



## wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 04:43 AM UTC

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)

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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:

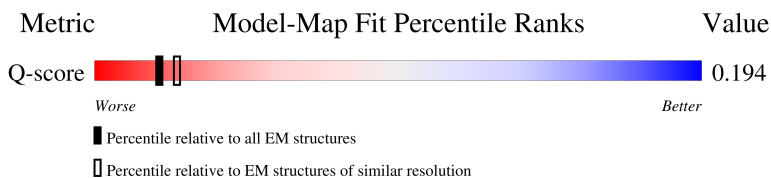
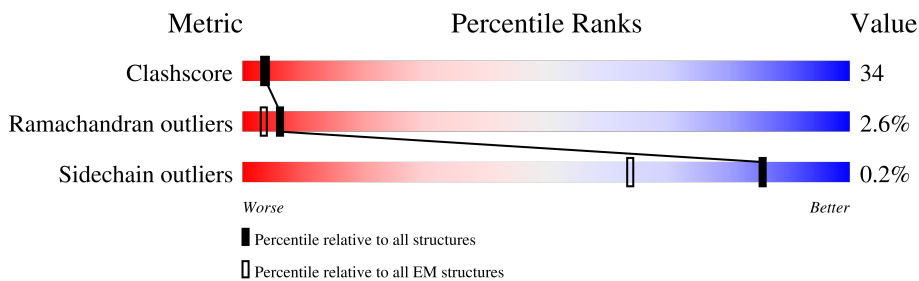
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 ( 3.91 - 4.90 )

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	<div style="display: flex; justify-content: space-between;"> <span>45%</span> <span>47%</span> <span>35%</span> <span>•</span> <span>14%</span> </div>
1	B	1440	<div style="display: flex; justify-content: space-between;"> <span>45%</span> <span>46%</span> <span>37%</span> <span>•</span> <span>14%</span> </div>
1	C	1440	<div style="display: flex; justify-content: space-between;"> <span>45%</span> <span>46%</span> <span>36%</span> <span>•</span> <span>14%</span> </div>
1	D	1440	<div style="display: flex; justify-content: space-between;"> <span>45%</span> <span>45%</span> <span>37%</span> <span>•</span> <span>14%</span> </div>

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Mol	Chain	Length	Quality of chain
1	E	1440	
1	F	1440	
1	G	1440	
1	H	1440	
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](#)

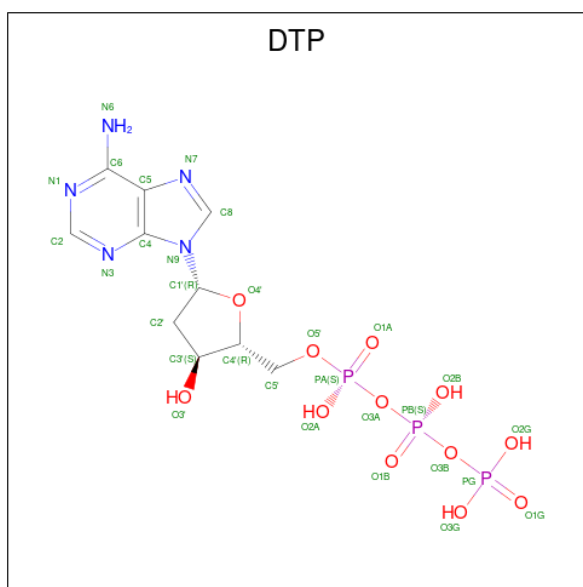
There are 2 unique types of molecules in this entry. The entry contains 161200 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ )



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	
2	N	1	Total	C	N	O	P	0
			30	10	5	12	3	

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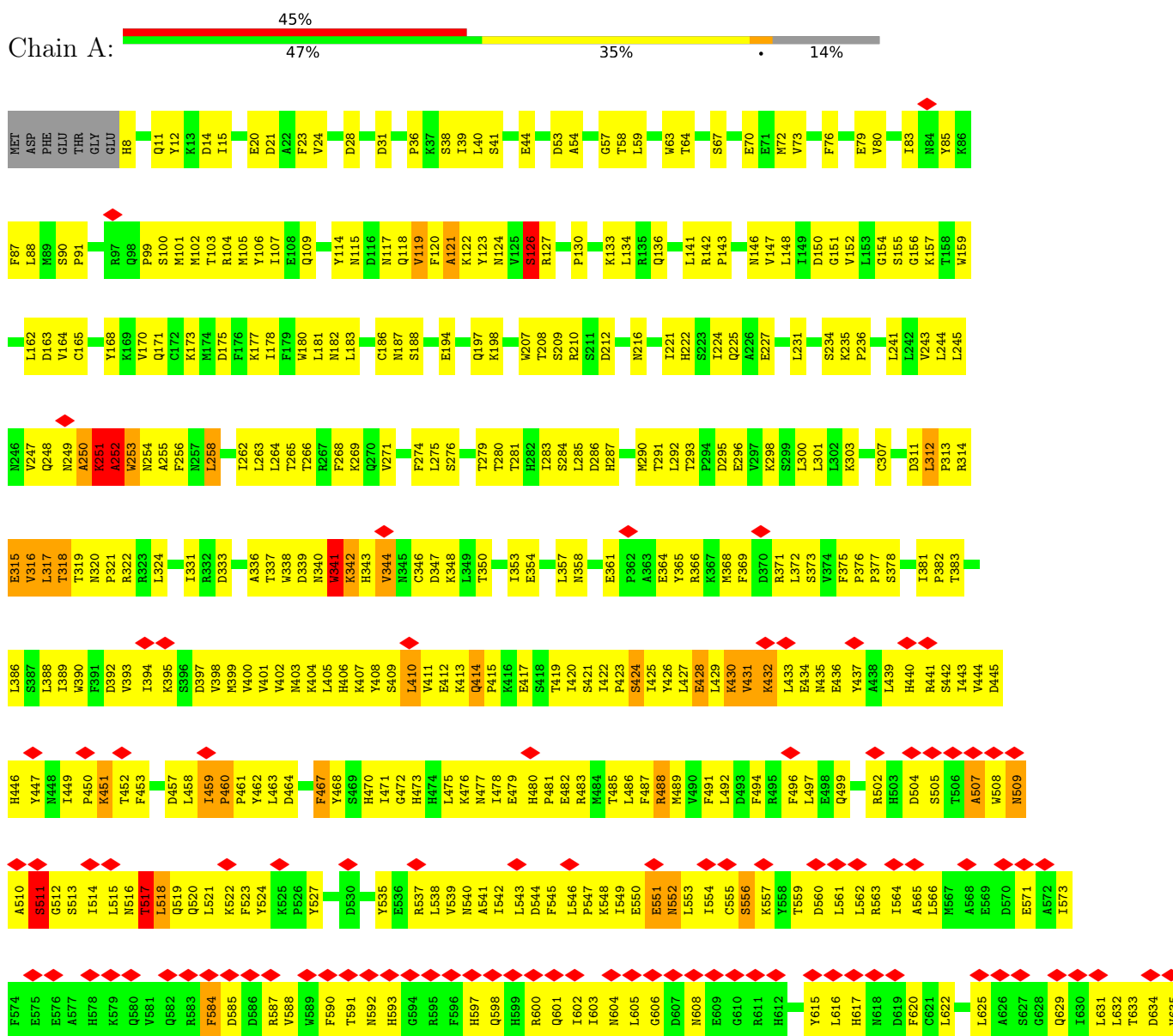
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	O	1	30	10	5	12	3	0
2	P	1	30	10	5	12	3	0

