



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2025 – 08:43 AM EDT

PDB ID : 5JUL / pdb_00005jul
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.

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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>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

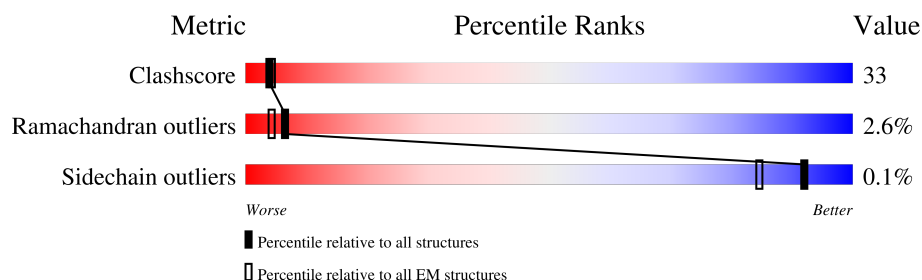
1 Overall quality at a glance

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	<div> <div>45%</div> <div>48%</div> <div>35%</div> <div>14%</div> </div>
1	B	1440	<div> <div>45%</div> <div>47%</div> <div>36%</div> <div>14%</div> </div>
1	C	1440	<div> <div>45%</div> <div>47%</div> <div>36%</div> <div>14%</div> </div>
1	D	1440	<div> <div>45%</div> <div>46%</div> <div>36%</div> <div>14%</div> </div>
1	E	1440	<div> <div>45%</div> <div>48%</div> <div>35%</div> <div>14%</div> </div>
1	F	1440	<div> <div>45%</div> <div>47%</div> <div>36%</div> <div>14%</div> </div>
1	G	1440	<div> <div>45%</div> <div>47%</div> <div>35%</div> <div>14%</div> </div>
1	H	1440	<div> <div>45%</div> <div>47%</div> <div>35%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	1440	<div> <div>45%</div> <div>47%</div> <div>36%</div> <div>14%</div> </div>
1	J	1440	<div> <div>45%</div> <div>48%</div> <div>35%</div> <div>14%</div> </div>
1	K	1440	<div> <div>45%</div> <div>47%</div> <div>36%</div> <div>14%</div> </div>
1	L	1440	<div> <div>45%</div> <div>47%</div> <div>36%</div> <div>14%</div> </div>
1	M	1440	<div> <div>45%</div> <div>47%</div> <div>36%</div> <div>14%</div> </div>
1	N	1440	<div> <div>45%</div> <div>47%</div> <div>35%</div> <div>14%</div> </div>
1	O	1440	<div> <div>45%</div> <div>47%</div> <div>36%</div> <div>14%</div> </div>
1	P	1440	<div> <div>45%</div> <div>47%</div> <div>35%</div> <div>14%</div> </div>

2 Entry composition

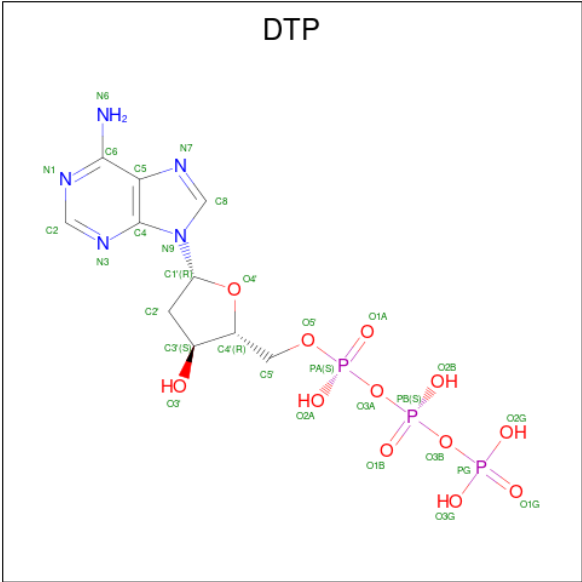
There are 2 unique types of molecules in this entry. The entry contains 161200 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



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

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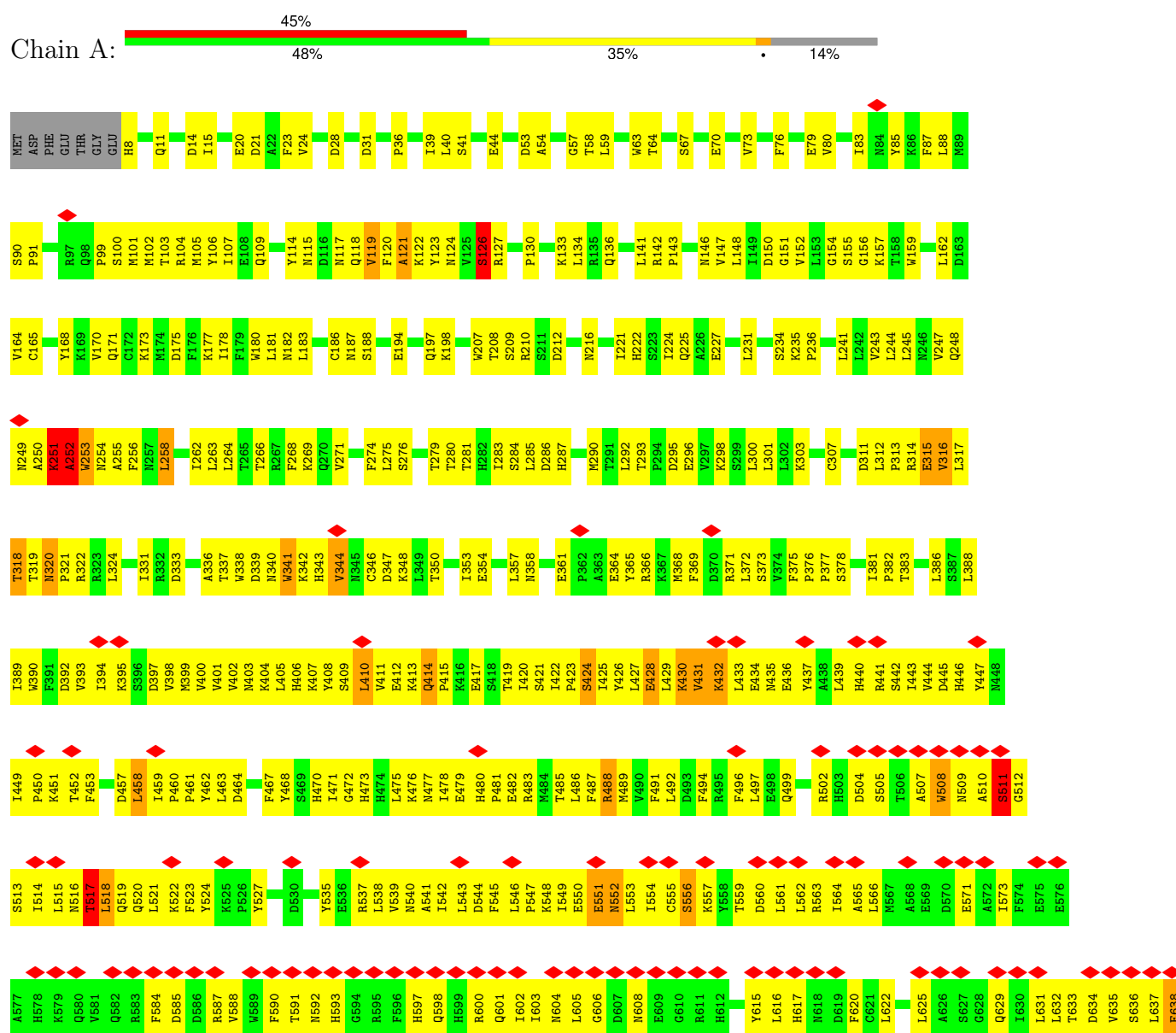
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Mol	Chain	Residues	Atoms					AltConf
2	O	1	Total	C	N	O	P	0
			30	10	5	12	3	
2	P	1	Total	C	N	O	P	0
			30	10	5	12	3	

3 Residue-property plots

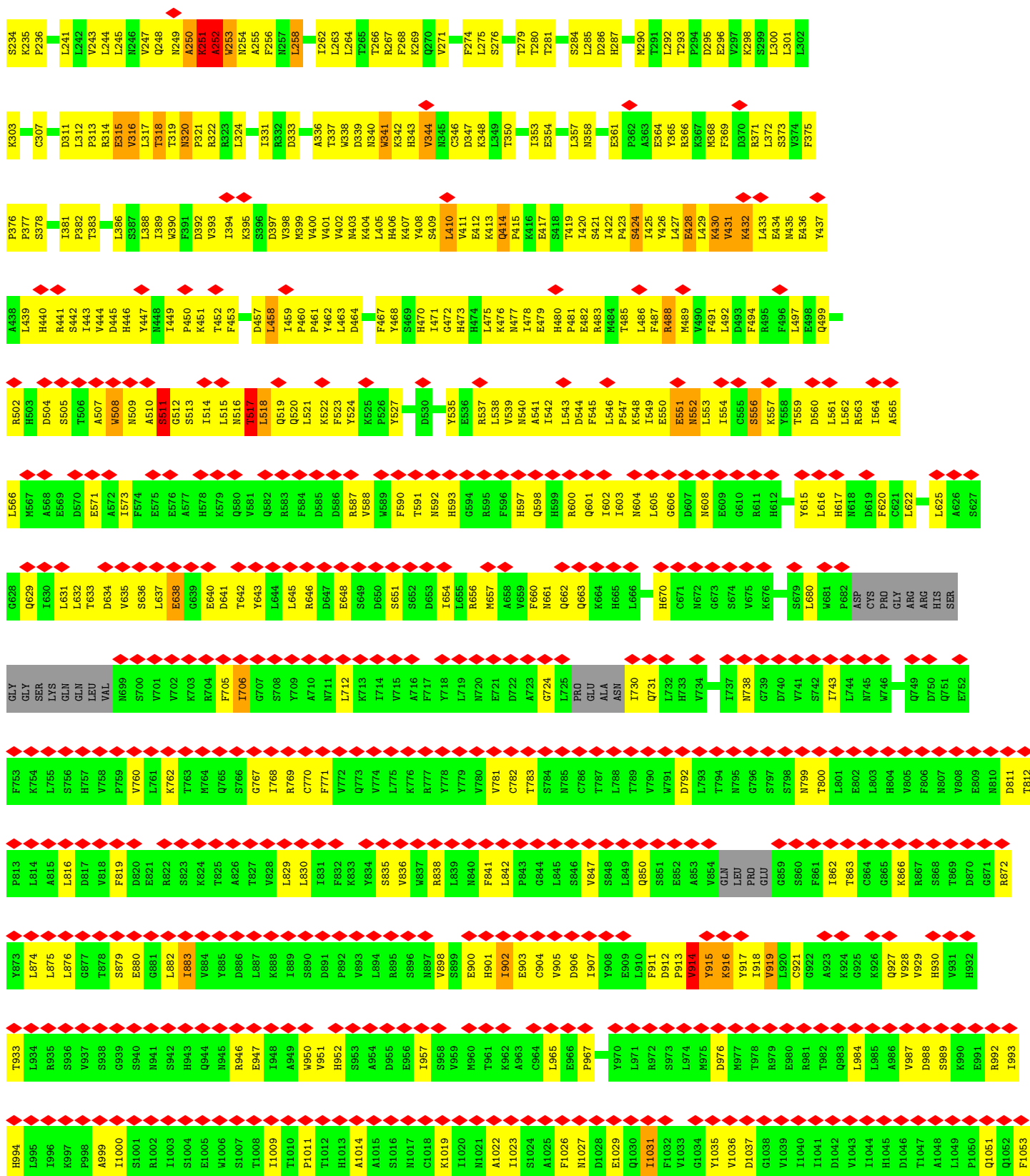
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

