Supplementary information

Polarity-determined triple partition of dual binding pockets unlocks mechanistic insights and novel antagonist design of NMDA receptor: a combined MD/DFT study

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Table S1. The molecular docking results of the lead compounds and modified ligands EVT01, EVT02.

ID	Docking scores	Glide energy /kcal·mol^{-1}	Molecular weight	Crucial residues
3689 (Ifenprodil)	-10.121	-99.797	325.4	GLU-236, GLN-110, SER-132, PHE-176
16110243 (Compound A)	-11.448	-93.320	353.4	GLU-236, SER-132, PHE-176, PHE-114
118207404 (Compound B)	-11.216	-98.296	368.4	GLU-236, GLN-110, PHE-176, PHE-114
156328 (Compound C)	-11.457	-87.595	402.5	GLU-236, GLN-110, SER-132, PHE-176
72941990 (EVT-101)	-10.545	-90.207	391.2	ASP-136, TYR-109
134493918 (Compound E)	-10.208	-85.476	370.3	ASP-136, TYR-109
9797323 (Compound F)	-10.206	-86.665	324.3	TYR-109, PHE-114
44415872 (Compound N)	-10.446	-88.502	412.5	ASP-136, PHE-114, SER-132
EVT01	-10.476	-86.404	362.41	ASP-136, PHE-114, TYR-109
EVT02	-10.662	-87.642	302.78	ASP-136, PHE-114, TYR-109, GLN-110

Table S2.

The docking results of 12 molecules through virtual screening.

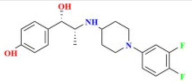
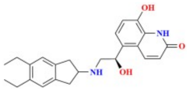
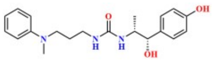
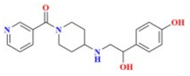
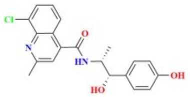
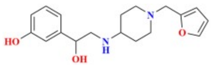
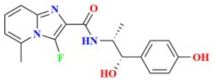
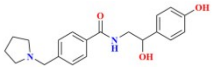
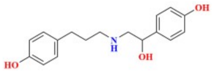
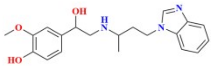
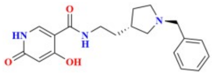
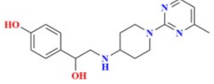
ID	Structure	Docking scores	Glide energy /kcal·mol^{-1}	Molecular weight	Crucial residues
132422327 (IF01)		-13.281	-92.586	362.42	GLU-236 GLN-110 SER-132 PHE-176
6918554 (IF02)		-11.954	-48.478	392.50	GLU-236 GLN-110 SER-132 PHE-176
121503195 (IF03)		-11.690	-99.451	357.45	GLU-236 GLN-110 PHE-176 PHE-114 SER-132
132409872 (IF04)		-11.526	-95.977	341.41	GLU-236 GLN-110 PHE-176 PHE-114
77080364 (IF05)		-11.517	-86.636	370.83	GLU-236 GLN-110 PHE-176 TYR-109
132414677 (IF06)		-11.265	-106.105	316.40	GLU-236 GLN-110 TYR-109 PHE-176 PHE-114
74246339 (IF07)		-10.583	-75.267	343.36	GLU-236 GLN-110 PHE-176
74240710 (IF08)		-10.536	-85.678	340.42	GLU-236 GLN-110 PHE-176 PHE-114
71751913 (IF09)		-10.492	-94.915	287.36	GLU-236 GLN-110 PHE-176 TYR-109
9802645 (IF10)		-10.264	-94.643	355.44	GLU-236 GLN-110 PHE-176 PHE-114
039-221-827 (IF11)		-10.258	-90.049	341.17	GLU-236 GLN-110 PHE-176 PHE-114 TYR-109
72869262 (IF12)		-10.106	-71.249	342.44	GLU-236 GLN-110 SER-132 PHE-176

Table S3.

Original results of G-terminal and central hydrogen bond energies through DFT calculations.

ID_ligand	ID_residue	$E_{complex}$ /Hartree	E_{ligand} /Hartree	$E_{residue}$ /Hartree	E_{H_bond}= $E_{complex}$-($E_{residue}$+E_{ligand}) /kcal·mol^{-1}	$E_{H\_bond\_average}$ /kcal·mol^{-1}
Ifenprodil	GLN-110_1 GLN-110_2 GLN-110_3 GLN-110_4 GLN-110_5	- 1478.690872158- 1478.731176221 - 1478.659689434- 1478.683091530 -1478.703444816	- 1022.126289018- 1022.154053324 - 1022.102123400- 1022.118478124 -1022.139115150	-456.551803341 -456.564701318 -456.547333212 -456.552178710 -456.551513154	-8.02 -7.79 -6.42 -7.80 -8.04	**-7.61**
	GLU-236_1 GLU-236_2 GLU-236_3 GLU-236_4 GLU-236_5	- 1498.103657473- 1498.144214074 - 1498.092144604- 1498.107278081 -1498.128953984	- 1022.126289018- 1022.154053324 - 1022.102123400- 1022.118478124 -1022.139115150	-475.971065259 -475.978687170 -475.978596432 -475.977975624 -475.979838793	-3.96 -7.20 -7.17 -6.79 -6.28	**-6.28**
	SER-132_1 SER-132_2 SER-132_3 SER-132_4 SER-132_5	-1345.877346911 -1345.889941413 -1345.838228793 -1345.860853615 -1345.883691368	-1022.126289018 -1022.154053324 -1022.102123400 -1022.118478124 -1022.139115150	-323.747270337 -323.733570817 -323.733234391 -323.739756625 -323.742625400	-2.38 -1.45 -1.80 -1.64 -1.22	**-1.70**
IF03	GLN-110_1 GLN-110_2 GLN-110_3 GLN-110_4 GLN-110_5	- 1624.912516391- 1624.919230360 -1624.937278926 -1624.914412568 -1624.925316236	-1168.354327950 -1168.353983569 - 1168.373533419- 1168.348189173 -1168.355662226	-456.549077508 -456.557416783 -456.557571066 -456.552140211 -456.560993308	-5.72 -6.91 -5.87 -8.84 -5.43	**-6.55**
	GLU-236_1 GLU-236_2 GLU-236_3 GLU-236_4 GLU-236_5	- 1644.344346462- 1644.330419324 -1644.353175876 - 1644.327813851- 1644.336958818	-1168.354327950 - 1168.353983569- 1168.373533419 - 1168.348189173- 1168.355662226	-475.980938284 -475.971852007 -475.968266202 -475.968857466 -475.979908669	-5.70 -2.88 -7.14 -6.76 -0.87	**-4.67**
	SER-132_1 SER-132_2	-1492.091880832 -1492.100596103	-1168.354327950 -1168.353983569	-323.732771068 -323.742368521	-3.00 -2.66	

	SER-132_3	-1492.117058818	-1168.373533419	-323.738247481	-3.31	
	SER-132_4	-1492.090714503	-1168.348189173	-323.739201884	-2.09	
	SER-132_5	-1492.098011682	-1168.355662226	-323.739339152	-1.89	
IF09	GLN-110_1 GLN-110_2 GLN-110_3 GLN-110_4 GLN-110_5	- 1437.228908753- 1437.242433484 - 1437.243047026- 1437.249190593 -1437.239209764	-980.662133617 -980.668708703 -980.669438507 -980.675069132 -980.670320617	-456.553176079 -456.560773375 -456.562647583 -456.559422132 -456.560000425	-8.53 -8.16 -6.88 -9.22 -5.58	**-7.67**
	GLU-236_1 GLU-236_2 GLU-236_3 GLU-236_4 GLU-236_5	- 1456.650334610- 1456.660586035 - 1456.651949086- 1456.665245108 -1456.656017762	-980.662133617 -980.668708703 -980.669438507 -980.675069132 -980.670320617	-475.980029331 -475.982594422 -475.973360297 -475.981357174 -475.976845510	-5.13 -5.83 -5.74 -5.53 -5.55	**-5.56**
	SER-132_1	-1304.412741528	-980.662133617	-323.745579707	-3.16	**-3.01**
	SER-132_2	-1304.414652552	-980.668708703	-323.740807311	-3.22	
	SER-132_3	-1304.407908329	-980.669438507	-323.734173247	-2.70	
	SER-132_4	-1304.423421588	-980.675069132	-323.744573360	-2.37	
	SER-132_5	-1304.419675710	-980.670320617	-323.743634833	-3.59	

Table S4.

Original results of N-terminal π-π stacking and hydrophobic interaction energies through DFT calculations.

ID_ligand	ID_residue	$E_{complex}$ /Hartree	E_{ligand} /Hartree	$E_{residue}$ /Hartree	$E_{pi\text{-}pi\_stacking}$= $E_{complex}$-($E_{residue}$+E_{ligand}) /kcal·mol^{-1}	$E_{pi\text{-}pi\_stacking\_average}$ /kcal·mol^{-1}
Ifenprodil	ARG-115_1 ARG-115_2 ARG-115_3 ARG-115_4 ARG-115_5	- 1553.939190972- 1553.924368674 - 1553.902292653- 1553.903559605 -1553.937861652	-1022.154053321 -1022.126289011 -1022.102123416 -1022.118478137 -1022.139115140	-531.783051396 -531.796195481 -531.797626573 -531.783762688 -531.797034892	-1.31 -1.18 -1.60 -0.83 -1.07	**-1.20**
	PHE-114_1	-1501.703763058	-1022.154053321	-479.546240293	-2.18	**-1.92**
	PHE-114_2	-1501.672031383	-1022.126289011	-479.542533331	-2.01	
	PHE-114_3	-1501.657210619	-1022.102123416	-479.551093529	-2.51	
	PHE-114_4	-1501.669957199	-1022.118478137	-479.549107024	-1.49	

	PHE-114_5	-1501.691257722	-1022.139115140	-479.549932836	-1.39	
	PHE-176_1	-1501.706159449	-1022.154053321	-479.543937817	-5.13	**-5.09**
	PHE-176_2	-1501.669701355	-1022.126289011	-479.535136244	-5.19	
	PHE-176_3	-1501.651571152	-1022.102123416	-479.540214696	-5.79	
	PHE-176_4	-1501.664735084	-1022.118478137	-479.540156715	-3.83	
	PHE-176_5	-1501.702303333	-1022.139115140	-479.554411309	-5.51	
Compound A	ARG-115_1	-1720.620654454	-1188.825262379	-531.793221340	-1.36	**-1.28**
	ARG-115_2	-1720.582585743	-1188.807938602	-531.774664776	-1.01	
	ARG-115_3	-1720.593719521	-1188.808317232	-531.783811144	-1.00	
	ARG-115_4	-1720.641692183	-1188.841772482	-531.798586310	-1.84	
	ARG-115_5	-1720.637202181	-1188.830595556	-531.804689226	-1.20	
	PHE-176_1	-1668.373019587	-1188.825262379	-479.538661217	-5.71	**-5.40**
	PHE-176_2	-1668.347916871	-1188.807938602	-479.530685102	-5.83	
	PHE-176_3	-1668.361428019	-1188.808317232	-479.546275538	-4.29	
	PHE-176_4	-1668.404056703	-1188.841772482	-479.553283266	-5.65	
	PHE-176_5	-1668.385814133	-1188.830595556	-479.546485239	-5.48	
IF03	PHE-114_1	-1647.912319123	-1168.354327945	-479.553561238	-2.78	**-2.64**
	PHE-114_2	-1647.913310448	-1168.353983564	-479.554176728	-3.23	
	PHE-114_3	-1647.932674576	-1168.373533419	-479.556250031	-1.81	
	PHE-114_4	-1647.898122994	-1168.348189165	-479.545816489	-2.58	
	PHE-114_5	-1647.909070225	-1168.355662228	-479.548948377	-2.80	

Table S5.

Original results of hybrid interaction energies in secondary binding pocket through DFT calculations.

ID_ligand	**ID_residue**	$E_{complex}$ **/Hartree**	E_{ligand} **/Hartree**	$E_{residue}$ **/Hartree**	$E_{pi\text{-}pi\_stacking} = E_{complex} - (E_{residue} + E_{ligand})$ **/kcal·mol^{-1}**	$E_{pi\text{-}pi\_stacking\_average}$ **/kcal·mol^{-1}**
EVT-101	TYR-109_1	-1691.426824500	-1136.603228731	-554.800343909	-7.18	**-6.92**
	TYR-109_2	-1691.420431739	-1136.606147368	-554.802358211	-8.66	
	TYR-109_3	-1691.417925636	-1136.597298944	-554.785091708	-6.01	
	TYR-109_4	-1691.397905795	-1136.614067386	-554.799736794	-5.24	
	TYR-109_5	-1691.405385270	-1136.610660221	-554.797034892	-7.50	
	ASP-138_1	-1573.285376699	-1136.603228731	-436.679218115	-3.78	**-2.66**
	ASP-138_2	-1573.282727571	-1136.606147368	-436.673226154	-2.01	
	ASP-138_3	-1573.275497623	-1136.597298944	-436.675210355	-2.69	
	ASP-138_4	-1573.291397032	-1136.614067386	-436.659338867	-2.79	

	ASP-138_5	-1573.290542676	-1136.610660221	-436.671509105	-2.04	
Compound F	ASP-136_1	-1615.468568047	-1178.797231744	-436.667824080	-2.35	**-1.89**
	ASP-136_2	-1615.453718588	-1178.791490118	-436.675037238	-1.28	
	ASP-136_3	-1615.462249565	-1178.785116924	-436.673750812	-1.24	
	ASP-136_4	-1615.458381456	-1178.786808047	-436.673033395	-2.13	
	ASP-136_5	-1615.468162257	-1178.796165852	-436.665208377	-2.43	
	ASP-138_1	-1615.474151490	-1178.797231744	-436.678172280	-0.50	**-1.48**
	ASP-138_2	-1615.472475640	-1178.791490118	-436.673307611	-2.42	
	ASP-138_3	-1615.460914293	-1178.785116924	-436.677131043	-0.93	
	ASP-138_4	-1615.476886436	-1178.786808047	-436.668956078	-0.46	
	ASP-138_5	-1615.44518642	-1178.796165852	-436.662205331	-3.11	
EVT02	GLN-110_1	-1776.096019321	-1319.550788844	-456.553934013	-6.22	**-8.63**
	GLN-110_2	-1776.126438243	-1319.542959500	-456.561496714	-8.69	
	GLN-110_3	-1776.105910380	-1319.558063512	-456.546757408	-5.86	
	GLN-110_4	-1776.111106857	-1319.542805108	-456.553819154	-13.52	
	GLN-110_5	-1776.125842287	-1319.532294638	-456.553614782	-8.88	

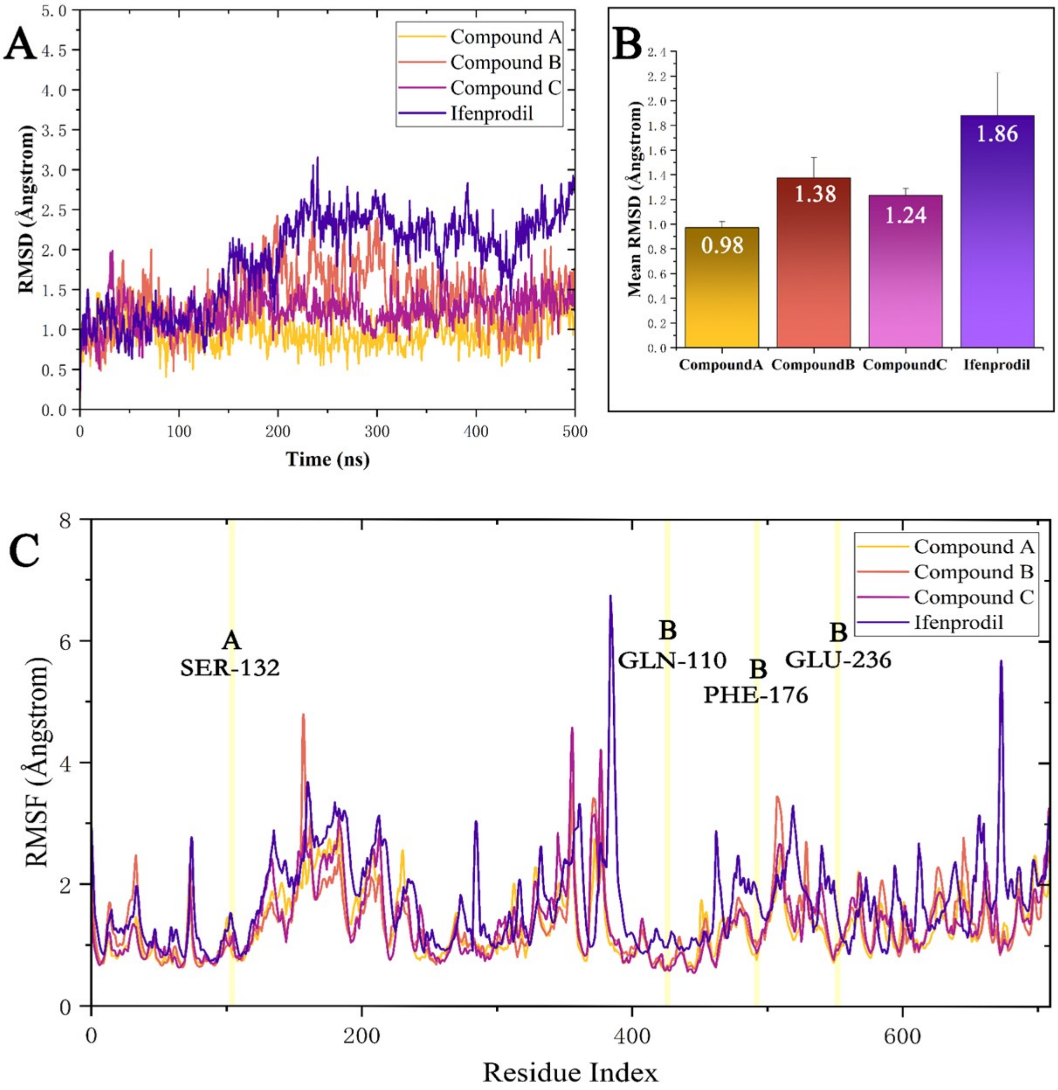


Fig.S1. RMSD and RMSF curves for ifenprodil, compound A, compound B and compound C during 500 ns MD simulations. (A) RMSD curves for ifenprodil, compound A, compound B and compound C. (B) Mean RMSD values, with error bars upon columns representing the standard errors. (C) Fluctuation of RMSF values for ifenprodil, compound A, compound B and compound C, with key residues we recognized highlighted. The chains where key residues located were marked upon.

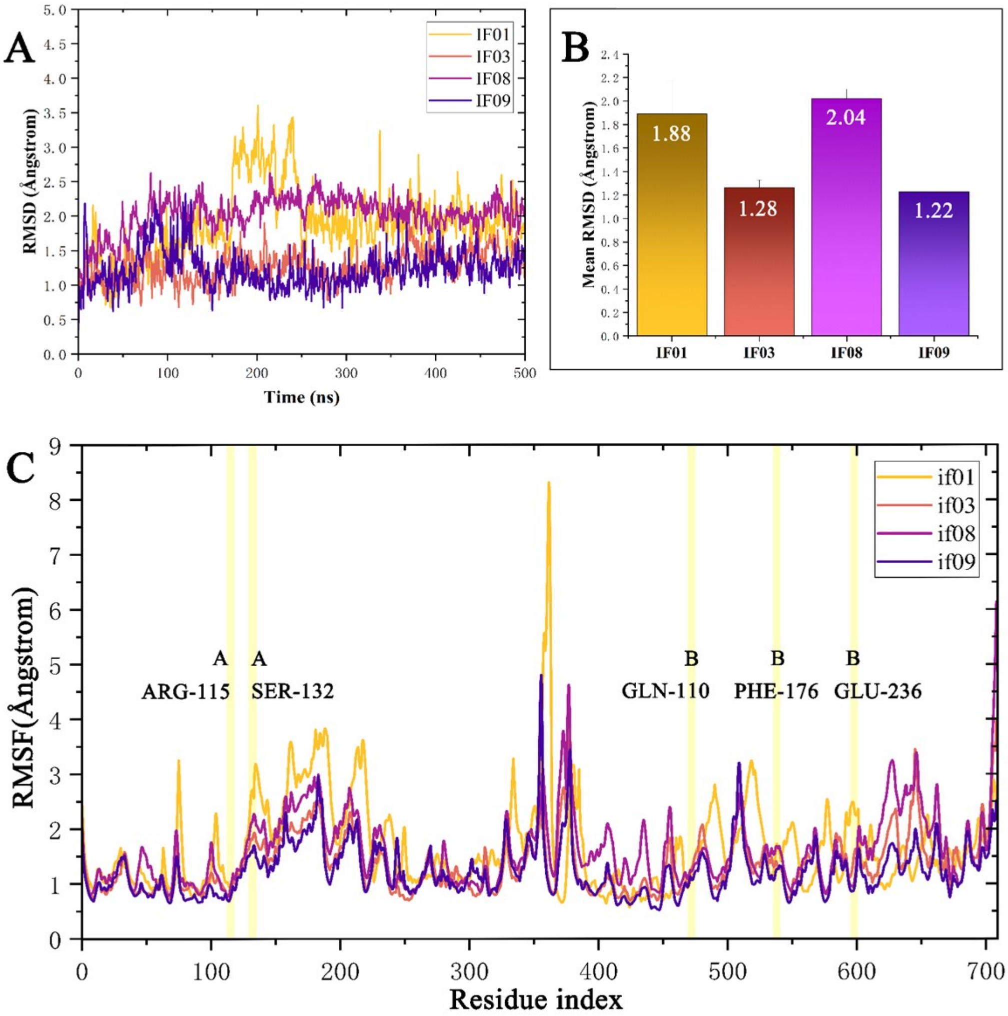


Fig.S2. RMSD and RMSF curves during 500 ns MD simulations. (A) RMSD curves for IF01, IF03, IF08 and IF09. (B) Mean RMSD values, with error bars upon columns representing the standard errors. (C) Fluctuation of RMSF values for IF01, IF03, IF08 and IF09, with key residues we recognized highlighted. The chains where key residues located were marked upon.

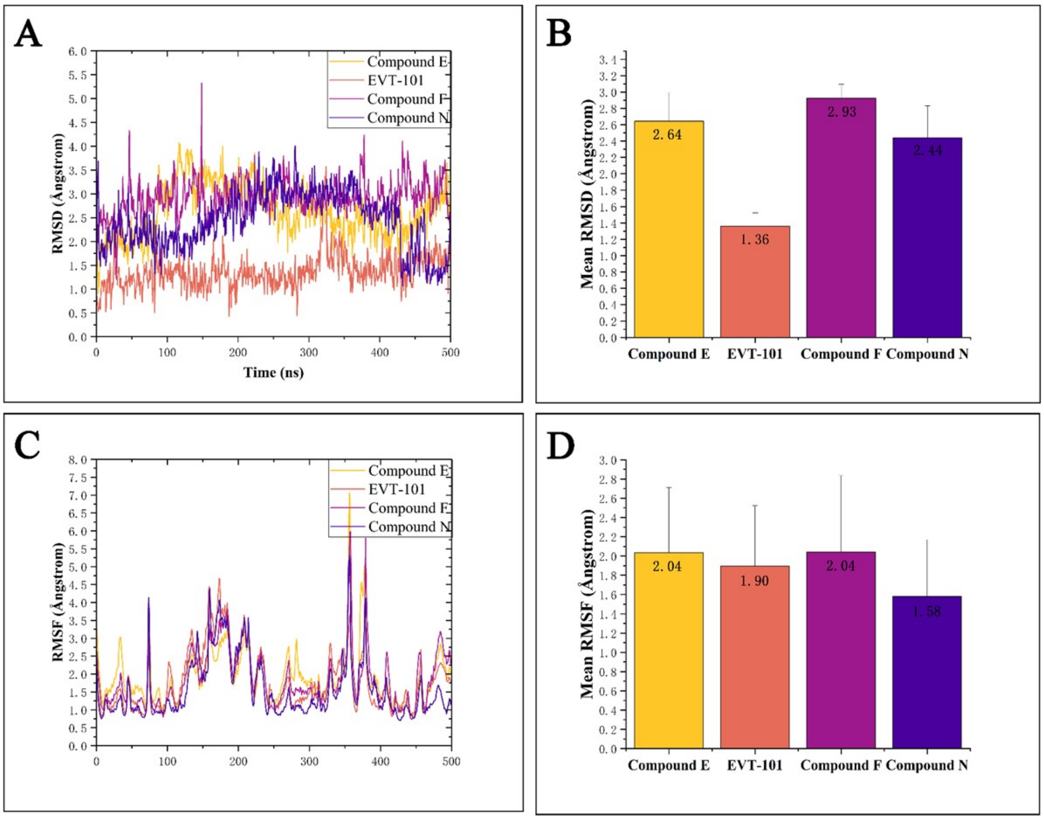


Fig.S3. RMSD and RMSF curves during 500 ns MD simulations. (A) RMSD curves for EVT-101, compound E, compound F, compound N. (B) Mean RMSD values, with error bars upon columns representing the standard errors. (C) Fluctuation of RMSF values for EVT-101, compound E, compound F, compound N. (D) Mean RMSF values, with error bars upon columns representing the standard errors.

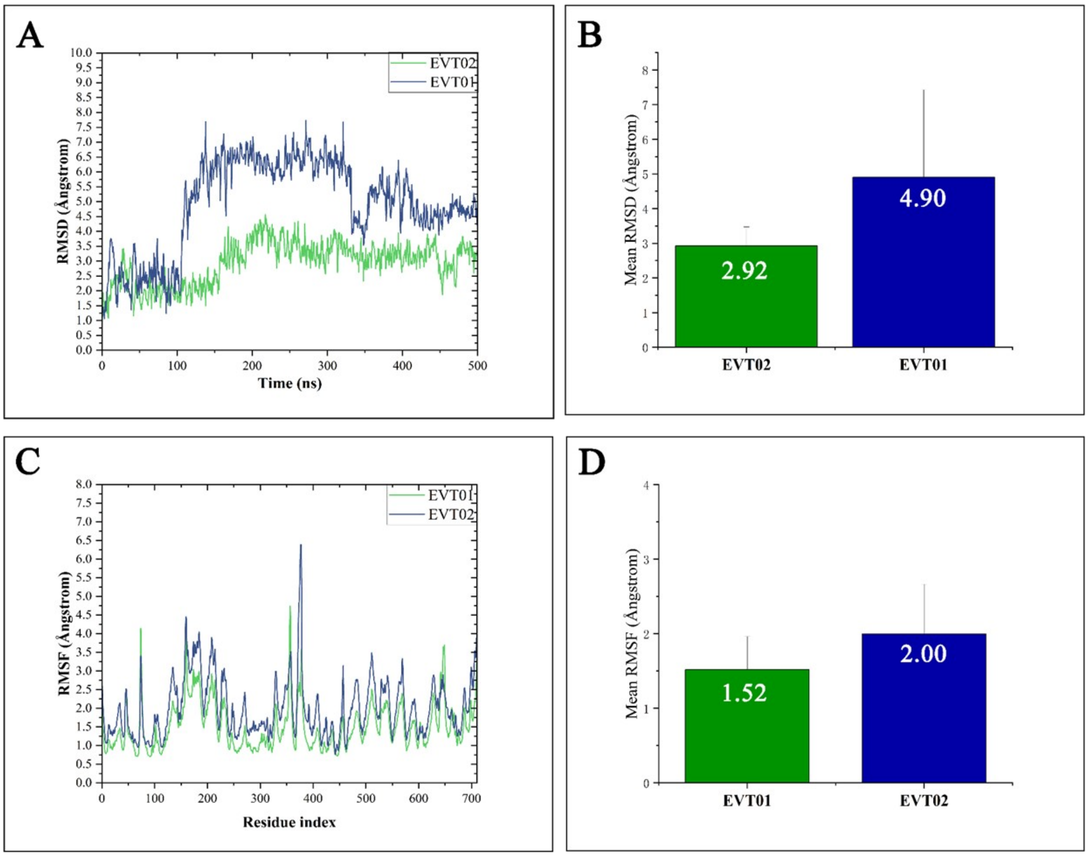


Fig.S4. RMSD and RMSF curves during 500 ns MD simulations. (A) RMSD curves for EVT01 and EVT02. (B) Mean RMSD values, with error bars upon columns representing the standard errors. (C) Fluctuation of RMSF values for EVT01 and EVT02. (D) Mean RMSF values, with error bars upon columns representing the standard errors.

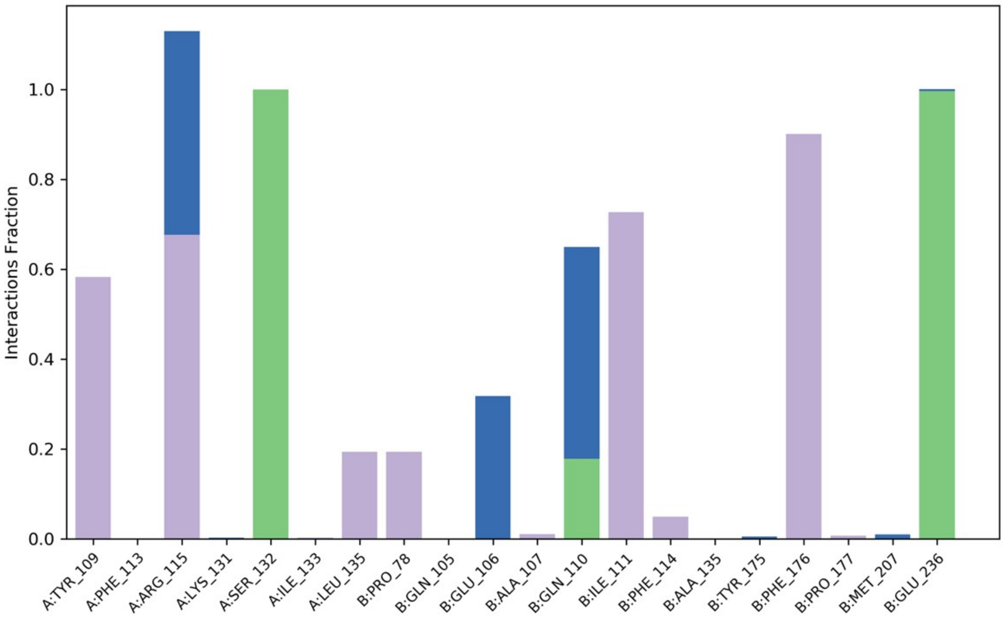


Fig.S5. Bar charts of protein contacts between 5EWJ and compound A during 500 ns MD simulation.

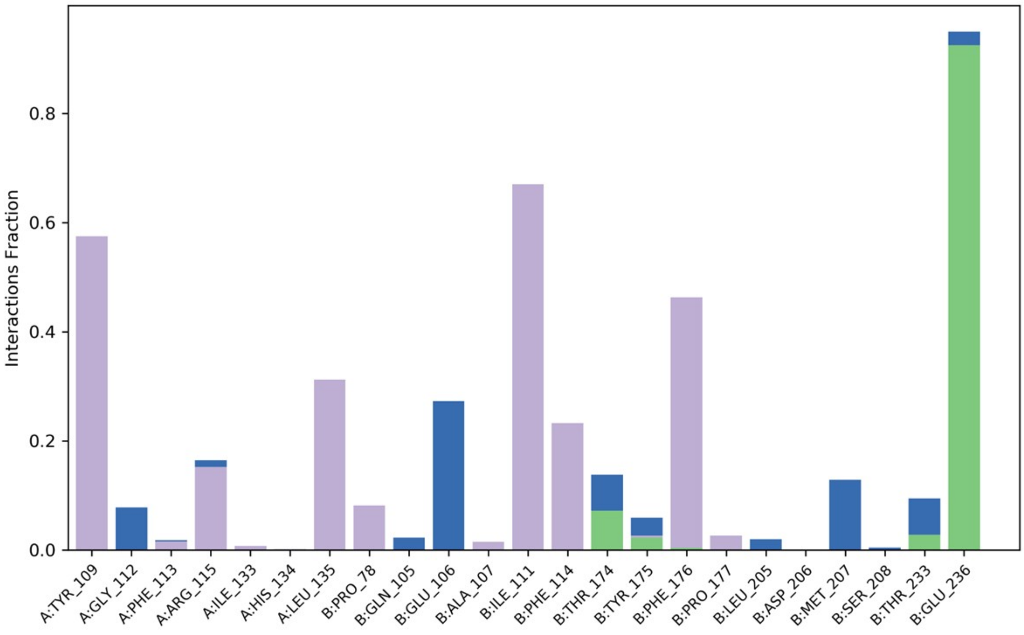


Fig.S6. Bar charts of protein contacts between 5EWJ and compound B during 500 ns MD simulation.

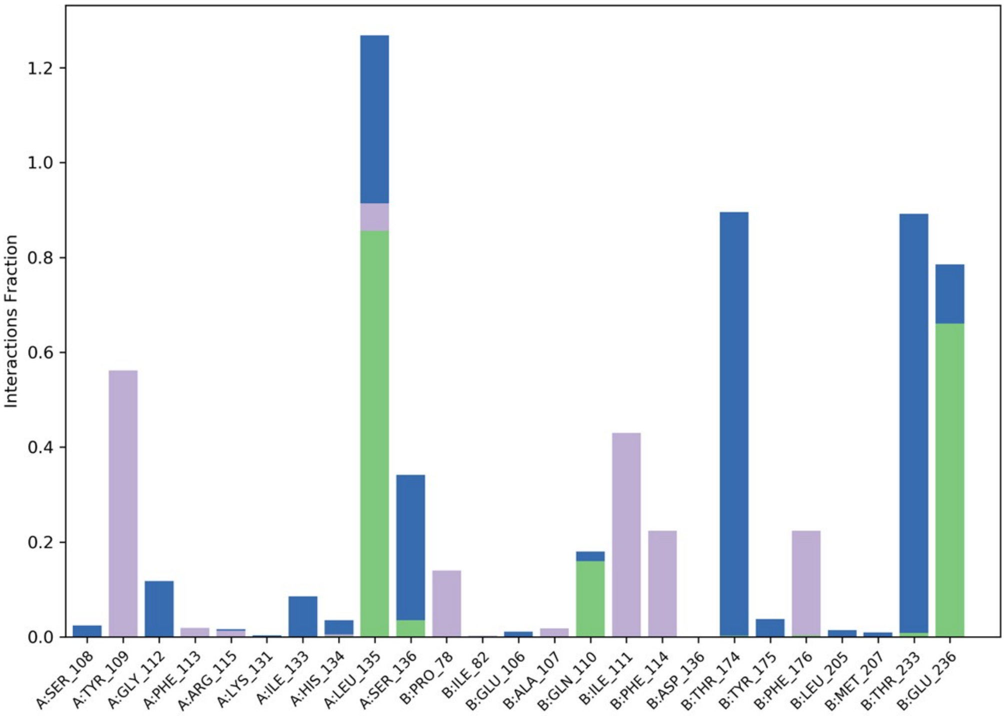


Fig.S7. Bar charts of protein contacts between 5EWJ and compound C during 500 ns MD simulation.

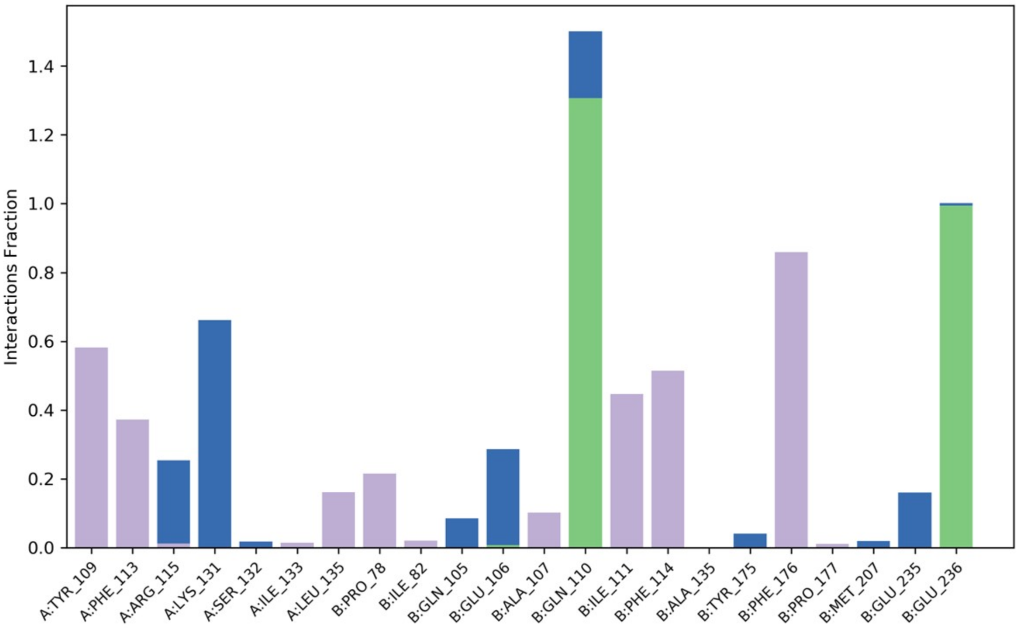


Fig.S8. Bar charts of protein contacts between 5EWJ and ifenprodil during 500 ns MD simulation.

