



## wwPDB EM Validation Summary Report ⓘ

Nov 1, 2022 – 03:14 PM EDT

PDB ID : 5JUL  
EMDB ID : EMD-8177  
Title : Near atomic structure of the Dark apoptosome  
Authors : Cheng, T.C.; Akey, I.V.; Yuan, S.; Yu, Z.; Ludtke, S.J.; Akey, C.W.  
Deposited on : 2016-05-10  
Resolution : 4.40 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

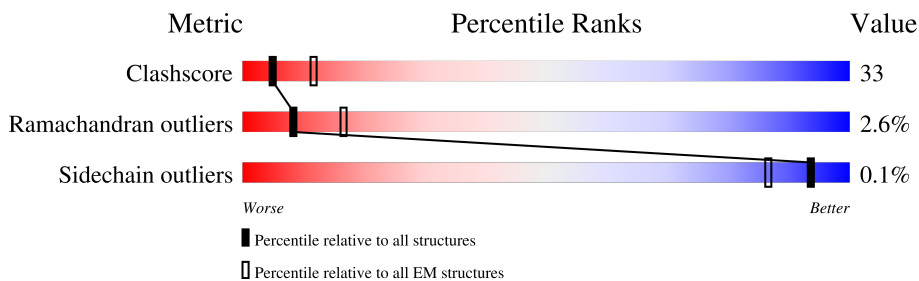
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1440	45% 
1	B	1440	45% 
1	C	1440	45% 
1	D	1440	45% 
1	E	1440	45% 
1	F	1440	45% 
1	G	1440	45% 
1	H	1440	45% 

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Mol	Chain	Length	Quality of chain
1	I	1440	
1	J	1440	
1	K	1440	
1	L	1440	
1	M	1440	
1	N	1440	
1	O	1440	
1	P	1440	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 161200 atoms, of which 0 are hydrogens and 0 are deuteriums.

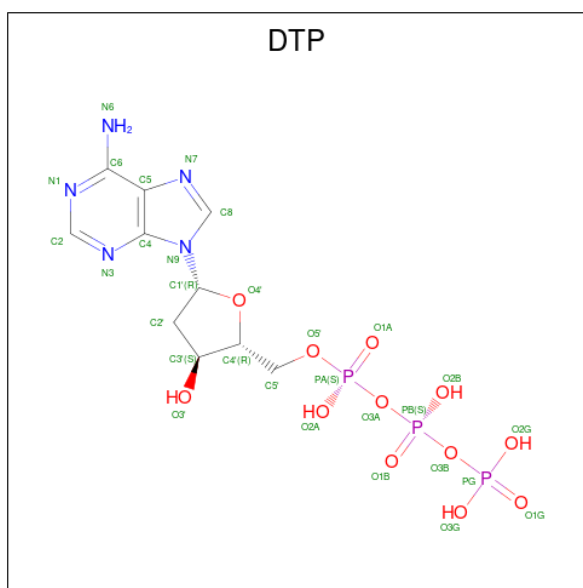
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Apaf-1 related killer DARK.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	1233	10045	6434	1698	1860	1	52	0	0
1	B	1233	10045	6434	1698	1860	1	52	0	0
1	C	1233	10045	6434	1698	1860	1	52	0	0
1	D	1233	10045	6434	1698	1860	1	52	0	0
1	E	1233	10045	6434	1698	1860	1	52	0	0
1	F	1233	10045	6434	1698	1860	1	52	0	0
1	G	1233	10045	6434	1698	1860	1	52	0	0
1	H	1233	10045	6434	1698	1860	1	52	0	0
1	I	1233	10045	6434	1698	1860	1	52	0	0
1	J	1233	10045	6434	1698	1860	1	52	0	0
1	K	1233	10045	6434	1698	1860	1	52	0	0
1	L	1233	10045	6434	1698	1860	1	52	0	0
1	M	1233	10045	6434	1698	1860	1	52	0	0
1	N	1233	10045	6434	1698	1860	1	52	0	0
1	O	1233	10045	6434	1698	1860	1	52	0	0
1	P	1233	10045	6434	1698	1860	1	52	0	0

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (for-

mula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
2	A	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	B	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	C	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	D	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	E	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	F	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	G	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	H	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	I	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	J	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	K	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	L	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	M	1	Total	C	N	O	P	0
			30	10	5	12	3	

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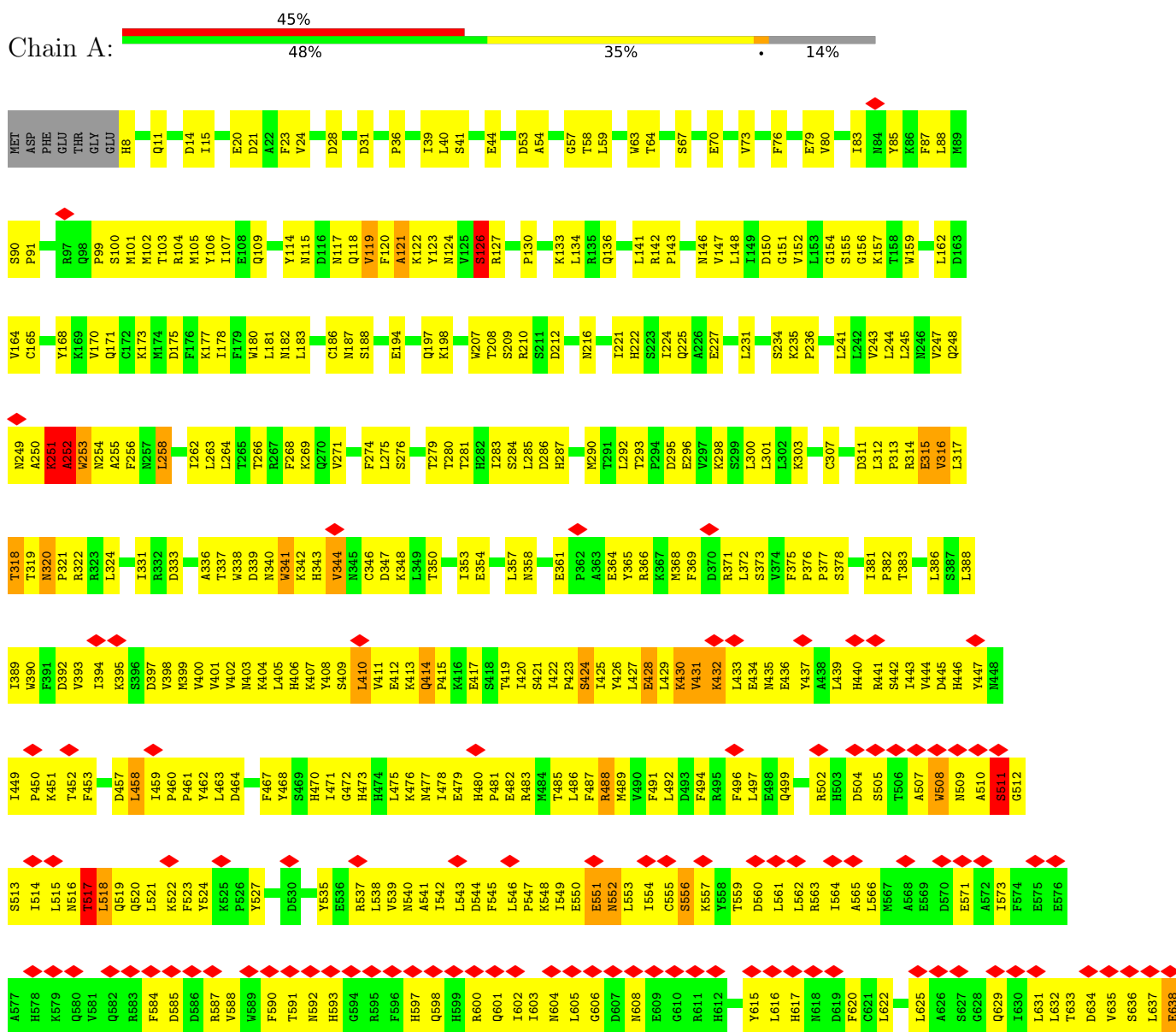
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	N	1	Total 30	10	5	12	3	0
2	O	1	Total 30	10	5	12	3	0
2	P	1	Total 30	10	5	12	3	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Apaf-1 related killer DARK

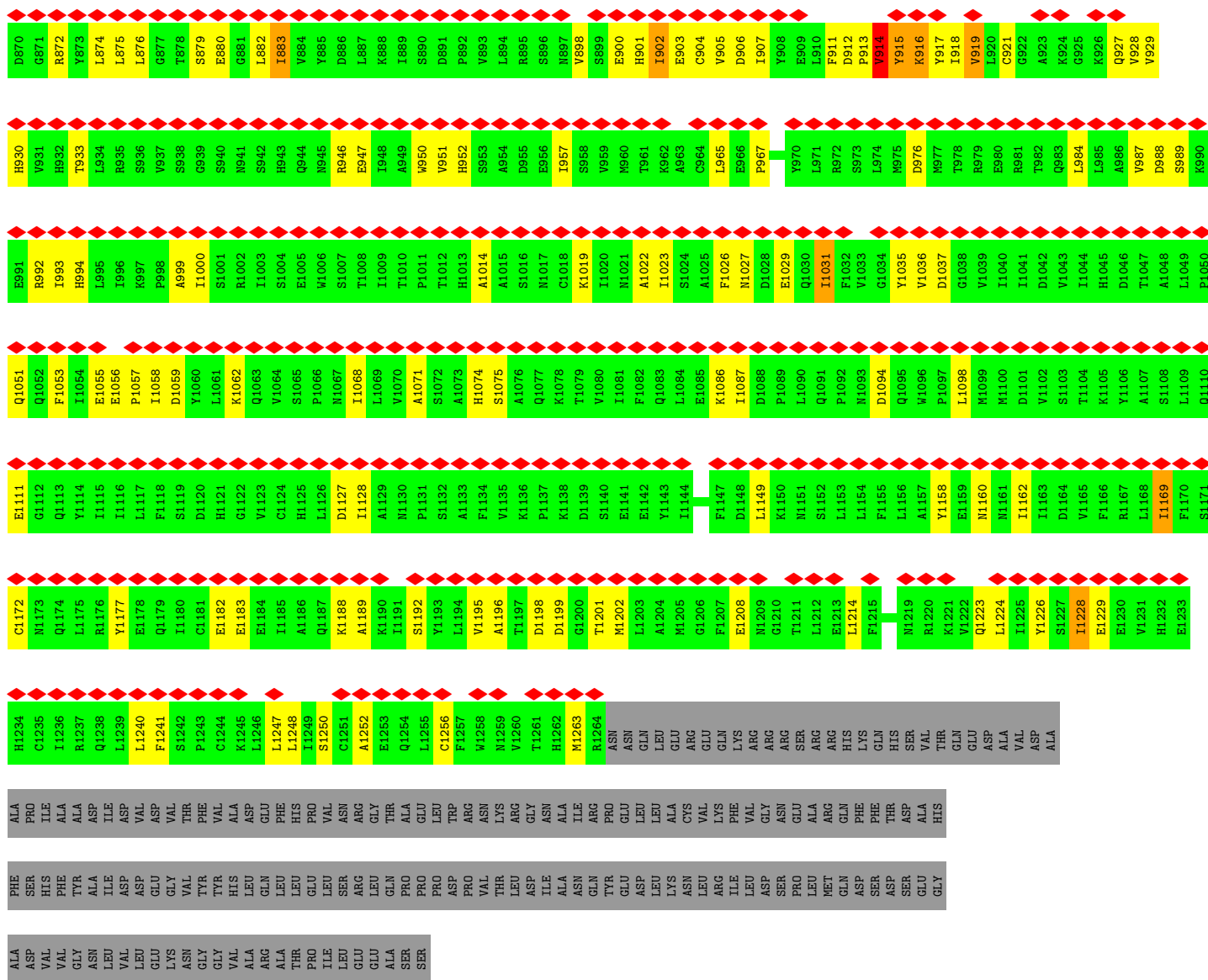




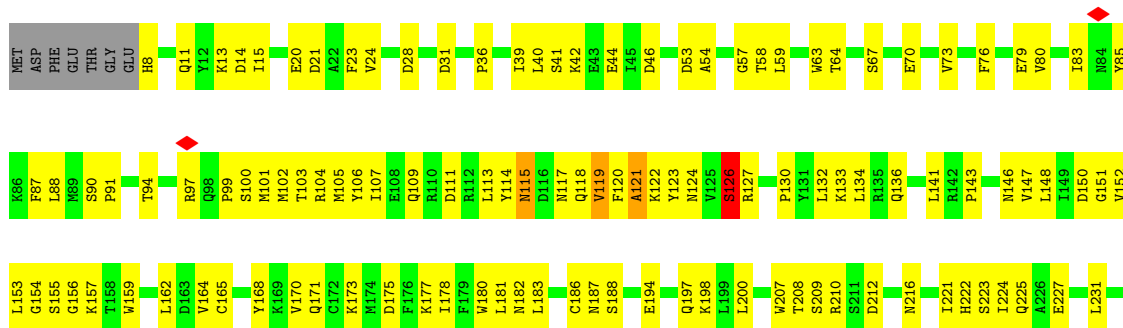


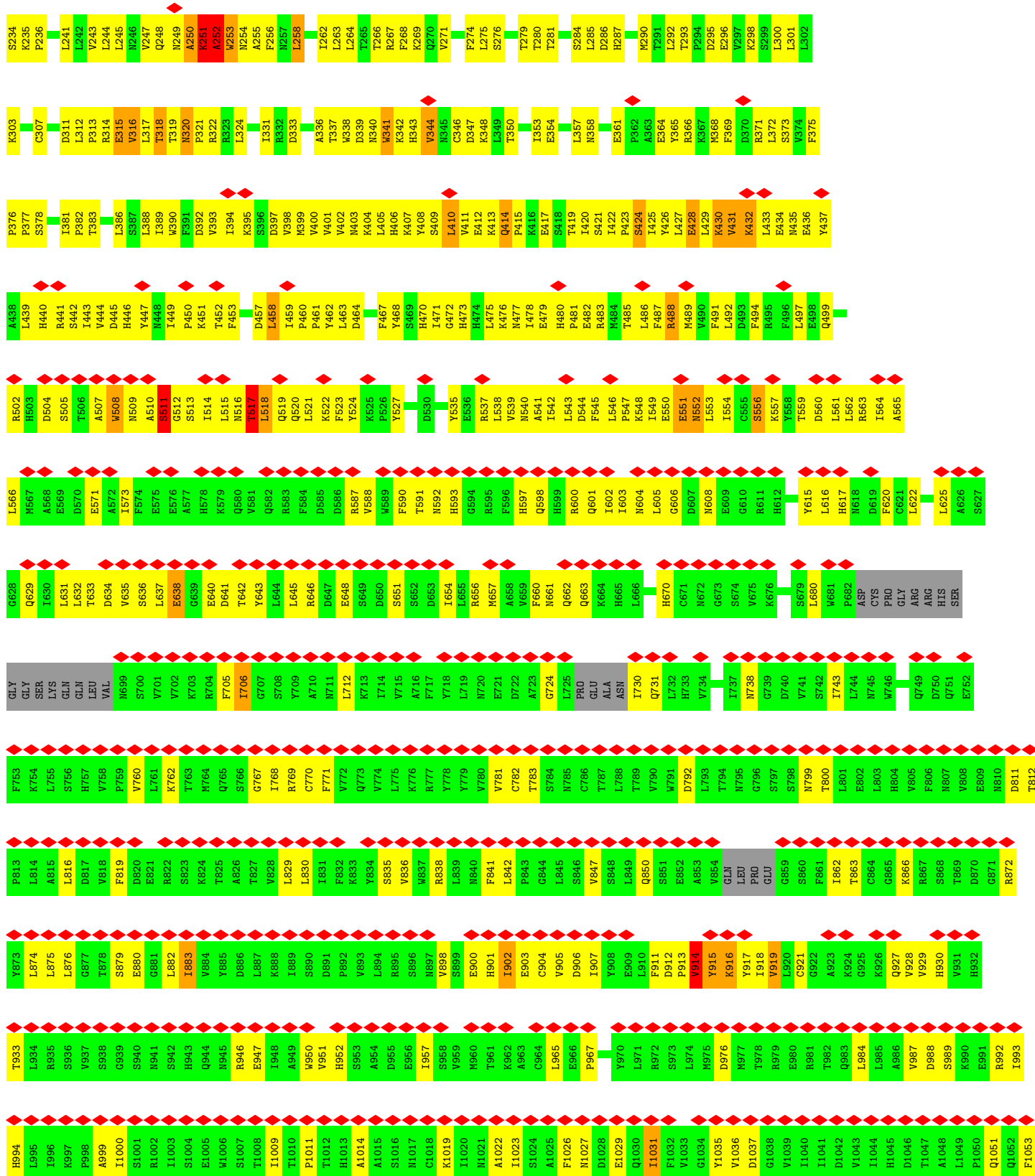


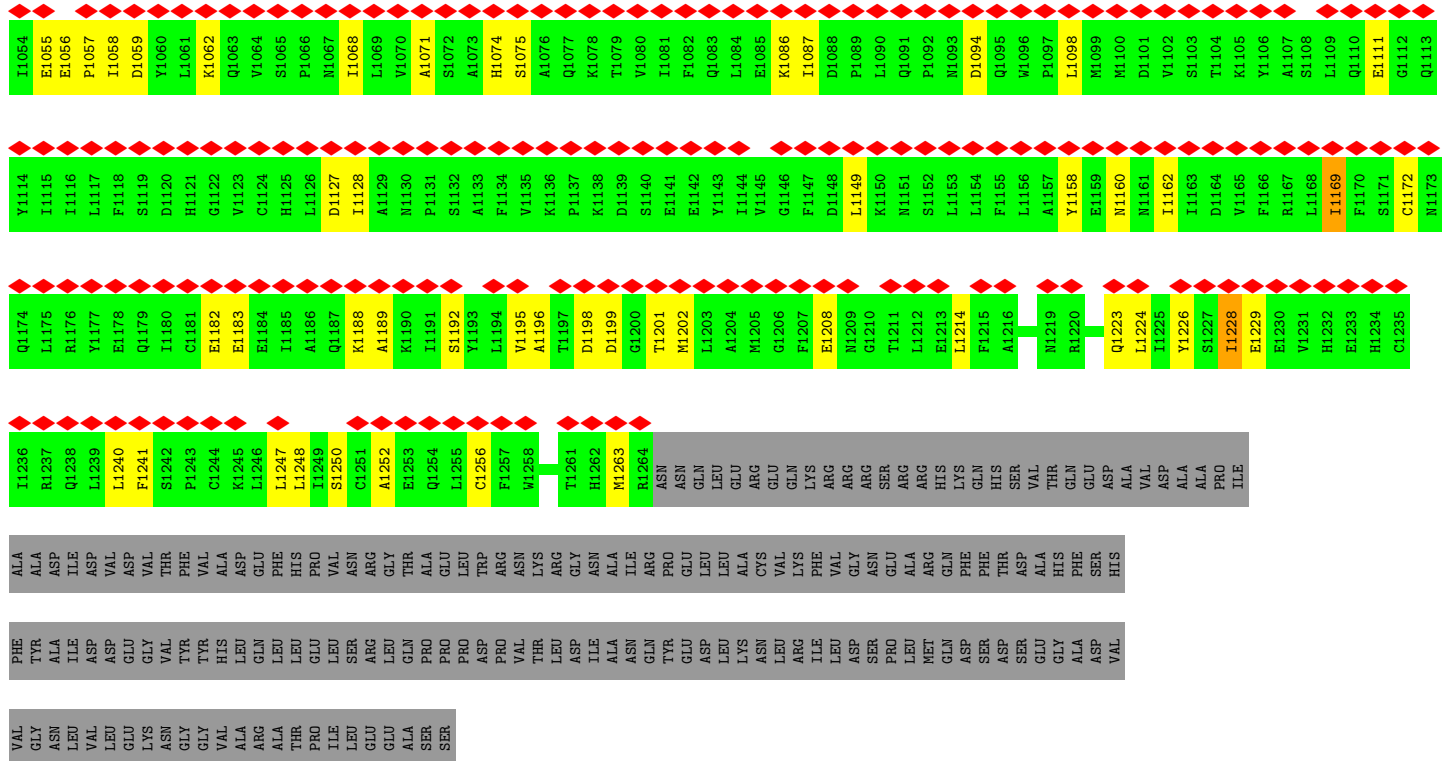
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Y85	K86	F87	L88	M89	S90	P91	I92	K93	T94	R97	Q98	P99	M100	M101	A102	T103	K104	M105	Y106	I107	E108	Q109	L113	Y114	N115	D116	N117	Q118	V119	A121	K122	I45	Y123	M124	V125	R126	R127	P130	Y131	L132	K133	T64	R135	Q136	L141	R142	P143	N146	V147	L148	I149	E226	L301	I83	M84					
L153	G154	G156	K157	W159	L162	D163	V164	C165	Y168	K169	V170	M101	Q171	M102	C172	A255	K173	M174	F176	I177	I178	Q109	L113	Y114	N115	D116	N117	Q118	V119	A121	K122	I45	Y123	M124	V125	R126	R127	P130	Y131	L132	K133	T64	R135	Q136	L141	R142	P143	N146	V147	L148	I149	E226	L301	I83	M84					
S234	K235	P236	L241	V243	L244	N246	Q248	N249	A250	K251	A252	W253	N254	A255	F256	M257	L258	I262	L263	L264	T265	T266	K267	F268	K269	Q270	V271	F274	L275	S276	T279	T280	T281	S284	L285	D286	H287	M290	T291	L292	T293	P294	D295	E296	Y297	K298	S299	L300	L301	L302										
K303	C307	R308	D311	L312	P313	R314	V315	L317	T318	T319	N320	P321	R322	K323	L324	I331	K332	D333	A336	T337	W338	D339	N340	K341	K342	H343	V344	K345	C346	D347	K348	L349	T350	T351	L352	L353	E354	S355	S356	L357	M358	E361	P362	A363	E364	Y365	R366	K367	M368	F369	D370	R371	L372							
S373	V374	P376	P377	S378	A379	H440	H441	I442	S443	V444	D445	H446	A447	M448	I449	P450	K451	T452	V453	D454	S455	D456	D457	L458	I459	Q460	P461	Y462	L463	D464	F467	Y468	S469	H470	I471	G472	H473	H474	L475	M476	M477	I478	E479	H480	P481	S482	E483	R484	M485	T485	L486	F487	R488	M489	V490	F491	L492	D493	F494	
R495	F496	L497	F498	Q499	R502	H503	D504	S505	T506	A507	M508	N509	A510	S511	G512	S513	I514	L515	M516	T517	L518	Q519	Q520	L521	K522	F523	Y524	K525	P526	Y527	Y535	E536	R537	L538	V539	N540	A541	L542	L543	D544	F545	L546	P547	K548	I549	E550	E551	N552	L553	E554	C555	S556	K557	T559	D560	L561				
L562	R563	I564	A565	L566	M567	A568	E569	D570	E571	I573	F574	N509	A510	S511	G512	S513	I514	L515	M516	T517	L518	Q519	Q520	L521	K522	F523	Y524	K525	P526	Y527	Y535	E536	R537	L538	V539	N540	A541	L542	L543	D544	F545	L546	P547	K548	I549	E550	E551	N552	L553	E554	C555	S556	K557	T559	D560	L561				
L625	A626	G627	G628	Q629	I630	L631	L632	T633	D634	V635	S636	L637	E638	G639	E640	D641	T642	Y643	L644	L645	R646	D647	S648	S649	D650	S651	S652	D653	I654	R655	R656	M657	A658	V659	F660	N661	Q662	Q663	K664	H665	H670	C671	N672	G673	S674	V675	K676	L680	M681	P682	ASP	CYS	PRO	GLY	ARG	ARG				
HIS	SER	GLY	GLY	SER	LYS	GLN	GLN	VAL	M699	S700	V701	V702	K703	R704	F705	I706	G707	S708	A710	M711	L712	K713	I714	V715	A716	F717	Y718	L719	M720	E721	D722	A723	G724	L725	PRO	GLU	ALA	ASN	I730	Q731	L732	H733	V734	I737	M738	G739	D740	S742	I743	L744	N745	W746	L803	C864	G865	K866	F806	N807	V808	E809
D750	Q751	E752	F753	K754	L755	S756	H757	V758	P759	V760	L761	K762	T763	M764	Q765	S766	I768	R769	C770	F771	V772	Q773	V774	L775	K776	R777	Y778	V779	W780	V781	C782	T783	S784	N785	C786	T787	L788	L849	W790	W791	D792	L793	T794	N795	G796	S797	V798	N799	T800	L801	E802	L803	C864	G865	K866	F806	N807	V808	E809	
D811	D812	F813	L814	A815	L816	D817	W818	F819	D820	E821	R822	S823	K824	T825	A826	T827	W828	L829	L830	L831	F832	K833	Y834	S835	V836	M837	R838	L839	H840	F841	P843	G844	L845	S846	V847	S848	L849	Q850	S851	E852	A853	V854	GLN	LEU	PRD	GLU	G859	S860	F861	I862	T863	C864	G865	K866	F806	N807	V808	E809		



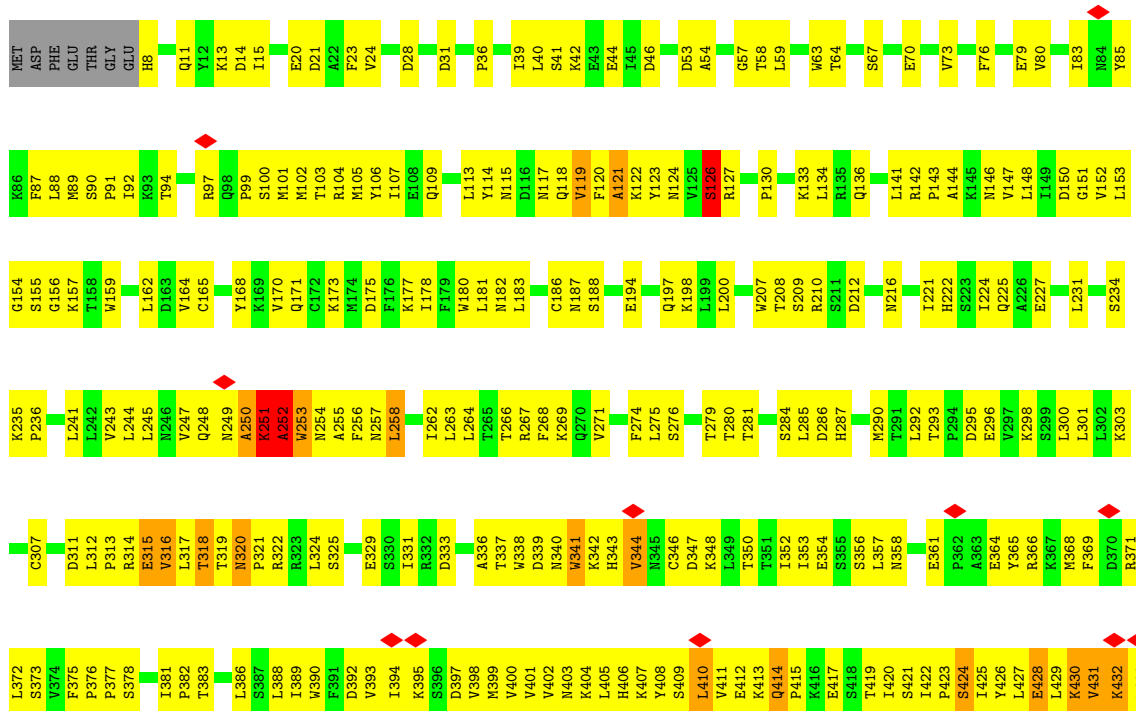
• Molecule 1: Apaf-1 related killer DARK