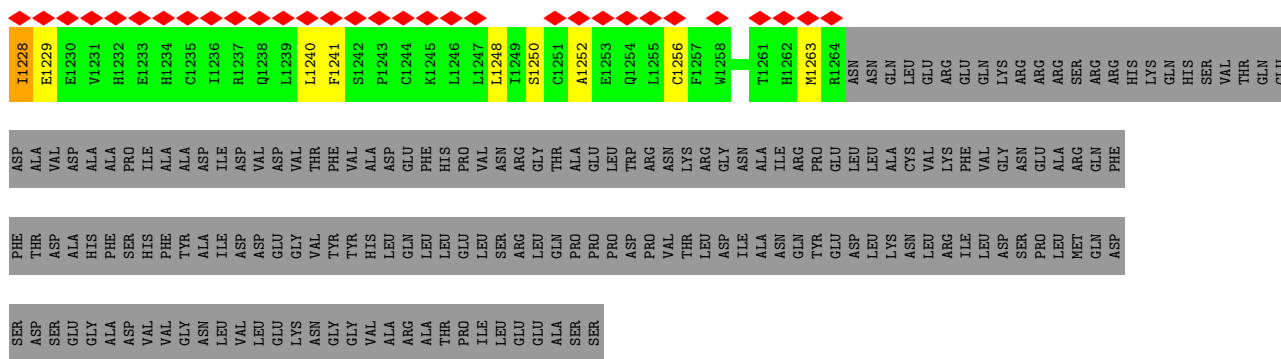


- Molecule 1: Apaf-1 related killer DARK

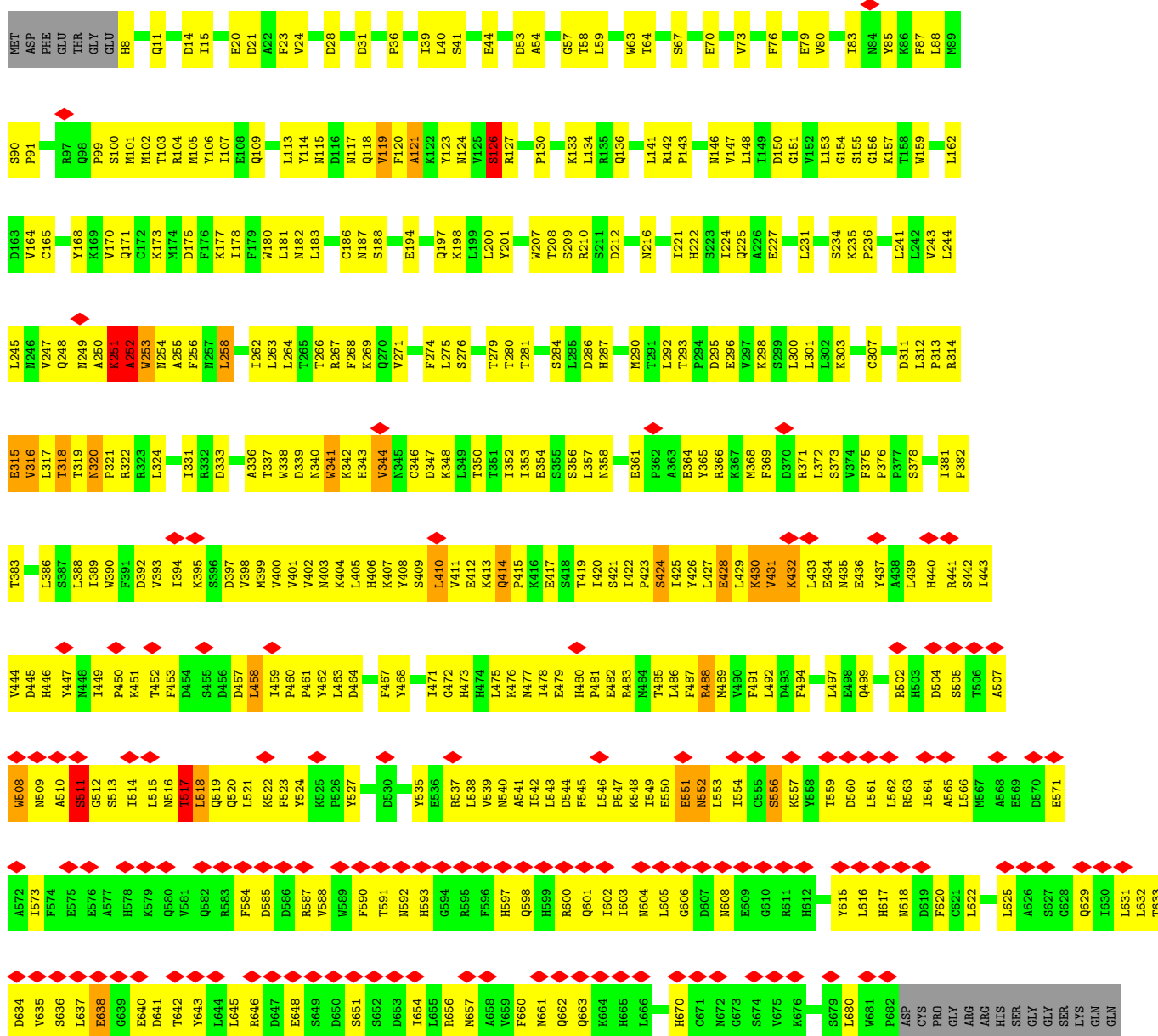




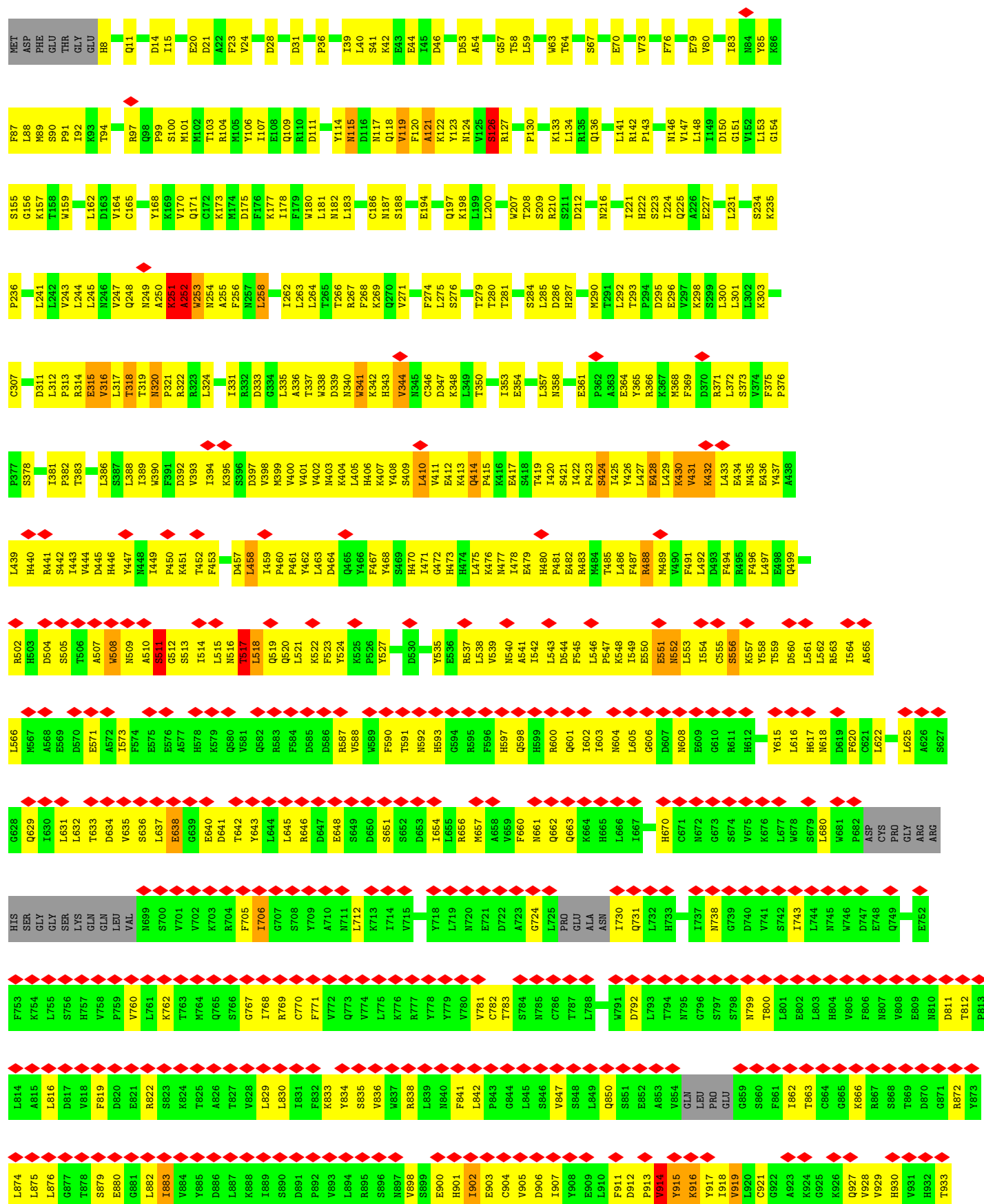
V1165	K1105	H1045	L985	G924	H804	L744	ASP	C821	D560	R495	E434
F1166	Y1106	D1046	A986	G925	V805	N745	CYS	L622	L561	F496	M435
R1167	A1107	T1047	V987	K926	F806	N746	PRO	GLY	L562	E497	E436
L1168	S1108	L1048	D988	Q927	N807	N747	ARG	L625	R563	E498	Y437
I1169	L1109	L1049	S989	Q928	V808	E748	ARG	A626	I564	Q499	A438
F1170	Q1110	P1050	K990	V929	E809	N749	HIS	S627	A565	R502	L439
S1171	E1111	Q1051	E991	H930	N810	D750	SER	G628	L566	H503	H440
C1172	Q1112	Q1052	R992	H932	D811	Q751	GLY	L630	M567	H504	R441
M1173	Q1113	F1053	R993	T933	T812	E752	GLY	L631	A568	D504	S442
L1174	Y1114	I1054	H994	L934	P813	F753	SER	L632	E569	S505	I443
L1175	I1115	E1055	L995	R935	L814	N754	GLN	T633	T506	T507	V444
R1176	I1116	E1056	I996	S936	L815	L755	GLN	D634	D570	A507	D445
Y1177	L1117	P1057	K997	V937	A815	S756	LEU	V635	E571	M508	H446
F1178	F1118	I1058	R998	S938	L816	N757	VAL	D635	A572	R448	Y447
S1179	S1119	D1059	A999	G939	D817	H757	N699	V636	F574	N509	H449
I1180	D1120	Y1060	I1000	S940	V818	F758	S700	A510	E575	A510	P450
C1181	H1121	L1061	R1001	N941	N819	F759	V701	G512	E576	S511	K451
E1182	G1122	K1062	S1002	S942	D820	N760	V702	E638	A577	S513	T452
E1183	V1123	Q1063	I1003	H943	E821	L761	K703	G639	H578	I514	D453
I1184	C1124	V1064	E1004	Q944	R822	K762	R704	D641	K379	L515	L454
L1185	H1125	S1065	E1005	Q945	S923	N763	F705	Y643	Q582	N516	S455
A1186	L1126	P1066	V1006	N946	K824	Q765	G707	L644	R583	T517	D456
Q1187	D1127	M1067	D886	R946	A826	S766	S708	L645	F584	L518	D457
K1188	I1128	I1068	L887	E947	T827	G767	V709	R646	D585	Q519	L458
A1189	I1129	L1069	K888	I948	V828	N768	A710	D647	D586	Q520	I459
K1190	M1130	V1070	T889	A949	L829	R769	N711	E648	R587	L521	P461
I1191	P1131	A1071	S890	W950	L830	C770	L712	D650	K525	F523	Y462
S1192	S1132	S1072	D891	H952	T831	F771	K713	S651	V588	Y524	D464
Y1193	A1133	H1013	P892	S953	R832	N772	A715	G552	W589	K526	F467
L1194	F1134	H1074	K893	A954	K833	Q773	A716	D653	F590	P526	Y468
V1195	V1135	S1075	L894	E955	Y834	N774	F717	I654	T591	D530	S469
A1196	K1136	A1076	R895	E956	S835	L775	Y718	L855	N592	Y535	I471
T1197	P1137	Q1077	S896	N957	V836	K776	L719	R656	H593	E536	G472
D1198	K1138	K1078	N897	I957	N837	N777	N720	M657	G594	R537	H474
D1199	D1139	T1079	S958	S958	R838	Y778	E721	A658	F596	L538	K476
G1200	S1140	V1080	W959	S899	L839	N779	D722	V659	H597	V539	M477
T1201	I1141	N1021	N960	S899	N840	V780	A723	F660	Q598	A541	I478
M1202	E1142	F1082	T961	H901	F841	N781	G724	N661	H599	I542	E479
L1203	Y1143	Q1083	K962	I902	L842	C782	L725	Q662	R600	L543	H480
A1204	I1144	L1084	C964	E903	P843	N783	PRO	Q663	Q601	D544	P481
M1205	G1145	E1085	L965	V905	G844	N785	ALA	H665	I602	F545	E482
G1206	K1146	K1086	E966	D906	L845	C786	ASN	L666	N604	L486	M484
F1207	D1147	I1087	P967	N907	S846	T787	I730	I667	L605	F487	L486
E1208	D1148	D1088	P967	I907	V847	L788	Q731	G606	G606	E550	R488
M1209	L1149	D1028	Y908	N908	S848	N789	L732	H670	D607	E551	M489
L1212	K1150	Q1030	E909	E909	L849	V790	H733	C671	N608	N552	V490
E1213	M1151	I1031	R972	F911	Q850	N791	V734	G672	N553	L553	F491
L1214	S1152	F1032	S973	D912	S851	D792	I737	G673	E509	I554	L492
F1215	L1153	P1033	L974	P913	E852	L793	N738	G674	G610	C555	D493
	L1154	G1034	N975	N914	A853	N794	I738	V675	R611	S556	F494
	F1155	Y1035	D976	Y915	V854	N795	G739	G676	H612	K557	
N1219	L1156	V1036	N977	K916	N854	N796	D740	K676	Y615	Y558	
R1220	A1157	D1037	Y978	Y917	GLN	G796	V741	L677	L616		
K1221	Y1158	L1098	R979	I918	LEU	N797	V741	N678	H617		
Q1223	E1159	M1099	V919	N919	PRO	S797	S742	G679	N618		
L1224	N1160	V1039	L920	C921	GLU	N798	I743	L680	D619		
I1225	M1161	I1040	G922	A923	GLU	T800		W681	F620		
Y1226	T1162	D1042	Q983			L801		P682			
S1227	I1163	V1043				L803					



● Molecule 1: Apaf-1 related killer DARK









E1056	P1057	I1058	D1059	Y1060	L1061	K1062	Q1063	S1064	V1065	P1066	N1067	L1068	I1069	V1070	A1071	S1072	A1073	H1074	S1075	A1076	Q1077	K1078	T1079	V1080	I1081	F1082	L1083	L1084	E1085	K1086	I1087	D1088	P1089	L1090	Q1091	P1092	N1093	D1094	Q1095	N1096	P1097	L1098	M1099	M1100	D1101	V1102	S1103	T1104	K1105	Y1106	A1107	S1108	L1109	Q1110	E1111	G1112	Q1113	Y1114	I1115	
1996	K997	P998	A999	I1000	S1001	I1002	I1003	S1004	E1005	P1006	S1007	T1008	I1009	A1010	P1011	T1012	A1013	A1014	A1015	S1016	Q1017	N1017	C1018	K1019	I1020	N1021	A1022	I1023	S1024	A1025	F1026	N1027	D1028	E1029	Q1030	I1031	F1032	V1033	G1034	Y1035	V1036	D1037	G1038	V1039	I1040	I1041	D1042	V1043	I1044	H1045	D1046	T1047	A1048	L1049	P1050	Q1051	Q1052	F1053	I1054	E1055
R935	S936	V937	S938	G939	S940	H941	S942	H943	S944	R945	R946	E947	I948	A949	V950	V951	H952	S953	A954	D955	E956	I957	S958	S959	H960	T961	K962	A963	C964	L965	E966	P967	Y970	L971	R972	S973	L974	M975	D976	M977	T978	S979	E980	R981	T982	Q983	L984	L985	A986	V987	D988	S989	K990	E991	R992	I993	H994	L995		
L875	L876	G877	T878	S879	E880	G881	L882	T883	H884	Y885	D886	L887	K888	T889	S890	D891	K892	V893	Y894	R895	S896	H897	V898	E899	E900	H901	I902	E903	C904	V905	D906	I907	Y908	E909	L910	F911	D912	P913	Y914	Y915	K916	Y917	PRO	GLU	G859	S860	F861	T862	T863	C864	S865	K866	R867	D868	T869	D870	S871	H872	Y873	L874
L755	S756	H757	V758	F759	V760	L761	K762	T763	M764	Q765	S766	G767	T768	R769	C770	F771	V772	Q773	V774	L775	K776	R777	V778	Y779	V780	H781	C782	T783	S784	M785	C786	T787	L788	T789	V790	H791	D792	L793	T794	M795	G796	S797	S798	M799	T800	L801	E802	L803	H804	V805	F806	H807	V808	E809	H810	D811	T812	P813	L814	
L631	L632	T633	D634	V635	S636	L637	E638	G639	E640	D641	Y642	Y643	L644	R645	R646	D647	E648	S649	D650	S651	S652	D653	I654	R655	L656	M657	A658	V659	F660	N661	Q662	Q663	K664	H665	L666	H670	C671	N672	G673	S674	V675	K676	S679	L680	W681	P682	ASP	CYS	PRO	GLY	ARG	ARG	HIS	SER	GLY	GLY	SER	Q629	I630	
E569	D570	E571	A572	I573	F574	E575	A576	A577	H578	K579	Q580	V581	Q582	R583	F584	D585	D586	R587	V588	W589	F590	T591	N592	H593	G594	R595	F596	H597	Q598	H599	R600	I602	I603	N604	L605	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	Q518	Q519	Q520	L521	K522	F523	Y524	K525	P526	Y527	D530	Y535	E536	R537	L538	V539	N540	A541	I542	D544	F545	L546	P547	K548	I549	E550	E551	N552	L553	I554	C555	S556	K557	Y558	D559	L561	L562	R563	I564	A565	L566	M567	A568					
L312	P313	R314	E315	V316	L317	T318	N319	N320	P321	R322	E323	L324	I331	R332	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	R371	L372	S373	M374	V375	P376	S377	I381								
P382	T383	L386	S387	L388	T389	W390	F391	D392	V393	F453	I394	K395	S396	D397	V398	M399	V400	V401	V402	M403	K404	L405	H406	K407	Y408	S409	L410	E412	K413	Q414	P415	K416	E417	T419	I420	S421	I422	P423	S424	I425	Y426	L427	E428	K430	V431	K432	L433	E434	S435	E436	V437	A438	L439	H440	R441	S442				
I443	V444	D445	H446	Y447	M448	I449	P450	K451	T452	R453	D454	S455	D456	L458	I459	P460	P461	Y462	L463	D464	F467	Y468	S469	H470	I471	G472	H473	H474	L475	K476	M477	I478	E479	H480	P481	E482	R483	M484	T485	L486	D487	R488	M489	V490	F491	L492	D493	F494	R495	F496	L497	E498	Q499	R502	H503	D504				





ILE	ASP	LEU	GLY	VAL	TYR	HIS	LEU	GLN	LEU	GLU	LEU	GLU	LEU	SER	ARG	GLU	GLN	PRO	PRO	ASP	VAL	THR	LEU	ASP	ILE	S41	ALA	ASN	GLN	TYR	GLU	ASP	LEU	LYS	ASN	LEU	ARG	ILE	LEU	LEU	ASP	PRO	MET	GLN	ASP	SER	ASP	GLY	ALA	VAL	VAL	GLY	ASN
LEU	VAL	LEU	GLU	GLY	ASN	GLY	VAL	ALA	ARG	ALA	THR	PRO	ILE	LEU	GLU	GLU	ALA	GLN	PRO	ASP	VAL	THR	LEU	ASP	ILE	S41	ALA	ASN	GLN	TYR	GLU	ASP	LEU	LYS	ASN	LEU	ARG	ILE	LEU	LEU	ASP	PRO	MET	GLN	ASP	SER	ASP	GLY	ALA	VAL	VAL	GLY	ASN

● Molecule 1: Apaf-1 related killer DARK



LYS	GLN	GLN	GLN	LEU	VAL	K699	S700	V701	V702	K703	R704	F705	I706	G707	S708	L709	A710	W711	L712	K713	I714	V715	A716	F717	Y718	L719	N720	E721	D722	A723	G724	L725	PRO	GLU	ALA	ASN	I730	Q731	L732	H733	V734	I737	N738	G739	D740	V741	S742	L743	I744	N745	W746	D747	ARG	ARG	HIS	SER	GLY	GLY	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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S90	P91	R97	Q98	P99	S100	M101	M102	T103	R104	M105	Y106	I107	E108	Q109	L113	Y114	M115	D116	N117	Q118	V119	F120	A121	K122	Y123	N124	V125	S126	R127	P130	K133	L134	R135	Q136	L141	R142	P143	N146	V147	L148	I149	D150	G151	V152	L153	G154	S155	G156	K157	T158	V159	L162							
D163	V164	C165	Y168	K169	V170	Q171	C172	M173	M174	D175	F176	K177	F178	L179	V180	L181	T266	R267	F268	L183	C186	N187	H188	E194	Q197	K198	L199	L200	W207	T208	S209	R210	S211	D212	N216	I221	H222	Q225	A226	E227	L231	S234	K235	P236	L241	V243	L244	L245	N246										
V247	Q248	N249	A250	K251	A252	W253	N254	A255	V256	N257	L258	I262	L263	L264	T265	T266	R267	F268	K269	Q270	H271	F274	S275	S276	T279	T280	T281	S284	L285	D286	H287	M290	T291	L292	T293	P294	D295	E296	V297	K298	S299	L300	L301	K303	L304	L305	D306	C307	D311	L312	P313	R314							
E315	V316	L317	T318	T319	N320	P321	R322	R323	L324	I331	R332	D333	A336	T337	W338	D339	N340	W341	K342	H343	V344	N345	C346	D347	K348	L349	T350	T351	L352	I353	E354	S355	S356	L357	N358	E361	P362	A363	E364	Y365	R366	K367	M368	F369	D370	L371	L372	L373	L374	L375	L376	L377	S378	I381	P382				
T383	L386	S387	L388	I389	W390	F391	R392	V393	L394	K395	S396	D397	V398	M399	V400	V401	V402	N403	K404	L405	H406	K407	Y408	S409	L410	V411	E412	K413	Q414	P415	R416	E417	S418	T419	P481	I420	S421	I422	P423	S424	I425	Y426	L427	E428	L429	K430	V431	K432	L433	E434	N435	A436	Y437	A438	H440	R441	D504	S505	T506
V444	D445	H446	Y447	M448	L449	P450	K451	T452	F453	D454	S455	D456	L457	L458	T459	P460	P461	Y462	L463	D464	F467	Y468	G471	G472	H473	H474	L475	K476	N477	L478	E479	H480	P481	I482	R483	M484	T485	L486	F487	R488	M489	V490	F491	L492	D493	F494	R495	F496	E498	Q499	R502	H503	D504	S505	T506				
A507	N508	N509	A510	S511	G512	S513	T514	L515	N516	T517	L518	Q519	W520	L521	K522	F523	Y524	K525	F526	Y527	D530	Y535	E536	R537	L538	V539	N540	A541	I542	L543	D544	F545	L546	P547	K548	I549	E550	E551	N552	L553	I554	C555	S556	K557	Y558	T559	D560	L561	L562	R563	I564	A565	C621	L622	L625	A568	E569	D570	
E571	A572	L573	F574	E575	E576	A577	H578	K579	Q580	V581	T582	L583	F584	D585	D586	E587	V588	N589	F590	T591	N592	H593	G594	R595	F596	H597	Q598	H599	R600	Q601	L602	L603	N604	L605	G606	D607	N608	E609	G610	H611	H612	Y615	L616	H617	N618	P619	F620	G621	L622	L625	A568	E569	D570						
T633	D634	V635	S636	L637	E638	G639	E640	D641	T642	V643	L644	L645	R646	D647	E648	S649	D650	S651	S652	D653	L654	L655	R656	M657	A658	V659	F660	N661	G662	Q663	K664	H665	L666	H670	C671	N672	G673	S674	V675	K676	S679	N681	C682	ASP	CYS	PRO	PRO	GLY	ARG	ARG	HIS	GLY	GLY	SER	GLY	GLN			
GLN	LEU	VAL	N699	S700	V701	K702	R703	R704	F705	L706	G707	S708	V709	A710	N711	L712	K713	T714	V715	A716	F717	L718	V719	W720	E721	K722	A723	G724	L725	PRO	GLU	ALA	ASN	W730	Q731	L732	H733	W734	L737	N738	G739	D740	V741	S742	L743	L744	N745	W746	D747	E748	Q749	D750	Q751	SER	GLY	GLN			
H757	V758	F759	V760	L761	K762	T763	H764	Q765	S766	G767	L768	R769	C770	F771	V772	Q773	V774	L775	K776	F777	V778	W779	V780	W781	C782	T783	S784	M785	G786	T787	L788	T789	W790	W791	D792	L793	T794	N795	G796	S797	S798	N799	T800	L801	E802	L803	H804	V805	F806	N807	W808	D809	C810	D811	T812	P813	L814	A815	L816
D817	V818	F819	D820	E821	R822	S823	K824	T825	L826	T827	V828	L829	R830	L831	Y834	S835	V836	R837	R838	S839	L839	H840	F841	L842	P843	G844	L845	S846	V847	S848	L849	Q850	S851	E852	A853	V854	GLN	LEU	PRO	GLU	G859	L920	C921	G922	F923	L924	K925	G926	Q927	V928	V929	H930	V931	H932	T933	L934	R935	S936	V937
T878	S879	E880	G881	L882	T883	H884	Y885	D886	L887	K888	L889	S890	D891	P892	H893	L894	D895	S896	V897	V898	S899	E900	H901	I902	E903	C904	V905	D906	I907	Y908	E909	L910	F911	D912	P913	V914	Y915	K916	Y917	I918	V919	L920	C921	G922	F923	L924	K925	G926	Q927	V928	V929	H930	V931	H932	T933	L934	R935	S936	V937
S938	Q939	S940	N941	S942	H943	Q944	Y945	R946	E947	L948	A949	W950	V951	H952	S953	A954	D955	E956	I957	S958	V959	M960	T961	K962	A963	C964	L965	E966	P967	Y970	L971	R972	S973	L974	M975	Y976	M977	I978	R979	E980	R981	G982	Q983	L984	L985	A986	V987	D988	S989	K990	E991	R992	I993	H994	L995	I996	K997	P998	

A999	D1059	S1119	Q1179	F1241	VAL
I1000	Y1060	D1120	I1180	S1242	ASP
S1001	L1061	H1121	C1181	P1243	GLY
R1002	K1062	G1122	E1182	C1244	VAL
I1003	V1063	G1123	E1183	K1245	THR
S1004	Q1064	C1124	E1184	L1246	TYR
E1005	S1065	H1125	I1185	L1247	HIS
W1006	P1066	L1126	A1186	L1248	LEU
S1007	N1067	D1127	Q1187	L1249	GLN
T1008	I1068	T1128	Q1188	C1250	LEU
I1009	L1069	A1129	A1189	C1251	PRO
T1010	V1070	N1130	K1190	A1252	VAL
P1011	A1071	P1131	K1191	E1253	ASN
H1013	S1072	S1132	I1192	Q1254	ARG
A1014	A1073	A1133	Y1193	L1255	GLY
A1015	H1074	F1134	L1194	C1256	THR
S1016	S1075	K1135	V1195	F1257	PRO
M1017	Q1077	P1137	T1197	W1258	LEU
C1018	K1078	K1138	D1198	T1261	ASP
K1019	T1079	D1139	G1200	M1263	GLU
I1020	V1080	S1140	I1201	R1264	VAL
M1021	I1081	E1141	M1202	ASN	ASN
A1022	F1082	E1142	I1203	GLN	GLN
I1023	Q1083	I1143	A1204	LEU	LEU
S1024	L1084	I1144	M1205	ARG	GLU
A1025	E1085	V1145	G1206	GLY	LEU
F1026	K1086	F1146	E1207	ASN	ASN
N1027	I1087	F1147	F1208	LYS	VAL
D1028	D1088	L1148	E1209	ARG	ARG
E1029	P1089	L1149	M1209	ARG	THR
Q1030	L1090	K1150	G1210	ARG	ASP
I1031	Q1091	M1151	T1211	ARG	GLY
F1032	P1092	S1152	L1212	ARG	PRO
V1033	N1093	L1153	E1213	HIS	LEU
G1034	D1094	L1154	L1214	LYS	MET
Y1035	W1095	F1155	F1215	GLN	GLN
W1036	W1096	L1156	N1219	HIS	ASP
D1037	P1097	A1157	R1220	VAL	THR
G1038	L1098	E1158	K1221	THR	ASP
V1039	M1099	E1159	V1222	GLN	ALA
I1040	M1100	N1160	Q1223	ASP	HIS
I1041	D1101	M1161	L1224	ALA	ASP
D1042	V1102	I1162	I1225	VAL	VAL
V1043	S1103	I1163	Y1226	ASP	PHE
I1044	T1104	D1164	S1227	ALA	TYR
H1045	K1105	V1165	I1228	ILE	ASN
T1046	Y1106	F1166	E1229	ALA	ILE
T1047	A1107	R1167	V1231	ALA	ASP
A1048	S1108	L1168	H1232	ASP	ILE
L1049	L1109	I1169	E1233	ASP	VAL
P1050	Q1110	S1171	H1234	C1235	
Q1051	E1111	C1172	I1236	I1237	
Q1052	G1112	M1173	Q1174	Q1238	
F1053	Y1113	L1175	L1239	L1240	
I1054	I1114	R1176			
E1055	I1115	Y1177			
E1056	I1116	E1178			
P1057	L1117				
I1058	F1118				

