Supplementary Information

Structural Insight into Inhibition of REV7 Protein Interaction Revealed by Docking, Molecular Dynamics and MM/PBSA Studies

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Table S1: The GAFF atom type, atom name, charge and mass for all the atoms of compound **7** generated using ACPYPE.

Atom number	Atom type	Atom name	Charge	Mass
1	c	C1	0.735099	12.01
2	n	N1	-0.3963	14.01
3	cc	C2	0.4898	12.01
4	nd	N2	-0.594101	14.01
5	cd	C3	0.1363	12.01
6	cc	C4	-0.2106	12.01
7	ss	S1	0.1372	32.06
8	cd	C5	-0.2111	12.01
9	cc	C6	-0.0605	12.01
10	o	O1	-0.595501	16
11	c3	C11	0.081	12.01
12	c3	C12	-0.0807	12.01
13	c3	C13	-0.1019	12.01
14	c3	C14	0.085	12.01
15	n	N3	-0.4648	14.01
16	c3	C15	0.085	12.01
17	c	C17	0.654101	12.01
18	c3	C16	-0.1019	12.01
19	o	O3	-0.603101	16
20	c3	C18	-0.1701	12.01
21	cc	C7	0.2932	12.01
22	os	O2	-0.3128	16
23	cc	C8	0.27	12.01
24	cd	C9	-0.2783	12.01
25	c3	C19	-0.1364	12.01
26	cd	C10	-0.2323	12.01
27	h5	H2	0.0538	1.008
28	h4	H5	0.181	1.008
29	h1	H112	0.0722	1.008
30	h1	H113	0.0722	1.008
31	hc	H12	0.0497	1.008
32	hc	H132	0.05695	1.008
33	hc	H133	0.05695	1.008
34	h1	H142	0.0587	1.008
35	h1	H143	0.0587	1.008
36	h1	H152	0.0587	1.008
37	h1	H153	0.0587	1.008
38	hc	H162	0.05695	1.008
39	hc	H163	0.05695	1.008
40	hc	H181	0.065367	1.008
41	hc	H182	0.065367	1.008

42	hc	H183	0.065367	1.008
43	ha	H9	0.159	1.008
44	hc	H191	0.060367	1.008
45	hc	H192	0.060367	1.008
46	hc	H193	0.060367	1.008
47	ha	H10	0.156	1.008

Table S2: The GAFF atom type, atom name, charge and mass for all the atoms of compound **13** generated using ACPYPE.

Atom number	Atom type	Atom name	Charge	Mass
1	c	C1	0.729101	12.01
2	n	N1	-0.3993	14.01
3	cc	C2	0.4908	12.01
4	nd	N2	-0.584101	14.01
5	cd	C3	0.1373	12.01
6	cc	C4	-0.2126	12.01
7	ss	S1	0.1512	32.06
8	cd	C5	-0.2101	12.01
9	cc	C6	-0.0645	12.01
10	o	O1	-0.610501	16
11	c3	C12	0.095	12.01
12	cy	C13	-0.1307	12.01
13	cy	C14	0.0635	12.01
14	n	N3	-0.4438	14.01
15	cy	C15	0.0635	12.01
16	c	C16	0.641101	12.01
17	c3	C17	-0.1721	12.01
18	o	O3	-0.592101	16
19	cc	C7	0.2962	12.01
20	os	O2	-0.3168	16
21	cc	C8	0.267	12.01
22	cd	C9	-0.2763	12.01
23	c3	C11	-0.1354	12.01
24	cd	C10	-0.2333	12.01
25	h5	H2	0.0578	1.008
26	h4	H5	0.182	1.008
27	h1	H122	0.0732	1.008
28	h1	H123	0.0732	1.008
29	hc	H13	0.0787	1.008
30	h1	H142	0.0697	1.008
31	h1	H143	0.0697	1.008
32	h1	H152	0.0697	1.008
33	h1	H153	0.0697	1.008
34	hc	H171	0.068033	1.008

35	hc	H172	0.068033	1.008
36	hc	H173	0.068033	1.008
37	ha	H9	0.16	1.008
38	hc	H111	0.060367	1.008
39	hc	H112	0.060367	1.008
40	hc	H113	0.060367	1.008
41	ha	H10	0.158	1.008

Table S3: The GAFF atom type, atom name, charge and mass for all the atoms of compound **14R** generated using ACPYPE.

