	3.605	1.629	H
HETATM	60	H	0	-2.623	2.541	-0.202	H
HETATM	61	F	0	1.775	2.768	-0.384	F

END

a3k.pdb

TITLE	a3k.pdb						
HETATM	1	Ru	0	-0.271	0.974	0.170	Ru
HETATM	2	C	0	-0.372	-3.236	-0.070	C
HETATM	3	C	0	1.147	-3.094	0.027	C
HETATM	4	H	0	-0.703	-3.623	-1.054	H
HETATM	5	H	0	1.684	-3.569	-0.813	H
HETATM	6	C	0	0.185	-0.959	0.068	C
HETATM	7	N	0	1.351	-1.642	0.003	N
HETATM	8	N	0	-0.831	-1.861	0.112	N
HETATM	9	Cl	0	-0.701	1.339	-2.187	Cl
HETATM	10	Cl	0	-0.080	0.922	2.606	Cl
HETATM	11	C	0	-1.890	2.715	0.425	C
HETATM	12	C	0	2.653	-1.073	-0.091	C
HETATM	13	C	0	3.442	-0.934	1.067	C
HETATM	14	C	0	3.131	-0.668	-1.353	C
HETATM	15	C	0	4.717	-0.374	0.940	C
HETATM	16	C	0	4.411	-0.108	-1.434	C
HETATM	17	C	0	5.214	0.051	-0.299	C
HETATM	18	H	0	5.335	-0.256	1.839	H
HETATM	19	H	0	4.788	0.212	-2.414	H
HETATM	20	C	0	-2.193	-1.444	-0.013	C
HETATM	21	C	0	-2.970	-1.264	1.153	C
HETATM	22	C	0	-2.745	-1.237	-1.294	C
HETATM	23	C	0	-4.269	-0.763	1.012	C
HETATM	24	C	0	-4.049	-0.738	-1.385	C
HETATM	25	C	0	-4.813	-0.471	-0.244	C
HETATM	26	H	0	-4.877	-0.611	1.914	H
HETATM	27	H	0	-4.475	-0.553	-2.379	H
HETATM	28	C	0	2.901	-1.313	2.410	C
HETATM	29	H	0	3.636	-1.111	3.207	H
HETATM	30	H	0	1.982	-0.740	2.644	H
HETATM	31	H	0	2.636	-2.384	2.476	H
HETATM	32	C	0	2.274	-0.812	-2.572	C
HETATM	33	H	0	1.840	-1.826	-2.659	H
HETATM	34	H	0	1.417	-0.108	-2.554	H
HETATM	35	H	0	2.849	-0.612	-3.491	H
HETATM	36	C	0	6.567	0.686	-0.401	C
HETATM	37	H	0	6.512	1.777	-0.223	H
HETATM	38	H	0	7.272	0.281	0.345	H
HETATM	39	H	0	7.013	0.552	-1.401	H
HETATM	40	C	0	-2.441	-1.649	2.499	C
HETATM	41	H	0	-3.206	-1.504	3.279	H
HETATM	42	H	0	-2.138	-2.712	2.524	H

HETATM	43	H	0	-1.555	-1.051	2.780	H
HETATM	44	C	0	-2.000	-1.609	-2.539	C
HETATM	45	H	0	-2.227	-2.655	-2.828	H
HETATM	46	H	0	-2.288	-0.964	-3.384	H
HETATM	47	H	0	-0.908	-1.516	-2.429	H
HETATM	48	C	0	-6.187	0.116	-0.366	C
HETATM	49	H	0	-6.146	1.222	-0.405	H
HETATM	50	H	0	-6.697	-0.212	-1.287	H
HETATM	51	H	0	-6.827	-0.147	0.493	H
HETATM	52	H	0	1.554	-3.523	0.963	H
HETATM	53	H	0	-0.795	-3.898	0.706	H
HETATM	54	C	0	-0.795	3.485	0.640	C
HETATM	55	C	0	1.414	1.636	0.007	C
HETATM	56	H	0	2.194	1.505	0.787	H
HETATM	57	H	0	1.700	2.257	-0.871	H
HETATM	58	H	0	-2.338	2.195	1.281	H
HETATM	59	H	0	-0.253	3.559	1.591	H
HETATM	60	H	0	-2.437	2.787	-0.521	H
HETATM	61	F	0	-0.335	4.308	-0.291	F

END

a3l.pdb

TITLE	a3l.pdb						
HETATM	1	Ru	0	-0.239	0.952	-0.163	Ru
HETATM	2	Cl	0	-0.674	0.713	-2.563	Cl
HETATM	3	Cl	0	0.049	1.406	2.194	Cl
HETATM	4	C	0	0.131	-1.030	0.029	C
HETATM	5	N	0	-0.900	-1.897	0.087	N
HETATM	6	C	0	-0.463	-3.276	0.300	C
HETATM	7	C	0	1.052	-3.170	0.107	C
HETATM	8	N	0	1.285	-1.720	0.092	N
HETATM	9	C	0	-2.241	-1.410	0.169	C
HETATM	10	C	0	-3.039	-1.382	-0.995	C
HETATM	11	C	0	-4.296	-0.776	-0.921	C
HETATM	12	C	0	-4.778	-0.223	0.273	C
HETATM	13	C	0	-3.995	-0.331	1.427	C
HETATM	14	C	0	-2.732	-0.934	1.403	C
HETATM	15	C	0	2.589	-1.139	0.052	C
HETATM	16	C	0	3.247	-0.864	1.264	C
HETATM	17	C	0	4.513	-0.271	1.214	C
HETATM	18	C	0	5.127	0.045	-0.003	C
HETATM	19	C	0	4.456	-0.261	-1.194	C
HETATM	20	C	0	3.189	-0.855	-1.189	C
HETATM	21	C	0	-2.585	-2.033	-2.264	C
HETATM	22	C	0	-6.098	0.485	0.307	C
HETATM	23	C	0	-1.991	-1.159	2.687	C
HETATM	24	C	0	2.589	-1.163	2.575	C
HETATM	25	C	0	6.464	0.721	-0.032	C
HETATM	26	C	0	2.475	-1.158	-2.470	C
HETATM	27	H	0	-0.947	-3.955	-0.424	H
HETATM	28	H	0	-0.744	-3.612	1.318	H
HETATM	29	H	0	1.392	-3.617	-0.847	H
HETATM	30	H	0	1.630	-3.647	0.918	H
HETATM	31	H	0	-4.914	-0.730	-1.827	H
HETATM	32	H	0	-4.376	0.058	2.380	H
HETATM	33	H	0	5.031	-0.048	2.156	H
HETATM	34	H	0	4.931	-0.034	-2.157	H
HETATM	35	H	0	-2.889	-3.099	-2.286	H
HETATM	36	H	0	-1.493	-1.988	-2.391	H
HETATM	37	H	0	-3.034	-1.547	-3.145	H
HETATM	38	H	0	-6.805	0.079	-0.436	H

HETATM	39	H	0	-5.979	1.561	0.076	H
HETATM	40	H	0	-6.573	0.426	1.301	H
HETATM	41	H	0	-2.341	-2.096	3.165	H
HETATM	42	H	0	-0.901	-1.231	2.555	H
HETATM	43	H	0	-2.167	-0.340	3.402	H
HETATM	44	H	0	2.202	-2.198	2.627	H
HETATM	45	H	0	1.725	-0.488	2.737	H
HETATM	46	H	0	3.288	-1.024	3.415	H
HETATM	47	H	0	7.077	0.463	0.848	H
HETATM	48	H	0	6.356	1.823	-0.030	H
HETATM	49	H	0	7.040	0.462	-0.937	H
HETATM	50	H	0	3.109	-0.931	-3.343	H
HETATM	51	H	0	1.541	-0.569	-2.569	H
HETATM	52	H	0	2.181	-2.222	-2.543	H
HETATM	53	C	0	1.247	1.964	-0.583	C
HETATM	54	H	0	1.607	2.068	-1.627	H
HETATM	55	H	0	1.838	2.471	0.205	H
HETATM	56	C	0	-1.683	2.537	-0.260	C
HETATM	57	C	0	-0.518	3.281	-0.536	C
HETATM	58	H	0	-2.322	2.256	-1.106	H
HETATM	59	H	0	-2.141	2.680	0.729	H
HETATM	60	H	0	-0.256	3.579	-1.561	H
HETATM	61	F	0	-0.066	4.138	0.381	F

END

a3NB.pdb

TITLE	a3NB.pdb						
HETATM	1	Ru	0	0.046	0.971	-0.140	Ru
HETATM	2	C	0	-0.857	-3.176	0.384	C
HETATM	3	C	0	0.662	-3.243	0.189	C
HETATM	4	H	0	-1.414	-3.759	-0.370	H
HETATM	5	H	0	0.959	-3.816	-0.709	H
HETATM	6	C	0	-0.032	-1.022	0.068	C
HETATM	7	N	0	1.038	-1.834	0.040	N
HETATM	8	N	0	-1.150	-1.747	0.234	N
HETATM	9	Cl	0	-0.872	0.638	-2.394	Cl
HETATM	10	Cl	0	0.967	1.411	2.028	Cl
HETATM	11	C	0	-1.231	2.471	-0.056	C
HETATM	12	H	0	-1.468	2.818	0.964	H
HETATM	13	C	0	2.384	-1.350	-0.009	C
HETATM	14	C	0	3.093	-1.170	1.194	C
HETATM	15	C	0	2.958	-1.031	-1.255	C
HETATM	16	C	0	4.374	-0.615	1.132	C
HETATM	17	C	0	4.243	-0.478	-1.269	C
HETATM	18	C	0	4.956	-0.248	-0.087	C
HETATM	19	H	0	4.923	-0.448	2.067	H
HETATM	20	H	0	4.698	-0.220	-2.235	H
HETATM	21	C	0	-2.468	-1.195	0.271	C
HETATM	22	C	0	-2.910	-0.549	1.442	C
HETATM	23	C	0	-3.303	-1.313	-0.857	C
HETATM	24	C	0	-4.181	0.034	1.441	C
HETATM	25	C	0	-4.566	-0.717	-0.812	C
HETATM	26	C	0	-5.014	-0.025	0.319	C
HETATM	27	H	0	-4.531	0.542	2.350	H
HETATM	28	H	0	-5.213	-0.786	-1.696	H
HETATM	29	C	0	2.503	-1.570	2.511	C
HETATM	30	H	0	2.945	-0.989	3.336	H
HETATM	31	H	0	1.414	-1.395	2.544	H
HETATM	32	H	0	2.685	-2.641	2.731	H
HETATM	33	C	0	2.214	-1.274	-2.531	C
HETATM	34	H	0	1.864	-2.320	-2.613	H

HETATM	35	H	0	1.311	-0.639	-2.619	H
HETATM	36	H	0	2.853	-1.070	-3.407	H
HETATM	37	C	0	6.307	0.399	-0.119	C
HETATM	38	H	0	6.232	1.485	0.081	H
HETATM	39	H	0	6.983	-0.014	0.649	H
HETATM	40	H	0	6.797	0.288	-1.101	H
HETATM	41	C	0	-2.052	-0.487	2.669	C
HETATM	42	H	0	-2.651	-0.223	3.556	H
HETATM	43	H	0	-1.550	-1.449	2.877	H
HETATM	44	H	0	-1.243	0.267	2.586	H
HETATM	45	C	0	-2.873	-2.076	-2.073	C
HETATM	46	H	0	-3.181	-3.139	-2.013	H
HETATM	47	H	0	-3.334	-1.659	-2.983	H
HETATM	48	H	0	-1.782	-2.039	-2.221	H
HETATM	49	C	0	-6.353	0.648	0.321	C
HETATM	50	H	0	-6.286	1.669	-0.100	H
HETATM	51	H	0	-7.091	0.103	-0.293	H
HETATM	52	H	0	-6.763	0.750	1.339	H
HETATM	53	H	0	1.189	-3.686	1.054	H
HETATM	54	H	0	-1.182	-3.527	1.382	H
HETATM	55	C	0	0.036	3.199	-0.611	C
HETATM	56	H	0	-0.287	3.674	-1.557	H
HETATM	57	C	0	1.248	2.291	-0.988	C
HETATM	58	H	0	2.143	2.564	-0.406	H
HETATM	59	H	0	1.402	2.182	-2.073	H
HETATM	60	H	0	-2.078	2.443	-0.758	H
HETATM	61	F	0	0.436	4.170	0.271	F

END

a3m.pdb

TITLE	a3m.pdb						
HETATM	1	Ru	0	-0.239	0.952	-0.163	Ru
HETATM	2	Cl	0	-0.674	0.713	-2.563	Cl
HETATM	3	Cl	0	0.049	1.406	2.194	Cl
HETATM	4	C	0	0.131	-1.030	0.029	C
HETATM	5	N	0	-0.900	-1.897	0.087	N
HETATM	6	C	0	-0.463	-3.276	0.300	C
HETATM	7	C	0	1.052	-3.170	0.107	C
HETATM	8	N	0	1.285	-1.720	0.092	N
HETATM	9	C	0	-2.241	-1.410	0.169	C
HETATM	10	C	0	-3.039	-1.382	-0.995	C
HETATM	11	C	0	-4.296	-0.776	-0.921	C
HETATM	12	C	0	-4.778	-0.223	0.273	C
HETATM	13	C	0	-3.995	-0.331	1.427	C
HETATM	14	C	0	-2.732	-0.934	1.403	C
HETATM	15	C	0	2.589	-1.139	0.052	C
HETATM	16	C	0	3.247	-0.864	1.264	C
HETATM	17	C	0	4.513	-0.271	1.214	C
HETATM	18	C	0	5.127	0.045	-0.003	C
HETATM	19	C	0	4.456	-0.261	-1.194	C
HETATM	20	C	0	3.189	-0.855	-1.189	C
HETATM	21	C	0	-2.585	-2.033	-2.264	C
HETATM	22	C	0	-6.098	0.485	0.307	C
HETATM	23	C	0	-1.991	-1.159	2.687	C
HETATM	24	C	0	2.589	-1.163	2.575	C
HETATM	25	C	0	6.464	0.721	-0.032	C
HETATM	26	C	0	2.475	-1.158	-2.470	C
HETATM	27	H	0	-0.947	-3.955	-0.424	H
HETATM	28	H	0	-0.744	-3.612	1.318	H
HETATM	29	H	0	1.392	-3.617	-0.847	H
HETATM	30	H	0	1.630	-3.647	0.918	H

HETATM	31	H	0	-4.914	-0.730	-1.827	H
HETATM	32	H	0	-4.376	0.058	2.380	H
HETATM	33	H	0	5.031	-0.048	2.156	H
HETATM	34	H	0	4.931	-0.034	-2.157	H
HETATM	35	H	0	-2.889	-3.099	-2.286	H
HETATM	36	H	0	-1.493	-1.988	-2.391	H
HETATM	37	H	0	-3.034	-1.547	-3.145	H
HETATM	38	H	0	-6.805	0.079	-0.436	H
HETATM	39	H	0	-5.979	1.561	0.076	H
HETATM	40	H	0	-6.573	0.426	1.301	H
HETATM	41	H	0	-2.341	-2.096	3.165	H
HETATM	42	H	0	-0.901	-1.231	2.555	H
HETATM	43	H	0	-2.167	-0.340	3.402	H
HETATM	44	H	0	2.202	-2.198	2.627	H
HETATM	45	H	0	1.725	-0.488	2.737	H
HETATM	46	H	0	3.288	-1.024	3.415	H
HETATM	47	H	0	7.077	0.463	0.848	H
HETATM	48	H	0	6.356	1.823	-0.030	H
HETATM	49	H	0	7.040	0.462	-0.937	H
HETATM	50	H	0	3.109	-0.931	-3.343	H
HETATM	51	H	0	1.541	-0.569	-2.569	H
HETATM	52	H	0	2.181	-2.222	-2.543	H
HETATM	53	C	0	1.247	1.964	-0.583	C
HETATM	54	H	0	1.607	2.068	-1.627	H
HETATM	55	H	0	1.838	2.471	0.205	H
HETATM	56	C	0	-1.683	2.537	-0.260	C
HETATM	57	C	0	-0.518	3.281	-0.536	C
HETATM	58	H	0	-2.322	2.256	-1.106	H
HETATM	59	H	0	-2.141	2.680	0.729	H
HETATM	60	H	0	-0.256	3.579	-1.561	H
HETATM	61	F	0	-0.066	4.138	0.381	F

END

a3n.pdb

TITLE	a3n.pdb						
HETATM	1	Ru	0	-0.271	0.974	0.170	Ru
HETATM	2	C	0	-0.372	-3.236	-0.070	C
HETATM	3	C	0	1.147	-3.094	0.027	C
HETATM	4	H	0	-0.703	-3.623	-1.054	H
HETATM	5	H	0	1.684	-3.569	-0.813	H
HETATM	6	C	0	0.185	-0.959	0.068	C
HETATM	7	N	0	1.351	-1.642	0.003	N
HETATM	8	N	0	-0.831	-1.861	0.112	N
HETATM	9	Cl	0	-0.701	1.339	-2.187	Cl
HETATM	10	Cl	0	-0.080	0.922	2.606	Cl
HETATM	11	C	0	-1.890	2.715	0.425	C
HETATM	12	C	0	2.653	-1.073	-0.091	C
HETATM	13	C	0	3.442	-0.934	1.067	C
HETATM	14	C	0	3.131	-0.668	-1.353	C
HETATM	15	C	0	4.717	-0.374	0.940	C
HETATM	16	C	0	4.411	-0.108	-1.434	C
HETATM	17	C	0	5.214	0.051	-0.299	C
HETATM	18	H	0	5.335	-0.256	1.839	H
HETATM	19	H	0	4.788	0.212	-2.414	H
HETATM	20	C	0	-2.193	-1.444	-0.013	C
HETATM	21	C	0	-2.970	-1.264	1.153	C
HETATM	22	C	0	-2.745	-1.237	-1.294	C
HETATM	23	C	0	-4.269	-0.763	1.012	C
HETATM	24	C	0	-4.049	-0.738	-1.385	C
HETATM	25	C	0	-4.813	-0.471	-0.244	C
HETATM	26	H	0	-4.877	-0.611	1.914	H