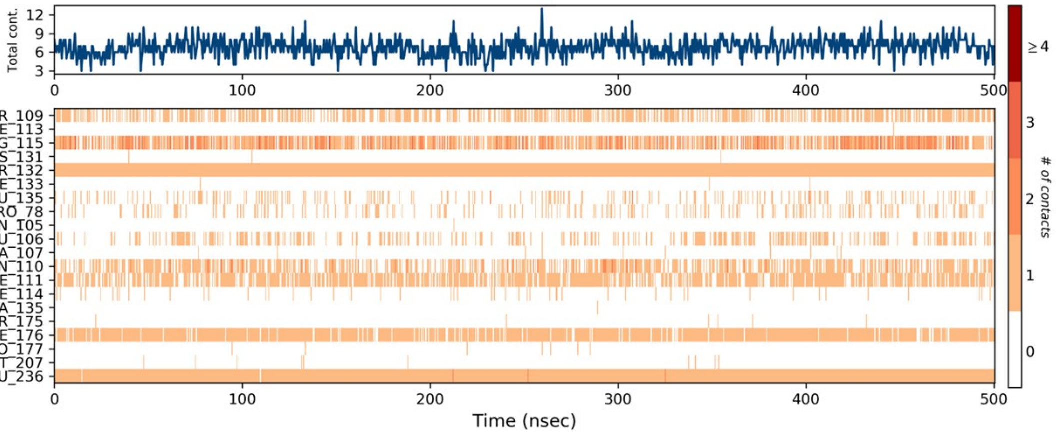


Fig.S9. protein-ligand contacts between 5EWJ and compound A during 500 ns MD simulation.

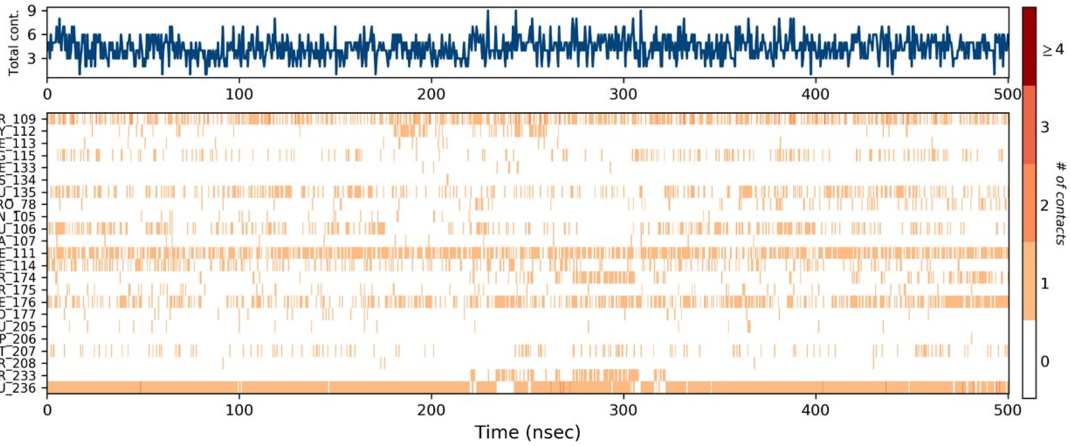


Fig.S10. protein-ligand contacts between 5EWJ and compound B during 500 ns MD simulation.

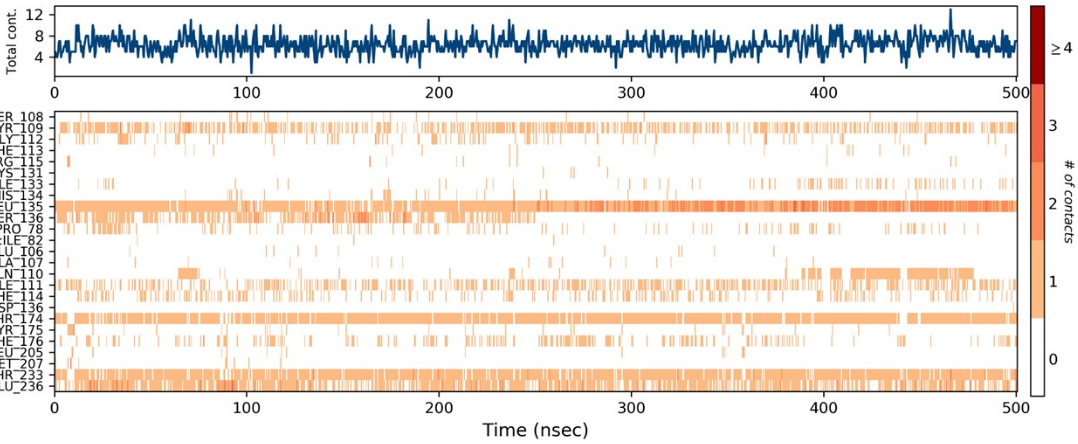


Fig.S11. protein-ligand contacts between 5EWJ and compound C during 500 ns MD simulation.

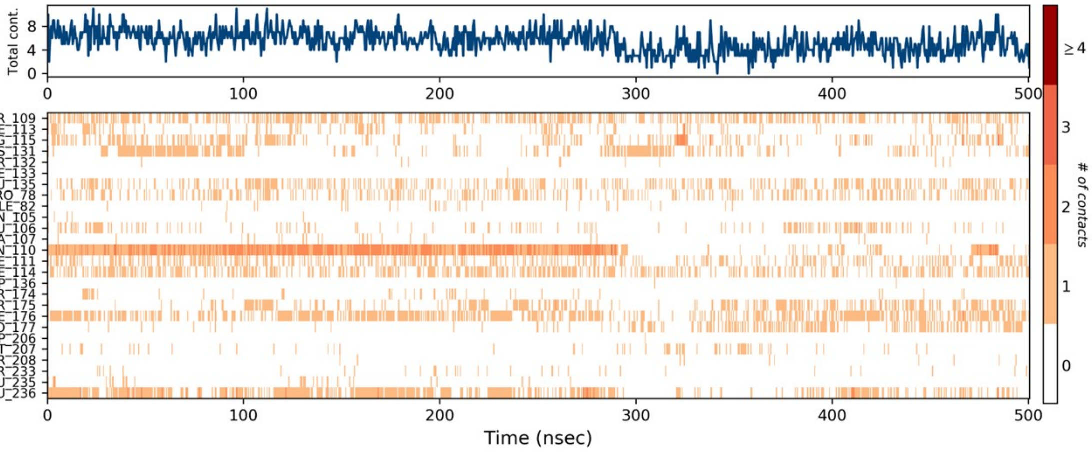


Fig.S12. protein-ligand contacts between 5EWJ and ifenprodil during 500 ns MD simulation.

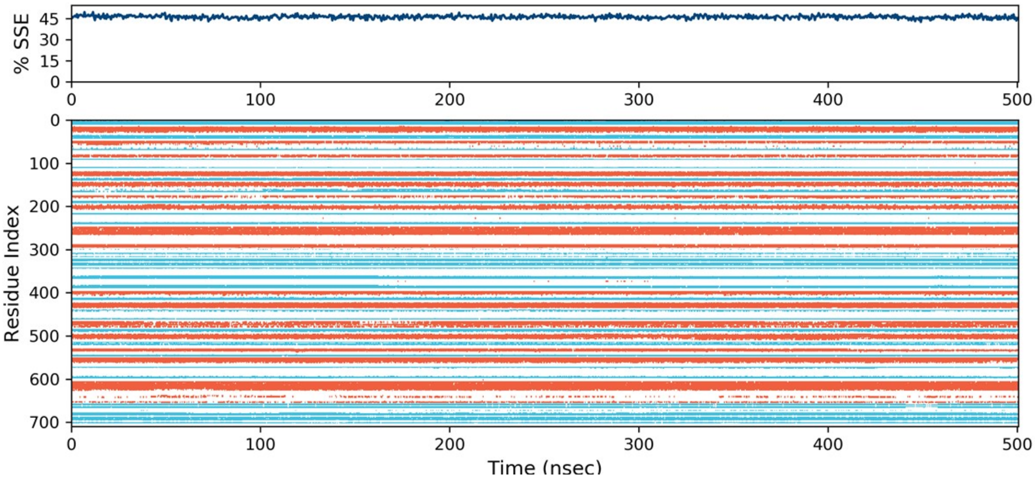


Fig.S13. SSE (Secondary structure element) timeline of 5EWJ/compound A complex during 500 ns MD simulation.

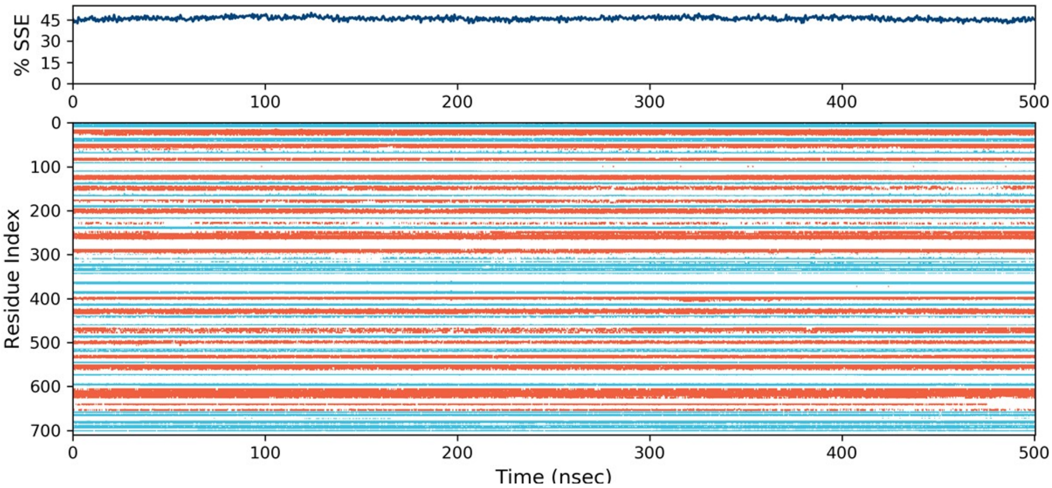


Fig.S14. SSE (Secondary structure element) timeline of 5EWJ/compound B complex during 500 ns MD simulation.

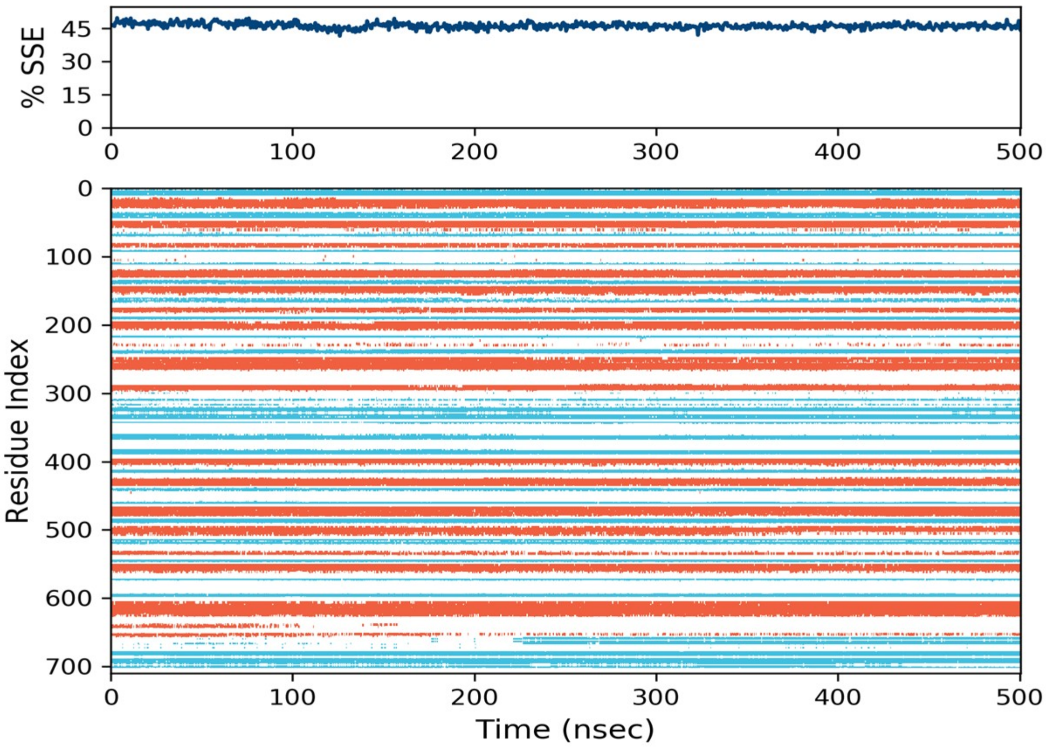


Fig.S15. SSE (Secondary structure element) timeline of 5EWJ/compound C complex during 500 ns MD simulation.

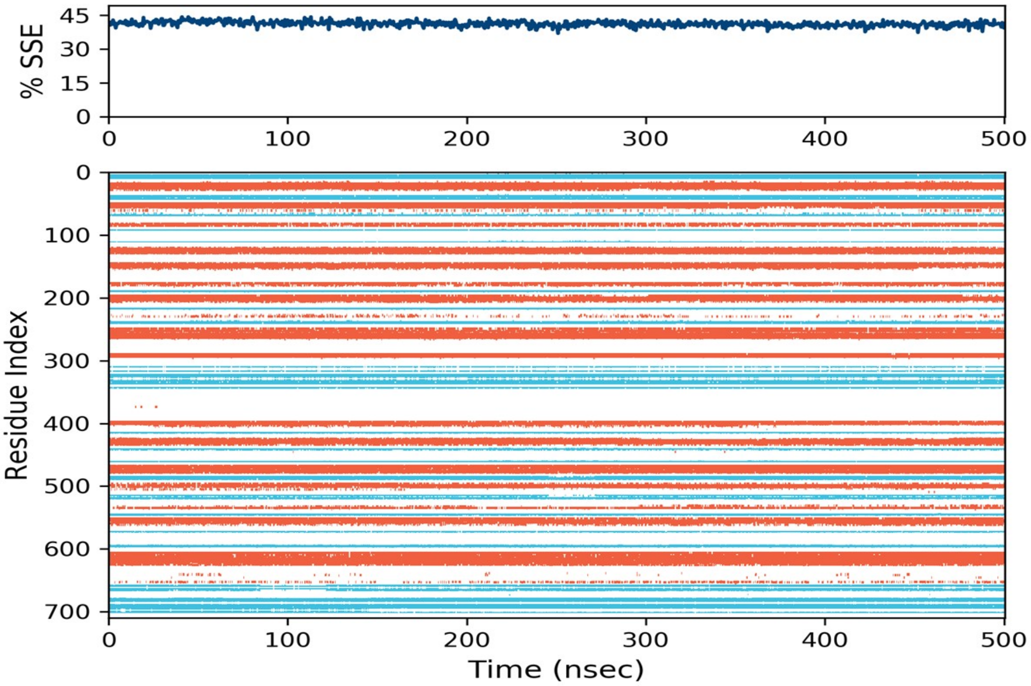


Fig.S16. SSE (Secondary structure element) timeline of 5EWJ/ifenprodil complex during 500 ns MD simulation.

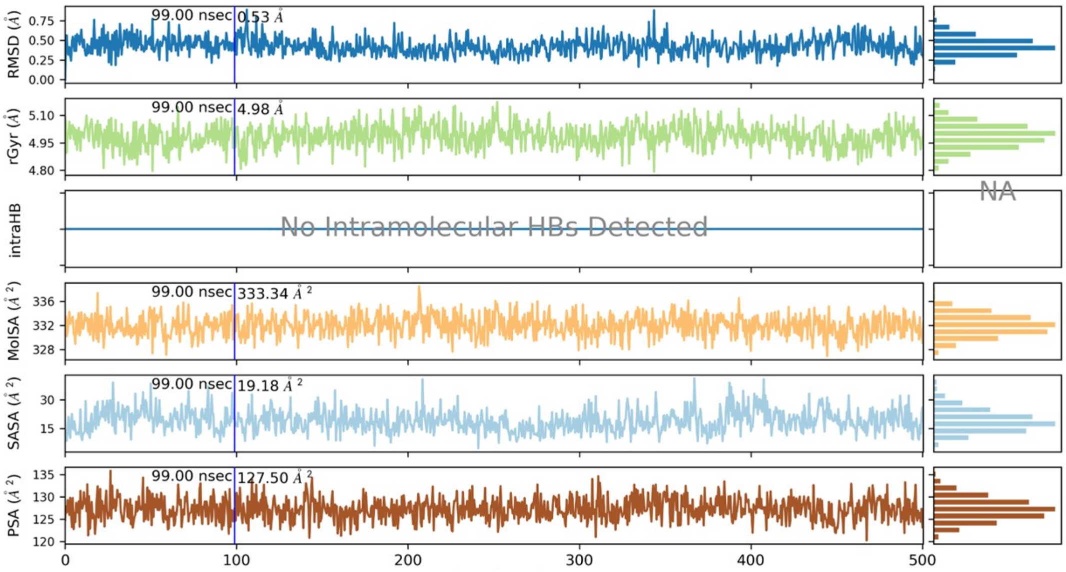


Fig.S17. Ligand properties of compound A during 500 ns MD simulation.

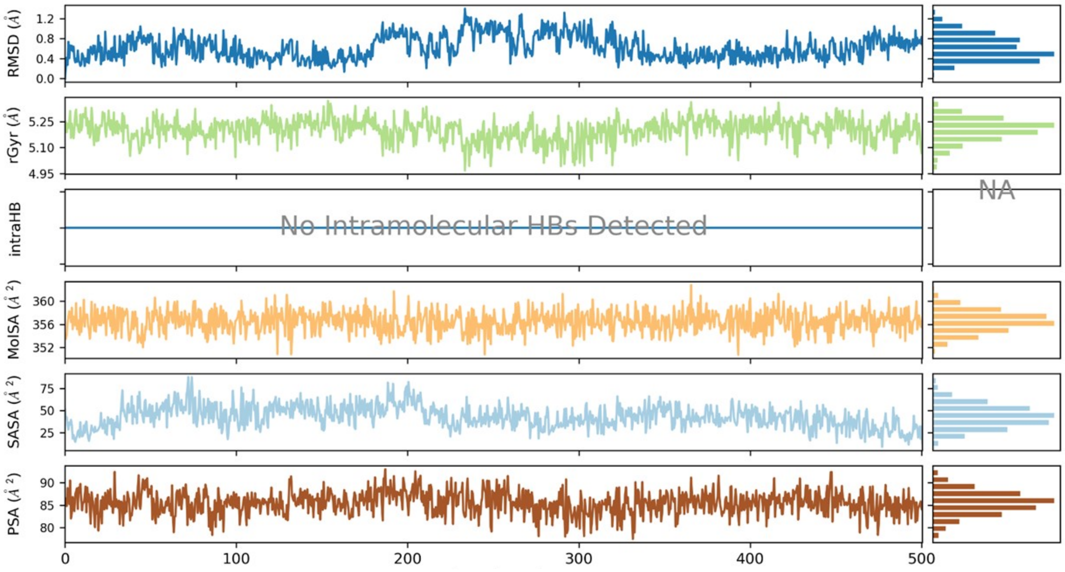


Fig.S18. Ligand properties of compound B during 500 ns MD simulation.

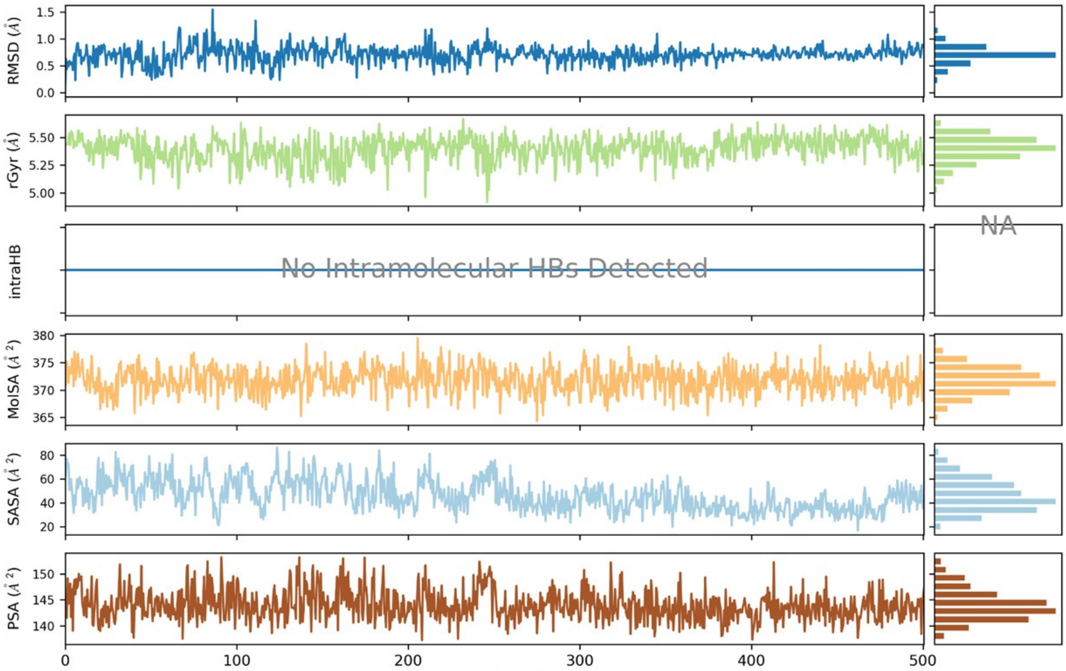


Fig.S19. Ligand properties of compound C during 500 ns MD simulation.

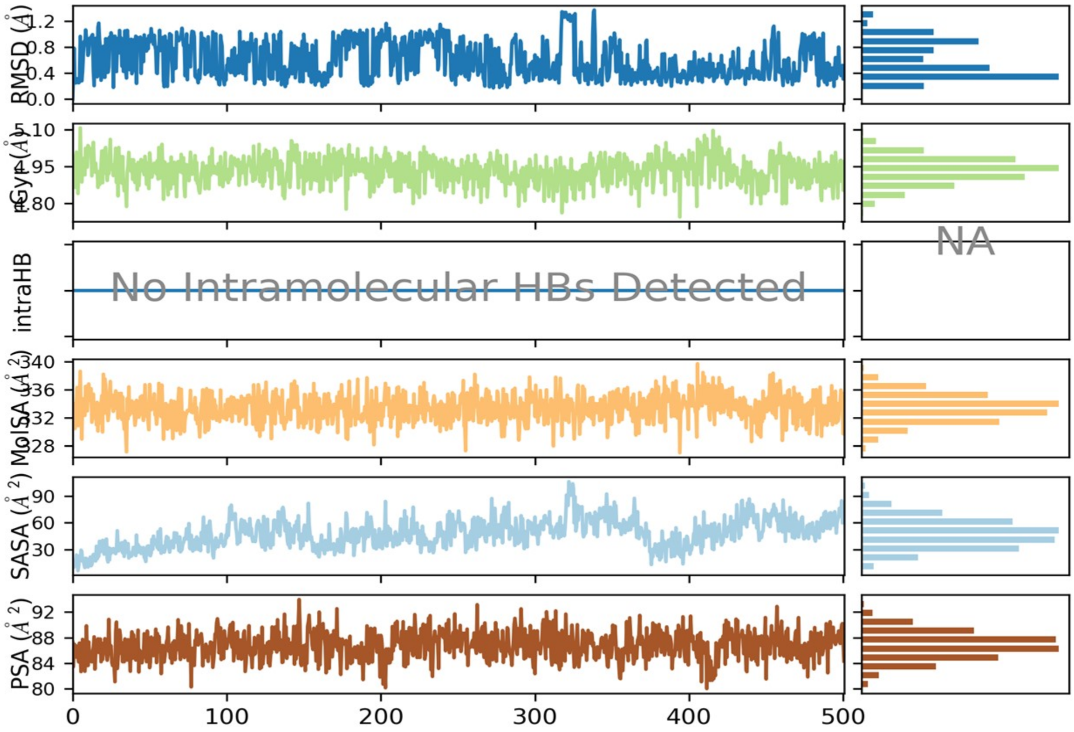


Fig.S20. Ligand properties of ifenprodil during 500 ns MD simulation.

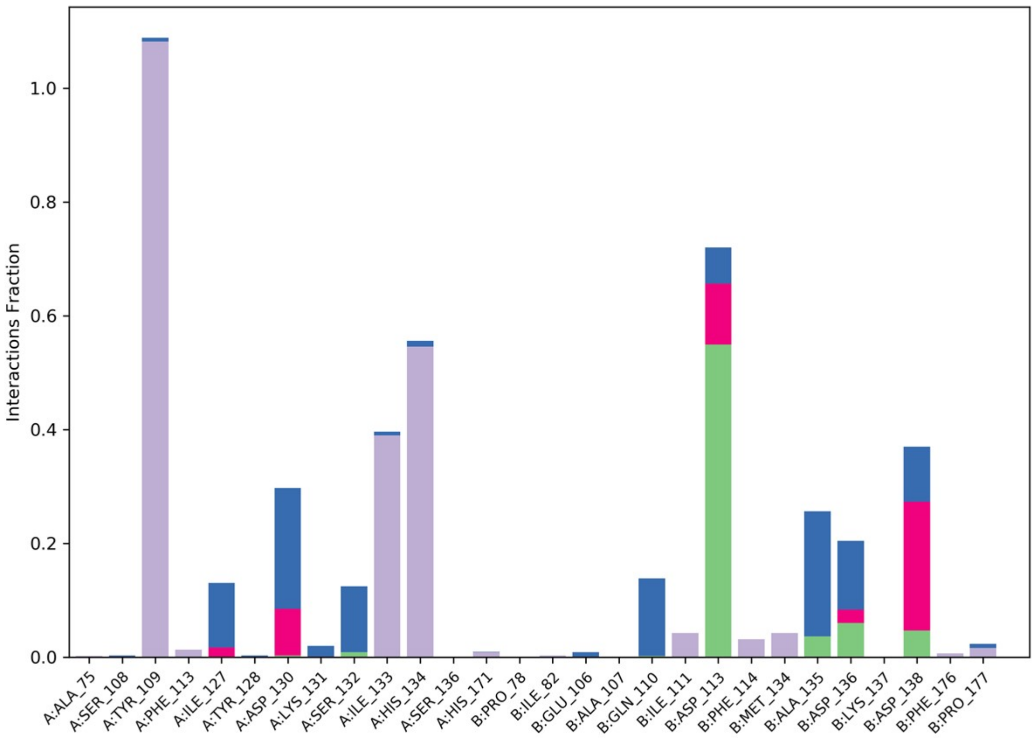


Fig.S21. Bar charts of protein contacts between 5EWJ and EVT-101 during 500 ns MD simulation.

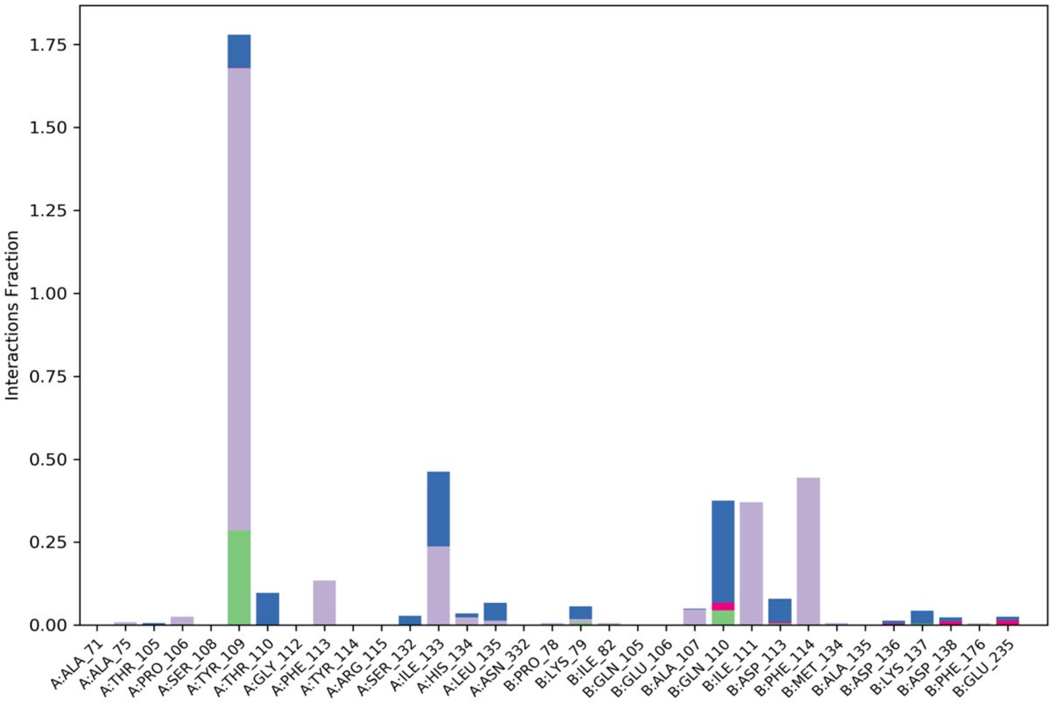


Fig.S22. Bar charts of protein contacts between 5EWJ and compound E during 500 ns MD simulation.

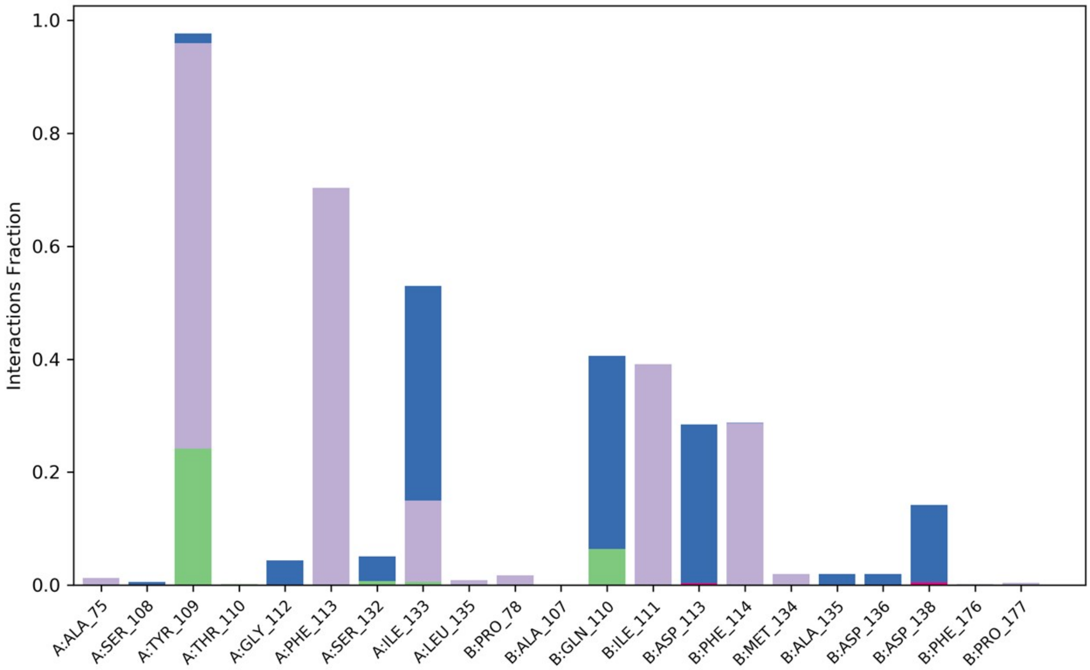


Fig.S23. Bar charts of protein contacts between 5EWJ and compound F during 500 ns MD simulation.

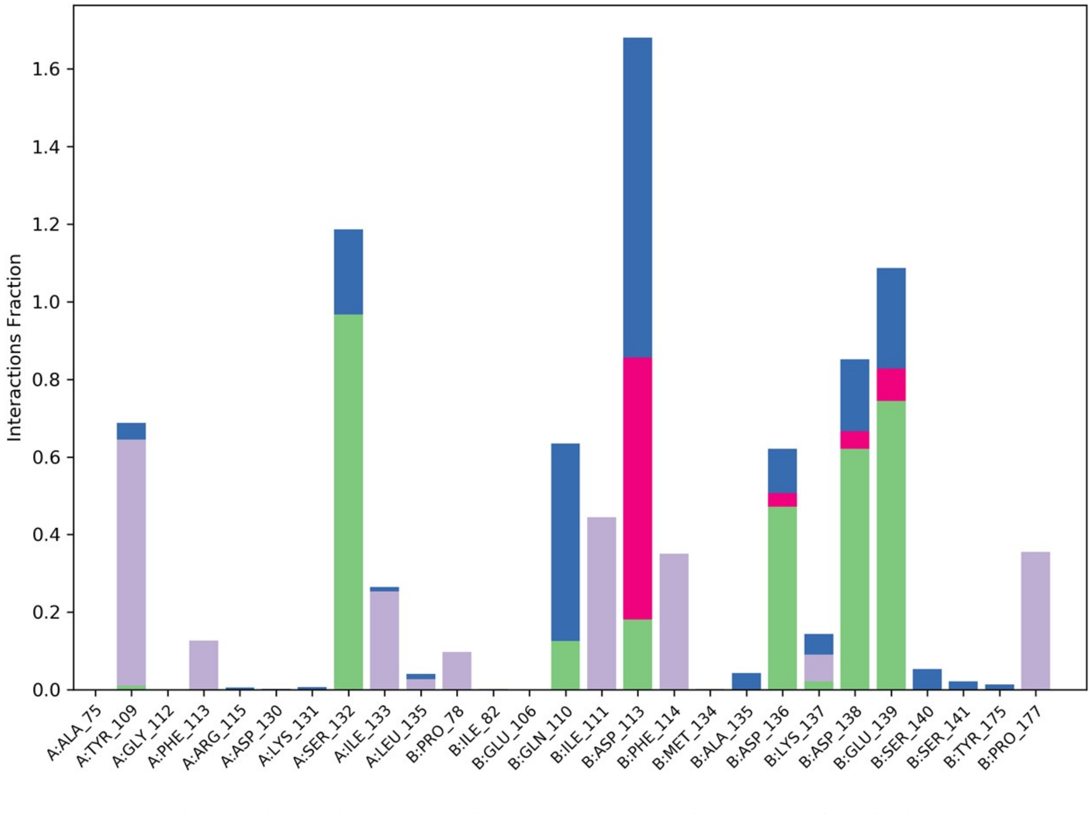


Fig.S24. Bar charts of protein contacts between 5EWJ and compound N during 500 ns MD simulation.

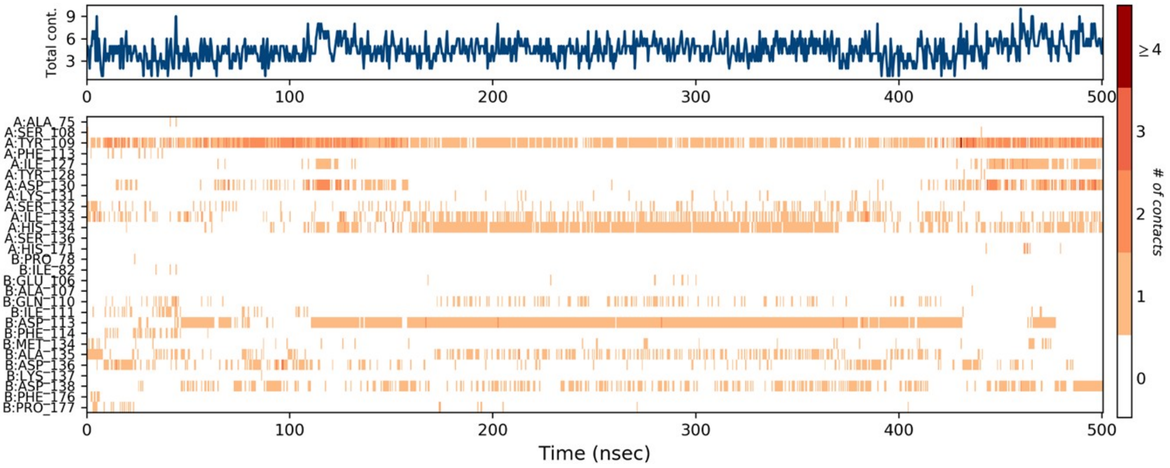


Fig.S25. protein-ligand contacts between 5EWJ and EVT-101 during 500 ns MD simulation.