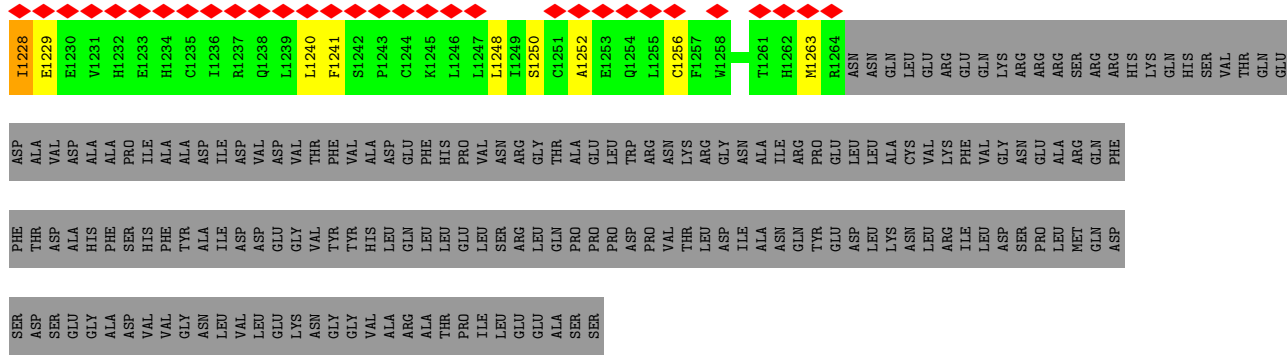




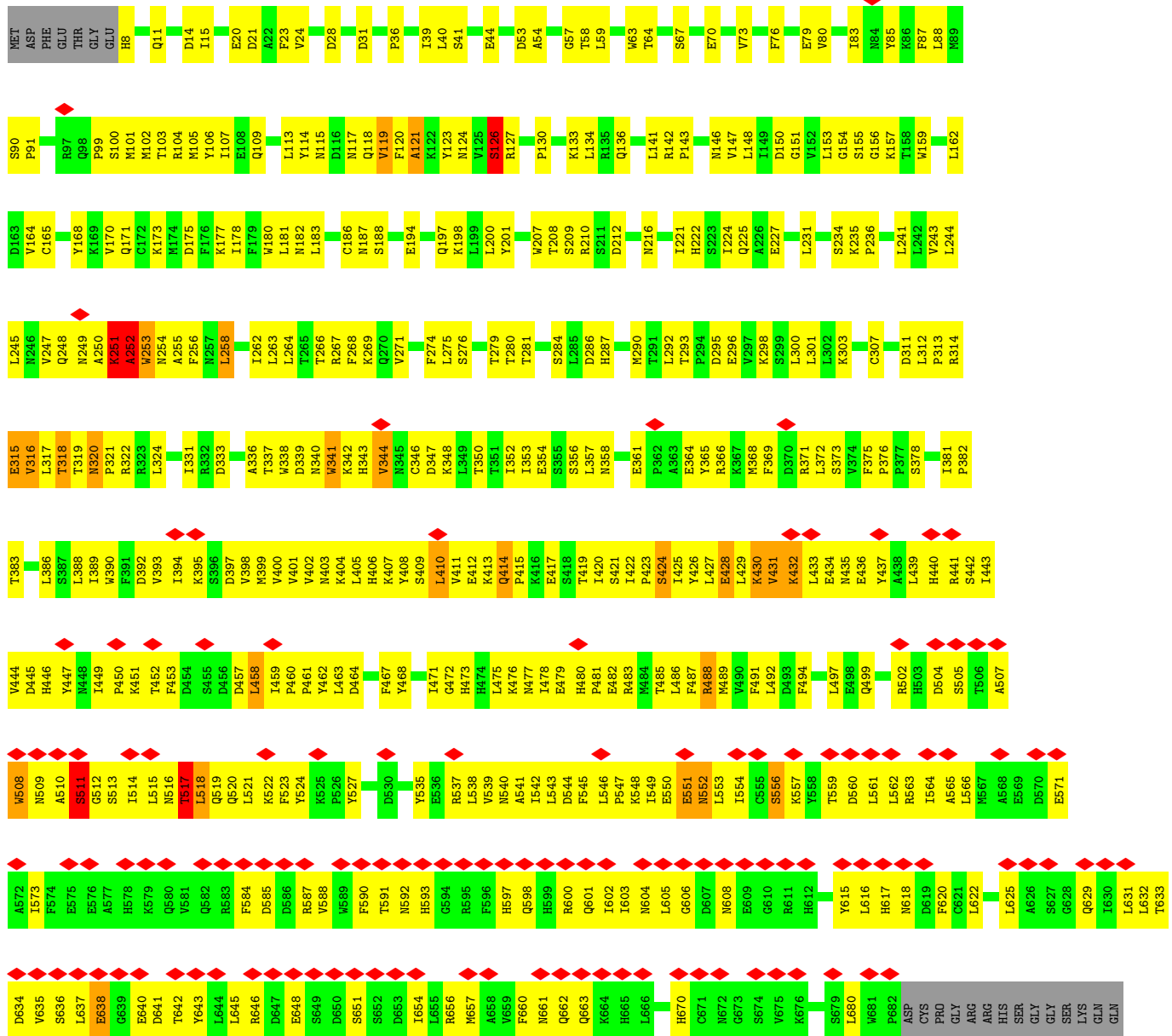
- Molecule 1: Apaf-1 related killer DARK



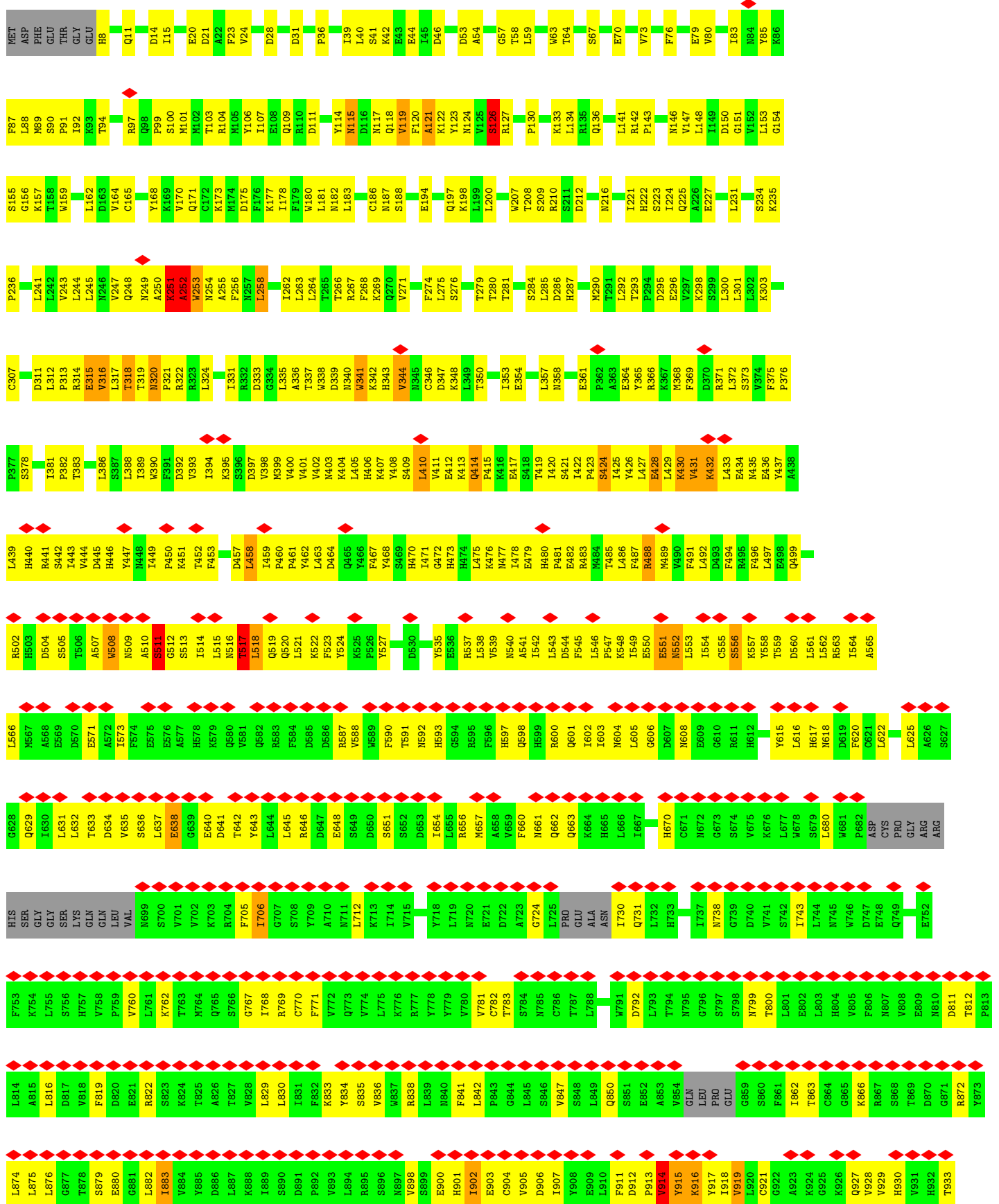
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R495	F496	L497	E498	Q499	R502	H503	D504	S505	I506	A507	M508	N509	A510	G511	S512	S513	I514	L515	M516	T517	L518	Q519	Q520	L521	K522	F523	Y524	K525	P526	Y527	D530	Y535	E536	R537	L538	V539	N540	A541	I542	L543	D544	F545	L546	P547	K548	I549	E550	E551	M552	L553	I554	G555	S556	K557	Y558	T559				
D560	L561	L562	R563	I564	A565	M567	A568	E569	D570	E571	A572	I573	F574	E575	G576	A577	H578	K579	Q580	S581	Q582	Q583	F584	D585	D586	R587	V588	M589	F590	T591	N592	H593	G594	R595	F596	H597	N598	Q599	R600	Q601	D602	D603	I604	I605	L606	L607	R608	N609	G610	R611	H612	Y615	L616	H617	N618	D619	F620			
C621	L622	L625	A626	S627	G628	Q629	L630	L631	L632	T633	D634	V635	S636	L637	E638	G639	D641	T642	Y643	L644	L645	R646	D647	E648	S649	D650	S651	R652	D653	I654	L655	R656	M657	A658	V659	F660	N661	Q662	Q663	H664	H665	L666	I667	H670	C671	N672	G673	S674	V675	K676	L677	H678	S679	L680	M681	P682				
ASP	CYS	PRO	GLY	ARG	ARG	HIS	SER	GLY	GLY	SER	LVS	GLN	GLN	LEU	VAL	M699	S700	V701	V702	K703	R704	F705	I706	G707	S708	Y709	A710	N711	L712	K713	I714	V715	A716	F717	Y718	L719	N720	E721	D722	A723	G724	L725	PRO	ALA	ASN	I730	Q731	L732	H733	V734	I737	N738	G739	D740	V741	S742	I743			
L744	N745	M746	D747	E748	Q749	D750	Q751	E752	F753	K754	L755	S756	H757	V758	F759	V760	L761	K762	M764	Q765	S766	G767	I768	R769	C770	F771	V772	Q773	V774	L775	K776	R777	Y778	Y779	V780	V781	C782	T783	S784	N785	C786	T787	L788	L789	N790	M791	D792	L793	T794	N795	G796	S797	S798	N799	T800	L801	E802	L803		
H804	V805	F806	N807	V808	E809	M810	D811	H812	L813	L814	A815	L816	D817	V818	F819	D820	E821	H822	S823	R824	T825	A826	T827	V828	L829	L830	T831	F832	K833	Y834	S835	V836	H837	R838	L839	N840	F841	L842	P843	G844	L845	S846	V847	S848	L849	Q850	S851	E852	A853	V854	GLN	LEU	PRO	GLU	G859	S860	F861	L862	T863	
C864	G865	R866	R867	S868	T869	D870	G871	R872	H873	L874	L875	L876	G877	T878	S879	E880	G881	L882	T883	H884	Y885	D886	L887	R888	S889	D891	H892	S893	A894	D895	E896	S897	V898	E900	H901	I902	E903	C904	V905	D906	I907	V908	E909	L910	F911	D912	P913	N914	Y915	K916	Y917	L918	I919	L920	C921	G922	A923			
K924	G925	K926	Q927	V928	V929	H930	V931	H932	T933	L934	H935	S936	K937	S938	G939	S940	N941	H942	H943	Q944	N945	R946	E947	I948	A949	N950	Y951	H952	S953	A954	D955	E956	I957	S958	V959	H960	T961	R962	C964	L965	E966	P967	N970	L971	H972	S973	L974	N975	D976	H977	T978	R979	E980	N981	G982	H983	L984			
L985	A986	V987	D988	S989	K990	E991	R992	I993	H994	L995	I996	K997	I998	A999	I1000	S1001	R1002	I1003	S1004	E1005	V1006	S1007	I1008	I1009	T1010	P1011	T1012	H1013	A1014	A1015	S1016	N1017	K1018	K1019	I1020	N1021	I1022	I1023	S1024	A1025	F1026	N1027	E1028	Q1030	I1031	F1032	P1033	M1034	G1035	V1036	Y1037	D1038	M1039	I1040	I1041	D1042	S1043	I1044		
H1045	D1046	T1047	A1048	L1049	P1050	Q1051	Q1052	F1053	I1054	E1055	E1056	P1057	I1058	D1059	Y1060	L1061	Q1063	V1064	S1065	P1066	M1067	I1068	L1069	V1070	A1071	S1072	A1073	H1074	S1075	A1076	Q1077	K1078	T1079	V1080	I1081	F1082	Q1083	L1084	E1085	K1086	I1087	D1088	P1089	L1090	Q1091	P1092	M1093	D1094	Q1095	V1096	D1097	L1098	M1099	M1100	D1101	V1102	S1103	T1104		
K1105	Y1106	A1107	S1108	L1109	Q1110	E1111	G1112	Q1113	Y1114	I1115	I1116	L1117	F1118	S1119	D1120	H1121	G1122	V1123	C1124	H1125	L1126	D1127	I1128	A1129	M1130	P1131	A1132	A1133	F1134	V1135	K1136	P1137	K1138	D1139	E1141	E1142	Y1143	I1144	V1145	G1146	F1147	D1148	L1149	K1150	M1151	S1152	L1153	L1154	F1155	L1156	Y1158	E1159	M1160	M1161	I1162	I1163	D1164			
V1165	F1166	R1167	L1168	I1169	F1170	S1171	C1172	M1173	Q1174	L1175	R1176	Y1177	E1178	Q1179	I1180	C1181	E1182	E1183	E1184	I1185	A1186	Q1187	K1188	A1189	K1190	I1191	S1192	Y1193	L1194	V1195	A1196	T1197	D1198	D1199	G1200	M1201	M1202	L1203	A1204	M1205	G1206	F1207	E1208	M1209	L1212	E1213	L1214	F1215	N1219	R1220	K1221	V1222	Q1223	L1224	I1225	Y1226	S1227			



● Molecule 1: Apaf-1 related killer DARK









L934	R935	S936	V937	S938	G939	S940	N941	S942	H943	Q944	N945	R946	E947	I948	A949	W950	V951	H952	S953	A954	D955	E956	I957	S958	V959	M960	T961	K962	A963	C964	L965	E966	P967	N968	V969	Y970	L971	R972	S973	L974	M975	D976	M977	T978	R979	E980	T982	Q983	L984	L985	A986	V987	D988	S989	K990	R992	I993		
H994	L995	I996	K997	P998	A999	I1000	S1001	R1002	I1003	S1004	E1005	W1006	S1007	T1008	I1009	T1010	P1011	T1012	H1013	A1014	A1015	S1016	M1017	C1018	K1019	I1020	M1021	A1022	I1023	S1024	F1025	F1026	M1027	D1028	E1029	Q1030	I1031	F1032	V1033	G1034	Y1035	W1036	D1037	G1038	V1039	I1040	I1041	D1042	V1043	I1044	H1045	D1046	T1047	A1048	L1049	P1050	Q1051	Q1052	F1053
I1054	E1055	E1056	P1057	I1058	D1059	Y1060	L1061	K1062	Q1063	V1064	S1065	P1066	N1067	I1068	L1069	V1070	A1071	S1072	A1073	H1074	S1075	A1076	Q1077	K1078	T1079	V1080	I1081	F1082	Q1083	L1084	E1085	K1086	I1087	D1088	P1089	L1090	Q1091	P1092	M1093	D1094	Q1095	W1096	P1097	L1098	M1099	M1100	D1101	V1102	S1103	T1104	K1105	Y1106	A1107	S1108	L1109	Q1110	E1111	G1112	Q1113
Y1114	I1115	I1116	L1117	F1118	S1119	D1120	H1121	K1122	V1123	C1124	H1125	L1126	D1127	I1128	A1129	M1130	P1131	S1132	A1133	F1134	V1135	K1136	P1137	K1138	D1139	S1140	E1141	Y1142	I1143	L1144	V1145	G1146	F1147	D1148	L1149	K1150	M1151	S1152	L1153	L1154	F1155	L1156	A1157	Y1158	E1159	M1160	M1161	I1162	D1164	V1165	F1166	R1167	L1168	I1169	F1170	S1171	C1172	M1173	
Q1174	L1175	R1176	Y1177	E1178	Q1179	I1180	C1181	E1182	E1183	E1184	I1185	A1186	Q1187	K1188	A1189	K1190	I1191	S1192	Y1193	L1194	V1195	A1196	T1197	D1198	D1199	G1200	T1201	M1202	L1203	A1204	M1205	G1206	F1207	E1208	H1209	L1212	E1213	L1214	F1215	A1216	M1219	R1220	Q1223	L1224	I1225	Y1226	S1227	I1228	E1229	E1230	V1231	H1232	E1233	H1234	C1235	I1236			
R1237	Q1238	L1239	L1240	F1241	S1242	P1243	C1244	K1245	L1246	L1247	L1248	I1249	S1250	C1251	A1252	E1253	Q1254	L1255	F1257	W1258	T1261	M1262	M1263	R1264	ASN	ASN	GLN	LEU	GLU	LEU	ALA	ARG	CYS	VAL	GLN	LYS	PHE	VAL	ARG	GLY	ASN	SER	ARG	GLU	ALA	ALA	ASP	VAL	VAL	ASP	ALA	ALA	PRO	PRO	ILE	ALA	ALA		
ALA	ASP	ILE	ASP	VAL	ASP	THR	PHE	VAL	GLU	ASP	HIS	VAL	ALA	ARG	LEU	PRO	LEU	VAL	ARG	GLY	THR	LEU	ALA	ALA	ILE	ASN	GLN	TYR	PRO	GLU	LEU	ILE	VAL	ARG	ASP	GLY	ASN	SER	ARG	GLU	ALA	ALA	ASP	VAL	VAL	ASP	ALA	ALA	PRO	PRO	ILE	ALA	ALA						
TYR	ALA	ILE	ASP	GLU	GLY	VAL	THR	TYR	VAL	GLY	HIS	VAL	ALA	ARG	LEU	PRO	LEU	VAL	ARG	GLY	THR	LEU	ALA	ALA	ILE	ASN	GLN	TYR	PRO	GLU	LEU	ILE	VAL	ARG	ASP	GLY	ASN	SER	ARG	GLU	ALA	ALA	ASP	VAL	VAL	ASP	ALA	ALA	PRO	PRO	ILE	ALA	ALA						
GLY	ASN	LEU	VAL	LEU	GLY	LYS	ASN	GLY	GLY	VAL	VAL	ALA	ARG	ALA	THR	THR	ILE	LEU	GLU	GLY	GLU	ALA	ALA	ALA	ASN	GLN	TYR	PRO	GLU	LEU	ILE	VAL	ARG	ASP	GLY	ASN	SER	ARG	GLU	ALA	ALA	ASP	VAL	VAL	ASP	ALA	ALA	PRO	PRO	ILE	ALA	ALA							

• Molecule 1: Apaf-1 related killer DARK



MET	ASP	PHE	GLU	THR	GLY	GLU	H8	Q11	D14	I15	E20	D21	F22	A23	V24	D28	D31	P36	I39	L40	S41	K42	E43	E44	I45	D46	D63	A64	G67	T68	L69	W63	T64	S67	E70	V73	F76	E79	V80	I83	N84	Y85	K86									
F87	L88	M89	P91	T94	R97	Q98	P99	S100	M101	M102	T103	R104	M105	Y106	I107	E108	Y114	M115	D116	Q118	V119	F120	K122	Y123	I124	D125	S126	R127	P130	K133	L134	E135	Q136	L141	R142	P143	A144	K145	V147	L148	I149	D150	G151	G154	S155	G156	K157					
T158	W159	L162	D163	V164	C165	Y168	K169	V170	Q171	S172	K173	M174	F176	K177	I178	F179	W180	L181	M182	L183	C186	M187	S188	E194	Q197	K198	L200	W207	T208	S209	R210	S211	D212	N216	I221	H222	S223	I224	Q225	A226	E227	L231	S234	K235	P236	L241						
L242	V243	L244	L245	N246	V247	Q248	N249	A250	A251	K252	W253	N254	A255	F256	N257	L258	T262	L263	L264	T265	T266	R267	F268	K269	Q270	V271	F274	L275	S276	T279	T280	T281	S284	L285	D286	H287	M290	T291	L292	T293	P294	D295	E296	V297	K298	S299	L300	L301	L302	K303	C307	D311

E1056	P1057	I1058	D1059	Y1060	L1061	K1062	Q1063	V1064	S1065	P1066	N1067	I1068	L1069	V1070	A1071	S1072	H1073	H1074	S1075	A1076	Q1077	K1078	T1079	V1080	I1081	F1082	L1083	E1085	K1086	I1087	D1088	P1089	L1090	Q1091	P1092	N1093	D1094	Q1095	W1096	P1097	L1098	M1099	M1100	D1101	V1102	S1103	T1104	K1105	Y1106	A1107	S1108	L1109	Q1110	E1111	G1112	Q1113	Y1114	I1115																																																																																																										
L875	L876	G877	T878	S879	E880	G881	I882	I883	V884	Y885	D886	L887	K888	I889	S890	D891	F892	V893	Y894	A895	D895	F896	I897	V898	S899	E900	H901	I902	E903	C904	V905	D906	I907	Y908	E909	L910	F911	D912	P913	Y914	K916	Y917	Y918	V919	L920	C921	G922	K924	G925	K926	Q927	V928	Y929	H930	V931	H932	T933	L934	R935	V936	T937	Y938	L939	R940	S941	S942	H943	Q944	Y945	R946	E947	I948	A949	V950	V951	H952	S953	A954	D955	Q956	I957	V958	Y959	M960	T961	Q962	A963	C964	L965	E966	I967	Y968	S969	E970	L971	F972	V973	N974	Y975	D976	M977	T978	V979	L980	E981	T982	C983	L984	S985	K986	R987	H988	S989	V990	V991	H992	T993	L994	L995																																													
A815	L816	D817	V818	F819	D820	E821	S822	S823	K824	T825	D826	T827	V828	L829	L830	I831	K832	K833	Y834	S835	V836	W837	R838	H839	H840	F841	L842	P843	C844	L845	S846	V847	S848	L849	L850	F851	D852	E853	Y854	GLN	LEU	PRO	GLU	G859	S880	F881	T882	T883	C884	S885	K886	R887	V888	Y889	H890	V891	H892	T893	L894	S895	V896	V897	H898	L899	V900	V901	H902	H903	L904	L905	A906	T907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999
L755	S756	H757	V758	F759	V760	L761	K762	T763	W764	Q765	S766	G767	L768	R769	C770	F771	V772	Q773	V774	L775	K776	R777	V778	Y779	W780	V781	C782	T783	S784	W785	C786	T787	L788	T789	V790	W791	D792	L793	T794	W795	G796	S797	S798	W799	T800	L801	E802	L803	H804	V805	F806	H807	W808	E809	H810	D811	T812	P813	L814																																																																																																									
L631	L632	T633	D634	V635	S636	L637	E638	E640	D641	T642	Y643	L644	L645	R646	D647	E648	S649	D650	S651	S652	D653	L654	R655	M656	M657	A658	V659	F660	N661	Q662	K664	H665	L666	H670	C671	N672	G673	S674	V675	K676	S679	L680	W681	P682	ASP	CYS	PRO	GLY	ARG	ARG	HIS	GLY	GLY	SER																																																																																																														
L631	L632	T633	D634	V635	S636	L637	E638	E640	D641	T642	Y643	L644	L645	R646	D647	E648	S649	D650	S651	S652	D653	L654	R655	M656	M657	A658	V659	F660	N661	Q662	K664	H665	L666	H670	C671	N672	G673	S674	V675	K676	S679	L680	W681	P682	ASP	CYS	PRO	GLY	ARG	ARG	HIS	GLY	GLY	SER																																																																																																														
L569	D570	E571	A572	I573	F574	E575	E576	A577	H578	K579	Q580	V581	Q582	F583	F584	D585	D586	R587	V588	W589	F590	T591	N592	H593	G594	R595	F596	H597	Q598	H599	R600	I602	I603	N604	L605	L606	G606	D607	N608	E609	G610	R611	H612	Y615	L616	H617	N618	D619	F620	C621	L622	L625	A626	S627	G628	Q629	I630																																																																																																											
S505	T506	A507	W508	N509	A510	S511	G512	S513	I514	L515	N516	T517	L518	Q520	L521	K522	F523	Y524	K525	P526	Y527	D530	Y535	R537	L538	V539	N540	A541	I542	L543	D544	F545	L546	I602	K548	I549	E550	E551	N552	L553	I554	C555	S556	K557	Y558	T559	D560	L561	L562	R563	I564	A565	L566	M567	A568																																																																																																													
E569	D570	E571	A572	I573	F574	E575	E576	A577	H578	K579	Q580	V581	Q582	F583	F584	D585	D586	R587	V588	W589	F590	T591	N592	H593	G594	R595	F596	H597	Q598	H599	R600	I602	I603	N604	L605	L606	G606	D607	N608	E609	G610	R611	H612	Y615	L616	H617	N618	D619	F620	C621	L622	L625	A626	S627	G628	Q629	I630																																																																																																											
L312	P313	R314	E315	V316	L317	T318	S319	N320	P321	R322	E323	L324	I331	D332	D333	A336	T337	W338	D339	N340	W341	K342	H343	V344	N345	C346	D347	K348	L349	T350	I353	E354	L357	N358	E361	P362	A363	E364	Y365	R366	K367	M368	F369	D370	K371	L372	S373	M374	V375	F376	P377	S378	I381																																																																																																															
P382	T383	L386	S387	L388	I389	W390	F391	D392	V393	R394	K395	S396	D397	V398	M399	V400	V401	V402	M403	K404	L405	H406	K407	Y408	S409	L410	V411	E412	K413	Q414	P415	K416	S417	T419	I420	S421	I422	P423	S424	I425	Y426	L427	E428	L429	V431	K432	L433	E434	M435	E436	F437	A438	L439	H440	R441	S442																																																																																																												
I443	V444	H446	H447	M448	I449	P450	K451	F452	F453	D454	S455	D456	D457	L458	I459	P460	P461	Y462	L463	D464	Y467	Y468	S469	H470	I471	G472	H473	H474	K476	M477	I478	E479	H480	I481	S482	R483	M484	T485	L486	F487	R488	L489	V490	F491	L492	D493	F494	R495	F496	L497	E498	Q499	R502	H503	D504																																																																																																													