HETATM	27	H	0	-4.475	-0.553	-2.379	H
HETATM	28	C	0	2.901	-1.313	2.410	C
HETATM	29	H	0	3.636	-1.111	3.207	H
HETATM	30	H	0	1.982	-0.740	2.644	H
HETATM	31	H	0	2.636	-2.384	2.476	H
HETATM	32	C	0	2.274	-0.812	-2.572	C
HETATM	33	H	0	1.840	-1.826	-2.659	H
HETATM	34	H	0	1.417	-0.108	-2.554	H
HETATM	35	H	0	2.849	-0.612	-3.491	H
HETATM	36	C	0	6.567	0.686	-0.401	C
HETATM	37	H	0	6.512	1.777	-0.223	H
HETATM	38	H	0	7.272	0.281	0.345	H
HETATM	39	H	0	7.013	0.552	-1.401	H
HETATM	40	C	0	-2.441	-1.649	2.499	C
HETATM	41	H	0	-3.206	-1.504	3.279	H
HETATM	42	H	0	-2.138	-2.712	2.524	H
HETATM	43	H	0	-1.555	-1.051	2.780	H
HETATM	44	C	0	-2.000	-1.609	-2.539	C
HETATM	45	H	0	-2.227	-2.655	-2.828	H
HETATM	46	H	0	-2.288	-0.964	-3.384	H
HETATM	47	H	0	-0.908	-1.516	-2.429	H
HETATM	48	C	0	-6.187	0.116	-0.366	C
HETATM	49	H	0	-6.146	1.222	-0.405	H
HETATM	50	H	0	-6.697	-0.212	-1.287	H
HETATM	51	H	0	-6.827	-0.147	0.493	H
HETATM	52	H	0	1.554	-3.523	0.963	H
HETATM	53	H	0	-0.795	-3.898	0.706	H
HETATM	54	C	0	-0.795	3.485	0.640	C
HETATM	55	C	0	1.414	1.636	0.007	C
HETATM	56	H	0	2.194	1.505	0.787	H
HETATM	57	H	0	1.700	2.257	-0.871	H
HETATM	58	H	0	-2.338	2.195	1.281	H
HETATM	59	H	0	-0.253	3.559	1.591	H
HETATM	60	H	0	-2.437	2.787	-0.521	H
HETATM	61	F	0	-0.335	4.308	-0.291	F

END

4a.pdb

TITLE	4a.pdb						
HETATM	1	Ru	0	-0.298	0.542	0.034	Ru
HETATM	2	C	0	0.227	-3.577	0.133	C
HETATM	3	C	0	1.710	-3.236	-0.020	C
HETATM	4	H	0	-0.153	-4.220	-0.682	H
HETATM	5	H	0	2.134	-3.579	-0.984	H
HETATM	6	C	0	0.493	-1.241	0.055	C
HETATM	7	N	0	1.736	-1.769	0.037	N
HETATM	8	N	0	-0.403	-2.263	0.088	N
HETATM	9	Cl	0	-0.725	0.715	-2.317	Cl
HETATM	10	Cl	0	-0.403	0.673	2.428	Cl
HETATM	11	C	0	-2.624	2.351	0.194	C
HETATM	12	C	0	2.972	-1.064	-0.035	C
HETATM	13	C	0	3.703	-0.858	1.150	C
HETATM	14	C	0	3.455	-0.626	-1.280	C
HETATM	15	C	0	4.942	-0.219	1.066	C
HETATM	16	C	0	4.693	0.027	-1.318	C
HETATM	17	C	0	5.449	0.233	-0.159	C
HETATM	18	H	0	5.518	-0.051	1.985	H
HETATM	19	H	0	5.079	0.375	-2.286	H
HETATM	20	C	0	-1.807	-2.011	0.012	C
HETATM	21	C	0	-2.558	-1.832	1.197	C
HETATM	22	C	0	-2.426	-1.951	-1.256	C

HETATM	23	C	0	-3.898	-1.448	1.078	C
HETATM	24	C	0	-3.769	-1.571	-1.323	C
HETATM	25	C	0	-4.508	-1.282	-0.170	C
HETATM	26	H	0	-4.480	-1.278	1.993	H
HETATM	27	H	0	-4.246	-1.488	-2.308	H
HETATM	28	C	0	3.114	-1.237	2.473	C
HETATM	29	H	0	3.820	-1.050	3.297	H
HETATM	30	H	0	2.195	-0.652	2.673	H
HETATM	31	H	0	2.820	-2.303	2.522	H
HETATM	32	C	0	2.655	-0.829	-2.529	C
HETATM	33	H	0	2.286	-1.867	-2.626	H
HETATM	34	H	0	1.756	-0.182	-2.554	H
HETATM	35	H	0	3.252	-0.600	-3.428	H
HETATM	36	C	0	6.762	0.955	-0.221	C
HETATM	37	H	0	6.636	2.035	-0.017	H
HETATM	38	H	0	7.478	0.574	0.527	H
HETATM	39	H	0	7.231	0.873	-1.216	H
HETATM	40	C	0	-1.985	-2.142	2.545	C
HETATM	41	H	0	-2.374	-1.457	3.315	H
HETATM	42	H	0	-2.266	-3.171	2.845	H
HETATM	43	H	0	-0.888	-2.064	2.571	H
HETATM	44	C	0	-1.700	-2.353	-2.502	C
HETATM	45	H	0	-1.872	-3.428	-2.717	H
HETATM	46	H	0	-2.055	-1.781	-3.374	H
HETATM	47	H	0	-0.613	-2.193	-2.434	H
HETATM	48	C	0	-5.918	-0.788	-0.268	C
HETATM	49	H	0	-5.944	0.317	-0.309	H
HETATM	50	H	0	-6.422	-1.150	-1.181	H
HETATM	51	H	0	-6.524	-1.086	0.604	H
HETATM	52	H	0	2.339	-3.662	0.782	H
HETATM	53	H	0	-0.002	-4.082	1.091	H
HETATM	54	C	0	-1.568	3.180	0.083	C
HETATM	55	C	0	1.238	1.524	-0.029	C
HETATM	56	F	0	-3.327	1.952	-0.835	F
HETATM	57	F	0	-3.141	1.999	1.342	F
HETATM	58	F	0	-0.952	3.689	1.122	F
HETATM	59	F	0	-1.178	3.685	-1.057	F
HETATM	60	F	0	2.186	1.599	0.877	F
HETATM	61	F	0	1.559	2.402	-0.959	F

END

4b.pdb

TITLE	4b.pdb						
HETATM	1	Ru	0	-0.144	0.637	-0.001	Ru
HETATM	2	C	0	-0.430	-3.665	0.169	C
HETATM	3	C	0	1.091	-3.544	0.011	C
HETATM	4	H	0	-0.899	-4.292	-0.609	H
HETATM	5	H	0	1.464	-3.996	-0.927	H
HETATM	6	C	0	0.153	-1.416	-0.015	C
HETATM	7	N	0	1.308	-2.091	-0.014	N
HETATM	8	N	0	-0.875	-2.274	0.047	N
HETATM	9	Cl	0	-0.999	0.478	-2.267	Cl
HETATM	10	Cl	0	0.717	0.585	2.256	Cl
HETATM	11	C	0	-1.617	2.029	0.447	C
HETATM	12	C	0	2.593	-1.469	-0.072	C
HETATM	13	C	0	3.370	-1.368	1.096	C
HETATM	14	C	0	3.051	-0.958	-1.303	C
HETATM	15	C	0	4.588	-0.683	1.024	C
HETATM	16	C	0	4.272	-0.276	-1.327	C
HETATM	17	C	0	5.044	-0.116	-0.170	C
HETATM	18	H	0	5.189	-0.580	1.936	H

HETATM	19	H	0	4.633	0.130	-2.281	H
HETATM	20	C	0	-2.222	-1.798	0.108	C
HETATM	21	C	0	-2.707	-1.224	1.301	C
HETATM	22	C	0	-3.013	-1.840	-1.059	C
HETATM	23	C	0	-3.961	-0.594	1.267	C
HETATM	24	C	0	-4.261	-1.219	-1.036	C
HETATM	25	C	0	-4.734	-0.558	0.107	C
HETATM	26	H	0	-4.330	-0.115	2.184	H
HETATM	27	H	0	-4.865	-1.213	-1.952	H
HETATM	28	C	0	2.935	-1.993	2.387	C
HETATM	29	H	0	3.297	-1.410	3.250	H
HETATM	30	H	0	1.838	-2.045	2.475	H
HETATM	31	H	0	3.342	-3.018	2.495	H
HETATM	32	C	0	2.259	-1.148	-2.561	C
HETATM	33	H	0	1.943	-2.199	-2.693	H
HETATM	34	H	0	1.328	-0.548	-2.580	H
HETATM	35	H	0	2.851	-0.864	-3.446	H
HETATM	36	C	0	6.322	0.666	-0.207	C
HETATM	37	H	0	6.816	0.602	-1.191	H
HETATM	38	H	0	6.138	1.740	-0.014	H
HETATM	39	H	0	7.038	0.325	0.560	H
HETATM	40	C	0	-1.989	-1.331	2.612	C
HETATM	41	H	0	-2.604	-1.909	3.328	H
HETATM	42	H	0	-1.005	-1.819	2.537	H
HETATM	43	H	0	-1.809	-0.340	3.062	H
HETATM	44	C	0	-2.520	-2.524	-2.296	C
HETATM	45	H	0	-2.662	-3.622	-2.240	H
HETATM	46	H	0	-3.061	-2.172	-3.188	H
HETATM	47	H	0	-1.448	-2.326	-2.467	H
HETATM	48	C	0	-6.020	0.206	0.066	C
HETATM	49	H	0	-5.847	1.231	-0.318	H
HETATM	50	H	0	-6.761	-0.260	-0.604	H
HETATM	51	H	0	-6.474	0.312	1.066	H
HETATM	52	H	0	1.652	-4.000	0.846	H
HETATM	53	H	0	-0.732	-4.069	1.154	H
HETATM	54	C	0	-0.506	2.880	0.087	C
HETATM	55	C	0	1.228	1.806	-0.530	C
HETATM	56	F	0	-2.692	2.056	-0.335	F
HETATM	57	F	0	-2.002	2.022	1.726	F
HETATM	58	F	0	-0.632	3.594	-1.027	F
HETATM	59	F	0	0.066	3.593	1.050	F
HETATM	60	F	0	1.464	2.212	-1.752	F
HETATM	61	F	0	2.188	2.273	0.223	F

END

4NA.pdb

TITLE	4NA.pdb						
HETATM	1	Ru	0	0.017	0.582	0.002	Ru
HETATM	2	C	0	-0.818	-3.603	0.081	C
HETATM	3	C	0	0.708	-3.626	-0.077	C
HETATM	4	H	0	-1.347	-4.108	-0.747	H
HETATM	5	H	0	1.041	-4.092	-1.023	H
HETATM	6	C	0	-0.023	-1.430	0.003	C
HETATM	7	N	0	1.065	-2.200	-0.069	N
HETATM	8	N	0	-1.133	-2.168	0.075	N
HETATM	9	Cl	0	-0.797	0.498	-2.270	Cl
HETATM	10	Cl	0	0.819	0.481	2.279	Cl
HETATM	11	C	0	-1.244	2.037	0.420	C
HETATM	12	C	0	2.393	-1.666	-0.108	C
HETATM	13	C	0	3.156	-1.628	1.077	C
HETATM	14	C	0	2.896	-1.157	-1.321	C

HETATM	15	C	0	4.393	-0.984	1.045	C
HETATM	16	C	0	4.143	-0.518	-1.303	C
HETATM	17	C	0	4.889	-0.400	-0.128	C
HETATM	18	H	0	4.980	-0.922	1.971	H
HETATM	19	H	0	4.537	-0.106	-2.240	H
HETATM	20	C	0	-2.450	-1.606	0.107	C
HETATM	21	C	0	-2.951	-1.091	1.319	C
HETATM	22	C	0	-3.211	-1.562	-1.079	C
HETATM	23	C	0	-4.195	-0.449	1.301	C
HETATM	24	C	0	-4.446	-0.913	-1.047	C
HETATM	25	C	0	-4.943	-0.331	0.126	C
HETATM	26	H	0	-4.589	-0.037	2.239	H
HETATM	27	H	0	-5.033	-0.851	-1.972	H
HETATM	28	C	0	2.679	-2.282	2.338	C
HETATM	29	H	0	3.096	-1.781	3.226	H
HETATM	30	H	0	1.582	-2.251	2.437	H
HETATM	31	H	0	2.999	-3.343	2.383	H
HETATM	32	C	0	2.151	-1.291	-2.613	C
HETATM	33	H	0	1.472	-2.160	-2.622	H
HETATM	34	H	0	1.512	-0.412	-2.822	H
HETATM	35	H	0	2.854	-1.396	-3.457	H
HETATM	36	C	0	6.182	0.356	-0.113	C
HETATM	37	H	0	6.021	1.400	0.219	H
HETATM	38	H	0	6.914	-0.085	0.584	H
HETATM	39	H	0	6.644	0.407	-1.113	H
HETATM	40	C	0	-2.202	-1.228	2.609	C
HETATM	41	H	0	-2.901	-1.272	3.462	H
HETATM	42	H	0	-1.570	-2.132	2.637	H
HETATM	43	H	0	-1.515	-0.380	2.789	H
HETATM	44	C	0	-2.737	-2.218	-2.339	C
HETATM	45	H	0	-3.076	-3.272	-2.394	H
HETATM	46	H	0	-3.139	-1.704	-3.227	H
HETATM	47	H	0	-1.639	-2.205	-2.432	H
HETATM	48	C	0	-6.239	0.419	0.115	C
HETATM	49	H	0	-6.075	1.482	-0.144	H
HETATM	50	H	0	-6.945	0.017	-0.631	H
HETATM	51	H	0	-6.733	0.405	1.101	H
HETATM	52	H	0	1.222	-4.146	0.751	H
HETATM	53	H	0	-1.164	-4.060	1.026	H
HETATM	54	C	0	0.060	2.876	-0.003	C
HETATM	55	C	0	1.331	1.986	-0.425	C
HETATM	56	F	0	-2.286	2.310	-0.356	F
HETATM	57	F	0	-1.612	2.293	1.674	F
HETATM	58	F	0	-0.269	3.659	-1.044	F
HETATM	59	F	0	0.421	3.648	1.035	F
HETATM	60	F	0	1.707	2.220	-1.681	F
HETATM	61	F	0	2.384	2.226	0.349	F

END

s5a.pdb

TITLE	s5a.pdb						
HETATM	1	Ru	0	-0.232	0.443	-0.028	Ru
HETATM	2	C	0	0.506	-3.629	0.239	C
HETATM	3	C	0	1.976	-3.214	0.130	C
HETATM	4	H	0	0.192	-4.312	-0.572	H
HETATM	5	H	0	2.459	-3.579	-0.796	H
HETATM	6	C	0	0.653	-1.288	0.086	C
HETATM	7	N	0	1.921	-1.747	0.115	N
HETATM	8	N	0	-0.190	-2.353	0.139	N
HETATM	9	Cl	0	-0.596	0.497	-2.394	Cl
HETATM	10	Cl	0	-0.375	0.687	2.355	Cl

HETATM	11	C	0	-2.698	2.255	-0.102	C
HETATM	12	C	0	3.117	-0.974	0.046	C
HETATM	13	C	0	3.794	-0.663	1.239	C
HETATM	14	C	0	3.613	-0.571	-1.206	C
HETATM	15	C	0	4.993	0.049	1.159	C
HETATM	16	C	0	4.808	0.160	-1.241	C
HETATM	17	C	0	5.510	0.472	-0.072	C
HETATM	18	H	0	5.526	0.298	2.085	H
HETATM	19	H	0	5.202	0.483	-2.213	H
HETATM	20	C	0	-1.602	-2.164	0.033	C
HETATM	21	C	0	-2.376	-1.957	1.197	C
HETATM	22	C	0	-2.203	-2.178	-1.247	C
HETATM	23	C	0	-3.725	-1.621	1.042	C
HETATM	24	C	0	-3.554	-1.841	-1.349	C
HETATM	25	C	0	-4.320	-1.526	-0.221	C
HETATM	26	H	0	-4.325	-1.423	1.939	H
HETATM	27	H	0	-4.018	-1.813	-2.344	H
HETATM	28	C	0	3.183	-1.007	2.561	C
HETATM	29	H	0	3.847	-0.732	3.397	H
HETATM	30	H	0	2.223	-0.469	2.698	H
HETATM	31	H	0	2.952	-2.084	2.662	H
HETATM	32	C	0	2.871	-0.895	-2.466	C
HETATM	33	H	0	2.607	-1.967	-2.529	H
HETATM	34	H	0	1.916	-0.339	-2.541	H
HETATM	35	H	0	3.470	-0.646	-3.357	H
HETATM	36	C	0	6.775	1.274	-0.131	C
HETATM	37	H	0	6.579	2.348	0.051	H
HETATM	38	H	0	7.502	0.955	0.636	H
HETATM	39	H	0	7.265	1.202	-1.117	H
HETATM	40	C	0	-1.818	-2.191	2.566	C
HETATM	41	H	0	-2.235	-1.483	3.299	H
HETATM	42	H	0	-2.080	-3.213	2.907	H
HETATM	43	H	0	-0.723	-2.088	2.607	H
HETATM	44	C	0	-1.440	-2.612	-2.460	C
HETATM	45	H	0	-1.515	-3.711	-2.589	H
HETATM	46	H	0	-1.840	-2.144	-3.373	H
HETATM	47	H	0	-0.371	-2.350	-2.406	H
HETATM	48	C	0	-5.740	-1.075	-0.363	C
HETATM	49	H	0	-5.791	0.022	-0.497	H
HETATM	50	H	0	-6.232	-1.523	-1.243	H
HETATM	51	H	0	-6.343	-1.314	0.530	H
HETATM	52	H	0	2.590	-3.565	0.979	H
HETATM	53	H	0	0.270	-4.124	1.201	H
HETATM	54	C	0	-1.642	3.090	-0.209	C
HETATM	55	C	0	1.246	1.512	-0.095	C
HETATM	56	F	0	-3.296	1.784	-1.182	F
HETATM	57	F	0	-1.085	3.675	0.819	F
HETATM	58	F	0	-1.162	3.499	-1.351	F
HETATM	59	F	0	2.161	1.685	0.831	F
HETATM	60	F	0	1.535	2.373	-1.052	F
HETATM	61	Cl	0	-3.497	1.946	1.372	Cl

END

s5b.pdb

TITLE	s5b.pdb						
HETATM	1	Ru	0	-0.232	0.443	-0.028	Ru
HETATM	2	C	0	0.506	-3.629	0.239	C
HETATM	3	C	0	1.976	-3.214	0.130	C
HETATM	4	H	0	0.192	-4.312	-0.572	H
HETATM	5	H	0	2.459	-3.579	-0.796	H
HETATM	6	C	0	0.653	-1.288	0.086	C

