

PDB files of morphine, hydromorphone and β -funaltrexamine bound with a lysine residue. The last two columns correspond to the partial charges and atom types (where lowercase letters indicate GAFF types), respectively.

Morphine

ATOM	1	C15	MOP	1	-1.125	0.355	1.934	-0.066620	c3
ATOM	2	C16	MOP	1	-2.268	-0.589	1.585	-0.088723	c3
ATOM	3	N1	MOP	1	-3.082	-0.058	0.431	-0.029428	n4
ATOM	4	C17	MOP	1	-4.241	-0.946	0.130	-0.323402	c3
ATOM	5	H17	MOP	1	-4.769	-0.563	-0.730	0.160897	hx
ATOM	6	H18	MOP	1	-4.896	-0.956	0.988	0.160897	hx
ATOM	7	H19	MOP	1	-3.890	-1.946	-0.065	0.160897	hx
ATOM	8	H20	MOP	1	-3.478	0.813	0.747	0.293233	hn
ATOM	9	H15	MOP	1	-2.952	-0.716	2.414	0.115384	hx
ATOM	10	H16	MOP	1	-1.903	-1.559	1.286	0.115384	hx
ATOM	11	H13	MOP	1	-1.513	1.253	2.410	0.060777	hc
ATOM	12	H14	MOP	1	-0.496	-0.144	2.661	0.060777	hc
ATOM	13	C7	MOP	1	-0.313	0.734	0.680	0.074811	c3
ATOM	14	C3	MOP	1	0.279	-0.498	0.056	-0.113238	ca
ATOM	15	C2	MOP	1	1.549	-0.652	0.538	0.237768	ca
ATOM	16	C1	MOP	1	2.324	-1.726	0.146	0.313162	ca
ATOM	17	O2	MOP	1	3.565	-1.850	0.639	-0.574943	oh
ATOM	18	H11	MOP	1	4.024	-2.583	0.249	0.451107	ho
ATOM	19	C6	MOP	1	1.743	-2.610	-0.763	-0.383211	ca
ATOM	20	H3	MOP	1	2.317	-3.457	-1.097	0.219704	ha
ATOM	21	C5	MOP	1	0.474	-2.408	-1.292	-0.175065	ca
ATOM	22	H2	MOP	1	0.105	-3.095	-2.032	0.172469	ha
ATOM	23	C4	MOP	1	-0.288	-1.319	-0.886	-0.005328	ca
ATOM	24	C10	MOP	1	-1.604	-0.882	-1.499	-0.007964	c3
ATOM	25	H5	MOP	1	-2.312	-1.700	-1.579	0.068668	hc
ATOM	26	H6	MOP	1	-1.422	-0.561	-2.520	0.068668	hc
ATOM	27	C9	MOP	1	-2.250	0.329	-0.796	-0.002790	c3
ATOM	28	H4	MOP	1	-2.975	0.771	-1.468	0.087316	hx
ATOM	29	C8	MOP	1	-1.257	1.413	-0.314	0.111395	c3
ATOM	30	H1	MOP	1	-1.848	2.176	0.197	0.033084	hc
ATOM	31	C14	MOP	1	-0.518	2.085	-1.439	-0.351845	c2
ATOM	32	H10	MOP	1	-1.059	2.278	-2.351	0.170786	ha
ATOM	33	C13	MOP	1	0.731	2.485	-1.318	-0.120674	c2
ATOM	34	H9	MOP	1	1.215	2.986	-2.138	0.176227	ha
ATOM	35	C12	MOP	1	1.604	2.337	-0.098	0.280651	c3
ATOM	36	O3	MOP	1	2.822	1.848	-0.568	-0.633473	oh
ATOM	37	H12	MOP	1	3.383	1.608	0.159	0.437959	ho
ATOM	38	H8	MOP	1	1.748	3.334	0.314	0.034773	h1
ATOM	39	C11	MOP	1	1.004	1.454	1.045	0.073973	c3
ATOM	40	H7	MOP	1	0.915	2.039	1.949	0.089080	h1
ATOM	41	O1	MOP	1	1.901	0.385	1.347	-0.353141	os
END									