I1116	R1176	Q1238	ASP	ASN
L1117	Y1177	L1239	ILE	LEU
F1118	E1178	L1240	ASP	VAL
S1119	Q1179	F1241	VAL	LEU
D1120	I1180	G1242	GLY	GLY
H1121	C1181	P1243	THR	LYS
H1122	E1182	C1244	PHE	ASN
V1123	E1183	K1245	VAL	GLY
C1124	I1184	L1246	ALA	VAL
H1125	I1185	L1247	LEU	ALA
L1126	A1186	L1248	GLN	ALA
D1127	Q1187	I1249	LEU	THR
I1128	K1188	S1250	PRO	PRO
A1129	A1189	C1251	VAL	ILE
M1130	K1190	A1252	SER	LEU
P1131	I1191	E1253	ARG	GLU
S1132	S1192	Q1254	GLY	LEU
A1133	I1193	L1255	THR	GLN
F1134	L1194	C1256	PRO	PRO
V1135	Y1195	F1257	ASP	ASP
K1136	A1196	W1258	TRP	PRO
P1137	T1197	T1261	ASN	VAL
K1138	D1198	H1262	ARG	THR
D1139	I1199	M1263	LEU	LEU
S1140	G1200	R1264	GLY	LEU
E1141	T1201	ASN	ASN	ASN
E1142	M1202	ASN	GLN	GLN
Y1143	L1203	LEU	LEU	GLU
I1144	A1204	GLU	LEU	LEU
V1145	M1205	GLU	LEU	LYS
G1146	G1206	GLN	VAL	ASN
F1147	F1207	LYS	ILE	ARG
D1148	E1208	ARG	PHE	ILE
L1149	N1209	ARG	VAL	VAL
K1150	G1210	SER	GLY	ASP
M1151	T1211	ARG	ASN	SER
S1152	L1212	ARG	GLU	PRO
L1153	H1213	HIS	ALA	LEU
L1154	L1214	GLN	GLN	MET
F1155	F1215	GLN	PHE	ASP
L1156	N1219	SER	PHE	SER
A1157	K1221	THR	THR	ASP
Y1158	E1159	GLN	ALA	THR
E1159	V1222	GLU	HIS	GLY
M1160	Q1223	ASP	ALA	ALA
N1161	N1160	VAL	VAL	VAL
I1162	I1162	ASP	ASP	VAL
I1163	I1163	ALA	ALA	ALA
D1164	Y1226	PRO	PRO	PRO
V1165	S1227	ILE	ILE	ILE
F1166	I1228	ALA	ALA	ALA
R1167	E1229	ALA	ALA	ALA
L1168	E1230	VAL	VAL	VAL
I1169	H1231	LEU	LEU	LEU
F1170	H1232	SER	SER	SER
S1171	E1233	SER	SER	SER
C1172	H1234	CYS	CYS	CYS
Q1174	C1235	LEU	LEU	LEU
L1175	I1236	ALA	ALA	ALA
	R1237	GLY	GLY	GLY

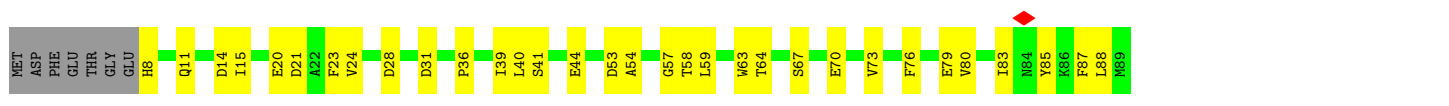
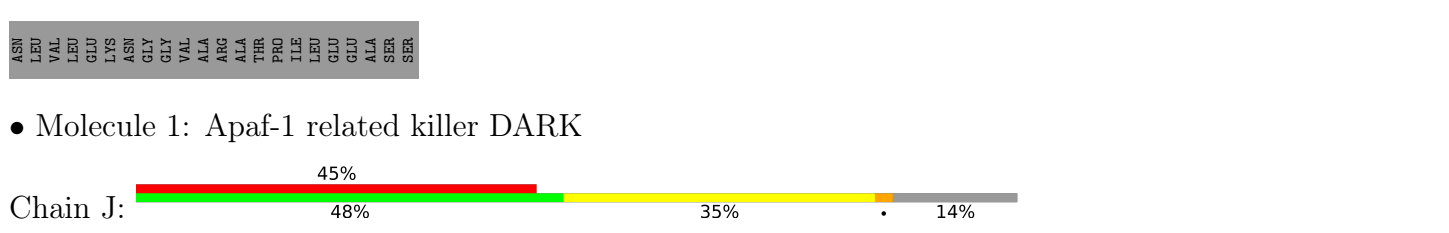
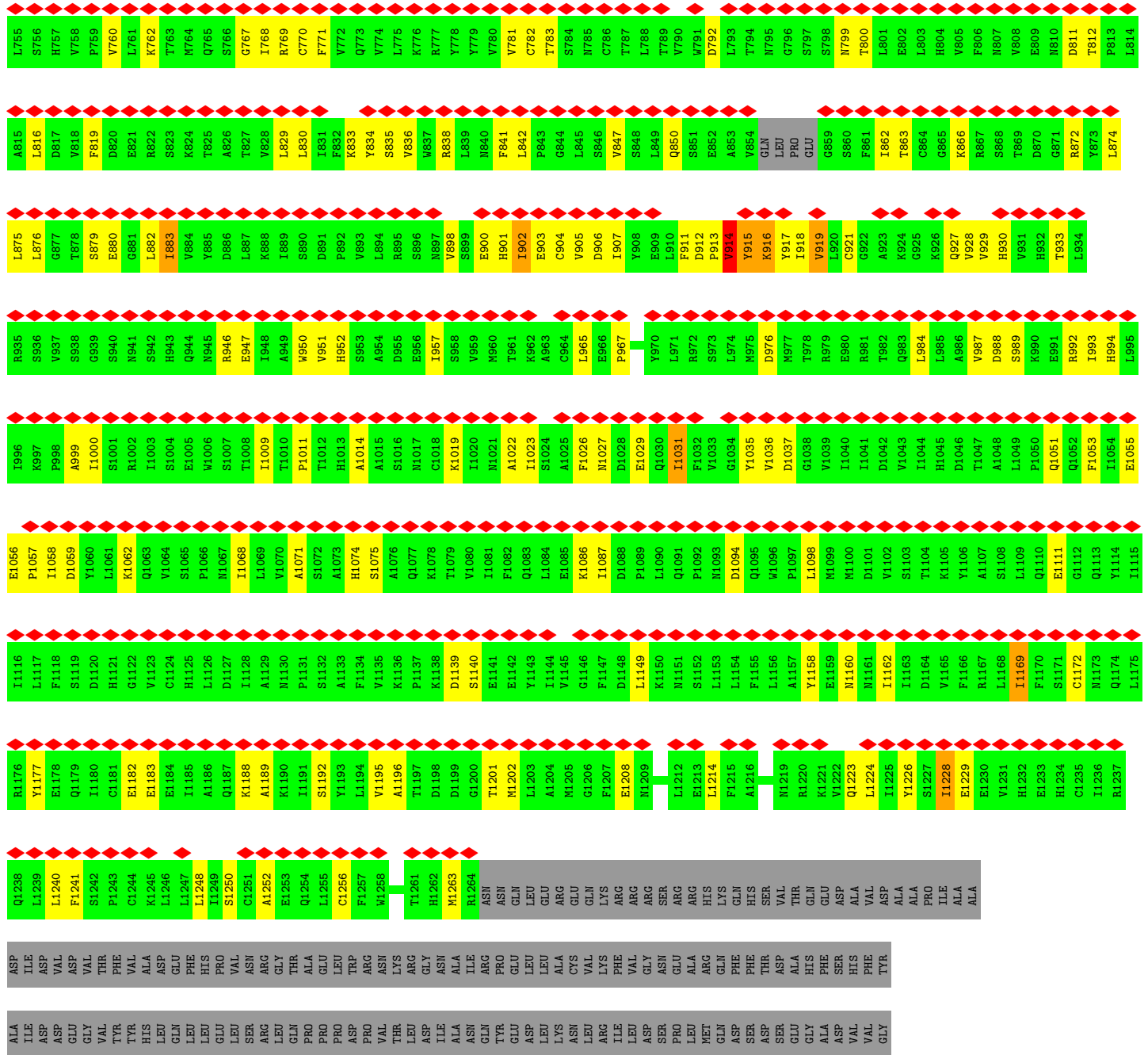
• Molecule 1: Apaf-1 related killer DARK

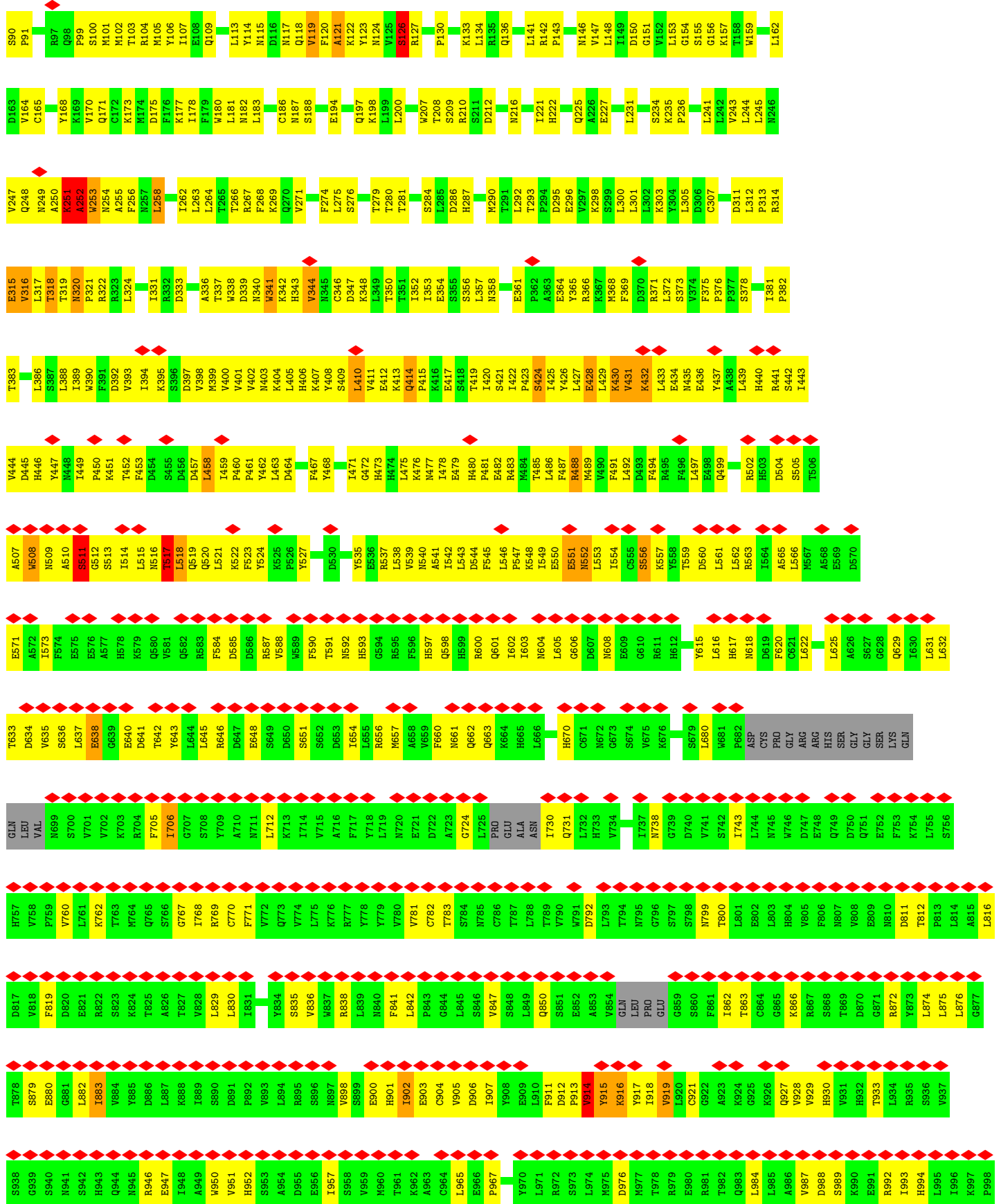


MET	K66	L245	I312	P382	I443
ASP	F87	M246	P313	T383	V444
PHE	L88	Q247	R314	L386	D445
THR	M89	Q248	E315	L387	H446
GLY	S90	N249	V316	L388	Y447
THR	P91	A250	L317	I389	H448
GLU	I92	K251	T318	W390	I449
H8	K93	A252	T319	M391	P450
	T94	W253	N320	F392	K451
	Q11	N254	P321	D392	T452
	Y12	A255	R322	V393	F453
	K13	F256	R323	I394	D454
	K13	M257	L324	K395	S455
	D14	L258	I331	D397	D456
	I15	I262	R332	V398	D457
	E20	K173	D333	M399	L458
	D21	L263	L336	V400	I459
	A22	L264	A336	V401	P460
	F23	T265	T337	V402	P461
	V24	R266	W338	M403	Y462
	D28	R267	D339	K404	L463
	D31	F179	N340	K404	D464
	P36	E108	L405	L405	F467
	I39	Q109	K342	H406	S469
	L40	L113	H343	K407	H470
	S41	Y114	V344	Y408	I471
	K42	M115	N345	S409	G472
	E43	N116	C346	L410	H473
	E44	D116	D347	V411	H474
	F45	M117	K348	E412	L475
	D46	Q118	L349	Q414	K476
	D53	V119	T279	P415	M477
	A54	F120	T280	K416	E417
	G57	A121	H282	E418	T419
	L59	K122	T281	S418	H480
	V63	Y123	I283	E419	P481
	T64	M124	S284	T419	I420
	S67	V125	L285	I420	S421
	E70	S126	D286	I422	I422
	V73	R127	H287	P423	P423
	F76	P130	M290	A424	T484
	E79	K133	L292	I425	T485
	V80	L134	T293	A426	L486
	I83	Q136	P294	L427	F487
	Y85	L141	H221	E428	M488
		R142	Q225	L429	M489
		P143	A226	K430	V490
		L146	E227	F369	F491
		V147	L300	K432	L492
		L148	L301	L433	D493
		V149	K302	E434	F495
		I149	K303	M435	F496
		D150	Y304	E436	L497
		G151	L305	Y437	E498
		I84	D306	A438	Q499
		S155	C307	L439	R502
			L242	H440	H503
			L244	R441	D504
				S442	

ILE	L1239	Y1177	L1117	P1057	K997	S936	L876	L816	S756	GLN	L631	E569	S505
ASP	L1240	E1178	F1118	I1058	P998	V937	Q877	D817	H757	GLN	L632	D570	T806
VAL	L1241	Q1179	S1119	D1059	A999	S938	T878	Y818	V758	LEU	T833	E571	A507
THR	S1242	I1180	D1120	Y1060	I1000	G939	S879	F819	P759	VAL	D634	A572	W608
PHE	C1243	C1181	H1121	K1061	S1001	S940	S879	D820	V760	THR	D635	I573	N609
VAL	C1244	E1182	G1122	K1062	R1002	S941	G881	E821	L761	VAL	D636	F574	A510
ALA	K1245	E1183	V1123	Q1063	I1003	S942	L882	R822	K762	THR	E838	E575	S611
ASP	L1246	F1184	C1124	V1064	S1004	H943	T883	S823	T763	GLY	G639	E576	G512
GLU	L1247	I1185	H1125	E1065	E1005	I944	W884	K824	M764	GLU	E640	A577	S513
PHE	L1248	A1186	L1126	S1066	W1006	I945	W885	T825	Q765	THR	E641	H578	I514
HIS	L1249	Q1187	D1127	M1067	S1007	R946	W886	A826	S766	GLY	D642	K579	L515
PRO	S1250	K1188	I1128	I1068	T1008	E947	L887	T827	G767	PRO	T641	Q580	N516
VAL	C1251	A1189	A1129	L1069	I1009	I948	X888	W828	I768	ASN	Y643	V581	T817
ASN	A1252	K1190	M1130	V1070	T1010	A949	L889	L829	R769	GLY	L844	Q582	L518
ARG	E1253	I1191	P1131	A1071	P1011	W950	S890	L830	C770	THR	L845	Q519	Q519
THR	Q1254	S1192	S1132	S1072	T1012	W951	D891	L830	C770	THR	R646	F584	Q520
ALA	L1255	L1193	A1133	A1073	H1013	H952	D891	L831	F771	ALA	D647	D585	L521
LEU	C1256	L1194	F1134	S1075	A1014	S953	R892	K833	V772	THR	S649	D586	K522
LEU	F1257	V1195	V1135	A1076	A1015	A954	W894	Y834	Q774	THR	D650	E648	Y524
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ARG	H1262	D1199	D1139	T1079	K1019	S958	W898	R839	I778	ARG	D653	N592	D530
GLY	M1263	G1200	S1140	V1080	I1020	W959	S899	L839	V779	GLY	I654	H593	Y535
ALA	R1264	T1201	E1141	I1081	M1021	W960	E900	N840	W780	ALA	R656	G594	E536
ARG	ASN	M1202	E1142	F1082	A1022	H961	H901	F841	V781	ARG	M657	G595	R637
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CYS	GLN	F1207	F1147	K1087	M1027	E966	D906	S846	C786	CYS	Q663	Q599	I543
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PHE	ARG	M1209	L1149	P1089	E1029	W970	Y908	S848	L788	PHE	H665	Q601	F545
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GLY	SER	L1212	N1151	I1031	I1031	L972	F911	Q850	V790	GLY	H670	I603	P547
ASN	ARG	E1213	S1152	F1032	F1032	A973	S851	S851	W791	ASN	C671	L605	K548
GLU	ARG	I1214	L1153	V1033	V1033	S973	D912	E852	D792	GLU	G672	L606	I549
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PHE	SER	R1220	L1156	D1037	D1037	N977	LEU	LEU	G796	PHE	V675	E609	I554
THR	VAL	K1221	A1157	P1097	P1097	N978	PRD	PRD	S797	THR	K676	R611	C555
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PHE	VAL	L1226	I1162	D1042	D1042	T982	A923	L862	L801	PHE	ASP	L617	D560
TYR	ALA	Y1226	I1163	V1043	V1043	T983	K925	T863	E802	TYR	CYS	H617	D560
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ALA	ALA	E1230	F1166	D1046	D1046	A986	Q927	K866	H804	ALA	ARG	F820	R563
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ALA	ASP	L1112	G1112	Q1052	Q1052	E992	T933	R872	W810	ALA	GLY	A826	A566
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ALA	ASP	L1115	L1115	L1115	L1115	L995	L875	R875	L754	ALA	LYS	Q629	A566
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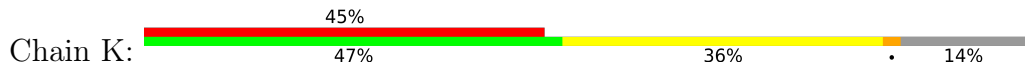






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VAL	ASP	VAL	THR	TYR	VAL	ALA	GLN	GLU	PRO	VAL	ASN	ARG	GLY	THR	PRO	THR	VAL	LYS	ARG	GLY	ALA	ALA	ASN	ILE	ASN	PRO	PRO	GLU	LEU	VAL	ARG	VAL	PHE	LEU	VAL	THR	ASP	ALA	HIS	ALA	ALA	ASP	ALA	ASP	VAL	PHE	TYR	ALA	ILE	ASP									
ASP	GLU	VAL	GLY	TYR	HIS	LEU	ARG	LEU	PRO	LEU	SER	ARG	LEU	GLN	PRO	ASP	THR	VAL	ASN	THR	LEU	ILE	ASN	GLN	TYR	GLU	LEU	VAL	ARG	ILE	LEU	ASP	GLY	SER	THR	ASP	GLU	GLY	ALA	ASP	VAL	PHE	ASN	LEU	LEU	VAL	ASP												
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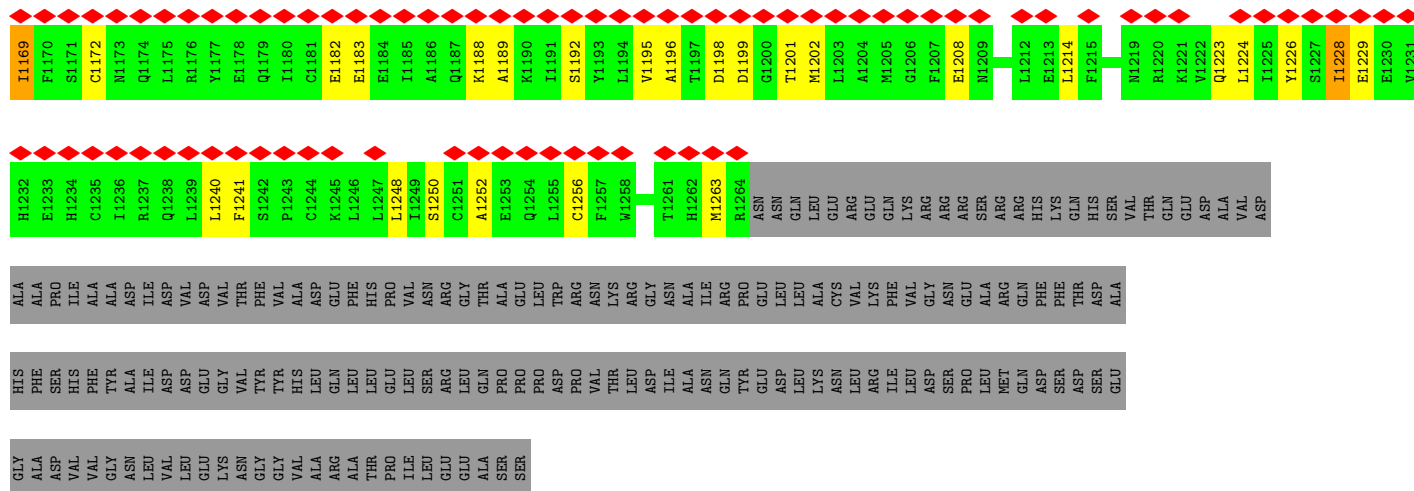
• Molecule 1: Apaf-1 related killer DARK



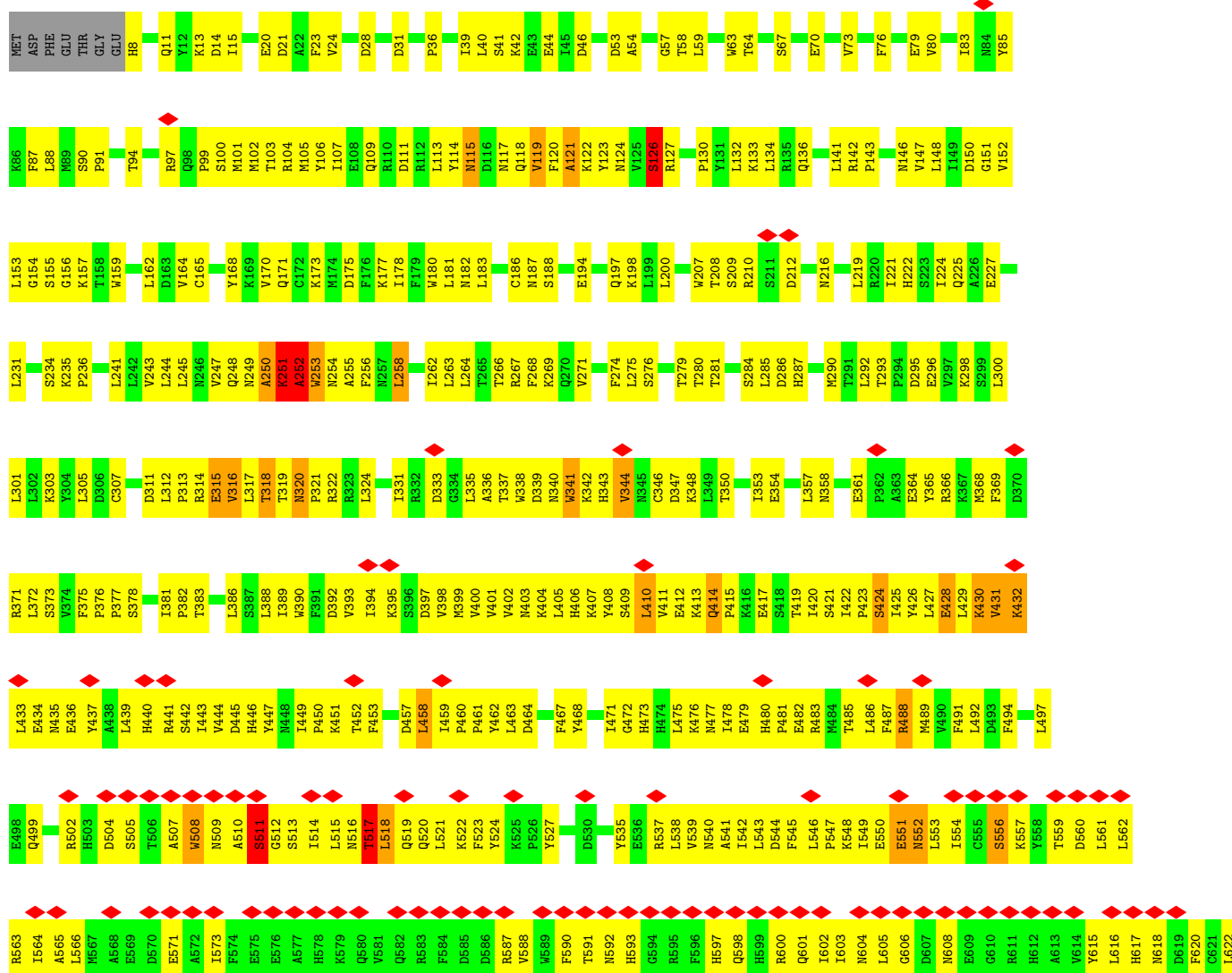
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K86	F87	L88	M89	S90	P91	I92	K93	T94	Q98	P99	S100	M101	M102	T103	R104	M105	Y106	I107	E108	Q109	L113	Y114	M115	N117	Q118	V119	A120	K122	L123	M124	V125	S126	R127	P130	K133	L134	R135	Q136	L141	R142	P143	A144	K145	M146	Q147	L148	I149	D150	G151	V152	L153	
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C307	D311	L312	P313	R314	E315	V316	L317	Q318	T319	N320	P321	R322	R323	L324	S325	E329	S330	I331	R332	D333	A336	T337	W338	D339	N340	W341	K342	H343	V344	N345	C346	D347	L349	K348	T350	I353	E354	L357	N358	E361	P362	A363	E364	Y365	R366	K367	M368	F369	D370	R371	L372	S373