HETATM	7	N	0	1.921	-1.747	0.115	N
HETATM	8	N	0	-0.190	-2.353	0.139	N
HETATM	9	Cl	0	-0.596	0.497	-2.394	Cl
HETATM	10	Cl	0	-0.375	0.687	2.355	Cl
HETATM	11	C	0	-2.698	2.255	-0.102	C
HETATM	12	C	0	3.117	-0.974	0.046	C
HETATM	13	C	0	3.794	-0.663	1.239	C
HETATM	14	C	0	3.613	-0.571	-1.206	C
HETATM	15	C	0	4.993	0.049	1.159	C
HETATM	16	C	0	4.808	0.160	-1.241	C
HETATM	17	C	0	5.510	0.472	-0.072	C
HETATM	18	H	0	5.526	0.298	2.085	H
HETATM	19	H	0	5.202	0.483	-2.213	H
HETATM	20	C	0	-1.602	-2.164	0.033	C
HETATM	21	C	0	-2.376	-1.957	1.197	C
HETATM	22	C	0	-2.203	-2.178	-1.247	C
HETATM	23	C	0	-3.725	-1.621	1.042	C
HETATM	24	C	0	-3.554	-1.841	-1.349	C
HETATM	25	C	0	-4.320	-1.526	-0.221	C
HETATM	26	H	0	-4.325	-1.423	1.939	H
HETATM	27	H	0	-4.018	-1.813	-2.344	H
HETATM	28	C	0	3.183	-1.007	2.561	C
HETATM	29	H	0	3.847	-0.732	3.397	H
HETATM	30	H	0	2.223	-0.469	2.698	H
HETATM	31	H	0	2.952	-2.084	2.662	H
HETATM	32	C	0	2.871	-0.895	-2.466	C
HETATM	33	H	0	2.607	-1.967	-2.529	H
HETATM	34	H	0	1.916	-0.339	-2.541	H
HETATM	35	H	0	3.470	-0.646	-3.357	H
HETATM	36	C	0	6.775	1.274	-0.131	C
HETATM	37	H	0	6.579	2.348	0.051	H
HETATM	38	H	0	7.502	0.955	0.636	H
HETATM	39	H	0	7.265	1.202	-1.117	H
HETATM	40	C	0	-1.818	-2.191	2.566	C
HETATM	41	H	0	-2.235	-1.483	3.299	H
HETATM	42	H	0	-2.080	-3.213	2.907	H
HETATM	43	H	0	-0.723	-2.088	2.607	H
HETATM	44	C	0	-1.440	-2.612	-2.460	C
HETATM	45	H	0	-1.515	-3.711	-2.589	H
HETATM	46	H	0	-1.840	-2.144	-3.373	H
HETATM	47	H	0	-0.371	-2.350	-2.406	H
HETATM	48	C	0	-5.740	-1.075	-0.363	C
HETATM	49	H	0	-5.791	0.022	-0.497	H
HETATM	50	H	0	-6.232	-1.523	-1.243	H
HETATM	51	H	0	-6.343	-1.314	0.530	H
HETATM	52	H	0	2.590	-3.565	0.979	H
HETATM	53	H	0	0.270	-4.124	1.201	H
HETATM	54	C	0	-1.642	3.090	-0.209	C
HETATM	55	C	0	1.246	1.512	-0.095	C
HETATM	56	F	0	-3.296	1.784	-1.182	F
HETATM	57	F	0	-1.085	3.675	0.819	F
HETATM	58	F	0	-1.162	3.499	-1.351	F
HETATM	59	F	0	2.161	1.685	0.831	F
HETATM	60	F	0	1.535	2.373	-1.052	F
HETATM	61	Cl	0	-3.497	1.946	1.372	Cl

END

s5PA.pdb

TITLE	s5PA.pdb						
HETATM	1	Ru	0	0.019	0.558	-0.081	Ru
HETATM	2	C	0	-0.479	-3.681	0.195	C

HETATM	3	C	0	1.042	-3.593	0.021	C
HETATM	4	H	0	-0.974	-4.271	-0.595	H
HETATM	5	H	0	1.397	-4.047	-0.923	H
HETATM	6	C	0	0.148	-1.456	0.021	C
HETATM	7	N	0	1.292	-2.146	-0.000	N
HETATM	8	N	0	-0.903	-2.276	0.109	N
HETATM	9	Cl	0	-0.755	0.191	-2.347	Cl
HETATM	10	Cl	0	0.932	0.671	2.148	Cl
HETATM	11	C	0	-1.414	1.892	0.203	C
HETATM	12	C	0	2.593	-1.549	-0.015	C
HETATM	13	C	0	3.325	-1.476	1.189	C
HETATM	14	C	0	3.114	-1.045	-1.221	C
HETATM	15	C	0	4.557	-0.821	1.174	C
HETATM	16	C	0	4.353	-0.390	-1.184	C
HETATM	17	C	0	5.076	-0.255	0.003	C
HETATM	18	H	0	5.121	-0.738	2.112	H
HETATM	19	H	0	4.765	0.012	-2.119	H
HETATM	20	C	0	-2.260	-1.818	0.113	C
HETATM	21	C	0	-2.795	-1.275	1.299	C
HETATM	22	C	0	-3.023	-1.898	-1.067	C
HETATM	23	C	0	-4.077	-0.720	1.252	C
HETATM	24	C	0	-4.299	-1.329	-1.066	C
HETATM	25	C	0	-4.829	-0.712	0.073	C
HETATM	26	H	0	-4.492	-0.274	2.165	H
HETATM	27	H	0	-4.888	-1.353	-1.992	H
HETATM	28	C	0	2.819	-2.098	2.454	C
HETATM	29	H	0	3.187	-1.552	3.338	H
HETATM	30	H	0	1.719	-2.098	2.513	H
HETATM	31	H	0	3.167	-3.146	2.555	H
HETATM	32	C	0	2.401	-1.204	-2.529	C
HETATM	33	H	0	1.711	-2.065	-2.538	H
HETATM	34	H	0	1.777	-0.326	-2.776	H
HETATM	35	H	0	3.125	-1.334	-3.351	H
HETATM	36	C	0	6.375	0.491	0.033	C
HETATM	37	H	0	6.234	1.517	0.421	H
HETATM	38	H	0	7.114	0.006	0.694	H
HETATM	39	H	0	6.821	0.584	-0.971	H
HETATM	40	C	0	-2.029	-1.308	2.587	C
HETATM	41	H	0	-2.674	-1.017	3.432	H
HETATM	42	H	0	-1.631	-2.317	2.804	H
HETATM	43	H	0	-1.160	-0.622	2.592	H
HETATM	44	C	0	-2.515	-2.598	-2.290	C
HETATM	45	H	0	-2.844	-3.656	-2.307	H
HETATM	46	H	0	-2.903	-2.125	-3.207	H
HETATM	47	H	0	-1.416	-2.578	-2.362	H
HETATM	48	C	0	-6.163	-0.033	0.024	C
HETATM	49	H	0	-6.046	1.043	-0.209	H
HETATM	50	H	0	-6.818	-0.457	-0.755	H
HETATM	51	H	0	-6.693	-0.090	0.990	H
HETATM	52	H	0	1.601	-4.061	0.850	H
HETATM	53	H	0	-0.782	-4.106	1.170	H
HETATM	54	C	0	-0.213	2.831	-0.249	C
HETATM	55	C	0	1.159	2.042	-0.662	C
HETATM	56	F	0	-2.435	1.982	-0.651	F
HETATM	57	F	0	-0.610	3.508	-1.338	F
HETATM	58	F	0	0.109	3.705	0.715	F
HETATM	59	F	0	1.464	2.250	-1.940	F
HETATM	60	F	0	2.193	2.461	0.054	F
HETATM	61	Cl	0	-2.038	2.216	1.820	Cl

END

TITLE	s5c.pdb						
HETATM	1	Ru	0	0.136	0.620	-0.075	Ru
HETATM	2	Cl	0	-0.541	0.212	-2.372	Cl
HETATM	3	Cl	0	0.948	0.759	2.194	Cl
HETATM	4	C	0	-0.013	-1.450	0.107	C
HETATM	5	N	0	-1.128	-2.192	0.122	N
HETATM	6	C	0	-0.830	-3.626	0.236	C
HETATM	7	C	0	0.696	-3.670	0.116	C
HETATM	8	N	0	1.061	-2.250	0.151	N
HETATM	9	C	0	-2.449	-1.650	0.101	C
HETATM	10	C	0	-3.207	-1.703	-1.083	C
HETATM	11	C	0	-4.466	-1.093	-1.090	C
HETATM	12	C	0	-4.982	-0.455	0.042	C
HETATM	13	C	0	-4.226	-0.465	1.221	C
HETATM	14	C	0	-2.964	-1.066	1.276	C
HETATM	15	C	0	2.393	-1.733	0.092	C
HETATM	16	C	0	3.121	-1.582	1.290	C
HETATM	17	C	0	4.363	-0.948	1.233	C
HETATM	18	C	0	4.894	-0.475	0.026	C
HETATM	19	C	0	4.185	-0.707	-1.155	C
HETATM	20	C	0	2.940	-1.349	-1.150	C
HETATM	21	C	0	-2.711	-2.415	-2.304	C
HETATM	22	C	0	-6.306	0.244	-0.009	C
HETATM	23	C	0	-2.191	-1.101	2.559	C
HETATM	24	C	0	2.596	-2.097	2.595	C
HETATM	25	C	0	6.179	0.294	0.009	C
HETATM	26	C	0	2.285	-1.688	-2.456	C
HETATM	27	H	0	-1.347	-4.188	-0.561	H
HETATM	28	H	0	-1.198	-4.010	1.207	H
HETATM	29	H	0	1.043	-4.122	-0.834	H
HETATM	30	H	0	1.184	-4.215	0.943	H
HETATM	31	H	0	-5.054	-1.110	-2.017	H
HETATM	32	H	0	-4.625	0.006	2.128	H
HETATM	33	H	0	4.920	-0.791	2.166	H
HETATM	34	H	0	4.605	-0.379	-2.115	H
HETATM	35	H	0	-3.090	-1.939	-3.223	H
HETATM	36	H	0	-1.611	-2.409	-2.371	H
HETATM	37	H	0	-3.055	-3.469	-2.320	H
HETATM	38	H	0	-6.181	1.317	-0.250	H
HETATM	39	H	0	-6.968	-0.180	-0.783	H
HETATM	40	H	0	-6.836	0.197	0.958	H
HETATM	41	H	0	-1.254	-0.510	2.520	H
HETATM	42	H	0	-1.894	-2.132	2.831	H
HETATM	43	H	0	-2.792	-0.699	3.391	H
HETATM	44	H	0	1.495	-2.077	2.641	H
HETATM	45	H	0	2.963	-1.490	3.438	H
HETATM	46	H	0	2.926	-3.140	2.773	H
HETATM	47	H	0	5.993	1.370	0.193	H
HETATM	48	H	0	6.875	-0.044	0.796	H
HETATM	49	H	0	6.694	0.221	-0.964	H
HETATM	50	H	0	2.322	-0.843	-3.163	H
HETATM	51	H	0	2.817	-2.533	-2.936	H
HETATM	52	H	0	1.224	-1.964	-2.358	H
HETATM	53	C	0	1.502	2.036	-0.752	C
HETATM	54	F	0	1.842	2.004	-2.038	F
HETATM	55	F	0	2.606	2.104	-0.008	F
HETATM	56	C	0	0.395	2.880	-0.372	C
HETATM	57	C	0	-1.369	1.711	0.178	C
HETATM	58	F	0	-0.240	3.520	-1.345	F
HETATM	59	F	0	0.534	3.645	0.697	F
HETATM	60	F	0	-2.238	2.039	-0.742	F
HETATM	61	Cl	0	-1.950	2.310	1.705	Cl

END

s5d.pdb

TITLE	s5d.pdb					
HETATM	1 Ru	0	-0.267	0.513	0.097	Ru
HETATM	2 C	0	0.099	-3.633	0.019	C
HETATM	3 C	0	1.589	-3.340	-0.133	C
HETATM	4 H	0	-0.308	-4.245	-0.806	H
HETATM	5 H	0	1.987	-3.634	-1.124	H
HETATM	6 C	0	0.445	-1.307	0.037	C
HETATM	7 N	0	1.669	-1.882	0.018	N
HETATM	8 N	0	-0.486	-2.298	0.008	N
HETATM	9 Cl	0	-0.774	0.760	-2.221	Cl
HETATM	10 Cl	0	-0.398	0.522	2.484	Cl
HETATM	11 C	0	-2.699	2.277	0.414	C
HETATM	12 C	0	2.934	-1.229	-0.046	C
HETATM	13 C	0	3.706	-1.140	1.128	C
HETATM	14 C	0	3.400	-0.718	-1.269	C
HETATM	15 C	0	4.962	-0.535	1.056	C
HETATM	16 C	0	4.656	-0.099	-1.293	C
HETATM	17 C	0	5.449	-0.003	-0.146	C
HETATM	18 H	0	5.568	-0.457	1.968	H
HETATM	19 H	0	5.025	0.311	-2.243	H
HETATM	20 C	0	-1.887	-2.030	-0.081	C
HETATM	21 C	0	-2.658	-1.891	1.095	C
HETATM	22 C	0	-2.488	-1.946	-1.357	C
HETATM	23 C	0	-4.002	-1.523	0.965	C
HETATM	24 C	0	-3.836	-1.591	-1.434	C
HETATM	25 C	0	-4.598	-1.342	-0.287	C
HETATM	26 H	0	-4.601	-1.385	1.876	H
HETATM	27 H	0	-4.300	-1.493	-2.424	H
HETATM	28 C	0	3.140	-1.599	2.436	C
HETATM	29 H	0	3.867	-1.471	3.256	H
HETATM	30 H	0	2.232	-1.021	2.696	H
HETATM	31 H	0	2.839	-2.663	2.424	H
HETATM	32 C	0	2.565	-0.800	-2.510	C
HETATM	33 H	0	2.108	-1.798	-2.643	H
HETATM	34 H	0	1.722	-0.081	-2.492	H
HETATM	35 H	0	3.165	-0.582	-3.409	H
HETATM	36 C	0	6.782	0.682	-0.188	C
HETATM	37 H	0	6.720	1.705	0.229	H
HETATM	38 H	0	7.539	0.146	0.411	H
HETATM	39 H	0	7.165	0.777	-1.217	H
HETATM	40 C	0	-2.109	-2.232	2.446	C
HETATM	41 H	0	-2.498	-1.553	3.222	H
HETATM	42 H	0	-2.414	-3.261	2.726	H
HETATM	43 H	0	-1.011	-2.174	2.493	H
HETATM	44 C	0	-1.739	-2.300	-2.604	C
HETATM	45 H	0	-1.903	-3.366	-2.862	H
HETATM	46 H	0	-2.085	-1.699	-3.460	H
HETATM	47 H	0	-0.654	-2.138	-2.515	H
HETATM	48 C	0	-6.015	-0.870	-0.399	C
HETATM	49 H	0	-6.054	0.233	-0.476	H
HETATM	50 H	0	-6.513	-1.266	-1.300	H
HETATM	51 H	0	-6.617	-1.150	0.481	H
HETATM	52 H	0	2.212	-3.841	0.629	H
HETATM	53 H	0	-0.144	-4.150	0.969	H
HETATM	54 C	0	-1.707	3.164	0.220	C
HETATM	55 C	0	1.282	1.450	0.128	C
HETATM	56 F	0	-3.431	1.815	-0.568	F
HETATM	57 F	0	-3.114	1.905	1.597	F

HETATM	58	F	0	-1.033	3.707	1.204	F
HETATM	59	F	0	-1.440	3.675	-0.951	F
HETATM	60	F	0	2.284	1.330	0.971	F
HETATM	61	Cl	0	1.607	2.859	-0.869	Cl

END

a5a.pdb

TITLE	a5a.pdb						
HETATM	1	Ru	0	-0.282	0.419	-0.032	Ru
HETATM	2	C	0	0.316	-3.675	0.338	C
HETATM	3	C	0	1.792	-3.314	0.154	C
HETATM	4	H	0	-0.055	-4.374	-0.434	H
HETATM	5	H	0	2.220	-3.715	-0.785	H
HETATM	6	C	0	0.533	-1.344	0.110	C
HETATM	7	N	0	1.787	-1.848	0.111	N
HETATM	8	N	0	-0.341	-2.380	0.220	N
HETATM	9	Cl	0	-0.696	0.433	-2.388	Cl
HETATM	10	Cl	0	-0.432	0.691	2.346	Cl
HETATM	11	C	0	-2.657	2.264	-0.029	C
HETATM	12	C	0	3.008	-1.122	0.007	C
HETATM	13	C	0	3.718	-0.822	1.183	C
HETATM	14	C	0	3.499	-0.757	-1.259	C
HETATM	15	C	0	4.944	-0.162	1.073	C
HETATM	16	C	0	4.723	-0.079	-1.325	C
HETATM	17	C	0	5.458	0.220	-0.173	C
HETATM	18	H	0	5.503	0.079	1.986	H
HETATM	19	H	0	5.113	0.215	-2.308	H
HETATM	20	C	0	-1.750	-2.162	0.131	C
HETATM	21	C	0	-2.505	-1.926	1.302	C
HETATM	22	C	0	-2.370	-2.188	-1.139	C
HETATM	23	C	0	-3.851	-1.571	1.162	C
HETATM	24	C	0	-3.718	-1.833	-1.228	C
HETATM	25	C	0	-4.462	-1.489	-0.094	C
HETATM	26	H	0	-4.436	-1.354	2.065	H
HETATM	27	H	0	-4.196	-1.817	-2.215	H
HETATM	28	C	0	3.116	-1.124	2.520	C
HETATM	29	H	0	3.798	-0.848	3.341	H
HETATM	30	H	0	2.172	-0.559	2.658	H
HETATM	31	H	0	2.860	-2.193	2.646	H
HETATM	32	C	0	2.721	-1.063	-2.502	C
HETATM	33	H	0	2.408	-2.123	-2.547	H
HETATM	34	H	0	1.789	-0.467	-2.565	H
HETATM	35	H	0	3.313	-0.850	-3.407	H
HETATM	36	C	0	6.754	0.967	-0.264	C
HETATM	37	H	0	6.607	2.050	-0.087	H
HETATM	38	H	0	7.483	0.623	0.489	H
HETATM	39	H	0	7.219	0.868	-1.260	H
HETATM	40	C	0	-1.929	-2.149	2.666	C
HETATM	41	H	0	-2.326	-1.427	3.396	H
HETATM	42	H	0	-2.197	-3.163	3.025	H
HETATM	43	H	0	-0.833	-2.057	2.688	H
HETATM	44	C	0	-1.636	-2.659	-2.356	C
HETATM	45	H	0	-1.775	-3.751	-2.487	H
HETATM	46	H	0	-2.012	-2.167	-3.267	H
HETATM	47	H	0	-0.553	-2.462	-2.307	H
HETATM	48	C	0	-5.881	-1.027	-0.222	C
HETATM	49	H	0	-5.927	0.074	-0.330	H
HETATM	50	H	0	-6.378	-1.452	-1.110	H
HETATM	51	H	0	-6.483	-1.282	0.667	H
HETATM	52	H	0	2.432	-3.671	0.981	H
HETATM	53	H	0	0.104	-4.127	1.326	H