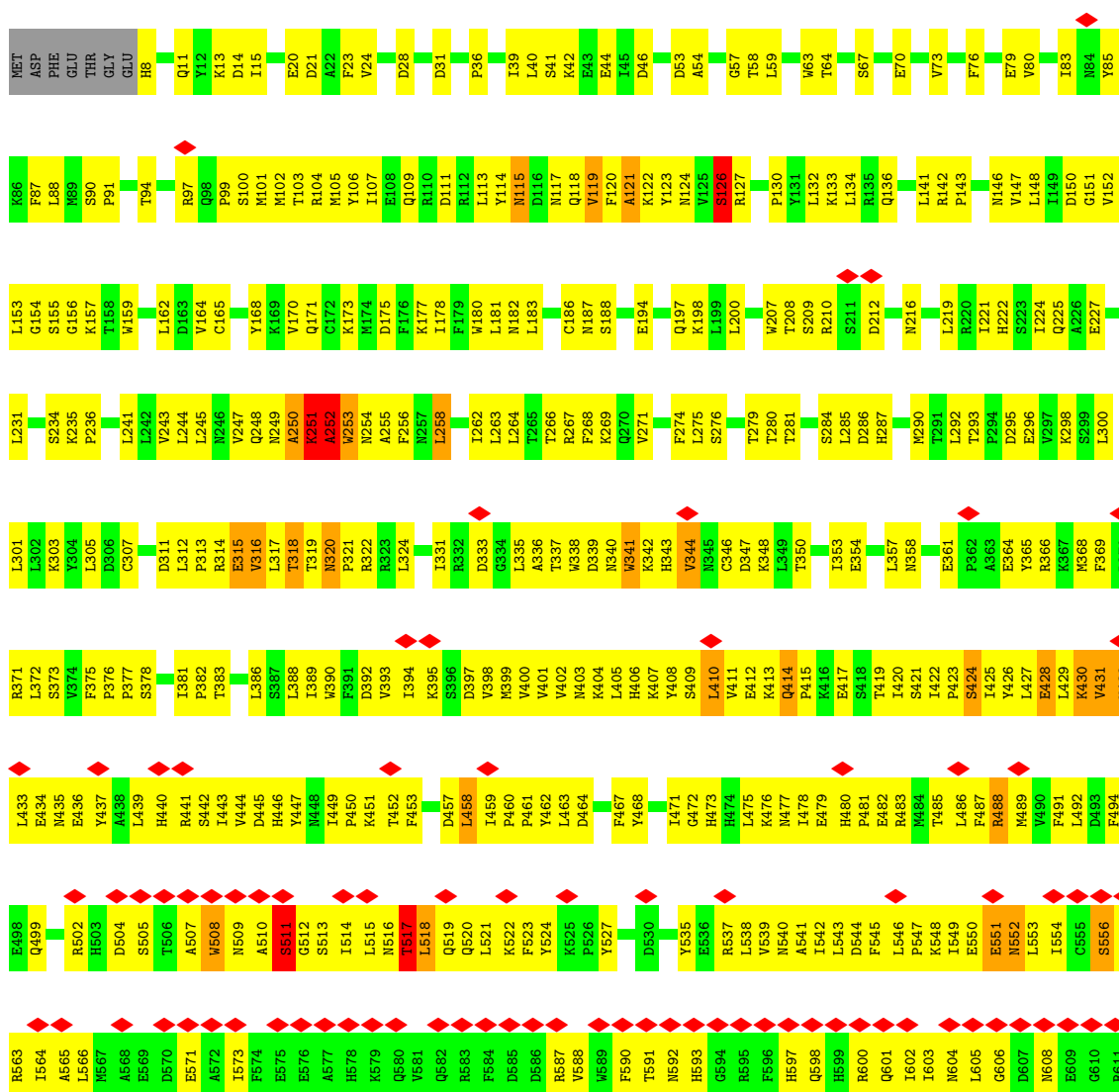
• Molecule 1: Apaf-1 related killer DARK



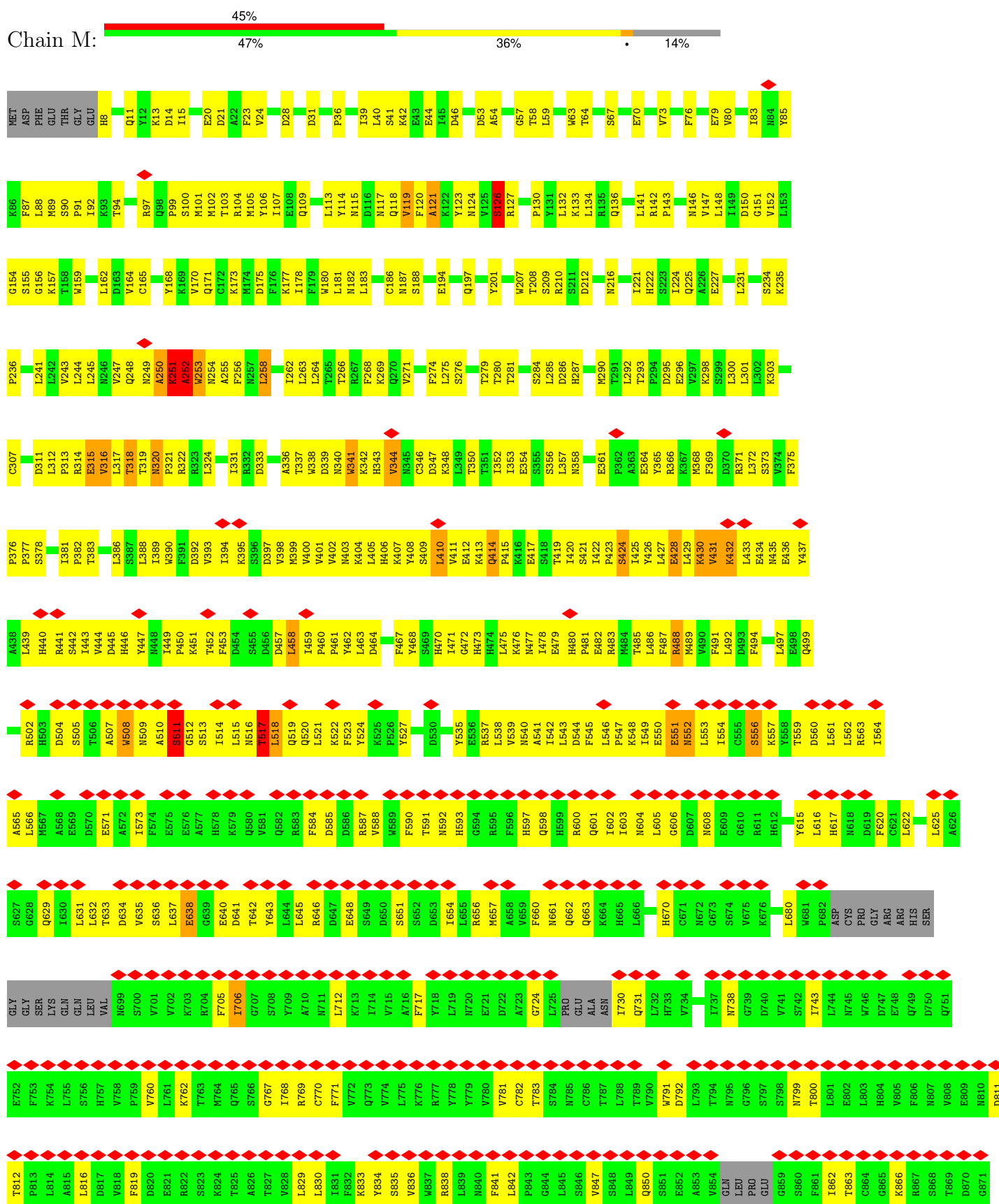
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ASP	F87	S155	P236	D311
PHE	L88	G156	L241	L312
GLU	M89	K157	L242	P313
THR	S90	T158	V243	R314
GLY	P91	W159	L244	E315
GLU	I92	L162	L245	V316
H8	K93	D163	N246	T317
Q11	T94	C165	N247	T318
Y12	Q95	Y168	N249	T319
K13	R97	K169	A250	N320
D14	Q98	V170	K251	P321
I15	P99	M101	A252	R322
E20	M102	T103	W253	R323
D21	T104	K173	N254	L324
A22	R104	W174	A255	S325
F23	M105	D175	F256	E329
V24	Y106	F176	N257	S330
D28	I107	K177	L258	I331
Q109	E108	I178	T262	R332
D31	L113	W180	L263	D333
P36	Y114	L181	L264	A336
I39	D116	N182	T265	T337
L40	N117	K183	R266	W338
S41	Q118	G186	F267	D339
K42	V119	N187	K268	N340
E43	A120	S188	Q270	W341
E44	K122	E194	F274	K342
L45	Y123	Q197	L275	H343
D46	N124	K198	S276	N344
D53	V125	L199	T279	W345
A54	R127	L200	T280	C346
G57	P130	W207	T281	D347
T58	L59	T208	S284	L349
L59	K133	S209	L285	T350
W63	L134	R210	H286	I353
T64	Q135	S211	H287	E354
S67	Q136	D212	M290	L357
E70	L141	N216	T291	N358
V73	P143	I221	L292	E361
F76	K145	H222	P293	P362
E79	N146	S223	P294	A363
V80	V147	I224	D295	E364
I83	L148	Q225	E296	Y365
N84	I149	A226	V297	R366
Y85	D150	E227	K298	K367
	G151	L231	S299	M368
	V152	S234	L300	F369
	L153		L301	D370
			K303	R371
				L372
				S373

L1109	Q1110	E1111	G1112	Q1113	Y1114	I1115	I1116	P1117	L1118	S1119	D1120	H1121	G1122	V1123	C1124	H1125	L1126	D1127	I1128	A1129	N1130	P1131	S1132	A1133	F1134	V1135	K1136	P1137	K1138	D1139	S1140	E1141	I1142	V1143	T1144	V1145	G1146	F1147	L1148	L1149	K1150	N1151	S1152	L1153	L1154	F1155	L1156	P1157	L1158	E1159	N1160	N1161	I1162	I1163	D1164	K1165	F1166	R1167		
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V928	V929	H930	V931	H932	T933	L934	R935	S936	V937	S938	Y939	S940	H941	S942	H943	Q944	H945	R946	E947	T948	A949	V950	V951	H952	S953	A954	D955	E956	Y957	S958	V959	N960	T961	R962	A963	C964	L965	E966	P967	Y970	L971	R972	S973	L974	H975	D976	H977	T978	R979	E980	R981	T982	Q983	L984	L985	A986	V987	D988		
R807	V808	E809	H810	D811	T812	P813	L814	A815	L816	D817	V818	F819	D820	E821	R822	S823	K824	T825	A826	T827	R828	V829	L830	R831	V832	S833	V834	S835	V836	H837	R838	L839	H840	F841	L842	P843	G844	L845	S846	V847	S848	L849	Q850	S851	E852	A853	V854	G1855	L856	C857	S858	R859	S860	F861	T862	T863	C864	C865	K866	F867
S868	T869	D870	G871	R872	H873	L874	L875	L876	G877	T878	S879	E880	G881	L882	T883	V884	V885	D886	L887	R888	T889	S890	D891	P892	H893	L894	R895	S896	Y897	V898	S899	N900	H901	I902	E903	C904	V905	D906	I907	Y908	E909	L910	F911	D912	P913	V914	Y915	K916	L917	I918	V919	L920	C921	G922	A923	K924	G925	K926	Q927	
W746	D747	E748	Q749	D750	Q751	E752	F753	K754	L755	S756	H757	V758	P759	V760	L761	R762	T763	M764	Q765	S766	G767	I768	R769	C770	F771	V772	Q773	W774	L775	K776	V777	V778	V779	V780	V781	C782	T783	S784	N785	C786	T787	L788	Y791	D792	G793	L794	N795	G796	S797	S798	N799	T800	L801	E802	L803	H804	V805	F806		
L625	A626	G627	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	L655	R656	M657	A658	V659	F660	N661	Q662	Q663	K664	H665	L666	I667	H670	C671	N672	G673	S674	V675	K676	L677	W678	S679	L680	W681	P682	ASP	CYS			
L562	R563	I564	A565	L566	M567	A568	E569	D570	E571	A572	I573	F574	E575	A577	H578	K579	Q580	V581	Q582	R583	F584	D585	D586	R587	V588	M589	F590	T591	N592	H593	Q594	R595	F596	H597	Q598	H599	R600	I601	I602	I603	N604	L605	G606	D607	N608	E609	G610	R611	H612	Y615	L616	H617	N618	D619	F620	C621	L622			
L497	E498	Q499	R502	H503	D504	S505	T506	A507	W508	N509	A510	S511	G512	S513	I514	L515	N516	T517	L518	Q519	Q520	L521	K522	F523	Y524	K525	P526	Y527	D530	Y535	E536	R537	L538	V539	N540	A541	I542	L543	L546	P547	K548	I549	E550	E551	N552	L553	I554	C555	S556	K557	Y558	T559	D560	L561						
E436	Y437	A438	L439	H440	R441	S442	I443	V444	D445	H446	Y447	M448	I449	P450	K451	T452	F453	D454	S455	D456	L457	A458	I459	P460	M461	Y462	L463	D464	F467	Y468	S469	H470	I471	G472	H473	H474	L475	K476	N477	E478	E479	H480	P481	E482	R483	M484	T485	L486	F487	R488	K489	V490	F491	L492	D493	F494	R495	F496		
V374	F375	P376	P377	S378	I381	P382	T383	L386	S387	L388	I389	W390	F391	D392	V393	I394	K395	S396	D397	V398	M399	V400	V401	M402	M403	K404	L405	H406	K407	Y408	S409	L410	V411	E412	K413	Q414	P415	K416	E417	S418	E419	I420	S421	I422	P423	S424	I425	Y426	L427	E428	L429	K430	V431	K432	L433	E434	M435			

- Molecule 1: Apaf-1 related killer DARK



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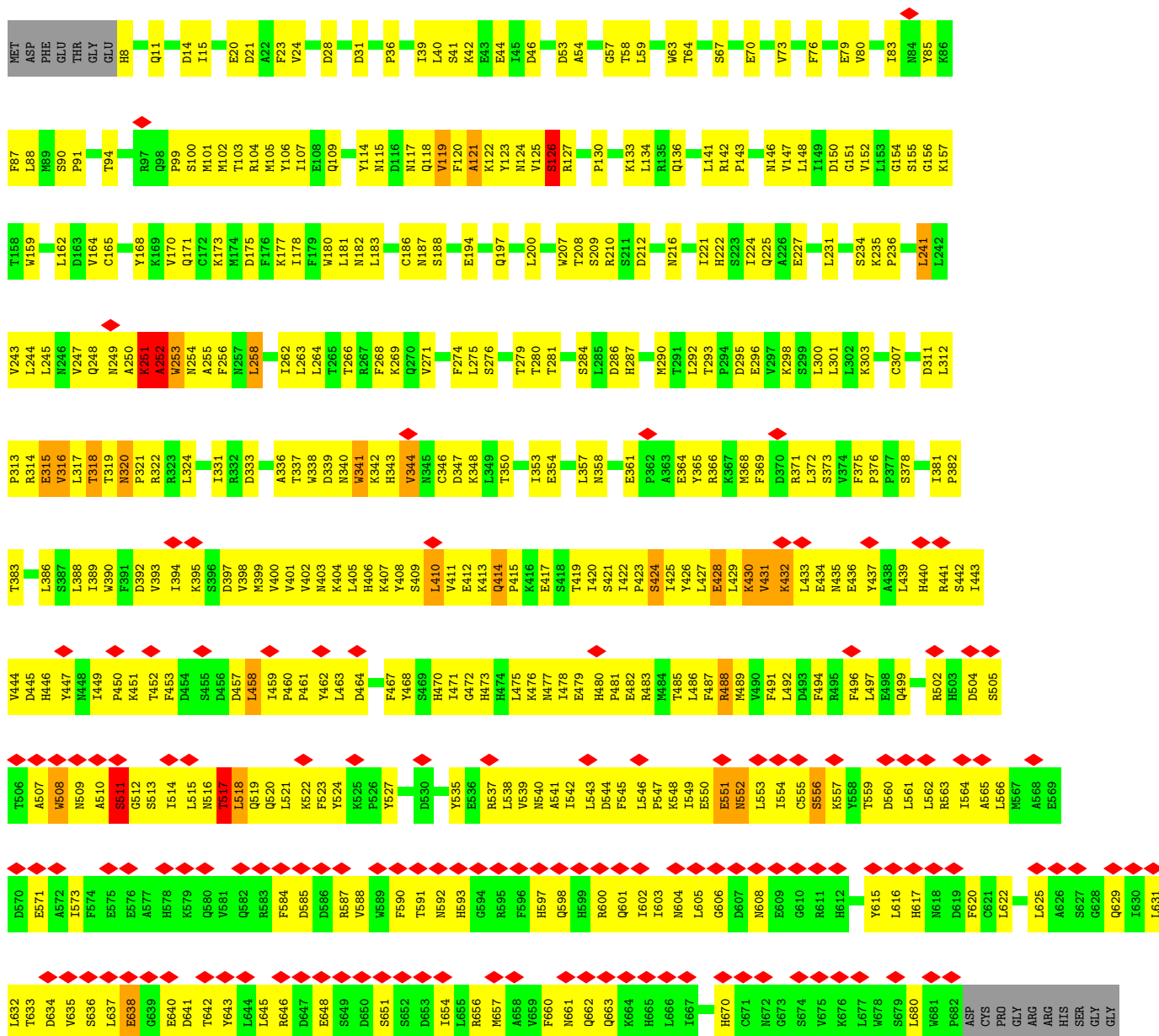


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H943	S1004	I883	S823	T763	W702	G639	A577	S513	P450	W390	T319	A250
Q944	E1005	W884	K824	W764	K703	E640	H578	I514	K451	F391	P321	K251
N945	W1006	Y885	T825	Q765	R704	D641	K579	M516	T452	V393	R322	W253
R946	S1007	D886	A826	S766	F705	T642	Q580	L515	D454	I394	H323	N254
E947	T1008	L887	T827	Y643	I706	Y643	V681	T517	P454	K395	L324	A255
I948	I1009	K888	W828	L644	G707	L644	Q582	L518	S455	S396	I331	F256
A949	T1010	L889	L829	L645	S708	L645	R583	Q520	D456	D397	R332	W257
W950	P1011	S890	L830	R646	W709	R646	F584	Q520	L458	V398	D333	L258
V951	T1012	D891	C770	D647	A710	D647	D585	L521	I459	W400	A336	I262
H952	H1013	P892	F771	E648	W711	E648	D586	K522	P460	V401	T337	L263
S953	A1014	K833	W772	S649	K713	S649	V588	F523	F461	V402	T337	L264
A954	L894	Y834	Q773	D650	W714	D650	V588	Y524	V461	M403	D339	T265
E955	S1016	R895	L775	S651	I714	S651	V588	K525	V462	K404	N340	T266
D956	W1017	W836	L776	S652	W715	S652	V588	F526	D464	L405	N340	R267
E956	E1018	H837	K777	D653	A716	D653	F590	Y527	D464	H406	W341	F268
I957	K1018	W837	W777	I654	F717	I654	T591	D530	F467	K407	H343	K342
W958	K1019	R838	Y778	L655	H593	L655	N592	Y535	Y468	Y408	V344	Q270
S958	I1020	L839	Y718	R656	G594	R656	H593	E536	H470	S409	N345	V271
V959	E1021	H840	W719	M657	R596	M657	G594	R537	I471	V411	C346	F274
M960	M1022	H901	L719	N720	R596	N720	R596	L538	G472	L410	D347	L275
A1021	A1021	I902	W781	A658	F596	A658	F596	V539	H473	K413	K348	S276
K962	I1023	E903	C782	W659	E721	W659	H597	N540	H474	Q414	L349	
S1024	S1024	C904	T783	F660	D722	F660	Q598	A541	L475	P415	T350	
C964	A1025	V905	S784	N661	A723	N661	H599	I542	E479	K416		
L965	F1026	D906	Q662	Q663	G724	Q662	R600	L543	L478	E417		
E966	N1027	W847	Q663	K664	L725	K664	Q601	D544	E479	T419		
P967	D1028	S848	L786	H665	GLU	H665	Q601	L546	H480	I420		
	E1029	L849	W788	L666	ASN	L666	I602	P547	P481	N358		
Y970	Q1030	Q850	V790	H670	I730	H670	L604	K548	E482	E361		
L971	I1031	S851	W791	C671	Q731	C671	L605	E550	R484	P362		
R972	F1032	E852	D791	N672	L732	N672	G606	B551	T485	A363		
S973	V1033	P913	D792	G673	L732	G673	D607	L552	L486	E364		
L974	G1034	W914	L793	S674	W734	S674	N608	L553	F487	Y365		
Y1035	Y1035	Y915	T794	K674	V734	K674	E609	M489	M489	R366		
V1036	V1036	K916	W795	S674		S674	E609	C555	Y490	K368		
D1037	D1037	L918	G796	V675		V675	G610	S556	F491	F369		
W977	W977	GLU	S797	K676		K676	R611	K557	L492	D370		
T978	T978	P918	S797				G610	Y588	D493	R371		
G1038	G1038	Q859	S798	S679	G739	S679	H612	T559	F494	L433		
V1039	V1039	S860	W799	L680	D740	L680	Y615	D560	R495	L300		
E980	I1040	C921	T800	W681	V741	W681	L616	L561	F496	E436		
R981	I1041	F861	S742	P682	S742	P682	L616	L562	Q499	Y437		
T982	D1042	L862	I743	ASP	I743	ASP	H617	R563	A438	P377		
Q983	V1043	T863	E802	CYS	L744	CYS	M618	R563	L439	S378		
L984	G925	C864	L803	PRO	W745	PRO	D619	I564	H503			
H985	H1044	G865	H804	GLY	N745	GLY	F620	A565	H440	I381		
A986	D1046	K866	V805	ARG	W746	ARG	G621	S505	D504	P382		
V987	T1047	R867	F806	HTS	D747	HTS	L622	M567	S505	T383		
D988	A1048	S868	N807	SER	Q749	SER		A568	V444			
W988	L1049	T869	V808	GLY	W750	GLY		E569	A507			
S989	P1050	D870	Q751	SER	Q751	SER		D570	W508			
Q990	Q1051	H871	E752	LYS	E752	LYS		E571	N509			
E991	Q1051	R872	N810	GLN	F753	GLN		A572				
R992	F1052	L811	D811	GLN	Q629	GLN		I573	AS10			
Q993	T053	Y873	T812	LEU	I630	LEU		F574				
I1054	I1054	L874	P813	VAL	L631	VAL						
E1055	E1055	L875	L814		L632							
E1056	E1056	L876	S756		T633							
P1057	P1057	L877	H757		D634							
K997	K997	G877	P758		V635							
I1058	I1058	T878	W759		S636							
D1059	D1059	S879	V760									
A999	A999	E880										
I1000	I1000											
S1001	S1001											