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● Molecule 1: Apaf-1 related killer DARK



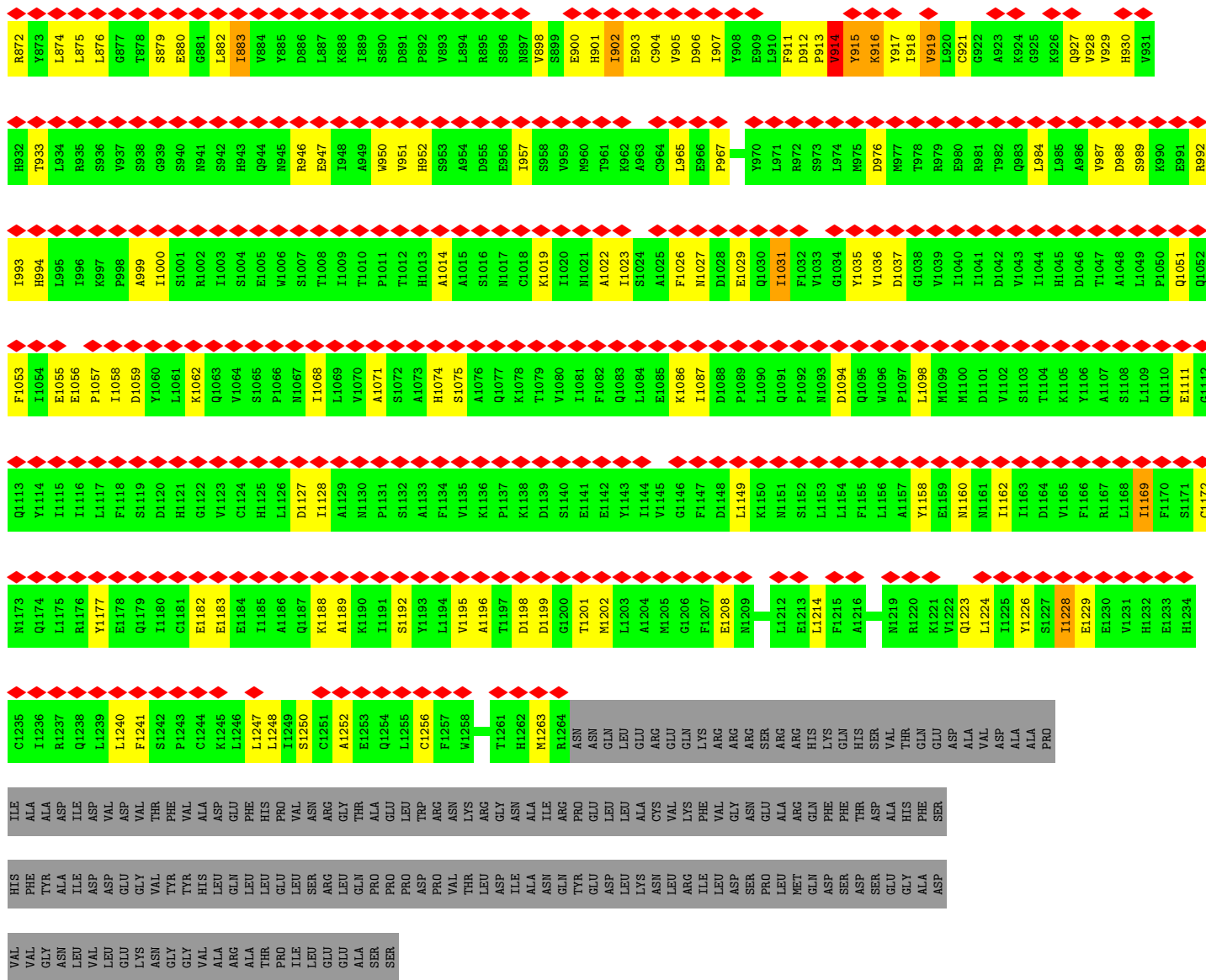
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VAL	VAL	PHE	ALA	I1236	Q1113	F1053	I993	H932	G871	N810	Q749	ARG	ARG	A626
ASN	ASN	TYR	ALA	R1237	Y1114	I1054	H994	T933	R872	D811	D750	SER	SER	G628
VAL	VAL	ILE	ILE	Q1238	I1115	E1055	L995	L934	Y873	T812	Q751	GLY	GLY	G629
VAL	VAL	ASP	ASP	L1239	I1116	E1056	I996	R835	L874	P813	F752	SER	SER	I630
GLU	GLU	ASP	VAL	L1240	L1117	P1057	K997	S936	L875	L814	K754	LYS	LYS	L631
LYS	LYS	GLY	THR	F1241	F1118	I1058	P998	V937	L876	A815	L755	GLN	GLN	L632
ASN	ASN	VAL	THR	S1242	S1119	D1059	A999	S938	G877	L816	S756	LEU	LEU	T633
VAL	VAL	THR	VAL	C1243	D1120	Y1060	I1000	G939	T878	D817	H757	VAL	VAL	D634
ALA	ALA	VAL	VAL	E1182	H1121	L1061	S1001	S940	S879	V818	V758			V635
ALA	ALA	LEU	ASP	E1183	G1122	K1062	R1002	N941	E880	F819	V759			S636
GLN	GLN	LEU	GLU	E1184	V1123	Q1063	I1003	S942	G881	D820	F760			L637
LEU	LEU	LEU	PHE	I1185	C1124	V1064	S1004	H943	L882	E821	V761			E639
THR	THR	GLU	PRO	I1186	H1125	S1065	I1005	Q944	O883	R822	K762			E640
LEU	LEU	LEU	VAL	Q1187	L1126	P1066	M1006	I945	D886	S823	T763			D641
ASN	ASN	VAL	VAL	Q1187	L1127	N1067	M1007	I946	L887	K824	M764			T642
ARG	ARG	ARG	ARG	K1188	D1127	N1067	S1007	E947	K888	T825	Q765			Y643
ARG	ARG	ARG	THR	A1189	I1128	I1068	T1008	E947	K888	A826	S766			L644
GLY	GLY	THR	THR	K1190	I1129	I1068	T1008	E947	L889	V828	G767			L645
GLY	GLY	THR	ALA	I1191	N1130	V1070	I1009	I949	I889	L829	I768			R646
GLU	GLU	ALA	GLU	S1192	P1131	A1071	T1010	A949	I889	L830	C770			D647
LEU	LEU	LEU	TRP	Y1193	S1132	S1072	P1011	A950	L894	I831	F771			E648
ASP	ASP	ASP	ASP	A1194	A1133	A1073	H1012	V951	R895	Y834	V772			S649
VAL	VAL	VAL	ASN	V1195	F1134	H1074	H1013	H952	S896	I714	Q773			D650
LEU	LEU	LEU	THR	A1196	V1135	S1075	A1014	V953	N897	V774	V774			S651
ASP	ASP	GLY	ARG	T1197	V1136	A1076	A1015	R895	V837	K776	L775			S652
ILE	ILE	ASN	GLY	D1198	K1136	Q1077	S1016	D955	S899	K777	V790			E653
ALA	ALA	ALA	ALA	D1199	X1138	K1078	M1017	S956	V837	I718	I654			L655
ASN	ASN	ASN	ARG	G1200	D1139	T1079	K1019	S958	S899	V778	V778			R656
PRO	PRO	PRO	PRO	T1201	S1140	V1080	I1020	V959	E900	N720	N720			M657
GLU	GLU	GLU	GLU	M1202	I1141	I1081	M1021	N960	H901	I778	I778			F660
LEU	LEU	LEU	LEU	L1203	E1142	F1082	A1022	V961	I902	F841	V781			M661
ALA	ALA	ALA	ALA	M1204	E1143	Q1083	I1023	T961	E903	P843	C782			Q662
GLN	GLN	GLN	CYS	G1206	Y1143	L1084	S1024	A963	C904	P843	C782			Q663
VAL	VAL	VAL	VAL	F1207	G1146	E1085	A1025	C964	V905	G844	C783			H665
LYS	LYS	LYS	LYS	E1208	F1147	K1086	F1026	L965	D906	L845	L783			L666
ARG	ARG	ARG	VAL	M1209	L1148	I1087	M1027	E966	I907	S846	S784			
ASP	ASP	ASP	VAL	L1149	L1149	D1088	D1028	P967	Y908	V847	L725			
GLY	GLY	GLY	GLY	K1150	K1150	P1089	E1029	Y970	E909	V847	PRO			
SER	SER	SER	GLU	N1151	N1151	L1090	Q1030	L971	L910	S848	GLU			
ALA	ALA	ALA	ALA	S1152	S1152	Q1091	I1031	R972	D912	S848	ALA			
ARG	ARG	ARG	ARG	L1153	L1153	P1092	F1032	F911	P913	L849	ASN			
HIS	HIS	HIS	HIS	L1154	L1154	M1093	F1032	S973	P913	Q850	ASN			
GLN	GLN	GLN	PHE	F1155	F1155	D1094	M1033	S973	Y914	S851	I730			
THR	THR	THR	THR	L1156	L1156	Q1095	V1033	L974	Y915	E852	L732			
ASP	ASP	ASP	ASP	A1157	A1157	M1096	Y1035	H975	K916	A853	H733			
ALA	ALA	ALA	ALA	Y1158	Y1158	M1097	V1036	D976	Y917	V854	V734			
ALA	ALA	ALA	ALA	E1159	E1159	L1098	D1037	H977	I918	GLN	L732			
VAL	VAL	VAL	VAL	M1160	M1160	M1099	G1038	T978	V919	PRO	H733			
VAL	VAL	VAL	VAL	N1161	N1161	M1100	V1039	S979	L920	GLU	V734			
ASP	ASP	ASP	ASP	I1162	I1162	D1101	I1040	E980	G922	GLU	V734			
ALA	ALA	ALA	ALA	Y1226	Y1226	V1102	I1041	A981	A923	S859	D740			
ALA	ALA	ALA	ALA	S1227	S1227	V1103	D1042	T982	K924	S860	L677			
PRO	PRO	PRO	PRO	I1228	I1228	T1104	V1043	Q983	G925	F861	S679			
				E1229	E1229	H1045	I1044	L984	K926	T863	L744			
				E1230	E1230	F1106	H1045	L985	Q927	C864	L744			
				V1231	V1231	R1167	D1046	A986	V928	G865	N745			
				H1232	H1232	A1107	T1047	V987	V929	K866	V746			
				E1233	E1233	S1108	A1048	D988	H930	R867	N807			
				H1234	H1234	L1109	L1049	S989		S868	V805			
						Q1110	P1050	K990		T869	V808			
						E1111	Q1051	E991						

• Molecule 1: Apaf-1 related killer DARK

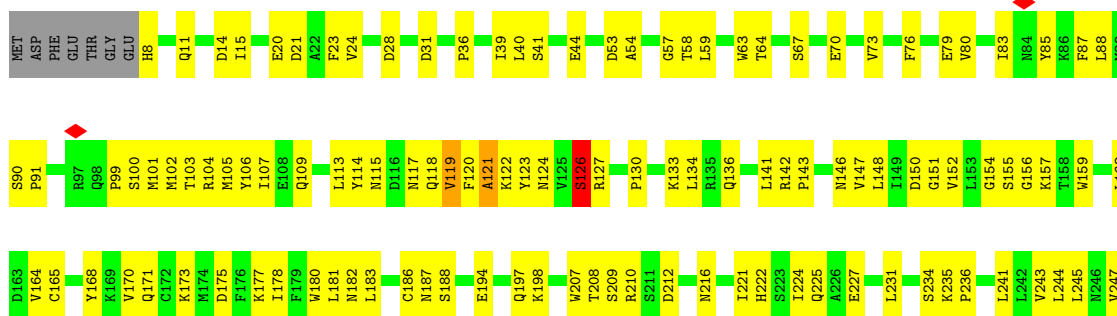


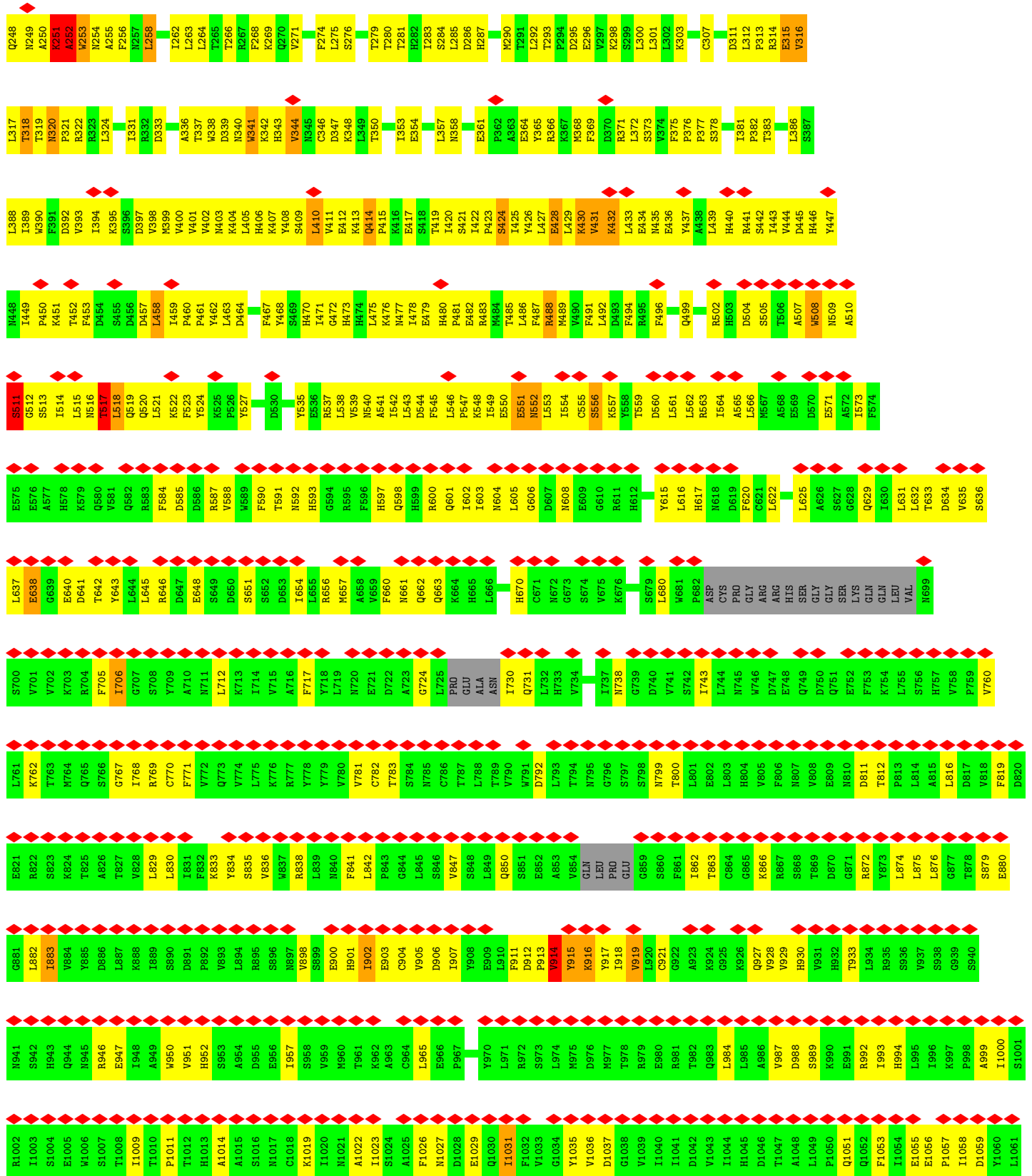


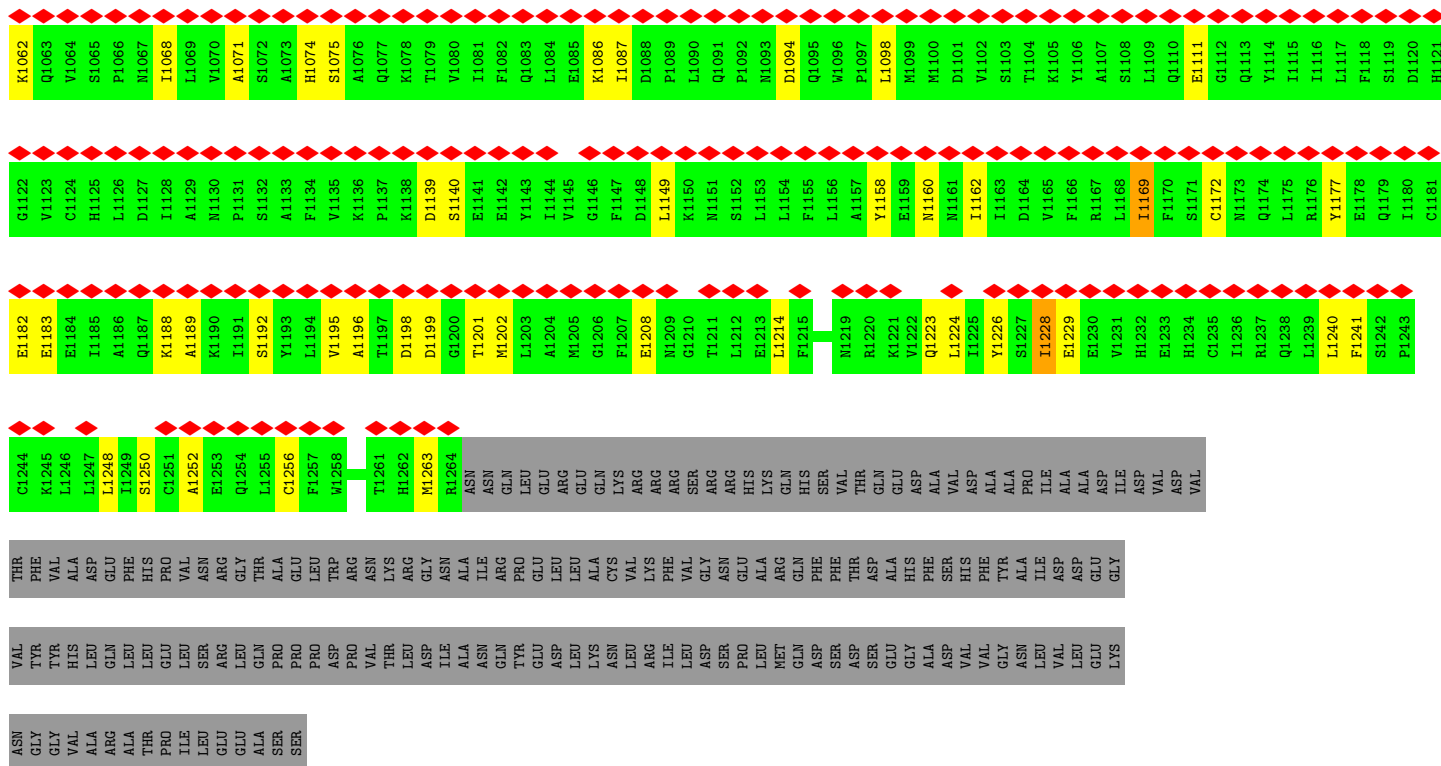
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K86	F87	M88	M89	S90	P91	I92	K93	T94	R97	Q98	P99	S100	M101	M102	T103	R104	M105	Y106	I107	E108	Q109	L113	Y114	N115	D116	N117	Q118	V119	F120	F121	K122	L275	Y123	N124	Y125	S126	R127	W207	T208	S209	R210	L132	K133	L134	R135	Q136	L141	R142	P143	N146	V147	L148	I149	D150	G151	V152	L153		
G154	S155	K156	K157	W158	W159	L162	D163	V164	C165	Y168	K169	V170	Q171	C172	K173	M174	F175	F176	K177	I178	W179	W180	L181	M182	L183	C186	M187	S188	E194	F274	L275	S276	T279	T280	T281	S284	L285	D286	H287	M290	T291	L292	T293	P294	D295	E296	Q225	A226	E227	L231	S234	K235							
P236	L241	V243	L244	L245	N246	V247	Q248	A250	K251	A252	W253	N254	A255	F256	M257	L258	I262	L263	L264	T265	T266	F268	T267	K269	Q270	V271	F274	L275	S276	T279	T280	T281	S284	L285	D286	H287	M290	T291	L292	T293	P294	D295	E296	Q225	A226	E227	L231	S234	K235										
C307	D311	L312	P313	R314	E315	V316	L317	T318	R319	N320	P321	R322	R323	L324	I331	R332	D333	A336	T337	W338	D339	M340	W341	K342	H343	V344	R345	C346	D347	K348	L349	T350	L351	I352	I353	E354	S355	S356	L357	N358	E361	F362	A363	Y364	E365	R366	K367	M368	F369	D370	R371	L372	S373	V374	F375				
P376	P377	S378	I381	P382	T383	L386	S387	L388	I389	K390	R391	D392	V393	I394	K395	S396	D397	V398	M399	V400	P401	M402	N403	K404	L405	H406	K407	Y408	S409	L410	V411	E412	K413	Q414	P415	E417	R418	T419	I420	S421	I422	S423	S424	I425	Y426	Y427	E428	L429	K430	V431	K432	L433	R434	E435	M436	E437	E438	Y439	
A438	L439	H440	R441	I442	I443	V444	D445	H446	Y447	N448	I449	P450	K451	T452	F453	D454	S455	D456	D457	L458	I459	P460	Y461	Y462	L463	D464	F467	Y468	S469	H470	I471	G472	H473	H474	L475	K476	M477	I478	E479	H480	P481	E482	R483	M484	T485	L486	F487	R488	M489	V490	F491	L492	D493	F494	L497	E498	Q499		
R502	H503	D504	S505	T506	A507	W508	N509	A510	G511	S513	I514	L515	M516	T517	L518	Q519	Q520	L521	K522	F523	Y524	K525	P526	Y527	D530	Y535	E536	R537	L538	V539	N540	A541	I542	L543	D544	F545	L546	P547	K548	I549	E550	E551	N552	L553	I554	C555	S556	R557	Y558	T559	D560	L561	L562	R563	I564				
A565	L566	M567	A568	E569	D570	E571	A572	I573	F574	E575	E576	A577	H578	K579	Q580	V581	Q582	L644	L645	R646	D647	E648	S649	D650	S651	S652	D653	I654	R655	M657	A658	V659	F660	N661	Q662	Q663	K664	H665	I603	I604	L605	G606	D607	N608	E609	G610	R611	H612	Y615	L616	H617	N618	D619	F620	C621	L622	L625	A626	
S627	G628	Q629	I630	L631	L632	T633	D634	V635	S636	L637	E638	G639	E640	D641	T642	Y643	L644	L645	R646	D647	E648	S649	D650	S651	S652	D653	I654	R655	M657	A658	V659	F660	N661	Q662	Q663	K664	H665	I603	I604	L605	G606	D607	N608	E609	G610	R611	H612	Y615	L616	H617	N618	D619	F620	C621	L622	L625	A626		
G628	Q629	I630	L631	L632	T633	D634	V635	S636	L637	E638	G639	E640	D641	T642	Y643	L644	L645	R646	D647	E648	S649	D650	S651	S652	D653	I654	R655	M657	A658	V659	F660	N661	Q662	Q663	K664	H665	I603	I604	L605	G606	D607	N608	E609	G610	R611	H612	Y615	L616	H617	N618	D619	F620	C621	L622	L625	A626			
GLY	GLY	SER	LYS	GLN	LEU	VAL	N699	S700	V701	W702	K703	R704	F705	I706	G707	S708	I709	A710	N711	L712	K713	I714	V715	A716	F717	Y718	L719	N720	E721	A722	A723	G724	L725	PRO	GLU	ALA	ASN	I730	Q731	L732	H733	V734	I737	W738	G739	D740	V741	S742	I743	L744	N745	W746	D747	E748	Q749	D750	Q751		
E752	F753	K754	L755	S756	H757	V758	P759	V760	L761	K762	T763	M764	Q765	S766	G767	I768	R769	C770	F771	V772	Q773	V774	L775	K776	R777	Y778	Y779	W780	V781	C782	T783	S784	N785	C786	L787	L788	L789	W790	W791	D792	L793	T794	W795	G796	S797	S798	N799	T800	L801	E802	L803	H804	G805	F806	N807	E808	D809	N810	D811
T812	P813	L814	A815	L816	D817	V818	F819	D820	E821	R822	S823	K824	T825	A826	T827	V828	L829	L830	F831	K832	K833	Y834	S835	V836	W837	R838	L839	N840	F841	L842	P843	L844	L845	S846	V847	S848	L849	Q850	S851	E852	A853	V854	GLN	LEU	PRO	GLU	G859	S860	L862	T863	C864	G865	K866	R867	S868	T869	D870	G871	