HETATM	54	C	0	-1.623	3.103	-0.254	C
HETATM	55	C	0	1.228	1.435	-0.134	C
HETATM	56	F	0	-3.365	1.750	-1.001	F
HETATM	57	F	0	-3.142	1.993	1.152	F
HETATM	58	F	0	-1.312	3.443	-1.490	F
HETATM	59	F	0	2.172	1.575	0.769	F
HETATM	60	F	0	1.508	2.299	-1.089	F
HETATM	61	Cl	0	-0.807	3.959	0.975	Cl

END

a5b.pdb

TITLE	a5b.pdb						
HETATM	1	Ru	0	-0.106	0.553	-0.060	Ru
HETATM	2	Cl	0	-0.988	0.141	-2.292	Cl
HETATM	3	Cl	0	0.790	0.661	2.169	Cl
HETATM	4	C	0	0.122	-1.502	0.082	C
HETATM	5	N	0	-0.915	-2.337	0.221	N
HETATM	6	C	0	-0.485	-3.724	0.422	C
HETATM	7	C	0	1.031	-3.638	0.216	C
HETATM	8	N	0	1.269	-2.192	0.097	N
HETATM	9	C	0	-2.264	-1.862	0.243	C
HETATM	10	C	0	-3.059	-2.019	-0.911	C
HETATM	11	C	0	-4.310	-1.405	-0.941	C
HETATM	12	C	0	-4.782	-0.643	0.138	C
HETATM	13	C	0	-4.006	-0.569	1.294	C
HETATM	14	C	0	-2.749	-1.186	1.380	C
HETATM	15	C	0	2.567	-1.600	0.002	C
HETATM	16	C	0	3.342	-1.445	1.166	C
HETATM	17	C	0	4.578	-0.800	1.057	C
HETATM	18	C	0	5.056	-0.325	-0.169	C
HETATM	19	C	0	4.285	-0.540	-1.317	C
HETATM	20	C	0	3.044	-1.184	-1.257	C
HETATM	21	C	0	-2.577	-2.820	-2.081	C
HETATM	22	C	0	-6.072	0.109	0.029	C
HETATM	23	C	0	-2.015	-1.161	2.687	C
HETATM	24	C	0	2.889	-1.974	2.492	C
HETATM	25	C	0	6.357	0.413	-0.248	C
HETATM	26	C	0	2.257	-1.436	-2.506	C
HETATM	27	H	0	-0.984	-4.394	-0.300	H
HETATM	28	H	0	-0.765	-4.058	1.440	H
HETATM	29	H	0	1.373	-4.152	-0.701	H
HETATM	30	H	0	1.609	-4.050	1.063	H
HETATM	31	H	0	-4.918	-1.487	-1.850	H
HETATM	32	H	0	-4.374	-0.008	2.163	H
HETATM	33	H	0	5.179	-0.653	1.964	H
HETATM	34	H	0	4.663	-0.209	-2.294	H
HETATM	35	H	0	-3.067	-2.494	-3.013	H
HETATM	36	H	0	-1.490	-2.714	-2.233	H
HETATM	37	H	0	-2.802	-3.898	-1.955	H
HETATM	38	H	0	-5.902	1.101	-0.432	H
HETATM	39	H	0	-6.533	0.290	1.015	H
HETATM	40	H	0	-6.807	-0.413	-0.607	H
HETATM	41	H	0	-1.773	-0.134	3.008	H
HETATM	42	H	0	-1.059	-1.707	2.663	H
HETATM	43	H	0	-2.644	-1.607	3.480	H
HETATM	44	H	0	1.791	-2.020	2.573	H
HETATM	45	H	0	3.244	-1.333	3.316	H
HETATM	46	H	0	3.293	-2.990	2.677	H
HETATM	47	H	0	6.209	1.498	-0.086	H
HETATM	48	H	0	7.072	0.075	0.521	H
HETATM	49	H	0	6.836	0.303	-1.236	H

HETATM	50	H	0	1.345	-0.813	-2.574	H
HETATM	51	H	0	2.865	-1.233	-3.403	H
HETATM	52	H	0	1.909	-2.484	-2.570	H
HETATM	53	C	0	1.212	1.704	-0.764	C
HETATM	54	F	0	1.384	2.034	-2.017	F
HETATM	55	F	0	2.240	2.164	-0.101	F
HETATM	56	C	0	-0.486	2.803	-0.190	C
HETATM	57	C	0	-1.593	1.944	0.230	C
HETATM	58	F	0	-0.683	3.368	-1.388	F
HETATM	59	Cl	0	0.161	3.930	0.973	Cl
HETATM	60	F	0	-2.669	1.937	-0.550	F
HETATM	61	F	0	-1.994	2.017	1.502	F

END

a5NA.pdb

TITLE	a5NA.pdb						
HETATM	1	Ru	0	0.026	0.493	-0.048	Ru
HETATM	2	C	0	-0.900	-3.662	0.361	C
HETATM	3	C	0	0.618	-3.734	0.147	C
HETATM	4	H	0	-1.471	-4.249	-0.379	H
HETATM	5	H	0	0.900	-4.261	-0.784	H
HETATM	6	C	0	-0.067	-1.522	0.073	C
HETATM	7	N	0	1.005	-2.320	0.058	N
HETATM	8	N	0	-1.190	-2.232	0.203	N
HETATM	9	Cl	0	-0.848	0.170	-2.289	Cl
HETATM	10	Cl	0	0.875	0.585	2.198	Cl
HETATM	11	C	0	-1.230	1.981	0.213	C
HETATM	12	C	0	2.346	-1.825	-0.016	C
HETATM	13	C	0	3.105	-1.724	1.168	C
HETATM	14	C	0	2.869	-1.419	-1.260	C
HETATM	15	C	0	4.362	-1.123	1.096	C
HETATM	16	C	0	4.136	-0.823	-1.281	C
HETATM	17	C	0	4.881	-0.642	-0.113	C
HETATM	18	H	0	4.946	-1.008	2.018	H
HETATM	19	H	0	4.545	-0.489	-2.244	H
HETATM	20	C	0	-2.498	-1.650	0.222	C
HETATM	21	C	0	-2.951	-0.992	1.381	C
HETATM	22	C	0	-3.299	-1.730	-0.937	C
HETATM	23	C	0	-4.188	-0.337	1.329	C
HETATM	24	C	0	-4.527	-1.069	-0.938	C
HETATM	25	C	0	-4.976	-0.346	0.176	C
HETATM	26	H	0	-4.542	0.191	2.224	H
HETATM	27	H	0	-5.143	-1.102	-1.845	H
HETATM	28	C	0	2.597	-2.263	2.470	C
HETATM	29	H	0	3.053	-1.733	3.322	H
HETATM	30	H	0	1.505	-2.152	2.570	H
HETATM	31	H	0	2.847	-3.337	2.586	H
HETATM	32	C	0	2.116	-1.612	-2.540	C
HETATM	33	H	0	1.416	-2.465	-2.496	H
HETATM	34	H	0	1.494	-0.735	-2.798	H
HETATM	35	H	0	2.812	-1.782	-3.378	H
HETATM	36	C	0	6.195	0.075	-0.147	C
HETATM	37	H	0	6.057	1.154	0.053	H
HETATM	38	H	0	6.893	-0.301	0.621	H
HETATM	39	H	0	6.687	-0.007	-1.131	H
HETATM	40	C	0	-2.170	-0.985	2.660	C
HETATM	41	H	0	-2.848	-1.075	3.526	H
HETATM	42	H	0	-1.430	-1.801	2.718	H
HETATM	43	H	0	-1.595	-0.051	2.792	H
HETATM	44	C	0	-2.865	-2.518	-2.135	C
HETATM	45	H	0	-3.182	-3.578	-2.058	H

HETATM	46	H	0	-3.314	-2.115	-3.057	H
HETATM	47	H	0	-1.772	-2.494	-2.275	H
HETATM	48	C	0	-6.271	0.405	0.119	C
HETATM	49	H	0	-6.160	1.340	-0.462	H
HETATM	50	H	0	-7.065	-0.179	-0.379	H
HETATM	51	H	0	-6.630	0.687	1.122	H
HETATM	52	H	0	1.151	-4.220	0.982	H
HETATM	53	H	0	-1.211	-3.996	1.368	H
HETATM	54	C	0	0.082	2.772	-0.298	C
HETATM	55	C	0	1.334	1.814	-0.678	C
HETATM	56	F	0	-2.263	2.218	-0.583	F
HETATM	57	F	0	-1.619	2.287	1.450	F
HETATM	58	F	0	-0.274	3.393	-1.440	F
HETATM	59	F	0	1.654	1.956	-1.962	F
HETATM	60	F	0	2.438	2.052	0.018	F
HETATM	61	Cl	0	0.595	3.972	0.909	Cl

END

a5d.pdb

TITLE	a5d.pdb						
HETATM	1	Ru	0	-0.106	0.553	-0.060	Ru
HETATM	2	Cl	0	-0.988	0.141	-2.292	Cl
HETATM	3	Cl	0	0.790	0.661	2.169	Cl
HETATM	4	C	0	0.122	-1.502	0.082	C
HETATM	5	N	0	-0.915	-2.337	0.221	N
HETATM	6	C	0	-0.485	-3.724	0.422	C
HETATM	7	C	0	1.031	-3.638	0.216	C
HETATM	8	N	0	1.269	-2.192	0.097	N
HETATM	9	C	0	-2.264	-1.862	0.243	C
HETATM	10	C	0	-3.059	-2.019	-0.911	C
HETATM	11	C	0	-4.310	-1.405	-0.941	C
HETATM	12	C	0	-4.782	-0.643	0.138	C
HETATM	13	C	0	-4.006	-0.569	1.294	C
HETATM	14	C	0	-2.749	-1.186	1.380	C
HETATM	15	C	0	2.567	-1.600	0.002	C
HETATM	16	C	0	3.342	-1.445	1.166	C
HETATM	17	C	0	4.578	-0.800	1.057	C
HETATM	18	C	0	5.056	-0.325	-0.169	C
HETATM	19	C	0	4.285	-0.540	-1.317	C
HETATM	20	C	0	3.044	-1.184	-1.257	C
HETATM	21	C	0	-2.577	-2.820	-2.081	C
HETATM	22	C	0	-6.072	0.109	0.029	C
HETATM	23	C	0	-2.015	-1.161	2.687	C
HETATM	24	C	0	2.889	-1.974	2.492	C
HETATM	25	C	0	6.357	0.413	-0.248	C
HETATM	26	C	0	2.257	-1.436	-2.506	C
HETATM	27	H	0	-0.984	-4.394	-0.300	H
HETATM	28	H	0	-0.765	-4.058	1.440	H
HETATM	29	H	0	1.373	-4.152	-0.701	H
HETATM	30	H	0	1.609	-4.050	1.063	H
HETATM	31	H	0	-4.918	-1.487	-1.850	H
HETATM	32	H	0	-4.374	-0.008	2.163	H
HETATM	33	H	0	5.179	-0.653	1.964	H
HETATM	34	H	0	4.663	-0.209	-2.294	H
HETATM	35	H	0	-3.067	-2.494	-3.013	H
HETATM	36	H	0	-1.490	-2.714	-2.233	H
HETATM	37	H	0	-2.802	-3.898	-1.955	H
HETATM	38	H	0	-5.902	1.101	-0.432	H
HETATM	39	H	0	-6.533	0.290	1.015	H
HETATM	40	H	0	-6.807	-0.413	-0.607	H
HETATM	41	H	0	-1.773	-0.134	3.008	H

HETATM	42	H	0	-1.059	-1.707	2.663	H
HETATM	43	H	0	-2.644	-1.607	3.480	H
HETATM	44	H	0	1.791	-2.020	2.573	H
HETATM	45	H	0	3.244	-1.333	3.316	H
HETATM	46	H	0	3.293	-2.990	2.677	H
HETATM	47	H	0	6.209	1.498	-0.086	H
HETATM	48	H	0	7.072	0.075	0.521	H
HETATM	49	H	0	6.836	0.303	-1.236	H
HETATM	50	H	0	1.345	-0.813	-2.574	H
HETATM	51	H	0	2.865	-1.233	-3.403	H
HETATM	52	H	0	1.909	-2.484	-2.570	H
HETATM	53	C	0	1.212	1.704	-0.764	C
HETATM	54	F	0	1.384	2.034	-2.017	F
HETATM	55	F	0	2.240	2.164	-0.101	F
HETATM	56	C	0	-0.486	2.803	-0.190	C
HETATM	57	C	0	-1.593	1.944	0.230	C
HETATM	58	F	0	-0.683	3.368	-1.388	F
HETATM	59	Cl	0	0.161	3.930	0.973	Cl
HETATM	60	F	0	-2.669	1.937	-0.550	F
HETATM	61	F	0	-1.994	2.017	1.502	F

END

sc5e.pdb

TITLE	sc5e.pdb						
HETATM	1	Ru	0	-0.171	0.481	0.078	Ru
HETATM	2	C	0	0.243	-3.646	-0.332	C
HETATM	3	C	0	1.731	-3.319	-0.404	C
HETATM	4	H	0	-0.126	-4.196	-1.217	H
HETATM	5	H	0	2.165	-3.507	-1.406	H
HETATM	6	C	0	0.545	-1.328	-0.086	C
HETATM	7	N	0	1.778	-1.882	-0.111	N
HETATM	8	N	0	-0.367	-2.322	-0.260	N
HETATM	9	Cl	0	-0.613	0.738	-2.251	Cl
HETATM	10	Cl	0	-0.371	0.468	2.457	Cl
HETATM	11	C	0	-2.638	2.331	0.521	C
HETATM	12	C	0	3.035	-1.212	-0.088	C
HETATM	13	C	0	3.759	-1.185	1.119	C
HETATM	14	C	0	3.542	-0.630	-1.262	C
HETATM	15	C	0	5.013	-0.571	1.130	C
HETATM	16	C	0	4.796	-0.009	-1.203	C
HETATM	17	C	0	5.543	0.027	-0.021	C
HETATM	18	H	0	5.583	-0.541	2.068	H
HETATM	19	H	0	5.200	0.454	-2.113	H
HETATM	20	C	0	-1.777	-2.111	-0.156	C
HETATM	21	C	0	-2.385	-2.095	1.119	C
HETATM	22	C	0	-2.552	-1.998	-1.331	C
HETATM	23	C	0	-3.755	-1.823	1.199	C
HETATM	24	C	0	-3.922	-1.751	-1.200	C
HETATM	25	C	0	-4.533	-1.629	0.052	C
HETATM	26	H	0	-4.228	-1.783	2.188	H
HETATM	27	H	0	-4.527	-1.643	-2.110	H
HETATM	28	C	0	3.143	-1.718	2.375	C
HETATM	29	H	0	3.848	-1.675	3.221	H
HETATM	30	H	0	2.247	-1.126	2.651	H
HETATM	31	H	0	2.803	-2.766	2.276	H
HETATM	32	C	0	2.749	-0.626	-2.532	C
HETATM	33	H	0	2.214	-1.578	-2.704	H
HETATM	34	H	0	1.963	0.154	-2.522	H
HETATM	35	H	0	3.394	-0.435	-3.405	H
HETATM	36	C	0	6.871	0.720	0.027	C
HETATM	37	H	0	6.777	1.738	0.450	H

HETATM	38	H	0	7.594	0.182	0.665	H
HETATM	39	H	0	7.316	0.831	-0.976	H
HETATM	40	C	0	-1.637	-2.486	2.358	C
HETATM	41	H	0	-1.967	-1.901	3.230	H
HETATM	42	H	0	-1.826	-3.555	2.586	H
HETATM	43	H	0	-0.549	-2.344	2.274	H
HETATM	44	C	0	-1.960	-2.214	-2.690	C
HETATM	45	H	0	-2.183	-3.239	-3.047	H
HETATM	46	H	0	-2.382	-1.512	-3.427	H
HETATM	47	H	0	-0.869	-2.075	-2.703	H
HETATM	48	C	0	-5.986	-1.286	0.164	C
HETATM	49	H	0	-6.128	-0.191	0.240	H
HETATM	50	H	0	-6.560	-1.621	-0.717	H
HETATM	51	H	0	-6.448	-1.726	1.064	H
HETATM	52	H	0	2.340	-3.881	0.326	H
HETATM	53	H	0	-0.024	-4.239	0.565	H
HETATM	54	C	0	-1.614	3.173	0.271	C
HETATM	55	C	0	1.379	1.412	0.177	C
HETATM	56	F	0	-2.970	2.023	1.758	F
HETATM	57	F	0	-0.889	3.704	1.223	F
HETATM	58	F	0	-1.341	3.647	-0.913	F
HETATM	59	F	0	2.349	1.285	1.054	F
HETATM	60	Cl	0	1.733	2.839	-0.788	Cl
HETATM	61	Cl	0	-3.681	1.741	-0.691	Cl

END

sc5f.pdb

TITLE	sc5f.pdb						
HETATM	1	Ru	0	-0.029	0.636	-0.046	Ru
HETATM	2	Cl	0	-0.815	0.196	-2.310	Cl
HETATM	3	Cl	0	0.770	0.700	2.227	Cl
HETATM	4	C	0	-0.010	-1.446	0.111	C
HETATM	5	N	0	-1.099	-2.220	0.224	N
HETATM	6	C	0	-0.753	-3.638	0.382	C
HETATM	7	C	0	0.770	-3.639	0.242	C
HETATM	8	N	0	1.090	-2.209	0.141	N
HETATM	9	C	0	-2.445	-1.743	0.132	C
HETATM	10	C	0	-3.137	-1.875	-1.085	C
HETATM	11	C	0	-4.418	-1.321	-1.180	C
HETATM	12	C	0	-5.018	-0.664	-0.101	C
HETATM	13	C	0	-4.328	-0.605	1.115	C
HETATM	14	C	0	-3.047	-1.150	1.258	C
HETATM	15	C	0	2.431	-1.716	0.058	C
HETATM	16	C	0	3.202	-1.621	1.234	C
HETATM	17	C	0	4.496	-1.106	1.137	C
HETATM	18	C	0	5.044	-0.717	-0.092	C
HETATM	19	C	0	4.280	-0.887	-1.249	C
HETATM	20	C	0	2.973	-1.385	-1.201	C
HETATM	21	C	0	-2.556	-2.614	-2.251	C
HETATM	22	C	0	-6.364	-0.022	-0.247	C
HETATM	23	C	0	-2.354	-1.137	2.587	C
HETATM	24	C	0	2.676	-2.089	2.556	C
HETATM	25	C	0	6.408	-0.103	-0.159	C
HETATM	26	C	0	2.194	-1.560	-2.467	C
HETATM	27	H	0	-1.261	-4.241	-0.391	H
HETATM	28	H	0	-1.099	-4.002	1.368	H
HETATM	29	H	0	1.125	-4.167	-0.663	H
HETATM	30	H	0	1.287	-4.083	1.110	H
HETATM	31	H	0	-4.956	-1.395	-2.134	H
HETATM	32	H	0	-4.797	-0.125	1.984	H
HETATM	33	H	0	5.093	-1.001	2.052	H