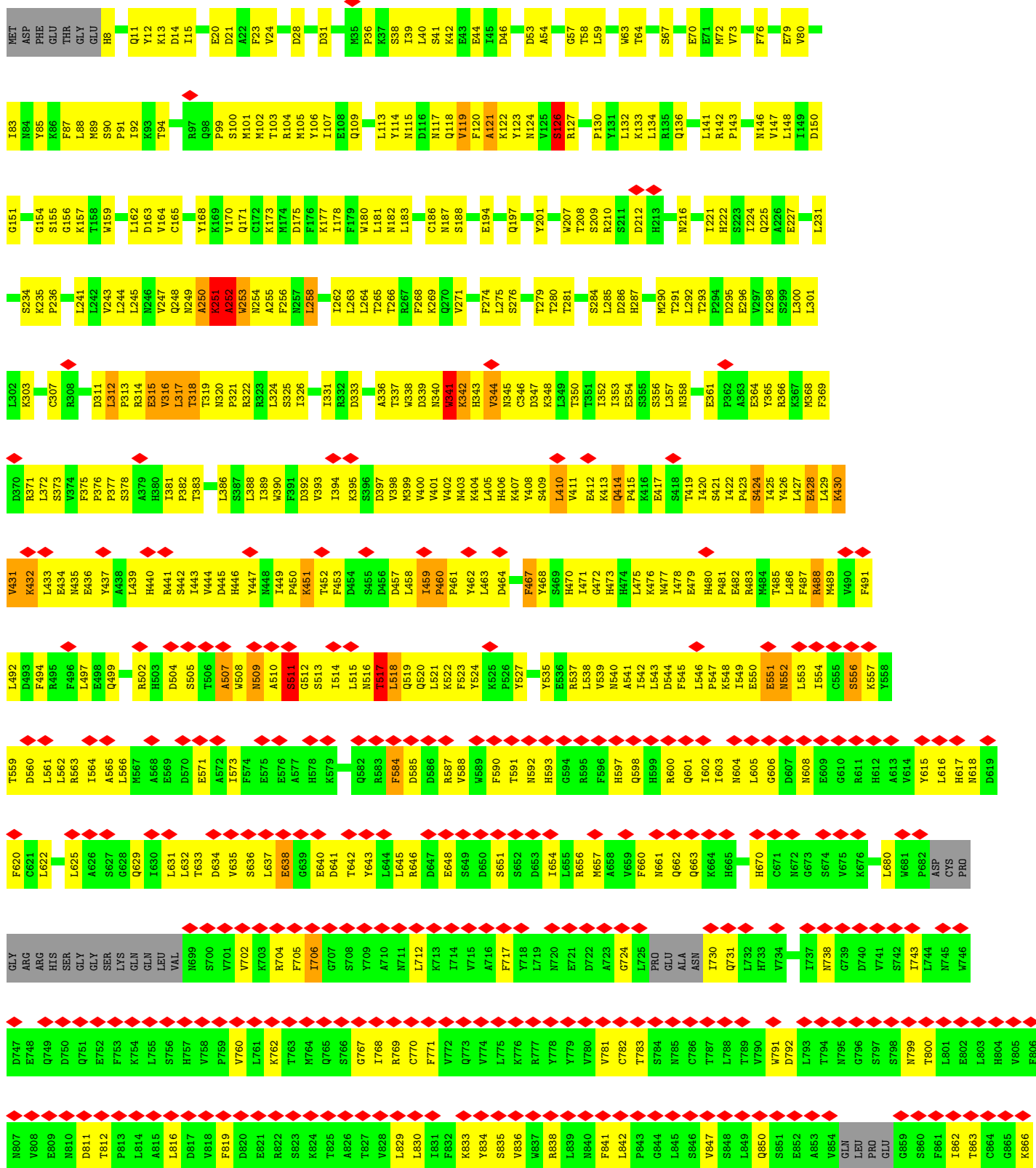
### 3 Residue-property plots

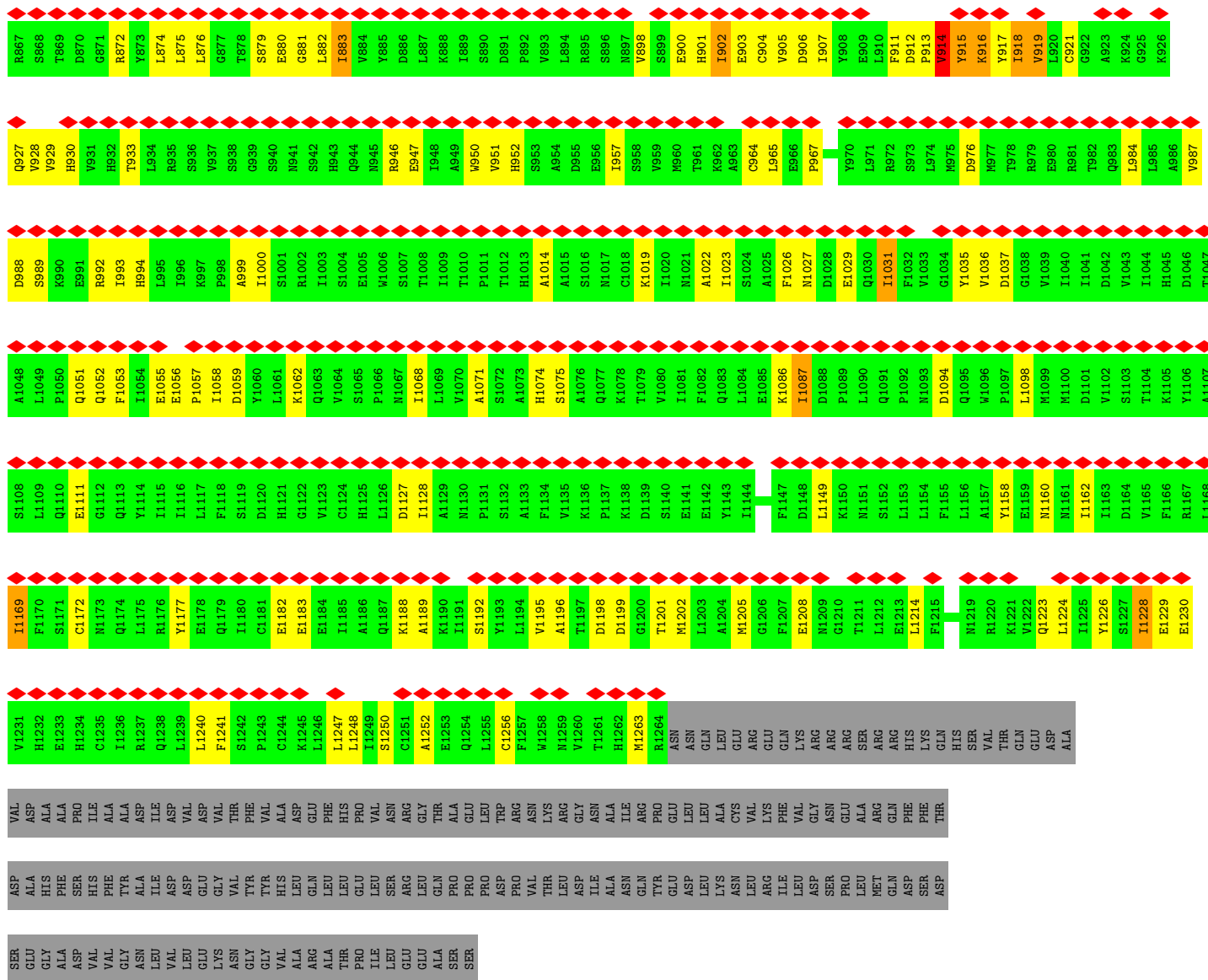
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

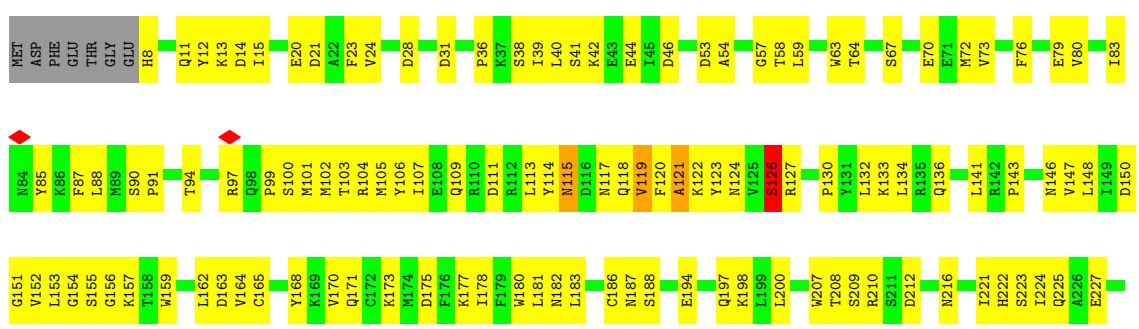
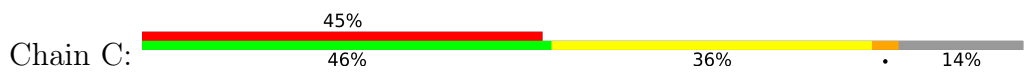