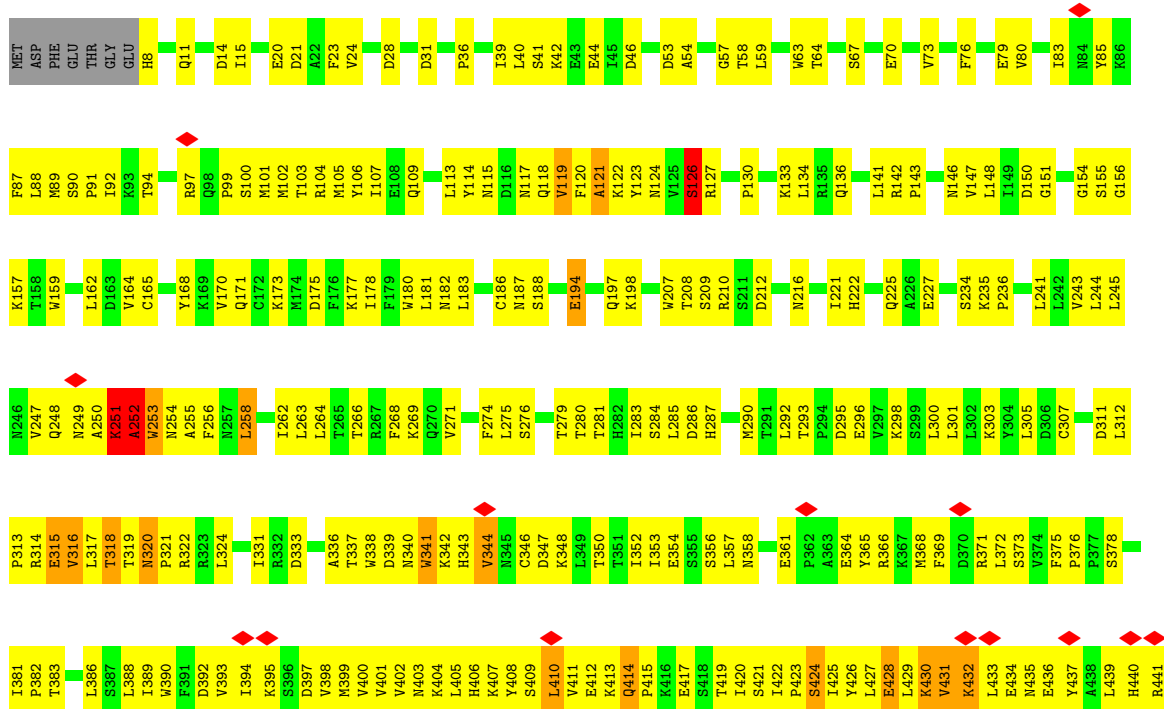
● Molecule 1: Apaf-1 related killer DARK







Molecule 1: Apaf-1 related killer DARK



R1176	E1056	I1116	I1056	H936	L875	A815	L755	LYS	I630	A568	D504	S442
Y1177	P1057	L1117	K997	S936	L876	L816	S756	GLN	L631	E569	S505	I443
E1178	I1058	F1118	P998	V937	G877	D817	H757	LEU	L632	D570	T506	V444
Q1179	D1059	S1119	A999	S938	T878	V818	V758	VAL	L633	E571	A507	D445
I1180	Y1060	D1120	I1000	G939	S879	F819	P759	M699	D634	A572	M508	H446
H1121	I1061	H1121	S1001	S940	E880	D820	V760	S700	V635	I573	M509	Y447
V1123	K1062	G1122	I1002	H941	G881	E821	L761	V701	S636	F574	I449	P450
C1124	Q1063	V1123	I1003	S942	L882	R822	K762	V702	L637	E575	A510	K451
H1125	W1064	C1124	E1005	H943	R883	S823	I763	K703	E638	E576	S511	T452
L1126	S1065	H1125	E1006	Q944	V884	K824	W764	R704	G639	H578	S513	F453
D1127	P1066	L1126	W1006	Q945	V885	T825	Q765	F705	E640	H579	I514	D454
K1187	M1067	D1127	S1007	R946	D886	A826	S766	I706	D641	K579	L515	S455
A1188	I1068	I1128	T1008	E947	L887	T827	G767	G707	T642	Q580	M516	D456
K1189	L1069	I1129	I1009	I948	R887	V828	I768	S708	Y643	V581	T517	L458
K1190	V1070	M1130	T1010	A949	L889	L829	R769	V709	L644	Q582	L518	I459
I1191	A1071	P1131	P1011	H950	S890	L830	C770	A710	L645	R583	Q519	P460
S1192	S1072	S1132	T1012	V951	D891	R831	F771	W711	R646	F584	L521	Y462
L1194	H1074	H1133	H1013	H952	R892	K833	V772	L712	E648	D585	K522	L463
V1195	S1075	V1135	A1014	S953	H893	X834	Q773	K713	S649	R587	Y524	D464
A1196	A1076	S1016	A1015	A954	L894	B834	V774	I714	D650	V588	K525	F467
T1197	Q1077	N1017	S1016	D955	R895	S835	L775	V715	S651	M589	P526	Y468
K1198	K1078	C1018	C1018	E957	S896	V836	K776	A716	S652	F590	Y527	S469
D1199	T1079	K1198	K1019	I958	R897	R837	R777	F717	D653	T591	D530	I471
G1200	V1080	E1140	I1020	V959	S898	R838	Y778	Y718	L855	H593	H535	G472
T1201	I1081	S1140	I1021	H960	E900	N840	Y779	L719	R856	G594	E536	H473
M1202	F1082	E1142	A1022	T961	H901	F841	C782	E721	M657	R595	E537	L475
L1203	Q1083	Y1143	I1023	K962	L902	L842	T783	D722	A658	L595	L638	K476
A1204	L1084	I1144	S1024	A963	E903	P843	I783	A723	F659	F596	V539	W477
M1205	E1085	G1145	A1025	C964	C904	G844	S784	G724	F660	H597	N540	I478
G1206	K1086	G1146	F1026	L965	V905	L845	W785	L725	N661	Q598	A541	E479
F1207	I1087	F1147	N1027	E966	D906	S846	C786	PR0	Q662	R600	I542	H480
E1208	D1028	L1148	D1028	P967	I907	V847	T787	GLU	Q663	I602	L543	P481
M1209	P1089	K1150	I1029	V970	V908	S848	L788	ALA	K664	G601	F545	E482
L1210	L1090	M1151	Q1030	H971	E909	L849	T789	I730	H665	I603	D544	T485
S1211	Q1091	S1152	I1031	L971	D912	Q850	V790	Q731	L666	M604	F545	L486
L1212	F1032	L1153	F1032	R972	F911	S851	W791	H733	H670	G606	E550	F487
L1214	V1033	L1154	V1033	S973	D913	E852	L792	H733	M672	D607	E551	M488
F1215	G1034	L1154	G1034	L974	V914	A853	L793	V734	G673	M608	N552	V490
A1216	Y1035	F1155	Y1035	H975	V915	V854	T794	V734	S674	E609	L553	L492
M1219	W1036	L1156	W1036	D976	K916	GLN	N795	I737	K676	G610	I554	F494
K1220	D1037	L1157	D1037	H977	V917	LEU	G796	N738	V675	R611	C555	F494
V1222	I1038	Y1158	I1038	T978	I918	GLU	S797	G739	K676	H512	S556	R496
L1223	V1039	E1159	V1039	R979	V919	G859	S798	D740	L880	Y615	K557	L497
I1225	I1040	M1160	I1040	E980	L920	S860	N799	V741	M681	Y615	E558	E498
Y1226	D1101	I1162	D1042	R981	G922	F861	T800	S742	P882	L616	T559	Q499
S1227	V1102	I1163	V1043	Q983	A923	T862	L801	I743	ASP	D560	D560	R502
I1228	T1104	L1164	I1044	T982	K924	T863	E802	L744	CYS	L617	L561	H503
E1229	K1105	V1165	H1045	L984	R926	C964	L803	W745	PRO	M618	L562	R563
I1230	W1106	F1166	H1046	L985	Q927	G865	H804	W746	GLY	D619	R563	I564
V1231	I1047	R1167	D1046	A986	Q928	K866	V805	D747	ARG	F620	I564	A565
H1232	A1048	S1108	A1048	V987	V928	R867	F806	E748	HIS	L622	L566	L667
E1233	L1108	I1168	L1049	D988	V929	S868	E807	Q749	GLY	L625	A626	S627
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C1235	Q1110	C1172	P1050	R990	V931	D870	E809	Q751	GLY	S627	G628	Q629
I1236	E1111	Q1174	Q1051	E991	H932	G871	N610	E752	SER	L625	A626	S627
R1237	G1112	L1175	F1053	I993	R933	R872	D811	F753	GLY	L625	A626	S627
	I1114		E1055	H994	L934	T873	T812	K754	SER	L625	A626	S627
	I1115		I1085	H994	L874	T874	P813	L814				







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D8	Depositor
Number of particles used	17769	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	432.0, 432.0, 432.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, APK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	B	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	C	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	D	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	E	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	F	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	G	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	H	0.51	6/10231 (0.1%)	0.62	10/13873 (0.1%)
1	I	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	J	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	K	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	L	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	M	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	N	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	O	0.51	6/10231 (0.1%)	0.62	9/13873 (0.1%)
1	P	0.51	6/10231 (0.1%)	0.62	10/13873 (0.1%)
All	All	0.51	96/163696 (0.1%)	0.62	146/221968 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
1	B	0	15
1	C	0	15
1	D	0	15
1	E	0	15
1	F	0	15
1	G	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	15
1	I	0	15
1	J	0	15
1	K	0	15
1	L	0	15
1	M	0	15
1	N	0	15
1	O	0	15
1	P	0	15
All	All	0	240

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	250	ALA	CA-CB	-10.19	1.31	1.52
1	J	250	ALA	CA-CB	-10.19	1.31	1.52
1	F	250	ALA	CA-CB	-10.18	1.31	1.52
1	L	250	ALA	CA-CB	-10.17	1.31	1.52
1	B	250	ALA	CA-CB	-10.16	1.31	1.52

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	559	THR	O-C-N	-7.67	110.42	122.70
1	L	559	THR	O-C-N	-7.66	110.44	122.70
1	N	559	THR	O-C-N	-7.66	110.44	122.70
1	J	559	THR	O-C-N	-7.65	110.46	122.70
1	D	559	THR	O-C-N	-7.65	110.46	122.70

There are no chirality outliers.

5 of 240 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	Peptide
1	A	123	TYR	Peptide
1	A	126	SER	Peptide
1	A	143	PRO	Peptide
1	A	8	HIS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10045	0	10046	666	0
1	B	10045	0	10046	684	0
1	C	10045	0	10046	679	0
1	D	10045	0	10046	692	0
1	E	10045	0	10046	670	0
1	F	10045	0	10046	692	0
1	G	10045	0	10046	683	0
1	H	10045	0	10046	661	0
1	I	10045	0	10046	671	0
1	J	10045	0	10046	666	0
1	K	10045	0	10046	694	0
1	L	10045	0	10046	686	0
1	M	10045	0	10045	674	0
1	N	10045	0	10046	662	0
1	O	10045	0	10046	666	0
1	P	10045	0	10046	672	0
2	A	30	0	9	6	0
2	B	30	0	9	7	0
2	C	30	0	9	6	0
2	D	30	0	9	6	0
2	E	30	0	9	6	0
2	F	30	0	9	6	0
2	G	30	0	9	6	0
2	H	30	0	9	6	0
2	I	30	0	9	6	0
2	J	30	0	9	6	0
2	K	30	0	9	6	0
2	L	30	0	9	6	0
2	M	30	0	9	6	0
2	N	30	0	9	6	0
2	O	30	0	9	6	0
2	P	30	0	9	6	0
All	All	161200	0	160879	10606	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 10606 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:875:LEU:HD11	1:I:911:PHE:CE2	1.25	1.72
1:E:875:LEU:HD11	1:E:911:PHE:CE2	1.25	1.72
1:J:875:LEU:HD11	1:J:911:PHE:CE2	1.25	1.71
1:F:875:LEU:HD11	1:F:911:PHE:CE2	1.25	1.71
1:C:875:LEU:HD11	1:C:911:PHE:CE2	1.25	1.71

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	B	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	C	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	D	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	E	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	F	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	G	1224/1440 (85%)	989 (81%)	202 (16%)	33 (3%)	5	34
1	H	1224/1440 (85%)	988 (81%)	204 (17%)	32 (3%)	5	35
1	I	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	J	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	K	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	L	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	M	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	N	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
1	O	1224/1440 (85%)	988 (81%)	203 (17%)	33 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	5	35
All	All	19584/23040 (85%)	15822 (81%)	3248 (17%)	514 (3%)	8	35

5 of 514 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ALA
1	A	315	GLU
1	A	517	THR
1	A	638	GLU
1	A	760	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	B	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	C	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	D	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	E	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	F	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	G	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	H	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	I	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	J	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	K	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	L	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	M	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	N	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
1	O	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	1138/1315 (86%)	1137 (100%)	1 (0%)	93	97
All	All	18208/21040 (86%)	18192 (100%)	16 (0%)	93	97

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	914	VAL
1	N	914	VAL
1	I	914	VAL
1	M	914	VAL
1	H	914	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 462 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1223	GLN
1	P	446	HIS
1	J	994	HIS
1	P	222	HIS
1	N	952	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

16 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	APK	H	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.98	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	APK	I	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	A	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	M	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	F	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	O	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	P	251	1	29,33,33	2.96	12 (41%)	28,47,47	3.00	7 (25%)
1	APK	K	251	1	29,33,33	2.98	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	E	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	C	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	J	251	1	29,33,33	2.96	12 (41%)	28,47,47	3.00	7 (25%)
1	APK	N	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	G	251	1	29,33,33	2.97	12 (41%)	28,47,47	3.00	7 (25%)
1	APK	L	251	1	29,33,33	2.98	12 (41%)	28,47,47	2.99	7 (25%)
1	APK	D	251	1	29,33,33	2.98	12 (41%)	28,47,47	3.00	7 (25%)
1	APK	B	251	1	29,33,33	2.97	12 (41%)	28,47,47	2.99	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	APK	H	251	1	-	9/15/37/37	0/3/3/3
1	APK	I	251	1	-	9/15/37/37	0/3/3/3
1	APK	A	251	1	-	9/15/37/37	0/3/3/3
1	APK	M	251	1	-	9/15/37/37	0/3/3/3
1	APK	F	251	1	-	9/15/37/37	0/3/3/3
1	APK	O	251	1	-	9/15/37/37	0/3/3/3
1	APK	P	251	1	-	9/15/37/37	0/3/3/3
1	APK	K	251	1	-	9/15/37/37	0/3/3/3
1	APK	E	251	1	-	9/15/37/37	0/3/3/3
1	APK	C	251	1	-	9/15/37/37	0/3/3/3
1	APK	J	251	1	-	9/15/37/37	0/3/3/3
1	APK	N	251	1	-	9/15/37/37	0/3/3/3
1	APK	G	251	1	-	9/15/37/37	0/3/3/3
1	APK	L	251	1	-	9/15/37/37	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	APK	D	251	1	-	9/15/37/37	0/3/3/3
1	APK	B	251	1	-	9/15/37/37	0/3/3/3

The worst 5 of 192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	APK	C2'-C3'	-8.14	1.31	1.53
1	B	251	APK	C2'-C3'	-8.13	1.31	1.53
1	K	251	APK	C2'-C3'	-8.13	1.31	1.53
1	G	251	APK	C2'-C3'	-8.12	1.31	1.53
1	N	251	APK	C2'-C3'	-8.12	1.31	1.53

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	251	APK	C1'-N9-C4	8.31	141.23	126.64
1	A	251	APK	C1'-N9-C4	8.30	141.23	126.64
1	D	251	APK	C1'-N9-C4	8.30	141.22	126.64
1	P	251	APK	C1'-N9-C4	8.30	141.22	126.64
1	B	251	APK	C1'-N9-C4	8.29	141.21	126.64

There are no chirality outliers.

5 of 144 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	251	APK	O-C-CA-CB
1	A	251	APK	CG-CD-CE-NZ
1	A	251	APK	C5'-O5'-P-O2P
1	A	251	APK	C4'-C5'-O5'-P
1	B	251	APK	O-C-CA-CB

There are no ring outliers.

16 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	251	APK	6	0
1	I	251	APK	6	0
1	A	251	APK	6	0
1	M	251	APK	6	0
1	F	251	APK	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	O	251	APK	5	0
1	P	251	APK	6	0
1	K	251	APK	7	0
1	E	251	APK	6	0
1	C	251	APK	7	0
1	J	251	APK	6	0
1	N	251	APK	6	0
1	G	251	APK	6	0
1	L	251	APK	7	0
1	D	251	APK	7	0
1	B	251	APK	6	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	DTP	L	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.74	7 (23%)
2	DTP	A	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.72	7 (23%)
2	DTP	P	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.74	7 (23%)
2	DTP	H	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.72	7 (23%)
2	DTP	I	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.74	7 (23%)
2	DTP	C	1501	-	26,32,32	3.68	8 (30%)	30,50,50	2.72	7 (23%)
2	DTP	M	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.75	7 (23%)
2	DTP	O	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.74	7 (23%)
2	DTP	G	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.72	7 (23%)
2	DTP	E	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.71	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DTP	J	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.74	7 (23%)
2	DTP	F	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.72	7 (23%)
2	DTP	D	1501	-	26,32,32	3.68	8 (30%)	30,50,50	2.72	7 (23%)
2	DTP	K	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.74	7 (23%)
2	DTP	N	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.74	7 (23%)
2	DTP	B	1501	-	26,32,32	3.67	8 (30%)	30,50,50	2.72	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	L	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	A	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	P	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	H	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	I	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	C	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	M	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	O	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	G	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	E	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	J	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	F	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	D	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	K	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	N	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	B	1501	-	-	3/18/34/34	0/3/3/3

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1501	DTP	C2'-C3'	-12.38	1.20	1.52
2	D	1501	DTP	C2'-C3'	-12.38	1.20	1.52
2	M	1501	DTP	C2'-C3'	-12.37	1.20	1.52
2	G	1501	DTP	C2'-C3'	-12.37	1.20	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1501	DTP	C2'-C3'	-12.37	1.20	1.52

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1501	DTP	C5-C6-N6	8.55	133.34	120.35
2	B	1501	DTP	C5-C6-N6	8.54	133.33	120.35
2	C	1501	DTP	C5-C6-N6	8.54	133.33	120.35
2	M	1501	DTP	C5-C6-N6	8.54	133.33	120.35
2	D	1501	DTP	C5-C6-N6	8.53	133.32	120.35

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

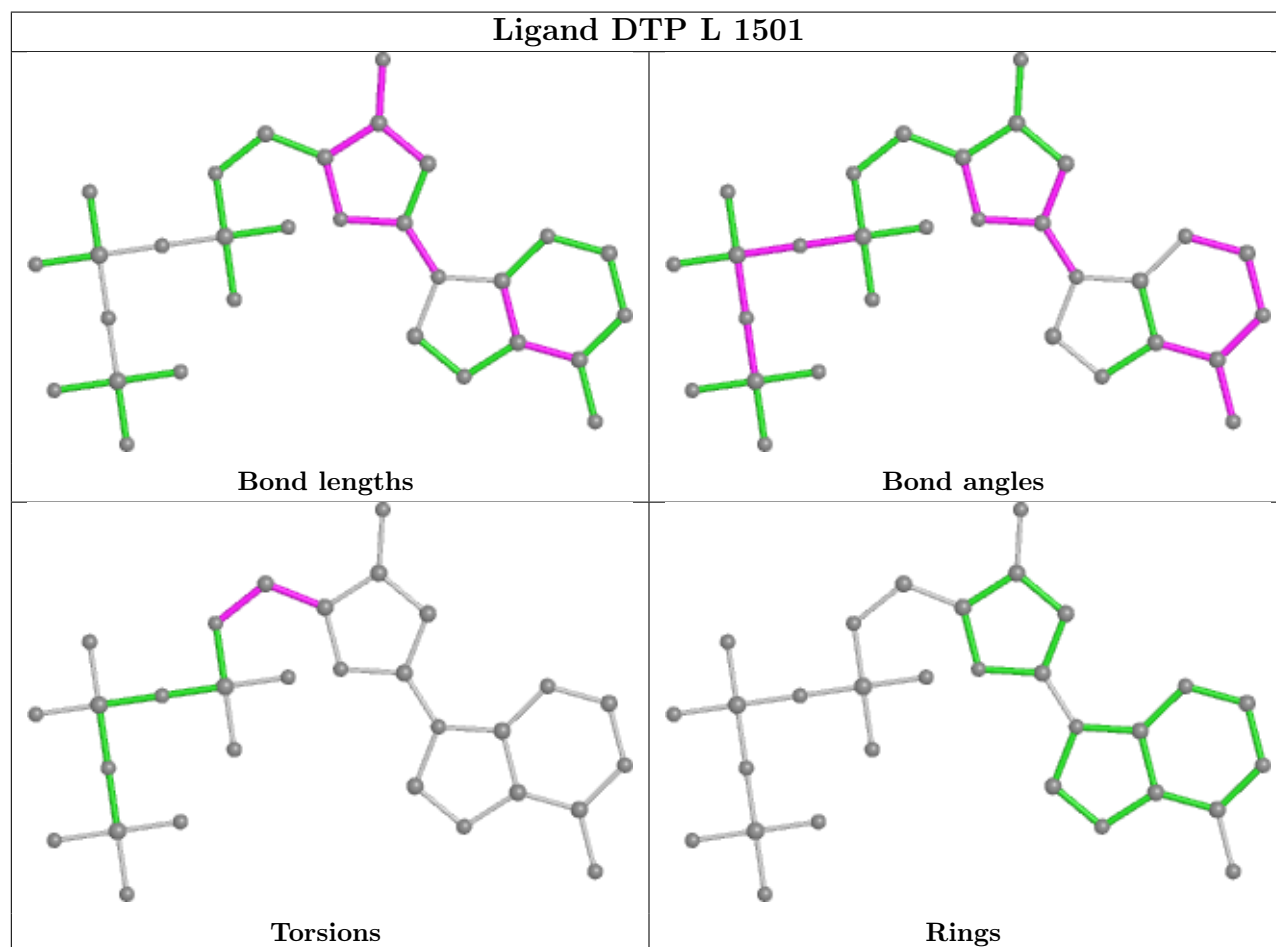
Mol	Chain	Res	Type	Atoms
2	A	1501	DTP	C3'-C4'-C5'-O5'
2	B	1501	DTP	C3'-C4'-C5'-O5'
2	C	1501	DTP	C3'-C4'-C5'-O5'
2	D	1501	DTP	C3'-C4'-C5'-O5'
2	E	1501	DTP	C3'-C4'-C5'-O5'

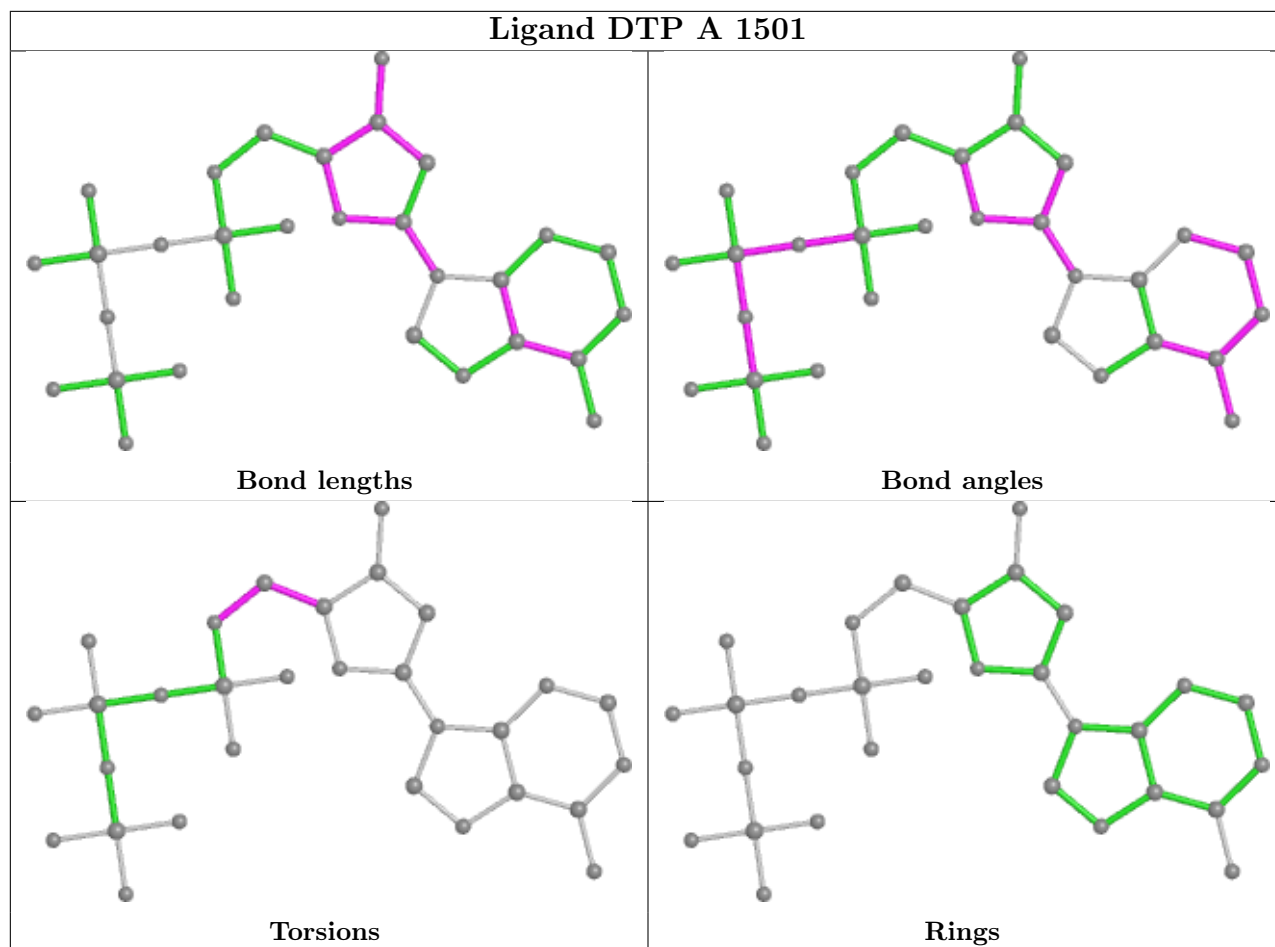
There are no ring outliers.