HETATM	34	H	0	4.706	-0.619	-2.225	H
HETATM	35	H	0	-2.888	-2.172	-3.205	H
HETATM	36	H	0	-1.455	-2.595	-2.257	H
HETATM	37	H	0	-2.884	-3.673	-2.255	H
HETATM	38	H	0	-6.941	-0.052	0.693	H
HETATM	39	H	0	-6.967	-0.501	-1.036	H
HETATM	40	H	0	-6.267	1.045	-0.524	H
HETATM	41	H	0	-1.401	-0.576	2.576	H
HETATM	42	H	0	-2.106	-2.162	2.923	H
HETATM	43	H	0	-2.994	-0.681	3.360	H
HETATM	44	H	0	1.582	-1.976	2.635	H
HETATM	45	H	0	3.120	-1.515	3.385	H
HETATM	46	H	0	2.926	-3.155	2.732	H
HETATM	47	H	0	6.355	0.992	-0.002	H
HETATM	48	H	0	6.885	-0.258	-1.142	H
HETATM	49	H	0	7.083	-0.500	0.618	H
HETATM	50	H	0	1.556	-0.684	-2.692	H
HETATM	51	H	0	2.870	-1.705	-3.326	H
HETATM	52	H	0	1.502	-2.419	-2.424	H
HETATM	53	C	0	-1.530	1.741	0.211	C
HETATM	54	F	0	-2.407	2.082	-0.697	F
HETATM	55	Cl	0	-2.122	2.268	1.761	Cl
HETATM	56	C	0	0.185	2.888	-0.296	C
HETATM	57	C	0	1.255	2.047	-0.817	C
HETATM	58	F	0	-0.460	3.605	-1.212	F
HETATM	59	F	0	0.396	3.609	0.793	F
HETATM	60	F	0	1.427	2.109	-2.143	F
HETATM	61	Cl	0	2.809	2.058	-0.010	Cl

END

sc5NB.pdb

TITLE	sc5NB.pdb						
HETATM	1	Ru	0	-0.006	0.518	-0.037	Ru
HETATM	2	C	0	-0.825	-3.644	0.489	C
HETATM	3	C	0	0.680	-3.686	0.208	C
HETATM	4	H	0	-1.415	-4.268	-0.204	H
HETATM	5	H	0	0.932	-4.194	-0.743	H
HETATM	6	C	0	-0.054	-1.492	0.127	C
HETATM	7	N	0	1.037	-2.263	0.116	N
HETATM	8	N	0	-1.158	-2.226	0.296	N
HETATM	9	Cl	0	-0.824	0.092	-2.284	Cl
HETATM	10	Cl	0	0.801	0.610	2.227	Cl
HETATM	11	C	0	-1.300	1.992	0.131	C
HETATM	12	C	0	2.377	-1.765	0.018	C
HETATM	13	C	0	3.160	-1.685	1.189	C
HETATM	14	C	0	2.895	-1.382	-1.235	C
HETATM	15	C	0	4.436	-1.128	1.095	C
HETATM	16	C	0	4.181	-0.830	-1.278	C
HETATM	17	C	0	4.952	-0.672	-0.125	C
HETATM	18	H	0	5.039	-1.032	2.007	H
HETATM	19	H	0	4.585	-0.512	-2.248	H
HETATM	20	C	0	-2.490	-1.705	0.195	C
HETATM	21	C	0	-3.063	-1.040	1.296	C
HETATM	22	C	0	-3.189	-1.860	-1.016	C
HETATM	23	C	0	-4.317	-0.441	1.125	C
HETATM	24	C	0	-4.444	-1.257	-1.136	C
HETATM	25	C	0	-5.008	-0.521	-0.088	C
HETATM	26	H	0	-4.764	0.097	1.970	H
HETATM	27	H	0	-4.985	-1.349	-2.086	H
HETATM	28	C	0	2.661	-2.206	2.502	C
HETATM	29	H	0	3.131	-1.672	3.344	H

HETATM	30	H	0	1.571	-2.085	2.614	H
HETATM	31	H	0	2.904	-3.280	2.627	H
HETATM	32	C	0	2.133	-1.560	-2.512	C
HETATM	33	H	0	1.308	-2.285	-2.424	H
HETATM	34	H	0	1.666	-0.618	-2.850	H
HETATM	35	H	0	2.807	-1.900	-3.318	H
HETATM	36	C	0	6.285	0.007	-0.185	C
HETATM	37	H	0	6.171	1.100	-0.049	H
HETATM	38	H	0	6.969	-0.342	0.607	H
HETATM	39	H	0	6.781	-0.137	-1.160	H
HETATM	40	C	0	-2.381	-1.011	2.629	C
HETATM	41	H	0	-3.029	-0.548	3.391	H
HETATM	42	H	0	-2.131	-2.031	2.979	H
HETATM	43	H	0	-1.431	-0.444	2.622	H
HETATM	44	C	0	-2.638	-2.671	-2.149	C
HETATM	45	H	0	-2.990	-3.721	-2.098	H
HETATM	46	H	0	-2.969	-2.269	-3.120	H
HETATM	47	H	0	-1.536	-2.678	-2.168	H
HETATM	48	C	0	-6.320	0.180	-0.269	C
HETATM	49	H	0	-6.172	1.187	-0.704	H
HETATM	50	H	0	-6.990	-0.365	-0.955	H
HETATM	51	H	0	-6.849	0.322	0.689	H
HETATM	52	H	0	1.259	-4.171	1.012	H
HETATM	53	H	0	-1.081	-3.950	1.520	H
HETATM	54	C	0	0.035	2.793	-0.317	C
HETATM	55	C	0	1.273	1.843	-0.733	C
HETATM	56	F	0	-2.269	2.165	-0.763	F
HETATM	57	F	0	-0.296	3.500	-1.410	F
HETATM	58	F	0	0.410	3.641	0.649	F
HETATM	59	F	0	1.511	1.942	-2.045	F
HETATM	60	Cl	0	2.780	2.176	0.109	Cl
HETATM	61	Cl	0	-1.941	2.473	1.702	Cl

END

sc5g.pdb

TITLE	sc5g.pdb						
HETATM	1	Ru	0	-0.029	0.636	-0.046	Ru
HETATM	2	Cl	0	-0.815	0.196	-2.310	Cl
HETATM	3	Cl	0	0.770	0.700	2.227	Cl
HETATM	4	C	0	-0.010	-1.446	0.111	C
HETATM	5	N	0	-1.099	-2.220	0.224	N
HETATM	6	C	0	-0.753	-3.638	0.382	C
HETATM	7	C	0	0.770	-3.639	0.242	C
HETATM	8	N	0	1.090	-2.209	0.141	N
HETATM	9	C	0	-2.445	-1.743	0.132	C
HETATM	10	C	0	-3.137	-1.875	-1.085	C
HETATM	11	C	0	-4.418	-1.321	-1.180	C
HETATM	12	C	0	-5.018	-0.664	-0.101	C
HETATM	13	C	0	-4.328	-0.605	1.115	C
HETATM	14	C	0	-3.047	-1.150	1.258	C
HETATM	15	C	0	2.431	-1.716	0.058	C
HETATM	16	C	0	3.202	-1.621	1.234	C
HETATM	17	C	0	4.496	-1.106	1.137	C
HETATM	18	C	0	5.044	-0.717	-0.092	C
HETATM	19	C	0	4.280	-0.887	-1.249	C
HETATM	20	C	0	2.973	-1.385	-1.201	C
HETATM	21	C	0	-2.556	-2.614	-2.251	C
HETATM	22	C	0	-6.364	-0.022	-0.247	C
HETATM	23	C	0	-2.354	-1.137	2.587	C
HETATM	24	C	0	2.676	-2.089	2.556	C
HETATM	25	C	0	6.408	-0.103	-0.159	C

HETATM	26	C	0	2.194	-1.560	-2.467	C
HETATM	27	H	0	-1.261	-4.241	-0.391	H
HETATM	28	H	0	-1.099	-4.002	1.368	H
HETATM	29	H	0	1.125	-4.167	-0.663	H
HETATM	30	H	0	1.287	-4.083	1.110	H
HETATM	31	H	0	-4.956	-1.395	-2.134	H
HETATM	32	H	0	-4.797	-0.125	1.984	H
HETATM	33	H	0	5.093	-1.001	2.052	H
HETATM	34	H	0	4.706	-0.619	-2.225	H
HETATM	35	H	0	-2.888	-2.172	-3.205	H
HETATM	36	H	0	-1.455	-2.595	-2.257	H
HETATM	37	H	0	-2.884	-3.673	-2.255	H
HETATM	38	H	0	-6.941	-0.052	0.693	H
HETATM	39	H	0	-6.967	-0.501	-1.036	H
HETATM	40	H	0	-6.267	1.045	-0.524	H
HETATM	41	H	0	-1.401	-0.576	2.576	H
HETATM	42	H	0	-2.106	-2.162	2.923	H
HETATM	43	H	0	-2.994	-0.681	3.360	H
HETATM	44	H	0	1.582	-1.976	2.635	H
HETATM	45	H	0	3.120	-1.515	3.385	H
HETATM	46	H	0	2.926	-3.155	2.732	H
HETATM	47	H	0	6.355	0.992	-0.002	H
HETATM	48	H	0	6.885	-0.258	-1.142	H
HETATM	49	H	0	7.083	-0.500	0.618	H
HETATM	50	H	0	1.556	-0.684	-2.692	H
HETATM	51	H	0	2.870	-1.705	-3.326	H
HETATM	52	H	0	1.502	-2.419	-2.424	H
HETATM	53	C	0	-1.530	1.741	0.211	C
HETATM	54	F	0	-2.407	2.082	-0.697	F
HETATM	55	Cl	0	-2.122	2.268	1.761	Cl
HETATM	56	C	0	0.185	2.888	-0.296	C
HETATM	57	C	0	1.255	2.047	-0.817	C
HETATM	58	F	0	-0.460	3.605	-1.212	F
HETATM	59	F	0	0.396	3.609	0.793	F
HETATM	60	F	0	1.427	2.109	-2.143	F
HETATM	61	Cl	0	2.809	2.058	-0.010	Cl

END

sc5h.pdb

TITLE	sc5h.pdb						
HETATM	1	Ru	0	-0.171	0.481	0.078	Ru
HETATM	2	C	0	0.243	-3.646	-0.332	C
HETATM	3	C	0	1.731	-3.319	-0.404	C
HETATM	4	H	0	-0.126	-4.196	-1.217	H
HETATM	5	H	0	2.165	-3.507	-1.406	H
HETATM	6	C	0	0.545	-1.328	-0.086	C
HETATM	7	N	0	1.778	-1.882	-0.111	N
HETATM	8	N	0	-0.367	-2.322	-0.260	N
HETATM	9	Cl	0	-0.613	0.738	-2.251	Cl
HETATM	10	Cl	0	-0.371	0.468	2.457	Cl
HETATM	11	C	0	-2.638	2.331	0.521	C
HETATM	12	C	0	3.035	-1.212	-0.088	C
HETATM	13	C	0	3.759	-1.185	1.119	C
HETATM	14	C	0	3.542	-0.630	-1.262	C
HETATM	15	C	0	5.013	-0.571	1.130	C
HETATM	16	C	0	4.796	-0.009	-1.203	C
HETATM	17	C	0	5.543	0.027	-0.021	C
HETATM	18	H	0	5.583	-0.541	2.068	H
HETATM	19	H	0	5.200	0.454	-2.113	H
HETATM	20	C	0	-1.777	-2.111	-0.156	C
HETATM	21	C	0	-2.385	-2.095	1.119	C

HETATM	22	C	0	-2.552	-1.998	-1.331	C
HETATM	23	C	0	-3.755	-1.823	1.199	C
HETATM	24	C	0	-3.922	-1.751	-1.200	C
HETATM	25	C	0	-4.533	-1.629	0.052	C
HETATM	26	H	0	-4.228	-1.783	2.188	H
HETATM	27	H	0	-4.527	-1.643	-2.110	H
HETATM	28	C	0	3.143	-1.718	2.375	C
HETATM	29	H	0	3.848	-1.675	3.221	H
HETATM	30	H	0	2.247	-1.126	2.651	H
HETATM	31	H	0	2.803	-2.766	2.276	H
HETATM	32	C	0	2.749	-0.626	-2.532	C
HETATM	33	H	0	2.214	-1.578	-2.704	H
HETATM	34	H	0	1.963	0.154	-2.522	H
HETATM	35	H	0	3.394	-0.435	-3.405	H
HETATM	36	C	0	6.871	0.720	0.027	C
HETATM	37	H	0	6.777	1.738	0.450	H
HETATM	38	H	0	7.594	0.182	0.665	H
HETATM	39	H	0	7.316	0.831	-0.976	H
HETATM	40	C	0	-1.637	-2.486	2.358	C
HETATM	41	H	0	-1.967	-1.901	3.230	H
HETATM	42	H	0	-1.826	-3.555	2.586	H
HETATM	43	H	0	-0.549	-2.344	2.274	H
HETATM	44	C	0	-1.960	-2.214	-2.690	C
HETATM	45	H	0	-2.183	-3.239	-3.047	H
HETATM	46	H	0	-2.382	-1.512	-3.427	H
HETATM	47	H	0	-0.869	-2.075	-2.703	H
HETATM	48	C	0	-5.986	-1.286	0.164	C
HETATM	49	H	0	-6.128	-0.191	0.240	H
HETATM	50	H	0	-6.560	-1.621	-0.717	H
HETATM	51	H	0	-6.448	-1.726	1.064	H
HETATM	52	H	0	2.340	-3.881	0.326	H
HETATM	53	H	0	-0.024	-4.239	0.565	H
HETATM	54	C	0	-1.614	3.173	0.271	C
HETATM	55	C	0	1.379	1.412	0.177	C
HETATM	56	F	0	-2.970	2.023	1.758	F
HETATM	57	F	0	-0.889	3.704	1.223	F
HETATM	58	F	0	-1.341	3.647	-0.913	F
HETATM	59	F	0	2.349	1.285	1.054	F
HETATM	60	Cl	0	1.733	2.839	-0.788	Cl
HETATM	61	Cl	0	-3.681	1.741	-0.691	Cl

END

st5e.pdb

TITLE	st5e.pdb						
HETATM	1	Ru	0	-0.152	0.454	0.002	Ru
HETATM	2	C	0	0.450	-3.656	0.156	C
HETATM	3	C	0	1.928	-3.281	0.064	C
HETATM	4	H	0	0.124	-4.329	-0.658	H
HETATM	5	H	0	2.399	-3.611	-0.882	H
HETATM	6	C	0	0.660	-1.315	0.066	C
HETATM	7	N	0	1.915	-1.815	0.122	N
HETATM	8	N	0	-0.212	-2.361	0.051	N
HETATM	9	Cl	0	-0.625	0.563	-2.327	Cl
HETATM	10	Cl	0	-0.340	0.609	2.378	Cl
HETATM	11	C	0	-3.004	2.061	0.130	C
HETATM	12	C	0	3.142	-1.092	0.063	C
HETATM	13	C	0	3.854	-0.876	1.256	C
HETATM	14	C	0	3.629	-0.640	-1.175	C
HETATM	15	C	0	5.079	-0.209	1.190	C
HETATM	16	C	0	4.853	0.042	-1.195	C
HETATM	17	C	0	5.590	0.261	-0.027	C

HETATM	18	H	0	5.638	-0.029	2.117	H
HETATM	19	H	0	5.242	0.402	-2.157	H
HETATM	20	C	0	-1.623	-2.180	-0.076	C
HETATM	21	C	0	-2.424	-2.023	1.076	C
HETATM	22	C	0	-2.204	-2.200	-1.365	C
HETATM	23	C	0	-3.785	-1.752	0.904	C
HETATM	24	C	0	-3.568	-1.927	-1.485	C
HETATM	25	C	0	-4.366	-1.667	-0.365	C
HETATM	26	H	0	-4.408	-1.599	1.795	H
HETATM	27	H	0	-4.016	-1.904	-2.486	H
HETATM	28	C	0	3.250	-1.261	2.571	C
HETATM	29	H	0	3.922	-1.017	3.410	H
HETATM	30	H	0	2.296	-0.721	2.732	H
HETATM	31	H	0	3.014	-2.339	2.638	H
HETATM	32	C	0	2.847	-0.848	-2.435	C
HETATM	33	H	0	2.456	-1.879	-2.521	H
HETATM	34	H	0	1.961	-0.184	-2.488	H
HETATM	35	H	0	3.464	-0.647	-3.325	H
HETATM	36	C	0	6.882	1.019	-0.069	C
HETATM	37	H	0	6.721	2.098	0.118	H
HETATM	38	H	0	7.591	0.669	0.701	H
HETATM	39	H	0	7.377	0.938	-1.052	H
HETATM	40	C	0	-1.887	-2.239	2.457	C
HETATM	41	H	0	-2.309	-1.512	3.169	H
HETATM	42	H	0	-2.167	-3.250	2.816	H
HETATM	43	H	0	-0.793	-2.145	2.516	H
HETATM	44	C	0	-1.404	-2.572	-2.575	C
HETATM	45	H	0	-1.429	-3.668	-2.736	H
HETATM	46	H	0	-1.811	-2.099	-3.483	H
HETATM	47	H	0	-0.348	-2.266	-2.498	H
HETATM	48	C	0	-5.803	-1.278	-0.516	C
HETATM	49	H	0	-5.912	-0.177	-0.478	H
HETATM	50	H	0	-6.226	-1.611	-1.478	H
HETATM	51	H	0	-6.431	-1.684	0.297	H
HETATM	52	H	0	2.534	-3.692	0.890	H
HETATM	53	H	0	0.189	-4.144	1.116	H
HETATM	54	C	0	-2.057	2.993	-0.089	C
HETATM	55	C	0	1.326	1.499	0.033	C
HETATM	56	F	0	-1.449	3.642	0.870	F
HETATM	57	F	0	-1.742	3.417	-1.283	F
HETATM	58	F	0	2.323	1.478	0.888	F
HETATM	59	Cl	0	1.520	2.925	-0.971	Cl
HETATM	60	F	0	-3.614	1.482	-0.891	F
HETATM	61	Cl	0	-3.623	1.687	1.672	Cl

END

st5f.pdb

TITLE	st5f.pdb						
HETATM	1	Ru	0	0.060	-0.585	-0.012	Ru
HETATM	2	Cl	0	0.810	-0.444	-2.303	Cl
HETATM	3	Cl	0	-0.661	-0.423	2.307	Cl
HETATM	4	C	0	-0.067	1.493	0.067	C
HETATM	5	N	0	0.999	2.297	0.155	N
HETATM	6	C	0	0.618	3.711	0.269	C
HETATM	7	C	0	-0.910	3.660	0.185	C
HETATM	8	N	0	-1.191	2.220	0.101	N
HETATM	9	C	0	2.343	1.821	0.021	C
HETATM	10	C	0	2.960	1.860	-1.244	C
HETATM	11	C	0	4.229	1.290	-1.378	C
HETATM	12	C	0	4.888	0.701	-0.294	C
HETATM	13	C	0	4.280	0.741	0.965	C