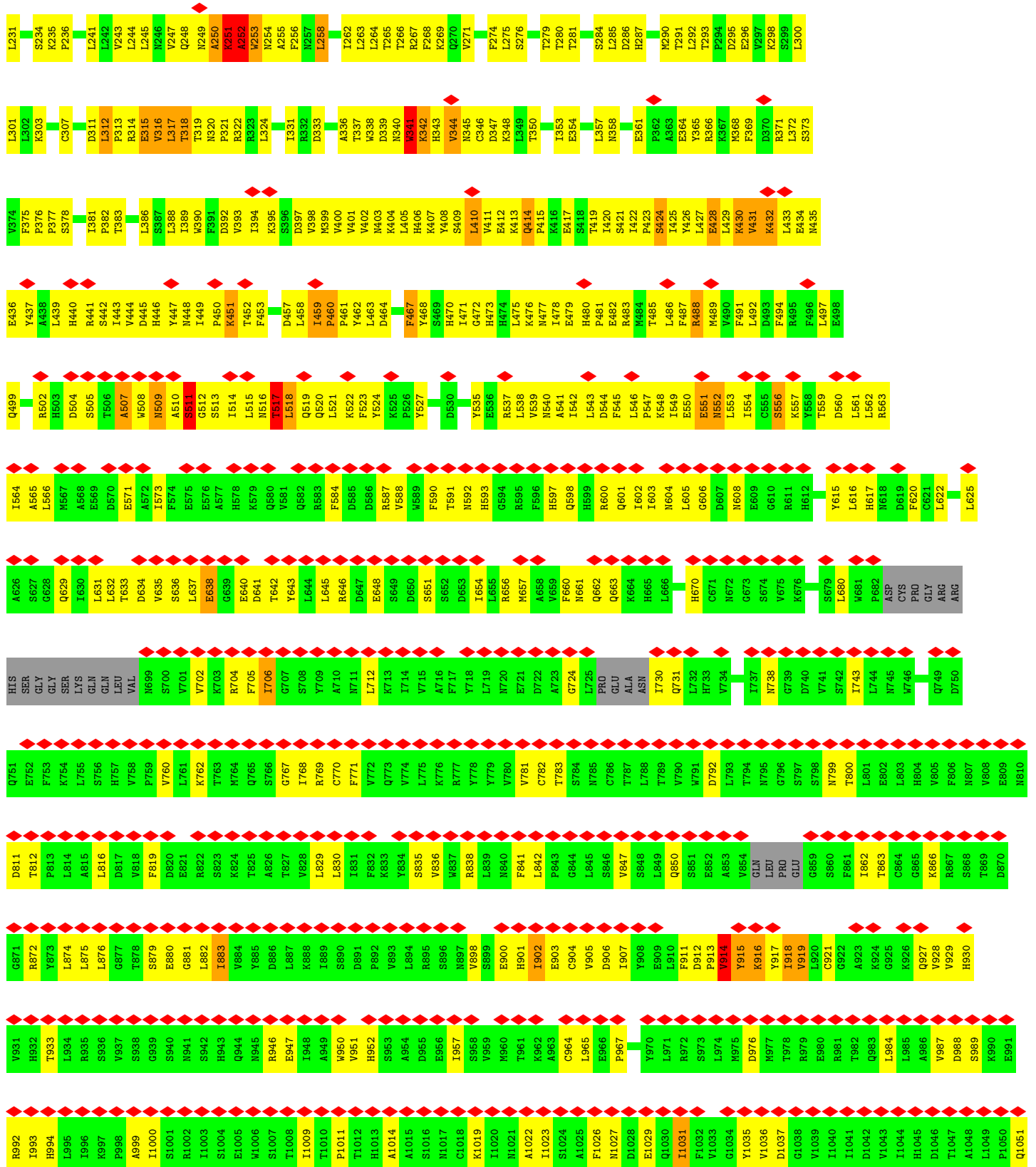






● Molecule 1: Apaf-1 related killer DARK



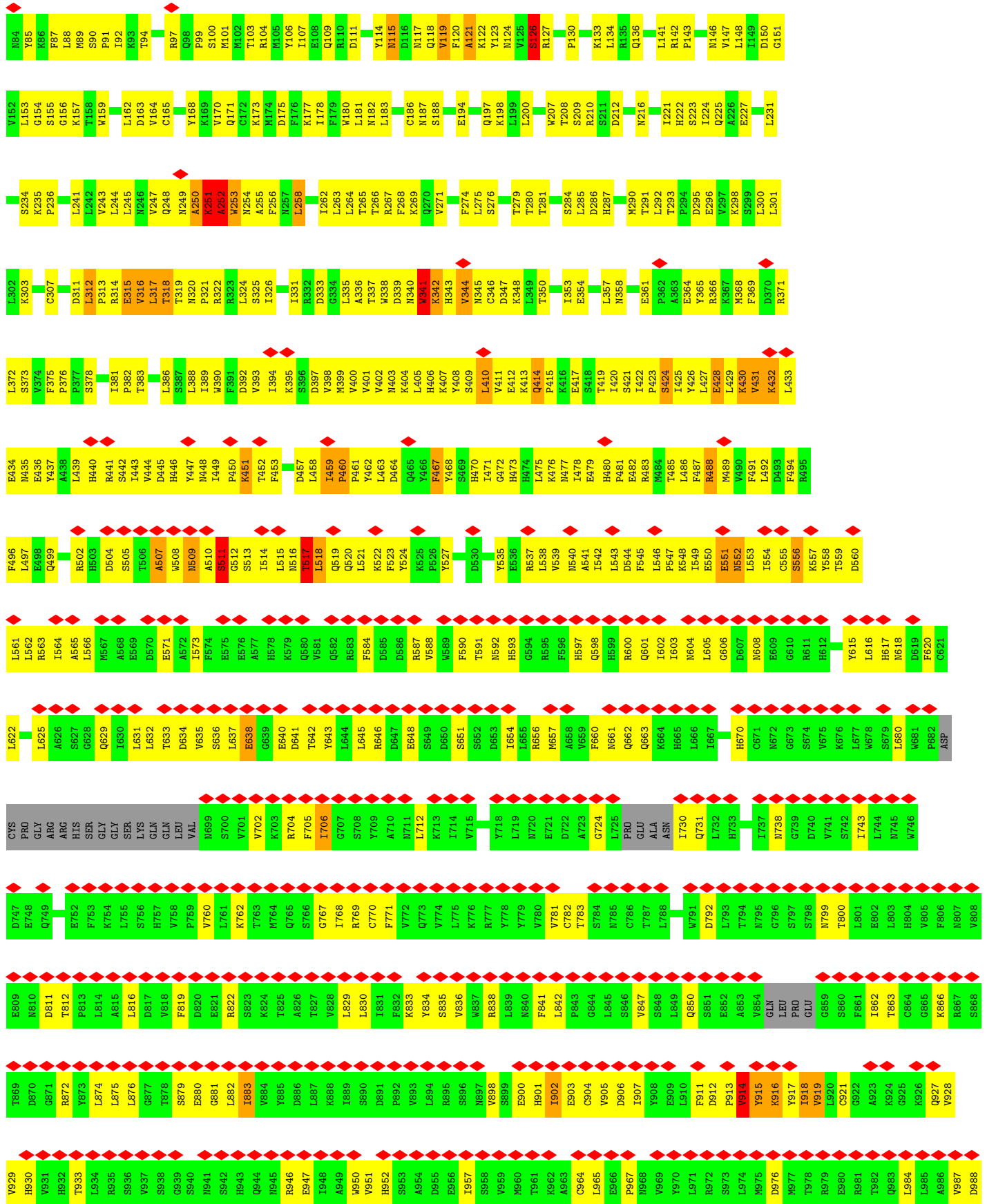




THR	I1225	V1102	D1042	T982	F861	L801	V741	L880	M618	K557	L492
GLN	Y1226	S1103	V1043	Q883	I862	E802	S742	W881	D619	Y558	D493
GLU	S1227	T1104	I1044	L984	T863	L803	I743	P882	F200	T559	F494
ALA	I1163	K1105	H1045	L985	C864	H804	L744	ASP	G821	D560	R495
VAL	V1165	K1106	D1046	A986	C865	V805	M745	PRO	L622	L561	F496
ASP	E1229	Y1107	T1047	P987	K866	F806	M746	GLY	L625	L562	L497
ALA	V1231	S1108	A1048	D988	R867	M807	M747	ARG	A626	I564	Q499
ALA	H1232	L1109	L1049	S989	S868	V808	D747	ARG	S827	A565	R502
ILE	I1169	Q1110	P1050	K990	T869	E809	E748	HIS	G828	L666	H503
ALA	F1170	E1111	Q1051	E991	D870	N810	Q749	SER	Q829	M567	D504
ASP	S1172	G1112	Q1052	R992	C871	D811	Q750	GLY	I830	A568	H504
ILE	M1173	Q1113	F1053	I993	R872	T812	Q751	LYS	E830	E569	S505
ASP	Q1174	Y1114	I1054	H994	T873	P813	E752	LYS	L632	D570	T506
VAL	L1175	I1115	E1055	L874	L874	L814	F753	GLN	T633	E571	A507
VAL	R1176	I1116	E1056	L875	L875	L814	K754	GLN	L634	A572	V508
THR	Y1177	L1117	P1057	K997	L876	A815	L755	LEU	D634	I573	N509
PHE	E1178	F1118	P1058	P998	L876	L816	S756	VAL	V635	F574	A510
VAL	Y1179	F1241	I1059	A999	C877	D817	H757	M899	S636	E575	S511
ALA	Q1180	D1120	D1059	E999	T878	V818	V758	S700	L637	E576	G512
ASP	C1181	H1121	Y1060	I1000	S879	F819	P759	V701	E638	A577	S513
GLU	P1243	H1122	K1061	S1001	E880	D820	V760	V702	G639	H578	I514
PHE	K1244	G1122	L1062	R1002	C881	E821	L761	K703	E640	K579	L515
PRO	E1182	G1123	Q1063	I1003	R882	R822	K762	R704	L641	Q580	L516
HIS	E1183	V1123	V1064	R1004	L883	S823	I763	F705	T642	Q581	N517
THR	E1184	C1124	V1064	S1004	V884	K824	M764	I706	Y643	Q582	L518
ASN	I1185	H1125	S1065	E1005	V885	T825	Q765	G707	L644	Q520	Q520
ARG	I1186	L1126	P1066	E1006	H886	T826	S766	S708	R646	L521	L521
GLY	Q1187	D1127	M1067	S1007	D887	T827	Q767	Y709	R646	K522	K522
THR	K1188	I1128	I1068	T1008	L887	T828	I768	I710	D647	F523	F523
ALA	A1189	A1129	V1070	I1009	K888	V828	R769	N711	E948	Y524	Y524
GLU	K1190	M1130	Y1070	T1010	R889	L829	C770	K713	S649	D585	D585
LEU	I1191	P1131	A1071	P1011	S890	L830	F771	L712	D850	R587	K525
TRP	S1192	S1072	S1072	T1012	D891	T831	V772	I714	S651	F526	F526
ARG	Y1193	A1073	H1013	H1013	P892	K833	Q773	V715	T591	Y527	Y527
ASN	L1194	H1074	A1014	A1014	H893	K834	V774	A716	N592	D530	D530
ALA	V1195	S1075	A1015	A1015	L894	Y834	L775	F717	H593	Y635	Y635
ILE	A1196	A1076	S1016	S1016	H895	S835	L776	Y718	G594	E536	E536
ARG	T1197	Q1077	Q1077	S1016	S896	V836	K776	L719	R656	R537	R537
PRO	D1198	K1078	C1018	C1018	S897	H637	R777	L719	R656	L538	L538
GLU	D1199	T1079	C1018	C1018	R897	R638	V778	N720	M657	V639	V639
LEU	G1200	V1080	I1020	I1020	S899	L839	Y779	E721	A658	N640	N640
ALA	T1201	E1141	M1021	M1021	E900	N840	V780	D722	F660	A541	A541
CYS	M1202	E1142	A1022	A1022	H901	N840	V780	G724	M661	I642	I642
VAL	L1203	E1143	I1023	I1023	I902	L842	T783	L725	Q662	L543	L543
LYS	A1204	Y1143	S1024	S1024	E903	P843	T784	PRO	Q663	F645	F645
PHE	M1205	I1144	C964	C964	C904	G844	S784	GLU	Q663	L546	L546
VAL	M1206	I1145	L965	L965	Y905	M785	M785	ALA	K664	P647	P647
GLY	G1206	G1146	F1026	F1026	D906	L845	C786	ASN	H665	K648	K648
ASN	F1207	F1147	F1027	F1027	D906	S846	C786	ASN	L666	I549	I549
GLU	E1208	D1148	N1027	N1027	I907	V847	T787	I730	I667	E550	E550
ALA	M1209	L1149	D1028	D1028	Y908	T788	T788	Q731	G606	E551	E551
ARG	S1210	K1149	P1089	P1089	S848	S848	T789	L732	D607	N652	N652
ARG	L1212	M1151	Q1030	Q1030	L849	L849	T789	H733	E608	L553	L553
ARG	L1213	L1152	I1031	I1031	Q850	Q850	V790	V734	N672	I554	I554
LYS	L1214	S1152	F1032	F1032	S851	S851	W791	G673	G610	C555	C555
GLN	F1215	L1153	V1033	V1033	E852	E852	D792	S674	R611	S556	S556
HIS	M1219	L1154	G1034	G1034	Y914	Y914	L793	N738	H612		
VAL	R1220	F1155	Y1035	Y1035	X915	X915	T794	G739	Y615		
ASP	K1221	L1156	Q1095	Q1095	K916	K916	M795	D740	L677		
ASP	Q1222	A1157	V1036	V1036	Y917	Y917	G796		W678		
VAL	L1224	Y1158	P1097	P1097	T918	T918	S797		S679		
VAL		E1159	G1038	G1038	Y919	Y919	S798				
VAL		M1160	V1039	V1039	L920	L920	N799				
VAL		N1161	I1040	I1040	S860	S860	T800				







SS89	L1049	L1109	II189	HI232	ALA	GLY	HIS
K990	P1060	Q1110	F1170	E1233	ALA	ALA	PHE
E991	Q1061	E1111	S1171	HI234	PRO	ASP	SER
R992	Q1062	G1112	C1172	C1235	ILE	VAL	HIS
I993	F1063	G1113	NI173	I1236	ALA	VAL	PHE
H994	I1064	Q1114	Q1174	R1237	ASP	ASN	TYR
L995	E1065	I1115	LI175	Q1238	ASP	LEU	ALA
I996	E1066	I1116	R1176	L1239	VAL	LEU	ASP
R997	P1067	L1117	Y1177	L1240	VAL	GLY	ASP
P998	I1068	F1118	E1178	F1241	THR	VAL	GLY
A999	D1069	S1119	Q1179	SI242	PHE	THR	TYR
I1000	Y1060	D1120	II180	P1243	VAL	TYR	TYR
S1001	L1061	H1121	C1181	C1244	ALA	VAL	HIS
R1002	K1062	G1122	E1182	K1245	GLU	ALA	LEU
I1003	Q1063	V1123	E1183	L1246	PHE	ARG	GLN
S1004	V1064	C1124	E1184	L1247	HIS	LEU	LEU
E1005	S1065	H1125	AI186	I1248	PRO	LEU	LEU
W1006	P1066	L1126	AI186	I1249	VAL	SER	LEU
S1007	N1067	D1127	Q1187	SI250	ARG	GLY	ARG
T1008	I1068	I1128	K1188	C1251	GLY	LEU	LEU
I1009	L1069	A1129	AI189	A1252	THR	ALA	GLN
T1010	I1070	M1130	K1190	E1253	ALA	PRO	PRO
P1011	A1071	P1131	II191	Q1254	GLU	PRO	PRO
T1012	S1072	S1132	SI192	L1255	TRP	ASP	TRP
H1013	A1073	S1133	Y1193	C1256	ARG	ARG	PRO
A1014	H1074	A1134	LI194	F1257	ASN	ASN	VAL
A1015	S1075	F1135	V1195	W1258	LYS	LYS	THR
S1016	A1076	K1136	AI196	T1261	ARG	ASP	LEU
W1017	Q1077	P1137	T1197	HI262	GLY	ILE	LEU
C1018	K1078	K1138	D1198	M1263	ALA	ALA	ALA
K1019	T1079	D1139	GI199	R1264	ILE	ASN	ASN
I1020	V1080	S1140	DI200	ASN	PRO	TYR	TYR
M1021	I1081	E1141	T1201	ASN	GLU	GLU	GLU
A1022	F1082	E1142	M1202	GLN	LEU	ASP	ASP
I1023	Q1083	E1143	L1203	LEU	LEU	LEU	LEU
S1024	L1084	Y1143	AI204	GLU	ALA	LYS	LYS
A1025	E1085	I1144	M1205	ARG	CYS	ASN	ASN
F1026	K1086	V1145	M1206	GLU	VAL	VAL	VAL
M1027	I1087	G1146	GI206	GLN	PHE	ILE	ILE
D1028	P1088	F1147	E1208	LYS	VAL	LEU	VAL
E1029	I1089	D1148	AI208	ARG	GLY	ASP	GLY
Q1030	L1090	L1149	M1209	ARG	ASN	SER	ASN
I1031	Q1091	K1150	L1212	SER	ALA	PRO	GLU
F1032	P1092	M1151	E1213	ARG	ALA	LEU	ALA
V1033	N1093	M1152	L1214	HIS	ARG	LEU	MET
G1034	D1094	L1153	F1215	LYS	GLN	GLN	GLN
Y1035	Q1095	L1154	AI216	HIS	THR	ASP	PHE
W1036	W1096	F1155	M1219	SER	VAL	THR	THR
D1037	P1097	L1156	R1220	VAL	GLN	GLU	GLU
G1038	L1098	A1157	Q1223	ASP	GLU	ASP	ASP
V1039	M1099	Y1158	L1224	ALA	ALA	VAL	ALA
I1040	M1100	E1159	Y1226	VAL	VAL	ASP	ASP
I1041	D1101	M1160	SI227	ASP	ASP	ASP	ASP
D1042	I1102	M1161	I1228	ASP	ASP	ASP	ASP
V1043	V1102	I1162	E1229	ASP	ASP	ASP	ASP
I1044	T1104	I1163	E1230	ASP	ASP	ASP	ASP
H1045	K1105	D1164	V1231	ASP	ASP	ASP	ASP
I1046	Y1106	V1165		ASP	ASP	ASP	ASP
D1047	A1107	F1166		ASP	ASP	ASP	ASP
A1048	S1108	R1167		ASP	ASP	ASP	ASP
		L1168		ASP	ASP	ASP	ASP