16 monomers are involved in 97 short contacts:

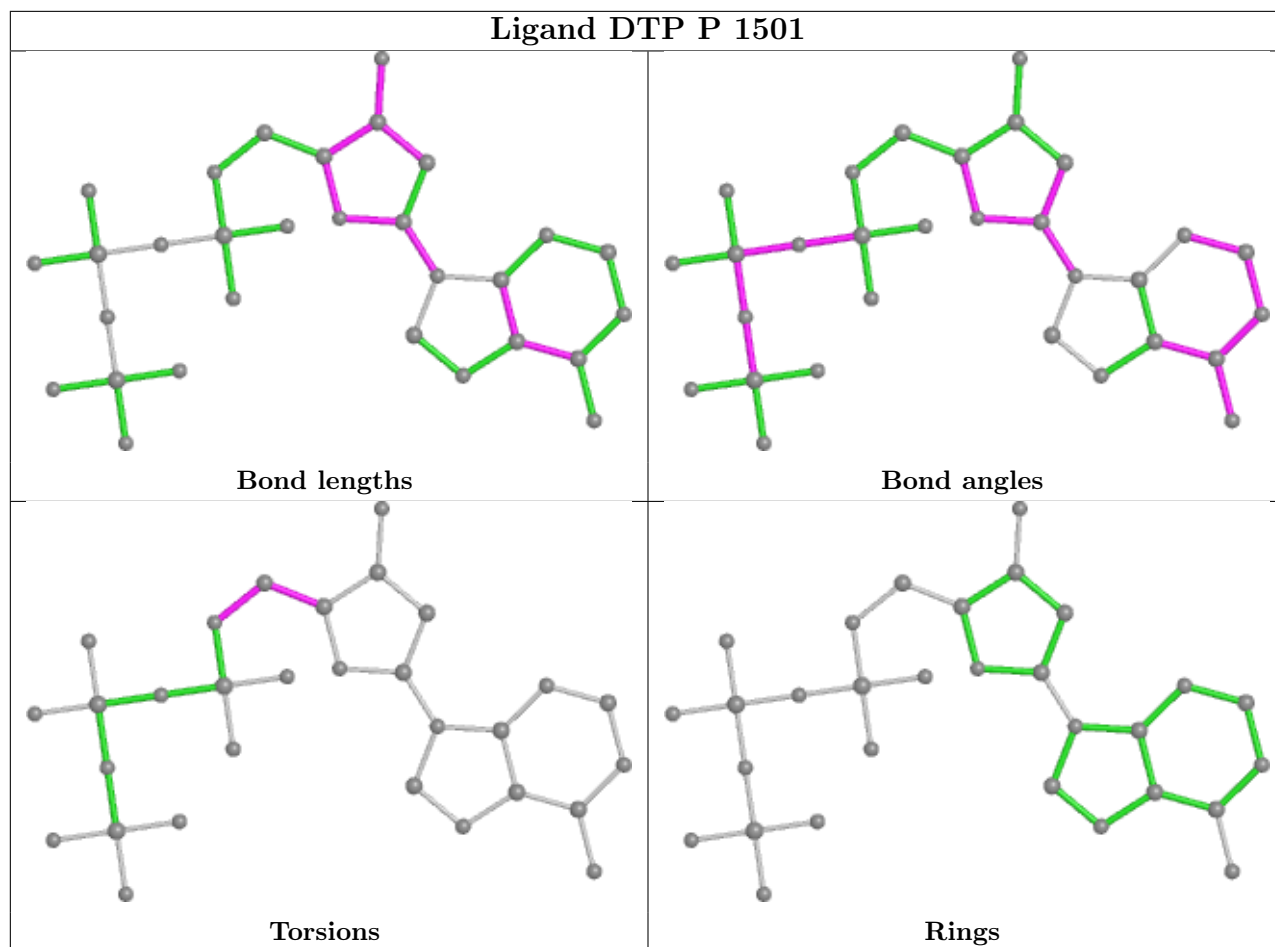
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1501	DTP	6	0
2	A	1501	DTP	6	0
2	P	1501	DTP	6	0
2	H	1501	DTP	6	0
2	I	1501	DTP	6	0
2	C	1501	DTP	6	0
2	M	1501	DTP	6	0
2	O	1501	DTP	6	0
2	G	1501	DTP	6	0
2	E	1501	DTP	6	0
2	J	1501	DTP	6	0
2	F	1501	DTP	6	0
2	D	1501	DTP	6	0
2	K	1501	DTP	6	0
2	N	1501	DTP	6	0
2	B	1501	DTP	7	0

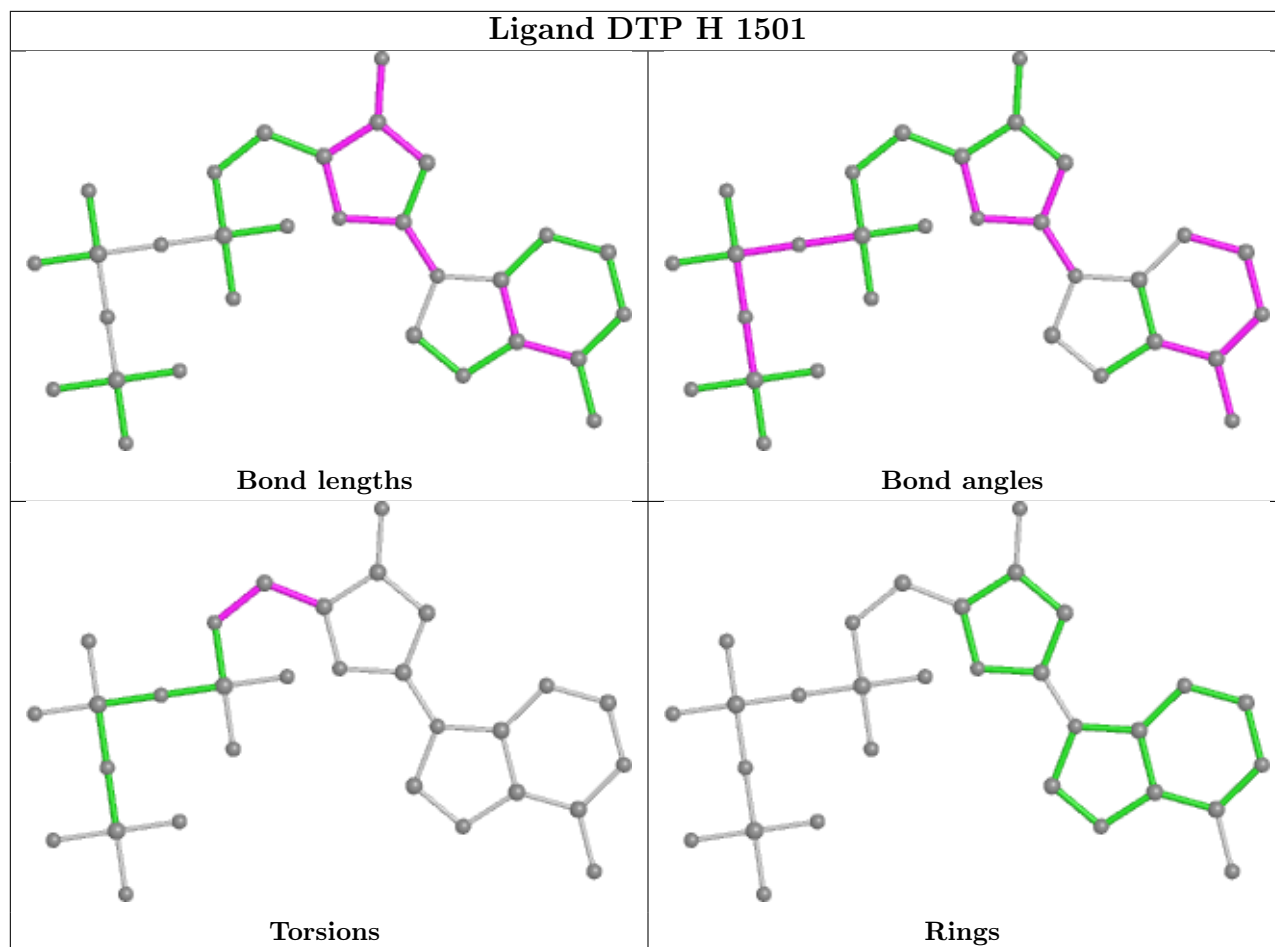
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