HETATM	14	C	0	3.014	1.307	1.151	C
HETATM	15	C	0	-2.508	1.666	0.057	C
HETATM	16	C	0	-3.270	1.579	1.237	C
HETATM	17	C	0	-4.522	0.958	1.170	C
HETATM	18	C	0	-5.026	0.445	-0.029	C
HETATM	19	C	0	-4.272	0.604	-1.197	C
HETATM	20	C	0	-3.018	1.224	-1.179	C
HETATM	21	C	0	2.301	2.510	-2.422	C
HETATM	22	C	0	6.207	0.016	-0.483	C
HETATM	23	C	0	2.409	1.393	2.519	C
HETATM	24	C	0	-2.793	2.163	2.532	C
HETATM	25	C	0	-6.339	-0.276	-0.060	C
HETATM	26	C	0	-2.252	1.431	-2.449	C
HETATM	27	H	0	1.080	4.294	-0.548	H
HETATM	28	H	0	0.988	4.126	1.225	H
HETATM	29	H	0	-1.314	4.174	-0.707	H
HETATM	30	H	0	-1.408	4.093	1.071	H
HETATM	31	H	0	4.703	1.285	-2.368	H
HETATM	32	H	0	4.798	0.315	1.833	H
HETATM	33	H	0	-5.113	0.864	2.090	H
HETATM	34	H	0	-4.667	0.240	-2.154	H
HETATM	35	H	0	2.579	2.001	-3.359	H
HETATM	36	H	0	1.201	2.485	-2.360	H
HETATM	37	H	0	2.613	3.569	-2.520	H
HETATM	38	H	0	6.061	-1.053	-0.730	H
HETATM	39	H	0	6.788	0.455	-1.311	H
HETATM	40	H	0	6.826	0.048	0.429	H
HETATM	41	H	0	3.109	1.013	3.281	H
HETATM	42	H	0	1.471	0.812	2.612	H
HETATM	43	H	0	2.161	2.437	2.787	H
HETATM	44	H	0	-1.695	2.212	2.591	H
HETATM	45	H	0	-3.132	1.558	3.389	H
HETATM	46	H	0	-3.195	3.186	2.678	H
HETATM	47	H	0	-6.202	-1.358	0.125	H
HETATM	48	H	0	-7.032	0.092	0.716	H
HETATM	49	H	0	-6.839	-0.182	-1.039	H
HETATM	50	H	0	-1.326	0.825	-2.499	H
HETATM	51	H	0	-2.864	1.164	-3.326	H
HETATM	52	H	0	-1.938	2.485	-2.570	H
HETATM	53	C	0	-1.403	-1.719	-0.357	C
HETATM	54	Cl	0	-2.007	-2.131	-1.934	Cl
HETATM	55	F	0	-2.263	-2.142	0.534	F
HETATM	56	C	0	0.340	-2.850	0.055	C
HETATM	57	C	0	1.484	-2.022	0.418	C
HETATM	58	F	0	0.460	-3.557	-1.059	F
HETATM	59	F	0	-0.220	-3.577	1.013	F
HETATM	60	F	0	2.490	-2.041	-0.466	F
HETATM	61	Cl	0	2.133	-2.144	2.041	Cl

END

st5NB.pdb

TITLE	st5NB.pdb						
HETATM	1	Ru	0	0.014	-0.500	0.006	Ru
HETATM	2	C	0	0.794	3.693	0.318	C
HETATM	3	C	0	-0.726	3.712	0.126	C
HETATM	4	H	0	1.336	4.263	-0.457	H
HETATM	5	H	0	-1.041	4.212	-0.809	H
HETATM	6	C	0	0.024	1.521	0.093	C
HETATM	7	N	0	-1.072	2.284	0.067	N
HETATM	8	N	0	1.127	2.265	0.211	N
HETATM	9	Cl	0	0.809	-0.373	-2.271	Cl

HETATM	10	Cl	0	-0.731	-0.341	2.304	Cl
HETATM	11	C	0	1.275	-1.972	0.380	C
HETATM	12	C	0	-2.404	1.757	0.023	C
HETATM	13	C	0	-3.165	1.693	1.207	C
HETATM	14	C	0	-2.922	1.305	-1.208	C
HETATM	15	C	0	-4.413	1.068	1.154	C
HETATM	16	C	0	-4.175	0.683	-1.209	C
HETATM	17	C	0	-4.919	0.530	-0.035	C
HETATM	18	H	0	-5.000	0.985	2.078	H
HETATM	19	H	0	-4.574	0.305	-2.159	H
HETATM	20	C	0	2.451	1.735	0.068	C
HETATM	21	C	0	3.094	1.160	1.183	C
HETATM	22	C	0	3.068	1.781	-1.195	C
HETATM	23	C	0	4.335	0.545	0.982	C
HETATM	24	C	0	4.313	1.165	-1.345	C
HETATM	25	C	0	4.945	0.520	-0.277	C
HETATM	26	H	0	4.837	0.078	1.839	H
HETATM	27	H	0	4.790	1.170	-2.333	H
HETATM	28	C	0	-2.689	2.308	2.487	C
HETATM	29	H	0	-3.043	1.733	3.358	H
HETATM	30	H	0	-1.591	2.346	2.556	H
HETATM	31	H	0	-3.080	3.339	2.599	H
HETATM	32	C	0	-2.176	1.508	-2.491	C
HETATM	33	H	0	-1.842	2.556	-2.609	H
HETATM	34	H	0	-1.268	0.879	-2.567	H
HETATM	35	H	0	-2.813	1.262	-3.356	H
HETATM	36	C	0	-6.217	-0.216	-0.045	C
HETATM	37	H	0	-6.051	-1.292	0.151	H
HETATM	38	H	0	-6.910	0.145	0.734	H
HETATM	39	H	0	-6.727	-0.147	-1.021	H
HETATM	40	C	0	2.490	1.232	2.552	C
HETATM	41	H	0	3.195	0.857	3.311	H
HETATM	42	H	0	2.226	2.271	2.826	H
HETATM	43	H	0	1.560	0.641	2.645	H
HETATM	44	C	0	2.438	2.488	-2.357	C
HETATM	45	H	0	2.795	3.535	-2.431	H
HETATM	46	H	0	2.693	1.991	-3.307	H
HETATM	47	H	0	1.337	2.507	-2.298	H
HETATM	48	C	0	6.243	-0.201	-0.480	C
HETATM	49	H	0	6.067	-1.267	-0.720	H
HETATM	50	H	0	6.824	0.222	-1.316	H
HETATM	51	H	0	6.874	-0.181	0.424	H
HETATM	52	H	0	-1.264	4.194	0.961	H
HETATM	53	H	0	1.113	4.079	1.304	H
HETATM	54	C	0	-0.070	-2.788	0.002	C
HETATM	55	C	0	-1.348	-1.869	-0.358	C
HETATM	56	F	0	2.248	-2.238	-0.493	F
HETATM	57	F	0	0.233	-3.586	-1.033	F
HETATM	58	F	0	-0.438	-3.548	1.043	F
HETATM	59	F	0	-2.335	-2.090	0.509	F
HETATM	60	Cl	0	-1.998	-2.112	-1.977	Cl
HETATM	61	Cl	0	1.904	-2.320	1.985	Cl

END

st5g.pdb

TITLE	st5g.pdb						
HETATM	1	Ru	0	0.060	-0.585	-0.012	Ru
HETATM	2	Cl	0	0.810	-0.444	-2.303	Cl
HETATM	3	Cl	0	-0.661	-0.423	2.307	Cl
HETATM	4	C	0	-0.067	1.493	0.067	C
HETATM	5	N	0	0.999	2.297	0.155	N

HETATM	6	C	0	0.618	3.711	0.269	C
HETATM	7	C	0	-0.910	3.660	0.185	C
HETATM	8	N	0	-1.191	2.220	0.101	N
HETATM	9	C	0	2.343	1.821	0.021	C
HETATM	10	C	0	2.960	1.860	-1.244	C
HETATM	11	C	0	4.229	1.290	-1.378	C
HETATM	12	C	0	4.888	0.701	-0.294	C
HETATM	13	C	0	4.280	0.741	0.965	C
HETATM	14	C	0	3.014	1.307	1.151	C
HETATM	15	C	0	-2.508	1.666	0.057	C
HETATM	16	C	0	-3.270	1.579	1.237	C
HETATM	17	C	0	-4.522	0.958	1.170	C
HETATM	18	C	0	-5.026	0.445	-0.029	C
HETATM	19	C	0	-4.272	0.604	-1.197	C
HETATM	20	C	0	-3.018	1.224	-1.179	C
HETATM	21	C	0	2.301	2.510	-2.422	C
HETATM	22	C	0	6.207	0.016	-0.483	C
HETATM	23	C	0	2.409	1.393	2.519	C
HETATM	24	C	0	-2.793	2.163	2.532	C
HETATM	25	C	0	-6.339	-0.276	-0.060	C
HETATM	26	C	0	-2.252	1.431	-2.449	C
HETATM	27	H	0	1.080	4.294	-0.548	H
HETATM	28	H	0	0.988	4.126	1.225	H
HETATM	29	H	0	-1.314	4.174	-0.707	H
HETATM	30	H	0	-1.408	4.093	1.071	H
HETATM	31	H	0	4.703	1.285	-2.368	H
HETATM	32	H	0	4.798	0.315	1.833	H
HETATM	33	H	0	-5.113	0.864	2.090	H
HETATM	34	H	0	-4.667	0.240	-2.154	H
HETATM	35	H	0	2.579	2.001	-3.359	H
HETATM	36	H	0	1.201	2.485	-2.360	H
HETATM	37	H	0	2.613	3.569	-2.520	H
HETATM	38	H	0	6.061	-1.053	-0.730	H
HETATM	39	H	0	6.788	0.455	-1.311	H
HETATM	40	H	0	6.826	0.048	0.429	H
HETATM	41	H	0	3.109	1.013	3.281	H
HETATM	42	H	0	1.471	0.812	2.612	H
HETATM	43	H	0	2.161	2.437	2.787	H
HETATM	44	H	0	-1.695	2.212	2.591	H
HETATM	45	H	0	-3.132	1.558	3.389	H
HETATM	46	H	0	-3.195	3.186	2.678	H
HETATM	47	H	0	-6.202	-1.358	0.125	H
HETATM	48	H	0	-7.032	0.092	0.716	H
HETATM	49	H	0	-6.839	-0.182	-1.039	H
HETATM	50	H	0	-1.326	0.825	-2.499	H
HETATM	51	H	0	-2.864	1.164	-3.326	H
HETATM	52	H	0	-1.938	2.485	-2.570	H
HETATM	53	C	0	-1.403	-1.719	-0.357	C
HETATM	54	Cl	0	-2.007	-2.131	-1.934	Cl
HETATM	55	F	0	-2.263	-2.142	0.534	F
HETATM	56	C	0	0.340	-2.850	0.055	C
HETATM	57	C	0	1.484	-2.022	0.418	C
HETATM	58	F	0	0.460	-3.557	-1.059	F
HETATM	59	F	0	-0.220	-3.577	1.013	F
HETATM	60	F	0	2.490	-2.041	-0.466	F
HETATM	61	Cl	0	2.133	-2.144	2.041	Cl

END

st5h.pdb

TITLE st5h.pdb
 REMARK 1 File created by GaussView 5.0.8

HETATM	1	Ru	0	-0.152	0.454	0.002	Ru
HETATM	2	C	0	0.450	-3.656	0.156	C
HETATM	3	C	0	1.928	-3.281	0.064	C
HETATM	4	H	0	0.124	-4.329	-0.658	H
HETATM	5	H	0	2.399	-3.611	-0.882	H
HETATM	6	C	0	0.660	-1.315	0.066	C
HETATM	7	N	0	1.915	-1.815	0.122	N
HETATM	8	N	0	-0.212	-2.361	0.051	N
HETATM	9	Cl	0	-0.625	0.563	-2.327	Cl
HETATM	10	Cl	0	-0.340	0.609	2.378	Cl
HETATM	11	C	0	-3.004	2.061	0.130	C
HETATM	12	C	0	3.142	-1.092	0.063	C
HETATM	13	C	0	3.854	-0.876	1.256	C
HETATM	14	C	0	3.629	-0.640	-1.175	C
HETATM	15	C	0	5.079	-0.209	1.190	C
HETATM	16	C	0	4.853	0.042	-1.195	C
HETATM	17	C	0	5.590	0.261	-0.027	C
HETATM	18	H	0	5.638	-0.029	2.117	H
HETATM	19	H	0	5.242	0.402	-2.157	H
HETATM	20	C	0	-1.623	-2.180	-0.076	C
HETATM	21	C	0	-2.424	-2.023	1.076	C
HETATM	22	C	0	-2.204	-2.200	-1.365	C
HETATM	23	C	0	-3.785	-1.752	0.904	C
HETATM	24	C	0	-3.568	-1.927	-1.485	C
HETATM	25	C	0	-4.366	-1.667	-0.365	C
HETATM	26	H	0	-4.408	-1.599	1.795	H
HETATM	27	H	0	-4.016	-1.904	-2.486	H
HETATM	28	C	0	3.250	-1.261	2.571	C
HETATM	29	H	0	3.922	-1.017	3.410	H
HETATM	30	H	0	2.296	-0.721	2.732	H
HETATM	31	H	0	3.014	-2.339	2.638	H
HETATM	32	C	0	2.847	-0.848	-2.435	C
HETATM	33	H	0	2.456	-1.879	-2.521	H
HETATM	34	H	0	1.961	-0.184	-2.488	H
HETATM	35	H	0	3.464	-0.647	-3.325	H
HETATM	36	C	0	6.882	1.019	-0.069	C
HETATM	37	H	0	6.721	2.098	0.118	H
HETATM	38	H	0	7.591	0.669	0.701	H
HETATM	39	H	0	7.377	0.938	-1.052	H
HETATM	40	C	0	-1.887	-2.239	2.457	C
HETATM	41	H	0	-2.309	-1.512	3.169	H
HETATM	42	H	0	-2.167	-3.250	2.816	H
HETATM	43	H	0	-0.793	-2.145	2.516	H
HETATM	44	C	0	-1.404	-2.572	-2.575	C
HETATM	45	H	0	-1.429	-3.668	-2.736	H
HETATM	46	H	0	-1.811	-2.099	-3.483	H
HETATM	47	H	0	-0.348	-2.266	-2.498	H
HETATM	48	C	0	-5.803	-1.278	-0.516	C
HETATM	49	H	0	-5.912	-0.177	-0.478	H
HETATM	50	H	0	-6.226	-1.611	-1.478	H
HETATM	51	H	0	-6.431	-1.684	0.297	H
HETATM	52	H	0	2.534	-3.692	0.890	H
HETATM	53	H	0	0.189	-4.144	1.116	H
HETATM	54	C	0	-2.057	2.993	-0.089	C
HETATM	55	C	0	1.326	1.499	0.033	C
HETATM	56	F	0	-1.449	3.642	0.870	F
HETATM	57	F	0	-1.742	3.417	-1.283	F
HETATM	58	F	0	2.323	1.478	0.888	F
HETATM	59	Cl	0	1.520	2.925	-0.971	Cl
HETATM	60	F	0	-3.614	1.482	-0.891	F
HETATM	61	Cl	0	-3.623	1.687	1.672	Cl

END

ac5e.pdb

TITLE	ac5e.pdb						
HETATM	1	Ru	0	-0.187	0.408	-0.114	Ru
HETATM	2	C	0	0.434	-3.628	0.719	C
HETATM	3	C	0	1.895	-3.198	0.824	C
HETATM	4	H	0	0.254	-4.343	-0.110	H
HETATM	5	H	0	2.575	-3.800	0.195	H
HETATM	6	C	0	0.614	-1.337	0.217	C
HETATM	7	N	0	1.874	-1.804	0.370	N
HETATM	8	N	0	-0.246	-2.366	0.455	N
HETATM	9	Cl	0	-0.600	0.166	-2.443	Cl
HETATM	10	Cl	0	-0.554	0.918	2.177	Cl
HETATM	11	C	0	-3.065	1.912	-0.405	C
HETATM	12	C	0	3.100	-1.095	0.219	C
HETATM	13	C	0	3.619	-0.334	1.280	C
HETATM	14	C	0	3.792	-1.223	-1.000	C
HETATM	15	C	0	4.853	0.304	1.094	C
HETATM	16	C	0	5.025	-0.584	-1.139	C
HETATM	17	C	0	5.568	0.186	-0.101	C
HETATM	18	H	0	5.267	0.904	1.914	H
HETATM	19	H	0	5.568	-0.674	-2.089	H
HETATM	20	C	0	-1.660	-2.240	0.303	C
HETATM	21	C	0	-2.457	-1.976	1.438	C
HETATM	22	C	0	-2.244	-2.426	-0.970	C
HETATM	23	C	0	-3.826	-1.762	1.251	C
HETATM	24	C	0	-3.616	-2.201	-1.107	C
HETATM	25	C	0	-4.414	-1.836	-0.017	C
HETATM	26	H	0	-4.447	-1.520	2.123	H
HETATM	27	H	0	-4.072	-2.306	-2.100	H
HETATM	28	C	0	2.862	-0.163	2.560	C
HETATM	29	H	0	3.535	0.111	3.390	H
HETATM	30	H	0	2.095	0.631	2.478	H
HETATM	31	H	0	2.306	-1.072	2.853	H
HETATM	32	C	0	3.163	-1.953	-2.146	C
HETATM	33	H	0	2.900	-2.999	-1.899	H
HETATM	34	H	0	2.220	-1.460	-2.455	H
HETATM	35	H	0	3.830	-1.978	-3.023	H
HETATM	36	C	0	6.875	0.897	-0.287	C
HETATM	37	H	0	6.740	1.848	-0.835	H
HETATM	38	H	0	7.349	1.148	0.677	H
HETATM	39	H	0	7.591	0.296	-0.874	H
HETATM	40	C	0	-1.889	-2.011	2.823	C
HETATM	41	H	0	-2.380	-1.275	3.479	H
HETATM	42	H	0	-2.050	-3.011	3.275	H
HETATM	43	H	0	-0.809	-1.797	2.848	H
HETATM	44	C	0	-1.449	-2.935	-2.132	C
HETATM	45	H	0	-1.526	-4.039	-2.194	H
HETATM	46	H	0	-1.823	-2.526	-3.084	H
HETATM	47	H	0	-0.380	-2.675	-2.071	H
HETATM	48	C	0	-5.858	-1.494	-0.209	C
HETATM	49	H	0	-5.977	-0.411	-0.407	H
HETATM	50	H	0	-6.301	-2.024	-1.069	H
HETATM	51	H	0	-6.463	-1.720	0.686	H
HETATM	52	H	0	2.282	-3.245	1.861	H
HETATM	53	H	0	0.050	-4.090	1.646	H
HETATM	54	C	0	-2.221	2.956	-0.497	C
HETATM	55	C	0	1.301	1.383	-0.431	C
HETATM	56	F	0	-3.631	1.545	0.715	F
HETATM	57	F	0	-1.721	3.322	-1.666	F