R1176	I1116	E1056	S1119	F1118	L1117	P1057	I0566	E1055	L1149	D1148	G1206	D1199	D1198	T1197	A1196	V1135	F1134	A1133	P1131	N1130	A1129	I1128	K1188	Q1187	A1186	S1065	V1064	Q1063	K1062	L1061	Y1060	A999	I0558	D1059	I0557	P1057	E1056	R1237	I1236	C1235	H1234	E1233	H1232	V1231	E1230	E1229	I1228	S1227	L1226	I1225	L1224	Q1223	V1222	K1221	R1220	M1219	A1216	F1215	L1214	S1213	E1212	L1212	N1209	E1208	F1207	G1206	K1086	F1026	A1025	L1084	L1083	Q1077	A1076	S1075	L1074	H1073	A1014	S953	H952	V951	W950	R895	L894	S893	R832	K833	Y834	I714	S649	E650	D589	V588	K525	P526	Y527	F467	Y468	S469	H470	I471	G472	H473	L474	K475	K476	L477	N478	E479	H480	P481	E482	R483	M484	L546	E551	N552	D607	G606	L605	N604	I603	P547	L546	T485	R488	O488	E550	S556	R495	F494	L492	F491	V490	M489	V490	E491	L492	D493	L493	N553	E509	G610	C555	S554	N552	E551	E550	R488	O488	F545	D544	L543	E541	N540	V539	L538	R537	E536	Y535	H593	E594	G594	H593	N592	T591	F590	P526	V589	K525	Y524	F523	D586	L712	E648	D647	R646	L645	R583	F584	Q520	P461	Q520	R583	F582	K522	F523	L463	L462	Y462	P461	Q520	P460	I459	L458	D457	N456	Q580	K579	H578	I514	S513	G512	S511	E575	A577	E576	E576	L637	A510	P450	K451	P450	A510	F574	I573	N509	M448	Y447	H446	D445	T506	S505	D504	S442
LVS	GLN	GLN	VAL	M699	S700	V701	V702	K703	R704	F705	I706	G707	S708	R709	A710	N711	L712	K713	I714	A716	F717	Y718	L719	R720	E721	D722	A723	G724	L725	PRD	GLU	ALA	ASN	I730	Q731	H733	V734	I737	N738	G739	D740	V741	S742	I743	L744	N745	M746	D747	Q749	D750	Q751	E752	F753	K754	LVS	GLN	GLN	VAL	M699	S700	V701	V702	K703	R704	F705	I706	G707	S708	R709	A710	N711	L712	E648	D647	R646	L645	R583	F584	Q520	P461	Q520	R583	F582	K522	F523	L463	L462	Y462	P461	Q520	P460	I459	L458	D457	N456	Q580	K579	H578	I514	S513	G512	S511	E575	A577	E576	E576	L637	A510	P450	K451	P450	A510	F574	I573	N509	M448	Y447	H446	D445	T506	S505	D504	LVS																																																																																																					
L755	S756	H757	V758	V759	V760	L761	K762	T763	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	T789	V790	W791	D792	L793	T794	N795	G796	S797	S798	N799	T800	L801	E802	L803	H804	V805	F806	N807	V808	E809	N810	D811	T812	P813	L814	L755	S756	H757	V758	V759	V760	L761	K762	T763	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	T789	V790	W791	D792	L793	T794	N795	G796	S797	S798	N799	T800	L801	E802	L803	H804	V805	F806	N807	V808	E809	N810	D811	T812	P813	L814	L755																																																																																																								
A815	L816	D817	V818	F819	D820	E821	R822	S823	K824	T825	A826	T827	V828	L829	L830	R831	K833	Y834	S835	V836	M837	R838	L839	N840	F841	L842	P843	G844	L845	S846	V847	S848	L849	Q850	S851	E852	A853	V854	GLN	LEU	PRO	GLU	G859	L920	C921	G922	A923	K924	G925	K926	Q927	V928	V929	H930	V931	D932	T933	L934	Y873	L874	A815	L816	D817	V818	F819	D820	E821	R822	S823	K824	T825	A826	T827	V828	L829	L830	R831	K833	Y834	S835	V836	M837	R838	L839	N840	F841	L842	P843	G844	L845	S846	V847	S848	L849	Q850	S851	E852	A853	V854	GLN	LEU	PRO	GLU	G859	L920	C921	G922	A923	K924	G925	K926	Q927	V928	V929	H930	V931	D932	T933	L934	Y873	L874	A815																																																																																																						
R935	S936	V937	S938	G939	S940	H941	S942	H943	Q944	S945	R946	E947	I948	A949	Y950	T951	H952	S953	A954	D955	E956	I957	S958	V959	H960	T961	K962	A963	C964	L965	E966	P967	V970	L971	R972	S973	L974	H975	D976	H977	T978	R979	E980	R981	T982	Q983	L984	L985	A986	V987	D988	S989	K990	E991	R992	I993	H994	L995	R935	S936	V937	S938	G939	S940	H941	S942	H943	Q944	S945	R946	E947	I948	A949	Y950	T951	H952	S953	A954	D955	E956	I957	S958	V959	H960	T961	K962	A963	C964	L965	E966	P967	V970	L971	R972	S973	L974	H975	D976	H977	T978	R979	E980	R981	T982	Q983	L984	L985	A986	V987	D988	S989	K990	E991	R992	I993	H994	L995	R935																																																																																																										
I996	K997	P998	A999	I1000	S1001	R1002	I1003	S1004	E1005	V1006	S1007	T1008	I1009	T1010	P1011	T1012	H1013	A1014	A1015	S1016	N1017	C1018	K1019	I1020	N1021	A1022	I1023	S1024	A1025	F1026	N1027	D1028	E1029	Q1030	I1031	F1032	V1033	G1034	Y1035	V1036	D1037	G1038	V1039	I1040	I1041	D1042	V1043	I1044	H1045	D1046	T1047	A1048	L1049	P1050	Q1051	Q1052	F1053	I1054	E1055	I996	K997	P998	A999	I1000	S1001	R1002	I1003	S1004	E1005	V1006	S1007	T1008	I1009	T1010	P1011	T1012	H1013	A1014	A1015	S1016	N1017	C1018	K1019	I1020	N1021	A1022	I1023	S1024	A1025	F1026	N1027	D1028	E1029	Q1030	I1031	F1032	V1033	G1034	Y1035	V1036	D1037	G1038	V1039	I1040	I1041	D1042	V1043	I1044	H1045	D1046	T1047	A1048	L1049	P1050	Q1051	Q1052	F1053	I1054	E1055	I996																																																																																																								
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	M1096	P1097	L1098	M1099	M1100	D1101	V1102	S1103	T1104	K1105	Y1106	A1107	S1108	L1109	Q1110	E1111	G1112	Q1113	Y1114	I1115	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	M1096	P1097	L1098	M1099	M1100	D1101	V1102	S1103	T1104	K1105	Y1106	A1107	S1108	L1109	Q1110	E1111	G1112	Q1113	Y1114	I1115	E1056																																																																																																								
R1176	Y1177	E1178	Q1179	C1181	E1182	E1183	E1184	I1185	A1186	Q1187	K1188	A1189	K1190	I1191	S1192	L1194	V1195	A1196	T1197	D1198	D1199	G1200	T1201	M1202	L1203	A1204	M1205	G1206	F1207	E1208	L1209	K1210	E1211	L1212	E1213	L1214	F1215	A1216	N1219	K1220	V1222	Q1223	I1225	Y1226	S1227	I1228	E1229	E1230	V1231	H1232	E1233	H1234	C1235	R1237	R1176	Y1177	E1178	Q1179	C1181	E1182	E1183	E1184	I1185	A1186	Q1187	K1188	A1189	K1190	I1191	S1192	L1194	V1195	A1196	T1197	D1198	D1199	G1200	T1201	M1202	L1203	A1204	M1205	G1206	F1207	E1208	L1209	K1210	E1211	L1212	E1213	L1214	F1215	A1216	N1219	K1220	V1222	Q1223	I1225	Y1226	S1227	I1228	E1229	E1230	V1231	H1232	E1233	H1234	C1235	R1237	R1176																																																																																																																		

- Molecule 1: Apaf-1 related killer DARK





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 ⓘ

5.1 Standard geometry ⓘ

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%)	4	26
1	B	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	C	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	D	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	E	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	F	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	G	1224/1440 (85%)	989 (81%)	202 (16%)	33 (3%)	4	26
1	H	1224/1440 (85%)	988 (81%)	204 (17%)	32 (3%)	4	26
1	I	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	J	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	K	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	L	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	M	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	N	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
1	O	1224/1440 (85%)	988 (81%)	203 (17%)	33 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	26
All	All	19584/23040 (85%)	15822 (81%)	3248 (17%)	514 (3%)	6	26

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 ⓘ

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%)	92	95
1	B	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	C	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	D	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	E	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	F	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	G	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	H	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	I	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	J	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	K	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	L	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	M	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	N	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
1	O	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	1138/1315 (86%)	1137 (100%)	1 (0%)	92	95
All	All	18208/21040 (86%)	18192 (100%)	16 (0%)	92	95

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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	A	251	1	28,33,33	2.93	11 (39%)	27,47,47	3.00	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	APK	D	251	1	28,33,33	2.93	11 (39%)	27,47,47	3.00	6 (22%)
1	APK	P	251	1	28,33,33	2.92	11 (39%)	27,47,47	3.00	6 (22%)
1	APK	J	251	1	28,33,33	2.92	11 (39%)	27,47,47	3.00	6 (22%)
1	APK	E	251	1	28,33,33	2.92	11 (39%)	27,47,47	2.99	6 (22%)
1	APK	G	251	1	28,33,33	2.92	11 (39%)	27,47,47	3.00	6 (22%)
1	APK	I	251	1	28,33,33	2.92	11 (39%)	27,47,47	2.99	6 (22%)
1	APK	L	251	1	28,33,33	2.93	11 (39%)	27,47,47	2.99	6 (22%)
1	APK	N	251	1	28,33,33	2.92	11 (39%)	27,47,47	3.00	6 (22%)
1	APK	F	251	1	28,33,33	2.92	11 (39%)	27,47,47	2.99	6 (22%)
1	APK	B	251	1	28,33,33	2.92	11 (39%)	27,47,47	2.99	6 (22%)
1	APK	H	251	1	28,33,33	2.93	11 (39%)	27,47,47	2.99	6 (22%)
1	APK	O	251	1	28,33,33	2.92	11 (39%)	27,47,47	3.00	6 (22%)
1	APK	M	251	1	28,33,33	2.92	11 (39%)	27,47,47	2.99	6 (22%)
1	APK	C	251	1	28,33,33	2.92	11 (39%)	27,47,47	3.00	6 (22%)
1	APK	K	251	1	28,33,33	2.93	11 (39%)	27,47,47	2.99	6 (22%)

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	A	251	1	-	8/15/37/37	0/3/3/3
1	APK	D	251	1	-	8/15/37/37	0/3/3/3
1	APK	P	251	1	-	8/15/37/37	0/3/3/3
1	APK	J	251	1	-	8/15/37/37	0/3/3/3
1	APK	E	251	1	-	8/15/37/37	0/3/3/3
1	APK	G	251	1	-	8/15/37/37	0/3/3/3
1	APK	I	251	1	-	8/15/37/37	0/3/3/3
1	APK	L	251	1	-	8/15/37/37	0/3/3/3
1	APK	N	251	1	-	8/15/37/37	0/3/3/3
1	APK	F	251	1	-	8/15/37/37	0/3/3/3
1	APK	B	251	1	-	8/15/37/37	0/3/3/3
1	APK	H	251	1	-	8/15/37/37	0/3/3/3
1	APK	O	251	1	-	8/15/37/37	0/3/3/3
1	APK	M	251	1	-	8/15/37/37	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	APK	C	251	1	-	8/15/37/37	0/3/3/3
1	APK	K	251	1	-	8/15/37/37	0/3/3/3

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	APK	C2'-C3'	-8.23	1.31	1.53
1	B	251	APK	C2'-C3'	-8.22	1.31	1.53
1	K	251	APK	C2'-C3'	-8.22	1.31	1.53
1	G	251	APK	C2'-C3'	-8.21	1.31	1.53
1	N	251	APK	C2'-C3'	-8.21	1.31	1.53

The worst 5 of 96 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 128 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	B	251	APK	O-C-CA-CB
1	B	251	APK	CG-CD-CE-NZ

There are no ring outliers.

16 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	251	APK	6	0
1	D	251	APK	7	0
1	P	251	APK	6	0
1	J	251	APK	6	0
1	E	251	APK	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	251	APK	6	0
1	I	251	APK	6	0
1	L	251	APK	7	0
1	N	251	APK	6	0
1	F	251	APK	6	0
1	B	251	APK	6	0
1	H	251	APK	6	0
1	O	251	APK	5	0
1	M	251	APK	6	0
1	C	251	APK	7	0
1	K	251	APK	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.37	6 (17%)
2	DTP	A	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.37	6 (17%)
2	DTP	H	1501	-	28,32,32	3.81	10 (35%)	35,50,50	2.37	6 (17%)
2	DTP	J	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.35	5 (14%)
2	DTP	C	1501	-	28,32,32	3.81	10 (35%)	35,50,50	2.37	6 (17%)
2	DTP	M	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.35	5 (14%)
2	DTP	N	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.35	5 (14%)
2	DTP	O	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.35	5 (14%)
2	DTP	P	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.35	5 (14%)
2	DTP	D	1501	-	28,32,32	3.81	10 (35%)	35,50,50	2.37	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DTP	K	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.35	5 (14%)
2	DTP	E	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.37	6 (17%)
2	DTP	G	1501	-	28,32,32	3.81	10 (35%)	35,50,50	2.37	6 (17%)
2	DTP	L	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.35	5 (14%)
2	DTP	F	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.37	6 (17%)
2	DTP	I	1501	-	28,32,32	3.80	10 (35%)	35,50,50	2.35	5 (14%)

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	B	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	A	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	H	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	J	1501	-	-	4/18/34/34	0/3/3/3
2	DTP	C	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	M	1501	-	-	4/18/34/34	0/3/3/3
2	DTP	N	1501	-	-	4/18/34/34	0/3/3/3
2	DTP	O	1501	-	-	4/18/34/34	0/3/3/3
2	DTP	P	1501	-	-	4/18/34/34	0/3/3/3
2	DTP	D	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	K	1501	-	-	4/18/34/34	0/3/3/3
2	DTP	E	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	G	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	L	1501	-	-	4/18/34/34	0/3/3/3
2	DTP	F	1501	-	-	3/18/34/34	0/3/3/3
2	DTP	I	1501	-	-	4/18/34/34	0/3/3/3

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1501	DTP	C2'-C3'	-12.88	1.20	1.52
2	D	1501	DTP	C2'-C3'	-12.88	1.20	1.52
2	M	1501	DTP	C2'-C3'	-12.88	1.20	1.52
2	G	1501	DTP	C2'-C3'	-12.87	1.20	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1501	DTP	C2'-C3'	-12.87	1.20	1.52

The worst 5 of 88 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	120.31
2	B	1501	DTP	C5-C6-N6	8.55	133.33	120.31
2	C	1501	DTP	C5-C6-N6	8.54	133.33	120.31
2	M	1501	DTP	C5-C6-N6	8.54	133.33	120.31
2	D	1501	DTP	C5-C6-N6	8.54	133.32	120.31

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

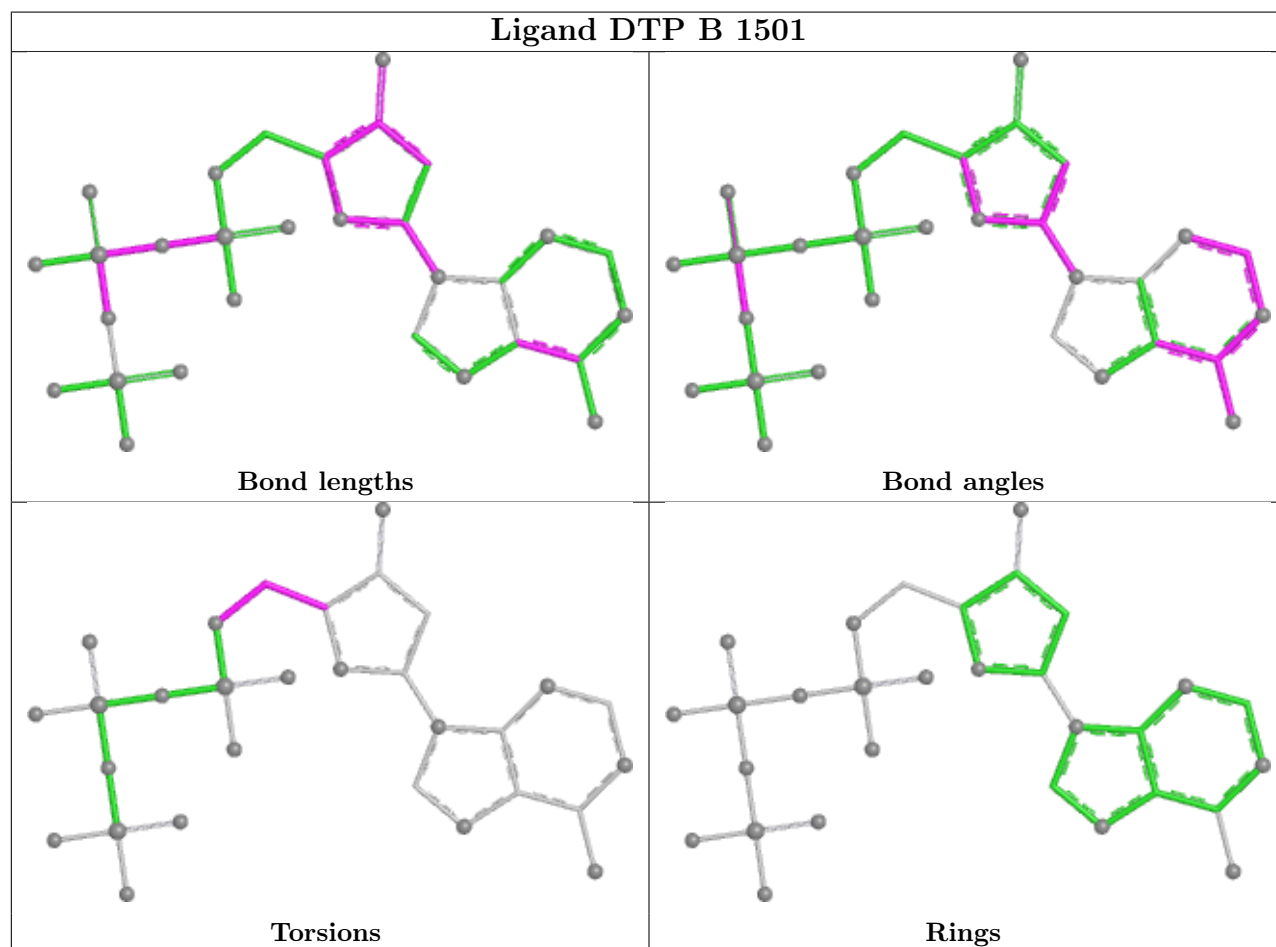
Mol	Chain	Res	Type	Atoms
2	A	1501	DTP	C3'-C4'-C5'-O5'
2	B	1501	DTP	C3'-C4'-C5'-O5'
2	C	1501	DTP	C3'-C4'-C5'-O5'
2	D	1501	DTP	C3'-C4'-C5'-O5'
2	E	1501	DTP	C3'-C4'-C5'-O5'

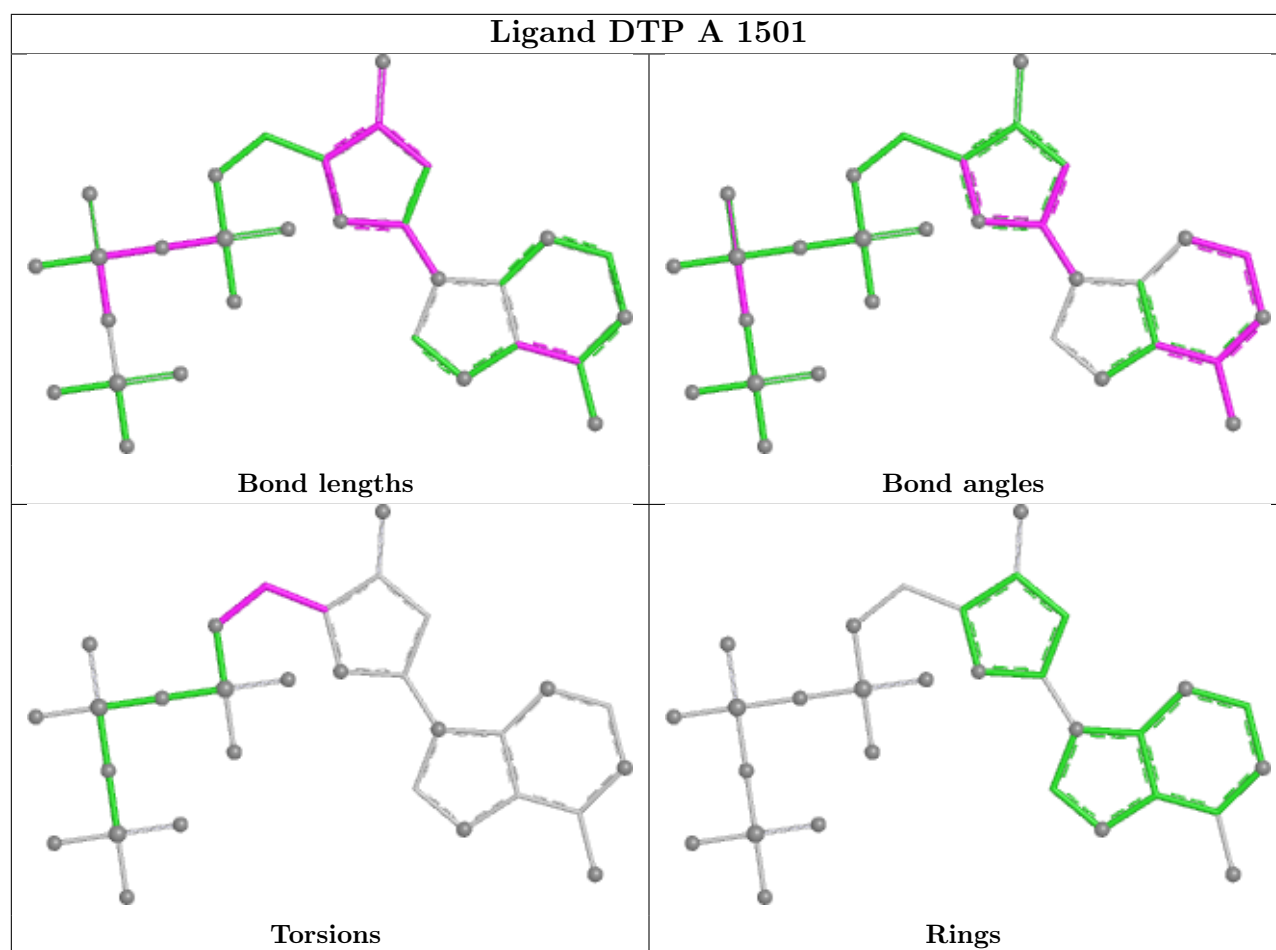
There are no ring outliers.