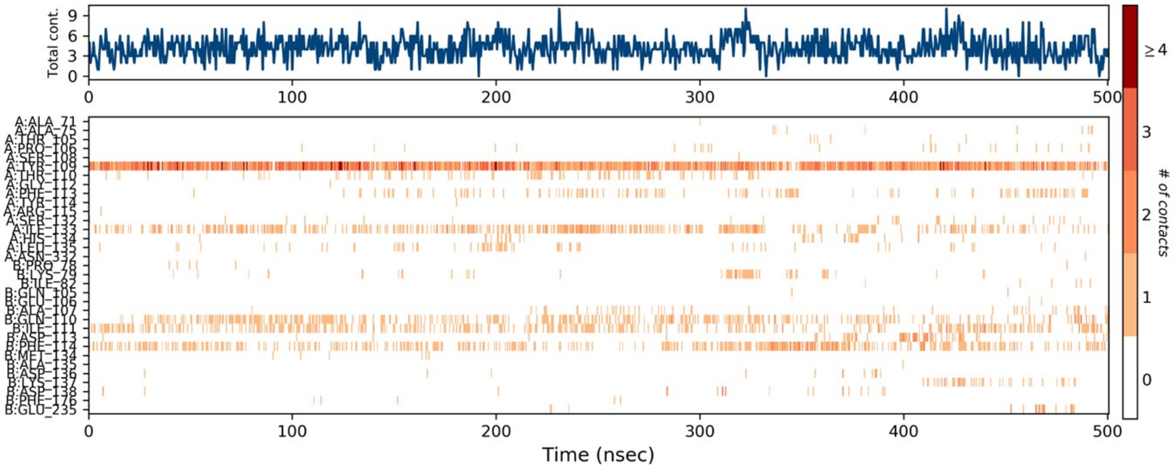


Fig.S26. protein-ligand contacts between 5EWJ and compound E during 500 ns MD simulation.

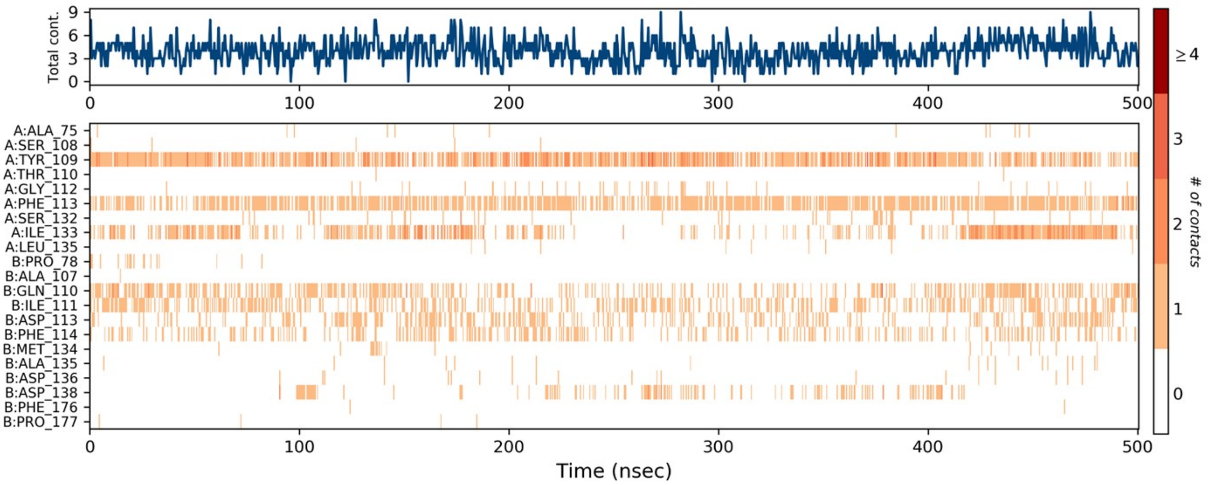


Fig.S27. protein-ligand contacts between 5EWJ and compound F during 500 ns MD simulation.

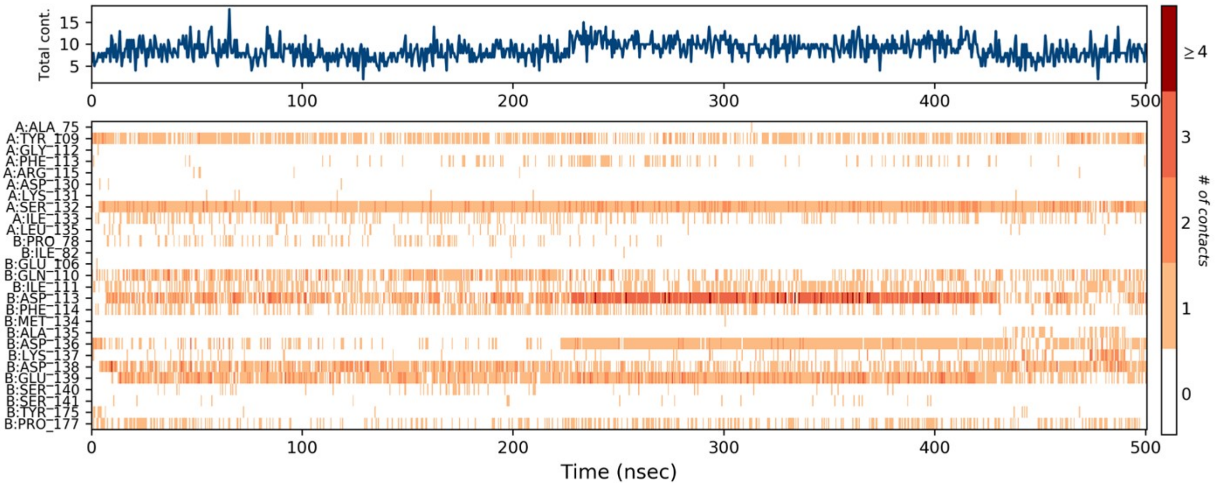


Fig.S28. protein-ligand contacts between 5EWJ and compound N during 500 ns MD simulation.

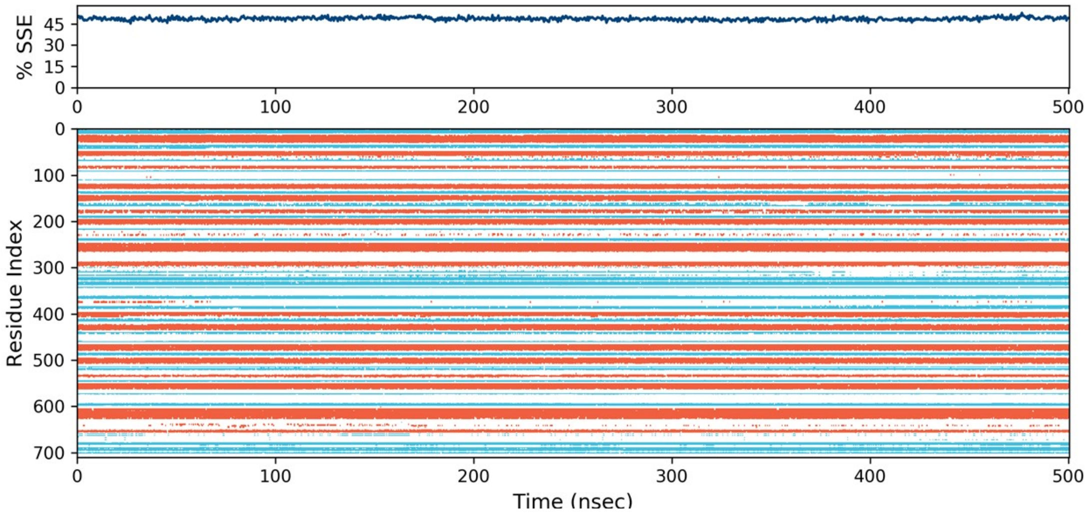


Fig.S29. SSE (Secondary structure element) timeline of 5EWJ/EVT-101 complex during 500 ns MD simulation.

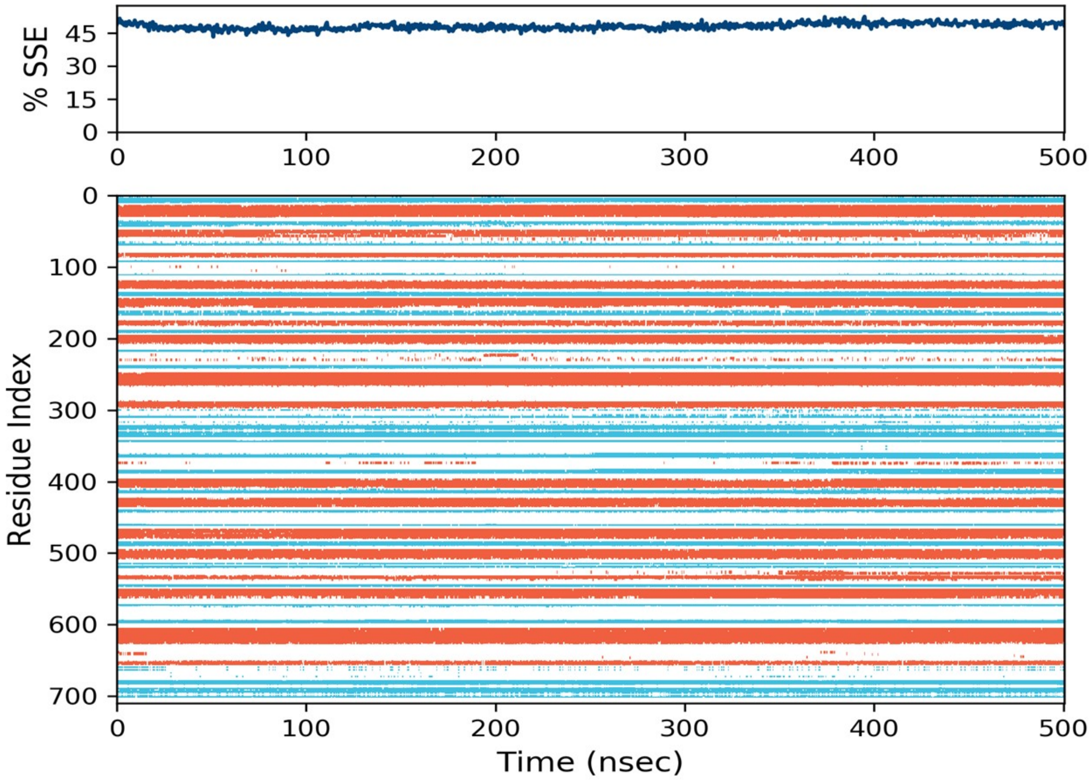


Fig.S30. SSE (Secondary structure element) timeline of 5EWJ/compound E complex during 500 ns MD simulation.

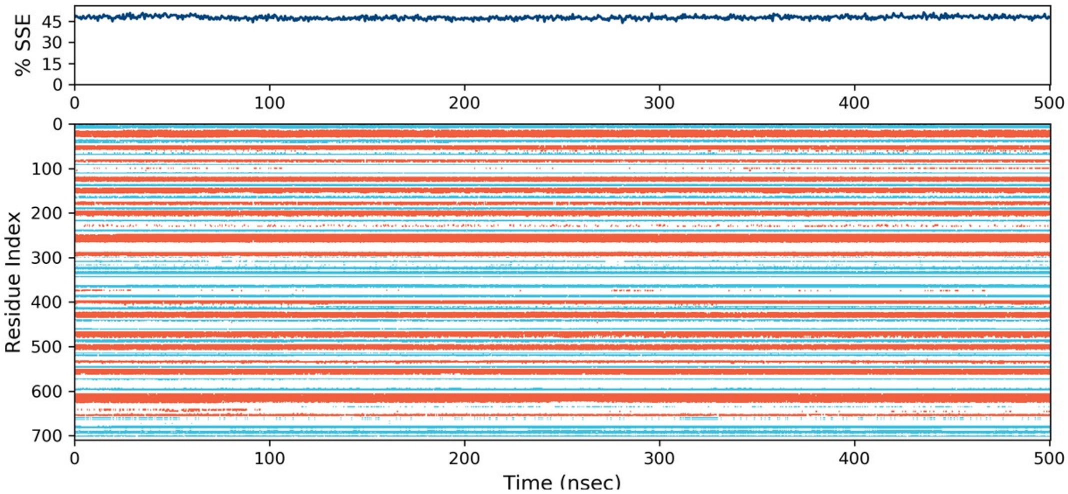


Fig.S31. SSE (Secondary structure element) timeline of 5EWJ/compound F complex during 500 ns MD simulation.

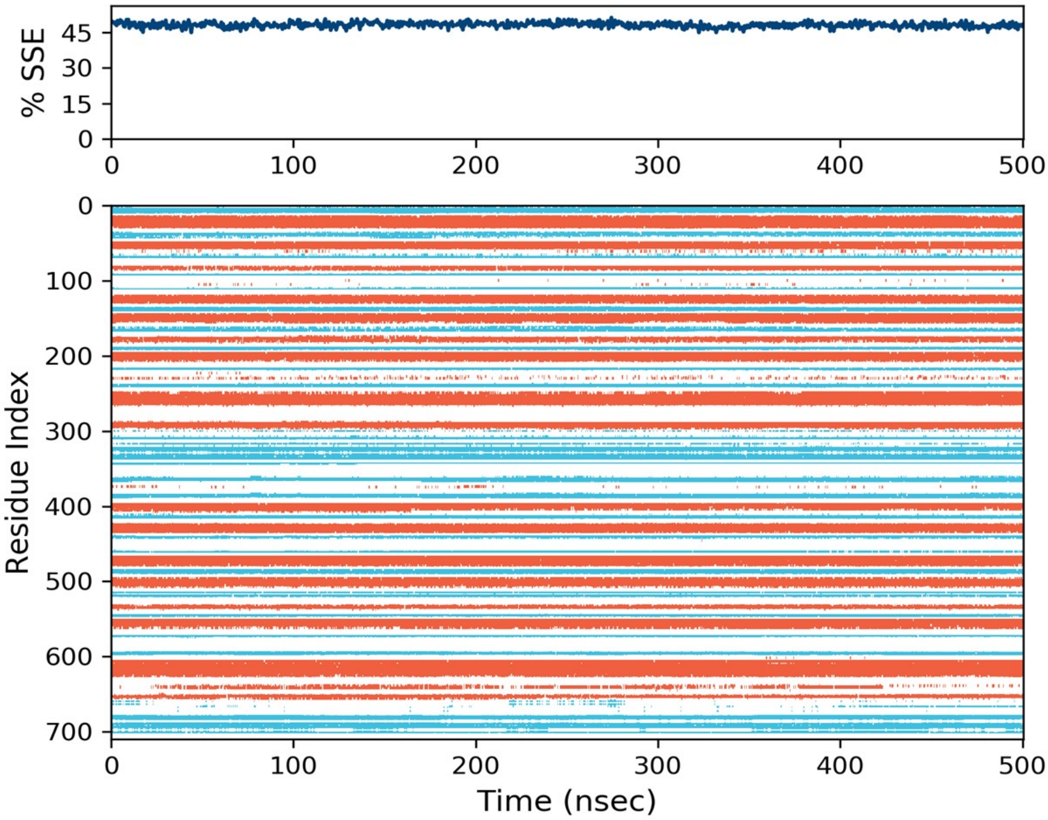


Fig.S32. SSE (Secondary structure element) timeline of 5EWJ/compound N complex during 500 ns MD simulation.

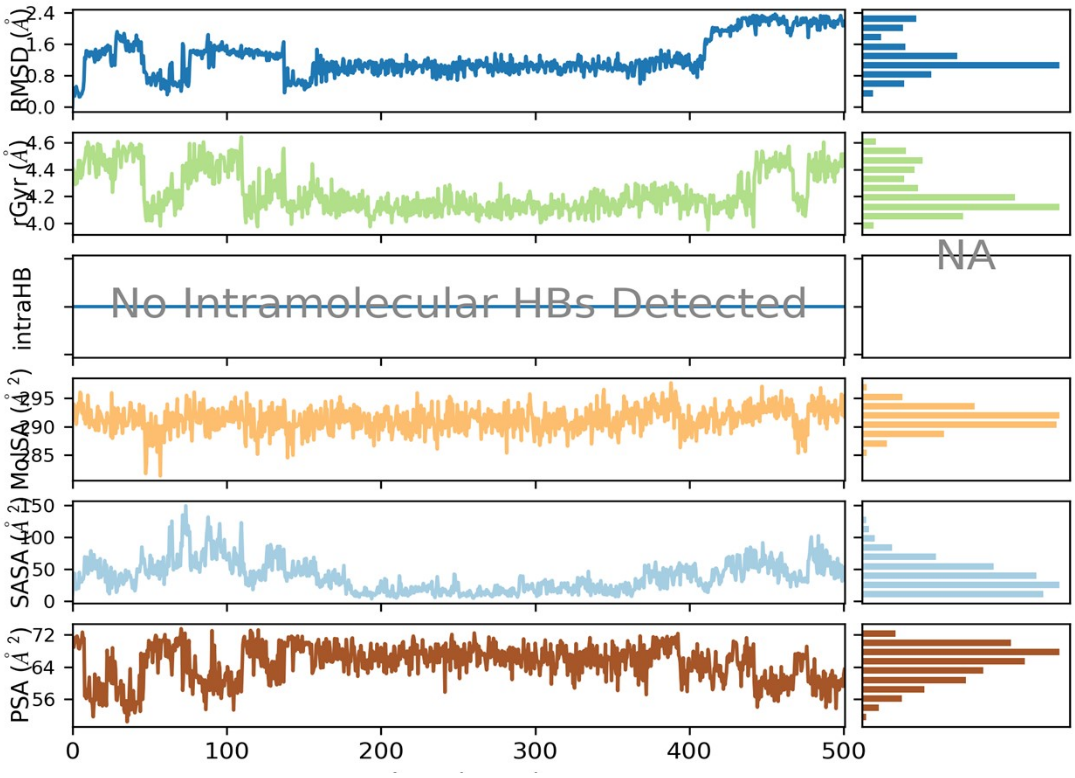


Fig.S33. Ligand properties of EVT-101 during 500 ns MD simulation.

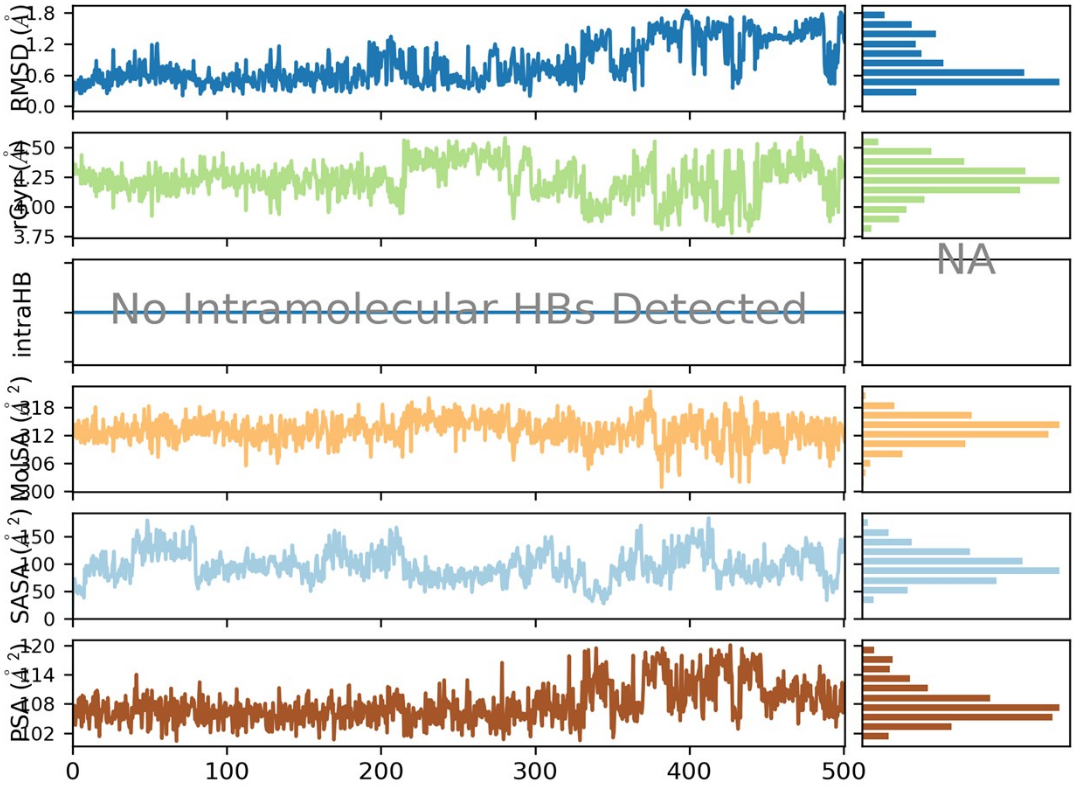


Fig.S34. Ligand properties of compound E during 500 ns MD simulation.

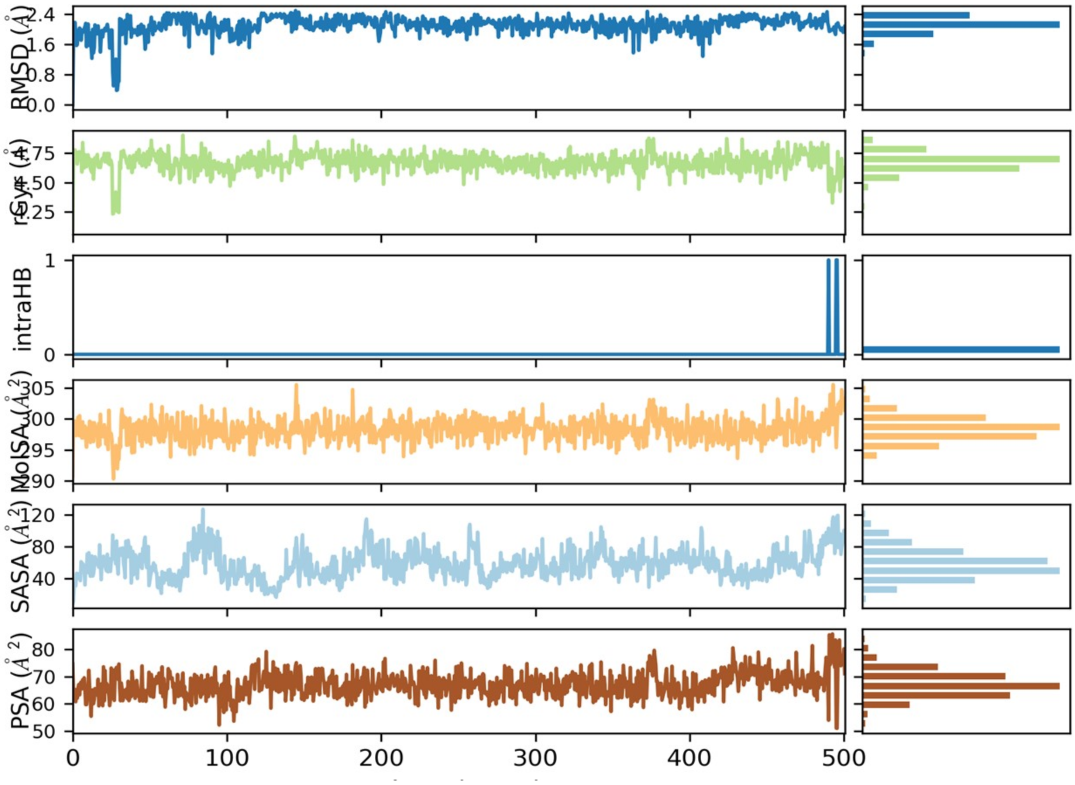


Fig.S35. Ligand properties of compound F during 500 ns MD simulation.

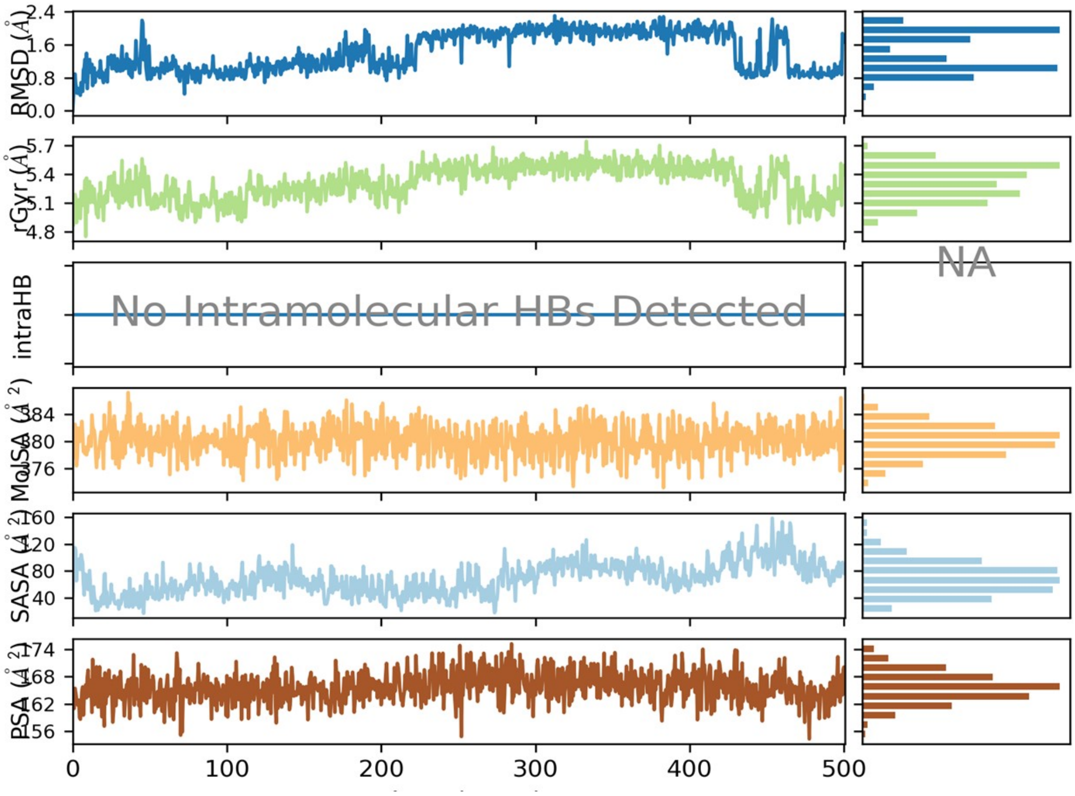


Fig.S36. Ligand properties of compound N during 500 ns MD simulation.

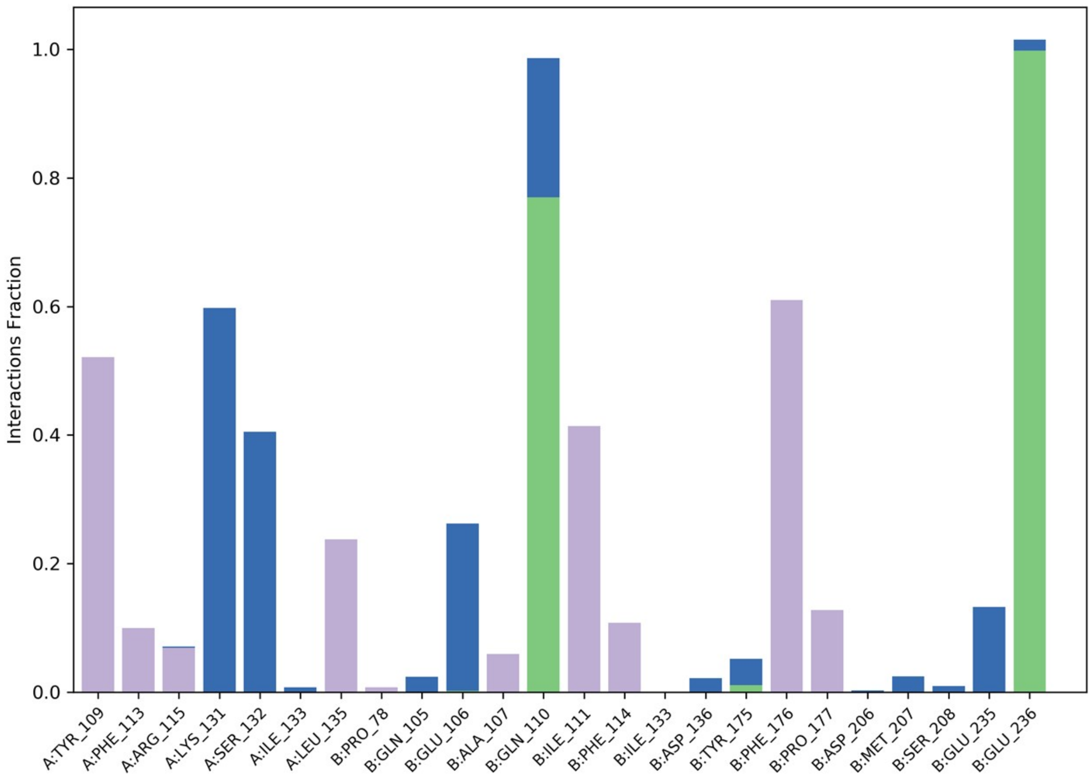


Fig.S37. Bar charts of protein contacts between 5EWJ and IF01 during 500 ns MD simulation.

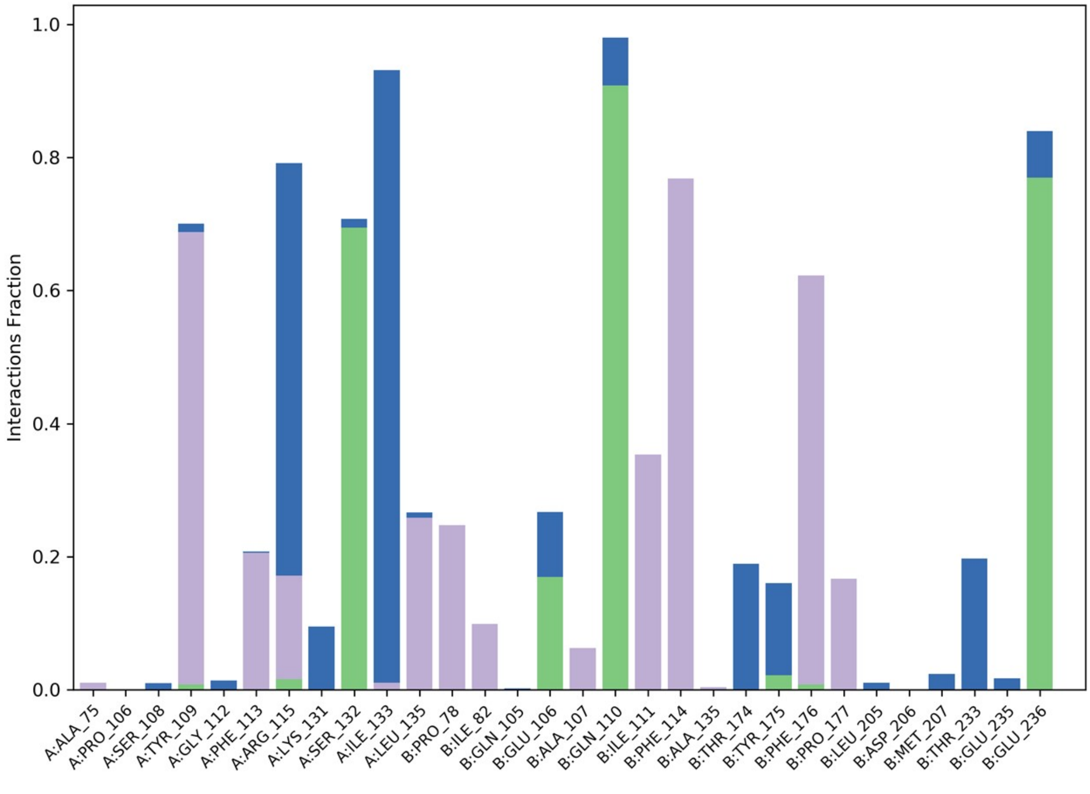


Fig.S38. Bar charts of protein contacts between 5EWJ and IF03 during 500 ns MD simulation.

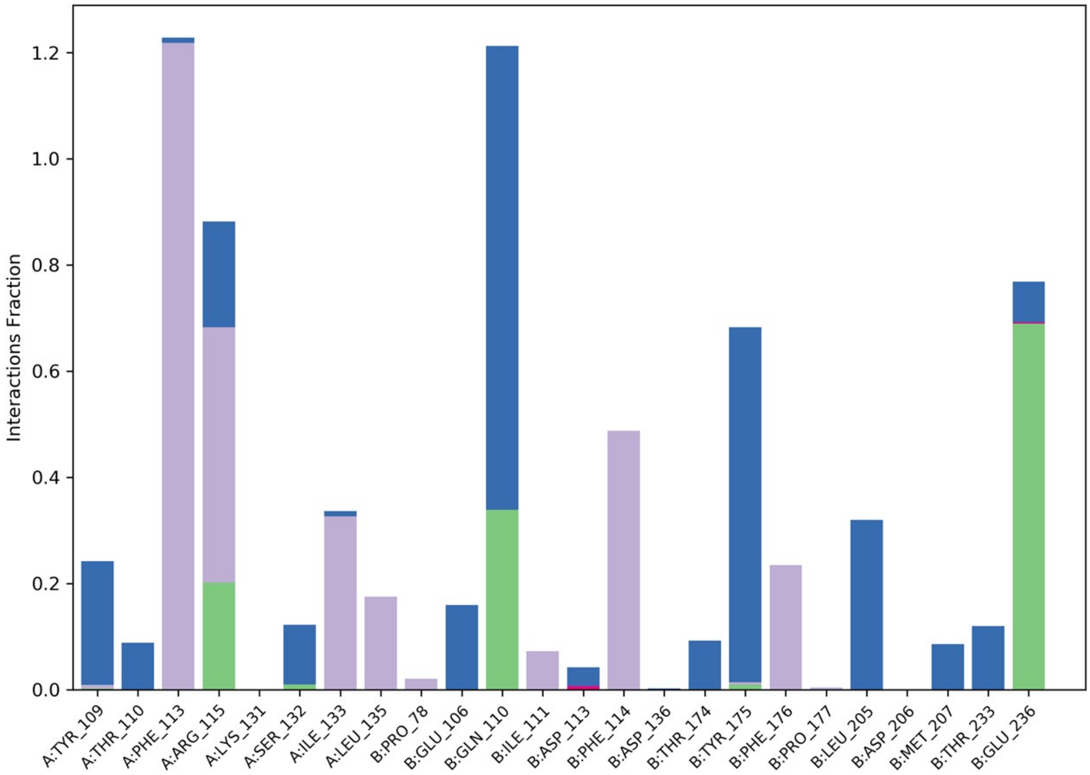


Fig.S39. Bar charts of protein contacts between 5EWJ and IF08 during 500 ns MD simulation.

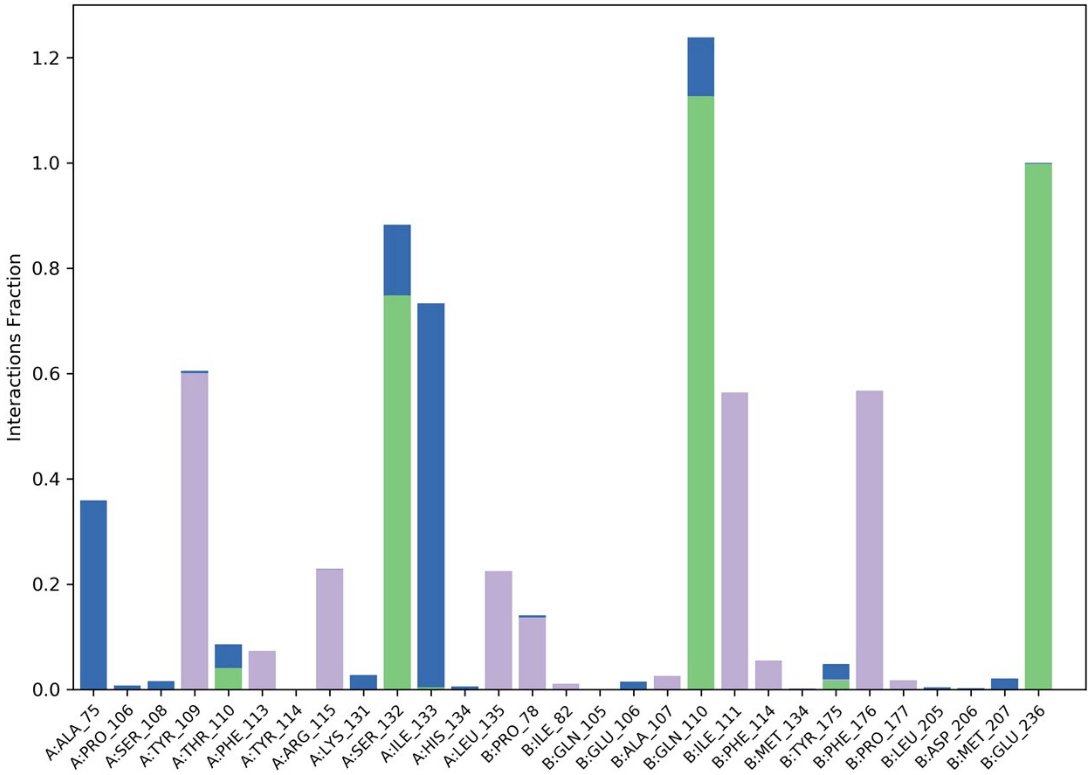


Fig.S40. Bar charts of protein contacts between 5EWJ and IF09 during 500 ns MD simulation.