Atom number	Atom type	Atom name	Charge	Mass
1	c	C1	0.732101	12.01
2	n	N1	-0.4003	14.01
3	cc	C2	0.4888	12.01
4	nd	N2	-0.593101	14.01
5	cd	C3	0.1343	12.01
6	cc	C4	-0.2106	12.01
7	ss	S1	0.1412	32.06
8	cd	C5	-0.2101	12.01
9	cc	C6	-0.0615	12.01
10	o	O1	-0.597501	16
11	c3	C12	0.095	12.01
12	c3	C13	-0.0977	12.01
13	c3	C14	0.09	12.01
14	n	N3	-0.4728	14.01
15	c	C15	0.656101	12.01
16	c3	C18	0.085	12.01
17	c3	C16	-0.1701	12.01
18	o	O3	-0.601101	16
19	c3	C17	-0.0894	12.01
20	cc	C7	0.2932	12.01
21	os	O2	-0.3148	16
22	cc	C8	0.27	12.01
23	cd	C9	-0.2773	12.01
24	c3	C11	-0.1364	12.01
25	cd	C10	-0.2313	12.01
26	h5	H2	0.0568	1.008
27	h4	H5	0.182	1.008
28	h1	H122	0.0702	1.008
29	h1	H123	0.0702	1.008
30	hc	H13	0.0877	1.008
31	h1	H142	0.0417	1.008

32	h1	H143	0.0417	1.008
33	h1	H182	0.0587	1.008
34	h1	H183	0.0587	1.008
35	hc	H161	0.066033	1.008
36	hc	H162	0.066033	1.008
37	hc	H163	0.066033	1.008
38	hc	H172	0.0572	1.008
39	hc	H173	0.0572	1.008
40	ha	H9	0.16	1.008
41	hc	H111	0.060367	1.008
42	hc	H112	0.060367	1.008
43	hc	H113	0.060367	1.008
44	ha	H10	0.157	1.008

Table S4: The GAFF atom type, atom name, charge and mass for all the atoms of compound **14S** generated using ACPYPE.

Atom number	Atom type	Atom name	Charge	Mass
1	o	O	-0.600501	16
2	cc	C	-0.0605	12.01
3	cd	C1	-0.2101	12.01
4	ss	S	0.1452	32.06
5	c	C2	0.7321	12.01
6	cc	C3	-0.2086	12.01
7	cd	C4	0.1333	12.01
8	nd	N	-0.591101	14.01
9	cc	C5	0.4868	12.01
10	n	N1	-0.3953	14.01
11	c3	C6	0.091	12.01
12	c3	C7	-0.0907	12.01
13	c3	C8	-0.0984	12.01
14	c3	C9	0.09	12.01
15	n	N2	-0.4738	14.01
16	c	C10	0.658101	12.01
17	c3	C11	0.095	12.01
18	c3	C12	-0.1701	12.01
19	o	O1	-0.601101	16
20	cc	C13	0.2932	12.01
21	cd	C14	-0.2313	12.01
22	cd	C15	-0.2773	12.01
23	cc	C16	0.269	12.01
24	c3	C17	-0.1354	12.01
25	os	O2	-0.3138	16
26	h4	HC	0.182	1.008

27	h5	HC1	0.0518	1.008
28	h1	HC2	0.0707	1.008
29	h1	HC3	0.0707	1.008
30	hc	HC4	0.0657	1.008
31	hc	HC5	0.0697	1.008
32	hc	HC6	0.0697	1.008
33	h1	HC7	0.0592	1.008
34	h1	HC8	0.0592	1.008
35	h1	HC9	0.0367	1.008
36	h1	HC10	0.0367	1.008
37	hc	HC11	0.0647	1.008
38	hc	HC12	0.0647	1.008
39	hc	HC13	0.0647	1.008
40	ha	HC14	0.157	1.008
41	ha	HC15	0.16	1.008
42	hc	HC16	0.060367	1.008
43	hc	HC17	0.060367	1.008
44	hc	HC18	0.060367	1.008

Table S5: The GAFF atom type, atom name, charge and mass for all the atoms of compound **15R** generated using ACPYPE.