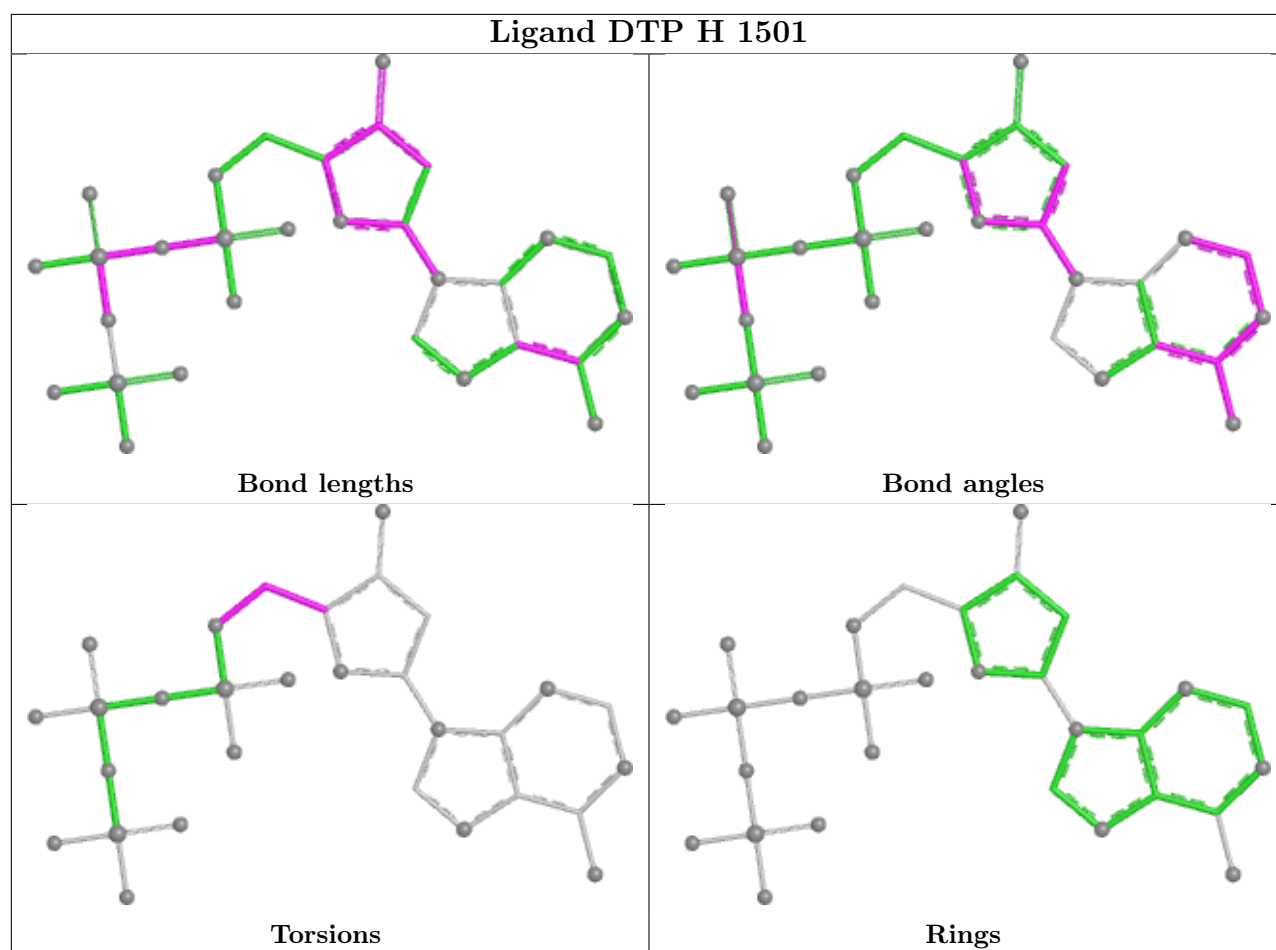
16 monomers are involved in 97 short contacts:

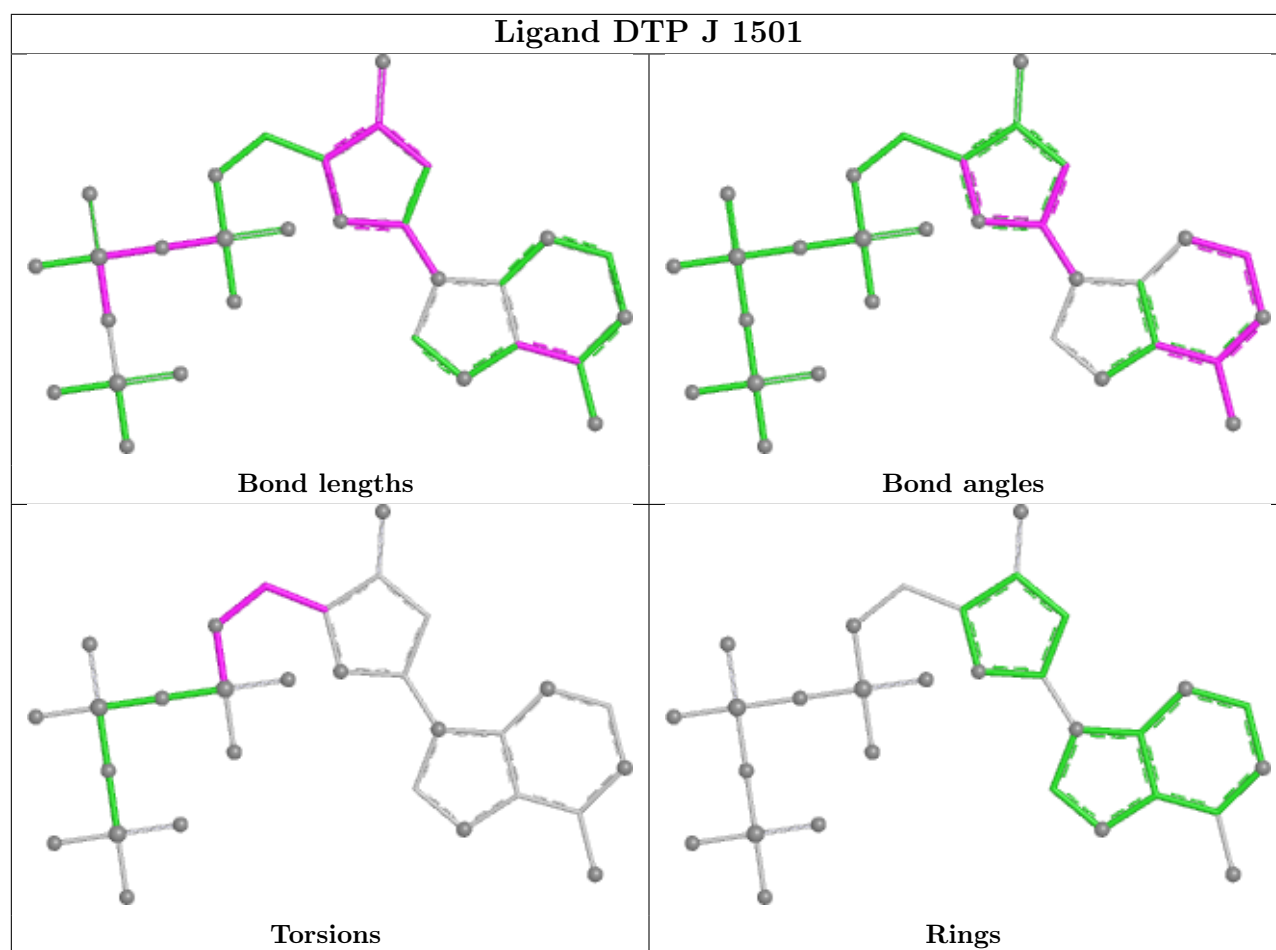
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1501	DTP	7	0
2	A	1501	DTP	6	0
2	H	1501	DTP	6	0
2	J	1501	DTP	6	0
2	C	1501	DTP	6	0
2	M	1501	DTP	6	0
2	N	1501	DTP	6	0
2	O	1501	DTP	6	0
2	P	1501	DTP	6	0
2	D	1501	DTP	6	0
2	K	1501	DTP	6	0
2	E	1501	DTP	6	0
2	G	1501	DTP	6	0
2	L	1501	DTP	6	0
2	F	1501	DTP	6	0
2	I	1501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

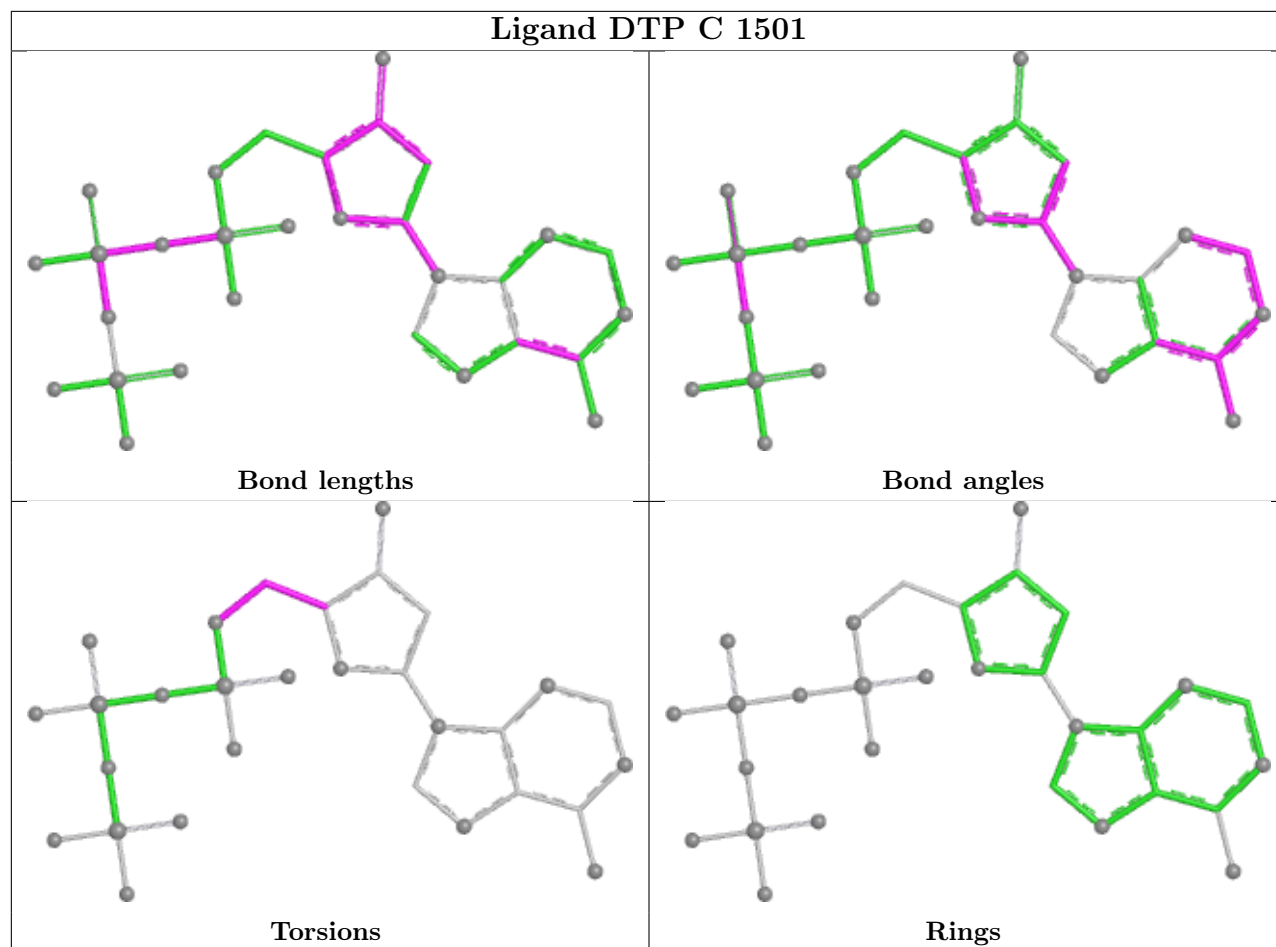
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