Hydromorphone

ATOM	1	C11	HMP	1	-2.182	-0.696	1.602	-0.102007	c3
ATOM	2	N1	HMP	1	-3.027	-0.170	0.470	-0.032172	n4
ATOM	3	C17	HMP	1	-4.188	-1.065	0.195	-0.378320	c3
ATOM	4	H17	HMP	1	-3.837	-2.063	-0.004	0.179936	hx
ATOM	5	H18	HMP	1	-4.735	-0.686	-0.655	0.179936	hx
ATOM	6	H19	HMP	1	-4.826	-1.075	1.066	0.179936	hx
ATOM	7	H20	HMP	1	-3.423	0.698	0.798	0.309383	hn
ATOM	8	H8	HMP	1	-2.844	-0.842	2.445	0.131026	hx
ATOM	9	H9	HMP	1	-1.806	-1.658	1.288	0.131026	hx
ATOM	10	C5	HMP	1	-1.050	0.268	1.933	-0.052704	c3
ATOM	11	H4	HMP	1	-0.397	-0.220	2.646	0.068612	hc
ATOM	12	H5	HMP	1	-1.448	1.156	2.419	0.068612	hc
ATOM	13	C1	HMP	1	-0.266	0.669	0.669	-0.024420	c3
ATOM	14	C2	HMP	1	0.351	-0.542	0.027	-0.185342	ca
ATOM	15	C6	HMP	1	1.635	-0.665	0.490	0.325508	ca
ATOM	16	O1	HMP	1	1.973	0.370	1.302	-0.341489	os
ATOM	17	C4	HMP	1	1.050	1.408	1.027	0.046939	c3
ATOM	18	H3	HMP	1	0.969	2.024	1.914	0.132615	h1
ATOM	19	C10	HMP	1	1.560	2.280	-0.131	0.465599	c
ATOM	20	O2	HMP	1	2.713	2.335	-0.395	-0.441300	o
ATOM	21	C15	HMP	1	0.499	3.028	-0.913	-0.001746	c3
ATOM	22	H13	HMP	1	0.002	3.745	-0.261	0.035543	hc
ATOM	23	H14	HMP	1	0.991	3.580	-1.702	0.035543	hc
ATOM	24	C9	HMP	1	-0.531	2.038	-1.478	-0.217214	c3
ATOM	25	H6	HMP	1	-0.027	1.328	-2.124	0.112013	hc
ATOM	26	H7	HMP	1	-1.256	2.567	-2.087	0.112013	hc
ATOM	27	C3	HMP	1	-1.238	1.327	-0.320	0.004780	c3
ATOM	28	H1	HMP	1	-1.821	2.090	0.199	0.043304	hc
ATOM	29	C8	HMP	1	-2.222	0.224	-0.772	-0.052664	c3
ATOM	30	H2	HMP	1	-2.966	0.647	-1.436	0.102963	hx
ATOM	31	C13	HMP	1	-1.571	-0.990	-1.472	0.021194	c3
ATOM	32	H10	HMP	1	-2.256	-1.829	-1.491	0.060800	hc
ATOM	33	H11	HMP	1	-1.451	-0.702	-2.512	0.060800	hc
ATOM	34	C7	HMP	1	-0.218	-1.376	-0.904	-0.005863	ca
ATOM	35	C14	HMP	1	0.563	-2.443	-1.328	-0.164792	ca
ATOM	36	H12	HMP	1	0.198	-3.140	-2.062	0.171593	ha
ATOM	37	C16	HMP	1	1.846	-2.618	-0.818	-0.378638	ca

ATOM	38	H15	HMP	1	2.432	-3.453	-1.162	0.217873	ha
ATOM	39	C12	HMP	1	2.423	-1.729	0.089	0.298415	ca
ATOM	40	O3	HMP	1	3.663	-1.846	0.577	-0.576910	oh
ATOM	41	H16	HMP	1	4.135	-2.560	0.170	0.459616	ho
END									