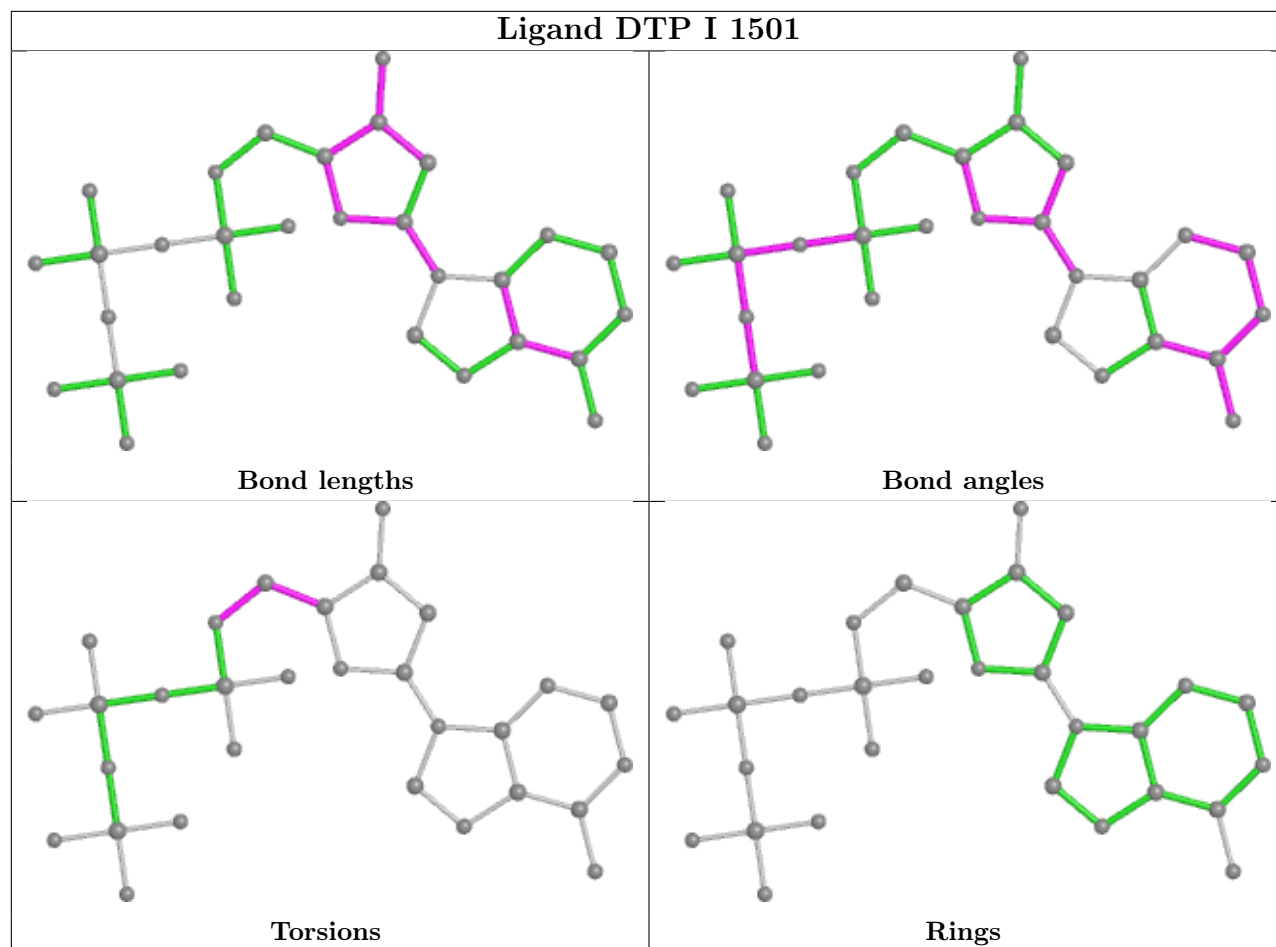


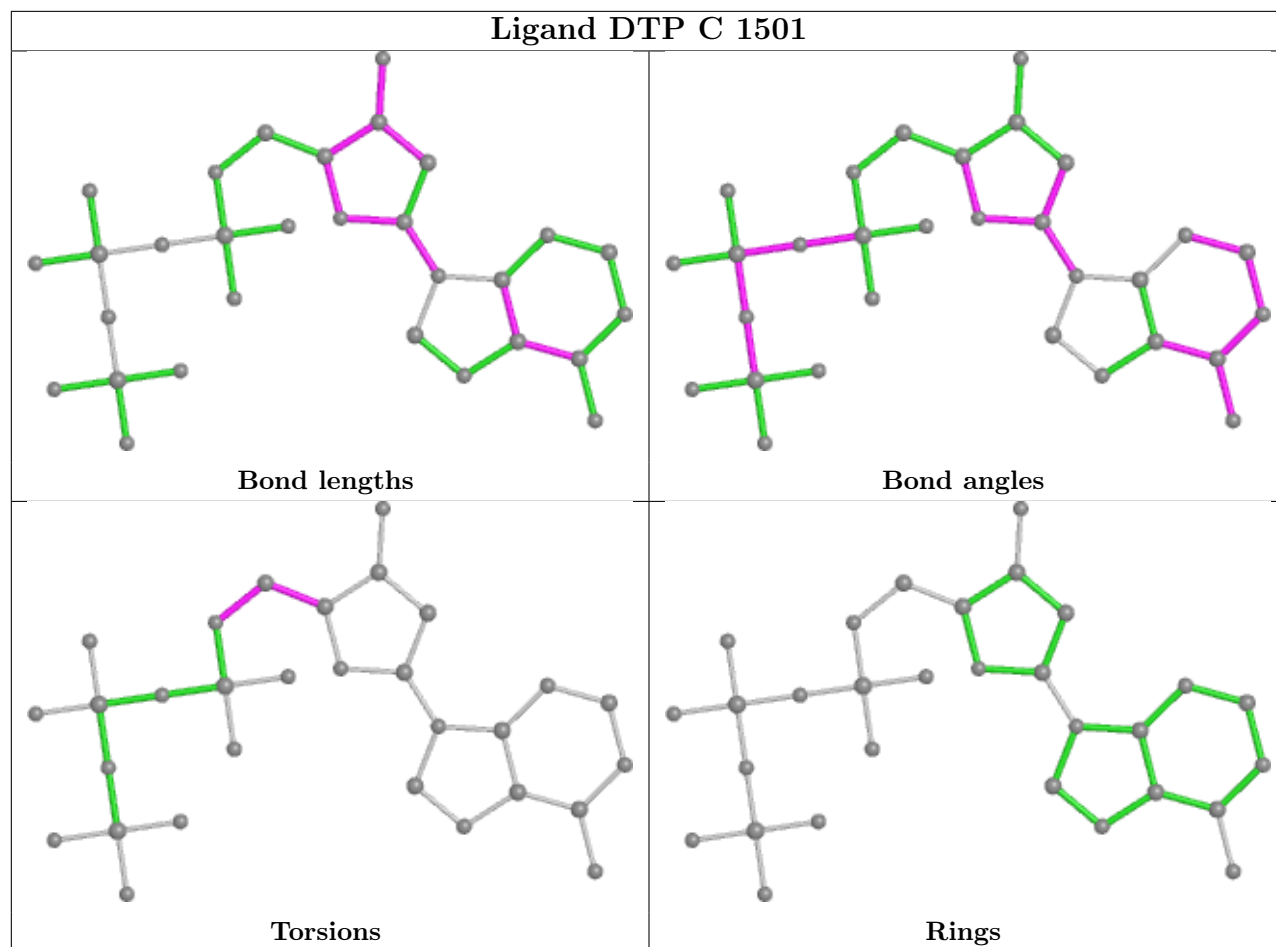


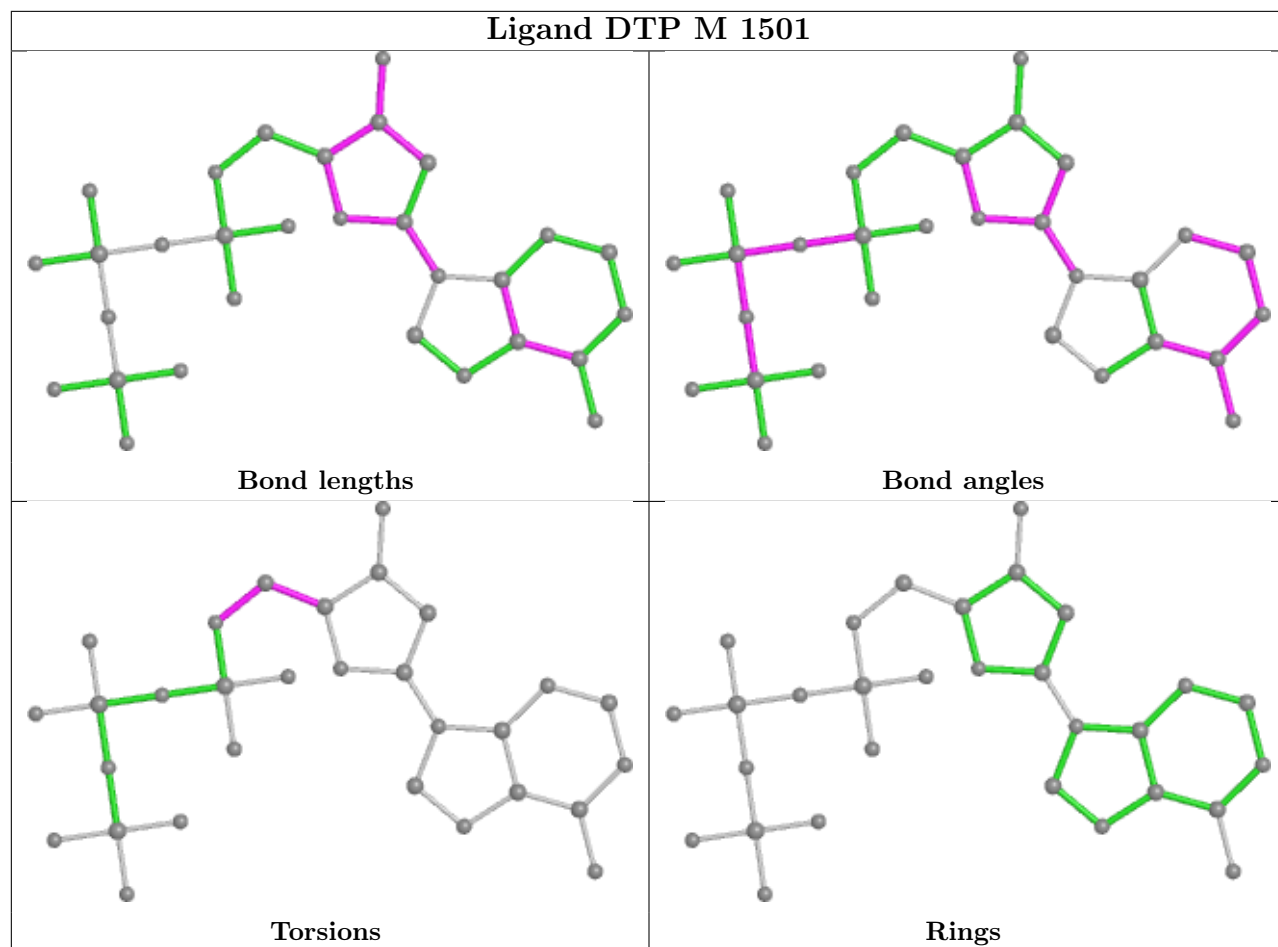


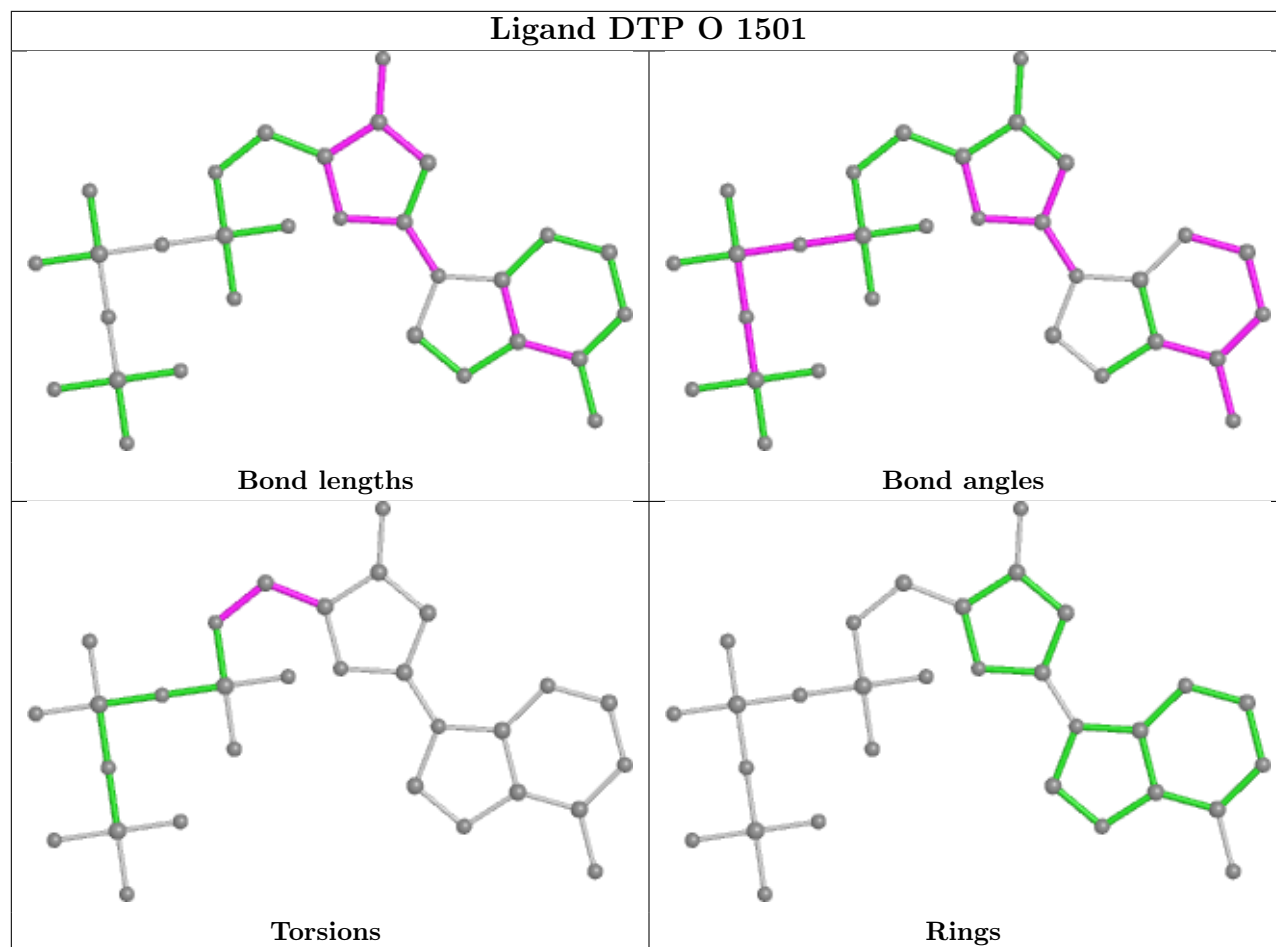


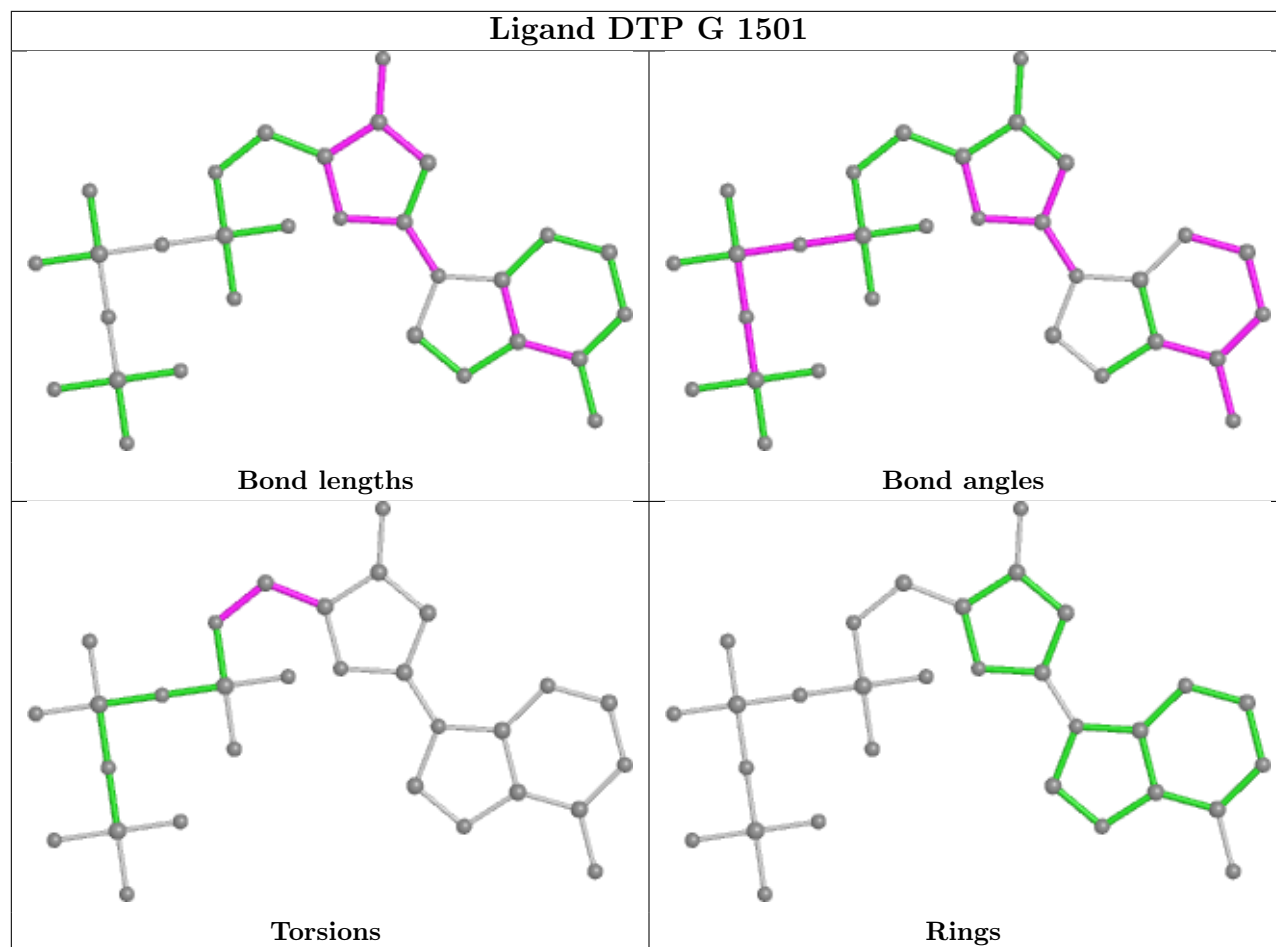


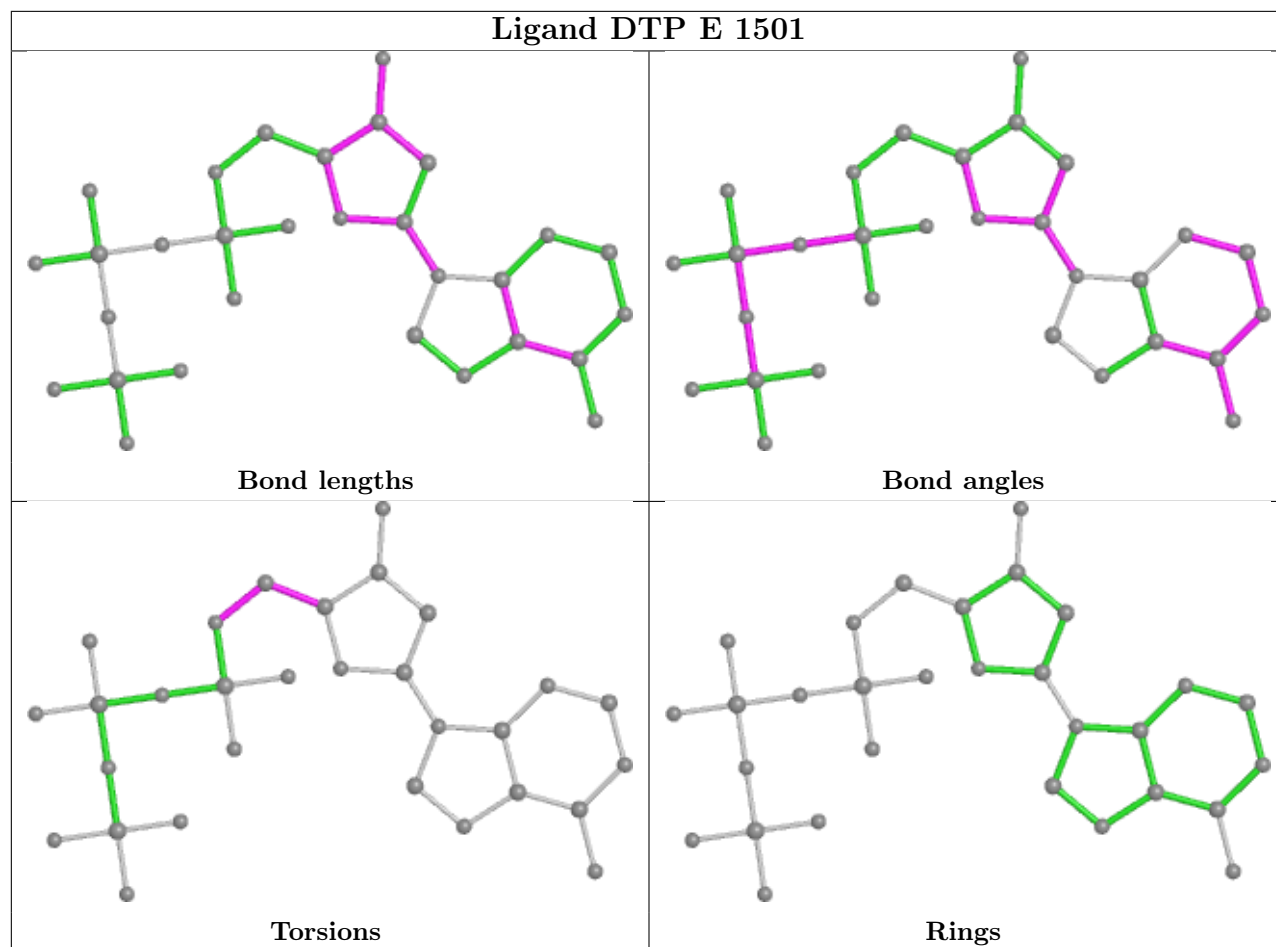




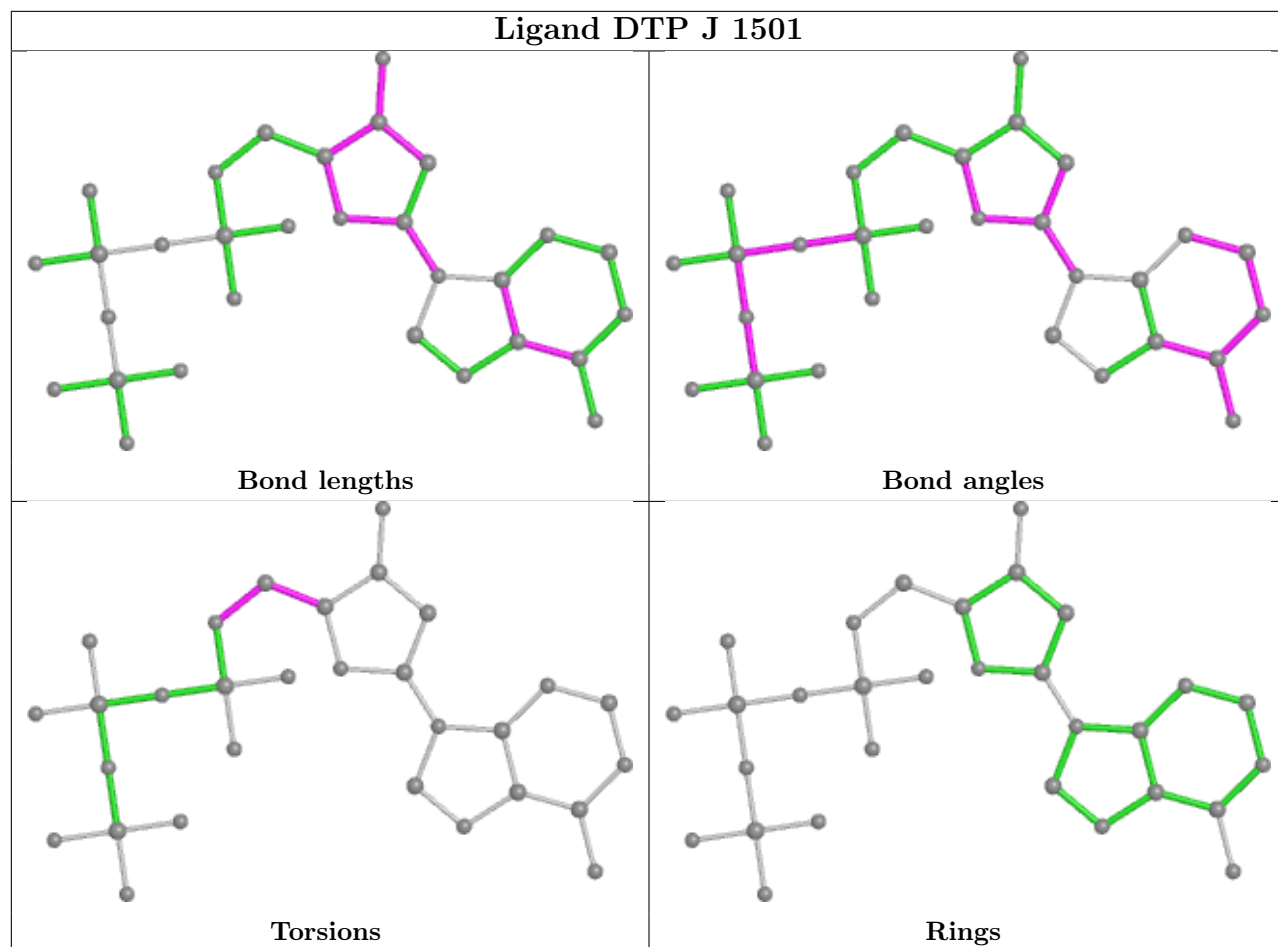


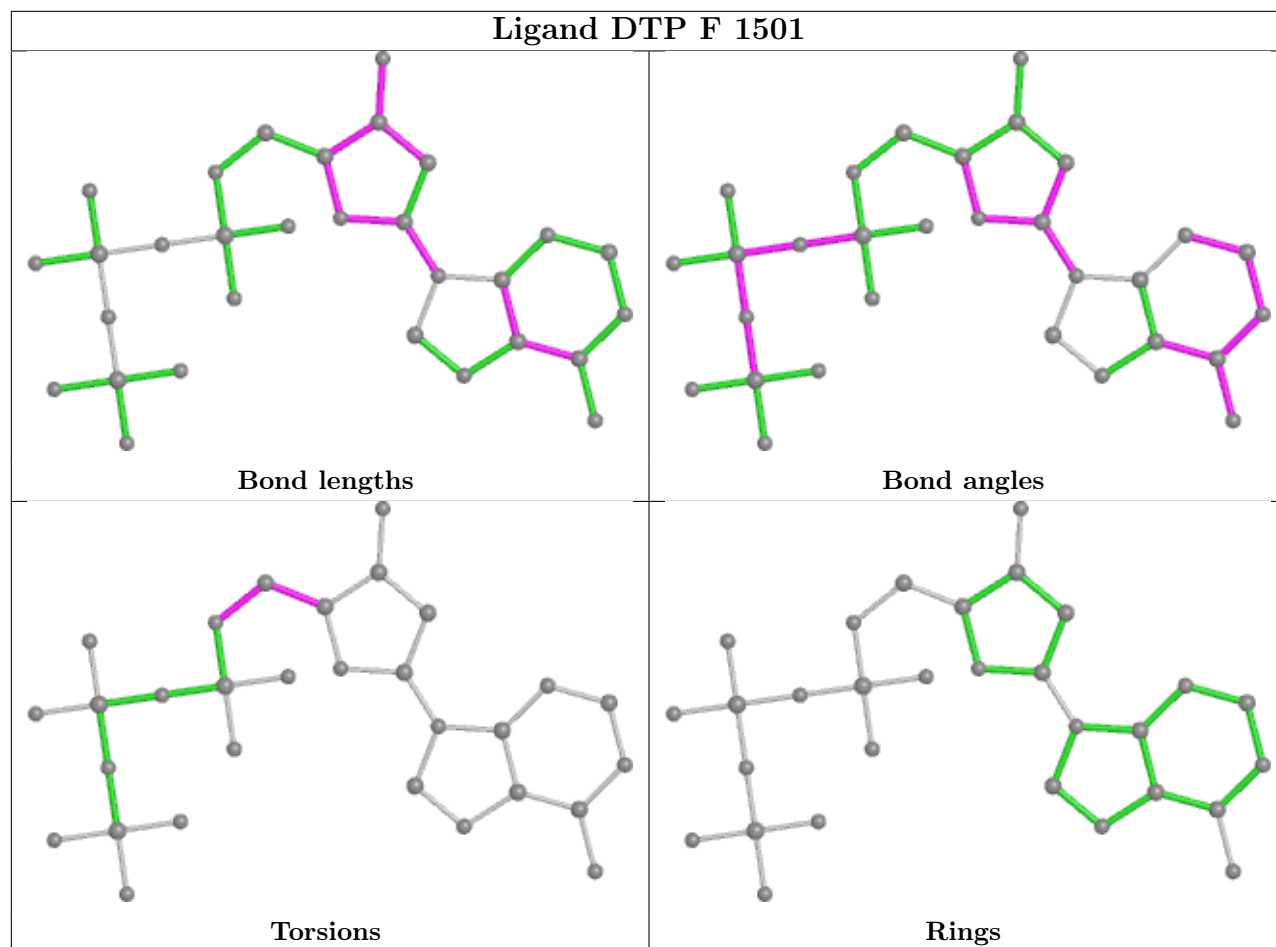


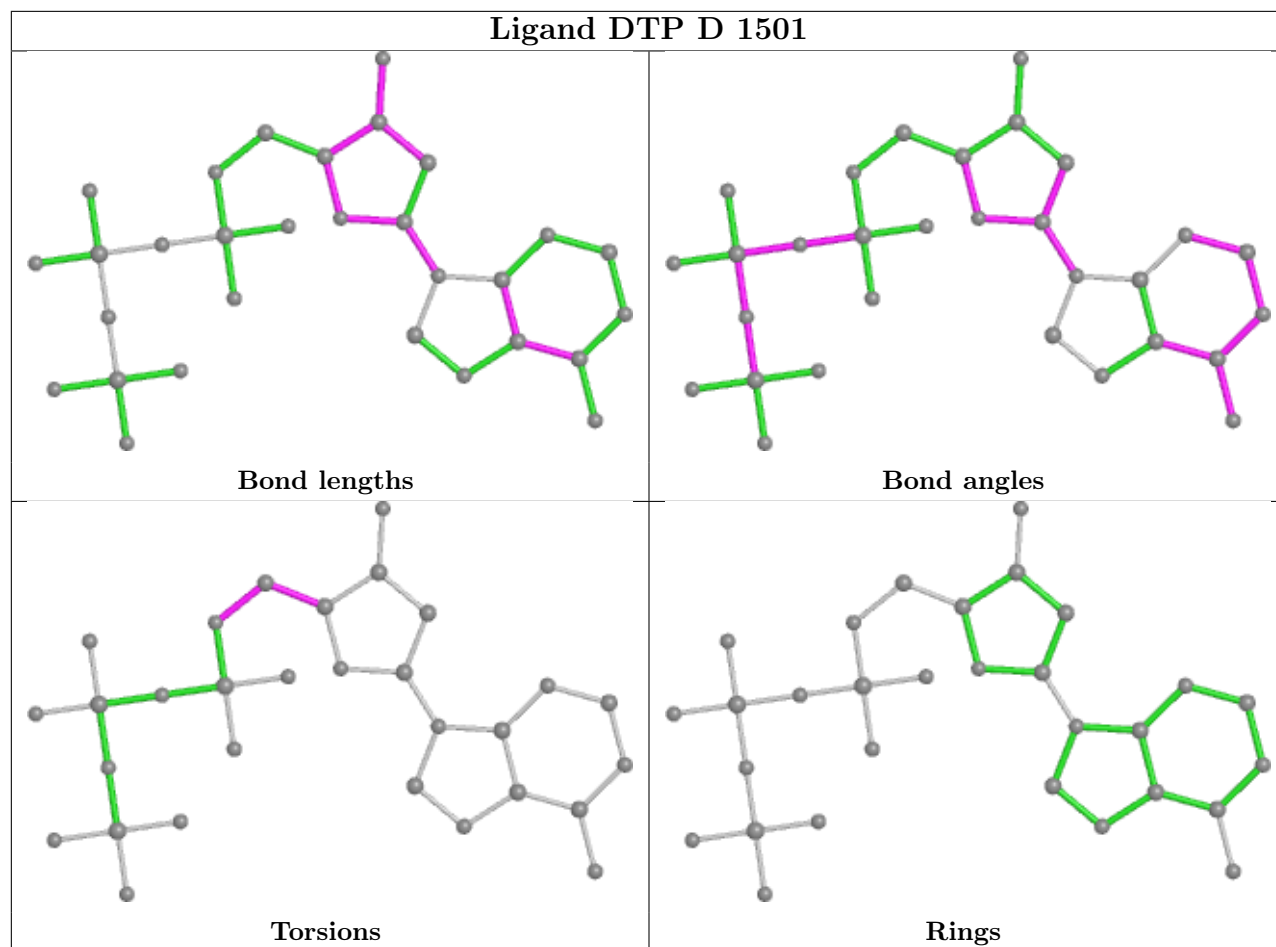


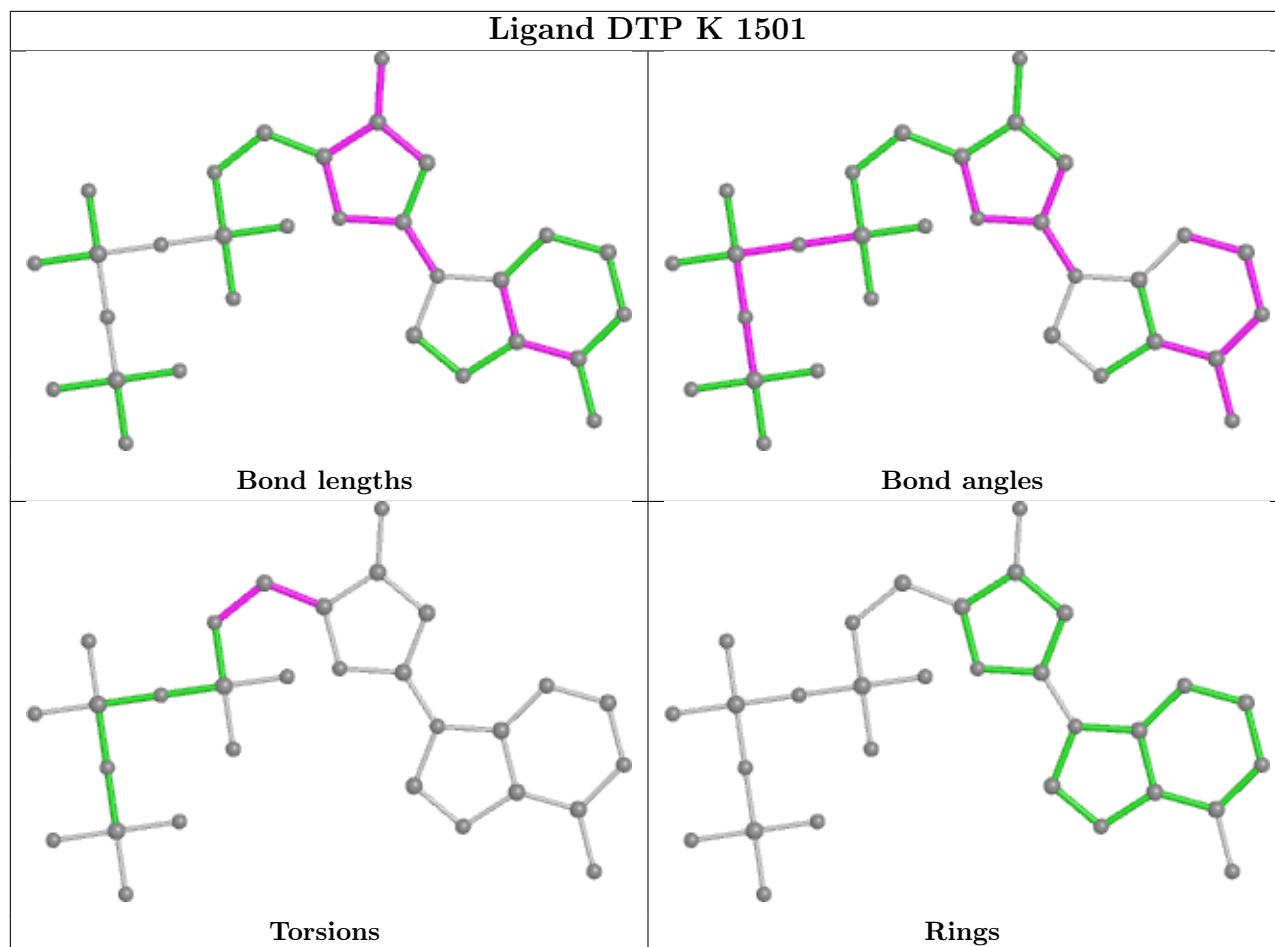


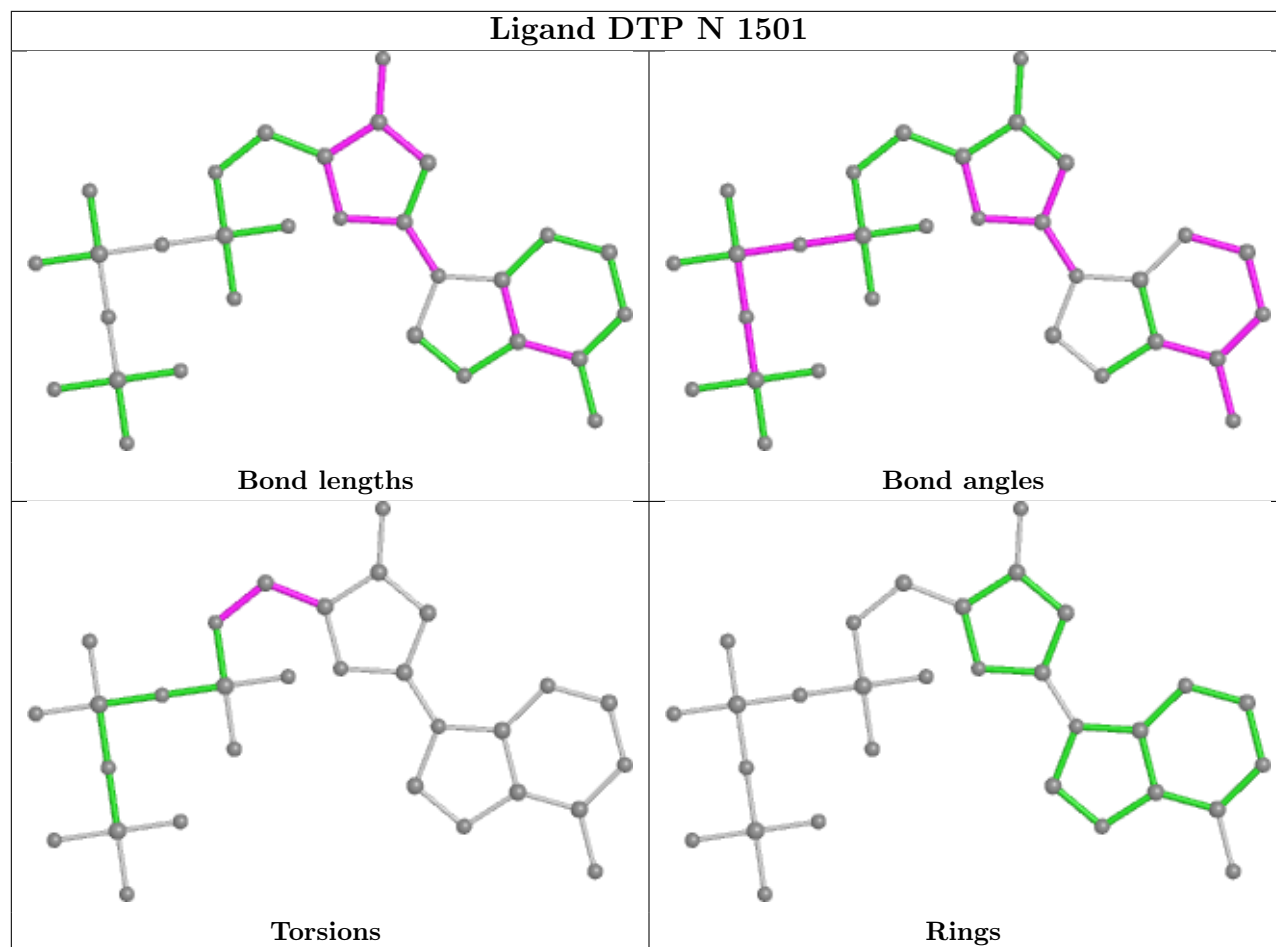


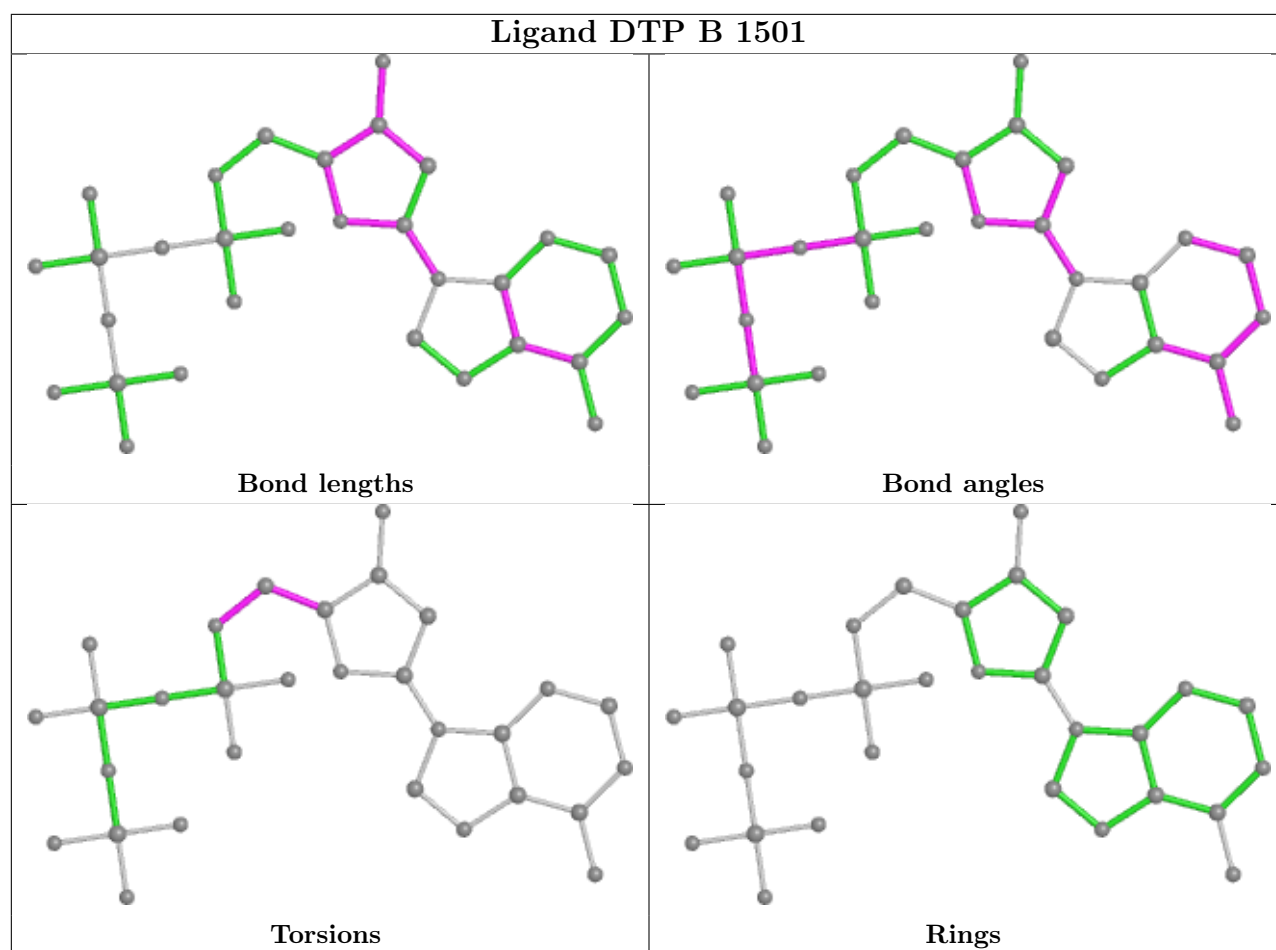












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

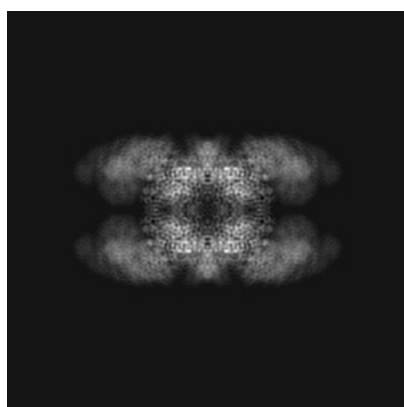
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8177. These allow visual inspection of the internal detail of the map and identification of artifacts.