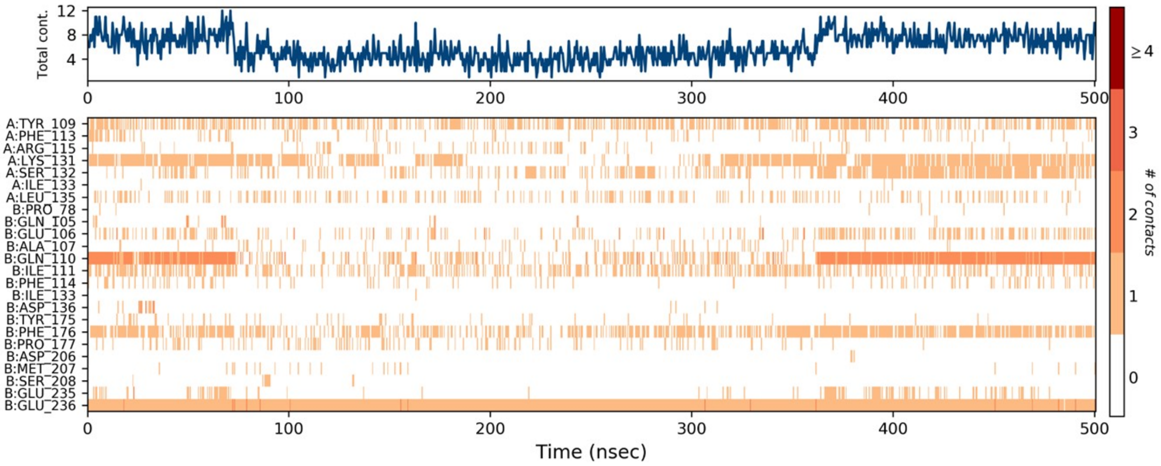


Fig.S41. protein-ligand contacts between 5EWJ and IF01 during 500 ns MD simulation.

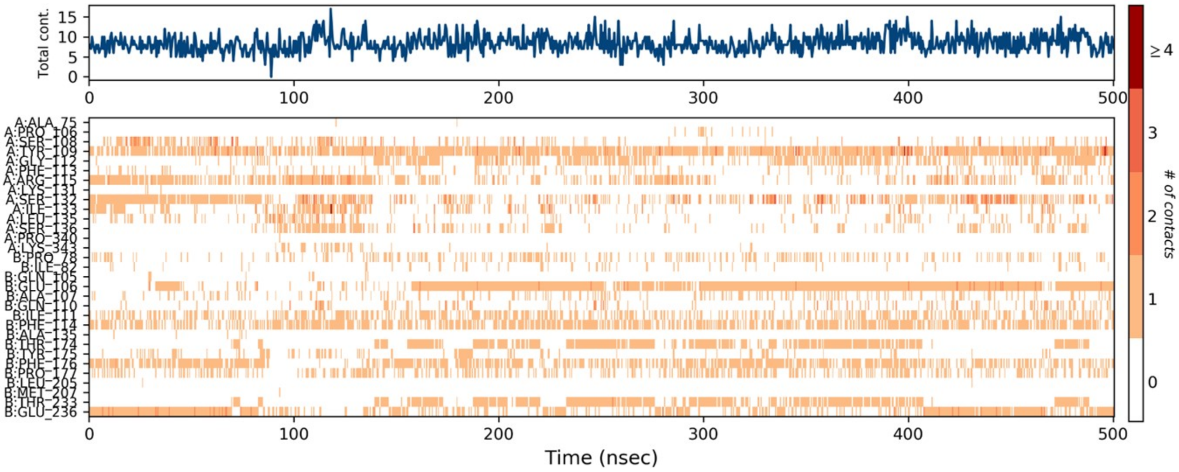


Fig.S42. protein-ligand contacts between 5EWJ and IF03 during 500 ns MD simulation.

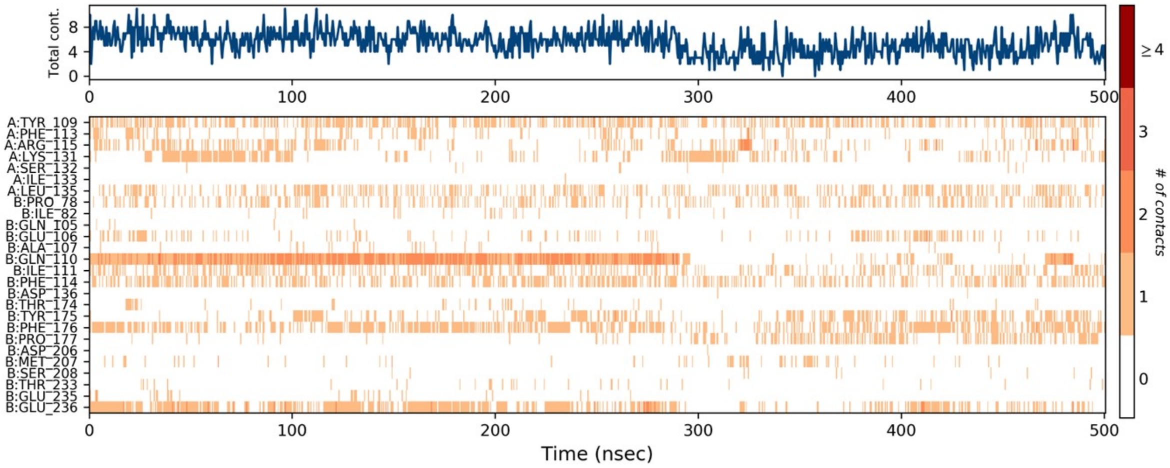


Fig.S43. protein-ligand contacts between 5EWJ and IF08 during 500 ns MD simulation.

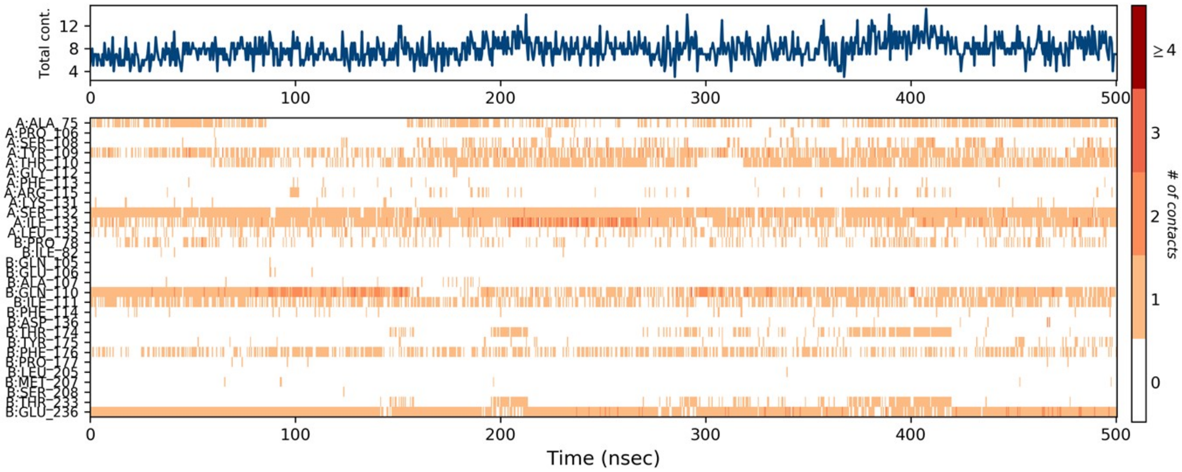


Fig.S44. protein-ligand contacts between 5EWJ and IF09 during 500 ns MD simulation.

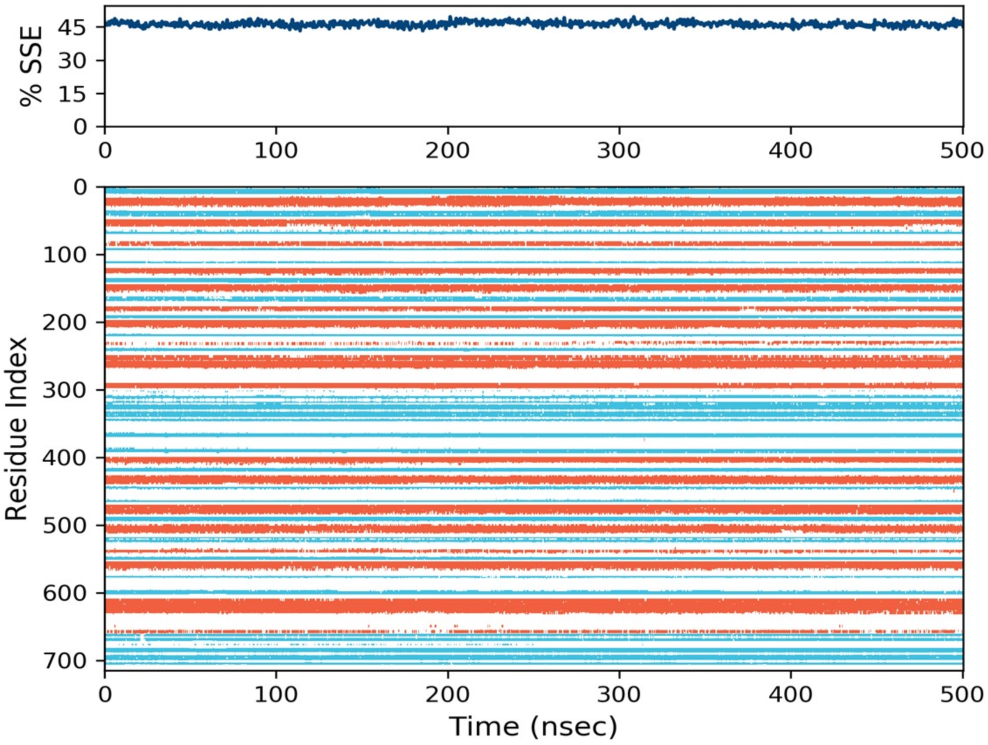


Fig.S45. SSE (Secondary structure element) timeline of 5EWJ/IF01 complex during 500 ns MD simulation.

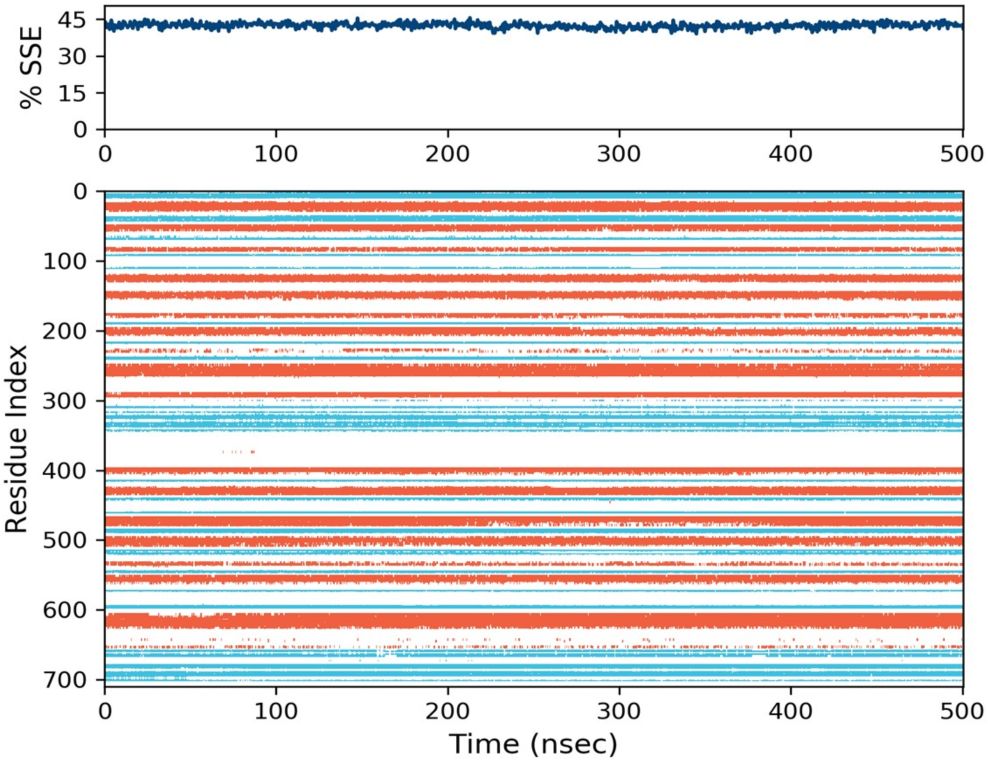


Fig.S46. SSE (Secondary structure element) timeline of 5EWJ/IF03 complex during 500 ns MD simulation.

Fig.S47. SSE (Secondary structure element) timeline of 5EWJ/IF08 complex during 500 ns MD simulation.

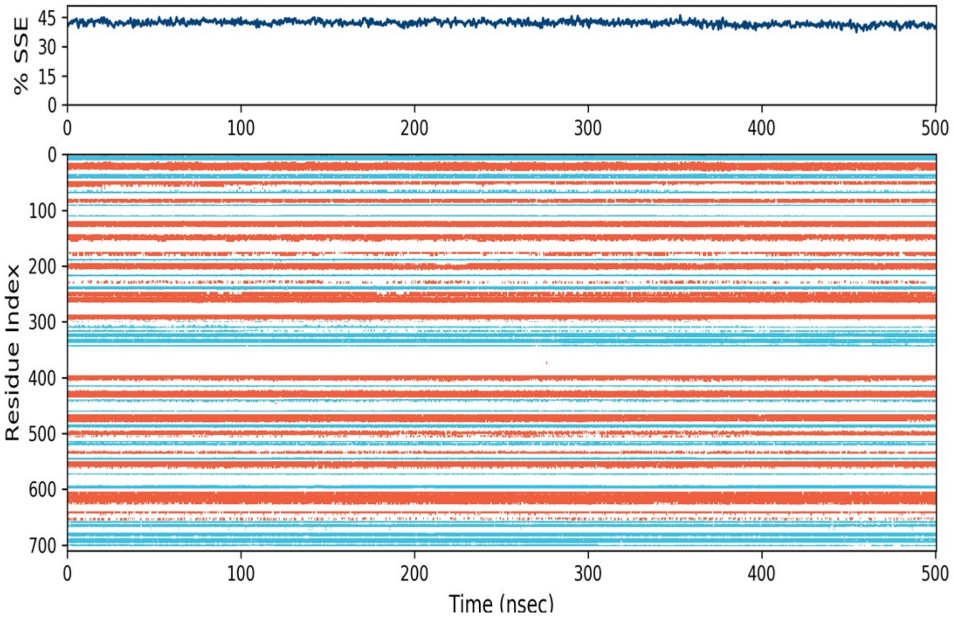


Fig.S48. SSE (Secondary structure element) timeline of 5EWJ/IF09 complex during 500 ns MD simulation.

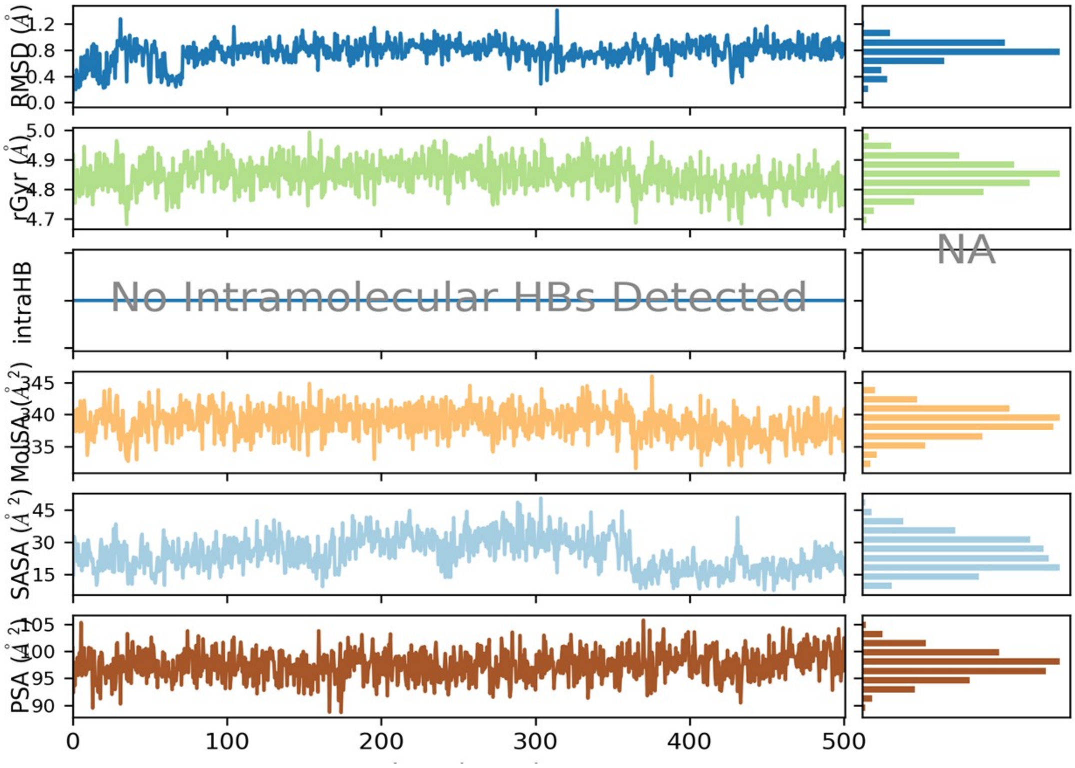


Fig.S49. Ligand properties of IF01 during 500 ns MD simulation.

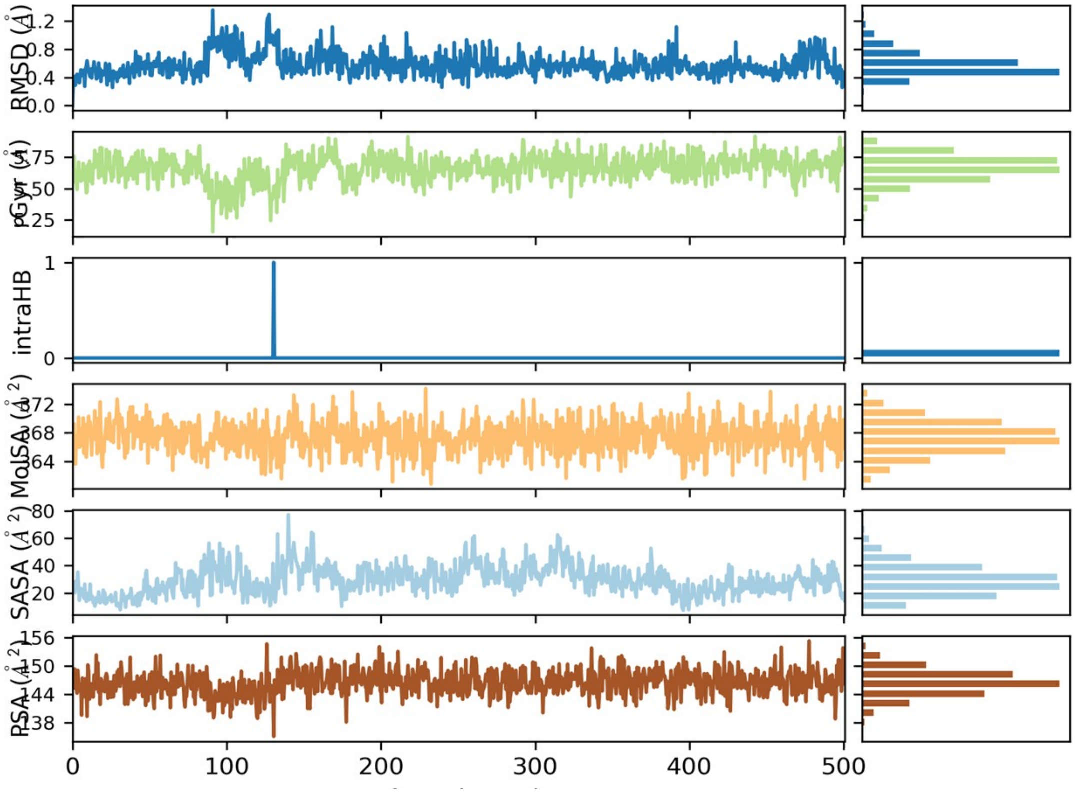


Fig.S50. Ligand properties of IF03 during 500 ns MD simulation.

Fig.S51. Ligand properties of IF08 during 500 ns MD simulation.

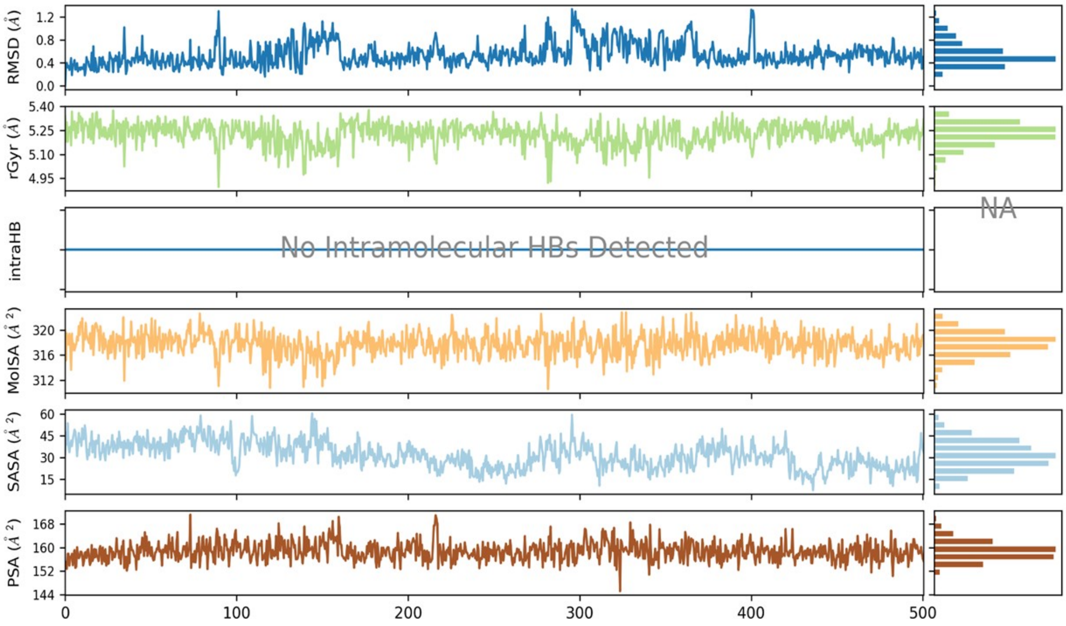


Fig.S52. Ligand properties of IF09 during 500 ns MD simulation.

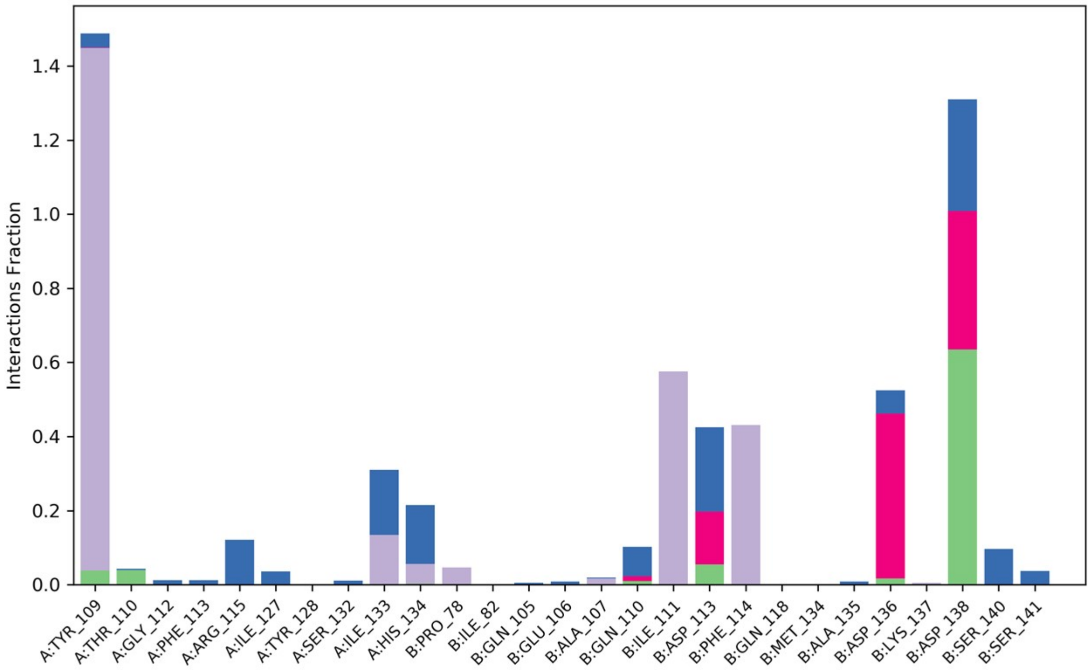


Fig.S53. Bar charts of protein contacts between 5EWJ and EVT01 during 500 ns MD simulation.

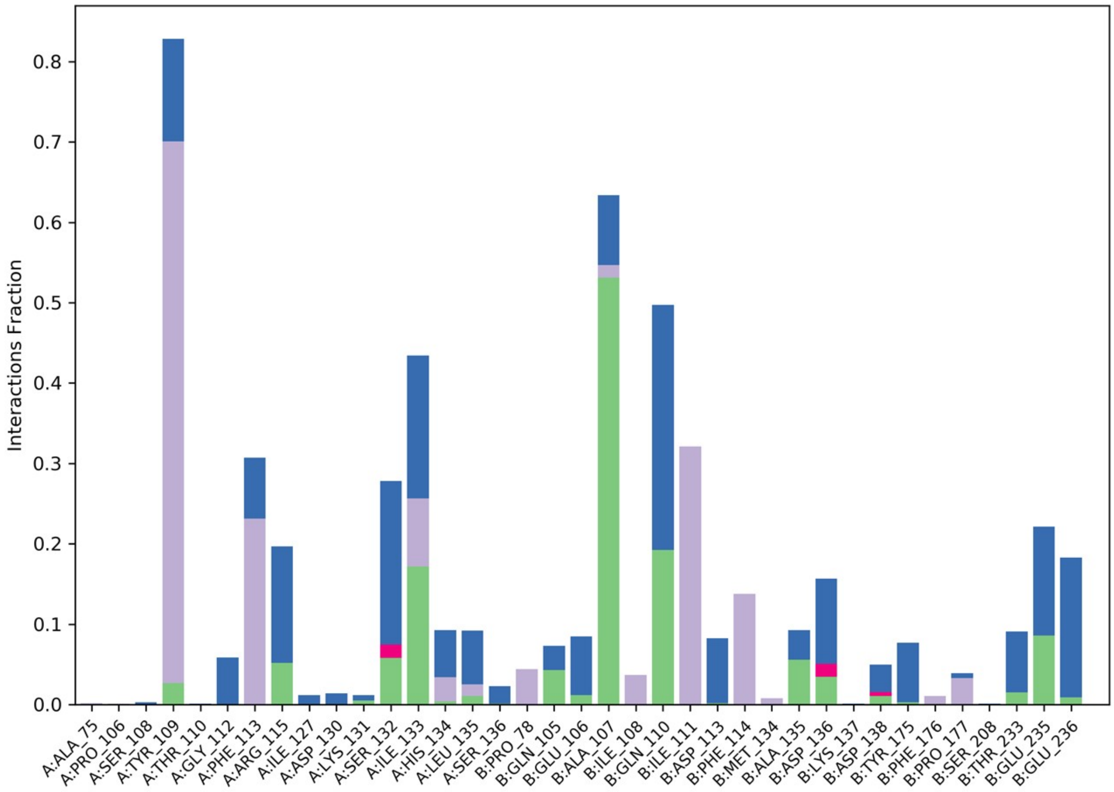


Fig.S54. Bar charts of protein contacts between 5EWJ and EVT02 during 500 ns MD simulation.

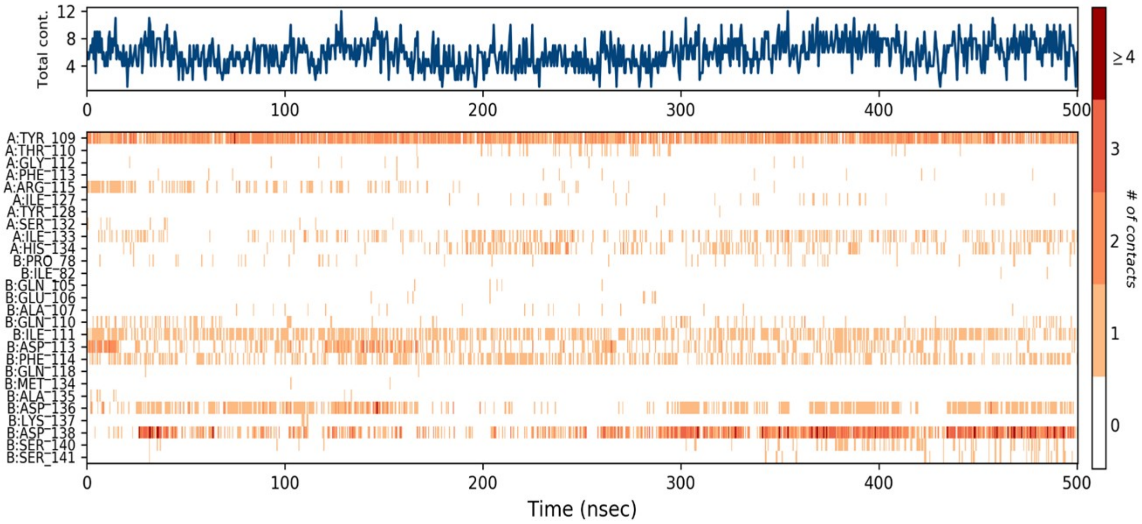


Fig.S55. protein-ligand contacts between 5EWJ and EVT01 during 500 ns MD simulation.

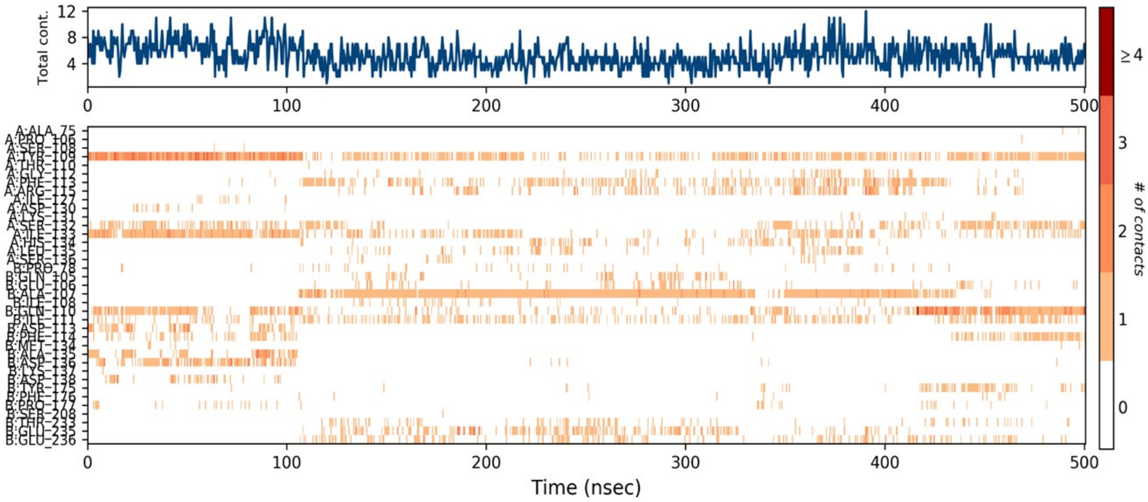


Fig.S56. protein-ligand contacts between 5EWJ and EVT02 during 500 ns MD simulation.

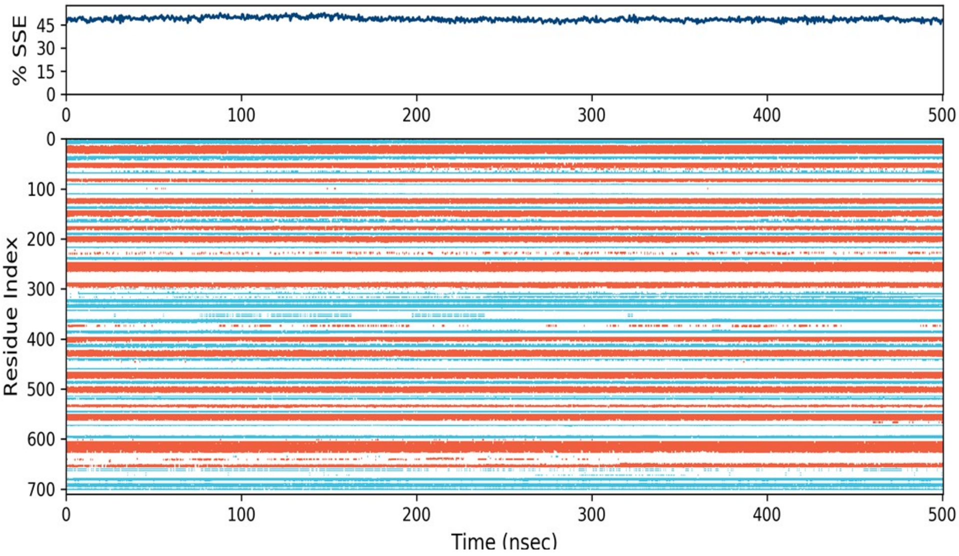


Fig.S57. SSE (Secondary structure element) timeline of 5EWJ/EVT01 complex during 500 ns MD simulation.

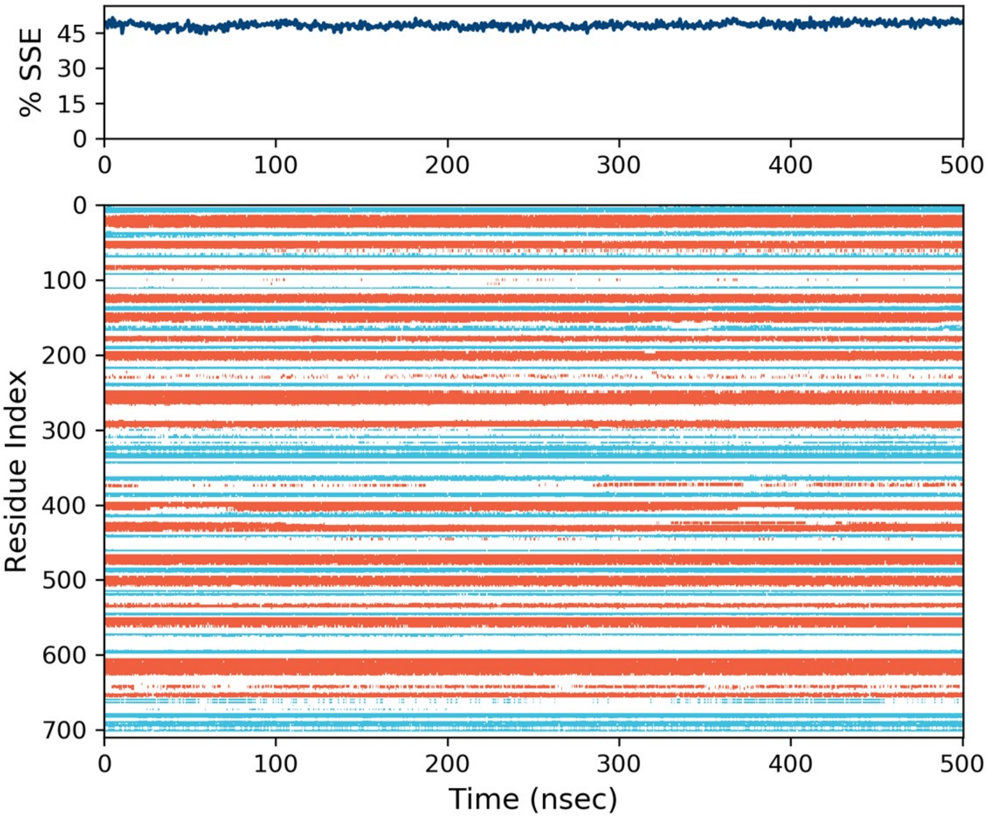


Fig.S58. SSE (Secondary structure element) timeline of 5EWJ/EVT02 complex during 500 ns MD simulation.