• Molecule 1: Apaf-1 related killer DARK

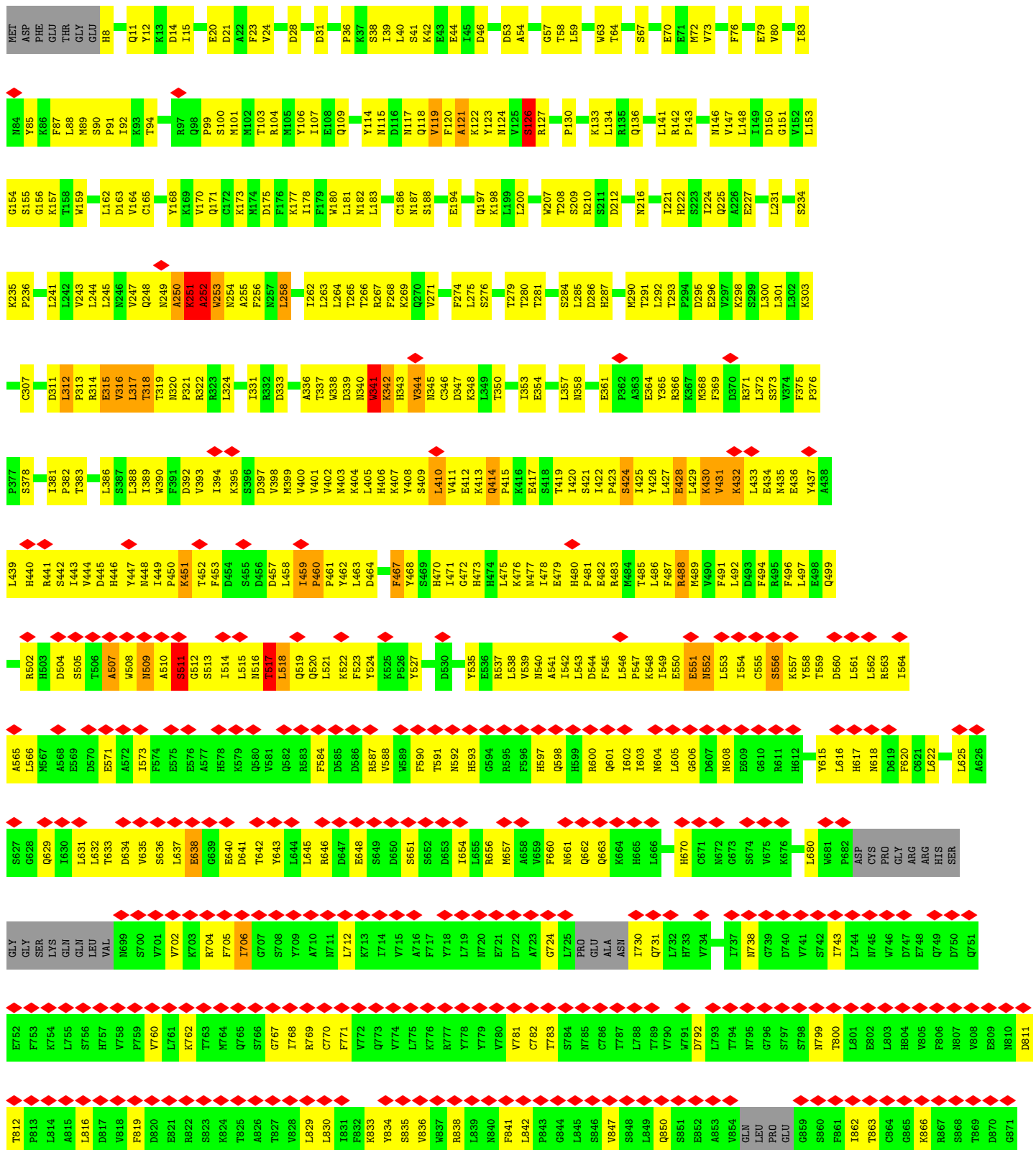


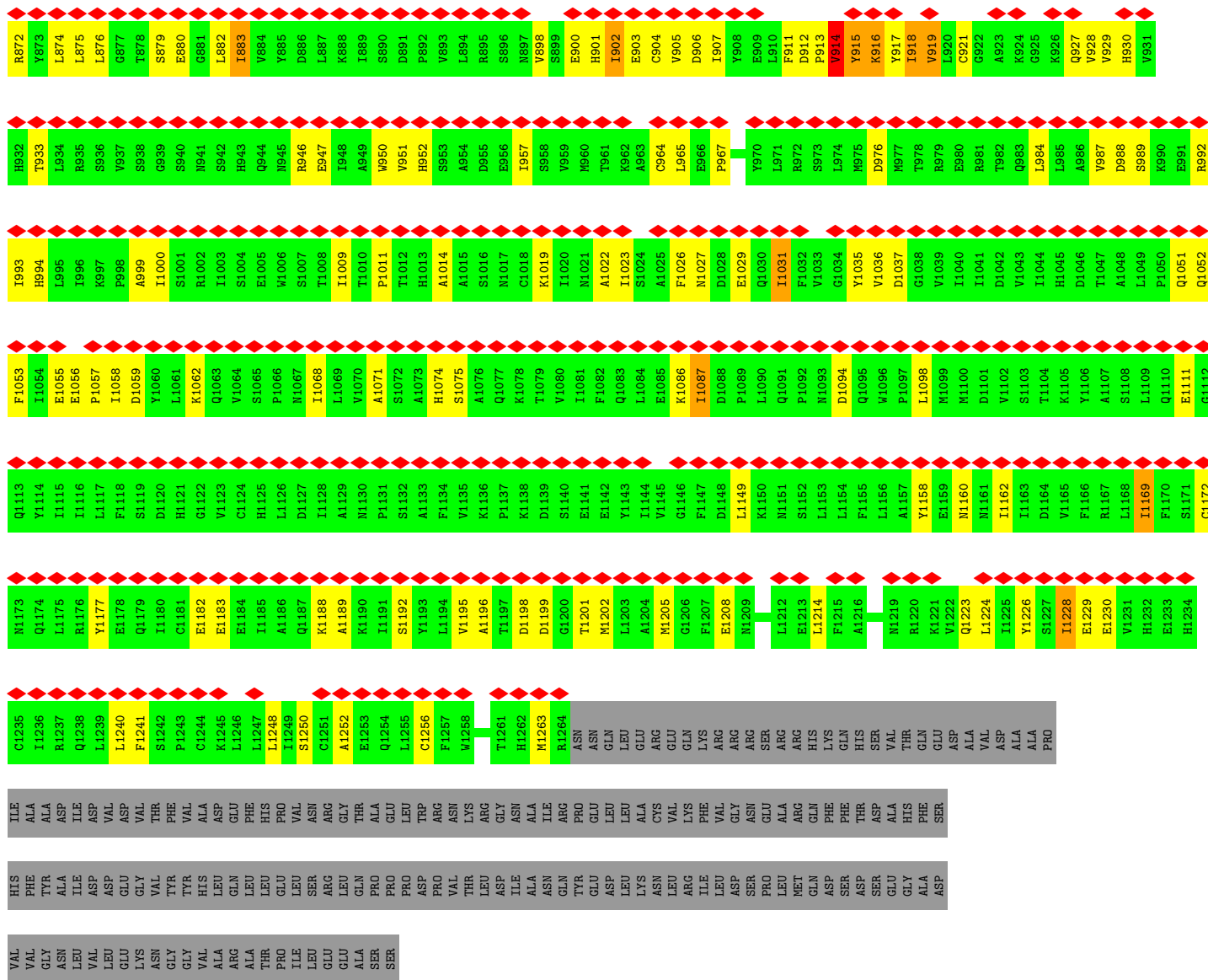
MET	Y84	Y168	Y177	Y178	Y179	Y180	Y181	Y182	Y183	Y184	Y185	Y186	Y187	Y188	Y189	Y190	Y191	Y192	Y193	Y194	Y195	Y196	Y197	Y198	Y199	Y200	Y201	Y202	Y203	Y204	Y205	Y206	Y207	Y208	Y209	Y210	Y211	Y212	Y213	Y214	Y215	Y216	Y217	Y218	Y219	Y220	Y221	Y222	Y223	Y224	Y225	Y226	Y227	Y228	Y229	Y230	Y231	Y232	Y233	Y234	Y235	Y236	Y237	Y238	Y239	Y240	Y241	Y242	Y243	Y244	Y245	Y246	Y247	Y248	Y249	Y250	Y251	Y252	Y253	Y254	Y255	Y256	Y257	Y258	Y259	Y260	Y261	Y262	Y263	Y264	Y265	Y266	Y267	Y268	Y269	Y270	Y271	Y272	Y273	Y274	Y275	Y276	Y277	Y278	Y279	Y280	Y281	Y282	Y283	Y284	Y285	Y286	Y287	Y288	Y289	Y290	Y291	Y292	Y293	Y294	Y295	Y296	Y297	Y298	Y299	Y300	Y301	Y302	Y303	Y304	Y305	Y306	Y307	Y308	Y309	Y310	Y311	Y312	Y313	Y314	Y315	Y316	Y317	Y318	Y319	Y320	Y321	Y322	Y323	Y324	Y325	Y326	Y327	Y328	Y329	Y330	Y331	Y332	Y333	Y334	Y335	Y336	Y337	Y338	Y339	Y340	Y341	Y342	Y343	Y344	Y345	Y346	Y347	Y348	Y349	Y350	Y351	Y352	Y353	Y354	Y355	Y356	Y357	Y358	Y359	Y360	Y361	Y362	Y363	Y364	Y365	Y366	Y367	Y368	Y369	Y370	Y371	Y372	Y373	Y374	Y375	Y376	Y377	Y378	Y379	Y380	Y381	Y382	Y383	Y384	Y385	Y386	Y387	Y388	Y389	Y390	Y391	Y392	Y393	Y394	Y395	Y396	Y397	Y398	Y399	Y400	Y401	Y402	Y403	Y404	Y405	Y406	Y407	Y408	Y409	Y410	Y411	Y412	Y413	Y414	Y415	Y416	Y417	Y418	Y419	Y420	Y421	Y422	Y423	Y424	Y425	Y426	Y427	Y428	Y429	Y430	Y431	Y432	Y433	Y434	Y435	Y436	Y437	Y438	Y439	Y440	Y441	Y442	Y443	Y444	Y445	Y446	Y447	Y448	Y449	Y450	Y451	Y452	Y453	Y454	Y455	Y456	Y457	Y458	Y459	Y460	Y461	Y462	Y463	Y464	Y465	Y466	Y467	Y468	Y469	Y470	Y471	Y472	Y473	Y474	Y475	Y476	Y477	Y478	Y479	Y480	Y481	Y482	Y483	Y484	Y485	Y486	Y487	Y488	Y489	Y490	Y491	Y492	Y493	Y494	Y495	Y496	Y497	Y498	Y499	Y500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702	Y703	Y704	Y705	Y706	Y707	Y708	Y709	Y710	Y711	Y712	Y713	Y714	Y715	Y716	Y717	Y718	Y719	Y720	Y721	Y722	Y723	Y724	Y725	Y726	Y727	Y728	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783	Y784	Y785	Y786	Y787	Y788	Y789	Y790	Y791	Y792	Y793	Y794	Y795	Y796	Y797	Y798	Y799	Y800	Y801	Y802	Y803	Y804	Y805	Y806	Y807	Y808	Y809	Y810	Y811	Y812	Y813	Y814	Y815	Y816	Y817	Y818	Y819	Y820	Y821	Y822	Y823	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y832	Y833	Y834	Y835	Y836	Y837	Y838	Y839	Y840	Y841	Y842	Y843	Y844	Y845	Y846	Y847	Y848	Y849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000
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Q1113	F1053	I993	H932	R872	T812	E752	GLY	G628	L566	R502	H440	S378
Y1114	I1054	H994	T933	W873	P813	F753	GLY	Q629	M667	H503	R441	I381
I1115	E1055	L995	L934	L874	L814	K754	SER	I630	A568	D504	S442	P382
I1116	E1056	I996	L935	L875	A815	L755	GLN	L631	E569	D505	I443	T383
L1117	P1057	K997	S936	L876	L816	S756	LEU	L632	D570	T506	V444	L386
F1118	I1058	P998	V937	L877	D817	H757	VAL	T633	E571	A507	H445	L387
S1119	D1059	A999	S938	T878	W818	W758	NG69	D634	I573	W508	H446	S387
D1120	Y1060	I1000	S939	S879	F819	P759	S700	G635	F574	N509	I388	L388
H1121	L1061	S1001	S940	E880	D820	V760	V701	L637	E575	A510	I389	L389
G1122	K1062	R1002	L882	C881	E821	L761	V702	E638	E576	S511	P450	F391
V1123	Q1063	I1003	S942	L883	R822	K762	K703	G639	A577	G512	K451	D392
C1124	V1064	S1004	H943	W884	S823	T763	R704	E640	K578	S513	T452	V993
L1125	S1065	E1005	Q944	W885	R824	W764	F705	E641	H579	I514	I394	I394