HETATM	58	F	0	2.250	1.154	-1.311	F
HETATM	59	F	0	-3.478	1.220	-1.435	F
HETATM	60	Cl	0	1.564	2.982	0.241	Cl
HETATM	61	Cl	0	-1.863	3.973	0.821	Cl

END

ac5f.pdb

TITLE	ac5f.pdb						
HETATM	1	Ru	0	-0.062	0.543	-0.063	Ru
HETATM	2	Cl	0	-0.905	0.150	-2.319	Cl
HETATM	3	Cl	0	0.676	0.603	2.215	Cl
HETATM	4	C	0	-0.078	-1.521	0.074	C
HETATM	5	N	0	-1.185	-2.264	0.193	N
HETATM	6	C	0	-0.875	-3.687	0.370	C
HETATM	7	C	0	0.646	-3.729	0.199	C
HETATM	8	N	0	1.006	-2.308	0.092	N
HETATM	9	C	0	-2.506	-1.717	0.211	C
HETATM	10	C	0	-3.293	-1.799	-0.958	C
HETATM	11	C	0	-4.539	-1.173	-0.962	C
HETATM	12	C	0	-5.024	-0.487	0.161	C
HETATM	13	C	0	-4.252	-0.481	1.323	C
HETATM	14	C	0	-2.995	-1.099	1.378	C
HETATM	15	C	0	2.355	-1.836	0.016	C
HETATM	16	C	0	3.117	-1.735	1.196	C
HETATM	17	C	0	4.409	-1.206	1.108	C
HETATM	18	C	0	4.956	-0.803	-0.114	C
HETATM	19	C	0	4.200	-0.978	-1.278	C
HETATM	20	C	0	2.902	-1.497	-1.239	C
HETATM	21	C	0	-2.832	-2.563	-2.161	C
HETATM	22	C	0	-6.334	0.237	0.102	C
HETATM	23	C	0	-2.251	-1.111	2.679	C
HETATM	24	C	0	2.586	-2.202	2.517	C
HETATM	25	C	0	6.308	-0.161	-0.176	C
HETATM	26	C	0	2.130	-1.689	-2.507	C
HETATM	27	H	0	-1.415	-4.292	-0.379	H
HETATM	28	H	0	-1.208	-4.019	1.372	H
HETATM	29	H	0	0.965	-4.268	-0.713	H
HETATM	30	H	0	1.168	-4.189	1.057	H
HETATM	31	H	0	-5.144	-1.206	-1.877	H
HETATM	32	H	0	-4.630	0.020	2.224	H
HETATM	33	H	0	4.997	-1.095	2.028	H
HETATM	34	H	0	4.628	-0.701	-2.250	H
HETATM	35	H	0	-3.244	-2.130	-3.087	H
HETATM	36	H	0	-1.735	-2.556	-2.265	H
HETATM	37	H	0	-3.169	-3.619	-2.118	H
HETATM	38	H	0	-6.212	1.236	-0.359	H
HETATM	39	H	0	-6.764	0.396	1.105	H
HETATM	40	H	0	-7.077	-0.302	-0.511	H
HETATM	41	H	0	-1.936	-0.096	2.978	H
HETATM	42	H	0	-1.333	-1.720	2.653	H
HETATM	43	H	0	-2.899	-1.500	3.485	H
HETATM	44	H	0	1.493	-2.077	2.595	H
HETATM	45	H	0	3.035	-1.635	3.348	H
HETATM	46	H	0	2.825	-3.271	2.690	H
HETATM	47	H	0	6.219	0.943	-0.177	H
HETATM	48	H	0	6.937	-0.429	0.690	H
HETATM	49	H	0	6.856	-0.432	-1.095	H
HETATM	50	H	0	1.361	-0.908	-2.662	H
HETATM	51	H	0	2.801	-1.672	-3.381	H
HETATM	52	H	0	1.581	-2.648	-2.522	H
HETATM	53	C	0	1.306	1.627	-0.784	C

HETATM	54	F	0	1.454	1.958	-2.044	F
HETATM	55	Cl	0	2.769	2.014	0.065	Cl
HETATM	56	C	0	-0.312	2.817	-0.209	C
HETATM	57	C	0	-1.486	1.991	0.128	C
HETATM	58	F	0	-0.433	3.415	-1.400	F
HETATM	59	Cl	0	0.290	3.906	1.010	Cl
HETATM	60	F	0	-2.513	2.075	-0.709	F
HETATM	61	F	0	-1.959	2.070	1.376	F

END

ac5PB.pdb

TITLE	ac5PB.pdb						
HETATM	1	Ru	0	-0.076	0.463	-0.035	Ru
HETATM	2	C	0	-0.927	-3.705	0.357	C
HETATM	3	C	0	0.591	-3.759	0.147	C
HETATM	4	H	0	-1.490	-4.308	-0.376	H
HETATM	5	H	0	0.882	-4.276	-0.787	H
HETATM	6	C	0	-0.116	-1.556	0.064	C
HETATM	7	N	0	0.966	-2.340	0.067	N
HETATM	8	N	0	-1.232	-2.281	0.182	N
HETATM	9	Cl	0	-0.895	0.093	-2.298	Cl
HETATM	10	Cl	0	0.643	0.552	2.245	Cl
HETATM	11	C	0	-1.376	1.908	0.145	C
HETATM	12	C	0	2.312	-1.855	-0.010	C
HETATM	13	C	0	3.079	-1.774	1.169	C
HETATM	14	C	0	2.848	-1.488	-1.261	C
HETATM	15	C	0	4.365	-1.235	1.085	C
HETATM	16	C	0	4.143	-0.960	-1.295	C
HETATM	17	C	0	4.903	-0.803	-0.133	C
HETATM	18	H	0	4.958	-1.137	2.003	H
HETATM	19	H	0	4.564	-0.658	-2.263	H
HETATM	20	C	0	-2.540	-1.700	0.215	C
HETATM	21	C	0	-2.990	-1.055	1.382	C
HETATM	22	C	0	-3.340	-1.755	-0.947	C
HETATM	23	C	0	-4.211	-0.367	1.329	C
HETATM	24	C	0	-4.554	-1.069	-0.946	C
HETATM	25	C	0	-4.991	-0.343	0.172	C
HETATM	26	H	0	-4.556	0.160	2.228	H
HETATM	27	H	0	-5.168	-1.081	-1.855	H
HETATM	28	C	0	2.556	-2.271	2.482	C
HETATM	29	H	0	3.016	-1.727	3.323	H
HETATM	30	H	0	1.465	-2.142	2.574	H
HETATM	31	H	0	2.790	-3.345	2.627	H
HETATM	32	C	0	2.076	-1.646	-2.534	C
HETATM	33	H	0	1.356	-2.482	-2.494	H
HETATM	34	H	0	1.471	-0.750	-2.766	H
HETATM	35	H	0	2.757	-1.818	-3.384	H
HETATM	36	C	0	6.248	-0.147	-0.187	C
HETATM	37	H	0	6.145	0.955	-0.171	H
HETATM	38	H	0	6.882	-0.422	0.672	H
HETATM	39	H	0	6.795	-0.396	-1.113	H
HETATM	40	C	0	-2.255	-1.122	2.687	C
HETATM	41	H	0	-2.915	-1.540	3.470	H
HETATM	42	H	0	-1.343	-1.738	2.646	H
HETATM	43	H	0	-1.935	-0.124	3.033	H
HETATM	44	C	0	-2.923	-2.550	-2.147	C
HETATM	45	H	0	-3.262	-3.602	-2.068	H
HETATM	46	H	0	-3.365	-2.137	-3.068	H
HETATM	47	H	0	-1.830	-2.549	-2.288	H
HETATM	48	C	0	-6.259	0.450	0.112	C
HETATM	49	H	0	-6.102	1.405	-0.426	H

HETATM	50	H	0	-7.057	-0.086	-0.431	H
HETATM	51	H	0	-6.637	0.704	1.116	H
HETATM	52	H	0	1.128	-4.245	0.980	H
HETATM	53	H	0	-1.235	-4.030	1.369	H
HETATM	54	C	0	-0.022	2.734	-0.318	C
HETATM	55	C	0	1.221	1.788	-0.697	C
HETATM	56	F	0	-2.360	2.153	-0.704	F
HETATM	57	F	0	-1.828	2.221	1.356	F
HETATM	58	F	0	-0.375	3.353	-1.461	F
HETATM	59	F	0	1.481	1.904	-2.003	F
HETATM	60	Cl	0	2.743	2.014	0.155	Cl
HETATM	61	Cl	0	0.368	3.950	0.916	Cl

END

ac5g.pdb

TITLE	ac5g.pdb						
HETATM	1	Ru	0	-0.071	0.533	-0.030	Ru
HETATM	2	Cl	0	0.690	0.599	2.255	Cl
HETATM	3	Cl	0	-0.920	0.176	-2.278	Cl
HETATM	4	C	0	-0.148	-1.513	0.136	C
HETATM	5	N	0	0.914	-2.325	0.139	N
HETATM	6	C	0	0.521	-3.734	0.269	C
HETATM	7	C	0	-0.997	-3.652	0.458	C
HETATM	8	N	0	-1.275	-2.219	0.296	N
HETATM	9	C	0	2.269	-1.881	0.015	C
HETATM	10	C	0	3.073	-1.804	1.170	C
HETATM	11	C	0	4.379	-1.326	1.036	C
HETATM	12	C	0	4.901	-0.950	-0.207	C
HETATM	13	C	0	4.100	-1.095	-1.342	C
HETATM	14	C	0	2.784	-1.564	-1.259	C
HETATM	15	C	0	-2.590	-1.656	0.235	C
HETATM	16	C	0	-3.320	-1.751	-0.966	C
HETATM	17	C	0	-4.560	-1.112	-1.040	C
HETATM	18	C	0	-5.087	-0.401	0.045	C
HETATM	19	C	0	-4.368	-0.380	1.244	C
HETATM	20	C	0	-3.126	-1.013	1.368	C
HETATM	21	C	0	2.566	-2.246	2.508	C
HETATM	22	C	0	6.275	-0.365	-0.317	C
HETATM	23	C	0	1.971	-1.717	-2.507	C
HETATM	24	C	0	-2.813	-2.539	-2.135	C
HETATM	25	C	0	-6.388	0.330	-0.083	C
HETATM	26	C	0	-2.410	-1.013	2.684	C
HETATM	27	H	0	1.042	-4.194	1.127	H
HETATM	28	H	0	0.818	-4.291	-0.640	H
HETATM	29	H	0	-1.328	-3.988	1.458	H
HETATM	30	H	0	-1.561	-4.233	-0.292	H
HETATM	31	H	0	5.003	-1.236	1.934	H
HETATM	32	H	0	4.505	-0.835	-2.329	H
HETATM	33	H	0	-5.122	-1.158	-1.981	H
HETATM	34	H	0	-4.788	0.133	2.119	H
HETATM	35	H	0	3.060	-1.689	3.322	H
HETATM	36	H	0	1.482	-2.084	2.620	H
HETATM	37	H	0	2.775	-3.321	2.682	H
HETATM	38	H	0	6.232	0.741	-0.303	H
HETATM	39	H	0	6.771	-0.647	-1.262	H
HETATM	40	H	0	6.927	-0.670	0.519	H
HETATM	41	H	0	2.617	-1.962	-3.367	H
HETATM	42	H	0	1.421	-0.792	-2.759	H
HETATM	43	H	0	1.199	-2.502	-2.420	H
HETATM	44	H	0	-1.713	-2.558	-2.184	H

HETATM	45	H	0	-3.166	-2.106	-3.085	H
HETATM	46	H	0	-3.178	-3.586	-2.101	H
HETATM	47	H	0	-6.237	1.334	-0.525	H
HETATM	48	H	0	-7.097	-0.199	-0.742	H
HETATM	49	H	0	-6.875	0.482	0.895	H
HETATM	50	H	0	-1.587	-0.275	2.724	H
HETATM	51	H	0	-3.105	-0.777	3.507	H
HETATM	52	H	0	-1.946	-1.991	2.906	H
HETATM	53	C	0	-1.400	1.872	0.225	C
HETATM	54	F	0	-1.776	2.278	1.420	F
HETATM	55	F	0	-2.340	2.223	-0.617	F
HETATM	56	C	0	0.173	2.771	-0.340	C
HETATM	57	C	0	1.298	1.833	-0.723	C
HETATM	58	Cl	0	0.500	3.936	0.936	Cl
HETATM	59	F	0	-0.309	3.391	-1.429	F
HETATM	60	Cl	0	2.834	1.911	0.123	Cl
HETATM	61	F	0	1.550	1.845	-2.040	F

END

ac5h.pdb

TITLE	ac5h.pdb						
HETATM	1	Ru	0	0.158	0.396	-0.076	Ru
HETATM	2	C	0	-0.503	-3.677	0.416	C
HETATM	3	C	0	-1.973	-3.260	0.496	C
HETATM	4	H	0	-0.158	-4.219	1.315	H
HETATM	5	H	0	-2.412	-3.431	1.498	H
HETATM	6	C	0	-0.673	-1.350	0.137	C
HETATM	7	N	0	-1.937	-1.823	0.207	N
HETATM	8	N	0	0.182	-2.396	0.293	N
HETATM	9	Cl	0	0.550	0.729	2.266	Cl
HETATM	10	Cl	0	0.256	0.327	-2.470	Cl
HETATM	11	C	0	2.661	2.090	-0.549	C
HETATM	12	C	0	-3.138	-1.058	0.146	C
HETATM	13	C	0	-3.814	-0.958	-1.084	C
HETATM	14	C	0	-3.637	-0.446	1.310	C
HETATM	15	C	0	-5.011	-0.239	-1.129	C
HETATM	16	C	0	-4.829	0.281	1.217	C
HETATM	17	C	0	-5.527	0.393	0.009	C
HETATM	18	H	0	-5.542	-0.152	-2.085	H
HETATM	19	H	0	-5.224	0.768	2.118	H
HETATM	20	C	0	1.596	-2.232	0.165	C
HETATM	21	C	0	2.186	-2.259	-1.119	C
HETATM	22	C	0	2.389	-2.080	1.325	C
HETATM	23	C	0	3.555	-1.993	-1.226	C
HETATM	24	C	0	3.755	-1.838	1.167	C
HETATM	25	C	0	4.348	-1.758	-0.099	C
HETATM	26	H	0	4.013	-1.979	-2.224	H
HETATM	27	H	0	4.373	-1.697	2.064	H
HETATM	28	C	0	-3.207	-1.532	-2.325	C
HETATM	29	H	0	-3.897	-1.464	-3.182	H
HETATM	30	H	0	-2.282	-0.984	-2.593	H
HETATM	31	H	0	-2.918	-2.593	-2.210	H
HETATM	32	C	0	-2.894	-0.543	2.607	C
HETATM	33	H	0	-2.628	-1.585	2.862	H
HETATM	34	H	0	-1.938	0.015	2.578	H
HETATM	35	H	0	-3.491	-0.138	3.440	H
HETATM	36	C	0	-6.786	1.203	-0.073	C
HETATM	37	H	0	-6.568	2.256	-0.332	H
HETATM	38	H	0	-7.472	0.823	-0.850	H
HETATM	39	H	0	-7.330	1.219	0.886	H
HETATM	40	C	0	1.415	-2.671	-2.336	C

HETATM	41	H	0	1.738	-2.109	-3.226	H
HETATM	42	H	0	1.586	-3.747	-2.541	H
HETATM	43	H	0	0.330	-2.512	-2.238	H
HETATM	44	C	0	1.814	-2.254	2.697	C
HETATM	45	H	0	2.011	-3.280	3.067	H
HETATM	46	H	0	2.270	-1.553	3.414	H
HETATM	47	H	0	0.728	-2.083	2.726	H
HETATM	48	C	0	5.800	-1.419	-0.241	C
HETATM	49	H	0	5.949	-0.322	-0.266	H
HETATM	50	H	0	6.399	-1.798	0.605	H
HETATM	51	H	0	6.230	-1.818	-1.174	H
HETATM	52	H	0	-2.615	-3.783	-0.235	H
HETATM	53	H	0	-0.286	-4.316	-0.463	H
HETATM	54	C	0	1.663	3.010	-0.527	C
HETATM	55	C	0	-1.361	1.408	-0.115	C
HETATM	56	F	0	3.045	1.551	-1.688	F
HETATM	57	F	0	1.068	3.364	-1.650	F
HETATM	58	F	0	-2.252	1.489	-1.076	F
HETATM	59	F	0	-1.721	2.300	0.785	F
HETATM	60	Cl	0	1.235	3.930	0.838	Cl
HETATM	61	Cl	0	3.621	1.681	0.796	Cl

END

at5e.pdb

TITLE	at5e.pdb						
HETATM	1	Ru	0	-0.255	0.409	0.015	Ru
HETATM	2	C	0	0.196	-3.726	0.216	C
HETATM	3	C	0	1.681	-3.408	0.055	C
HETATM	4	H	0	-0.193	-4.388	-0.580	H
HETATM	5	H	0	2.098	-3.768	-0.906	H
HETATM	6	C	0	0.488	-1.396	0.090	C
HETATM	7	N	0	1.725	-1.941	0.094	N
HETATM	8	N	0	-0.420	-2.407	0.133	N
HETATM	9	Cl	0	-0.716	0.482	-2.324	Cl
HETATM	10	Cl	0	-0.448	0.561	2.394	Cl
HETATM	11	C	0	-2.744	2.168	0.124	C
HETATM	12	C	0	2.975	-1.262	0.022	C
HETATM	13	C	0	3.700	-1.057	1.210	C
HETATM	14	C	0	3.478	-0.853	-1.225	C
HETATM	15	C	0	4.949	-0.438	1.130	C
HETATM	16	C	0	4.725	-0.216	-1.259	C
HETATM	17	C	0	5.473	-0.006	-0.096	C
HETATM	18	H	0	5.519	-0.269	2.053	H
HETATM	19	H	0	5.123	0.115	-2.226	H
HETATM	20	C	0	-1.827	-2.175	0.038	C
HETATM	21	C	0	-2.595	-1.989	1.209	C
HETATM	22	C	0	-2.435	-2.169	-1.238	C
HETATM	23	C	0	-3.946	-1.652	1.068	C
HETATM	24	C	0	-3.789	-1.837	-1.326	C
HETATM	25	C	0	-4.549	-1.542	-0.189	C
HETATM	26	H	0	-4.542	-1.477	1.973	H
HETATM	27	H	0	-4.260	-1.800	-2.317	H
HETATM	28	C	0	3.092	-1.412	2.532	C
HETATM	29	H	0	3.785	-1.204	3.363	H
HETATM	30	H	0	2.167	-0.829	2.708	H
HETATM	31	H	0	2.805	-2.478	2.600	H
HETATM	32	C	0	2.691	-1.068	-2.480	C
HETATM	33	H	0	2.334	-2.110	-2.574	H
HETATM	34	H	0	1.786	-0.430	-2.519	H
HETATM	35	H	0	3.294	-0.839	-3.374	H
HETATM	36	C	0	6.794	0.699	-0.152	C