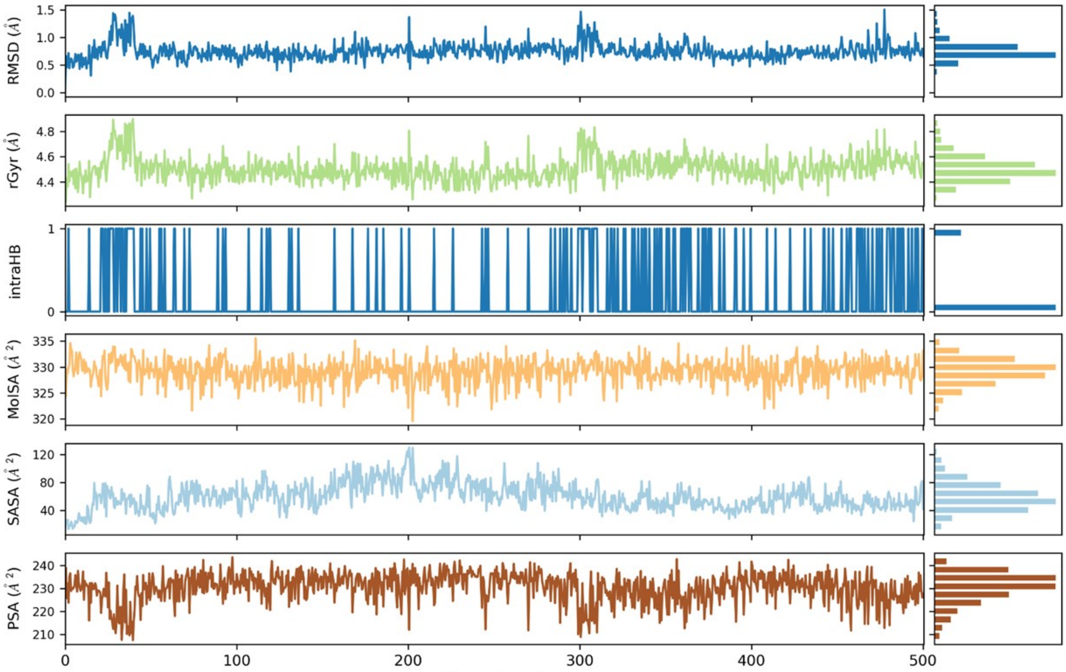


Fig.S59. Ligand properties of EVT01 during 500 ns MD simulation.

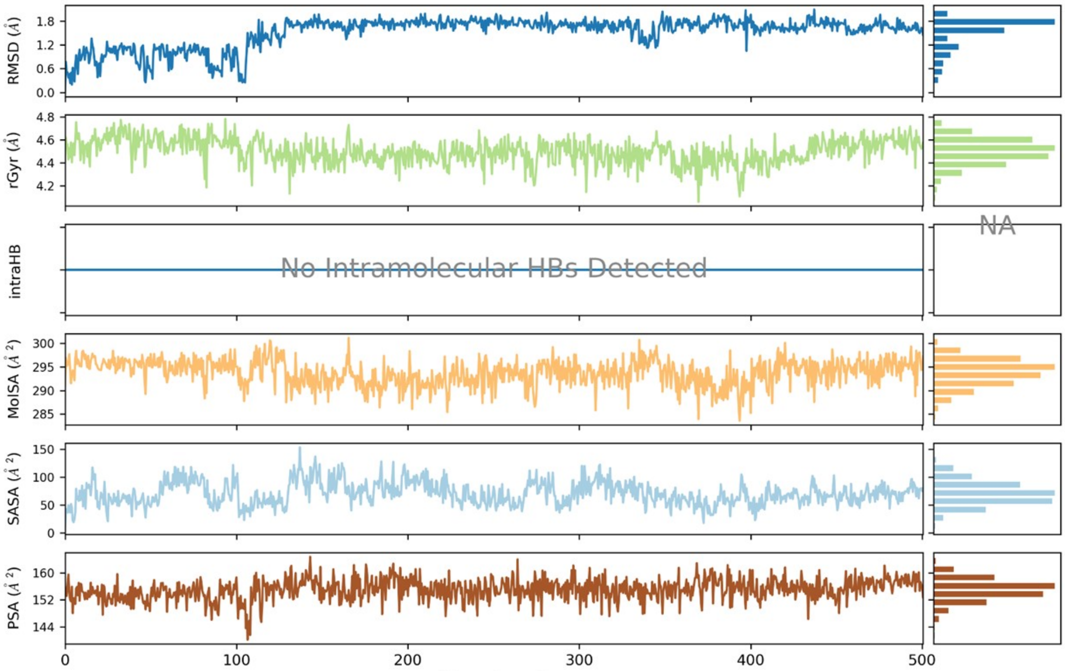


Fig.S60. Ligand properties of EVT02 during 500 ns MD simulation.

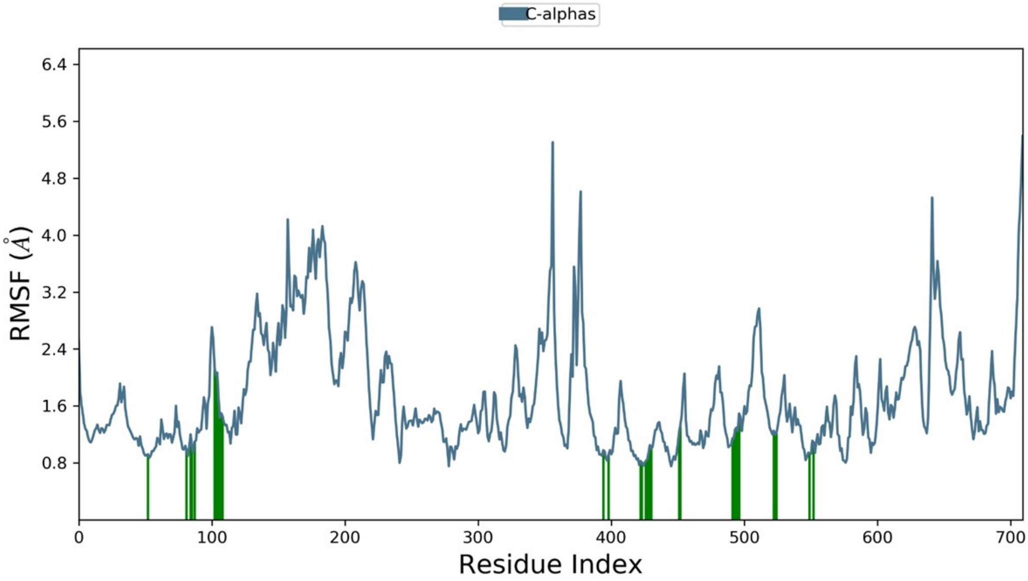


Fig.S61. RMSF curve for IF02 during 500 ns MD simulation.

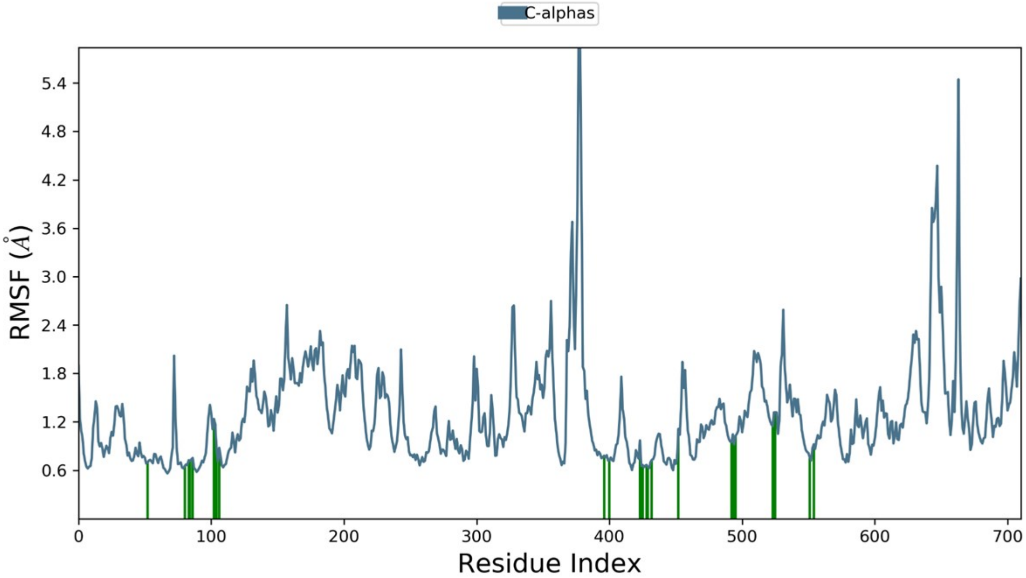


Fig.S62. RMSF curve for IF04 during 500 ns MD simulation.

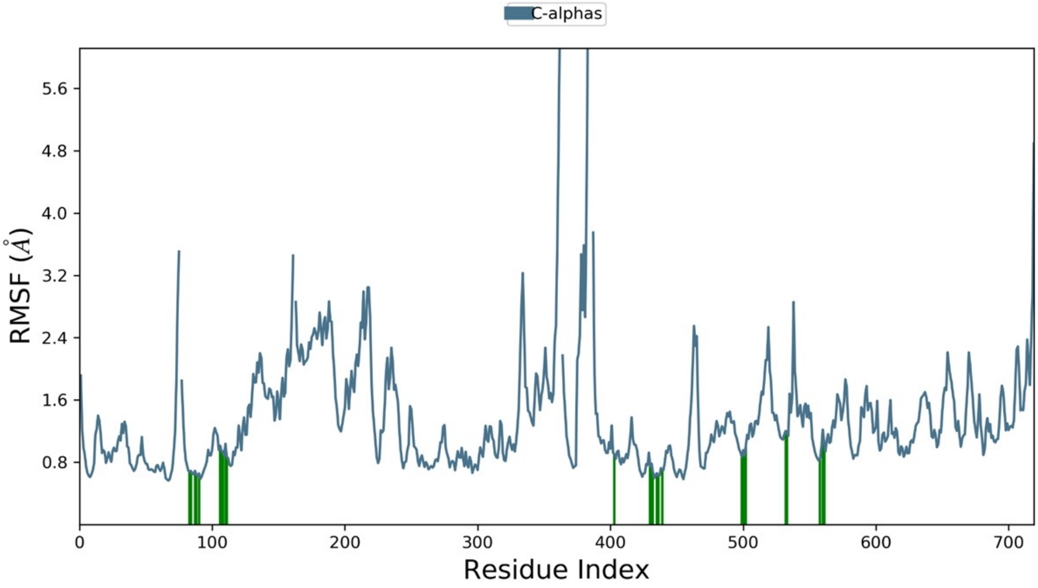


Fig.S63. RMSF curve for IF05 during 500 ns MD simulation.

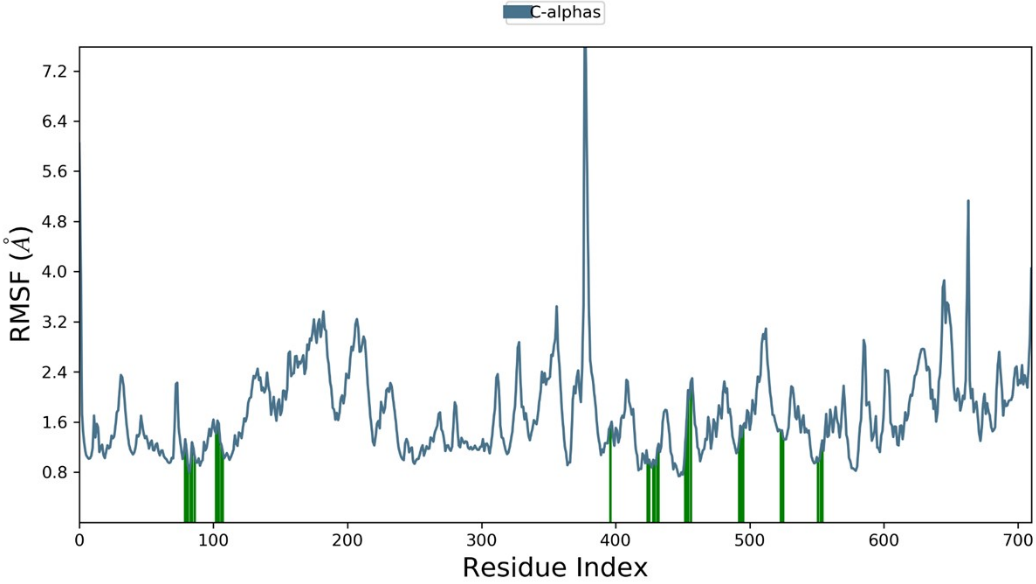


Fig.S64. RMSF curve for IF06 during 500 ns MD simulation.

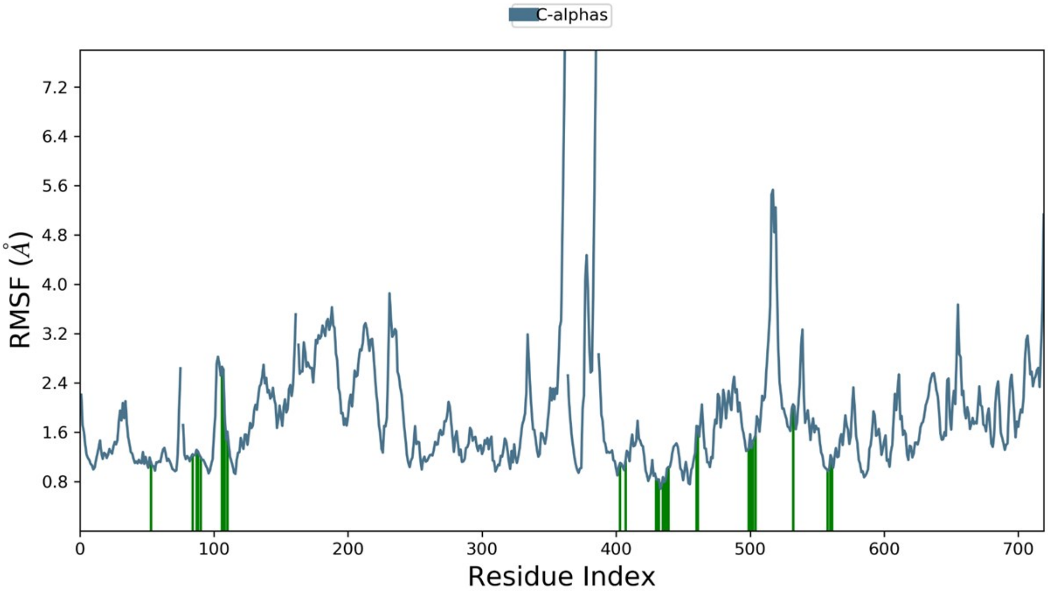


Fig.S65. RMSF curve for IF07 during 500 ns MD simulation.

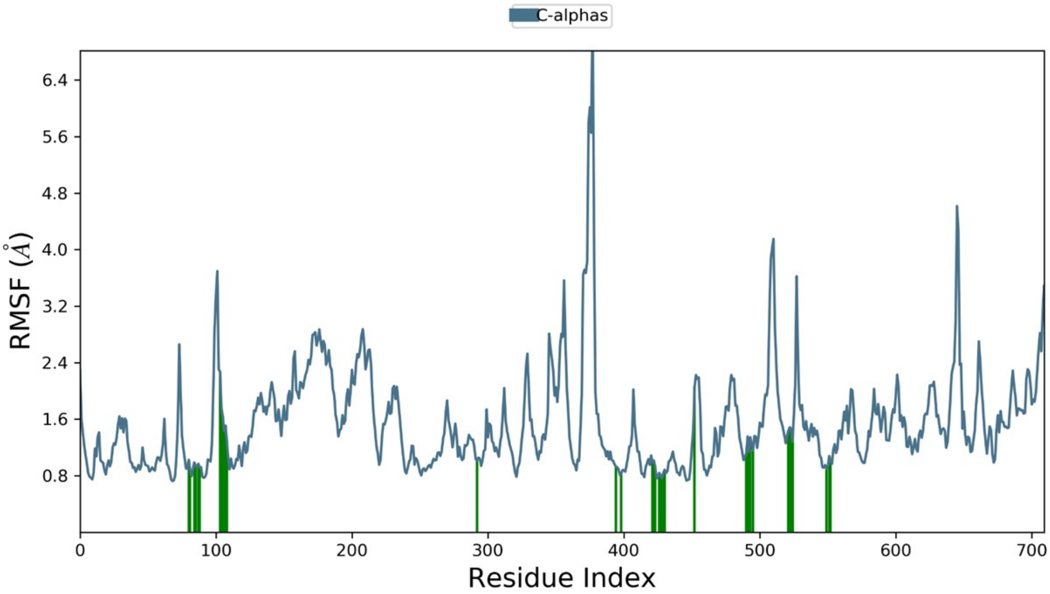


Fig.S66. RMSF curve for IF10 during 500 ns MD simulation.

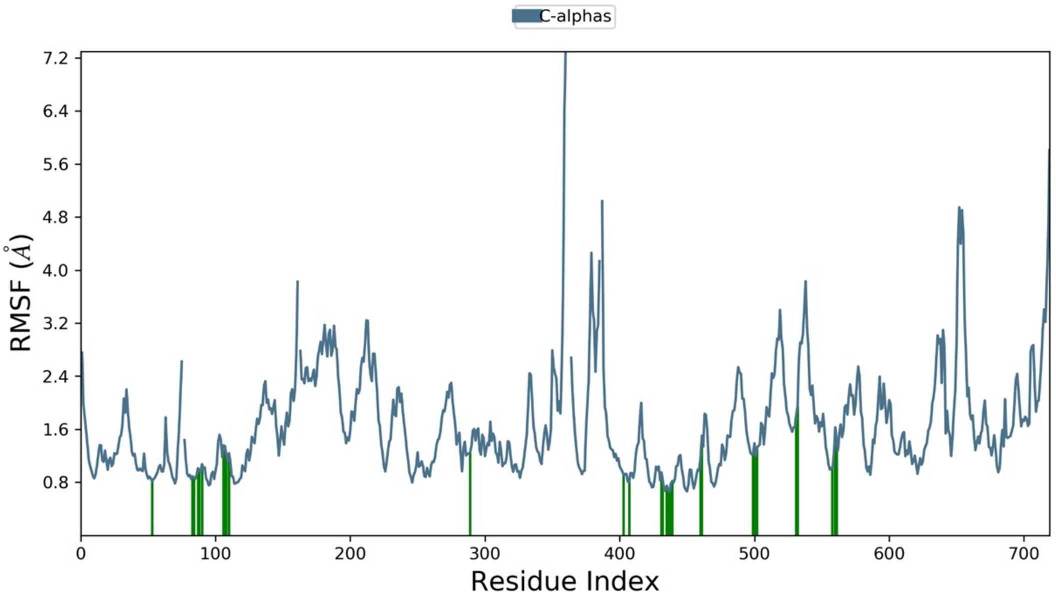


Fig.S67. RMSF curve for IF11 during 500 ns MD simulation.

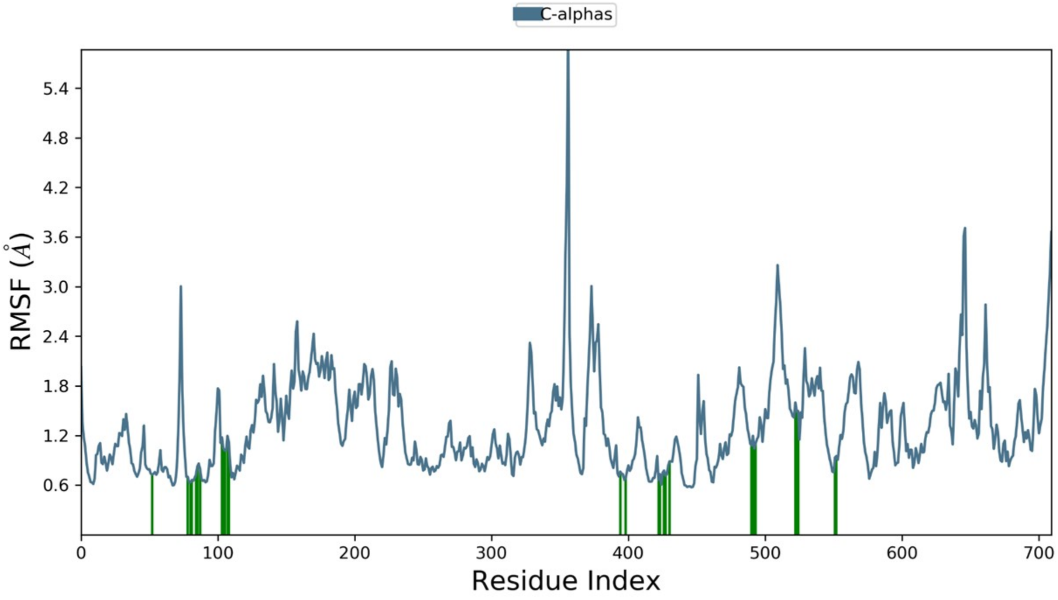


Fig.S68. RMSF curve for IF12 during 500 ns MD simulation.

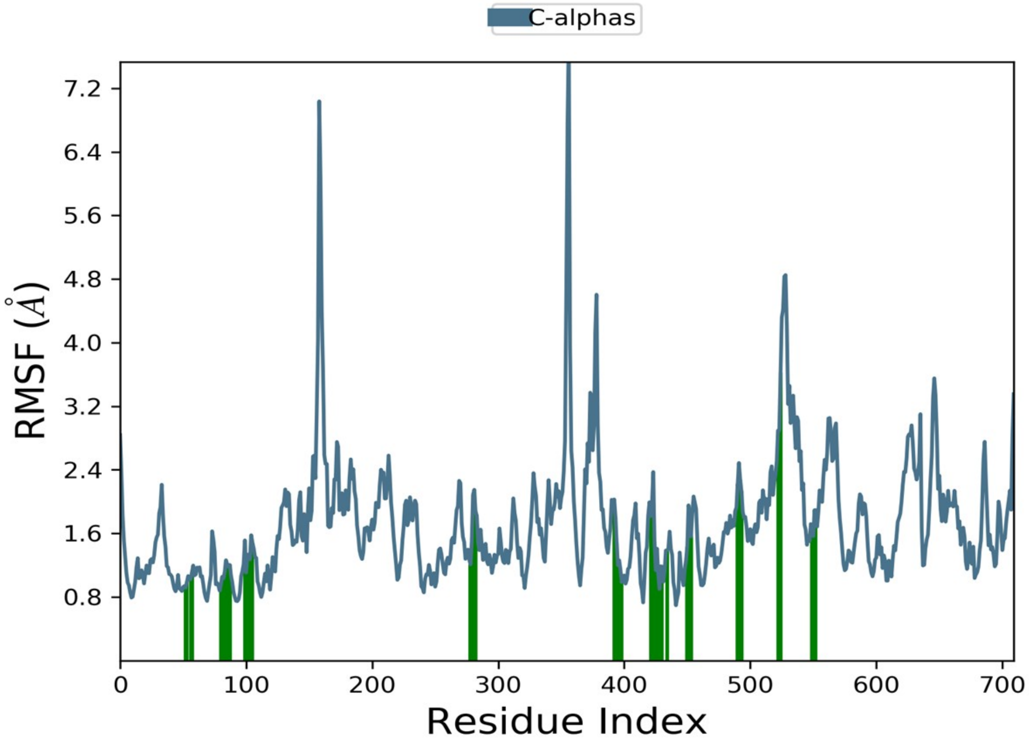


Fig.S69. RMSF curve for ANG01 during 500 ns MD simulation.

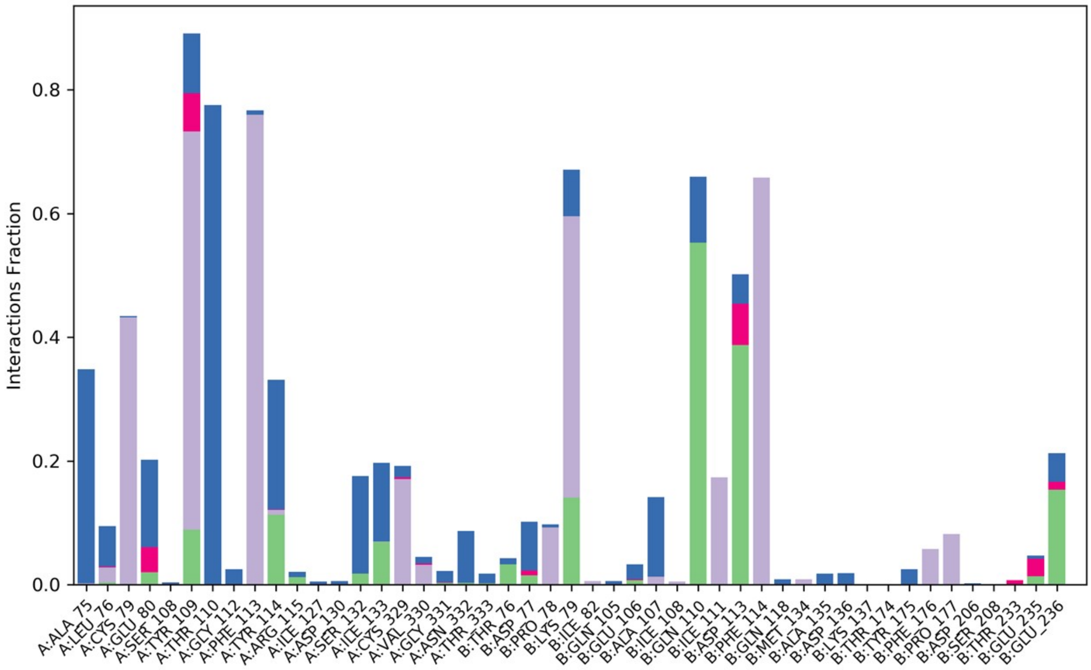


Fig.S70. Bar charts of protein contacts between 5EWJ and ANG01 during 500 ns MD simulation.

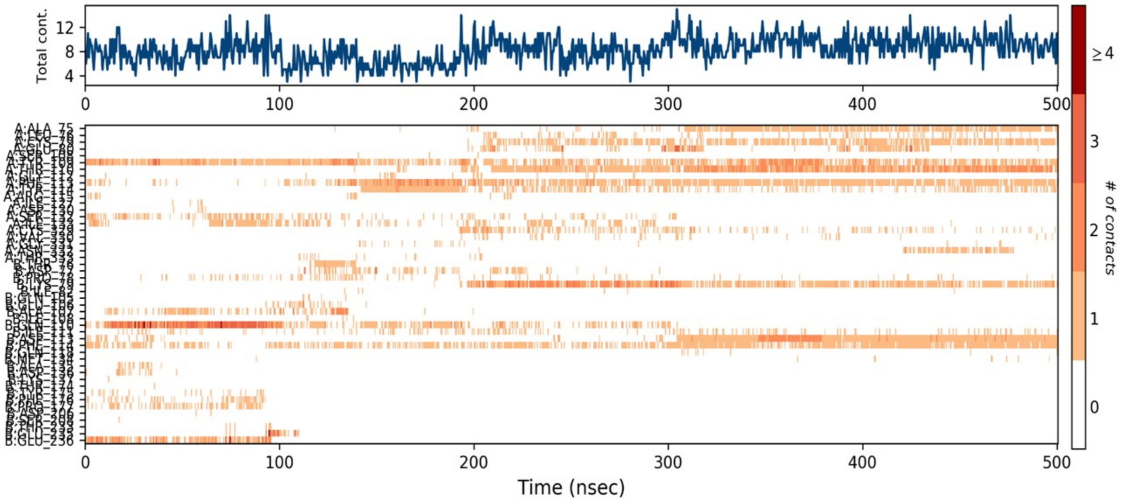


Fig.S71. protein-ligand contacts between 5EWJ and ANG01 during 500 ns MD simulation.

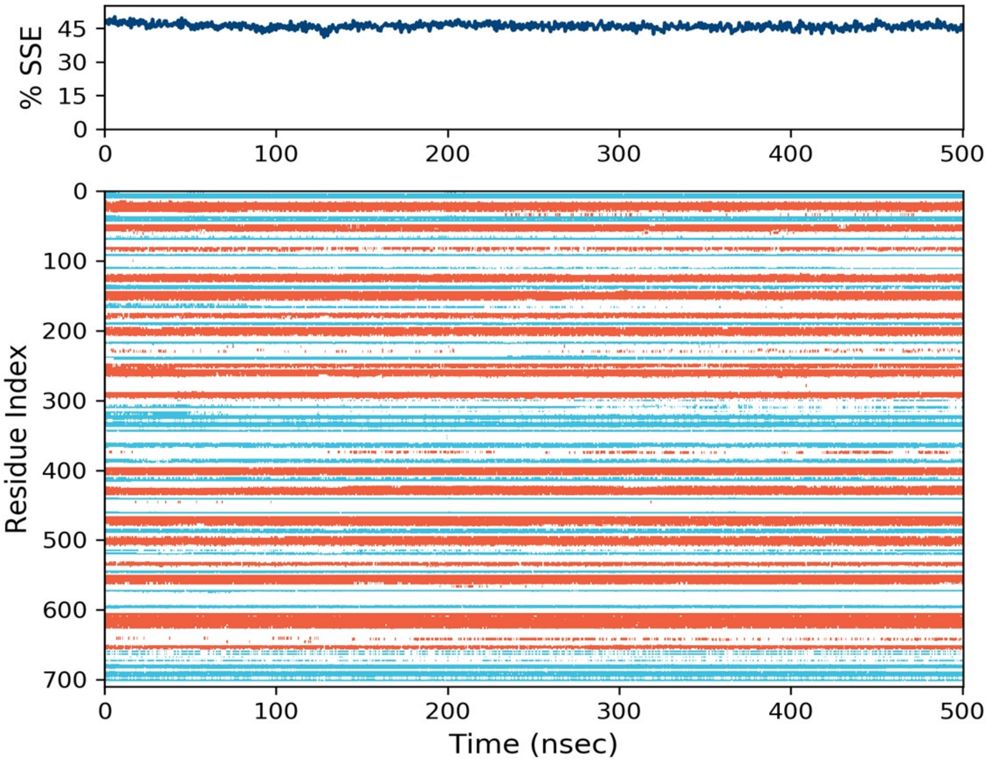


Fig.S72. SSE (Secondary structure element) timeline of 5EWJ/ANG01 complex during 500 ns MD simulation.

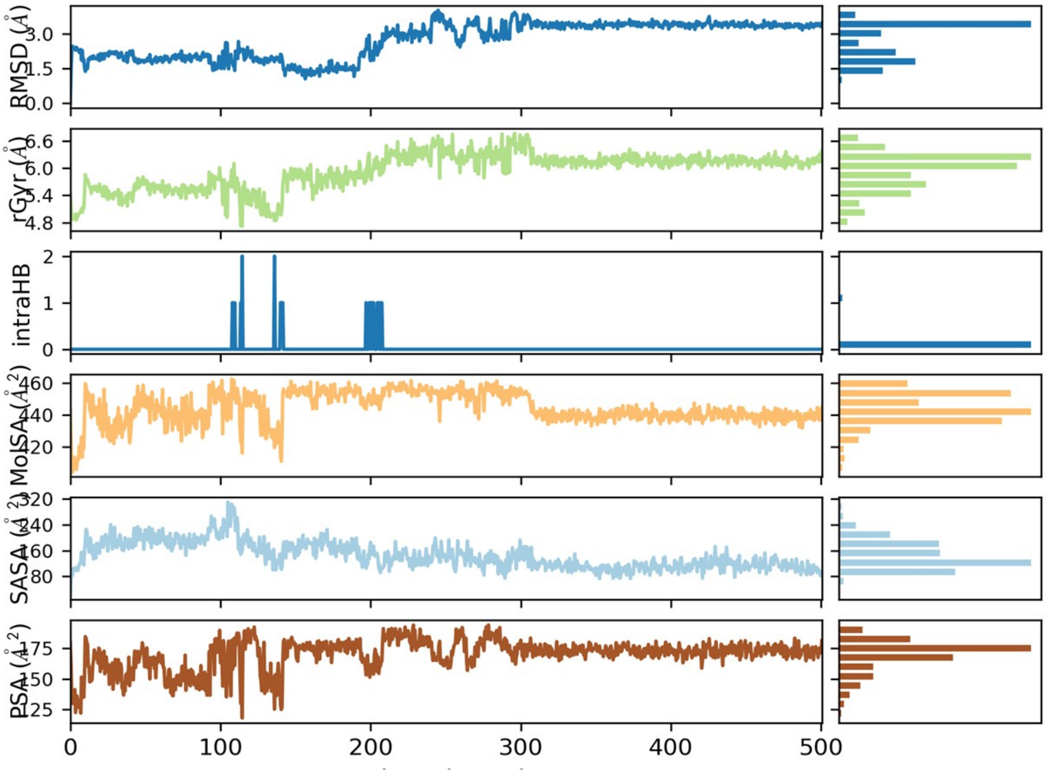


Fig.S73. Ligand properties of ANG01 during 500 ns MD simulation.

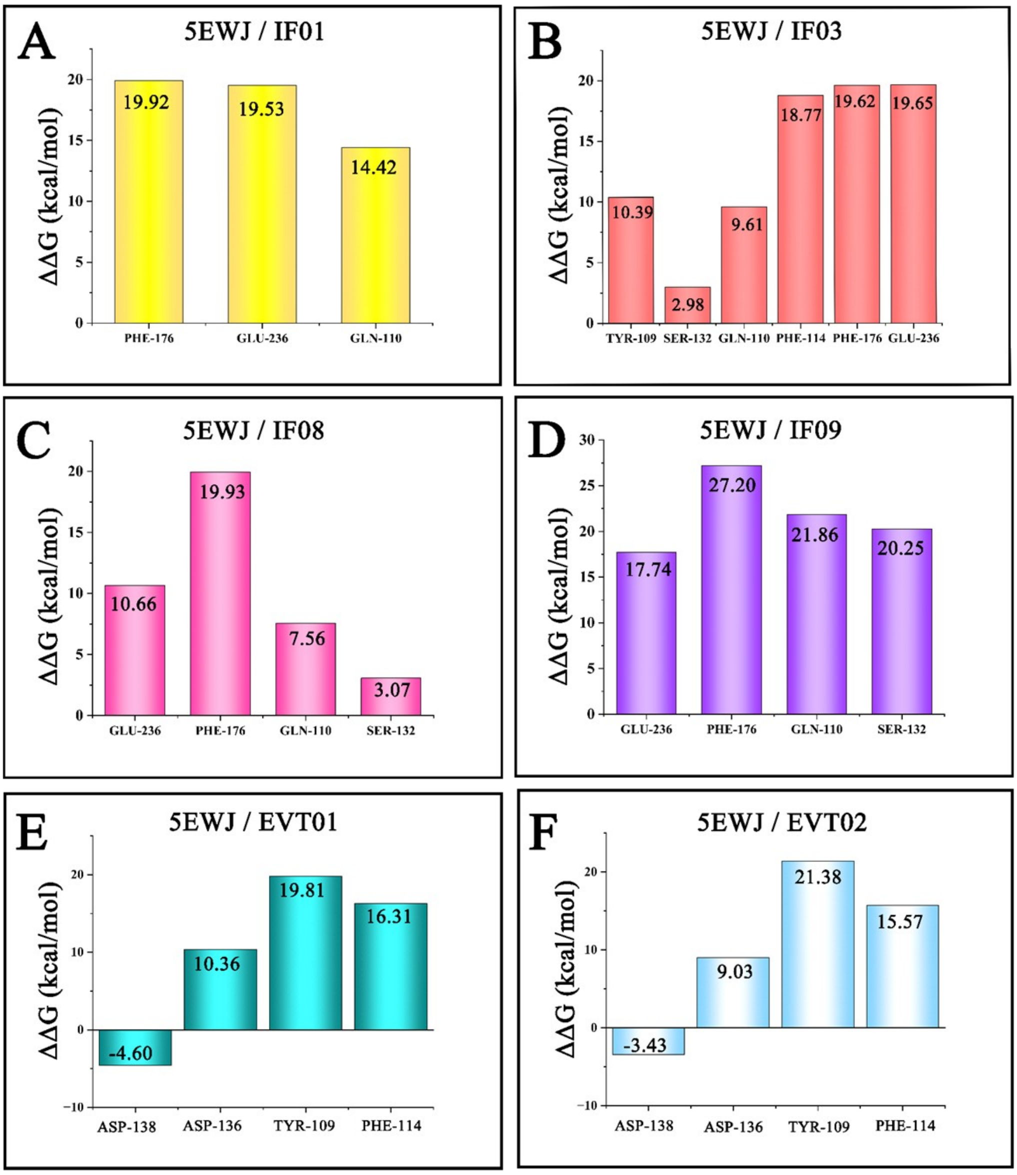


Fig.S74. Static analine scanning mutagenesis analysis of ligands we identified. (A) 5EWJ/IF01, (B) 5EWJ/IF03, (C) 5EWJ/IF08, (D) 5EWJ/IF09, (E) 5EWJ/EVT01, (F) 5EWJ/EVT02.