H1126	P1066	W1006	N945	Y885	T825	Q765	I706	T642	Q580	L515	D454	K396
D1127	M1067	S1007	R946	Y886	A826	S766	G707	E643	V581	N516	S455	S396
I1128	I1068	T1008	E947	D887	T827	G767	L644	L644	Q582	T517	D457	D397
A1129	L1069	I1009	I948	L888	W828	I768	L645	L645	L519	Q519	L458	V398
V1130	V1070	T1010	A949	R889	L829	R769	F709	R646	Q520	Q520	I469	M399
P1131	A1071	W950	W950	S890	L830	C770	A710	D647	L521	K522	P461	V401
S1132	S1072	V951	H952	D891	L831	F771	L712	E648	D585	F523	L463	M403
F1134	A1073	H1013	H953	P892	F832	W772	K713	S649	D588	Y524	D464	M404
A1135	H1074	A1014	K833	W893	K833	Q773	I714	D650	W589	K525	H406	M405
V1136	S1075	A1015	Y834	L894	Y834	W774	K715	S651	F590	P526	K407	M406
K1136	A1076	S1016	S835	L895	S835	W775	V715	S652	F591	Y527	Y408	M407
P1137	Q1077	N1017	W836	R895	W836	L775	A716	D653	T591	D530	Y409	M408
K1138	Q1078	C1018	W837	S896	W837	K776	F717	I654	N592	D530	I410	M409
D1139	T1079	K1019	R838	W898	R838	Y776	V718	L655	W593	Y535	I411	M410
S1140	V1080	I1020	L839	S899	L839	Y779	L719	G594	E536	E536	E412	M411
E1141	I1081	N1021	E900	E900	E900	W780	N720	G594	R537	R537	E413	M412
E1142	F1082	T961	H901	H901	F841	W781	E721	R595	L538	L538	H474	M413
Y1143	Q1083	I1023	I902	I902	L842	C782	D722	F596	V539	V539	H475	M414
T1144	L1084	S1024	E903	E903	P843	T783	A723	A658	N540	N540	K476	M415
V1145	E1085	A1025	C904	C904	Q844	W784	G724	W659	E541	E541	I478	M416
G1146	K1086	F1026	V905	V905	L845	C786	L725	F660	L546	L546	E479	M417
F1147	I1087	N1027	D906	D906	S846	W787	PRD	Q662	I602	I602	H480	M418
D1148	D1088	D1028	Y908	Y908	Y847	T788	ALA	K664	I603	I603	E482	M419
K1150	P1089	E1029	E909	E909	S848	L788	ASN	L866	N604	N604	E428	M420
N1151	L1090	Q1030	L910	L910	L849	W790	I730	H670	L605	L605	E429	M421
S1152	Q1091	I1031	F911	F911	Q850	W791	L732	C671	E551	E551	K430	M422
L1153	P1092	F1032	D912	D912	S851	N791	H733	N672	N552	N552	V431	M423
L1154	M1093	S973	P913	P913	E852	W792	V734	G673	L553	L553	K432	M424
V1155	D1094	G1034	L914	L914	A853	L793	I737	S674	I554	I554	L433	M425
F1156	Q1095	Y1035	Y915	Y915	W854	T794	I737	S674	C555	C555	E434	M426
L1156	M1096	V1036	K916	K916	GLN	W795	N738	W675	R611	R611	E436	M427
A1157	P1097	D1037	Y917	Y917	LEU	G796	G739	G676	H612	H612	Y437	M428
Y1158	L1098	G1038	Y918	Y918	PRD	W797	D740	L666	Y558	Y558	L438	M429
E1159	M1099	V1039	L919	L919	GLU	S798	V741	S679	T559	T559	A437	M430
N1160	M1100	I1040	L920	L920	PRD	W799	V741	L680	D560	D560	E438	M431
N1161	D1101	I1041	C921	C921	GLU	N799	S742	W681	L561	L561	L439	M432
I1162	D1102	D1042	G922	G922	GLU	T800	I743	P682	L562	L562	Y437	M433
I1163	S1103	V1043	A923	A923	L862	L801	L744	ASP	S627	S627	L433	M434
D1164	S1103	I1043	K924	K924	T863	E802	N745	CYS	F620	F620	E434	M435
V1165	T1104	L1044	G925	G925	C864	L803	W746	PRD	L622	L622	W435	M436
F1166	K1105	H1045	R926	R926	C864	H804	D747	GLY	L625	L625	E436	M437
F1167	Y1106	D1046	Q927	Q927	K866	W805	E748	ARG	A626	A626	Y437	M438
R1167	A1107	T1047	V928	V928	R867	F806	Q749	HIS	S627	S627	L433	M439
L1168	A1107	A1048	V929	V929	S868	N807	D750	SER			L433	M440
I1169	L1109	L1049	V930	V930	S868	W808	Q751				L433	M441
F1170	Q1110	P1050	H931	H931	D870	E809					L433	M442
S1171	E1111	Q1051	G871	G871	D870	E809					L433	M443
C1172	G1112	Q1052	R992	R992	D870	E809					L433	M444

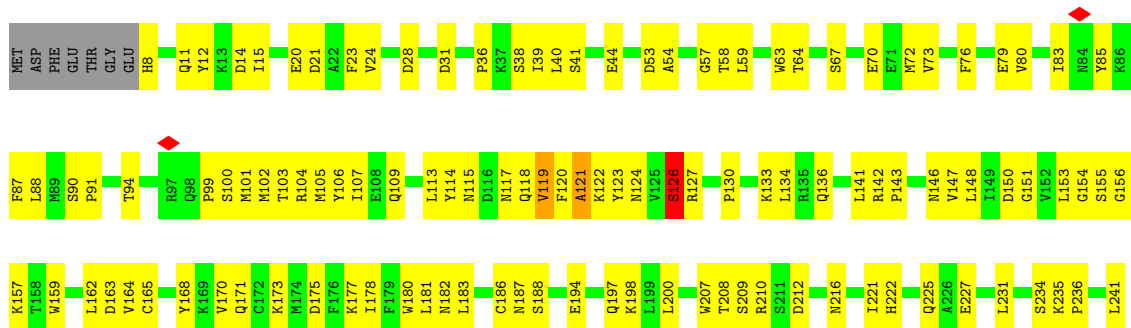
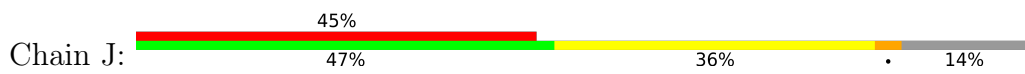