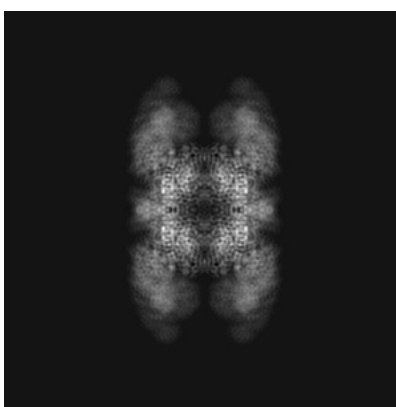
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

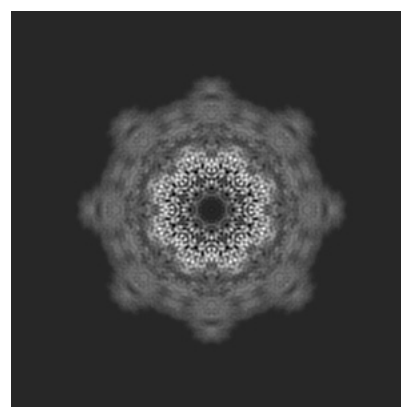
#### 6.1.1 Primary map



X



Y

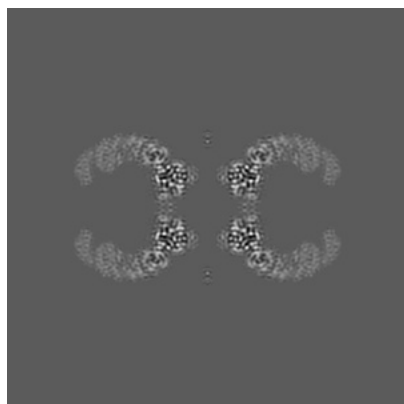


Z

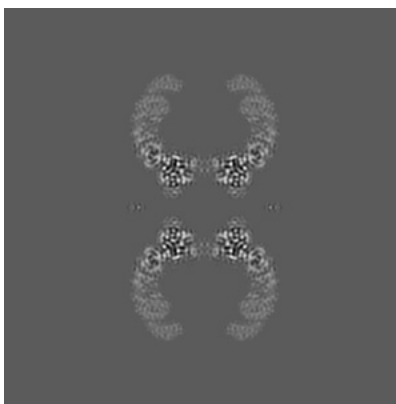
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 160



Y Index: 160

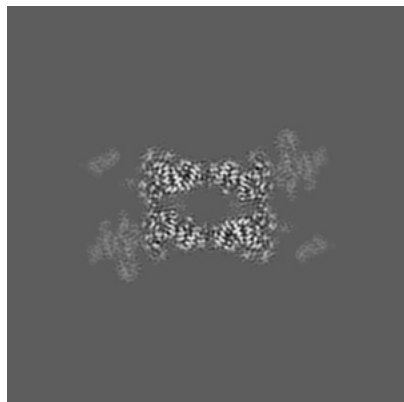


Z Index: 160

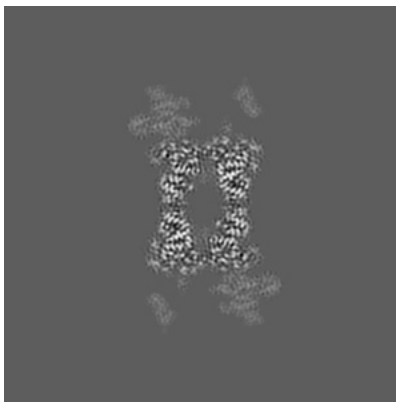
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

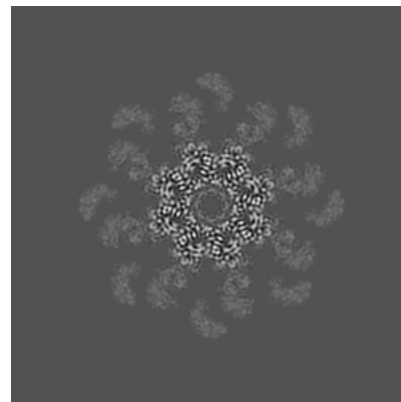
### 6.3.1 Primary map



X Index: 143



Y Index: 143

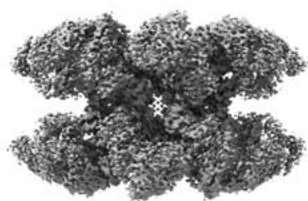


Z Index: 185

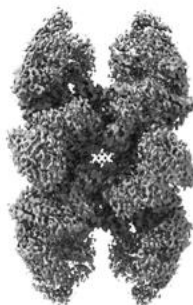
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

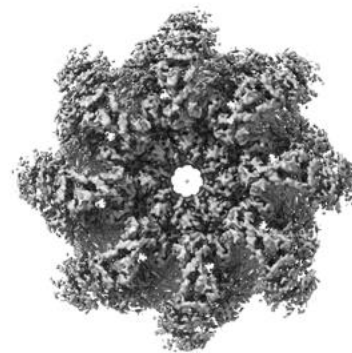
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



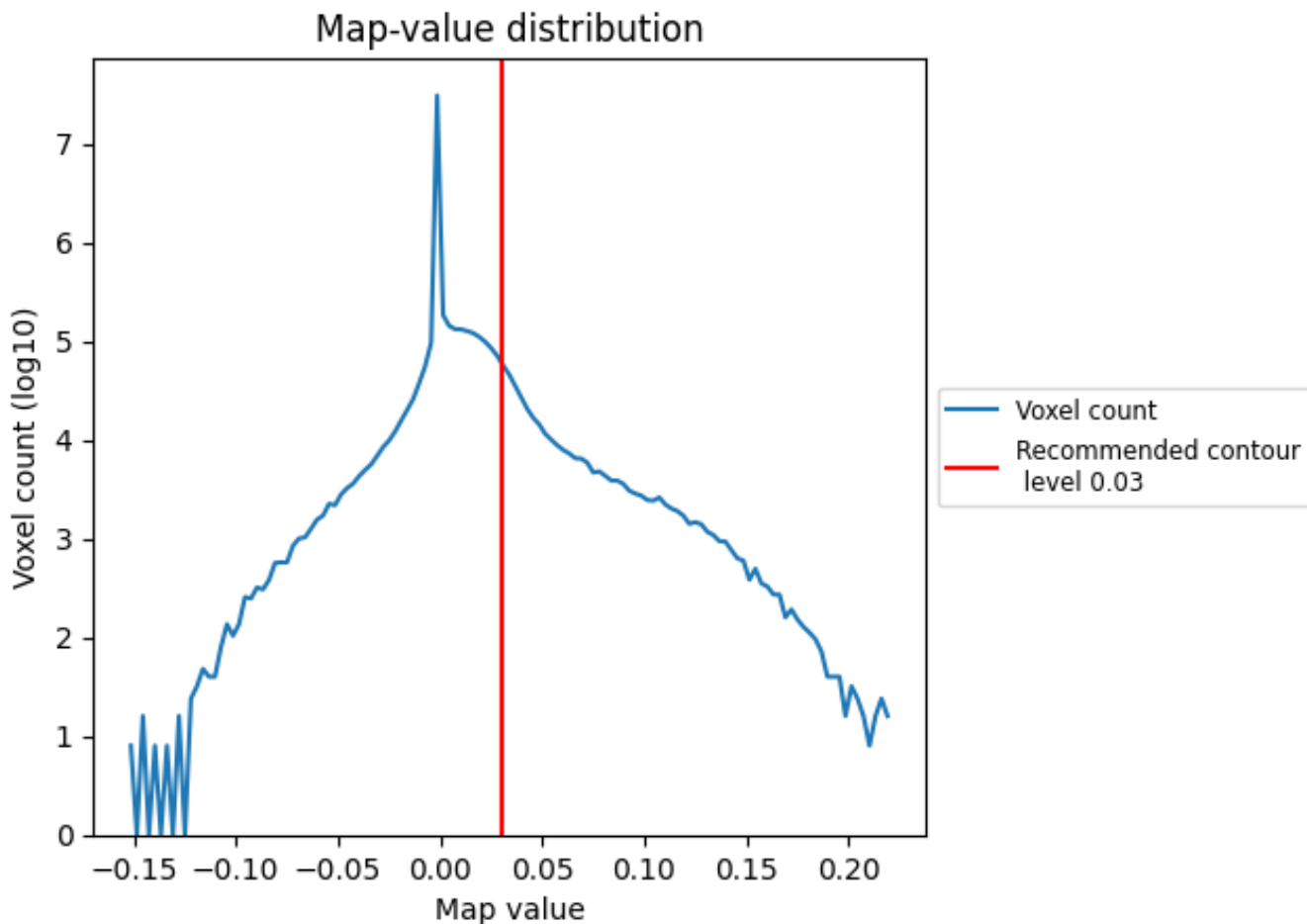
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

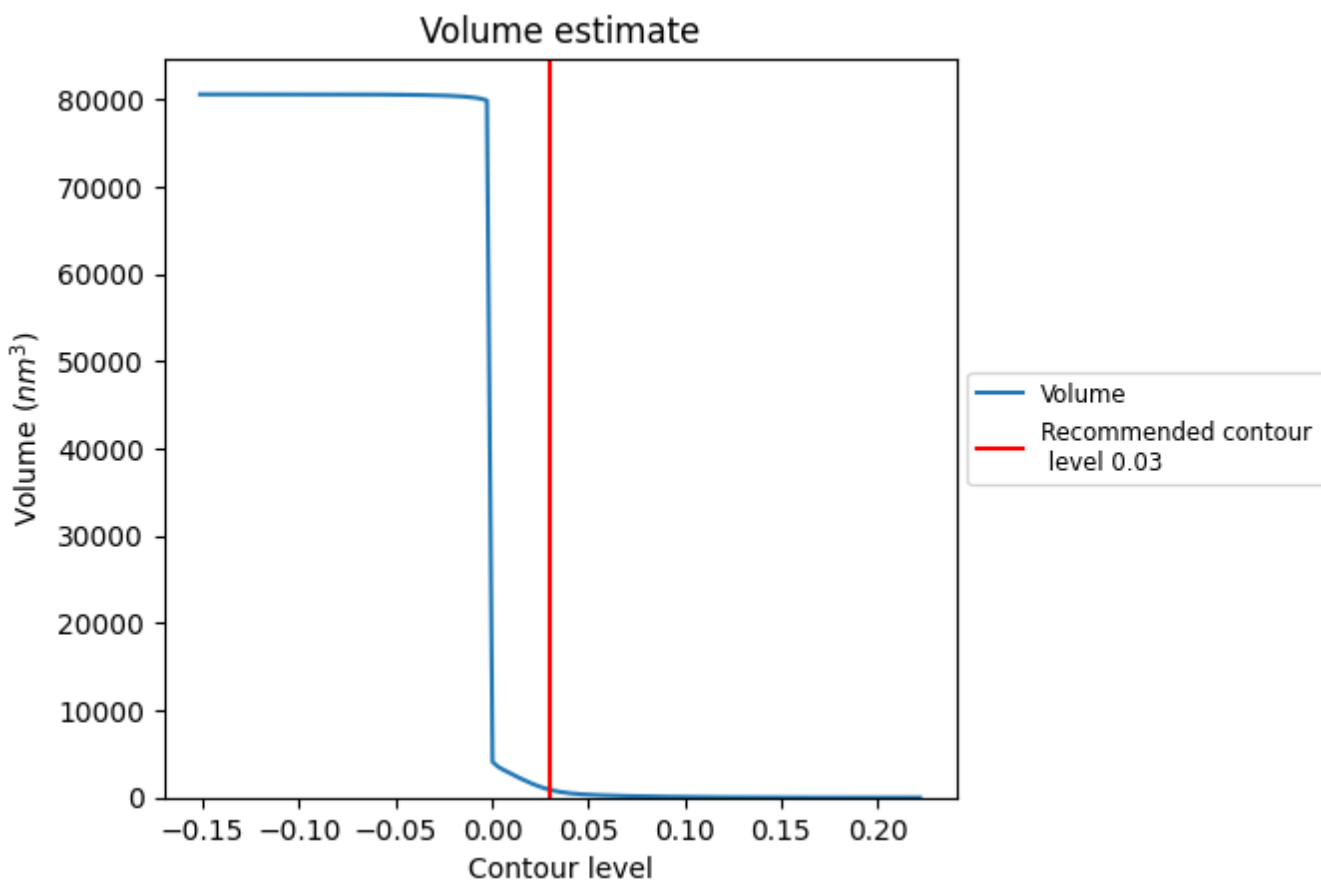
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

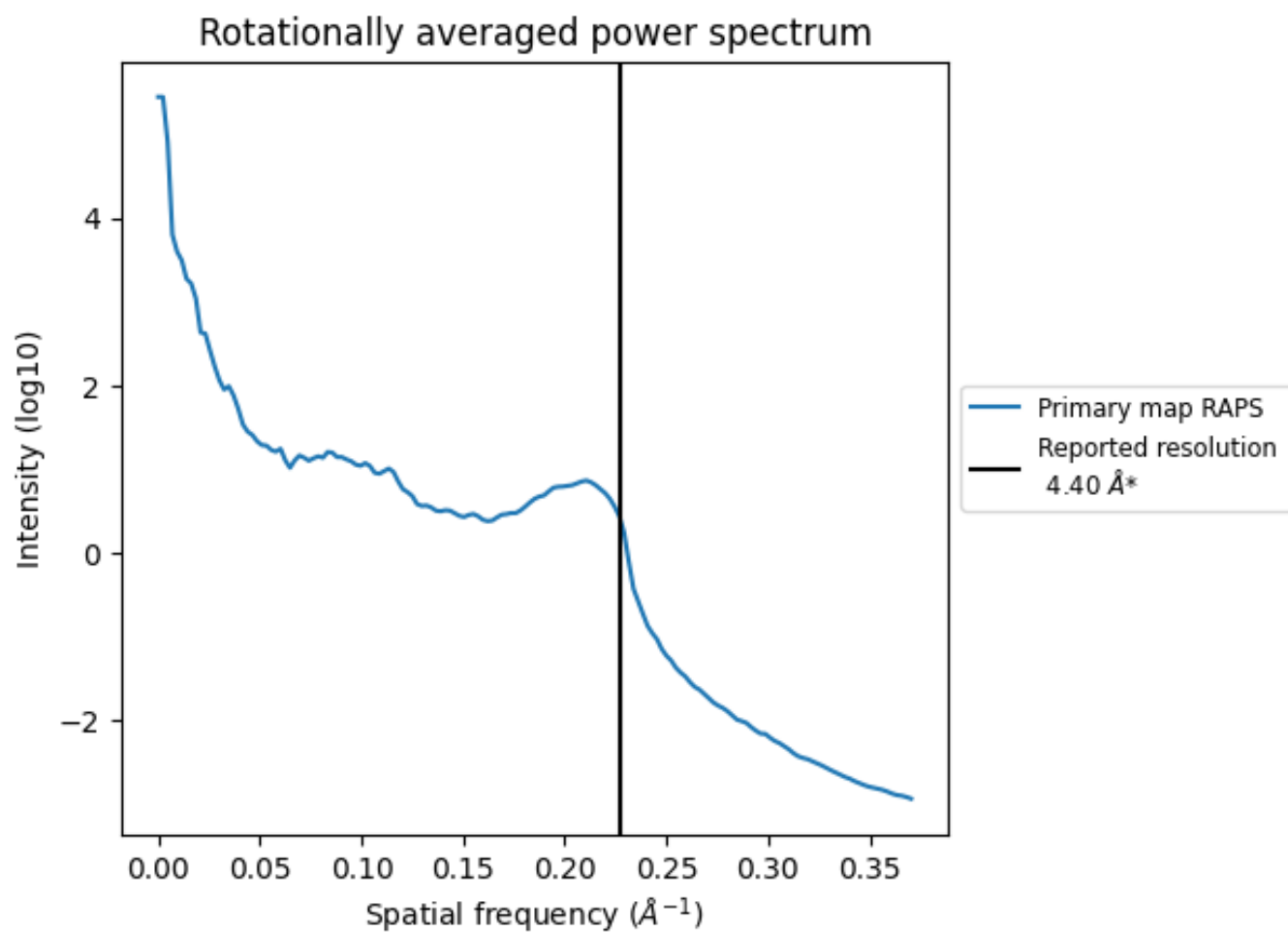
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 904 nm<sup>3</sup>; this corresponds to an approximate mass of 817 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.227 \text{\AA}^{-1}$

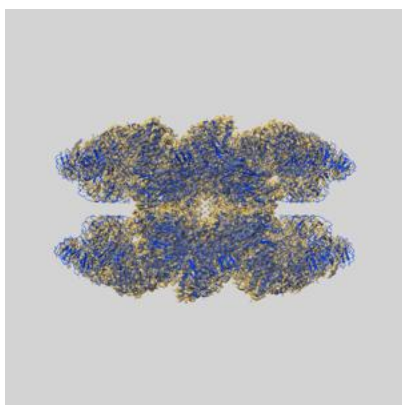
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

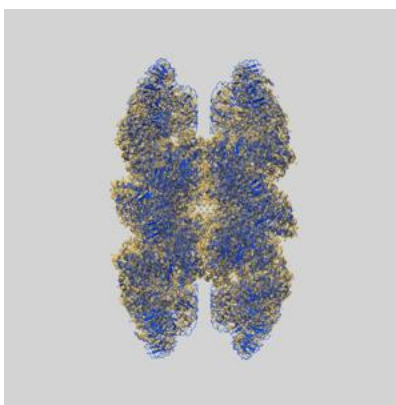
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8177 and PDB model 5JUL. Per-residue inclusion information can be found in section 3 on page 7.

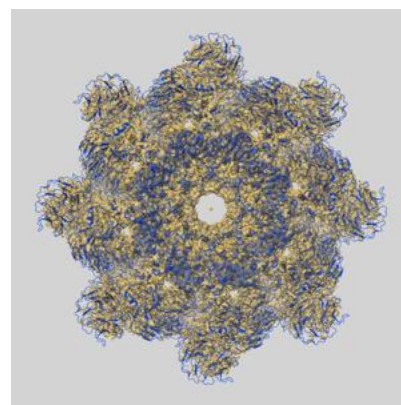
### 9.1 Map-model overlay [i](#)



X



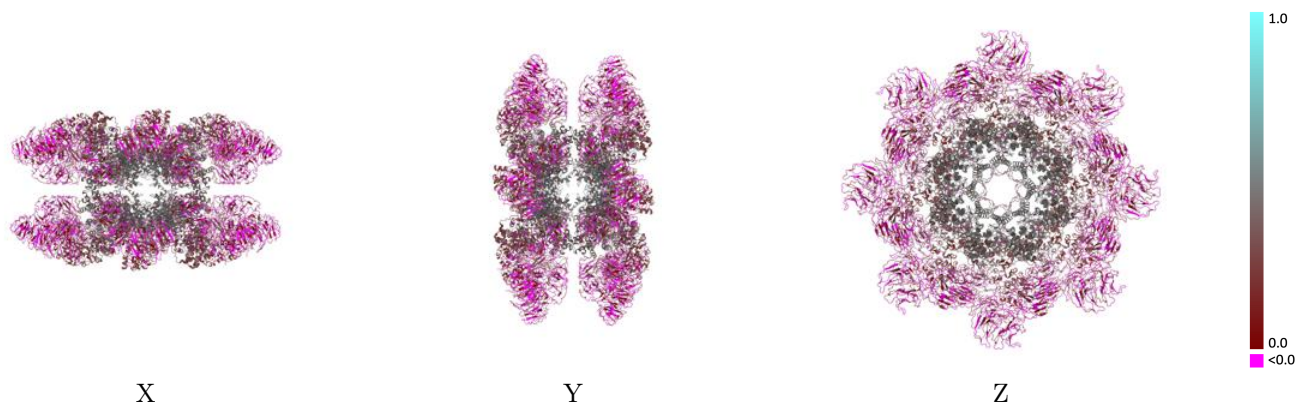
Y



Z

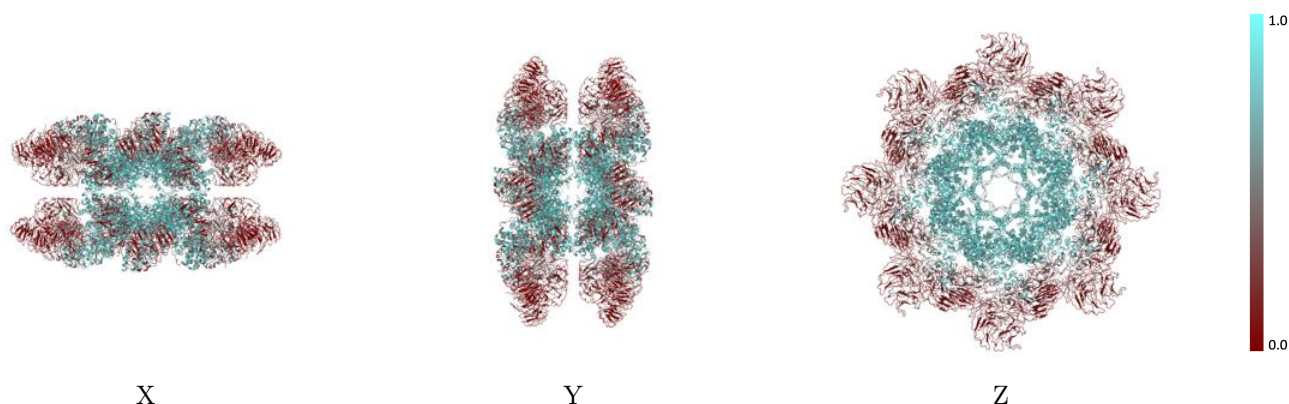
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



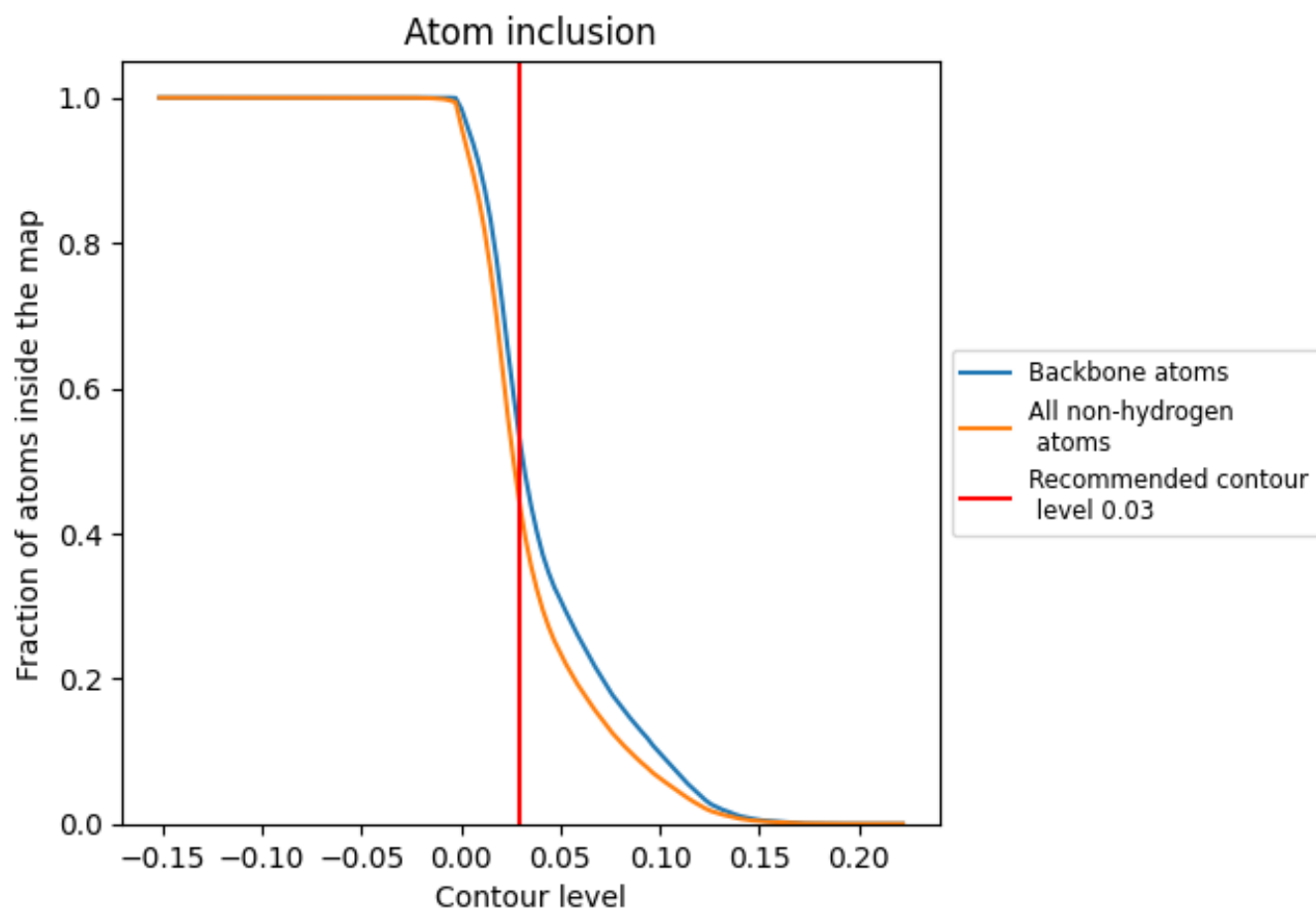
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4340	0.1940
A	0.4360	0.1950
B	0.4303	0.1890
C	0.4314	0.1900
D	0.4335	0.1960
E	0.4366	0.1950
F	0.4284	0.1900
G	0.4361	0.1940
H	0.4358	0.1950
I	0.4354	0.1950
J	0.4370	0.1950
K	0.4338	0.1960
L	0.4285	0.1880
M	0.4355	0.1950
N	0.4371	0.1950
O	0.4353	0.1950
P	0.4334	0.1960