Supplementary Section

Supplementary Section S1. ADMET prediction of identified ligands for primary and secondary binding pocket

ADMET prediction has been widely used to predict the physical and chemical properties of the potentially active compounds, as well as potential toxicity, to reduce the possible losses and risks in clinical phase. Four ligands screened out for primary binding pocket, two ligands modified for secondary binding pocket and ANG01 were involved to evaluate their further potential in pharmacological and clinical study.

S1.1. ADME prediction

In terms of absorption, water solubility (LogS) values could be divided into two ranges, -6 to -4 and -4 to -2. The compounds within the former range are considered to show low solubility, while the later with high solubility. Five of the six compounds were highly soluble in water. Caco-2 permeability will be optimal when the value is higher than -5.15 log unit, which was shown in IF01, IF03, IF09 and EVT02. All these molecules showed high gastrointestinal absorption and bioavailability, which was quantified as 0.55. For distribution, volume of distribution (VD) was used to assess whether drug was appropriately distributed in vivo, both in blood and tissue, with the optimal value within 0.04-20 L/kg. All the compounds fell within this range except EVT02. Blood-brain barrier (BBB) is a defensive function to prevent those undesired substances from the brain, while the entrance of drugs might also be forbidden. The drugs designed for NMDA receptors are required to cross the BBB because neurodegenerative disease occurs in the central nervous system. Plasma protein binding (PPB) will be optimal when the value is less than 0.9, or drugs with high protein-bound may have a low therapeutic index. All these compounds except EVT01 were not likely to inhibit CYP1A2, while IF03 and IF09 possibly inhibited CYP2C9. Values of half-life estimated the possibility to have long half-life, which is longer than three hours. IF01 showed the shortest half-life and EVT01 the longest.

Table S6.
ADME predictions of the compounds.

ID	**Absorption**				**Distribution**				**Metabolism**		**Excretion**
	Water Solubility (log mol/L)	GI Absorption	Caco-2 Permeability		VD Human (log L/kg)	BBB Penetration	PPB		CYP2C9 Inhibitor	CYP1A2 Inhibitor	$T_{1/2}$
IF01	-4.17	High	-5.119		3.373	Yes	0.699		No	No	0.069
IF03	-3.29	High	-5.150		0.847	Yes	0.688		Yes	No	0.796
IF08	-3.11	High	-5.690		3.857	Yes	0.515		No	No	0.397
IF09	-3.38	High	-5.010		2.425	Yes	0.616		Yes	No	0.701
EVT01	-3.93	High	-5.095		0.610	No	0.938		No	Yes	1.078
EVT02	-3.08	High	-5.258		-0.161	No	0.967		No	No	0.797
ANG01	-3.64	High	-5.899		1.709	No	0.939		No	No	0.923

Table S7.
Toxicity prediction of six compounds.

ID	**hERG Blockers**	**Human Hepatotoxicity**	**DILI**	**AMES Toxicity**	**FDAMDD**	**Eye Irritation**	**IGC_{50}**	**$LC_{50}FM$**	**$LC_{50}DM$**
IF01	0.782	0.916	0.033	0.124	0.832	0.011	3.678	3.893	6.854
IF03	0.085	0.087	0.139	0.108	0.040	0.015	3.149	3.716	3.009
IF08	0.815	0.163	0.028	0.024	0.771	0.011	3.581	3.692	5.082
IF09	0.048	0.284	0.058	0.398	0.641	0.009	4.932	5.473	6.978
EVT01	0.304	0.872	0.997	0.979	0.984	0.000	3.939	4.681	5.078
EVT02	0.037	0.996	0.997	0.944	0.160	0.578	2.983	3.478	4.262
ANG01	0.320	0.024	0.046	0.542	0.945	0.038	4.808	5.392	6.538

S1.2. Toxicity prediction

For the former six indicators, possibility that a molecule exhibited such toxic activity was proportional to its value, ranging from 0 to 1. Proteins encoded by the hERG gene[1] constitutes a potassium channel in the heart, whose blockage would prolong the action potential duration of cardiomyocytes and induce fatal arrhythmias. DILI is drug induced liver injury and FDAMDD indicates maximum recommended daily dose. AMES assay[2] has been widely accepted as a biometric method for assessing the mutagenicity of compounds. Both IF01 and IF08 showed high possibility to be hERG blockers, and IF01 showed high risk of hepatotoxicity. EVT01 and EVT02 showed high risks in human hepatotoxicity, DILI and AMES toxicity. The unit of the later three parameters is -log10[(mg/L)/(1000*MW)], indicating tetrahymena pyriformis 50 percent growth inhibition concentration, 96-hour fathead minnow 50 percent lethal concentration and 48-hour daphnia magna 50 percent lethal concentration respectively. IF03 and IF09 were evaluated to be safe through toxicity prediction.

S1.3. Computational ADMET profiling and advantages over clinical reference

Ifenprodil remains a clinically used NMDA antagonist but suffers from two critical limitations. Studies showed its blood-brain barrier (BBB) permeability was suboptimal (brain/plasma ratio = 0.15), reducing therapeutic efficacy in CNS disorders[3]. 28% incidence of liver enzyme elevation (ALT >3×ULN)[4] at therapeutic doses was also reported in clinical trials. ADMET properties of Ifenprodil as a clinical reference were predicted to evaluate the drug-likeness and translational potential of the identified hits (IF03, IF09) in Table S8. Key metrics that behaved better than Ifenprodil were listed.

Table S8.

Comparison of key ADMET properties between IF03, IF09 and Ifenprodil.

ID	BBB penetration	CYP1A2 inhibitor	CYP2D6 inhibitor	$T_{1/2}$	FDAMDD	hERG blockers	Human hepatotoxicity
Ifenprodil	0.574	0.424	0.990	0.375	0.795	0.828	0.406
IF03	0.758	0.286	0.419	0.796	0.040	0.085	0.087
IF09	0.611	0.304	0.620	0.701	0.641	0.048	0.284

ADMETlab gave the possibility of such properties ranging from 0 to 1. In terms of two crucial problems found in clinical trials, IF03 and IF09 showed enhanced BBB permeability (0.758 and 0.611) compared to Ifenprodil (0.574) and significantly reduced hepatotoxicity (reduced by half and five times less than Ifenprodil). Both hits showed lower CYP1A2 and CYP2D6 inhibition risks, suggesting their metabolic stability. IF03 and IF09 exhibited a 10-fold and 20-fold reduction in hERG blockade activity compared to Ifenprodil respectively, as well as a reduced FDAMDD, indicating their highly improved safety. Furthermore, IF03 and IF09 exhibited a two-fold extension in elimination half-life ($T_{1/2}$ = 0.796 and 0.701) compared to Ifenprodil ($T_{1/2}$ =0.375), significantly reducing dosing frequency while maintaining therapeutic efficacy. Collectively, multi-dimensional advancement in ADMET properties addressed critical barriers in NMDA antagonist therapy, positioning IF03 and IF09 as promising candidates for experimental development.

Supplementary Section S2. Binding free energy calculation via MMGBSA

Binding free energy of the ligand-protein complexes for primary binding pocket were also calculated via method of the molecular mechanics-generalized born surface area (MM-GBSA)[5], which differentiated between the ligands and receptors in each image after the molecular dynamics trajectory was divided into shots of twenty frames. The equation for calculating the MM_GBSA are expressed as:

$$\Delta G_{bind} = G_{complex} - (G_{protein} + G_{ligand}) = \Delta G_{MM} + \Delta G_{sol} - T\Delta S$$

in which two parameters can be elaborated as:

$$\Delta G_{MM} = \Delta G_{ele} + \Delta G_{vdw}$$

$$\Delta G_{sol} = \Delta G_{ele,\, sol} + \Delta G_{nonpol,\, sol}$$

$$\Delta G_{nonpol,\, sol} = \gamma SASA + b$$

ΔG_{bind} indicates the strength of the non-bonding interactions between protein and ligand, the absolute value of which is proportional to the stability of the binding complex. γ is surface tension which was set as 0.0072 kcal/mol $Å^{-2}$. All the four optimized complex systems derived from MD simulations, namely 5EWJ/IF01, 5EWJ/IF03, 5EWJ/IF08 and 5EWJ/IF09 were subjected to rotamer-group conformational search algorithms and GBSA continuous solvation method. MM-GBSA method was performed during the first 200ns as the state of stability had reached within this period. 200 frames were sampled in total for binding free energy calculation with the step length of 2. Fluctuations of ΔG_{bind}, $\Delta G_{coulomb}$, $\Delta G_{covalent}$, ΔG_{Hbond}, ΔG_{lipo}, ΔG_{solv} and ΔG_{vdW} were recorded (Fig.S75).

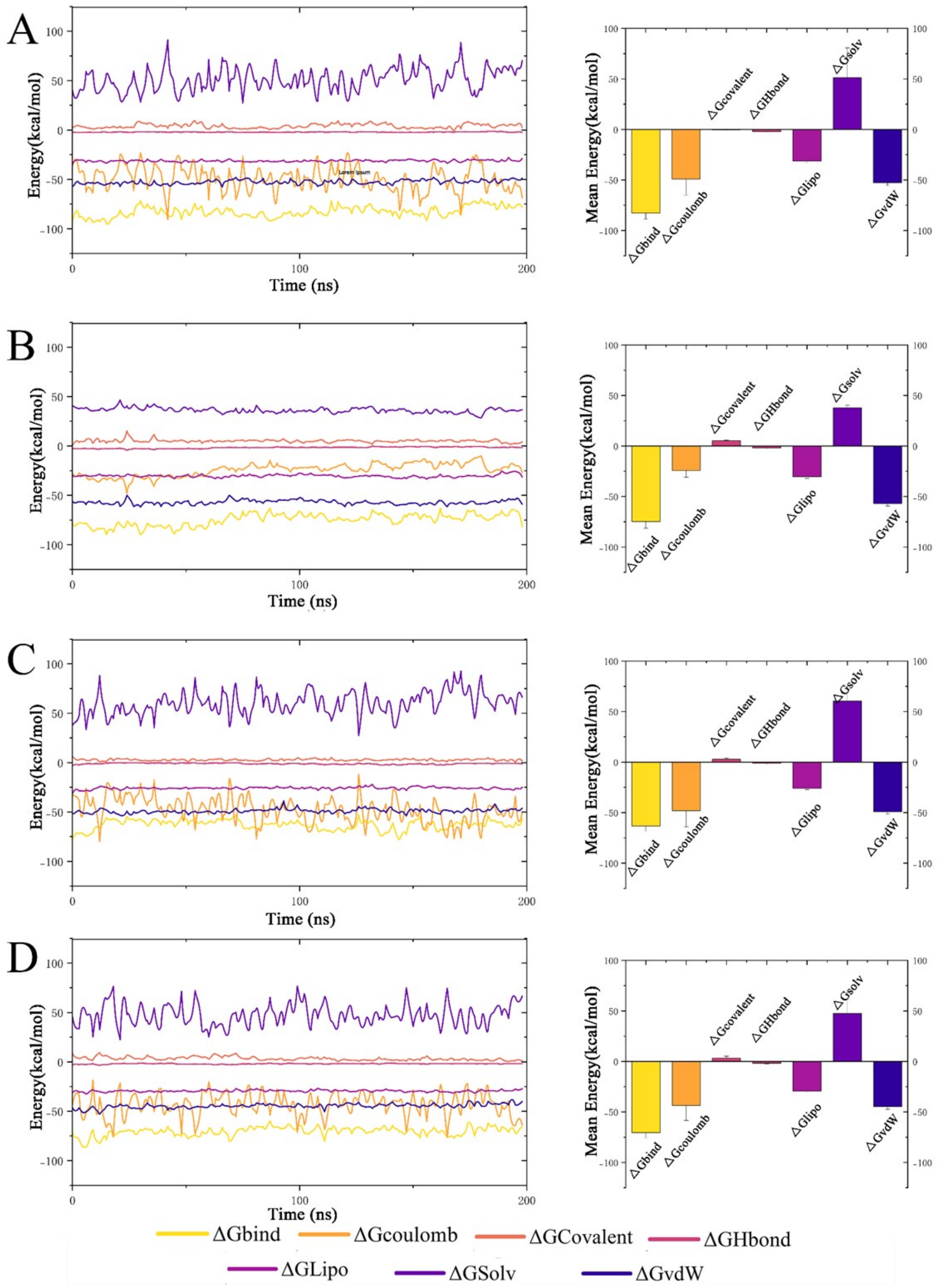


Fig.S75. Spectrum of binding free energies determined by MM-GBSA calculation during the first 200ns MD simulations. (A) 5EWJ/IF01, (B) 5EWJ/IF03, (C) 5EWJ/IF08, (D) 5EWJ/IF09.

Binding affinities between 5EWJ and IF01, 03, 09 were better than that of IF08 due to their lower ΔG_{bind}, which could be possibly attributed to the optimal van der Waals force interactions of IF01, 03 and stronger hydrogen bonds of IF01, 09. Coulomb interaction also stabilized the protein-ligand complexes of IF01 and IF09.

The lowest ΔG_{lipo} of IF01 and IF03 indicated higher binding affinity of their hydrophobic groups with the hydrophobic binding pocket, which aligned with their strong π-π stacking. IF08 was found to show the weakest binding affinity while the ΔG_{solv} of IF08 was highest, indicating the solvation energy would significantly offset the other interactions that stabilized the complex.

Table S9.

Average and standard deviations of binding free energy calculated by MM-GBSA method.

ID	**ΔG_{bind} /kcal • mol^{-1}**	**$\Delta G_{coulomb}$ /kcal • mol^{-1}**	**$\Delta G_{covalent}$ /kcal • mol^{-1}**	**ΔG_{Hbond} /kcal • mol^{-1}**	**ΔG_{lipo} /kcal • mol^{-1}**	**ΔG_{solv} /kcal • mol^{-1}**	**ΔG_{vdW} /kcal • mol^{-1}**	**σ（ΔG_{bind}） /kcal • mol^{-1}**
IF01	-82.79	-49.00	-0.35	-2.11	-31.33	51.35	-52.79	6.056
IF03	-74.79	-24.17	5.20	-1.77	-30.40	37.83	-56.95	6.469
IF08	-63.22	-48.06	2.80	-1.16	-25.92	60.54	-49.05	5.493
IF09	-70.39	-43.49	3.28	-2.01	-29.51	47.50	-44.61	5.287

Supplementary Section S3. Dynamic cross-correlation matrix analysis on primary binding pocket

The stability of the four protein-ligand complexes was compared by dynamic cross-correlation matrix[6], which was plotted in R studio 2024 by the function dccm() in bio3d package[7] after the trajectory and complex documents were loaded. Cross-correlation mapping of protein motions revealed coordinated dynamics patterns, with cyan domains (positive phase) indicating regions of synergistic movement and pink domains (negative phase) marking anti-phase dynamical relationships. Strong positive correlated movement along the diagonal arise from persistent conformational propagation, where displacements initiated at individual residues induce directionally conserved movements in adjacent atoms through bonded potential energy terms[8].

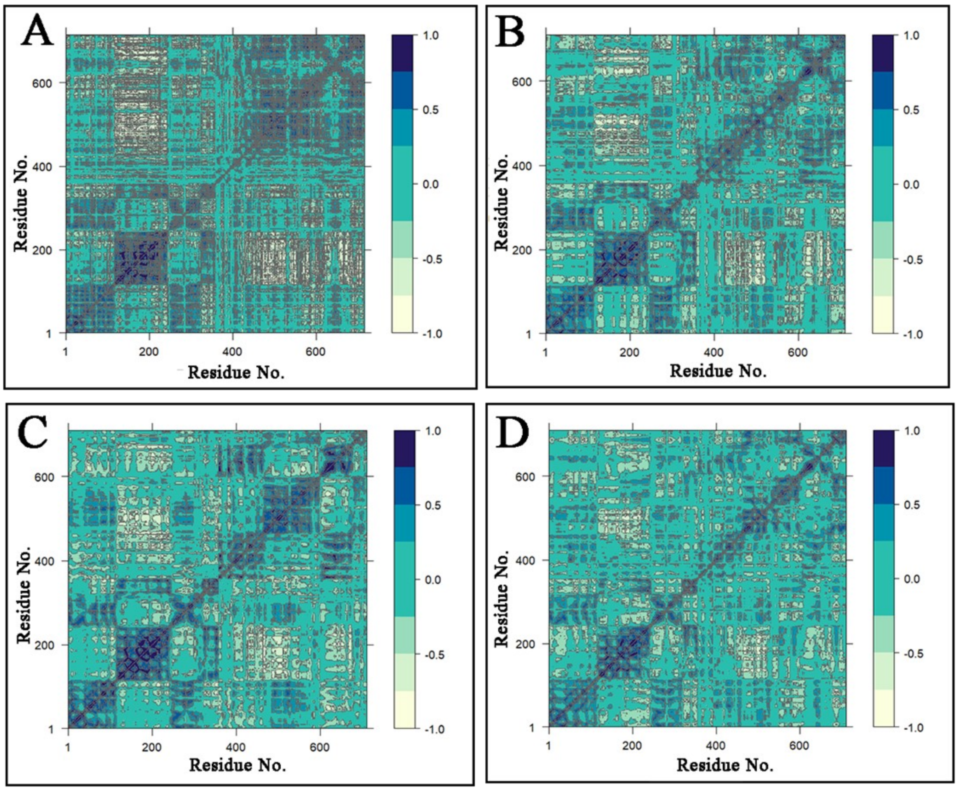


Fig.S76. Dynamic cross-correlation analysis of the four compounds. (A) 5EWJ/IF01, (B) 5EWJ/IF03, (C) 5EWJ/IF08, (D) 5EWJ/IF09.

Among the complex systems, positive movement in the complex of IF01 was found to be strongest. 5EWJ/IF03 and 5EWJ/IF08 systems exhibited relatively mild positive correlated movement in contrast, while the complex of IF09 showed most negative movement. The similarities in the distribution patterns of positive correlated movement along the diagonals of these four complexes verified the virtual screening we have made. Positive movement in residues GLU-236, GLN-110 and PHE-176 were found to be significantly stronger, which were in correspondence with the key amino acids. Notably, the two complex systems with higher stability (5EWJ/IF01 and 5EWJ/IF09) during MD simulations had stronger positive or negative correlated movement, suggesting the flexibility of the protein contributed to the system of protein-ligand complex.

Supplementary materials

Supplementary materials S1. Input structural files of the complex systems for ABFE/RBFE calculations

The input structural files of all the complex systems for ABFE/RBFE calculations have been uploaded as independent files.

Supplementary materials S2. Original co-crystallized complex structure

the original co-crystallized complex structure has been uploaded.