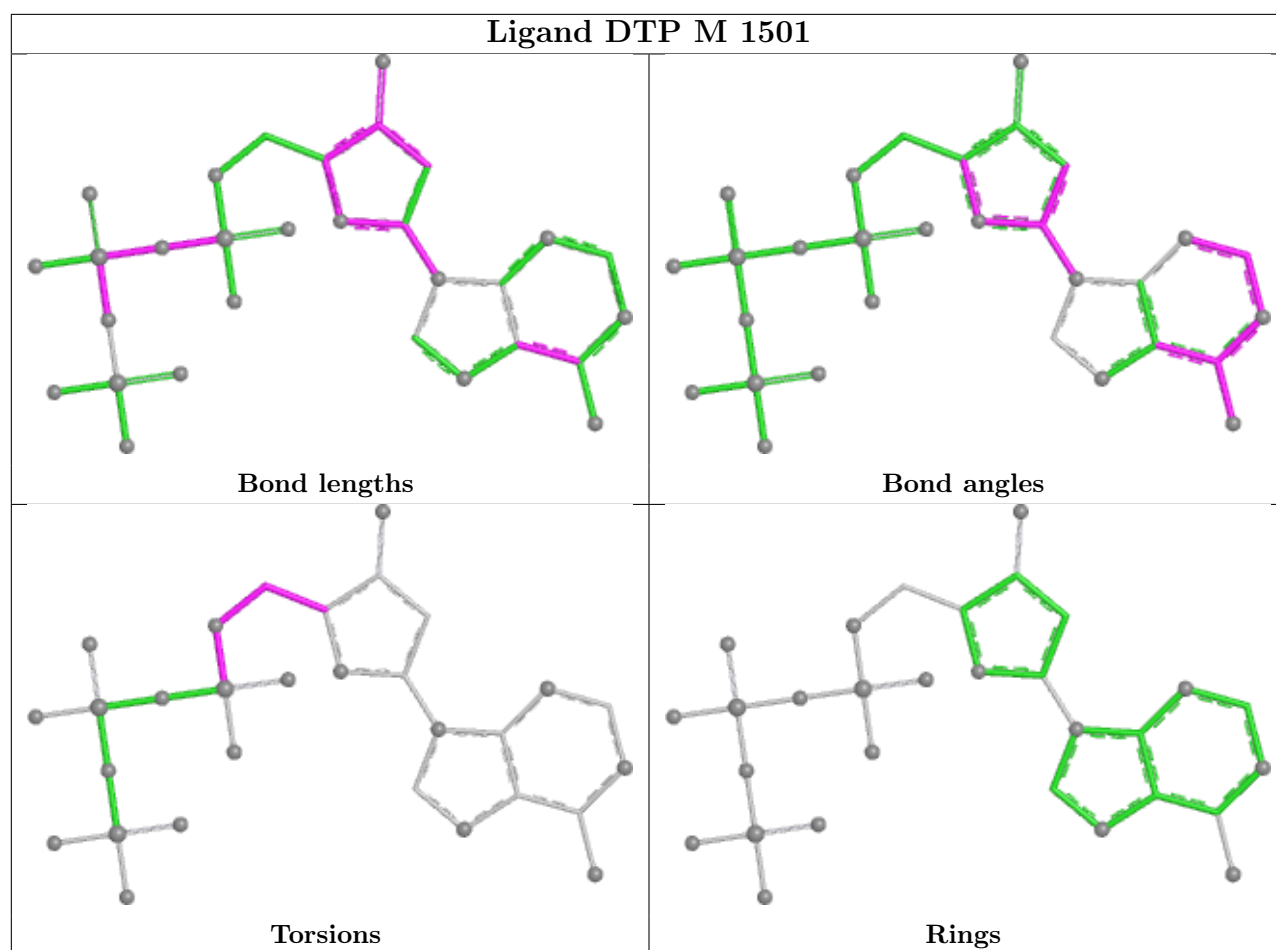


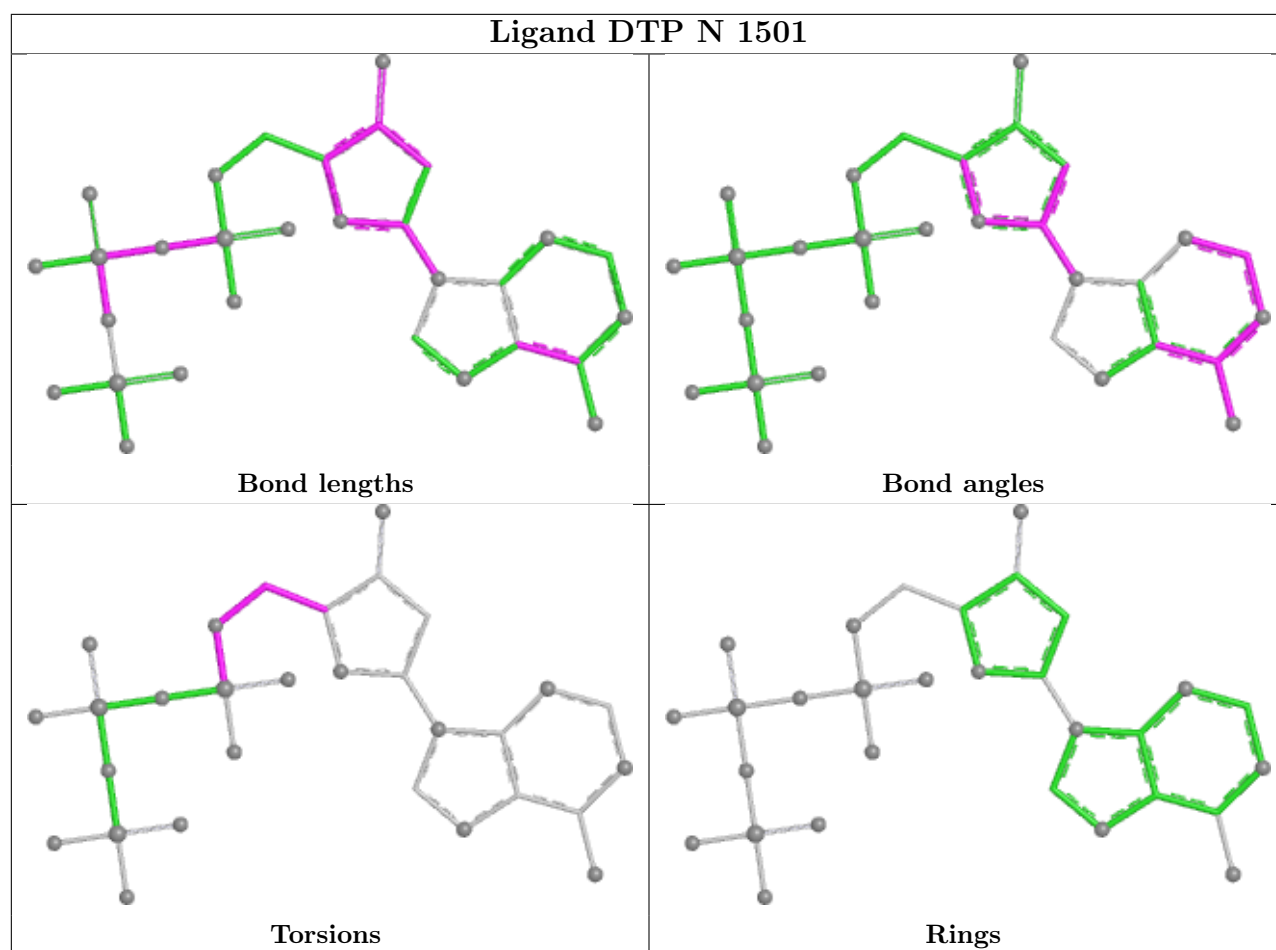


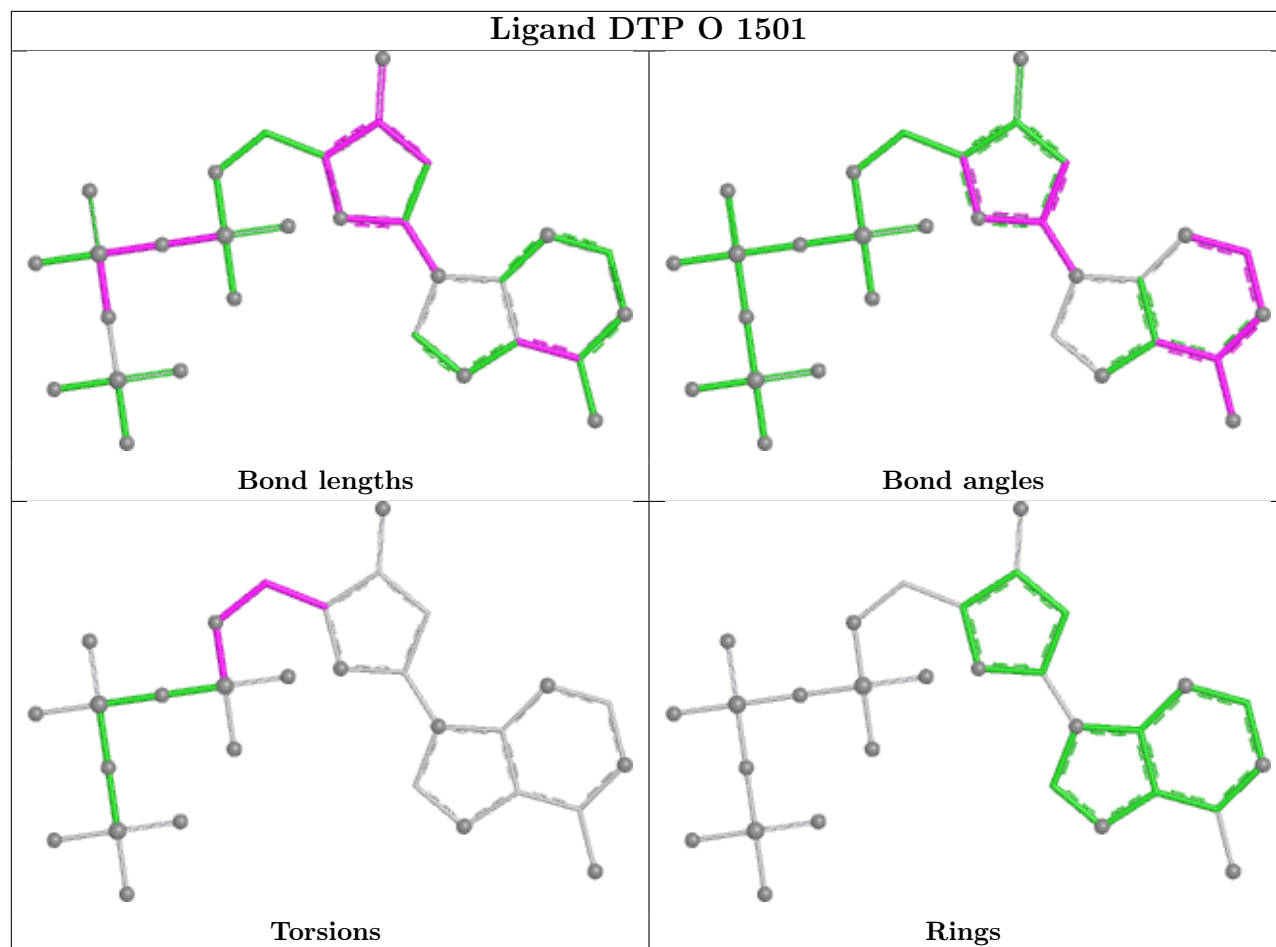


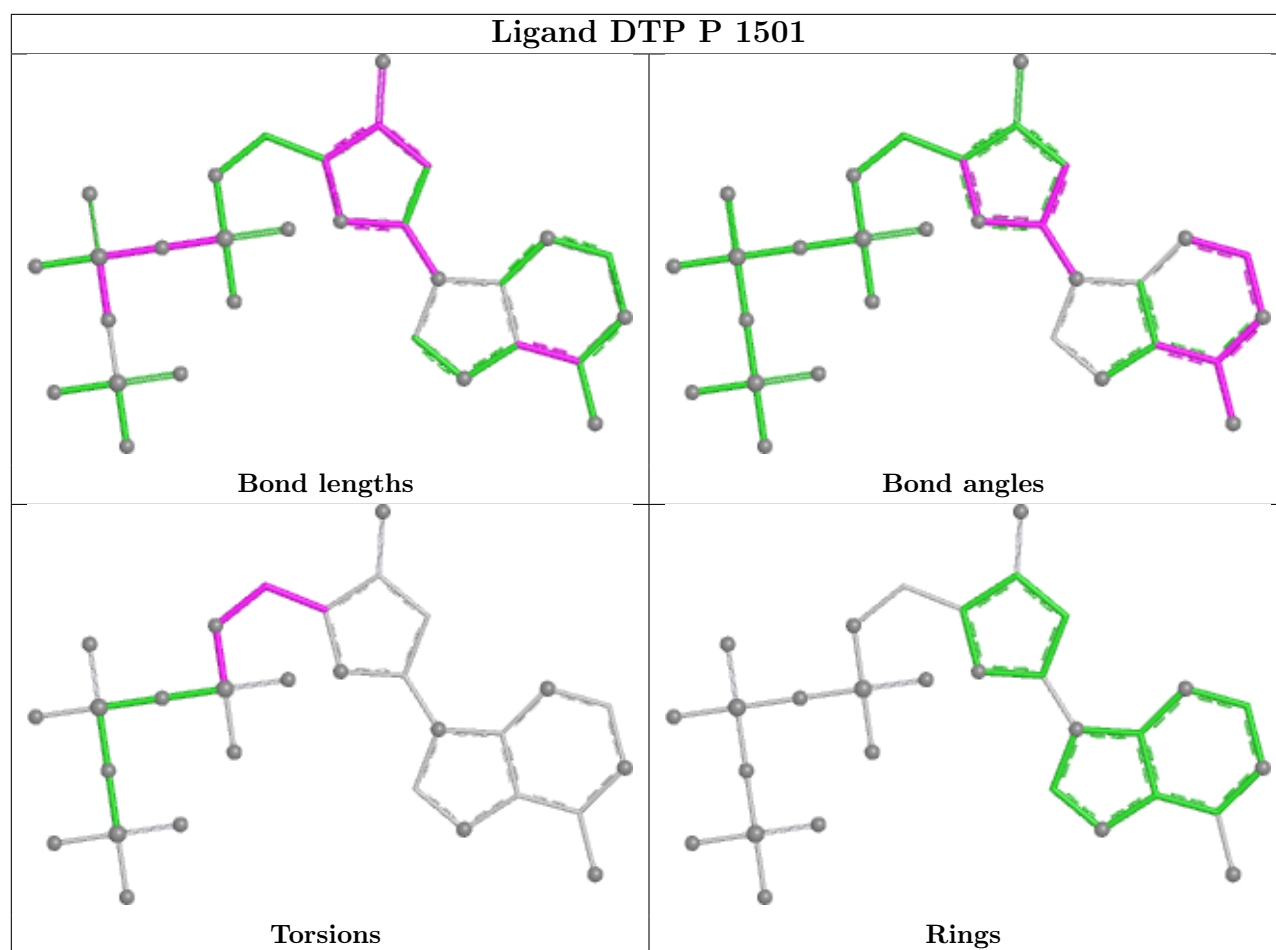


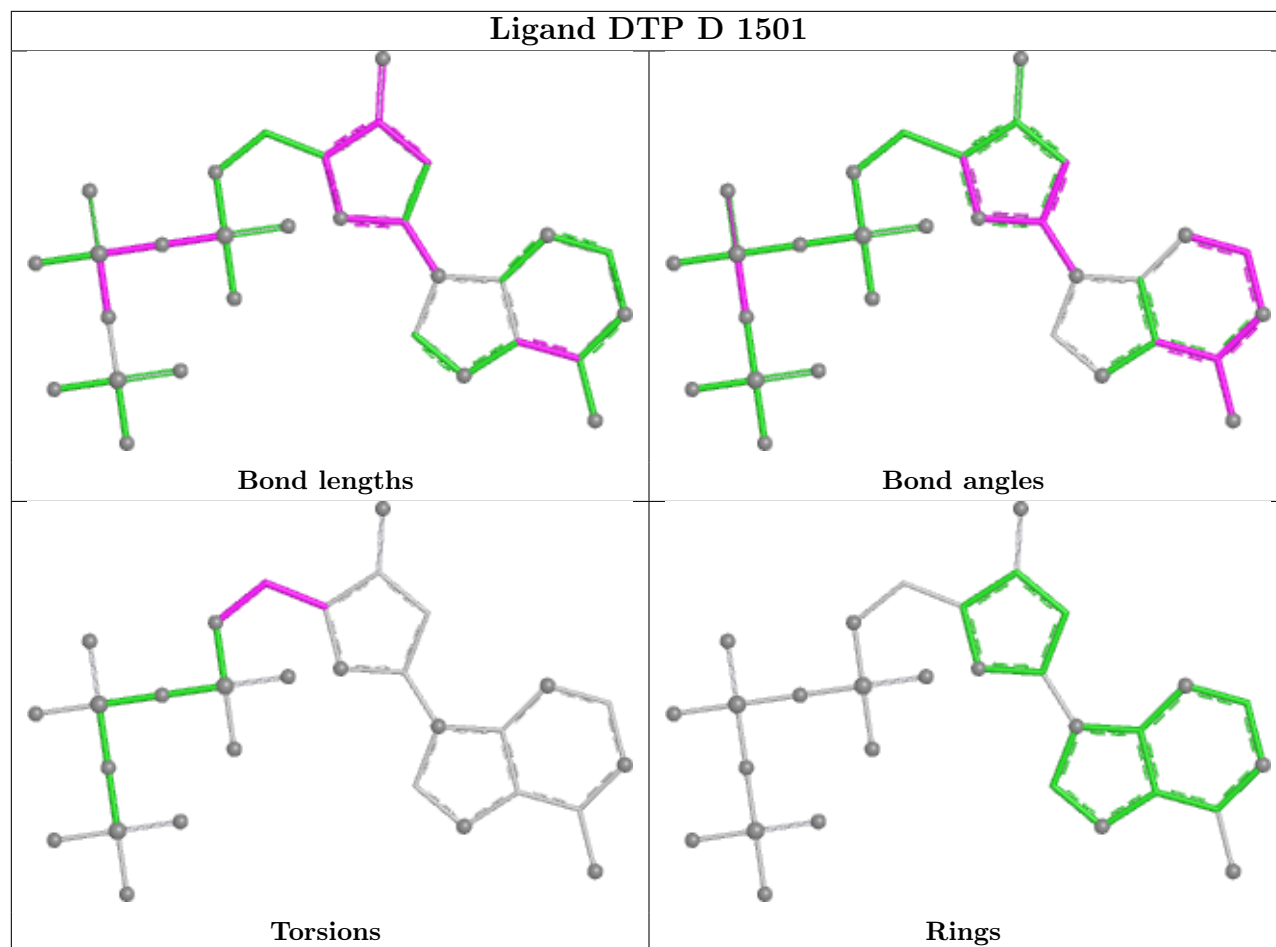


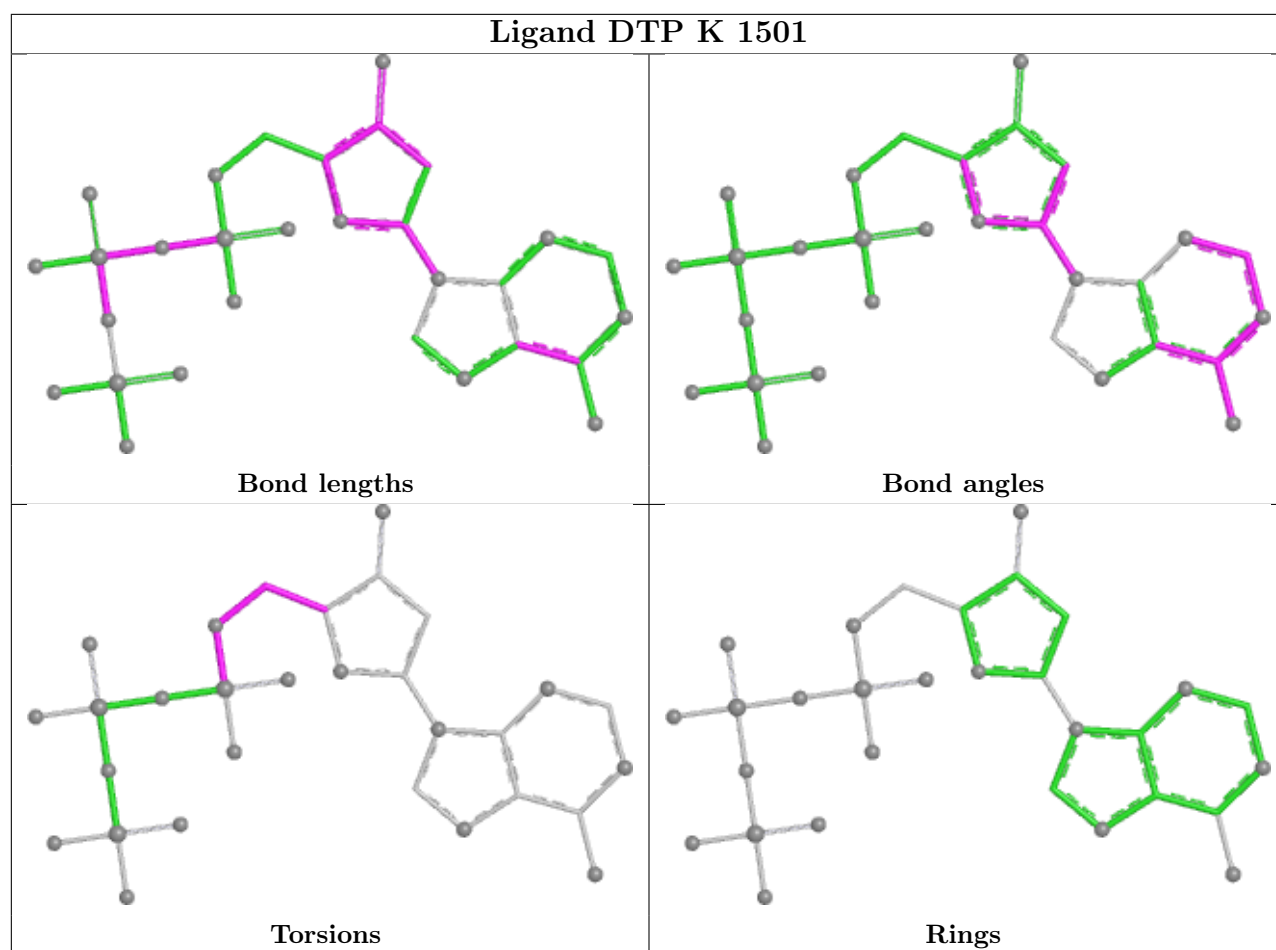


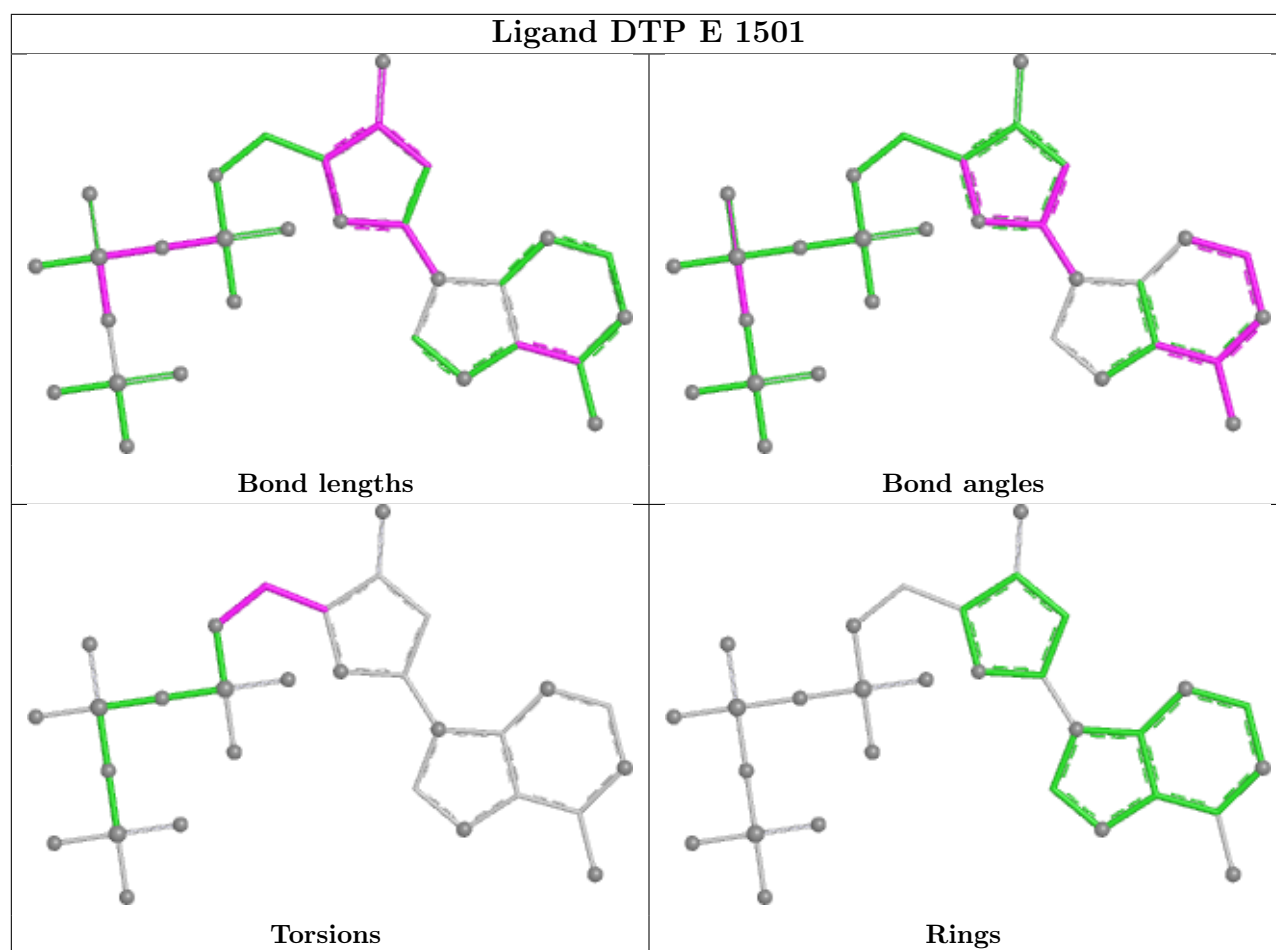


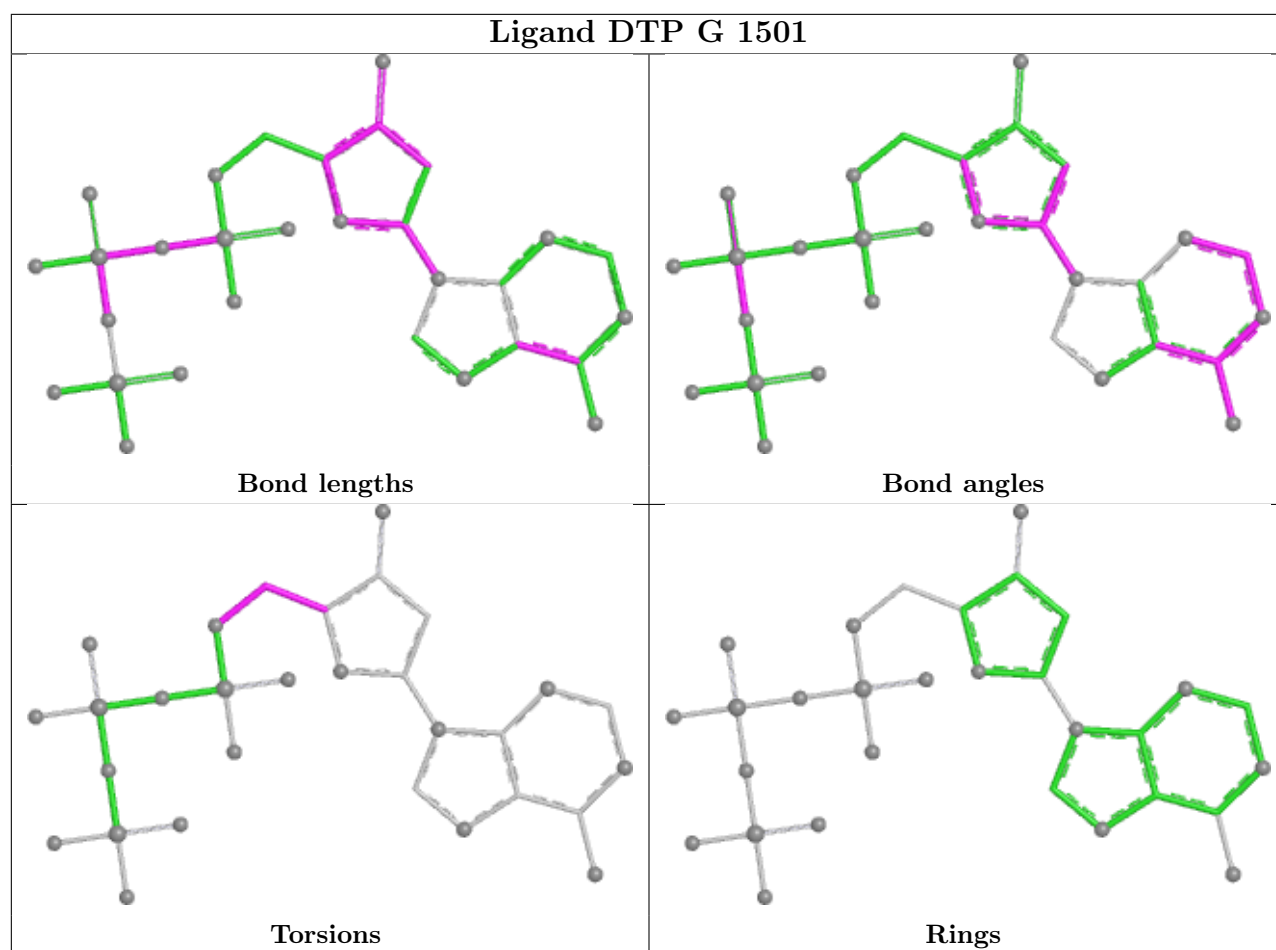


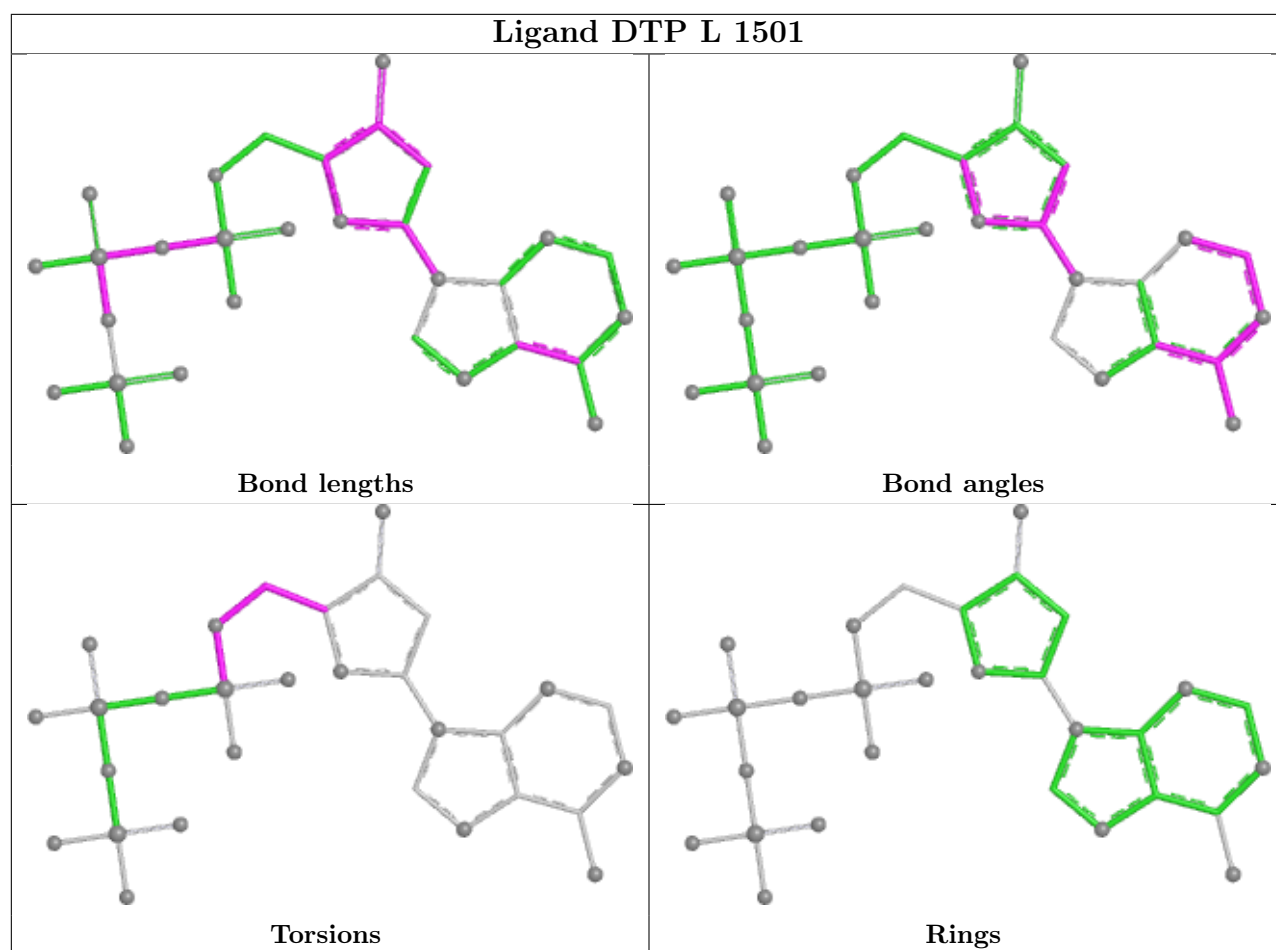


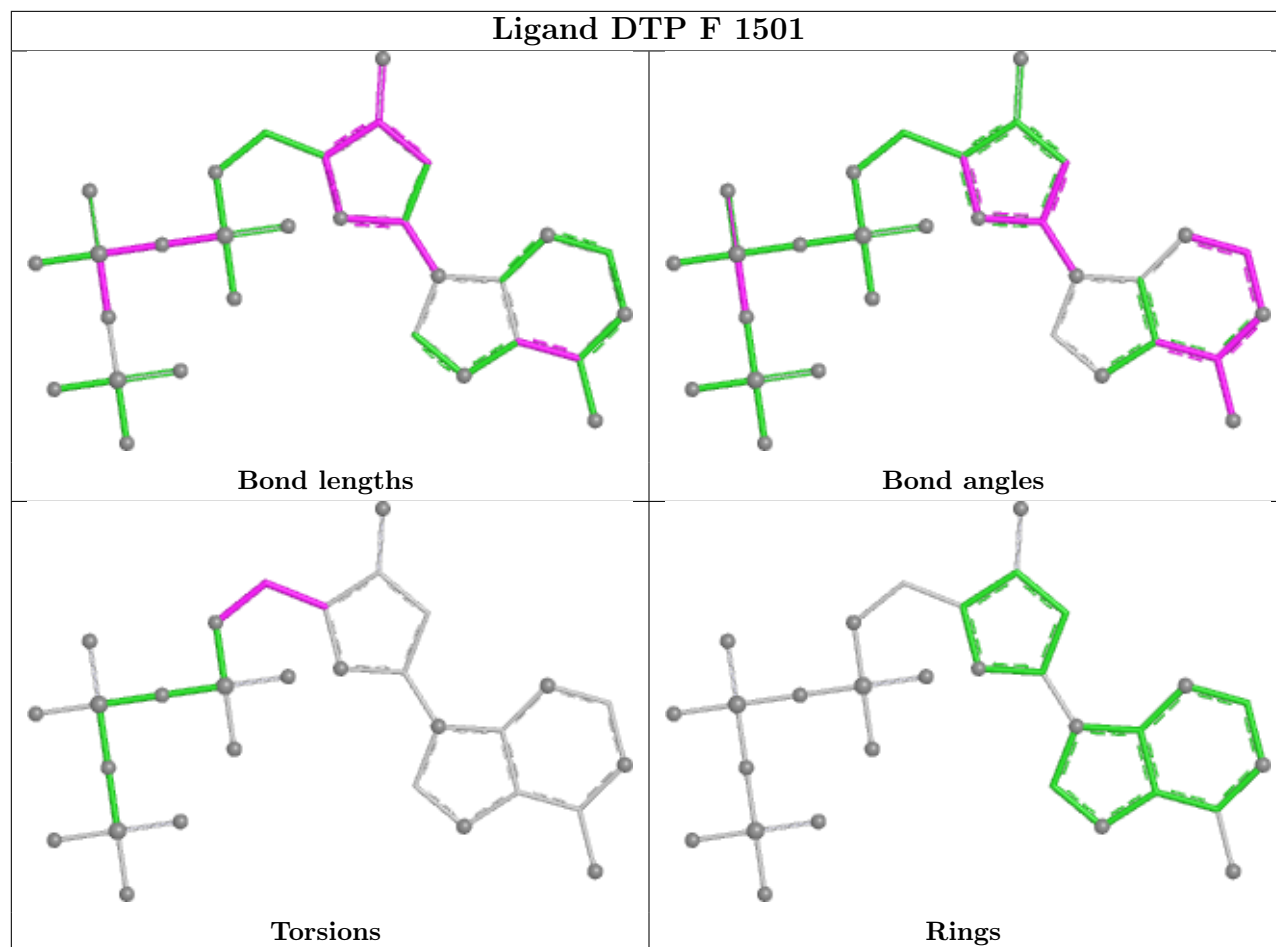


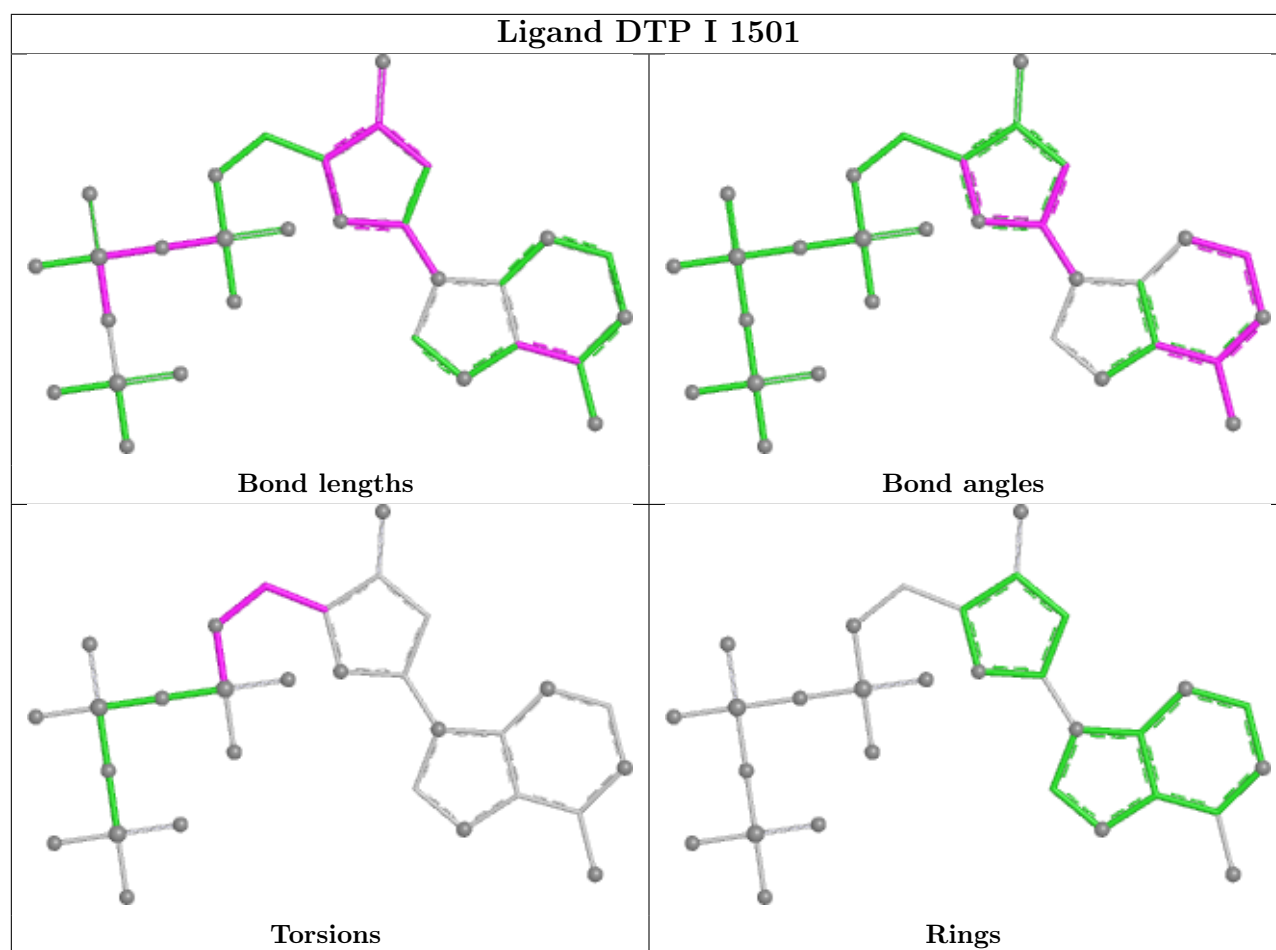












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

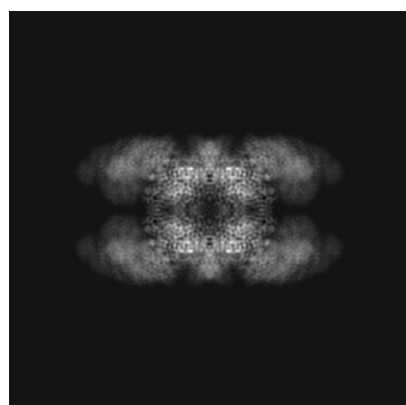
6 Map visualisation [i](#)

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.

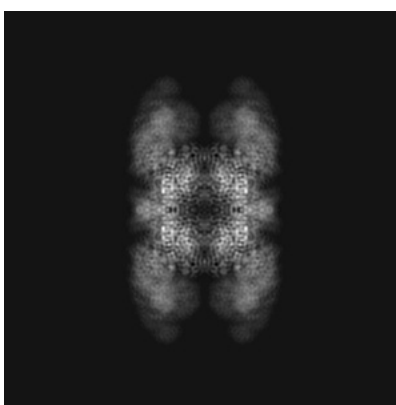