Atom number	Atom type	Atom name	Charge	Mass
1	c	C1	0.731102	12.01
2	n	N1	-0.4003	14.01
3	cc	C2	0.4858	12.01
4	nd	N2	-0.593101	14.01
5	cd	C3	0.1323	12.01
6	cc	C4	-0.2096	12.01
7	ss	S1	0.1412	32.06
8	cd	C5	-0.2101	12.01
9	cc	C6	-0.0605	12.01
10	o	O1	-0.593501	16
11	c3	C12	0.089	12.01
12	c3	C13	-0.1127	12.01
13	c3	C14	0.087	12.01
14	n	N3	-0.4588	14.01
15	c	C15	0.653101	12.01
16	c3	C17	0.076	12.01
17	c3	C16	-0.1711	12.01
18	o	O3	-0.602101	16
19	c3	C18	-0.1034	12.01
20	c3	C19	-0.0744	12.01

21	cc	C7	0.2922	12.01
22	os	O2	-0.3138	16
23	cc	C8	0.27	12.01
24	cd	C9	-0.2773	12.01
25	c3	C11	-0.1364	12.01
26	cd	C10	-0.2313	12.01
27	h5	H2	0.0548	1.008
28	h4	H5	0.182	1.008
29	h1	H122	0.0717	1.008
30	h1	H123	0.0717	1.008
31	hc	H13	0.0797	1.008
32	h1	H142	0.0477	1.008
33	h1	H143	0.0477	1.008
34	h1	H172	0.0667	1.008
35	h1	H173	0.0667	1.008
36	hc	H161	0.067033	1.008
37	hc	H162	0.067033	1.008
38	hc	H163	0.067033	1.008
39	hc	H182	0.0547	1.008
40	hc	H183	0.0547	1.008
41	hc	H192	0.0462	1.008
42	hc	H193	0.0462	1.008
43	ha	H9	0.16	1.008
44	hc	H111	0.0607	1.008
45	hc	H112	0.0607	1.008
46	hc	H113	0.0607	1.008
47	ha	H10	0.157	1.008

Table S6: The GAFF atom type, atom name, charge and mass for all the atoms of compound **15S** generated using ACPYPE.

Atom number	Atom type	Atom name	Charge	Mass
1	nc	N	-0.594101	14.01
2	cd	C	0.4908	12.01
3	n	N1	-0.3963	14.01
4	cc	C1	0.1383	12.01
5	cd	C2	-0.2116	12.01
6	c	C3	0.732103	12.01
7	ss	S	0.1362	32.06
8	cc	C4	-0.2091	12.01
9	cd	C5	-0.0635	12.01
10	o	O	-0.600501	16
11	c3	C6	0.09	12.01
12	c3	C7	-0.1077	12.01

13	c3	C8	0.076	12.01
14	n	N2	-0.4568	14.01
15	c	C9	0.652101	12.01
16	c3	C10	0.083	12.01
17	c3	C11	-0.1691	12.01
18	o	O1	-0.609101	16
19	c3	C12	-0.1034	12.01
20	c3	C13	-0.0774	12.01
21	cd	C14	0.2962	12.01
22	cc	C15	-0.2343	12.01
23	cc	C16	-0.2773	12.01
24	cd	C17	0.268	12.01
25	os	O2	-0.3148	16
26	c3	C18	-0.1354	12.01
27	h5	HC	0.0598	1.008
28	h4	HC1	0.181	1.008
29	h1	HC2	0.0727	1.008
30	h1	HC3	0.0727	1.008
31	hc	HC4	0.0677	1.008
32	h1	HC5	0.0642	1.008
33	h1	HC6	0.0642	1.008
34	h1	HC7	0.0522	1.008
35	h1	HC8	0.0522	1.008
36	hc	HC9	0.066033	1.008
37	hc	HC10	0.066033	1.008
38	hc	HC11	0.066033	1.008
39	hc	HC12	0.0502	1.008
40	hc	HC13	0.0502	1.008
41	hc	HC14	0.0582	1.008
42	hc	HC15	0.0582	1.008
43	ha	HC16	0.157	1.008
44	ha	HC17	0.159	1.008
45	hc	HC18	0.060033	1.008
46	hc	HC19	0.060033	1.008
47	hc	HC20	0.060033	1.008