Supplementary materials S3. Original input files for DFT calculation

```
Ifenprodil-ligand
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Ifenprodil-ligand + GLN-110
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Ifenprodil-GLN-110

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Ifenprodil-ligand + GLU-236

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C	-31.13210000	-32.02340000	-15.98800000
C	-29.28750000	-34.26270000	-15.97520000
C	-31.24450000	-33.19040000	-16.93150000
C	-30.05120000	-34.85480000	-18.34540000
C	-30.32210000	-31.22910000	-13.76870000
C	-28.64410000	-34.82090000	-19.16930000
C	-30.41940000	-36.23960000	-17.70930000
C	-30.85900000	-31.33800000	-12.33110000
C	-28.59440000	-35.67830000	-20.43340000
C	-30.43560000	-32.38510000	-11.43100000
C	-31.75100000	-30.38770000	-11.80990000
C	-29.54840000	-35.49440000	-21.48230000
C	-27.59300000	-36.67440000	-20.55520000
C	-31.12550000	-32.52540000	-10.18100000
C	-32.44820000	-30.55750000	-10.57560000
C	-29.38050000	-36.21190000	-22.67300000
C	-27.49390000	-37.37890000	-21.76790000
C	-32.11920000	-31.70400000	-9.76970000
C	-28.37990000	-37.14570000	-22.83580000
H	-26.76600000	-34.85160000	-18.85030000
H	-27.61290000	-38.45210000	-24.14240000
H	-29.31830000	-33.05750000	-17.58710000
H	-31.19210000	-33.17160000	-14.26080000
H	-28.83230000	-33.70480000	-14.14630000
H	-28.22990000	-32.52770000	-15.05140000
H	-30.56250000	-31.19780000	-16.41460000
H	-32.12290000	-31.65950000	-15.71610000
H	-28.24370000	-34.55320000	-16.09440000
H	-29.74260000	-35.19140000	-15.63080000
H	-31.80220000	-34.01590000	-16.48920000
H	-31.75640000	-32.93030000	-17.85800000

H	-30.88770000	-34.62880000	-19.00670000
H	-30.85100000	-30.37530000	-14.19220000
H	-29.30390000	-30.85910000	-13.64860000
H	-28.48240000	-33.81330000	-19.55220000
H	-31.24820000	-36.13590000	-17.00890000
H	-30.83580000	-36.91860000	-18.45340000
H	-29.57360000	-36.68080000	-17.18200000
H	-29.61180000	-33.03700000	-11.68150000
H	-31.89320000	-29.47520000	-12.36990000
H	-30.18210000	-34.62020000	-21.46020000
H	-26.88080000	-36.84320000	-19.76100000
H	-30.78600000	-33.37930000	-9.61360000
H	-33.18740000	-29.80150000	-10.35530000
H	-30.03340000	-36.13010000	-23.52940000
H	-26.72920000	-38.14100000	-21.79740000
H	-32.66270000	-31.86620000	-8.85060000
H	-21.03750000	-43.29330000	-23.08200000
H	-23.66110000	-42.40920000	-20.52110000

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N	-22.85840000	-42.44010000	-21.13340000
C	-23.21740000	-43.15740000	-22.38740000
C	-21.97140000	-43.82960000	-23.00100000
O	-22.05080000	-44.98920000	-23.40010000
C	-23.82370000	-42.07930000	-23.37440000
C	-25.20060000	-41.29280000	-22.95710000
C	-25.32430000	-39.92620000	-23.63300000
O	-24.37300000	-39.27520000	-24.02830000
O	-26.53500000	-39.55060000	-23.84550000
H	-22.54430000	-41.48080000	-21.16790000
H	-23.92640000	-43.96240000	-22.19400000
H	-23.97880000	-42.66770000	-24.27870000
H	-23.02890000	-41.34740000	-23.51830000
H	-25.21200000	-40.96850000	-21.91650000
H	-26.09770000	-41.90270000	-23.06340000
H	-21.03750000	-43.29330000	-23.08200000
H	-23.66110000	-42.40920000	-20.52110000

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N	-34.56330000	-36.84770000	-24.37880000
C	-33.41800000	-36.11060000	-24.00960000
C	-33.63720000	-35.62060000	-22.56580000

O	-32.75890000	-35.75750000	-21.70710000
C	-33.28340000	-34.83900000	-24.89960000
O	-32.10590000	-34.12370000	-24.59750000
H	-35.45050000	-36.37970000	-24.49640000
H	-32.55200000	-36.77060000	-23.95900000
H	-34.15850000	-34.20600000	-24.75240000
H	-33.19090000	-35.06220000	-25.96250000
H	-31.36800000	-34.66450000	-24.83400000
H	-34.57540000	-35.15160000	-22.30860000
H	-34.40400000	-37.29390000	-25.27080000
O	-27.53030000	-35.09860000	-18.35240000
O	-28.37490000	-37.92740000	-23.94980000
N	-29.89340000	-33.82350000	-17.26680000
C	-30.51800000	-32.41710000	-14.66650000
C	-29.15310000	-33.10480000	-14.99790000
C	-31.13210000	-32.02340000	-15.98800000
C	-29.28750000	-34.26270000	-15.97520000
C	-31.24450000	-33.19040000	-16.93150000
C	-30.05120000	-34.85480000	-18.34540000
C	-30.32210000	-31.22910000	-13.76870000
C	-28.64410000	-34.82090000	-19.16930000
C	-30.41940000	-36.23960000	-17.70930000
C	-30.85900000	-31.33800000	-12.33110000
C	-28.59440000	-35.67830000	-20.43340000
C	-30.43560000	-32.38510000	-11.43100000
C	-31.75100000	-30.38770000	-11.80990000
C	-29.54840000	-35.49440000	-21.48230000
C	-27.59300000	-36.67440000	-20.55520000
C	-31.12550000	-32.52540000	-10.18100000
C	-32.44820000	-30.55750000	-10.57560000
C	-29.38050000	-36.21190000	-22.67300000
C	-27.49390000	-37.37890000	-21.76790000
C	-32.11920000	-31.70400000	-9.76970000
C	-28.37990000	-37.14570000	-22.83580000
H	-26.76600000	-34.85160000	-18.85030000
H	-27.61290000	-38.45210000	-24.14240000
H	-29.31830000	-33.05750000	-17.58710000
H	-31.19210000	-33.17160000	-14.26080000
H	-28.83230000	-33.70480000	-14.14630000
H	-28.22990000	-32.52770000	-15.05140000
H	-30.56250000	-31.19780000	-16.41460000
H	-32.12290000	-31.65950000	-15.71610000
H	-28.24370000	-34.55320000	-16.09440000
H	-29.74260000	-35.19140000	-15.63080000

H	-31.80220000	-34.01590000	-16.48920000
H	-31.75640000	-32.93030000	-17.85800000
H	-30.88770000	-34.62880000	-19.00670000
H	-30.85100000	-30.37530000	-14.19220000
H	-29.30390000	-30.85910000	-13.64860000
H	-28.48240000	-33.81330000	-19.55220000
H	-31.24820000	-36.13590000	-17.00890000
H	-30.83580000	-36.91860000	-18.45340000
H	-29.57360000	-36.68080000	-17.18200000
H	-29.61180000	-33.03700000	-11.68150000
H	-31.89320000	-29.47520000	-12.36990000
H	-30.18210000	-34.62020000	-21.46020000
H	-26.88080000	-36.84320000	-19.76100000
H	-30.78600000	-33.37930000	-9.61360000
H	-33.18740000	-29.80150000	-10.35530000
H	-30.03340000	-36.13010000	-23.52940000
H	-26.72920000	-38.14100000	-21.79740000
H	-32.66270000	-31.86620000	-8.85060000

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N	-34.56330000	-36.84770000	-24.37880000
C	-33.41800000	-36.11060000	-24.00960000
C	-33.63720000	-35.62060000	-22.56580000
O	-32.75890000	-35.75750000	-21.70710000
C	-33.28340000	-34.83900000	-24.89960000
O	-32.10590000	-34.12370000	-24.59750000
H	-35.45050000	-36.37970000	-24.49640000
H	-32.55200000	-36.77060000	-23.95900000
H	-34.15850000	-34.20600000	-24.75240000
H	-33.19090000	-35.06220000	-25.96250000
H	-31.36800000	-34.66450000	-24.83400000
H	-34.57540000	-35.15160000	-22.30860000
H	-34.40400000	-37.29390000	-25.27080000

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O	1.94650000	-18.95470000	-26.82070000
O	3.91110000	-18.00510000	-22.68720000
O	-1.37980000	-13.84320000	-28.19690000
N	2.79880000	-19.30900000	-24.21630000
N	9.01750000	-22.00370000	-21.67670000
N	4.75200000	-19.93890000	-23.37490000
C	1.79170000	-18.27560000	-24.54430000

C	1.94000000	-17.83990000	-25.98030000
C	6.79230000	-21.06470000	-22.66640000
C	8.00990000	-20.85480000	-21.76490000
C	0.94620000	-16.73710000	-26.40540000
C	6.08120000	-19.71260000	-22.79380000
C	0.32830000	-18.68470000	-24.12620000
C	3.82250000	-19.02450000	-23.41940000
C	-0.08260000	-17.08670000	-27.31220000
C	0.97260000	-15.45680000	-25.83800000
C	8.70770000	-23.31840000	-21.34380000
C	10.46230000	-21.69000000	-21.44430000
C	-0.91100000	-16.10370000	-27.90930000
C	0.08050000	-14.43170000	-26.33600000
C	-0.75820000	-14.76990000	-27.48560000
C	7.46690000	-23.69490000	-20.78310000
C	9.61720000	-24.32060000	-21.68600000
C	7.19070000	-25.05960000	-20.56000000
C	9.39730000	-25.61010000	-21.26840000
C	8.16580000	-26.05480000	-20.81070000
H	1.14100000	-19.40190000	-26.61020000
H	-1.08320000	-12.96500000	-28.01260000
H	2.75300000	-20.22280000	-24.64420000
H	4.51480000	-20.85500000	-23.72790000
H	1.89280000	-17.42240000	-23.87350000
H	2.95630000	-17.45150000	-26.04600000
H	6.11390000	-21.81040000	-22.25200000
H	7.06370000	-21.40670000	-23.66510000
H	8.40230000	-19.88860000	-22.08190000
H	7.79340000	-20.70050000	-20.70780000
H	5.84620000	-19.20750000	-21.85690000
H	6.59680000	-19.05940000	-23.49780000
H	0.25940000	-18.54660000	-23.04720000
H	-0.47370000	-18.12640000	-24.60920000
H	0.08370000	-19.71250000	-24.39470000
H	-0.18700000	-18.11860000	-27.61320000
H	1.55980000	-15.24840000	-24.95590000
H	11.01380000	-21.48810000	-22.36260000
H	10.54440000	-20.77280000	-20.86120000
H	11.06340000	-22.39410000	-20.86900000
H	-1.69010000	-16.32140000	-28.62490000
H	0.06790000	-13.39950000	-26.01870000
H	6.71570000	-22.99080000	-20.45690000
H	10.58050000	-24.10810000	-22.12550000
H	6.27430000	-25.31960000	-20.05110000

H	10.29710000	-26.19350000	-21.39630000
H	8.08880000	-27.08790000	-20.50560000

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N	4.07080000	-20.57560000	-16.83850000
C	4.13610000	-21.70590000	-17.82170000
C	5.40280000	-22.63740000	-17.60780000
O	5.24970000	-23.84380000	-17.76730000
C	4.07710000	-21.16030000	-19.33810000
C	3.01590000	-20.01230000	-19.63270000
C	1.54100000	-20.40170000	-19.87760000
O	0.68780000	-19.53450000	-20.05900000
N	1.21750000	-21.66270000	-20.04380000
H	4.10580000	-19.60740000	-17.12400000
H	3.25680000	-22.32460000	-17.64270000
H	3.88820000	-21.95870000	-20.05580000
H	5.06490000	-20.83660000	-19.66600000
H	3.28150000	-19.34170000	-20.44990000
H	3.11280000	-19.39130000	-18.74210000
H	0.29740000	-21.90190000	-20.38460000
H	1.88430000	-22.41920000	-20.10010000
O	1.94650000	-18.95470000	-26.82070000
O	3.91110000	-18.00510000	-22.68720000
O	-1.37980000	-13.84320000	-28.19690000
N	2.79880000	-19.30900000	-24.21630000
N	9.01750000	-22.00370000	-21.67670000
N	4.75200000	-19.93890000	-23.37490000
C	1.79170000	-18.27560000	-24.54430000
C	1.94000000	-17.83990000	-25.98030000
C	6.79230000	-21.06470000	-22.66640000
C	8.00990000	-20.85480000	-21.76490000
C	0.94620000	-16.73710000	-26.40540000
C	6.08120000	-19.71260000	-22.79380000
C	0.32830000	-18.68470000	-24.12620000
C	3.82250000	-19.02450000	-23.41940000
C	-0.08260000	-17.08670000	-27.31220000
C	0.97260000	-15.45680000	-25.83800000
C	8.70770000	-23.31840000	-21.34380000
C	10.46230000	-21.69000000	-21.44430000
C	-0.91100000	-16.10370000	-27.90930000
C	0.08050000	-14.43170000	-26.33600000
C	-0.75820000	-14.76990000	-27.48560000
C	7.46690000	-23.69490000	-20.78310000

C	9.61720000	-24.32060000	-21.68600000
C	7.19070000	-25.05960000	-20.56000000
C	9.39730000	-25.61010000	-21.26840000
C	8.16580000	-26.05480000	-20.81070000
H	1.14100000	-19.40190000	-26.61020000
H	-1.08320000	-12.96500000	-28.01260000
H	2.75300000	-20.22280000	-24.64420000
H	4.51480000	-20.85500000	-23.72790000
H	1.89280000	-17.42240000	-23.87350000
H	2.95630000	-17.45150000	-26.04600000
H	6.11390000	-21.81040000	-22.25200000
H	7.06370000	-21.40670000	-23.66510000
H	8.40230000	-19.88860000	-22.08190000
H	7.79340000	-20.70050000	-20.70780000
H	5.84620000	-19.20750000	-21.85690000
H	6.59680000	-19.05940000	-23.49780000
H	0.25940000	-18.54660000	-23.04720000
H	-0.47370000	-18.12640000	-24.60920000
H	0.08370000	-19.71250000	-24.39470000
H	-0.18700000	-18.11860000	-27.61320000
H	1.55980000	-15.24840000	-24.95590000
H	11.01380000	-21.48810000	-22.36260000
H	10.54440000	-20.77280000	-20.86120000
H	11.06340000	-22.39410000	-20.86900000
H	-1.69010000	-16.32140000	-28.62490000
H	0.06790000	-13.39950000	-26.01870000
H	6.71570000	-22.99080000	-20.45690000
H	10.58050000	-24.10810000	-22.12550000
H	6.27430000	-25.31960000	-20.05110000
H	10.29710000	-26.19350000	-21.39630000
H	8.08880000	-27.08790000	-20.50560000
H	3.20160000	-20.62410000	-16.32630000
H	6.37170000	-22.24770000	-17.33260000

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N	4.07080000	-20.57560000	-16.83850000
C	4.13610000	-21.70590000	-17.82170000
C	5.40280000	-22.63740000	-17.60780000
O	5.24970000	-23.84380000	-17.76730000
C	4.07710000	-21.16030000	-19.33810000
C	3.01590000	-20.01230000	-19.63270000
C	1.54100000	-20.40170000	-19.87760000
O	0.68780000	-19.53450000	-20.05900000

N	1.21750000	-21.66270000	-20.04380000
H	4.10580000	-19.60740000	-17.12400000
H	3.25680000	-22.32460000	-17.64270000
H	3.88820000	-21.95870000	-20.05580000
H	5.06490000	-20.83660000	-19.66600000
H	3.28150000	-19.34170000	-20.44990000
H	3.11280000	-19.39130000	-18.74210000
H	0.29740000	-21.90190000	-20.38460000
H	1.88430000	-22.41920000	-20.10010000
H	3.20160000	-20.62410000	-16.32630000
H	6.37170000	-22.24770000	-17.33260000

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-1 1

N	0.65800000	-7.94970000	-27.42560000
C	-0.38990000	-7.56630000	-28.39490000
C	-0.80540000	-6.09220000	-28.12210000
O	-1.00170000	-5.36980000	-29.08690000
C	-1.63340000	-8.54790000	-28.35190000
C	-1.53150000	-9.76440000	-29.29120000
C	-0.40280000	-10.63320000	-28.95980000
O	-0.36690000	-11.16980000	-27.80230000
O	0.39370000	-10.91310000	-29.85790000
H	0.42100000	-8.42480000	-26.56640000
H	-0.04980000	-7.62910000	-29.42860000
H	-2.47590000	-7.92330000	-28.64890000
H	-1.77590000	-8.85550000	-27.31600000
H	-1.49340000	-9.47710000	-30.34200000
H	-2.45170000	-10.34840000	-29.27030000
O	1.94650000	-18.95470000	-26.82070000
O	3.91110000	-18.00510000	-22.68720000
O	-1.37980000	-13.84320000	-28.19690000
N	2.79880000	-19.30900000	-24.21630000
N	9.01750000	-22.00370000	-21.67670000
N	4.75200000	-19.93890000	-23.37490000
C	1.79170000	-18.27560000	-24.54430000
C	1.94000000	-17.83990000	-25.98030000
C	6.79230000	-21.06470000	-22.66640000
C	8.00990000	-20.85480000	-21.76490000
C	0.94620000	-16.73710000	-26.40540000
C	6.08120000	-19.71260000	-22.79380000
C	0.32830000	-18.68470000	-24.12620000
C	3.82250000	-19.02450000	-23.41940000
C	-0.08260000	-17.08670000	-27.31220000

C	0.97260000	-15.45680000	-25.83800000
C	8.70770000	-23.31840000	-21.34380000
C	10.46230000	-21.69000000	-21.44430000
C	-0.91100000	-16.10370000	-27.90930000
C	0.08050000	-14.43170000	-26.33600000
C	-0.75820000	-14.76990000	-27.48560000
C	7.46690000	-23.69490000	-20.78310000
C	9.61720000	-24.32060000	-21.68600000
C	7.19070000	-25.05960000	-20.56000000
C	9.39730000	-25.61010000	-21.26840000
C	8.16580000	-26.05480000	-20.81070000
H	1.14100000	-19.40190000	-26.61020000
H	-1.08320000	-12.96500000	-28.01260000
H	2.75300000	-20.22280000	-24.64420000
H	4.51480000	-20.85500000	-23.72790000
H	1.89280000	-17.42240000	-23.87350000
H	2.95630000	-17.45150000	-26.04600000
H	6.11390000	-21.81040000	-22.25200000
H	7.06370000	-21.40670000	-23.66510000
H	8.40230000	-19.88860000	-22.08190000
H	7.79340000	-20.70050000	-20.70780000
H	5.84620000	-19.20750000	-21.85690000
H	6.59680000	-19.05940000	-23.49780000
H	0.25940000	-18.54660000	-23.04720000
H	-0.47370000	-18.12640000	-24.60920000
H	0.08370000	-19.71250000	-24.39470000
H	-0.18700000	-18.11860000	-27.61320000
H	1.55980000	-15.24840000	-24.95590000
H	11.01380000	-21.48810000	-22.36260000
H	10.54440000	-20.77280000	-20.86120000
H	11.06340000	-22.39410000	-20.86900000
H	-1.69010000	-16.32140000	-28.62490000
H	0.06790000	-13.39950000	-26.01870000
H	6.71570000	-22.99080000	-20.45690000
H	10.58050000	-24.10810000	-22.12550000
H	6.27430000	-25.31960000	-20.05110000
H	10.29710000	-26.19350000	-21.39630000
H	8.08880000	-27.08790000	-20.50560000
H	-0.92170000	-5.70110000	-27.12210000
H	1.31360000	-8.57740000	-27.86850000

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-1 1

N	0.65800000	-7.94970000	-27.42560000

C	-0.38990000	-7.56630000	-28.39490000
C	-0.80540000	-6.09220000	-28.12210000
O	-1.00170000	-5.36980000	-29.08690000
C	-1.63340000	-8.54790000	-28.35190000
C	-1.53150000	-9.76440000	-29.29120000
C	-0.40280000	-10.63320000	-28.95980000
O	-0.36690000	-11.16980000	-27.80230000
O	0.39370000	-10.91310000	-29.85790000
H	0.42100000	-8.42480000	-26.56640000
H	-0.04980000	-7.62910000	-29.42860000
H	-2.47590000	-7.92330000	-28.64890000
H	-1.77590000	-8.85550000	-27.31600000
H	-1.49340000	-9.47710000	-30.34200000
H	-2.45170000	-10.34840000	-29.27030000
H	-0.92170000	-5.70110000	-27.12210000
H	1.31360000	-8.57740000	-27.86850000

IF03-ligand + SER-132
0 1

N	-1.69230000	-21.00670000	-29.96670000
C	-2.04130000	-20.59850000	-28.60870000
C	-0.95930000	-21.04600000	-27.62460000
O	-0.58990000	-20.39020000	-26.66080000
C	-3.37490000	-21.32490000	-28.24820000
O	-3.62960000	-22.52890000	-28.88120000
H	-1.78940000	-22.00130000	-30.11260000
H	-2.16880000	-19.51680000	-28.56530000
H	-4.25500000	-20.71690000	-28.45720000
H	-3.43260000	-21.72100000	-27.23430000
H	-2.80320000	-22.91860000	-29.12280000
H	-2.29700000	-20.53750000	-30.62570000
H	-0.51410000	-22.00930000	-27.82490000
O	1.94650000	-18.95470000	-26.82070000
O	3.91110000	-18.00510000	-22.68720000
O	-1.37980000	-13.84320000	-28.19690000
N	2.79880000	-19.30900000	-24.21630000
N	9.01750000	-22.00370000	-21.67670000
N	4.75200000	-19.93890000	-23.37490000
C	1.79170000	-18.27560000	-24.54430000
C	1.94000000	-17.83990000	-25.98030000
C	6.79230000	-21.06470000	-22.66640000
C	8.00990000	-20.85480000	-21.76490000
C	0.94620000	-16.73710000	-26.40540000
C	6.08120000	-19.71260000	-22.79380000

C	0.32830000	-18.68470000	-24.12620000
C	3.82250000	-19.02450000	-23.41940000
C	-0.08260000	-17.08670000	-27.31220000
C	0.97260000	-15.45680000	-25.83800000
C	8.70770000	-23.31840000	-21.34380000
C	10.46230000	-21.69000000	-21.44430000
C	-0.91100000	-16.10370000	-27.90930000
C	0.08050000	-14.43170000	-26.33600000
C	-0.75820000	-14.76990000	-27.48560000
C	7.46690000	-23.69490000	-20.78310000
C	9.61720000	-24.32060000	-21.68600000
C	7.19070000	-25.05960000	-20.56000000
C	9.39730000	-25.61010000	-21.26840000
C	8.16580000	-26.05480000	-20.81070000
H	1.14100000	-19.40190000	-26.61020000
H	-1.08320000	-12.96500000	-28.01260000
H	2.75300000	-20.22280000	-24.64420000
H	4.51480000	-20.85500000	-23.72790000
H	1.89280000	-17.42240000	-23.87350000
H	2.95630000	-17.45150000	-26.04600000
H	6.11390000	-21.81040000	-22.25200000
H	7.06370000	-21.40670000	-23.66510000
H	8.40230000	-19.88860000	-22.08190000
H	7.79340000	-20.70050000	-20.70780000
H	5.84620000	-19.20750000	-21.85690000
H	6.59680000	-19.05940000	-23.49780000
H	0.25940000	-18.54660000	-23.04720000
H	-0.47370000	-18.12640000	-24.60920000
H	0.08370000	-19.71250000	-24.39470000
H	-0.18700000	-18.11860000	-27.61320000
H	1.55980000	-15.24840000	-24.95590000
H	11.01380000	-21.48810000	-22.36260000
H	10.54440000	-20.77280000	-20.86120000
H	11.06340000	-22.39410000	-20.86900000
H	-1.69010000	-16.32140000	-28.62490000
H	0.06790000	-13.39950000	-26.01870000
H	6.71570000	-22.99080000	-20.45690000
H	10.58050000	-24.10810000	-22.12550000
H	6.27430000	-25.31960000	-20.05110000
H	10.29710000	-26.19350000	-21.39630000
H	8.08880000	-27.08790000	-20.50560000

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0 1

N	-1.69230000	-21.00670000	-29.96670000
C	-2.04130000	-20.59850000	-28.60870000
C	-0.95930000	-21.04600000	-27.62460000
O	-0.58990000	-20.39020000	-26.66080000
C	-3.37490000	-21.32490000	-28.24820000
O	-3.62960000	-22.52890000	-28.88120000
H	-1.78940000	-22.00130000	-30.11260000
H	-2.16880000	-19.51680000	-28.56530000
H	-4.25500000	-20.71690000	-28.45720000
H	-3.43260000	-21.72100000	-27.23430000
H	-2.80320000	-22.91860000	-29.12280000
H	-2.29700000	-20.53750000	-30.62570000
H	-0.51410000	-22.00930000	-27.82490000

IF09-ligand
1 1

O	15.17230000	37.94810000	19.79560000
O	18.77280000	48.11890000	21.24210000
O	14.11260000	33.35740000	15.50320000
N	15.50820000	40.34420000	18.57240000
C	15.91430000	41.57260000	17.95290000
C	16.06010000	42.66290000	19.07920000
C	15.78650000	44.09160000	18.51440000
C	15.27480000	39.14980000	17.71950000
C	14.50220000	38.15930000	18.57180000
C	17.15130000	41.61200000	17.05780000
C	16.49320000	45.21670000	19.26640000
C	14.29300000	36.80160000	17.74990000
C	17.36830000	46.01060000	18.51600000
C	16.33090000	45.47010000	20.64630000
C	13.59920000	36.81760000	16.53220000
C	14.97150000	35.60750000	18.19560000
C	18.12980000	47.07240000	19.14710000
C	17.11310000	46.43110000	21.28330000
C	13.55250000	35.63200000	15.79040000
C	14.86700000	34.43840000	17.51690000
C	18.05850000	47.18250000	20.55200000
C	14.16600000	34.45470000	16.31720000
H	14.86270000	37.17140000	20.23600000
H	18.40590000	48.33940000	22.08460000
H	13.55850000	33.38460000	14.73820000
H	14.59790000	40.56800000	18.94850000
H	16.12200000	40.08700000	19.33210000
H	15.04500000	41.78960000	17.33220000

H	17.10240000	42.72220000	19.39250000
H	15.40800000	42.43620000	19.92270000
H	14.74070000	44.38680000	18.42960000
H	16.13900000	44.03470000	17.48450000
H	16.13850000	38.80660000	17.14990000
H	14.70480000	39.40710000	16.82680000
H	13.51150000	38.54220000	18.81680000
H	17.48650000	42.56880000	16.65740000
H	18.00380000	41.27330000	17.64660000
H	16.98540000	40.92640000	16.22680000
H	17.45460000	45.88150000	17.44730000
H	15.67340000	44.96400000	21.33760000
H	13.29350000	37.74540000	16.07140000
H	15.49290000	35.55530000	19.13990000
H	18.80620000	47.80820000	18.73790000
H	17.02140000	46.52430000	22.35530000
H	13.13550000	35.68200000	14.79540000
H	15.29750000	33.50910000	17.85950000

IF09-ligand + GLN-110

1 1

N	10.74410000	45.61600000	21.04950000
C	11.79680000	44.91510000	21.79100000
C	12.83160000	46.03780000	22.16590000
O	13.53960000	45.93690000	23.17380000
C	12.41570000	43.72620000	20.93160000
C	11.35650000	42.68920000	20.33880000
C	11.90350000	41.73630000	19.22720000
O	13.09120000	41.34740000	19.20090000
N	11.00220000	41.46110000	18.35700000
H	10.89770000	45.68490000	20.05360000
H	11.39760000	44.49780000	22.71550000
H	13.19590000	43.20150000	21.48300000
H	12.94550000	44.05070000	20.03590000
H	10.48580000	43.22140000	19.95580000
H	10.85070000	42.04980000	21.06230000
H	11.18890000	40.99350000	17.48140000
H	10.01840000	41.65720000	18.47410000
O	15.17230000	37.94810000	19.79560000
O	18.77280000	48.11890000	21.24210000
O	14.11260000	33.35740000	15.50320000
N	15.50820000	40.34420000	18.57240000
C	15.91430000	41.57260000	17.95290000
C	16.06010000	42.66290000	19.07920000

C	15.78650000	44.09160000	18.51440000
C	15.27480000	39.14980000	17.71950000
C	14.50220000	38.15930000	18.57180000
C	17.15130000	41.61200000	17.05780000
C	16.49320000	45.21670000	19.26640000
C	14.29300000	36.80160000	17.74990000
C	17.36830000	46.01060000	18.51600000
C	16.33090000	45.47010000	20.64630000
C	13.59920000	36.81760000	16.53220000
C	14.97150000	35.60750000	18.19560000
C	18.12980000	47.07240000	19.14710000
C	17.11310000	46.43110000	21.28330000
C	13.55250000	35.63200000	15.79040000
C	14.86700000	34.43840000	17.51690000
C	18.05850000	47.18250000	20.55200000
C	14.16600000	34.45470000	16.31720000
H	14.86270000	37.17140000	20.23600000
H	18.40590000	48.33940000	22.08460000
H	13.55850000	33.38460000	14.73820000
H	14.59790000	40.56800000	18.94850000
H	16.12200000	40.08700000	19.33210000
H	15.04500000	41.78960000	17.33220000
H	17.10240000	42.72220000	19.39250000
H	15.40800000	42.43620000	19.92270000
H	14.74070000	44.38680000	18.42960000
H	16.13900000	44.03470000	17.48450000
H	16.13850000	38.80660000	17.14990000
H	14.70480000	39.40710000	16.82680000
H	13.51150000	38.54220000	18.81680000
H	17.48650000	42.56880000	16.65740000
H	18.00380000	41.27330000	17.64660000
H	16.98540000	40.92640000	16.22680000
H	17.45460000	45.88150000	17.44730000
H	15.67340000	44.96400000	21.33760000
H	13.29350000	37.74540000	16.07140000
H	15.49290000	35.55530000	19.13990000
H	18.80620000	47.80820000	18.73790000
H	17.02140000	46.52430000	22.35530000
H	13.13550000	35.68200000	14.79540000
H	15.29750000	33.50910000	17.85950000
H	12.91910000	46.90580000	21.52920000
H	9.86560000	45.13350000	21.17390000

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N	10.74410000	45.61600000	21.04950000
C	11.79680000	44.91510000	21.79100000
C	12.83160000	46.03780000	22.16590000
O	13.53960000	45.93690000	23.17380000
C	12.41570000	43.72620000	20.93160000
C	11.35650000	42.68920000	20.33880000
C	11.90350000	41.73630000	19.22720000
O	13.09120000	41.34740000	19.20090000
N	11.00220000	41.46110000	18.35700000
H	10.89770000	45.68490000	20.05360000
H	11.39760000	44.49780000	22.71550000
H	13.19590000	43.20150000	21.48300000
H	12.94550000	44.05070000	20.03590000
H	10.48580000	43.22140000	19.95580000
H	10.85070000	42.04980000	21.06230000
H	11.18890000	40.99350000	17.48140000
H	10.01840000	41.65720000	18.47410000
H	12.91910000	46.90580000	21.52920000
H	9.86560000	45.13350000	21.17390000

IF09-ligand + GLU-236

0 1

N	10.85090000	35.53200000	8.66390000
C	10.85940000	34.07880000	8.74030000
C	9.85550000	33.55590000	7.67660000
O	10.24250000	32.72600000	6.84810000
C	10.60830000	33.61830000	10.14990000
C	11.89180000	33.64910000	11.06700000
C	11.64060000	33.89900000	12.53880000
O	10.50280000	34.29660000	12.93730000
O	12.54210000	33.71510000	13.41240000
H	10.05450000	35.98930000	9.08420000
H	11.77430000	33.60940000	8.37880000
H	10.10180000	32.65380000	10.18670000
H	9.83650000	34.23690000	10.60790000
H	12.46450000	34.52480000	10.76160000
H	12.48310000	32.73850000	10.96990000
O	15.17230000	37.94810000	19.79560000
O	18.77280000	48.11890000	21.24210000
O	14.11260000	33.35740000	15.50320000
N	15.50820000	40.34420000	18.57240000
C	15.91430000	41.57260000	17.95290000
C	16.06010000	42.66290000	19.07920000

C	15.78650000	44.09160000	18.51440000
C	15.27480000	39.14980000	17.71950000
C	14.50220000	38.15930000	18.57180000
C	17.15130000	41.61200000	17.05780000
C	16.49320000	45.21670000	19.26640000
C	14.29300000	36.80160000	17.74990000
C	17.36830000	46.01060000	18.51600000
C	16.33090000	45.47010000	20.64630000
C	13.59920000	36.81760000	16.53220000
C	14.97150000	35.60750000	18.19560000
C	18.12980000	47.07240000	19.14710000
C	17.11310000	46.43110000	21.28330000
C	13.55250000	35.63200000	15.79040000
C	14.86700000	34.43840000	17.51690000
C	18.05850000	47.18250000	20.55200000
C	14.16600000	34.45470000	16.31720000
H	14.86270000	37.17140000	20.23600000
H	18.40590000	48.33940000	22.08460000
H	13.55850000	33.38460000	14.73820000
H	14.59790000	40.56800000	18.94850000
H	16.12200000	40.08700000	19.33210000
H	15.04500000	41.78960000	17.33220000
H	17.10240000	42.72220000	19.39250000
H	15.40800000	42.43620000	19.92270000
H	14.74070000	44.38680000	18.42960000
H	16.13900000	44.03470000	17.48450000
H	16.13850000	38.80660000	17.14990000
H	14.70480000	39.40710000	16.82680000
H	13.51150000	38.54220000	18.81680000
H	17.48650000	42.56880000	16.65740000
H	18.00380000	41.27330000	17.64660000
H	16.98540000	40.92640000	16.22680000
H	17.45460000	45.88150000	17.44730000
H	15.67340000	44.96400000	21.33760000
H	13.29350000	37.74540000	16.07140000
H	15.49290000	35.55530000	19.13990000
H	18.80620000	47.80820000	18.73790000
H	17.02140000	46.52430000	22.35530000
H	13.13550000	35.68200000	14.79540000
H	15.29750000	33.50910000	17.85950000
H	8.83410000	33.90610000	7.65360000
H	11.66670000	35.89910000	9.13270000

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-1 1

N	10.85090000	35.53200000	8.66390000
C	10.85940000	34.07880000	8.74030000
C	9.85550000	33.55590000	7.67660000
O	10.24250000	32.72600000	6.84810000
C	10.60830000	33.61830000	10.14990000
C	11.89180000	33.64910000	11.06700000
C	11.64060000	33.89900000	12.53880000
O	10.50280000	34.29660000	12.93730000
O	12.54210000	33.71510000	13.41240000
H	10.05450000	35.98930000	9.08420000
H	11.77430000	33.60940000	8.37880000
H	10.10180000	32.65380000	10.18670000
H	9.83650000	34.23690000	10.60790000
H	12.46450000	34.52480000	10.76160000
H	12.48310000	32.73850000	10.96990000
H	8.83410000	33.90610000	7.65360000
H	11.66670000	35.89910000	9.13270000

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N	16.53650000	32.79530000	21.74520000
C	15.30270000	33.52070000	21.59340000
C	15.52590000	35.06590000	21.89020000
O	14.66320000	35.83570000	21.40280000
C	14.20700000	32.99230000	22.56620000
O	14.52810000	33.22300000	23.93040000
H	16.80320000	32.68710000	22.71330000
H	14.91750000	33.44170000	20.57680000
H	14.08260000	31.91590000	22.44720000
H	13.25570000	33.49000000	22.37790000
H	15.46210000	33.25760000	24.07000000
H	16.34640000	35.46920000	22.46500000
H	16.43700000	31.87340000	21.34470000
O	15.17230000	37.94810000	19.79560000
O	18.77280000	48.11890000	21.24210000
O	14.11260000	33.35740000	15.50320000
N	15.50820000	40.34420000	18.57240000
C	15.91430000	41.57260000	17.95290000
C	16.06010000	42.66290000	19.07920000
C	15.78650000	44.09160000	18.51440000
C	15.27480000	39.14980000	17.71950000
C	14.50220000	38.15930000	18.57180000
C	17.15130000	41.61200000	17.05780000

C	16.49320000	45.21670000	19.26640000
C	14.29300000	36.80160000	17.74990000
C	17.36830000	46.01060000	18.51600000
C	16.33090000	45.47010000	20.64630000
C	13.59920000	36.81760000	16.53220000
C	14.97150000	35.60750000	18.19560000
C	18.12980000	47.07240000	19.14710000
C	17.11310000	46.43110000	21.28330000
C	13.55250000	35.63200000	15.79040000
C	14.86700000	34.43840000	17.51690000
C	18.05850000	47.18250000	20.55200000
C	14.16600000	34.45470000	16.31720000
H	14.86270000	37.17140000	20.23600000
H	18.40590000	48.33940000	22.08460000
H	13.55850000	33.38460000	14.73820000
H	14.59790000	40.56800000	18.94850000
H	16.12200000	40.08700000	19.33210000
H	15.04500000	41.78960000	17.33220000
H	17.10240000	42.72220000	19.39250000
H	15.40800000	42.43620000	19.92270000
H	14.74070000	44.38680000	18.42960000
H	16.13900000	44.03470000	17.48450000
H	16.13850000	38.80660000	17.14990000
H	14.70480000	39.40710000	16.82680000
H	13.51150000	38.54220000	18.81680000
H	17.48650000	42.56880000	16.65740000
H	18.00380000	41.27330000	17.64660000
H	16.98540000	40.92640000	16.22680000
H	17.45460000	45.88150000	17.44730000
H	15.67340000	44.96400000	21.33760000
H	13.29350000	37.74540000	16.07140000
H	15.49290000	35.55530000	19.13990000
H	18.80620000	47.80820000	18.73790000
H	17.02140000	46.52430000	22.35530000
H	13.13550000	35.68200000	14.79540000
H	15.29750000	33.50910000	17.85950000

IF09-SER-132
0 1

N	16.53650000	32.79530000	21.74520000
C	15.30270000	33.52070000	21.59340000
C	15.52590000	35.06590000	21.89020000
O	14.66320000	35.83570000	21.40280000
C	14.20700000	32.99230000	22.56620000

O	14.52810000	33.22300000	23.93040000
H	16.80320000	32.68710000	22.71330000
H	14.91750000	33.44170000	20.57680000
H	14.08260000	31.91590000	22.44720000
H	13.25570000	33.49000000	22.37790000
H	15.46210000	33.25760000	24.07000000
H	16.34640000	35.46920000	22.46500000
H	16.43700000	31.87340000	21.34470000

Ifenprodil-ligand + ARG-115

2 1

N	-7.86990000	-53.61170000	41.17770000
C	-8.39380000	-52.92230000	40.01220000
C	-9.42600000	-53.71840000	39.15800000
O	-9.60320000	-53.42880000	37.95940000
C	-7.29590000	-52.19940000	39.05790000
C	-6.06970000	-51.68770000	39.75530000
C	-6.25350000	-50.52100000	40.76880000
N	-5.10210000	-49.54580000	40.87170000
C	-4.03470000	-49.57550000	41.70110000
N	-3.88640000	-50.63530000	42.45890000
N	-3.17440000	-48.53120000	41.54030000
H	-8.13520000	-53.25460000	42.08450000
H	-8.99990000	-52.09990000	40.39240000
H	-7.80730000	-51.45690000	38.44540000
H	-6.96630000	-52.97820000	38.37020000
H	-5.41340000	-51.28850000	38.98200000
H	-5.56450000	-52.47750000	40.31140000
H	-6.32510000	-50.70980000	41.84000000
H	-7.12210000	-49.97110000	40.40640000
H	-5.27630000	-48.72370000	40.31140000
H	-2.95540000	-50.88760000	42.75840000
H	-4.62690000	-51.27920000	42.69810000
H	-2.26690000	-48.54540000	41.98330000
H	-3.46670000	-47.68300000	41.07640000
H	-8.17770000	-54.57360000	41.16710000
H	-9.98840000	-54.52330000	39.60790000
O	-3.56390000	-47.23370000	47.12930000
O	-4.29040000	-43.21100000	42.13090000
N	-6.07110000	-48.38010000	47.72020000
C	-6.43470000	-50.49530000	49.73680000
C	-5.14260000	-50.28410000	48.97610000
C	-7.40950000	-49.25660000	49.65750000
C	-5.23670000	-49.61850000	47.59630000

C	-7.41760000	-48.69380000	48.22380000
C	-5.97860000	-47.51370000	46.52850000
C	-6.10960000	-50.97910000	51.16050000
C	-4.72750000	-46.56420000	46.65180000
C	-6.17420000	-48.33510000	45.18120000
C	-7.32060000	-51.60640000	51.88590000
C	-4.59320000	-45.76900000	45.39930000
C	-7.65480000	-52.91400000	51.52230000
C	-8.02100000	-50.92630000	52.87470000
C	-5.61290000	-44.83860000	45.14410000
C	-3.47040000	-45.85090000	44.59890000
C	-8.69130000	-53.57730000	52.21750000
C	-9.05010000	-51.60310000	53.57160000
C	-5.59160000	-43.99570000	44.07250000
C	-3.37290000	-44.93430000	43.51490000
C	-9.38820000	-52.91360000	53.22240000
C	-4.40030000	-44.03520000	43.24330000
H	-3.39220000	-47.89210000	46.47350000
H	-3.57040000	-43.43000000	41.55930000
H	-5.62910000	-47.75480000	48.37880000
H	-6.91040000	-51.34560000	49.24830000
H	-4.66100000	-51.24280000	48.78330000
H	-4.40840000	-49.72770000	49.55870000
H	-7.13570000	-48.42020000	50.30070000
H	-8.40090000	-49.59830000	49.95490000
H	-4.24330000	-49.53030000	47.15630000
H	-5.74080000	-50.16670000	46.80030000
H	-7.86410000	-49.37780000	47.50220000
H	-8.08760000	-47.83430000	48.20100000
H	-6.85660000	-46.86900000	46.56770000
H	-5.69620000	-50.09670000	51.64880000
H	-5.35450000	-51.76170000	51.08610000
H	-4.96870000	-45.86580000	47.45310000
H	-7.11050000	-48.89240000	45.20850000
H	-6.25390000	-47.68940000	44.30670000
H	-5.40600000	-49.03780000	44.85840000
H	-7.15510000	-53.50170000	50.76650000
H	-7.79380000	-49.93750000	53.24500000
H	-6.43790000	-44.77990000	45.83860000
H	-2.69550000	-46.55350000	44.86780000
H	-8.91120000	-54.61940000	52.03860000
H	-9.72080000	-51.17580000	54.30230000
H	-6.45640000	-43.38100000	43.87090000
H	-2.50920000	-44.98210000	42.86820000

H	-10.14290000	-53.39880000	53.82370000

Ifenprodil-ARG-115

1 1

N	-7.86990000	-53.61170000	41.17770000
C	-8.39380000	-52.92230000	40.01220000
C	-9.42600000	-53.71840000	39.15800000
O	-9.60320000	-53.42880000	37.95940000
C	-7.29590000	-52.19940000	39.05790000
C	-6.06970000	-51.68770000	39.75530000
C	-6.25350000	-50.52100000	40.76880000
N	-5.10210000	-49.54580000	40.87170000
C	-4.03470000	-49.57550000	41.70110000
N	-3.88640000	-50.63530000	42.45890000
N	-3.17440000	-48.53120000	41.54030000
H	-8.13520000	-53.25460000	42.08450000
H	-8.99990000	-52.09990000	40.39240000
H	-7.80730000	-51.45690000	38.44540000
H	-6.96630000	-52.97820000	38.37020000
H	-5.41340000	-51.28850000	38.98200000
H	-5.56450000	-52.47750000	40.31140000
H	-6.32510000	-50.70980000	41.84000000
H	-7.12210000	-49.97110000	40.40640000
H	-5.27630000	-48.72370000	40.31140000
H	-2.95540000	-50.88760000	42.75840000
H	-4.62690000	-51.27920000	42.69810000
H	-2.26690000	-48.54540000	41.98330000
H	-3.46670000	-47.68300000	41.07640000
H	-8.17770000	-54.57360000	41.16710000
H	-9.98840000	-54.52330000	39.60790000

Ifenprodil-ligand + PHE-114

1 1

N	-8.22310000	-48.65510000	58.21680000
C	-9.60930000	-49.22020000	58.15250000
C	-9.84040000	-50.19530000	59.35480000
O	-10.82770000	-50.04200000	60.05410000
C	-9.75940000	-49.91500000	56.76340000
C	-10.87790000	-50.88330000	56.58810000
C	-12.19400000	-50.40640000	56.41930000
C	-10.64150000	-52.27730000	56.52620000
C	-13.27550000	-51.29840000	56.30920000
C	-11.77530000	-53.18140000	56.31280000
C	-13.01280000	-52.64460000	56.09550000

H	-7.52670000	-48.97700000	57.56000000
H	-10.45190000	-48.53320000	58.23140000
H	-8.86210000	-50.49390000	56.54470000
H	-9.80710000	-49.10750000	56.03280000
H	-12.36370000	-49.33990000	56.42790000
H	-9.64120000	-52.68260000	56.56720000
H	-14.20260000	-50.83590000	56.00430000
H	-11.50050000	-54.22570000	56.33220000