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

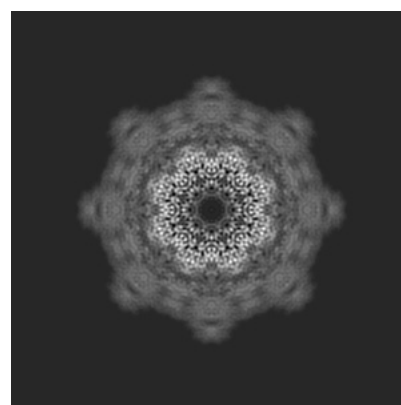
6.1.1 Primary map



X



Y

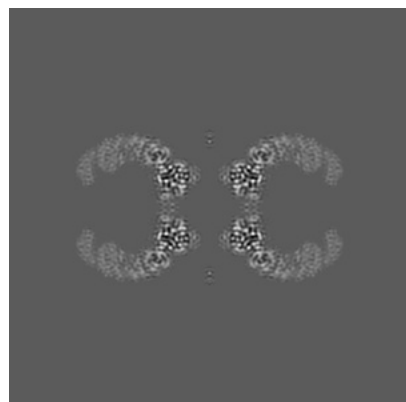


Z

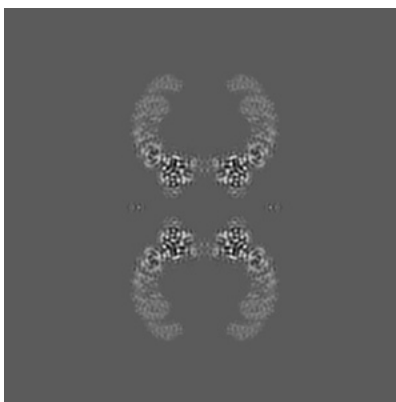
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

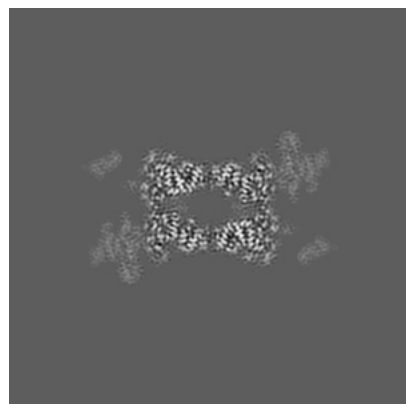


Z Index: 160

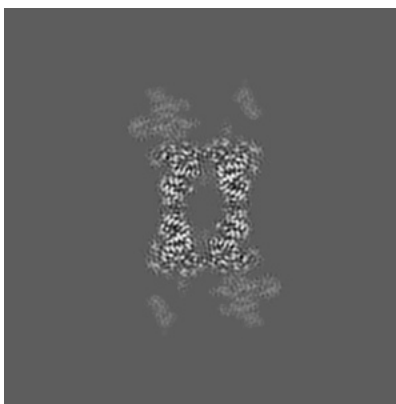
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

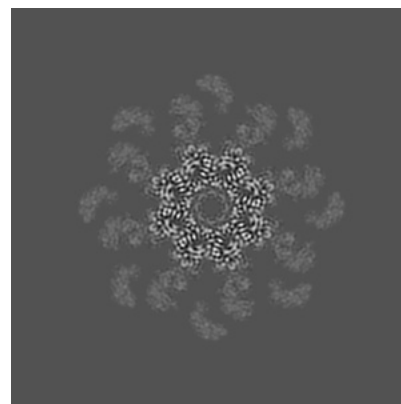
6.3.1 Primary map



X Index: 143



Y Index: 143

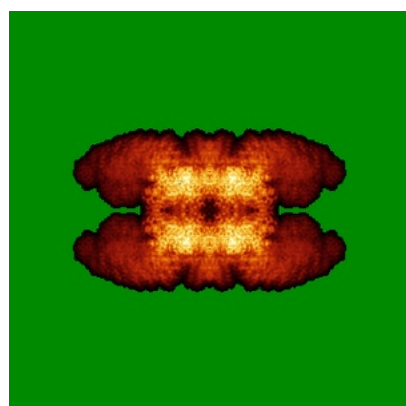


Z Index: 185

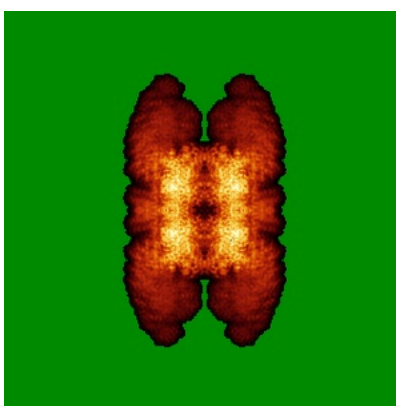
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