β-funaltrexamine bound with a lysine residue

ATOM	1	C14	FNA	1	3.537	1.423	-0.000	-0.054441	ca
ATOM	2	C13	FNA	1	3.160	2.295	1.052	0.023335	c3
ATOM	3	C23	FNA	1	2.107	3.304	0.627	0.049989	c3
ATOM	4	O4	FNA	1	1.729	4.148	1.714	-0.628897	oh
ATOM	5	H34	FNA	1	1.058	4.780	1.414	0.453703	ho
ATOM	6	C24	FNA	1	2.647	4.125	-0.546	-0.312925	c3
ATOM	7	C25	FNA	1	3.913	4.852	-0.179	0.047599	c3
ATOM	8	H37	FNA	1	3.745	5.507	0.649	0.059762	hc
ATOM	9	H38	FNA	1	4.276	5.460	-0.981	0.059762	hc
ATOM	10	H35	FNA	1	1.907	4.841	-0.838	0.162338	hc
ATOM	11	H36	FNA	1	2.868	3.453	-1.349	0.162338	hc
ATOM	12	C12	FNA	1	2.669	1.427	2.226	-0.039475	c3
ATOM	13	H25	FNA	1	3.428	0.730	2.509	0.098965	hc
ATOM	14	H26	FNA	1	2.442	2.031	3.078	0.098965	hc
ATOM	15	C11	FNA	1	1.437	0.688	1.744	-0.133176	c3
ATOM	16	H23	FNA	1	1.716	0.064	0.921	0.100085	hx
ATOM	17	H24	FNA	1	1.064	0.121	2.571	0.100085	hx
ATOM	18	N3	FNA	1	0.374	1.566	1.313	0.021925	n4
ATOM	19	C10	FNA	1	-0.752	0.705	0.870	-0.212710	c3
ATOM	20	C9	FNA	1	-2.072	1.409	0.429	-0.148288	cx
ATOM	21	C7	FNA	1	-2.146	2.382	-0.756	-0.232305	cx
ATOM	22	C8	FNA	1	-2.642	0.957	-0.913	-0.232305	cx
ATOM	23	H17	FNA	1	-2.093	0.265	-1.519	0.150308	hc
ATOM	24	H18	FNA	1	-3.561	0.510	-1.229	0.150308	hc
ATOM	25	H15	FNA	1	-2.844	3.193	-0.740	0.150308	hc
ATOM	26	H16	FNA	1	-1.442	2.999	-1.273	0.150308	hc
ATOM	27	H19	FNA	1	-2.389	1.492	1.448	0.147834	hc
ATOM	28	H20	FNA	1	-0.405	0.127	0.038	0.171814	hx
ATOM	29	H21	FNA	1	-1.022	0.143	1.739	0.171814	hx
ATOM	30	H22	FNA	1	0.003	2.186	2.033	0.332167	hn
ATOM	31	C22	FNA	1	0.967	2.408	0.228	-0.040438	c3
ATOM	32	H33	FNA	1	0.039	2.907	0.043	0.091490	hx
ATOM	33	C21	FNA	1	1.481	1.773	-1.113	-0.085212	c3
ATOM	34	H31	FNA	1	1.628	2.561	-1.822	0.053877	hc
ATOM	35	H32	FNA	1	0.738	1.069	-1.425	0.053877	hc
ATOM	36	C20	FNA	1	2.695	1.056	-0.988	0.092724	ca
ATOM	37	C19	FNA	1	3.126	0.169	-1.952	-0.136750	ca
ATOM	38	H30	FNA	1	2.562	-0.081	-2.777	0.183367	ha
ATOM	39	C18	FNA	1	4.384	-0.357	-1.712	-0.463536	ca
ATOM	40	H29	FNA	1	4.810	-1.002	-2.396	0.289683	ha
ATOM	41	C17	FNA	1	5.079	-0.019	-0.551	0.605046	ca
ATOM	42	O3	FNA	1	6.344	-0.493	-0.409	-0.762200	oh