● Molecule 1: Apaf-1 related killer DARK







ALA	E1229	F1166	Y1106	D1046	A986	G925	H604	I743	P882	F620	T559	F494
VAL	E1230	R1167	A1107	T1047	V987	K866	V605	L744	ASP	C821	D560	R495
ASP	V1231	L1168	S1108	A1048	D988	R867	F806	M745	CYS	L622	L561	F496
ALA	H1232	I1169	L1109	L1049	S989	S868	N807	W746	GLY	L625	R563	L497
PRO	H1233	F1170	Q1051	P1050	K990	T869	V608	D747	ARG	A626	I564	Q499
ILE	H1234	S1171	Q1052	Q1051	E991	D870	E809	E748	HIS	G828	A565	R502
ALA	C1235	C1172	F1053	F1053	R992	G871	N810	Q749	SER	Q829	L566	H503
ASP	M1173	M1173	I1054	I1054	I993	R872	D811	D750	GLY	I830	M567	D504
ILE	Q1174	Q1174	I1115	I1115	I994	Y873	T812	Q751	GLY	E830	A568	S505
VAL	L1175	L1175	I1116	I1116	L995	L874	P813	E752	SER	L631	E569	A506
ASP	R1176	R1176	E1056	E1056	I996	L875	L814	F753	LYS	L632	D570	O507
VAL	Y1177	Y1177	P1057	P1057	K997	L876	L815	K754	GLN	T633	E571	M508
THR	F1241	F1178	L1118	L1118	K998	L877	L816	L755	LEU	D634	A572	N509
VAL	S1242	Q1179	S1119	D1059	A999	G878	D817	S756	VAL	V635	I573	A510
ALA	P1243	I1180	D1120	Y1060	I1000	T878	V618	H757	N699	S636	F574	A511
ASP	C1244	C1181	H1121	L1061	S1001	S879	F619	V758	S700	L637	E575	G512
GLU	K1245	E1182	G1122	K1062	R1002	E880	E820	P759	V701	E838	E576	S513
PHE	L1246	E1183	V1123	Q1063	I1003	G881	E821	W760	W702	G639	A577	I514
PRO	L1247	E1184	C1124	V1064	S1004	L882	R822	K761	K703	E840	H578	L515
VAL	L1248	E1185	H1125	S1065	E1005	S823	S824	T763	F705	D841	K579	M516
ASN	S1250	I1186	L1126	P1066	W1006	Y884	K824	T764	I706	T642	Q580	L518
ARG	C1251	Q1187	D1127	M1067	W1007	Y886	T825	M764	I706	Y643	Q582	L519
GLY	C1251	Q1187	D1127	M1067	W1007	D886	A826	Q765	G707	L845	Q583	Q520
THR	ALA	K1188	I1128	I1068	T1098	L887	T827	S766	Y709	D647	F584	L521
ALA	A11252	A1189	A1129	V1070	I1009	K888	V828	Q767	A710	E848	D585	K522
GLU	K1190	K1190	M1130	V1070	I1010	L889	E828	I768	A710	E848	D586	Y524
LEU	N1190	N1190	N1130	A1071	T1011	S890	L829	R769	M711	S649	R587	K525
TRP	P1191	P1191	P1131	S1072	T1012	D891	L830	C770	L712	D650	V588	K526
ARG	S1192	S1192	S1132	S1072	H1013	P892	L831	F771	K713	S651	M589	Y527
LYS	Y1193	Y1193	A1133	H1074	H1013	R893	Y834	V772	I714	S652	F590	D530
ARG	L1194	L1194	F1134	S1075	A1014	L894	S835	Q773	I714	D653	T591	Y535
ASN	V1195	V1195	V1135	S1075	A1014	R894	S835	W774	A716	I654	N592	E536
ASN	A1196	A1196	K1136	Q1076	S1016	R895	V636	K776	L718	R656	H593	R537
ILE	T1197	T1197	P1137	Q1077	S1017	S896	W637	R777	L719	M657	L538	L539
PRO	D1198	D1198	K1138	K1078	C1018	S897	R838	Y778	N720	V659	N640	N640
GLU	D1199	D1199	D1139	T1079	K1018	R898	R838	W780	E721	F660	A541	I542
LEU	G1200	G1200	S1140	V1080	I1020	S899	L839	V781	D722	N661	Q598	L543
LEU	T1201	T1201	E1141	I1081	M1021	E900	N840	C782	G724	Q662	R600	D544
ALA	M1202	M1202	E1142	F1082	A1022	H901	F841	T783	L725	Q663	Q601	F545
VAL	L1203	L1203	Y1143	Q1083	I1023	1902	L842	W784	PRD	K664	I602	L546
LYS	A1204	A1204	Y1144	L1084	S1024	E903	P843	S785	ALA	H665	I603	K648
PHE	M1205	M1205	V1145	E1085	A1025	C904	G844	N785	ALA	L666	I603	K648
VAL	G1206	G1206	G1146	K1086	F1026	V905	L845	W786	ASN	I667	N604	I549
GLY	F1207	F1207	F1147	I1087	M1027	D906	V847	T787	I730	G606	L605	E550
ASN	E1208	E1208	L1148	D1088	D1028	1907	S848	W788	I730	Q731	L605	E551
ALA	M1209	M1209	L1149	P1089	Q1030	Y908	L849	L788	Q731	H670	G066	N552
ARG	L1212	L1212	K1150	L1090	Q1030	L910	Q850	W791	L732	C671	D607	L553
ARG	H1213	H1213	N1151	Q1091	I1031	F911	S851	D792	H733	M872	N608	L553
LYS	L1214	L1214	S1152	P1092	F1032	D912	H733	Q792	H733	G673	E909	I554
GLN	L1215	L1215	L1153	M1093	V1033	F913	S852	L793	W734	G673	G810	C555
HIS	F1215	F1215	D1094	D1094	G1034	R914	A853	T794	I737	S674	R611	S556
SER	F1155	F1155	Q1095	Q1095	Y1035	Y915	V854	T795	N738	V675	H612	K557
VAL	M1219	M1219	L1156	W1096	Y1036	K916	V854	W796	N738	K676	H612	Y558
THR	R1220	R1220	A1157	P1097	D1037	Y917	GLN	S797	G739	V675	L616	L616
GLU	K1221	K1221	Y1158	L1098	G1038	1918	PRD	S797	D740	L677	H617	H617
ASP	Q1223	Q1223	E1159	M1099	V1039	Y919	GLU	S798	V741	S679	M618	M618
L1224	L1224	L1224	M1160	M1100	I1040	L920	G859	S798	V741	S679	L680	L680
I1225	I1225	I1225	N1161	D1101	I1041	C921	S860	S799	S742	L680	W681	W681
Y1226	Y1226	Y1226	N1163	I1102	I1042	G922	S861	N799	S742	L680	L619	L619
S1227	S1227	S1227	I1163	S1103	D1043	A923	T863	T800	S742	L680	L619	L619
I1228	I1228	I1228	V1165	T1104	I1044	K924	C864	L803	S742	L680	L619	L619

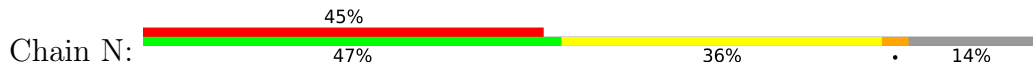






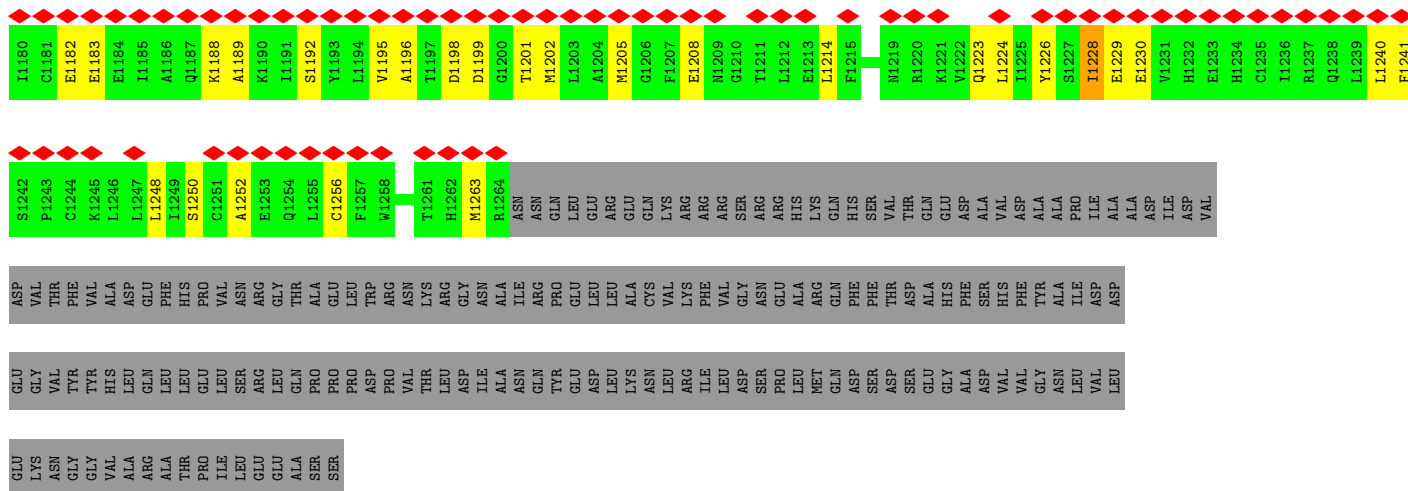
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R990	P1050	Q1110	F1170	H1232	ALA	HIS	GLY
E991	Q1051	E1111	S1171	E1233	ALA	PHE	ALA
R992	Q1052	G1112	C1172	H1234	PRO	SER	ASP
I993	F1053	G1113	N1173	I1235	ILE	HIS	VAL
H994	I1054	Y1114	Q1174	I1236	ALA	PHE	VAL
L995	E1055	Y1115	Q1175	I1237	ASP	TYR	GLY
I996	E1056	I1116	L1175	R1237	ASP	ILE	ASN
R997	P1057	I1117	R1176	Q1238	VAL	ASP	VAL
P998	I1058	L1117	Y1177	L1239	ASP	GLY	GLU
A999	D1059	F1118	A1178	L1240	VAL	VAL	LYS
I1000	Y1060	S1119	Q1179	F1241	THR	THR	ASN
S1001	L1061	D1120	I1180	S1242	PHE	TYR	GLY
R1002	K1062	H1121	C1181	P1243	TYR	TYR	GLY
I1003	Q1063	G1122	E1182	C1244	ALA	HIS	VAL
S1004	V1064	V1123	E1183	K1245	ASP	ALA	ALA
E1005	S1065	C1124	E1184	L1246	GLU	GLN	ARG
W1006	P1066	C1124	E1185	L1247	PHE	LEU	ALA
S1007	N1067	L1126	I1186	L1248	HIS	LEU	THR
T1008	N1067	D1127	A1186	I1249	LEU	GLU	PRO
I1009	I1068	I1128	Q1187	S1250	ASN	ARG	LEU
T1010	L1069	I1129	K1188	C1251	ARG	GLY	GLU
P1011	L1070	M1130	A1189	A1252	GLY	GLN	ALA
T1012	A1071	P1131	K1190	E1253	THR	GLN	ALA
H1013	A1072	P1132	I1191	L1255	PRO	PRO	SER
A1014	A1073	S1132	S1192	L1256	LEU	PRO	SER
A1015	H1074	F1133	Y1193	C1256	PRO	ARG	PRO
S1016	S1075	F1134	L1194	F1257	VAL	ASN	VAL
M1017	Q1077	V1135	V1195	W1258	THR	LYS	THR
C1018	K1078	K1136	A1196	T1261	ASP	GLY	LEU
K1019	T1079	P1137	T1197	H1262	ALA	ALA	ALA
I1020	I1080	D1139	D1199	M1263	ASN	ILE	ASN
M1021	I1081	S1140	G1200	R1264	PRO	TYR	GLY
I1023	F1082	E1141	T1201	ASN	LEU	ASP	LEU
S1024	Q1083	E1142	M1202	GLN	LEU	LEU	LEU
A1025	I1084	Y1143	L1203	ASN	ALA	ALA	ALA
F1026	E1085	I1144	A1204	GLN	CYS	VAL	VAL
M1027	K1086	V1145	M1205	ARG	VAL	ARG	LYS
D1028	I1087	G1146	G1206	GLN	GLN	PHE	THR
E1029	P1088	F1147	F1207	LYS	LYS	VAL	VAL
Q1030	P1089	D1148	E1208	ARG	ARG	GLY	GLY
I1031	Q1091	L1149	M1209	ARG	ASN	ASN	ASP
F1032	Q1091	K1150	L1212	ARG	ALA	ALA	ALA
V1033	N1093	M1151	E1213	ARG	SER	SER	SER
G1034	D1094	S1152	L1214	HIS	ALA	ALA	GLN
Y1035	Q1095	L1153	F1215	GLN	GLN	GLN	GLN
W1036	W1096	F1155	A1216	HIS	HIS	THR	THR
D1037	P1097	L1156	M1219	SER	SER	VAL	VAL
V1039	L1098	A1157	R1220	THR	THR	THR	THR
I1040	M1099	Y1158	K1221	GLN	GLN	GLN	GLN
I1041	M1100	E1159	V1221	GLU	GLU	GLU	GLU
D1042	D1101	M1160	Q1223	ASP	ASP	ALA	ALA
I1043	D1102	M1161	L1224	VAL	VAL	VAL	VAL
I1044	S1103	I1162	Y1226	VAL	VAL	VAL	VAL
I1045	T1104	I1163	S1227	ASP	ASP	ASP	ASP
D1046	K1105	V1165	I1228	THR	THR	SER	SER
T1047	Y1106	F1166	E1229	SER	SER	SER	SER
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	L1108	L1168					