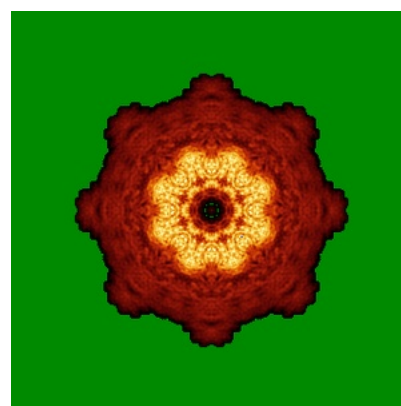
6.4.1 Primary map



X



Y

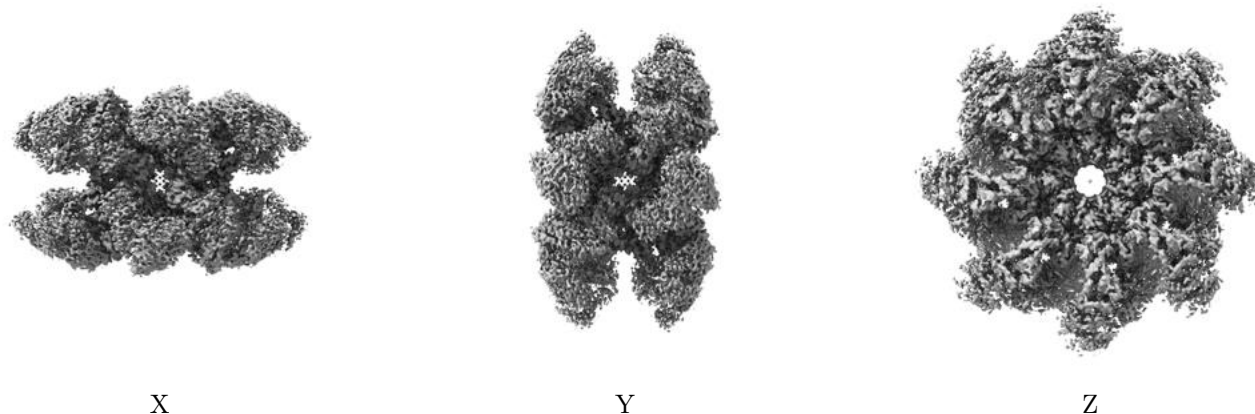


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

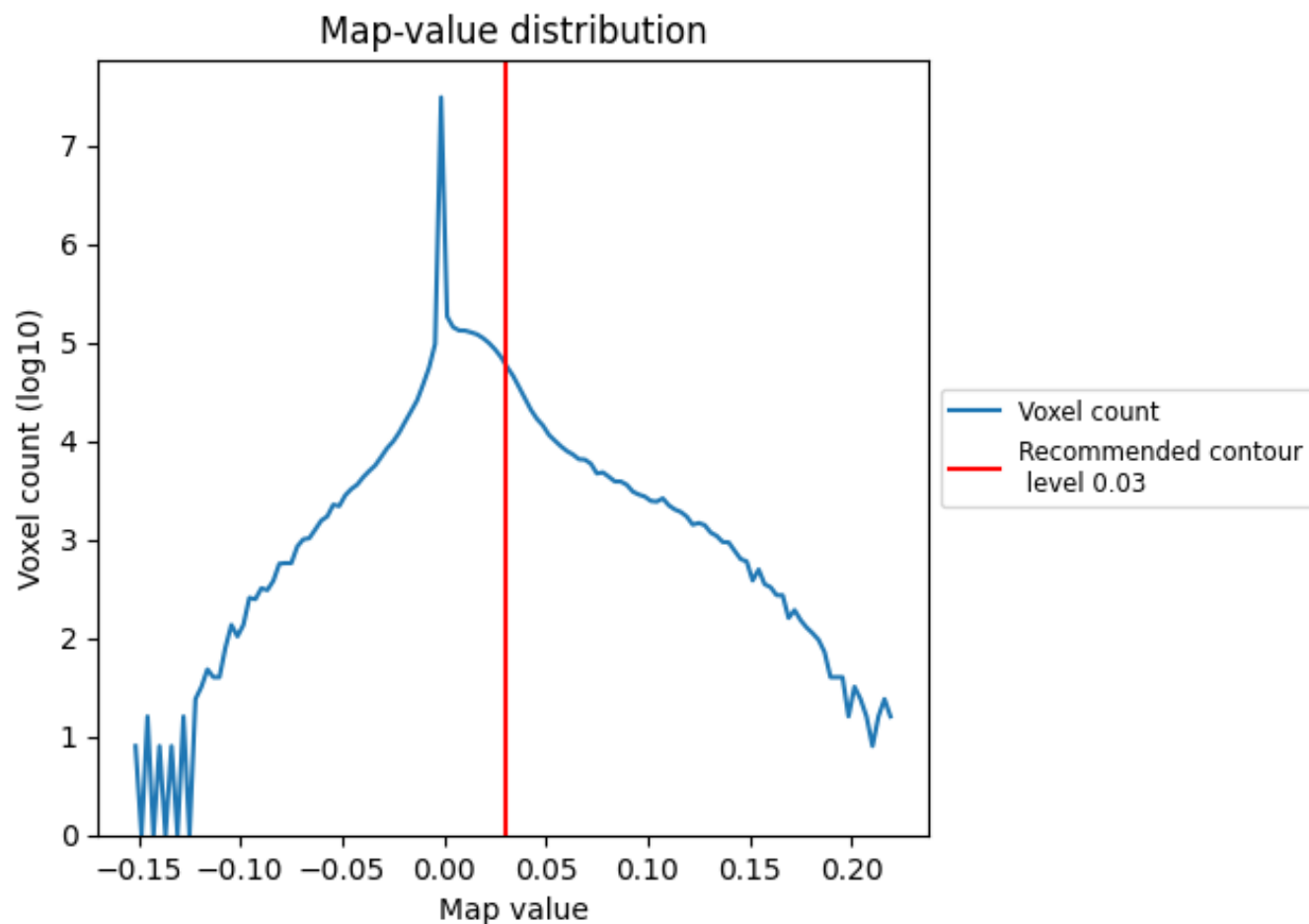
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

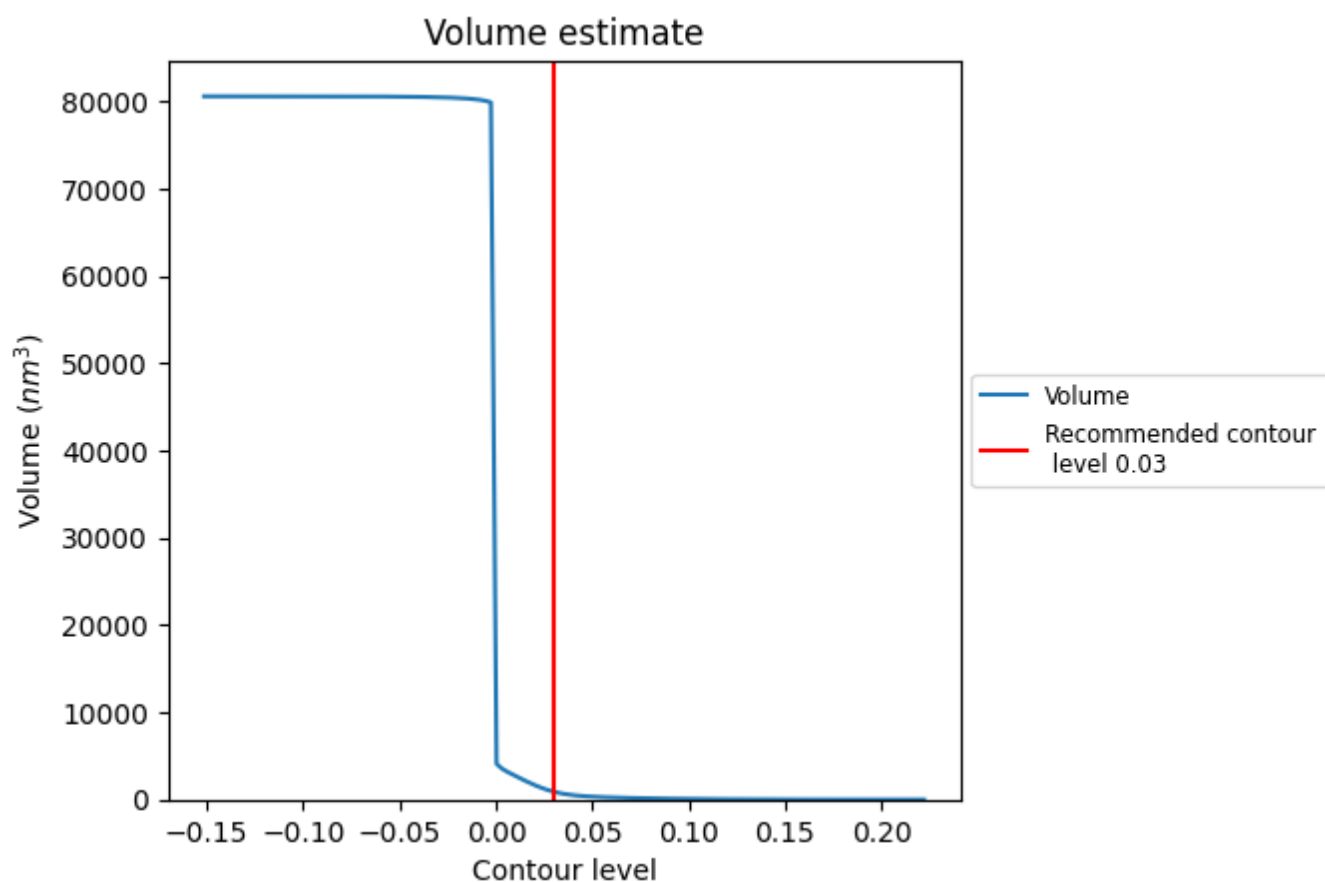
This section contains the results of statistical analysis of the map.

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.

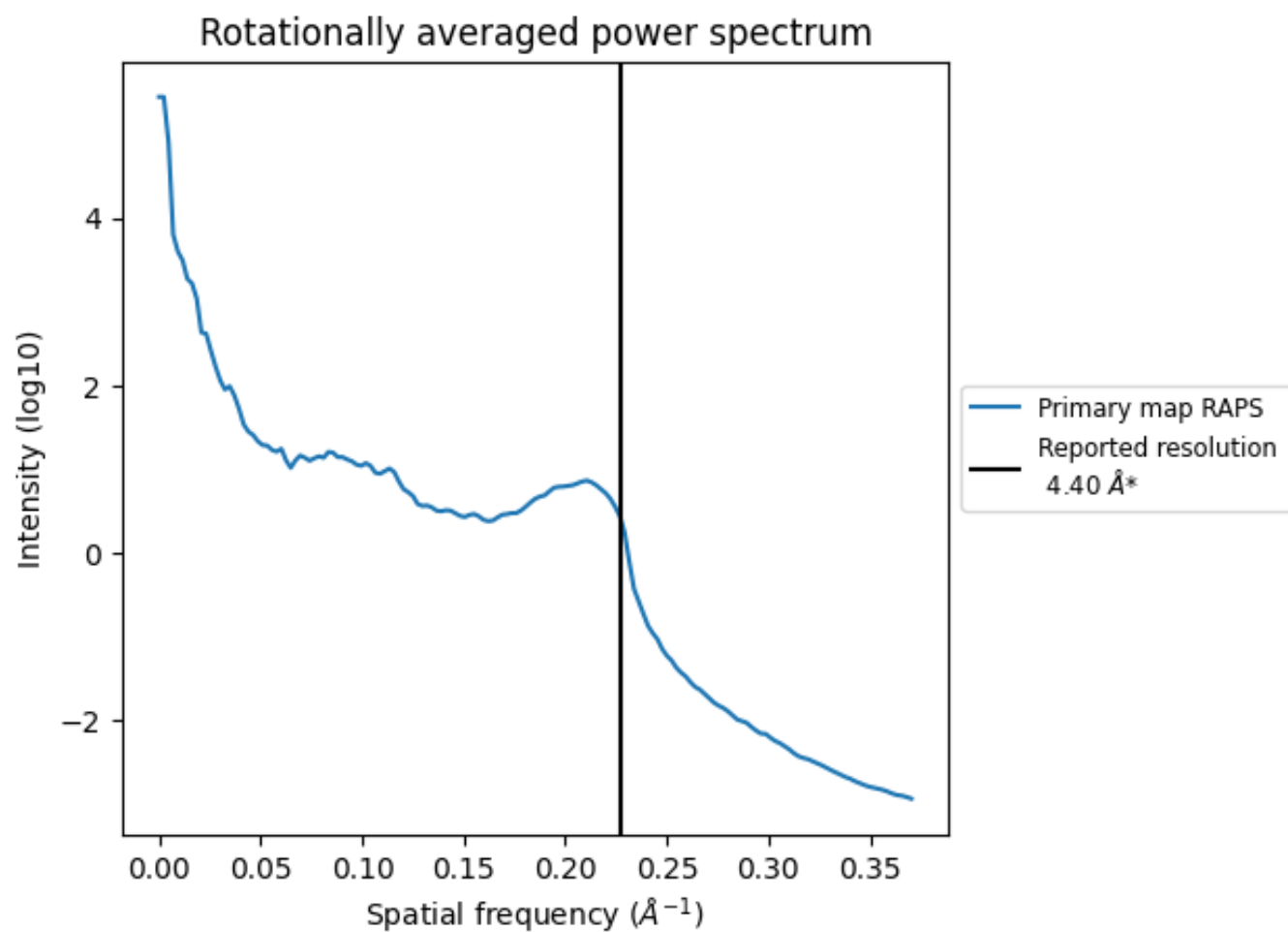
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 904 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

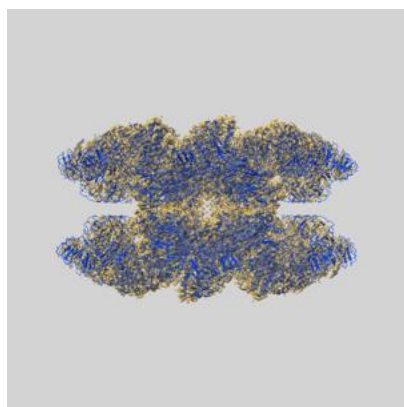
8 Fourier-Shell correlation

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

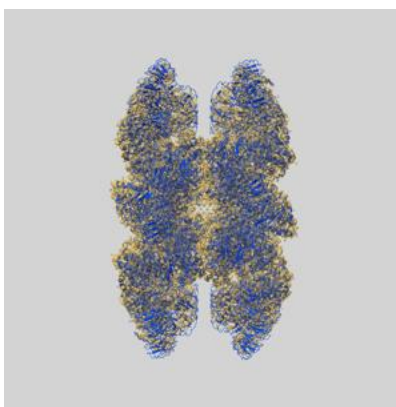
9 Map-model fit [i](#)

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](#).

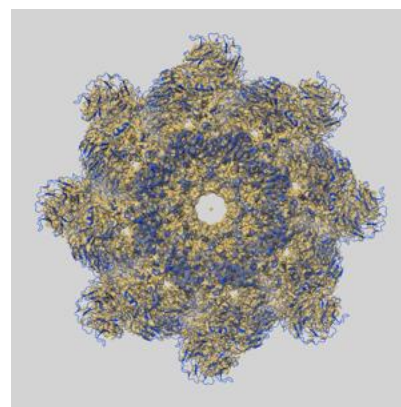
9.1 Map-model overlay [i](#)



X



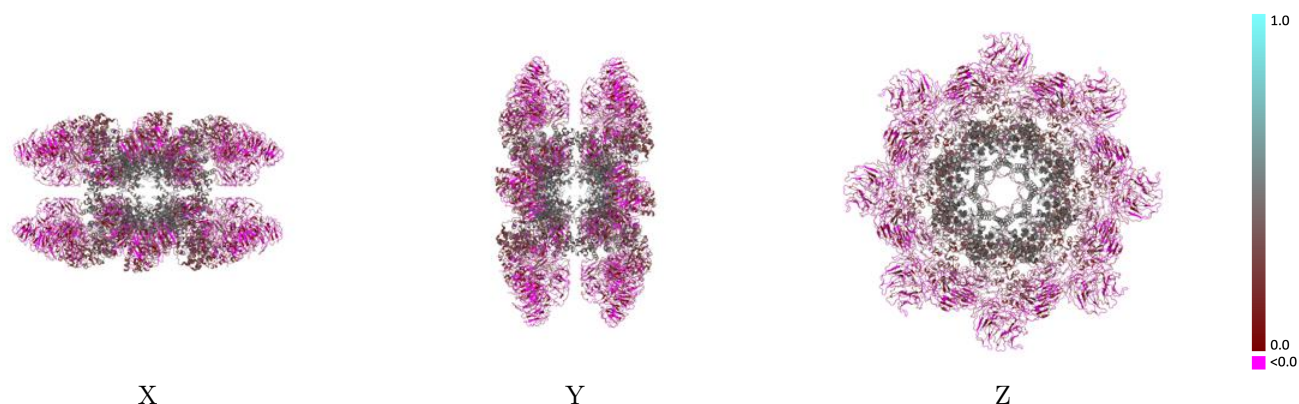
Y



Z

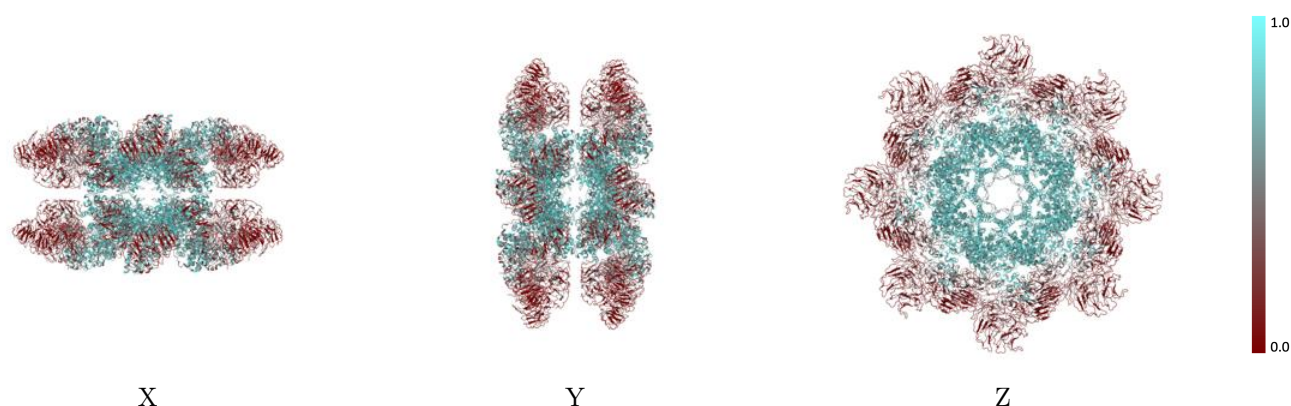
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



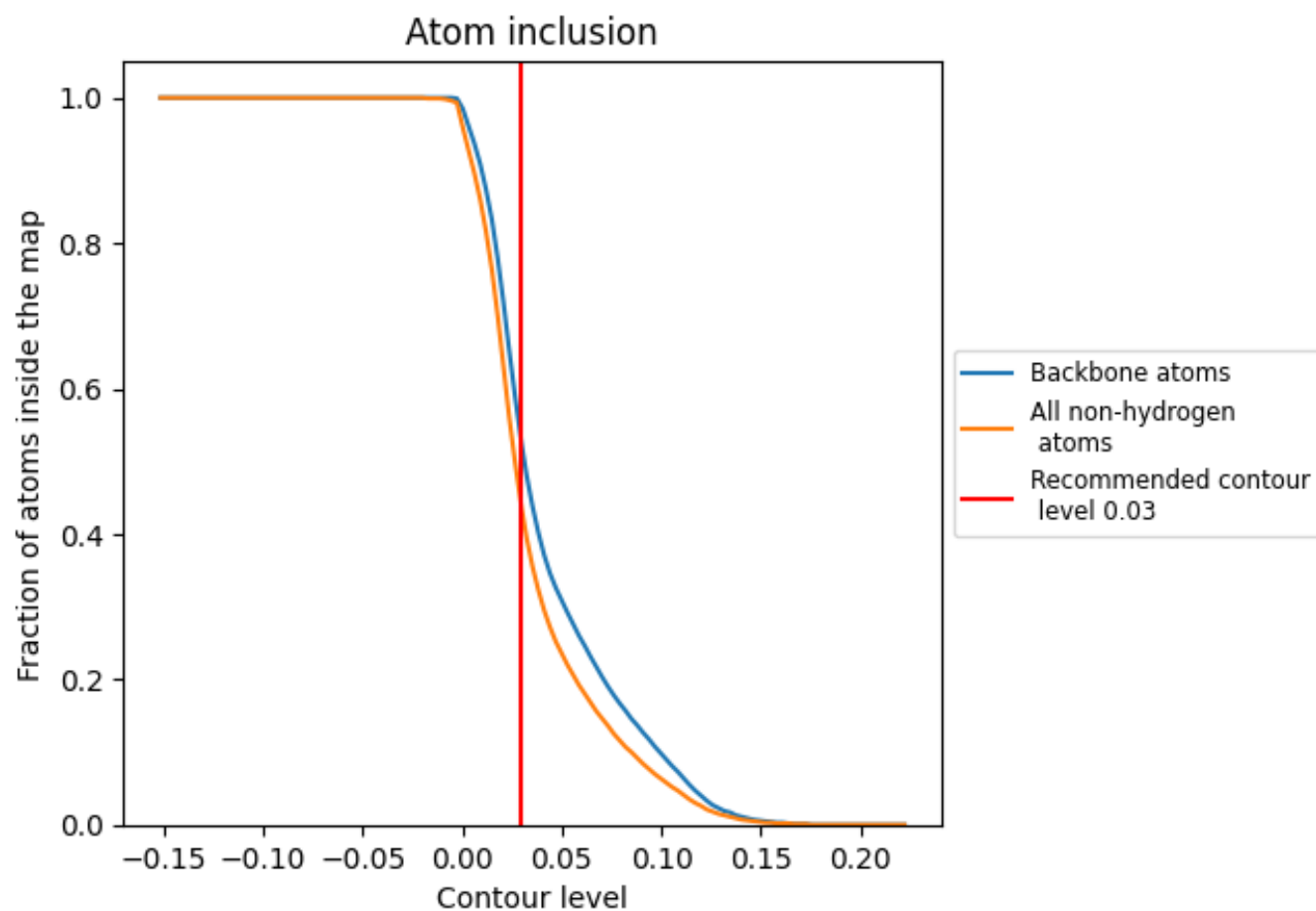
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ

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	<div></div> 0.4340	<div></div> 0.1940
A	<div></div> 0.4360	<div></div> 0.1950
B	<div></div> 0.4300	<div></div> 0.1890
C	<div></div> 0.4310	<div></div> 0.1900
D	<div></div> 0.4330	<div></div> 0.1960
E	<div></div> 0.4370	<div></div> 0.1950
F	<div></div> 0.4280	<div></div> 0.1900
G	<div></div> 0.4360	<div></div> 0.1940
H	<div></div> 0.4360	<div></div> 0.1950
I	<div></div> 0.4350	<div></div> 0.1950
J	<div></div> 0.4370	<div></div> 0.1950
K	<div></div> 0.4340	<div></div> 0.1960
L	<div></div> 0.4280	<div></div> 0.1880
M	<div></div> 0.4350	<div></div> 0.1950
N	<div></div> 0.4370	<div></div> 0.1950
O	<div></div> 0.4350	<div></div> 0.1950
P	<div></div> 0.4330	<div></div> 0.1960

1.0

0.0

<0.0