ATOM	43	H28	FNA	1	6.839	-0.285	0.359	0.471284	ho
ATOM	44	C16	FNA	1	4.836	1.046	0.191	-0.020055	ca
ATOM	45	O2	FNA	1	5.096	1.530	1.435	-0.325941	os
ATOM	46	C15	FNA	1	4.397	2.837	1.359	-0.021906	c3
ATOM	47	H27	FNA	1	4.464	3.487	2.206	0.204935	H1
ATOM	48	C26	FNA	1	4.933	3.716	0.213	-0.001066	c3
ATOM	49	H39	FNA	1	5.054	3.113	-0.662	0.103220	h1
ATOM	50	N4	FNA	1	6.244	4.266	0.600	-0.364572	n
ATOM	51	H40	FNA	1	6.587	4.099	1.508	0.289737	hn
ATOM	52	C27	FNA	1	6.984	4.992	-0.259	0.400043	c
ATOM	53	O5	FNA	1	6.665	5.225	-1.424	-0.452648	o
ATOM	54	C28	FNA	1	8.322	5.499	0.281	-0.000412	c3
ATOM	55	C29	FNA	1	8.661	6.801	-0.465	-0.350893	c3
ATOM	56	C30	FNA	1	7.578	7.884	-0.289	0.829129	c
ATOM	57	O6	FNA	1	7.369	8.704	-1.185	-0.531225	o
ATOM	58	O7	FNA	1	6.894	7.864	0.888	-0.413207	os
ATOM	59	C31	FNA	1	5.925	8.920	0.893	-0.043416	c3
ATOM	60	H44	FNA	1	5.387	8.906	1.818	0.104030	h1
ATOM	61	H45	FNA	1	5.243	8.782	0.081	0.104030	h1
ATOM	62	H46	FNA	1	6.423	9.860	0.785	0.104030	h1
ATOM	63	H42	FNA	1	9.588	7.180	-0.089	0.129991	hc
ATOM	64	H43	FNA	1	8.722	6.571	-1.508	0.129991	hc
ATOM	65	H41	FNA	1	8.278	5.650	1.339	0.101629	hx
ATOM	66	N2	FNA	1	9.376	4.488	-0.092	-0.113705	n4
ATOM	67	H13	FNA	1	10.287	4.946	-0.073	0.317124	hn
ATOM	68	H14	FNA	1	9.149	4.136	-1.022	0.317124	hn
ATOM	69	C6	FNA	1	9.409	3.310	0.845	-0.090484	c3
ATOM	70	H11	FNA	1	8.484	3.281	1.381	0.110937	hx
ATOM	71	H12	FNA	1	10.256	3.451	1.485	0.110937	hx
ATOM	72	C5	FNA	1	9.606	1.949	0.145	-0.047900	c3
ATOM	73	H9	FNA	1	9.446	2.076	-0.906	0.060869	hc
ATOM	74	H10	FNA	1	8.904	1.261	0.569	0.060869	hc
ATOM	75	CG	FNA	1	11.011	1.371	0.363	0.018700	CT
ATOM	76	HG2	FNA	1	11.188	1.302	1.415	0.010300	HC
ATOM	77	HG3	FNA	1	11.699	2.031	-0.124	0.010300	HC
ATOM	78	CB	FNA	1	11.210	-0.028	-0.259	-0.009400	CT
ATOM	79	HB2	FNA	1	12.258	-0.170	-0.422	0.036200	HC

ATOM	80	HB3	FNA	1	10.628	-0.035	-1.157	0.036200	HC
ATOM	81	CA	FNA	1	10.697	-1.208	0.585	-0.240000	CT
ATOM	82	N	FNA	1	11.221	-1.147	1.949	-0.347900	N
ATOM	83	H	FNA	1	12.235	-1.250	1.929	0.274700	H
ATOM	84	HA	FNA	1	9.631	-1.133	0.643	0.142600	H1
ATOM	85	C	FNA	1	11.041	-2.552	-0.084	0.734101	C
ATOM	86	O	FNA	1	10.214	-3.128	-0.798	-0.589401	O

END