H	-13.83120000	-53.33580000	55.95790000
H	-9.14460000	-50.99270000	59.57020000
H	-8.25930000	-47.65610000	58.07320000
O	-3.56390000	-47.23370000	47.12930000
O	-4.29040000	-43.21100000	42.13090000
N	-6.07110000	-48.38010000	47.72020000
C	-6.43470000	-50.49530000	49.73680000
C	-5.14260000	-50.28410000	48.97610000
C	-7.40950000	-49.25660000	49.65750000
C	-5.23670000	-49.61850000	47.59630000
C	-7.41760000	-48.69380000	48.22380000
C	-5.97860000	-47.51370000	46.52850000
C	-6.10960000	-50.97910000	51.16050000
C	-4.72750000	-46.56420000	46.65180000
C	-6.17420000	-48.33510000	45.18120000
C	-7.32060000	-51.60640000	51.88590000
C	-4.59320000	-45.76900000	45.39930000
C	-7.65480000	-52.91400000	51.52230000
C	-8.02100000	-50.92630000	52.87470000
C	-5.61290000	-44.83860000	45.14410000
C	-3.47040000	-45.85090000	44.59890000
C	-8.69130000	-53.57730000	52.21750000
C	-9.05010000	-51.60310000	53.57160000
C	-5.59160000	-43.99570000	44.07250000
C	-3.37290000	-44.93430000	43.51490000
C	-9.38820000	-52.91360000	53.22240000
C	-4.40030000	-44.03520000	43.24330000
H	-3.39220000	-47.89210000	46.47350000
H	-3.57040000	-43.43000000	41.55930000
H	-5.62910000	-47.75480000	48.37880000
H	-6.91040000	-51.34560000	49.24830000
H	-4.66100000	-51.24280000	48.78330000
H	-4.40840000	-49.72770000	49.55870000
H	-7.13570000	-48.42020000	50.30070000
H	-8.40090000	-49.59830000	49.95490000
H	-4.24330000	-49.53030000	47.15630000

H	-5.74080000	-50.16670000	46.80030000
H	-7.86410000	-49.37780000	47.50220000
H	-8.08760000	-47.83430000	48.20100000
H	-6.85660000	-46.86900000	46.56770000
H	-5.69620000	-50.09670000	51.64880000
H	-5.35450000	-51.76170000	51.08610000
H	-4.96870000	-45.86580000	47.45310000
H	-7.11050000	-48.89240000	45.20850000
H	-6.25390000	-47.68940000	44.30670000
H	-5.40600000	-49.03780000	44.85840000
H	-7.15510000	-53.50170000	50.76650000
H	-7.79380000	-49.93750000	53.24500000
H	-6.43790000	-44.77990000	45.83860000
H	-2.69550000	-46.55350000	44.86780000
H	-8.91120000	-54.61940000	52.03860000
H	-9.72080000	-51.17580000	54.30230000
H	-6.45640000	-43.38100000	43.87090000
H	-2.50920000	-44.98210000	42.86820000
H	-10.14290000	-53.39880000	53.82370000

Ifenprodil-PHE-114
0 1

N	-8.22310000	-48.65510000	58.21680000
C	-9.60930000	-49.22020000	58.15250000
C	-9.84040000	-50.19530000	59.35480000
O	-10.82770000	-50.04200000	60.05410000
C	-9.75940000	-49.91500000	56.76340000
C	-10.87790000	-50.88330000	56.58810000
C	-12.19400000	-50.40640000	56.41930000
C	-10.64150000	-52.27730000	56.52620000
C	-13.27550000	-51.29840000	56.30920000
C	-11.77530000	-53.18140000	56.31280000
C	-13.01280000	-52.64460000	56.09550000
H	-7.52670000	-48.97700000	57.56000000
H	-10.45190000	-48.53320000	58.23140000
H	-8.86210000	-50.49390000	56.54470000
H	-9.80710000	-49.10750000	56.03280000
H	-12.36370000	-49.33990000	56.42790000
H	-9.64120000	-52.68260000	56.56720000
H	-14.20260000	-50.83590000	56.00430000
H	-11.50050000	-54.22570000	56.33220000
H	-13.83120000	-53.33580000	55.95790000
H	-9.14460000	-50.99270000	59.57020000
H	-8.25930000	-47.65610000	58.07320000

IF03-ligand + PHE-114

0 1

N	5.39170000	-26.68030000	-15.91340000
C	6.21370000	-27.71810000	-16.48400000
C	6.99210000	-28.51410000	-15.42630000
O	6.80450000	-29.74360000	-15.31260000
C	7.16980000	-27.05760000	-17.56920000
C	8.25490000	-27.96900000	-18.04020000
C	8.04450000	-29.21910000	-18.64690000
C	9.57180000	-27.51240000	-17.93940000
C	9.08670000	-29.95940000	-19.25340000
C	10.62010000	-28.22050000	-18.57000000
C	10.38070000	-29.46880000	-19.17760000
H	5.62240000	-25.71060000	-16.07660000
H	5.60520000	-28.45010000	-17.01500000
H	7.53590000	-26.07690000	-17.26530000
H	6.52410000	-26.74780000	-18.39090000
H	7.01650000	-29.50960000	-18.80590000
H	9.70830000	-26.52000000	-17.53590000
H	8.93800000	-30.90420000	-19.75520000
H	11.63490000	-27.85620000	-18.50700000
H	11.15620000	-30.12220000	-19.54910000
H	4.44720000	-26.76960000	-16.25970000
H	7.70000000	-28.01400000	-14.78200000
O	1.94650000	-18.95470000	-26.82070000
O	3.91110000	-18.00510000	-22.68720000
O	-1.37980000	-13.84320000	-28.19690000
N	2.79880000	-19.30900000	-24.21630000
N	9.01750000	-22.00370000	-21.67670000
N	4.75200000	-19.93890000	-23.37490000
C	1.79170000	-18.27560000	-24.54430000
C	1.94000000	-17.83990000	-25.98030000
C	6.79230000	-21.06470000	-22.66640000
C	8.00990000	-20.85480000	-21.76490000
C	0.94620000	-16.73710000	-26.40540000
C	6.08120000	-19.71260000	-22.79380000
C	0.32830000	-18.68470000	-24.12620000
C	3.82250000	-19.02450000	-23.41940000
C	-0.08260000	-17.08670000	-27.31220000
C	0.97260000	-15.45680000	-25.83800000
C	8.70770000	-23.31840000	-21.34380000
C	10.46230000	-21.69000000	-21.44430000
C	-0.91100000	-16.10370000	-27.90930000

C	0.08050000	-14.43170000	-26.33600000
C	-0.75820000	-14.76990000	-27.48560000
C	7.46690000	-23.69490000	-20.78310000
C	9.61720000	-24.32060000	-21.68600000
C	7.19070000	-25.05960000	-20.56000000
C	9.39730000	-25.61010000	-21.26840000
C	8.16580000	-26.05480000	-20.81070000
H	1.14100000	-19.40190000	-26.61020000
H	-1.08320000	-12.96500000	-28.01260000
H	2.75300000	-20.22280000	-24.64420000
H	4.51480000	-20.85500000	-23.72790000
H	1.89280000	-17.42240000	-23.87350000
H	2.95630000	-17.45150000	-26.04600000
H	6.11390000	-21.81040000	-22.25200000
H	7.06370000	-21.40670000	-23.66510000
H	8.40230000	-19.88860000	-22.08190000
H	7.79340000	-20.70050000	-20.70780000
H	5.84620000	-19.20750000	-21.85690000
H	6.59680000	-19.05940000	-23.49780000
H	0.25940000	-18.54660000	-23.04720000
H	-0.47370000	-18.12640000	-24.60920000
H	0.08370000	-19.71250000	-24.39470000
H	-0.18700000	-18.11860000	-27.61320000
H	1.55980000	-15.24840000	-24.95590000
H	11.01380000	-21.48810000	-22.36260000
H	10.54440000	-20.77280000	-20.86120000
H	11.06340000	-22.39410000	-20.86900000
H	-1.69010000	-16.32140000	-28.62490000
H	0.06790000	-13.39950000	-26.01870000
H	6.71570000	-22.99080000	-20.45690000
H	10.58050000	-24.10810000	-22.12550000
H	6.27430000	-25.31960000	-20.05110000
H	10.29710000	-26.19350000	-21.39630000
H	8.08880000	-27.08790000	-20.50560000

IF03-PHE-114
0 1

N	5.39170000	-26.68030000	-15.91340000
C	6.21370000	-27.71810000	-16.48400000
C	6.99210000	-28.51410000	-15.42630000
O	6.80450000	-29.74360000	-15.31260000
C	7.16980000	-27.05760000	-17.56920000
C	8.25490000	-27.96900000	-18.04020000
C	8.04450000	-29.21910000	-18.64690000

C	9.57180000	-27.51240000	-17.93940000
C	9.08670000	-29.95940000	-19.25340000
C	10.62010000	-28.22050000	-18.57000000
C	10.38070000	-29.46880000	-19.17760000
H	5.62240000	-25.71060000	-16.07660000
H	5.60520000	-28.45010000	-17.01500000
H	7.53590000	-26.07690000	-17.26530000
H	6.52410000	-26.74780000	-18.39090000
H	7.01650000	-29.50960000	-18.80590000
H	9.70830000	-26.52000000	-17.53590000
H	8.93800000	-30.90420000	-19.75520000
H	11.63490000	-27.85620000	-18.50700000
H	11.15620000	-30.12220000	-19.54910000
H	4.44720000	-26.76960000	-16.25970000
H	7.70000000	-28.01400000	-14.78200000

Compound A-ligand
0 1

O	3.90150000	16.70810000	-16.90070000
C	3.42490000	15.45000000	-16.70540000
C	3.65820000	14.66040000	-15.53700000
C	3.03480000	13.37810000	-15.39130000
C	2.25940000	12.81640000	-16.43330000
N	1.65020000	11.58780000	-16.66730000
C	1.20310000	11.65380000	-17.91240000
N	1.33570000	12.86050000	-18.38090000
C	2.14090000	13.61820000	-17.59030000
C	2.68650000	14.86630000	-17.75040000
C	0.45140000	10.61120000	-18.73330000
O	-0.46760000	10.98070000	-19.43310000
N	0.85010000	9.31120000	-18.65250000
C	-0.08360000	8.22040000	-19.05800000
C	-0.17360000	7.22430000	-17.90630000
C	1.16620000	6.68220000	-17.51180000
C	1.06820000	5.68440000	-16.29420000
C	0.97490000	4.21660000	-16.60580000
C	2.13300000	3.39290000	-16.55820000
C	2.03990000	2.06840000	-16.93770000
C	0.83240000	1.50560000	-17.27870000
F	0.82200000	0.19490000	-17.51040000
C	-0.29310000	2.29020000	-17.33840000
C	-0.29350000	3.68810000	-17.03450000
C	2.19450000	7.75900000	-17.22940000
C	2.24930000	8.88000000	-18.28010000

H	0.93790000	13.06890000	-19.28560000
H	4.37570000	17.13770000	-16.20520000
H	4.17860000	15.02880000	-14.66540000
H	3.18860000	12.87590000	-14.44760000
H	2.55800000	15.30950000	-18.72680000
H	-1.11100000	8.53420000	-19.24240000
H	0.22400000	7.73450000	-19.98400000
H	-0.72550000	7.66420000	-17.07560000
H	-0.69620000	6.37010000	-18.33670000
H	1.54170000	6.13670000	-18.37760000
H	1.96000000	5.72550000	-15.66880000
H	0.19610000	5.84380000	-15.66010000
H	3.11430000	3.76530000	-16.30370000
H	3.00520000	1.60660000	-16.79170000
H	-1.21290000	1.83430000	-17.67380000
H	-1.13540000	4.35770000	-17.13040000
H	3.20840000	7.37460000	-17.11770000
H	1.84040000	8.08260000	-16.25060000
H	2.57070000	8.43350000	-19.22110000
H	2.97160000	9.65430000	-18.02140000

Compound A-ligand + ARG-115

1 1

N	10.55420000	8.41590000	-17.94880000
C	10.92550000	9.50620000	-18.90220000
C	11.99810000	8.93200000	-19.86140000
O	12.80090000	9.68740000	-20.51140000
C	11.30800000	10.92210000	-18.26020000
C	10.07490000	11.79740000	-17.89010000
C	9.40040000	11.35750000	-16.64870000
N	8.58390000	12.45260000	-16.04640000
C	7.53280000	12.29310000	-15.22670000
N	6.91090000	11.08230000	-15.02210000
N	7.03500000	13.31860000	-14.65440000
H	9.85790000	7.76070000	-18.27420000
H	10.03460000	9.63510000	-19.51690000
H	11.94280000	11.40490000	-19.00320000
H	12.07810000	10.84530000	-17.49270000
H	9.41830000	11.75540000	-18.75910000
H	10.36660000	12.84690000	-17.85140000
H	10.09850000	10.90740000	-15.94300000
H	8.77670000	10.49970000	-16.90000000
H	8.99190000	13.37110000	-16.14600000
H	6.17410000	10.94640000	-14.34480000

H	7.36000000	10.26370000	-15.40700000
H	6.27720000	13.28820000	-13.98740000
H	7.30510000	14.25670000	-14.91380000
H	12.05630000	7.85940000	-19.97310000
H	11.37320000	7.86730000	-17.72850000
O	3.90150000	16.70810000	-16.90070000
C	3.42490000	15.45000000	-16.70540000
C	3.65820000	14.66040000	-15.53700000
C	3.03480000	13.37810000	-15.39130000
C	2.25940000	12.81640000	-16.43330000
N	1.65020000	11.58780000	-16.66730000
C	1.20310000	11.65380000	-17.91240000
N	1.33570000	12.86050000	-18.38090000
C	2.14090000	13.61820000	-17.59030000
C	2.68650000	14.86630000	-17.75040000
C	0.45140000	10.61120000	-18.73330000
O	-0.46760000	10.98070000	-19.43310000
N	0.85010000	9.31120000	-18.65250000
C	-0.08360000	8.22040000	-19.05800000
C	-0.17360000	7.22430000	-17.90630000
C	1.16620000	6.68220000	-17.51180000
C	1.06820000	5.68440000	-16.29420000
C	0.97490000	4.21660000	-16.60580000
C	2.13300000	3.39290000	-16.55820000
C	2.03990000	2.06840000	-16.93770000
C	0.83240000	1.50560000	-17.27870000
F	0.82200000	0.19490000	-17.51040000
C	-0.29310000	2.29020000	-17.33840000
C	-0.29350000	3.68810000	-17.03450000
C	2.19450000	7.75900000	-17.22940000
C	2.24930000	8.88000000	-18.28010000
H	0.93790000	13.06890000	-19.28560000
H	4.37570000	17.13770000	-16.20520000
H	4.17860000	15.02880000	-14.66540000
H	3.18860000	12.87590000	-14.44760000
H	2.55800000	15.30950000	-18.72680000
H	-1.11100000	8.53420000	-19.24240000
H	0.22400000	7.73450000	-19.98400000
H	-0.72550000	7.66420000	-17.07560000
H	-0.69620000	6.37010000	-18.33670000
H	1.54170000	6.13670000	-18.37760000
H	1.96000000	5.72550000	-15.66880000
H	0.19610000	5.84380000	-15.66010000
H	3.11430000	3.76530000	-16.30370000

H	3.00520000	1.60660000	-16.79170000
H	-1.21290000	1.83430000	-17.67380000
H	-1.13540000	4.35770000	-17.13040000
H	3.20840000	7.37460000	-17.11770000
H	1.84040000	8.08260000	-16.25060000
H	2.57070000	8.43350000	-19.22110000
H	2.97160000	9.65430000	-18.02140000

Compound A-ARG-115

1 1

N	10.55420000	8.41590000	-17.94880000
C	10.92550000	9.50620000	-18.90220000
C	11.99810000	8.93200000	-19.86140000
O	12.80090000	9.68740000	-20.51140000
C	11.30800000	10.92210000	-18.26020000
C	10.07490000	11.79740000	-17.89010000
C	9.40040000	11.35750000	-16.64870000
N	8.58390000	12.45260000	-16.04640000
C	7.53280000	12.29310000	-15.22670000
N	6.91090000	11.08230000	-15.02210000
N	7.03500000	13.31860000	-14.65440000
H	9.85790000	7.76070000	-18.27420000
H	10.03460000	9.63510000	-19.51690000
H	11.94280000	11.40490000	-19.00320000
H	12.07810000	10.84530000	-17.49270000
H	9.41830000	11.75540000	-18.75910000
H	10.36660000	12.84690000	-17.85140000
H	10.09850000	10.90740000	-15.94300000
H	8.77670000	10.49970000	-16.90000000
H	8.99190000	13.37110000	-16.14600000
H	6.17410000	10.94640000	-14.34480000
H	7.36000000	10.26370000	-15.40700000
H	6.27720000	13.28820000	-13.98740000
H	7.30510000	14.25670000	-14.91380000
H	12.05630000	7.85940000	-19.97310000
H	11.37320000	7.86730000	-17.72850000

Compound A-ligand + PHE-176

0 1

N	0.82810000	18.54400000	-18.21690000
C	0.20610000	17.50660000	-17.39090000
C	-1.24920000	17.52030000	-17.79030000
O	-1.92540000	18.56280000	-17.83460000
C	0.48980000	17.84450000	-15.85590000

C	-0.21120000	16.77730000	-14.98940000
C	0.15160000	15.38230000	-15.08180000
C	-1.37890000	17.04420000	-14.29230000
C	-0.49050000	14.34610000	-14.45380000
C	-2.09670000	16.03910000	-13.69610000
C	-1.56180000	14.70590000	-13.70470000
H	1.06260000	19.41270000	-17.75810000
H	0.71580000	16.54960000	-17.50280000
H	0.33850000	18.90910000	-15.67750000
H	1.55890000	17.79700000	-15.64870000
H	0.95240000	15.07700000	-15.73900000
H	-1.68960000	18.06950000	-14.15570000
H	-0.17950000	13.31210000	-14.43000000
H	-2.99620000	16.35240000	-13.18710000
H	-2.12670000	13.93310000	-13.20470000
H	1.69530000	18.19530000	-18.59970000
H	-1.70070000	16.57260000	-18.04410000
O	3.90150000	16.70810000	-16.90070000
C	3.42490000	15.45000000	-16.70540000
C	3.65820000	14.66040000	-15.53700000
C	3.03480000	13.37810000	-15.39130000
C	2.25940000	12.81640000	-16.43330000
N	1.65020000	11.58780000	-16.66730000
C	1.20310000	11.65380000	-17.91240000
N	1.33570000	12.86050000	-18.38090000
C	2.14090000	13.61820000	-17.59030000
C	2.68650000	14.86630000	-17.75040000
C	0.45140000	10.61120000	-18.73330000
O	-0.46760000	10.98070000	-19.43310000
N	0.85010000	9.31120000	-18.65250000
C	-0.08360000	8.22040000	-19.05800000
C	-0.17360000	7.22430000	-17.90630000
C	1.16620000	6.68220000	-17.51180000
C	1.06820000	5.68440000	-16.29420000
C	0.97490000	4.21660000	-16.60580000
C	2.13300000	3.39290000	-16.55820000
C	2.03990000	2.06840000	-16.93770000
C	0.83240000	1.50560000	-17.27870000
F	0.82200000	0.19490000	-17.51040000
C	-0.29310000	2.29020000	-17.33840000
C	-0.29350000	3.68810000	-17.03450000
C	2.19450000	7.75900000	-17.22940000
C	2.24930000	8.88000000	-18.28010000
H	0.93790000	13.06890000	-19.28560000

H	4.37570000	17.13770000	-16.20520000
H	4.17860000	15.02880000	-14.66540000
H	3.18860000	12.87590000	-14.44760000
H	2.55800000	15.30950000	-18.72680000
H	-1.11100000	8.53420000	-19.24240000
H	0.22400000	7.73450000	-19.98400000
H	-0.72550000	7.66420000	-17.07560000
H	-0.69620000	6.37010000	-18.33670000
H	1.54170000	6.13670000	-18.37760000
H	1.96000000	5.72550000	-15.66880000
H	0.19610000	5.84380000	-15.66010000
H	3.11430000	3.76530000	-16.30370000
H	3.00520000	1.60660000	-16.79170000
H	-1.21290000	1.83430000	-17.67380000
H	-1.13540000	4.35770000	-17.13040000
H	3.20840000	7.37460000	-17.11770000
H	1.84040000	8.08260000	-16.25060000
H	2.57070000	8.43350000	-19.22110000
H	2.97160000	9.65430000	-18.02140000

Compound A-PHE-176
0 1

N	0.82810000	18.54400000	-18.21690000
C	0.20610000	17.50660000	-17.39090000
C	-1.24920000	17.52030000	-17.79030000
O	-1.92540000	18.56280000	-17.83460000
C	0.48980000	17.84450000	-15.85590000
C	-0.21120000	16.77730000	-14.98940000
C	0.15160000	15.38230000	-15.08180000
C	-1.37890000	17.04420000	-14.29230000
C	-0.49050000	14.34610000	-14.45380000
C	-2.09670000	16.03910000	-13.69610000
C	-1.56180000	14.70590000	-13.70470000
H	1.06260000	19.41270000	-17.75810000
H	0.71580000	16.54960000	-17.50280000
H	0.33850000	18.90910000	-15.67750000
H	1.55890000	17.79700000	-15.64870000
H	0.95240000	15.07700000	-15.73900000
H	-1.68960000	18.06950000	-14.15570000
H	-0.17950000	13.31210000	-14.43000000
H	-2.99620000	16.35240000	-13.18710000
H	-2.12670000	13.93310000	-13.20470000
H	1.69530000	18.19530000	-18.59970000
H	-1.70070000	16.57260000	-18.04410000

EVT101-ligand
1 1

F	-12.32800000	-27.38900000	41.63110000
F	-10.48630000	-30.07540000	38.98570000
F	-10.75370000	-27.94650000	39.19630000
N	-19.00710000	-31.88280000	37.00540000
N	-19.22160000	-30.86580000	35.07640000
N	-16.75660000	-33.84940000	38.71050000
N	-15.50150000	-33.89890000	39.16440000
C	-18.67060000	-32.79650000	37.98260000
C	-17.35960000	-32.65120000	38.60160000
C	-15.38620000	-31.53450000	39.57410000
C	-14.55720000	-30.41890000	40.00530000
C	-18.62200000	-31.97200000	35.68250000
C	-16.73510000	-31.49220000	39.09250000
C	-19.94360000	-30.86180000	37.16160000
C	-13.16970000	-30.30380000	39.67900000
C	-12.43760000	-29.17490000	40.06600000
C	-15.13690000	-29.41100000	40.77110000
C	-14.85170000	-32.84890000	39.57220000
C	-17.82690000	-33.00090000	34.96070000
C	-20.00220000	-30.16110000	35.98780000
C	-13.07100000	-28.28050000	40.96510000
C	-14.38280000	-28.41680000	41.38630000
C	-10.94710000	-29.08600000	39.78760000
H	-18.95930000	-30.51660000	34.16580000
H	-18.84990000	-33.76590000	37.51760000
H	-19.40690000	-32.84520000	38.78480000
H	-17.26110000	-30.54900000	39.09500000
H	-20.36200000	-30.66190000	38.13700000
H	-12.75560000	-31.09090000	39.06630000
H	-16.20620000	-29.42550000	40.92180000
H	-13.93710000	-33.05290000	40.10910000
H	-18.07690000	-33.20580000	33.91970000
H	-16.77040000	-32.73820000	35.01400000
H	-17.93050000	-33.92890000	35.52310000
H	-20.47120000	-29.21100000	35.77880000
H	-14.87840000	-27.69910000	42.02330000
H	-10.35020000	-29.16360000	40.69630000

EVT101-ligand + ASP-138
0 1

N	-22.76530000	-30.90960000	33.75110000

C	-23.99490000	-30.10530000	33.90560000
C	-24.49450000	-29.92620000	32.47680000
O	-23.59530000	-29.76410000	31.59210000
C	-23.81030000	-28.79660000	34.67150000
C	-23.61800000	-28.98760000	36.17360000
O	-23.18840000	-28.00650000	36.85130000
O	-24.01230000	-30.03540000	36.69300000
H	-21.97160000	-30.33190000	33.51380000
H	-24.75290000	-30.69320000	34.42320000
H	-24.67340000	-28.13830000	34.57260000
H	-22.96880000	-28.21470000	34.29520000
H	-25.53660000	-29.93080000	32.19300000
H	-22.56410000	-31.38780000	34.61770000
F	-12.32800000	-27.38900000	41.63110000
F	-10.48630000	-30.07540000	38.98570000
F	-10.75370000	-27.94650000	39.19630000
N	-19.00710000	-31.88280000	37.00540000
N	-19.22160000	-30.86580000	35.07640000
N	-16.75660000	-33.84940000	38.71050000
N	-15.50150000	-33.89890000	39.16440000
C	-18.67060000	-32.79650000	37.98260000
C	-17.35960000	-32.65120000	38.60160000
C	-15.38620000	-31.53450000	39.57410000
C	-14.55720000	-30.41890000	40.00530000
C	-18.62200000	-31.97200000	35.68250000
C	-16.73510000	-31.49220000	39.09250000
C	-19.94360000	-30.86180000	37.16160000
C	-13.16970000	-30.30380000	39.67900000
C	-12.43760000	-29.17490000	40.06600000
C	-15.13690000	-29.41100000	40.77110000
C	-14.85170000	-32.84890000	39.57220000
C	-17.82690000	-33.00090000	34.96070000
C	-20.00220000	-30.16110000	35.98780000
C	-13.07100000	-28.28050000	40.96510000
C	-14.38280000	-28.41680000	41.38630000
C	-10.94710000	-29.08600000	39.78760000
H	-18.95930000	-30.51660000	34.16580000
H	-18.84990000	-33.76590000	37.51760000
H	-19.40690000	-32.84520000	38.78480000
H	-17.26110000	-30.54900000	39.09500000
H	-20.36200000	-30.66190000	38.13700000
H	-12.75560000	-31.09090000	39.06630000
H	-16.20620000	-29.42550000	40.92180000
H	-13.93710000	-33.05290000	40.10910000

H	-18.07690000	-33.20580000	33.91970000
H	-16.77040000	-32.73820000	35.01400000
H	-17.93050000	-33.92890000	35.52310000
H	-20.47120000	-29.21100000	35.77880000
H	-14.87840000	-27.69910000	42.02330000
H	-10.35020000	-29.16360000	40.69630000

EVT101-ASP-138
0 2

N	-22.76530000	-30.90960000	33.75110000
C	-23.99490000	-30.10530000	33.90560000
C	-24.49450000	-29.92620000	32.47680000
O	-23.59530000	-29.76410000	31.59210000
C	-23.81030000	-28.79660000	34.67150000
C	-23.61800000	-28.98760000	36.17360000
O	-23.18840000	-28.00650000	36.85130000
O	-24.01230000	-30.03540000	36.69300000
H	-21.97160000	-30.33190000	33.51380000
H	-24.75290000	-30.69320000	34.42320000
H	-24.67340000	-28.13830000	34.57260000
H	-22.96880000	-28.21470000	34.29520000
H	-25.53660000	-29.93080000	32.19300000
H	-22.56410000	-31.38780000	34.61770000

EVT101-ligand + TYR-109
1 1

N	-15.37980000	-23.30060000	41.50360000
C	-14.34040000	-23.98960000	40.64520000
C	-12.88730000	-23.52270000	40.85050000
O	-11.94640000	-24.27800000	40.71270000
C	-14.65870000	-23.89660000	39.15940000
C	-15.46740000	-25.11200000	38.57620000
C	-16.88970000	-25.16850000	38.78410000
C	-14.80140000	-26.21000000	37.99740000
C	-17.65540000	-26.32920000	38.50210000
C	-15.57660000	-27.40090000	37.66980000
C	-16.99720000	-27.37460000	37.91810000
O	-17.78270000	-28.48010000	37.54990000
H	-15.99680000	-22.72800000	40.94540000
H	-14.29500000	-25.04390000	40.91820000
H	-13.72030000	-24.02420000	38.61960000
H	-15.17230000	-22.96270000	38.93130000
H	-17.38750000	-24.32460000	39.23860000
H	-13.72220000	-26.20100000	37.95720000

H	-18.72750000	-26.39920000	38.61200000
H	-15.14240000	-28.22540000	37.12370000
H	-17.30790000	-29.11580000	37.00940000
H	-12.71670000	-22.49210000	41.12440000
H	-15.93400000	-23.99470000	41.98430000
F	-12.32800000	-27.38900000	41.63110000
F	-10.48630000	-30.07540000	38.98570000
F	-10.75370000	-27.94650000	39.19630000
N	-19.00710000	-31.88280000	37.00540000
N	-19.22160000	-30.86580000	35.07640000
N	-16.75660000	-33.84940000	38.71050000
N	-15.50150000	-33.89890000	39.16440000
C	-18.67060000	-32.79650000	37.98260000
C	-17.35960000	-32.65120000	38.60160000
C	-15.38620000	-31.53450000	39.57410000
C	-14.55720000	-30.41890000	40.00530000
C	-18.62200000	-31.97200000	35.68250000
C	-16.73510000	-31.49220000	39.09250000
C	-19.94360000	-30.86180000	37.16160000
C	-13.16970000	-30.30380000	39.67900000
C	-12.43760000	-29.17490000	40.06600000
C	-15.13690000	-29.41100000	40.77110000
C	-14.85170000	-32.84890000	39.57220000
C	-17.82690000	-33.00090000	34.96070000
C	-20.00220000	-30.16110000	35.98780000
C	-13.07100000	-28.28050000	40.96510000
C	-14.38280000	-28.41680000	41.38630000
C	-10.94710000	-29.08600000	39.78760000
H	-18.95930000	-30.51660000	34.16580000
H	-18.84990000	-33.76590000	37.51760000
H	-19.40690000	-32.84520000	38.78480000
H	-17.26110000	-30.54900000	39.09500000
H	-20.36200000	-30.66190000	38.13700000
H	-12.75560000	-31.09090000	39.06630000
H	-16.20620000	-29.42550000	40.92180000
H	-13.93710000	-33.05290000	40.10910000
H	-18.07690000	-33.20580000	33.91970000
H	-16.77040000	-32.73820000	35.01400000
H	-17.93050000	-33.92890000	35.52310000
H	-20.47120000	-29.21100000	35.77880000
H	-14.87840000	-27.69910000	42.02330000
H	-10.35020000	-29.16360000	40.69630000

EVT101-TYR-109

0 1

N	-15.37980000	-23.30060000	41.50360000
C	-14.34040000	-23.98960000	40.64520000
C	-12.88730000	-23.52270000	40.85050000
O	-11.94640000	-24.27800000	40.71270000
C	-14.65870000	-23.89660000	39.15940000
C	-15.46740000	-25.11200000	38.57620000
C	-16.88970000	-25.16850000	38.78410000
C	-14.80140000	-26.21000000	37.99740000
C	-17.65540000	-26.32920000	38.50210000
C	-15.57660000	-27.40090000	37.66980000
C	-16.99720000	-27.37460000	37.91810000
O	-17.78270000	-28.48010000	37.54990000
H	-15.99680000	-22.72800000	40.94540000
H	-14.29500000	-25.04390000	40.91820000
H	-13.72030000	-24.02420000	38.61960000
H	-15.17230000	-22.96270000	38.93130000
H	-17.38750000	-24.32460000	39.23860000
H	-13.72220000	-26.20100000	37.95720000
H	-18.72750000	-26.39920000	38.61200000
H	-15.14240000	-28.22540000	37.12370000
H	-17.30790000	-29.11580000	37.00940000
H	-12.71670000	-22.49210000	41.12440000
H	-15.93400000	-23.99470000	41.98430000

Compound F -ligand

1 1

F	16.54270000	-8.03150000	-22.21480000
F	14.47870000	-8.53670000	-21.83650000
F	14.91210000	-6.52270000	-21.63510000
O	21.13130000	-2.36560000	-30.60930000
O	14.99040000	-7.48120000	-23.69590000
N	18.24880000	-3.13050000	-27.53360000
N	19.02370000	-5.27510000	-28.21760000
C	18.76570000	-2.69670000	-30.01910000
C	18.90210000	-2.29180000	-28.53240000
C	19.85590000	-2.71200000	-30.94990000
C	17.42860000	-5.17160000	-26.41490000
C	18.26180000	-4.48420000	-27.46550000
C	17.47280000	-3.12230000	-30.38910000
C	17.48530000	-4.90500000	-25.04990000
C	16.61270000	-6.29100000	-26.79470000
C	19.55640000	-3.18390000	-32.25660000
C	17.28890000	-3.75740000	-31.57450000

C	15.79640000	-6.69220000	-24.48440000
C	18.31930000	-3.70930000	-32.56600000
C	16.67800000	-5.61690000	-24.11610000
C	15.85790000	-7.01350000	-25.85250000
C	21.51470000	-1.02180000	-30.84750000
C	15.29730000	-7.58870000	-22.33580000
H	17.69460000	-2.62370000	-26.85820000
H	18.95840000	-6.25610000	-27.98620000
H	19.20450000	-4.88770000	-29.13260000
H	19.97160000	-2.19430000	-28.34590000
H	18.50090000	-1.28250000	-28.44060000
H	16.68340000	-3.17070000	-29.65360000
H	18.17020000	-4.14370000	-24.70660000
H	16.57570000	-6.44460000	-27.86310000
H	20.36600000	-3.28790000	-32.96380000
H	16.35660000	-4.28590000	-31.70890000
H	18.13520000	-4.11720000	-33.54890000
H	16.75300000	-5.35030000	-23.07220000
H	15.19080000	-7.77220000	-26.23420000
H	22.58570000	-1.02320000	-31.05000000
H	21.01320000	-0.58220000	-31.70970000
H	21.50920000	-0.37060000	-29.97350000

Compound F -ligand + ASP-136
0 1

F	16.54270000	-8.03150000	-22.21480000
F	14.47870000	-8.53670000	-21.83650000
F	14.91210000	-6.52270000	-21.63510000
O	21.13130000	-2.36560000	-30.60930000
O	14.99040000	-7.48120000	-23.69590000
N	18.24880000	-3.13050000	-27.53360000
N	19.02370000	-5.27510000	-28.21760000
C	18.76570000	-2.69670000	-30.01910000
C	18.90210000	-2.29180000	-28.53240000
C	19.85590000	-2.71200000	-30.94990000
C	17.42860000	-5.17160000	-26.41490000
C	18.26180000	-4.48420000	-27.46550000
C	17.47280000	-3.12230000	-30.38910000
C	17.48530000	-4.90500000	-25.04990000
C	16.61270000	-6.29100000	-26.79470000
C	19.55640000	-3.18390000	-32.25660000
C	17.28890000	-3.75740000	-31.57450000
C	15.79640000	-6.69220000	-24.48440000
C	18.31930000	-3.70930000	-32.56600000

C	16.67800000	-5.61690000	-24.11610000
C	15.85790000	-7.01350000	-25.85250000
C	21.51470000	-1.02180000	-30.84750000
C	15.29730000	-7.58870000	-22.33580000
H	17.69460000	-2.62370000	-26.85820000
H	18.95840000	-6.25610000	-27.98620000
H	19.20450000	-4.88770000	-29.13260000
H	19.97160000	-2.19430000	-28.34590000
H	18.50090000	-1.28250000	-28.44060000
H	16.68340000	-3.17070000	-29.65360000
H	18.17020000	-4.14370000	-24.70660000
H	16.57570000	-6.44460000	-27.86310000
H	20.36600000	-3.28790000	-32.96380000
H	16.35660000	-4.28590000	-31.70890000
H	18.13520000	-4.11720000	-33.54890000
H	16.75300000	-5.35030000	-23.07220000
H	15.19080000	-7.77220000	-26.23420000
H	22.58570000	-1.02320000	-31.05000000
H	21.01320000	-0.58220000	-31.70970000
H	21.50920000	-0.37060000	-29.97350000
N	13.60150000	-7.48600000	-17.58620000
C	14.94030000	-7.89480000	-17.74320000
C	15.87170000	-6.86380000	-18.40430000
O	17.07830000	-7.10340000	-18.55210000
C	15.25230000	-9.31170000	-18.29220000
C	14.80160000	-10.48850000	-17.38030000
O	14.92440000	-11.69470000	-17.70920000
O	14.27450000	-10.26930000	-16.26410000
H	13.40190000	-7.13930000	-16.65880000
H	15.20630000	-7.86550000	-16.68650000
H	16.30710000	-9.40030000	-18.55240000
H	14.70170000	-9.33810000	-19.23250000
H	13.39610000	-6.74540000	-18.24160000
H	15.46290000	-5.92270000	-18.74120000

Compound F -ASP-136
-1 1

N	13.60150000	-7.48600000	-17.58620000
C	14.94030000	-7.89480000	-17.74320000
C	15.87170000	-6.86380000	-18.40430000
O	17.07830000	-7.10340000	-18.55210000
C	15.25230000	-9.31170000	-18.29220000
C	14.80160000	-10.48850000	-17.38030000
O	14.92440000	-11.69470000	-17.70920000

O	14.27450000	-10.26930000	-16.26410000
H	13.40190000	-7.13930000	-16.65880000
H	15.20630000	-7.86550000	-16.68650000
H	16.30710000	-9.40030000	-18.55240000
H	14.70170000	-9.33810000	-19.23250000
H	13.39610000	-6.74540000	-18.24160000
H	15.46290000	-5.92270000	-18.74120000

Compound F-ligand + ASP-138

0 1

N	18.01070000	-3.01980000	-18.39130000
C	18.89660000	-2.26880000	-17.47700000
C	18.14530000	-1.01130000	-17.17490000
O	17.49860000	-0.28520000	-17.93970000
C	20.25340000	-1.93040000	-18.17980000
C	21.33020000	-3.07260000	-18.23590000
O	21.01600000	-4.22220000	-18.03880000
O	22.50790000	-2.74290000	-18.44280000
H	18.01620000	-2.70600000	-19.35130000
H	19.08710000	-2.87690000	-16.59260000
H	20.72640000	-1.10820000	-17.64270000
H	20.17370000	-1.63270000	-19.22530000
H	18.28670000	-3.99120000	-18.40580000
H	18.21970000	-0.76130000	-16.12690000
F	16.54270000	-8.03150000	-22.21480000
F	14.47870000	-8.53670000	-21.83650000
F	14.91210000	-6.52270000	-21.63510000
O	21.13130000	-2.36560000	-30.60930000
O	14.99040000	-7.48120000	-23.69590000
N	18.24880000	-3.13050000	-27.53360000
N	19.02370000	-5.27510000	-28.21760000
C	18.76570000	-2.69670000	-30.01910000
C	18.90210000	-2.29180000	-28.53240000
C	19.85590000	-2.71200000	-30.94990000
C	17.42860000	-5.17160000	-26.41490000
C	18.26180000	-4.48420000	-27.46550000
C	17.47280000	-3.12230000	-30.38910000
C	17.48530000	-4.90500000	-25.04990000
C	16.61270000	-6.29100000	-26.79470000
C	19.55640000	-3.18390000	-32.25660000
C	17.28890000	-3.75740000	-31.57450000
C	15.79640000	-6.69220000	-24.48440000
C	18.31930000	-3.70930000	-32.56600000
C	16.67800000	-5.61690000	-24.11610000

C	15.85790000	-7.01350000	-25.85250000
C	21.51470000	-1.02180000	-30.84750000
C	15.29730000	-7.58870000	-22.33580000
H	17.69460000	-2.62370000	-26.85820000
H	18.95840000	-6.25610000	-27.98620000
H	19.20450000	-4.88770000	-29.13260000
H	19.97160000	-2.19430000	-28.34590000
H	18.50090000	-1.28250000	-28.44060000
H	16.68340000	-3.17070000	-29.65360000
H	18.17020000	-4.14370000	-24.70660000
H	16.57570000	-6.44460000	-27.86310000
H	20.36600000	-3.28790000	-32.96380000
H	16.35660000	-4.28590000	-31.70890000
H	18.13520000	-4.11720000	-33.54890000
H	16.75300000	-5.35030000	-23.07220000
H	15.19080000	-7.77220000	-26.23420000
H	22.58570000	-1.02320000	-31.05000000
H	21.01320000	-0.58220000	-31.70970000
H	21.50920000	-0.37060000	-29.97350000

Compound F-ASP-138
-1 1

N	18.01070000	-3.01980000	-18.39130000
C	18.89660000	-2.26880000	-17.47700000
C	18.14530000	-1.01130000	-17.17490000
O	17.49860000	-0.28520000	-17.93970000
C	20.25340000	-1.93040000	-18.17980000
C	21.33020000	-3.07260000	-18.23590000
O	21.01600000	-4.22220000	-18.03880000
O	22.50790000	-2.74290000	-18.44280000
H	18.01620000	-2.70600000	-19.35130000
H	19.08710000	-2.87690000	-16.59260000
H	20.72640000	-1.10820000	-17.64270000
H	20.17370000	-1.63270000	-19.22530000
H	18.28670000	-3.99120000	-18.40580000
H	18.21970000	-0.76130000	-16.12690000

EVT02-ligand
1 1

C	29.08370000	27.55050000	-8.25300000
N	30.97690000	21.94400000	-10.71980000
N	30.31260000	20.98950000	-8.68860000
C	33.10950000	20.59030000	-11.46870000
C	31.58340000	20.91580000	-11.53690000

C	34.10810000	21.57800000	-11.44660000
C	30.02580000	23.35340000	-9.06920000
C	30.50770000	22.04330000	-9.45220000
C	33.48890000	19.26130000	-11.60360000
C	28.67060000	23.78700000	-8.91070000
C	31.05280000	24.32100000	-8.84510000
C	35.48610000	21.26080000	-11.43260000
C	34.81030000	18.95130000	-11.74950000
C	29.39550000	26.04170000	-8.52970000
C	35.82830000	19.89400000	-11.62870000
C	28.35320000	25.12100000	-8.71710000
C	30.72470000	25.69770000	-8.73960000
C	28.44670000	28.24890000	-9.47330000
N	27.64360000	29.32210000	-9.29110000
O	28.58140000	27.79000000	-10.57950000
Cl	27.32220000	22.70750000	-9.30160000
H	30.03240000	28.06540000	-8.10170000
H	28.51030000	27.56690000	-7.32610000
H	30.68670000	22.76180000	-11.23660000
H	29.93620000	21.09450000	-7.75730000
H	30.50760000	20.06680000	-9.05030000
H	31.32290000	21.24390000	-12.54310000
H	30.99210000	20.00190000	-11.59220000
H	33.97560000	22.64860000	-11.49800000
H	32.73520000	18.48970000	-11.54950000
H	32.11450000	24.20630000	-9.00700000
H	36.29000000	21.97920000	-11.36960000
H	35.17040000	17.93350000	-11.72030000
H	36.85550000	19.56370000	-11.67590000
H	27.33290000	25.46960000	-8.65460000
H	31.63830000	26.25330000	-8.58840000
H	27.11200000	29.88410000	-9.94040000
H	27.73190000	29.63360000	-8.33440000

EVT02-ligand + GLN-110

1 1

N	31.03260000	25.00280000	-15.61130000
C	31.49280000	25.00840000	-14.25830000
C	32.98350000	24.58810000	-14.24940000
O	33.70650000	25.02320000	-13.32520000
C	30.56200000	24.15080000	-13.43480000
C	29.07430000	24.61300000	-13.57830000
C	28.15930000	23.44430000	-13.25670000
O	28.60840000	22.50400000	-12.64670000

N	26.91640000	23.39550000	-13.65160000
H	30.40940000	24.22460000	-15.77290000
H	31.49840000	26.02200000	-13.85740000
H	30.83440000	24.33720000	-12.39600000
H	30.74880000	23.10200000	-13.66560000
H	28.68160000	25.02260000	-14.50890000
H	28.90300000	25.30560000	-12.75420000
H	26.40260000	22.55930000	-13.41310000
H	26.54080000	24.13420000	-14.22880000
H	33.40430000	23.94230000	-15.00590000
H	30.53790000	25.86230000	-15.80260000
C	29.08370000	27.55050000	-8.25300000
N	30.97690000	21.94400000	-10.71980000
N	30.31260000	20.98950000	-8.68860000
C	33.10950000	20.59030000	-11.46870000
C	31.58340000	20.91580000	-11.53690000
C	34.10810000	21.57800000	-11.44660000
C	30.02580000	23.35340000	-9.06920000
C	30.50770000	22.04330000	-9.45220000
C	33.48890000	19.26130000	-11.60360000
C	28.67060000	23.78700000	-8.91070000
C	31.05280000	24.32100000	-8.84510000
C	35.48610000	21.26080000	-11.43260000
C	34.81030000	18.95130000	-11.74950000
C	29.39550000	26.04170000	-8.52970000
C	35.82830000	19.89400000	-11.62870000
C	28.35320000	25.12100000	-8.71710000
C	30.72470000	25.69770000	-8.73960000
C	28.44670000	28.24890000	-9.47330000
N	27.64360000	29.32210000	-9.29110000
O	28.58140000	27.79000000	-10.57950000
Cl	27.32220000	22.70750000	-9.30160000
H	30.03240000	28.06540000	-8.10170000
H	28.51030000	27.56690000	-7.32610000
H	30.68670000	22.76180000	-11.23660000
H	29.93620000	21.09450000	-7.75730000
H	30.50760000	20.06680000	-9.05030000
H	31.32290000	21.24390000	-12.54310000
H	30.99210000	20.00190000	-11.59220000
H	33.97560000	22.64860000	-11.49800000
H	32.73520000	18.48970000	-11.54950000
H	32.11450000	24.20630000	-9.00700000
H	36.29000000	21.97920000	-11.36960000
H	35.17040000	17.93350000	-11.72030000

H	36.85550000	19.56370000	-11.67590000
H	27.33290000	25.46960000	-8.65460000
H	31.63830000	26.25330000	-8.58840000
H	27.11200000	29.88410000	-9.94040000
H	27.73190000	29.63360000	-8.33440000

EVT02-GLN-110
0 1

N	31.03260000	25.00280000	-15.61130000
C	31.49280000	25.00840000	-14.25830000
C	32.98350000	24.58810000	-14.24940000
O	33.70650000	25.02320000	-13.32520000
C	30.56200000	24.15080000	-13.43480000
C	29.07430000	24.61300000	-13.57830000
C	28.15930000	23.44430000	-13.25670000
O	28.60840000	22.50400000	-12.64670000
N	26.91640000	23.39550000	-13.65160000
H	30.40940000	24.22460000	-15.77290000
H	31.49840000	26.02200000	-13.85740000
H	30.83440000	24.33720000	-12.39600000
H	30.74880000	23.10200000	-13.66560000
H	28.68160000	25.02260000	-14.50890000
H	28.90300000	25.30560000	-12.75420000
H	26.40260000	22.55930000	-13.41310000
H	26.54080000	24.13420000	-14.22880000
H	33.40430000	23.94230000	-15.00590000
H	30.53790000	25.86230000	-15.80260000

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