• Molecule 1: Apaf-1 related killer DARK

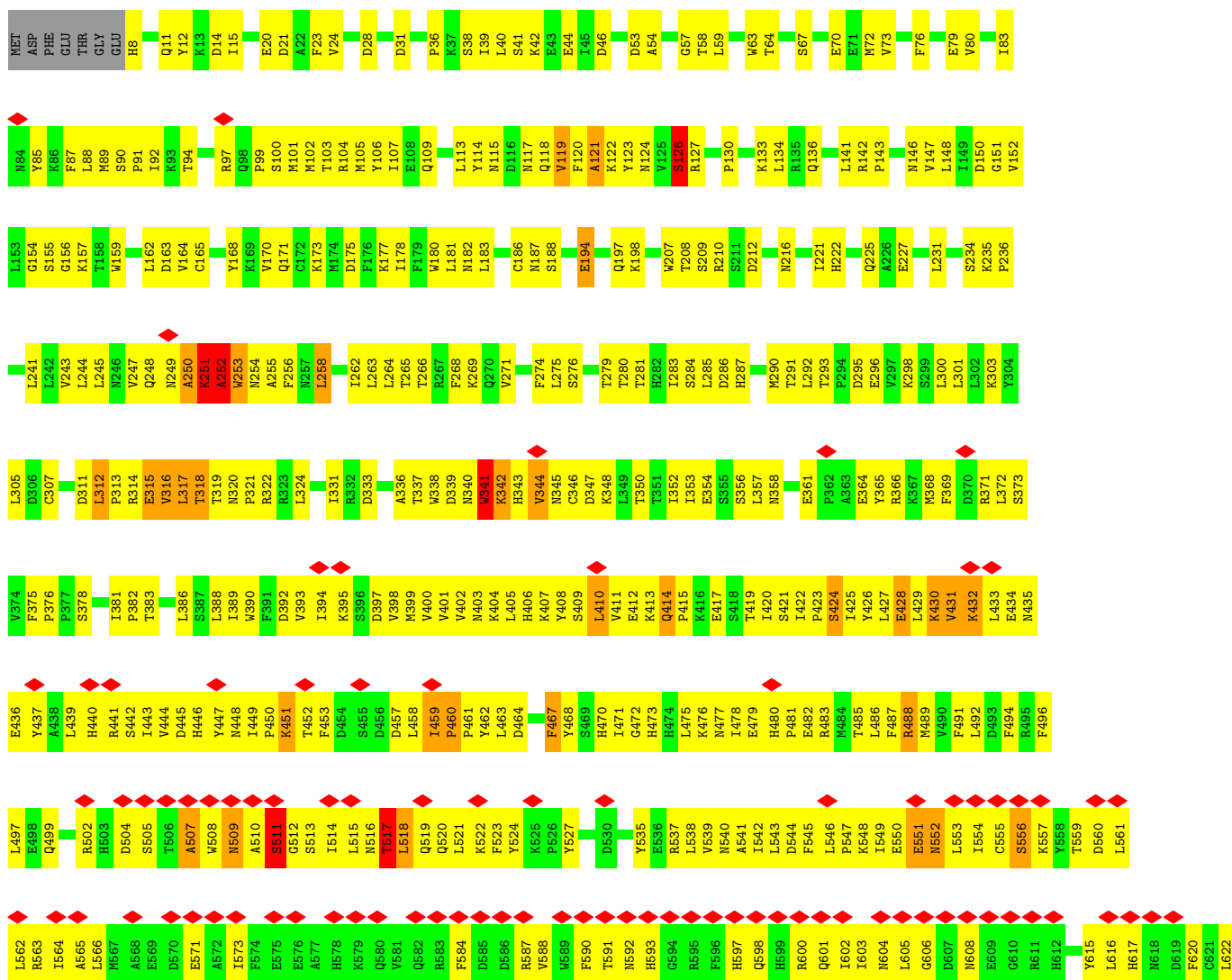


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ASP	L88	K169	T262	V247	V316
GLU	M89	V170	K177	Q248	L317
THR	P91	S100	I178	N249	T318
GLY	H8	M101	E108	A950	T319
GLU	Q98	M102	Q109	K251	N320
	P99	M102	L113	A952	P321
	S100	M102	Y114	W253	N320
	Y112	M102	Y114	N254	N320
	K13	M102	Y114	A255	P321
	D14	M102	Y114	F256	N320
	I15	M102	Y114	R257	P321
	E20	M105	D116	L258	I331
	D21	Y106	N117	T262	D333
	A22	I107	Q118	L263	A336
	F23	E108	F119	L264	T337
	V24	Q109	W180	T265	W338
	D28	L113	L181	T266	D339
	M115	Y114	M182	R267	N340
	D116	Y114	L183	F268	W341
	N117	D116	C186	K269	K342
	Q118	N117	M187	Q270	H343
	F119	Q118	S188	V271	V344
	A121	F120	E194	F274	N345
	S41	Q122	Q197	L275	C346
	E44	Y123	K198	S276	D347
	D53	M124	W207	T279	K348
	A54	V125	T208	T280	L349
	G57	S126	R210	H281	T350
	T58	R127	L285	H282	I353
	L59	P130	D286	H287	E354
	W63	K133	N216	M290	L357
	T64	L134	I221	T291	N358
	S67	R135	H222	L292	E361
	E70	Q136	S223	T293	P362
	M72	L141	I224	P294	A363
	V73	R142	Q225	D295	E364
	F76	P143	A226	E296	Y365
	E79	M146	E227	W297	R366
	V80	V147	L231	K298	K367
	I83	L148	S234	S299	F369
	N84	L149	K235	L300	D370
	Y85	G151	P236	L302	R371
	K86	G154	L241	K303	L372
		S155	L242	C307	S373
		G156	L243	D311	V374
		K157	L244	L312	F375
		T158	L245	P313	P376
		W159		R314	P377
					S378
					I381
					P382
					T383