HETATM	37	H	0	6.679	1.781	0.047	H
HETATM	38	H	0	7.501	0.313	0.602	H
HETATM	39	H	0	7.269	0.607	-1.144	H
HETATM	40	C	0	-2.033	-2.250	2.572	C
HETATM	41	H	0	-2.430	-1.541	3.315	H
HETATM	42	H	0	-2.316	-3.269	2.905	H
HETATM	43	H	0	-0.936	-2.170	2.607	H
HETATM	44	C	0	-1.689	-2.590	-2.466	C
HETATM	45	H	0	-1.845	-3.671	-2.657	H
HETATM	46	H	0	-2.043	-2.045	-3.355	H
HETATM	47	H	0	-0.605	-2.414	-2.392	H
HETATM	48	C	0	-5.976	-1.104	-0.315	C
HETATM	49	H	0	-6.042	-0.003	-0.408	H
HETATM	50	H	0	-6.462	-1.526	-1.211	H
HETATM	51	H	0	-6.575	-1.383	0.568	H
HETATM	52	H	0	2.307	-3.832	0.860	H
HETATM	53	H	0	-0.040	-4.200	1.189	H
HETATM	54	C	0	-1.757	3.064	-0.088	C
HETATM	55	C	0	1.279	1.374	0.002	C
HETATM	56	F	0	-3.200	1.841	1.302	F
HETATM	57	F	0	-1.484	3.456	-1.317	F
HETATM	58	F	0	-3.429	1.637	-0.855	F
HETATM	59	Cl	0	-0.969	3.916	1.160	Cl
HETATM	60	F	0	2.239	1.369	0.902	F
HETATM	61	Cl	0	1.631	2.666	-1.130	Cl

END

at5f.pdb

TITLE	at5f.pdb						
HETATM	1	Ru	0	0.131	0.511	-0.009	Ru
HETATM	2	Cl	0	0.955	0.365	2.265	Cl
HETATM	3	Cl	0	-0.603	0.383	-2.309	Cl
HETATM	4	C	0	-0.015	-1.555	-0.058	C
HETATM	5	N	0	1.061	-2.346	-0.149	N
HETATM	6	C	0	0.697	-3.758	-0.308	C
HETATM	7	C	0	-0.828	-3.731	-0.162	C
HETATM	8	N	0	-1.129	-2.295	-0.089	N
HETATM	9	C	0	2.392	-1.823	-0.116	C
HETATM	10	C	0	3.104	-1.863	1.101	C
HETATM	11	C	0	4.343	-1.228	1.165	C
HETATM	12	C	0	4.887	-0.563	0.056	C
HETATM	13	C	0	4.192	-0.598	-1.153	C
HETATM	14	C	0	2.947	-1.236	-1.271	C
HETATM	15	C	0	-2.450	-1.754	-0.023	C
HETATM	16	C	0	-3.228	-1.672	-1.192	C
HETATM	17	C	0	-4.488	-1.069	-1.106	C
HETATM	18	C	0	-4.983	-0.567	0.102	C
HETATM	19	C	0	-4.206	-0.711	1.258	C
HETATM	20	C	0	-2.944	-1.311	1.220	C
HETATM	21	C	0	2.552	-2.575	2.297	C
HETATM	22	C	0	6.172	0.195	0.183	C
HETATM	23	C	0	2.297	-1.319	-2.619	C
HETATM	24	C	0	-2.755	-2.235	-2.497	C
HETATM	25	C	0	-6.308	0.130	0.158	C
HETATM	26	C	0	-2.147	-1.497	2.475	C
HETATM	27	H	0	1.197	-4.373	0.462	H
HETATM	28	H	0	1.033	-4.123	-1.297	H
HETATM	29	H	0	-1.184	-4.237	0.754	H
HETATM	30	H	0	-1.354	-4.187	-1.019	H
HETATM	31	H	0	4.887	-1.224	2.118	H
HETATM	32	H	0	4.622	-0.118	-2.041	H

HETATM	33	H	0	-5.094	-0.980	-2.017	H
HETATM	34	H	0	-4.589	-0.348	2.220	H
HETATM	35	H	0	2.999	-2.190	3.228	H
HETATM	36	H	0	1.460	-2.443	2.387	H
HETATM	37	H	0	2.765	-3.662	2.258	H
HETATM	38	H	0	5.992	1.201	0.609	H
HETATM	39	H	0	6.665	0.343	-0.793	H
HETATM	40	H	0	6.885	-0.308	0.858	H
HETATM	41	H	0	2.031	-0.322	-3.009	H
HETATM	42	H	0	1.364	-1.904	-2.618	H
HETATM	43	H	0	2.992	-1.778	-3.346	H
HETATM	44	H	0	-1.657	-2.264	-2.568	H
HETATM	45	H	0	-3.114	-1.627	-3.344	H
HETATM	46	H	0	-3.141	-3.263	-2.652	H
HETATM	47	H	0	-6.182	1.229	0.124	H
HETATM	48	H	0	-6.854	-0.094	1.091	H
HETATM	49	H	0	-6.956	-0.143	-0.692	H
HETATM	50	H	0	-1.213	-0.902	2.487	H
HETATM	51	H	0	-2.733	-1.203	3.362	H
HETATM	52	H	0	-1.843	-2.552	2.612	H
HETATM	53	C	0	-1.330	1.620	0.428	C
HETATM	54	Cl	0	-1.855	2.092	2.013	Cl
HETATM	55	F	0	-2.247	1.989	-0.429	F
HETATM	56	C	0	0.425	2.794	-0.054	C
HETATM	57	C	0	1.553	1.947	-0.422	C
HETATM	58	F	0	0.576	3.410	1.118	F
HETATM	59	Cl	0	-0.248	3.832	-1.276	Cl
HETATM	60	F	0	2.619	2.008	0.372	F
HETATM	61	F	0	1.969	1.963	-1.689	F

END

at5PB.pdb

TITLE	at5PB.pdb						
HETATM	1	Ru	0	0.029	0.454	-0.012	Ru
HETATM	2	C	0	1.048	-3.700	-0.147	C
HETATM	3	C	0	-0.475	-3.801	0.007	C
HETATM	4	H	0	1.601	-4.214	0.659	H
HETATM	5	H	0	-0.784	-4.292	0.949	H
HETATM	6	C	0	0.149	-1.570	-0.022	C
HETATM	7	N	0	-0.901	-2.394	0.013	N
HETATM	8	N	0	1.294	-2.255	-0.083	N
HETATM	9	Cl	0	0.857	0.319	2.260	Cl
HETATM	10	Cl	0	-0.707	0.337	-2.301	Cl
HETATM	11	C	0	1.246	1.930	-0.384	C
HETATM	12	C	0	-2.258	-1.934	0.008	C
HETATM	13	C	0	-2.976	-1.912	-1.203	C
HETATM	14	C	0	-2.835	-1.490	1.215	C
HETATM	15	C	0	-4.251	-1.341	-1.202	C
HETATM	16	C	0	-4.114	-0.926	1.165	C
HETATM	17	C	0	-4.822	-0.817	-0.037	C
HETATM	18	H	0	-4.805	-1.288	-2.148	H
HETATM	19	H	0	-4.562	-0.554	2.095	H
HETATM	20	C	0	2.586	-1.640	-0.107	C
HETATM	21	C	0	3.064	-1.068	-1.302	C
HETATM	22	C	0	3.349	-1.605	1.079	C
HETATM	23	C	0	4.282	-0.376	-1.263	C
HETATM	24	C	0	4.558	-0.911	1.067	C
HETATM	25	C	0	5.028	-0.269	-0.088	C
HETATM	26	H	0	4.657	0.082	-2.187	H
HETATM	27	H	0	5.145	-0.856	1.992	H
HETATM	28	C	0	-2.417	-2.509	-2.458	C

HETATM	29	H	0	-2.834	-2.016	-3.351	H
HETATM	30	H	0	-1.321	-2.405	-2.520	H
HETATM	31	H	0	-2.668	-3.586	-2.535	H
HETATM	32	C	0	-2.119	-1.633	2.522	C
HETATM	33	H	0	-1.741	-2.661	2.673	H
HETATM	34	H	0	-1.242	-0.963	2.608	H
HETATM	35	H	0	-2.791	-1.398	3.364	H
HETATM	36	C	0	-6.151	-0.129	-0.080	C
HETATM	37	H	0	-6.025	0.953	-0.279	H
HETATM	38	H	0	-6.798	-0.525	-0.881	H
HETATM	39	H	0	-6.693	-0.213	0.877	H
HETATM	40	C	0	2.338	-1.197	-2.606	C
HETATM	41	H	0	3.049	-1.424	-3.419	H
HETATM	42	H	0	1.566	-1.984	-2.595	H
HETATM	43	H	0	1.811	-0.267	-2.884	H
HETATM	44	C	0	2.902	-2.316	2.320	C
HETATM	45	H	0	3.281	-3.357	2.345	H
HETATM	46	H	0	3.284	-1.812	3.223	H
HETATM	47	H	0	1.805	-2.347	2.412	H
HETATM	48	C	0	6.297	0.526	-0.051	C
HETATM	49	H	0	6.115	1.542	0.346	H
HETATM	50	H	0	7.056	0.065	0.605	H
HETATM	51	H	0	6.738	0.648	-1.055	H
HETATM	52	H	0	-0.962	-4.337	-0.826	H
HETATM	53	H	0	1.414	-4.100	-1.112	H
HETATM	54	C	0	-0.127	2.732	0.070	C
HETATM	55	C	0	-1.367	1.783	0.417	C
HETATM	56	F	0	2.251	2.262	0.414	F
HETATM	57	F	0	1.642	2.190	-1.626	F
HETATM	58	F	0	0.226	3.427	1.167	F
HETATM	59	F	0	-2.394	1.917	-0.421	F
HETATM	60	Cl	0	-1.998	2.002	2.048	Cl
HETATM	61	Cl	0	-0.592	3.857	-1.223	Cl

END

at5g.pdb

TITLE	at5g.pdb						
HETATM	1	Ru	0	0.017	0.510	-0.021	Ru
HETATM	2	Cl	0	-0.733	0.381	-2.308	Cl
HETATM	3	Cl	0	0.837	0.370	2.258	Cl
HETATM	4	C	0	0.159	-1.548	-0.013	C
HETATM	5	N	0	-0.882	-2.386	0.032	N
HETATM	6	C	0	-0.454	-3.790	0.040	C
HETATM	7	C	0	1.072	-3.684	-0.063	C
HETATM	8	N	0	1.306	-2.235	-0.056	N
HETATM	9	C	0	-2.243	-1.940	0.006	C
HETATM	10	C	0	-2.947	-1.938	-1.214	C
HETATM	11	C	0	-4.235	-1.398	-1.231	C
HETATM	12	C	0	-4.833	-0.885	-0.074	C
HETATM	13	C	0	-4.135	-0.966	1.135	C
HETATM	14	C	0	-2.843	-1.499	1.202	C
HETATM	15	C	0	2.602	-1.629	-0.078	C
HETATM	16	C	0	3.357	-1.564	1.109	C
HETATM	17	C	0	4.578	-0.886	1.080	C
HETATM	18	C	0	5.065	-0.295	-0.092	C
HETATM	19	C	0	4.325	-0.435	-1.270	C
HETATM	20	C	0	3.098	-1.108	-1.290	C
HETATM	21	C	0	-2.356	-2.521	-2.461	C
HETATM	22	C	0	-6.183	-0.240	-0.135	C
HETATM	23	C	0	-2.136	-1.621	2.518	C
HETATM	24	C	0	2.901	-2.231	2.371	C

HETATM	25	C	0	6.347	0.480	-0.080	C
HETATM	26	C	0	2.359	-1.278	-2.582	C
HETATM	27	H	0	-0.910	-4.329	-0.809	H
HETATM	28	H	0	-0.794	-4.284	0.969	H
HETATM	29	H	0	1.477	-4.127	-0.992	H
HETATM	30	H	0	1.598	-4.156	0.787	H
HETATM	31	H	0	-4.780	-1.363	-2.183	H
HETATM	32	H	0	-4.602	-0.599	2.058	H
HETATM	33	H	0	5.160	-0.808	2.007	H
HETATM	34	H	0	4.715	-0.021	-2.208	H
HETATM	35	H	0	-2.774	-2.040	-3.360	H
HETATM	36	H	0	-1.263	-2.388	-2.509	H
HETATM	37	H	0	-2.577	-3.605	-2.541	H
HETATM	38	H	0	-6.093	0.840	-0.360	H
HETATM	39	H	0	-6.816	-0.677	-0.926	H
HETATM	40	H	0	-6.724	-0.320	0.823	H
HETATM	41	H	0	-2.812	-1.367	3.350	H
HETATM	42	H	0	-1.255	-0.957	2.596	H
HETATM	43	H	0	-1.768	-2.650	2.690	H
HETATM	44	H	0	1.803	-2.290	2.442	H
HETATM	45	H	0	3.247	-1.677	3.259	H
HETATM	46	H	0	3.310	-3.258	2.449	H
HETATM	47	H	0	6.166	1.541	0.176	H
HETATM	48	H	0	6.844	0.471	-1.065	H
HETATM	49	H	0	7.059	0.092	0.668	H
HETATM	50	H	0	1.573	-0.512	-2.727	H
HETATM	51	H	0	3.049	-1.207	-3.438	H
HETATM	52	H	0	1.840	-2.251	-2.645	H
HETATM	53	C	0	1.342	1.809	-0.419	C
HETATM	54	F	0	1.701	2.126	-1.642	F
HETATM	55	F	0	2.278	2.246	0.386	F
HETATM	56	C	0	-0.270	2.763	0.099	C
HETATM	57	C	0	-1.419	1.864	0.440	C
HETATM	58	Cl	0	-0.583	3.846	-1.249	Cl
HETATM	59	F	0	0.219	3.432	1.150	F
HETATM	60	F	0	-2.449	1.902	-0.411	F
HETATM	61	Cl	0	-2.052	1.975	2.076	Cl

END

at5h.pdb

TITLE	at5h.pdb						
HETATM	1	Ru	0	-0.173	0.349	0.033	Ru
HETATM	2	C	0	0.681	-3.713	0.118	C
HETATM	3	C	0	2.137	-3.242	0.072	C
HETATM	4	H	0	0.416	-4.376	-0.726	H
HETATM	5	H	0	2.661	-3.550	-0.853	H
HETATM	6	C	0	0.745	-1.364	0.054	C
HETATM	7	N	0	2.028	-1.779	0.115	N
HETATM	8	N	0	-0.059	-2.460	0.041	N
HETATM	9	Cl	0	-0.688	0.595	-2.285	Cl
HETATM	10	Cl	0	-0.222	0.398	2.430	Cl
HETATM	11	C	0	-2.867	2.097	0.210	C
HETATM	12	C	0	3.194	-0.964	0.026	C
HETATM	13	C	0	3.916	-0.672	1.196	C
HETATM	14	C	0	3.616	-0.498	-1.233	C
HETATM	15	C	0	5.083	0.088	1.085	C
HETATM	16	C	0	4.782	0.273	-1.298	C
HETATM	17	C	0	5.527	0.572	-0.152	C
HETATM	18	H	0	5.651	0.326	1.995	H
HETATM	19	H	0	5.119	0.643	-2.275	H
HETATM	20	C	0	-1.474	-2.331	-0.103	C

HETATM	21	C	0	-2.297	-2.233	1.039	C
HETATM	22	C	0	-2.027	-2.296	-1.404	C
HETATM	23	C	0	-3.659	-1.975	0.850	C
HETATM	24	C	0	-3.390	-2.027	-1.541	C
HETATM	25	C	0	-4.212	-1.828	-0.425	C
HETATM	26	H	0	-4.302	-1.866	1.734	H
HETATM	27	H	0	-3.816	-1.952	-2.549	H
HETATM	28	C	0	3.388	-1.091	2.532	C
HETATM	29	H	0	4.069	-0.794	3.346	H
HETATM	30	H	0	2.402	-0.624	2.725	H
HETATM	31	H	0	3.235	-2.184	2.610	H
HETATM	32	C	0	2.822	-0.798	-2.468	C
HETATM	33	H	0	2.543	-1.866	-2.537	H
HETATM	34	H	0	1.870	-0.230	-2.497	H
HETATM	35	H	0	3.387	-0.539	-3.378	H
HETATM	36	C	0	6.759	1.422	-0.240	C
HETATM	37	H	0	6.523	2.490	-0.071	H
HETATM	38	H	0	7.509	1.142	0.519	H
HETATM	39	H	0	7.235	1.356	-1.233	H
HETATM	40	C	0	-1.776	-2.475	2.422	C
HETATM	41	H	0	-2.212	-1.765	3.143	H
HETATM	42	H	0	-2.049	-3.496	2.758	H
HETATM	43	H	0	-0.684	-2.368	2.495	H
HETATM	44	C	0	-1.190	-2.590	-2.610	C
HETATM	45	H	0	-1.147	-3.682	-2.799	H
HETATM	46	H	0	-1.609	-2.116	-3.511	H
HETATM	47	H	0	-0.155	-2.227	-2.507	H
HETATM	48	C	0	-5.645	-1.427	-0.593	C
HETATM	49	H	0	-5.732	-0.325	-0.652	H
HETATM	50	H	0	-6.084	-1.829	-1.522	H
HETATM	51	H	0	-6.271	-1.751	0.256	H
HETATM	52	H	0	2.737	-3.607	0.924	H
HETATM	53	H	0	0.432	-4.251	1.053	H
HETATM	54	C	0	-1.906	3.049	0.251	C
HETATM	55	C	0	1.294	1.435	-0.022	C
HETATM	56	F	0	-3.435	1.745	-0.925	F
HETATM	57	F	0	-1.394	3.451	1.396	F
HETATM	58	F	0	2.181	1.638	0.926	F
HETATM	59	F	0	1.610	2.270	-0.992	F
HETATM	60	Cl	0	-1.392	3.917	-1.120	Cl
HETATM	61	Cl	0	-3.553	1.406	1.609	Cl

END