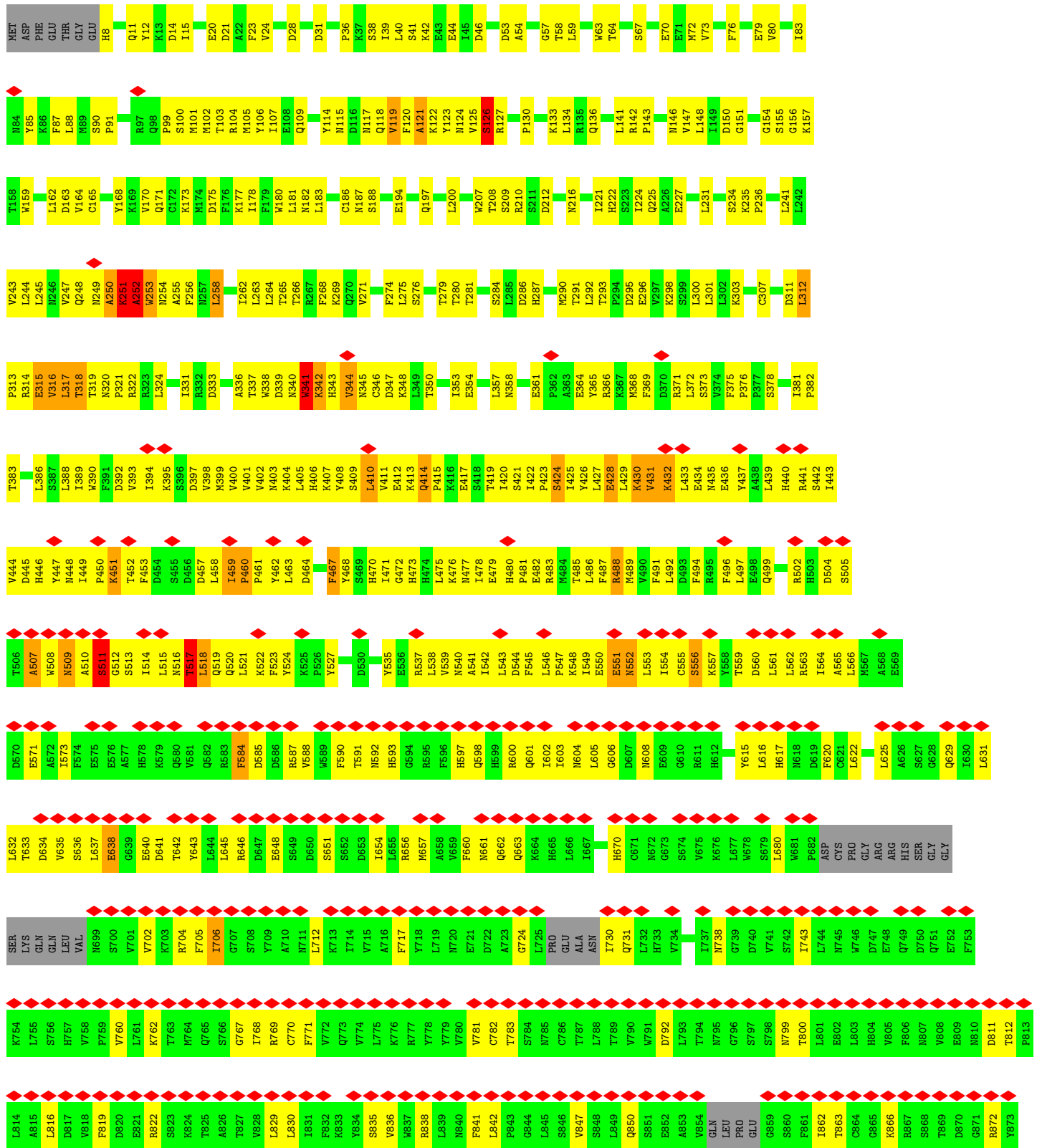
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Y1060	L1061	K1062	Q1063	V1064	S1065	P1066	M1067	I1068	L1069	V1070	A1071	S1072	A1073	H1074	S1075	A1076	A1077	Q1078	T1079	V1080	I1081	F1082	Q1083	L1084	E1085	K1086	I1087	D1088	P1089	L1090	Q1091	P1092	M1093	D1094	Q1095	M1096	P1097	L1098	M1099	M1100	D1101	V1102	S1103	T1104	K1105	F1106	A1107	S1108	L1109	Q1110	E1111	Q1112	Q1113	Y1114	I1115	L1116	Y1117	E1118	S1119	
G939	S940	R941	S942	H943	Q944	R945	R946	E947	I948	A949	W950	W951	H952	S953	A954	D955	E956	I957	S958	W959	W960	T961	K962	A963	C964	L965	E966	P967	Y970	L971	R972	S973	L974	Y975	D976	M977	T978	R979	E980	R981	T982	Q983	L984	L985	A986	V987	D988	S989	R990	H991	H992	T993	L994	R995	H996	L997	L998	K999	P998	A999
S879	E880	C881	L882	I883	W884	Y885	D886	L887	K888	I889	S890	D891	P892	W893	L894	R895	S896	R897	W898	S899	E900	H901	I902	E903	C904	Y905	D906	I907	Y908	E909	L910	F911	D912	P913	Y914	R915	R916	Y917	I918	Y919	L920	C921	G922	K923	G924	G925	K926	Q927	V928	V929	H930	V931	H932	T933	L934	R935	S936	V937	S938	
F819	D820	E821	R822	S823	K824	T825	A826	R827	W828	L829	L830	I831	K833	Y834	S835	W836	R837	R838	L839	W840	F841	L842	P843	C844	L845	S846	W847	S848	L849	Q850	S851	E852	A853	W854	G1N	PRO	GLU	G859	S860	F861	T862	T863	C864	G865	K866	R867	S868	T869	D870	G871	R872	T873	L874	L875	L876	G877	T878			
F759	W760	L761	K762	I763	W764	Q765	S766	G767	I768	R769	C770	F771	V772	Q773	W774	L775	K776	R777	W778	Y779	W780	W781	C782	I783	S784	M785	C786	I787	L788	W789	W790	W791	D792	L793	W794	M795	G796	S797	S798	N799	T800	L801	E802	L803	H804	W805	F806	R807	W808	E809	Q751	E752	F753	K754	L755	L814	L815	L816	D817	W818
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	M661	Q662	Q663	K664	H665	L666	H670	C671	M672	G673	S674	V675	K676	S679	L680	W681	P682	CYS	PRO	GLY	ARG	HIS	SER	GLY	LYS	GLN	LEU	A626	S627	G628	Q629	I630	L631	T632	T633	D634
V659	F674	E675	E676	A677	H678	K679	Q680	V681	Q682	R683	F684	D685	D686	R687	V688	W689	F690	T691	N692	H693	G694	R695	F696	H697	Q698	R600	Q601	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	L631	T632	T633	D634				
H446	Y447	M448	I449	P450	K451	T452	F453	D454	S455	D456	D457	L458	M399	V400	V401	V402	P461	Y462	L463	L404	L405	H406	K407	Y408	S409	L410	I471	C472	H473	H474	L475	K476	M477	I478	E479	H480	P481	S421	I422	R483	M484	T485	L486	F487	R488	M489	V490	F491	L492	F494	F496	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	D544	F545	L546	P547	K548	I549	E550	E551	N552	L553	I554	C555	S556	K557	V558	T559	D560	L561	L562	R563	I564	A565	L566	M567	A568	E569	D570	E571	A572			
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VAL	N699	S700	V701	W702	K703	R704	F705	I706	G707	S708	Y709	A710	M711	L712	K713	I714	W715	A716	F717	V718	L719	N720	E721	A723	G724	L725	PRO	GLU	ALA	ASN	I730	Q731	L732	H733	W734	I737	N738	G739	D740	V741	S742	I743	L744	N745	W746	D747	E748	Q749	D750	Q751	E752	F753	K754	L755	S756	H757	V758			



• 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
1	B	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
1	C	0.54	9/10231 (0.1%)	0.87	31/13873 (0.2%)
1	D	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
1	E	0.54	9/10231 (0.1%)	0.87	31/13873 (0.2%)
1	F	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
1	G	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
1	H	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
1	I	0.54	8/10231 (0.1%)	0.87	30/13873 (0.2%)
1	J	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
1	K	0.54	9/10231 (0.1%)	0.87	31/13873 (0.2%)
1	L	0.54	9/10231 (0.1%)	0.87	31/13873 (0.2%)
1	M	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
1	N	0.54	9/10231 (0.1%)	0.87	31/13873 (0.2%)
1	O	0.54	7/10231 (0.1%)	0.87	31/13873 (0.2%)
1	P	0.54	8/10231 (0.1%)	0.87	31/13873 (0.2%)
All	All	0.54	132/163696 (0.1%)	0.87	495/221968 (0.2%)

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 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	559	THR	C-N	11.28	1.49	1.33
1	M	559	THR	C-N	11.28	1.49	1.33
1	D	559	THR	C-N	11.27	1.49	1.33
1	L	559	THR	C-N	11.26	1.49	1.33
1	N	559	THR	C-N	11.26	1.49	1.33

The worst 5 of 495 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	414	GLN	O-C-N	13.80	135.52	121.30
1	I	414	GLN	O-C-N	13.78	135.50	121.30
1	P	414	GLN	O-C-N	13.78	135.49	121.30
1	C	414	GLN	O-C-N	13.77	135.49	121.30
1	K	414	GLN	O-C-N	13.77	135.49	121.30

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 [i](#)

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	695	0
1	B	10045	0	10046	708	0
1	C	10045	0	10046	708	0
1	D	10045	0	10046	719	0
1	E	10045	0	10046	696	0
1	F	10045	0	10046	720	0
1	G	10045	0	10046	706	0
1	H	10045	0	10046	682	0
1	I	10045	0	10046	697	0
1	J	10045	0	10046	693	0
1	K	10045	0	10046	721	0
1	L	10045	0	10046	715	0
1	M	10045	0	10045	700	0
1	N	10045	0	10046	690	0
1	O	10045	0	10046	687	0
1	P	10045	0	10046	694	0
2	A	30	0	9	6	0
2	B	30	0	9	6	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	11007	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 34.

The worst 5 of 11007 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	25
1	B	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	C	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	D	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	E	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	F	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	G	1224/1440 (85%)	989 (81%)	202 (16%)	33 (3%)	4	25
1	H	1224/1440 (85%)	988 (81%)	204 (17%)	32 (3%)	4	25
1	I	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	J	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	K	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	L	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	M	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	N	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
1	O	1224/1440 (85%)	988 (81%)	203 (17%)	33 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	1224/1440 (85%)	989 (81%)	203 (17%)	32 (3%)	4	25
All	All	19584/23040 (85%)	15822 (81%)	3248 (17%)	514 (3%)	6	25

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%)	1136 (100%)	2 (0%)	87	85
1	B	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	C	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	D	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	E	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	F	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	G	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	H	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	I	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	J	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	K	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	L	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	M	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	N	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
1	O	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	1138/1315 (86%)	1136 (100%)	2 (0%)	87	85
All	All	18208/21040 (86%)	18176 (100%)	32 (0%)	85	85

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	258	LEU
1	O	914	VAL
1	G	258	LEU
1	F	914	VAL
1	P	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 490 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	618	ASN
1	O	592	ASN
1	J	592	ASN
1	O	287	HIS
1	P	592	ASN

### 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	P	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.30	16 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	APK	N	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.29	16 (39%)
1	APK	B	251	1	32,33,33	2.84	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	J	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.29	16 (39%)
1	APK	E	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	L	251	1	32,33,33	2.84	13 (40%)	41,47,47	3.29	16 (39%)
1	APK	M	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.29	16 (39%)
1	APK	A	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	H	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	D	251	1	32,33,33	2.84	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	I	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	F	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	C	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	K	251	1	32,33,33	2.84	13 (40%)	41,47,47	3.30	16 (39%)
1	APK	O	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.29	16 (39%)
1	APK	G	251	1	32,33,33	2.83	13 (40%)	41,47,47	3.30	16 (39%)

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	P	251	1	-	11/19/37/37	0/3/3/3
1	APK	N	251	1	-	11/19/37/37	0/3/3/3
1	APK	B	251	1	-	11/19/37/37	0/3/3/3
1	APK	J	251	1	-	11/19/37/37	0/3/3/3
1	APK	E	251	1	-	11/19/37/37	0/3/3/3
1	APK	L	251	1	-	11/19/37/37	0/3/3/3
1	APK	M	251	1	-	11/19/37/37	0/3/3/3
1	APK	A	251	1	-	11/19/37/37	0/3/3/3
1	APK	H	251	1	-	11/19/37/37	0/3/3/3
1	APK	D	251	1	-	11/19/37/37	0/3/3/3
1	APK	I	251	1	-	11/19/37/37	0/3/3/3
1	APK	F	251	1	-	11/19/37/37	0/3/3/3
1	APK	C	251	1	-	11/19/37/37	0/3/3/3
1	APK	K	251	1	-	11/19/37/37	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	APK	O	251	1	-	11/19/37/37	0/3/3/3
1	APK	G	251	1	-	11/19/37/37	0/3/3/3

The worst 5 of 208 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 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	251	APK	C5-C4-N3	-7.58	116.28	126.72
1	E	251	APK	C5-C4-N3	-7.57	116.29	126.72
1	K	251	APK	C5-C4-N3	-7.57	116.29	126.72
1	B	251	APK	C5-C4-N3	-7.57	116.29	126.72
1	I	251	APK	C5-C4-N3	-7.56	116.31	126.72

There are no chirality outliers.

5 of 176 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 109 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	251	APK	7	0
1	M	251	APK	6	0
1	A	251	APK	7	0
1	H	251	APK	7	0
1	D	251	APK	7	0
1	I	251	APK	7	0
1	F	251	APK	7	0
1	C	251	APK	7	0
1	K	251	APK	7	0
1	O	251	APK	6	0
1	G	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	M	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.18	12 (26%)
2	DTP	A	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.20	13 (28%)
2	DTP	E	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.19	13 (28%)
2	DTP	G	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.19	13 (28%)
2	DTP	L	1501	-	31,32,32	3.89	14 (45%)	46,50,50	2.19	12 (26%)
2	DTP	O	1501	-	31,32,32	3.89	14 (45%)	46,50,50	2.18	12 (26%)
2	DTP	N	1501	-	31,32,32	3.89	14 (45%)	46,50,50	2.18	12 (26%)
2	DTP	P	1501	-	31,32,32	3.89	14 (45%)	46,50,50	2.18	12 (26%)
2	DTP	C	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.20	13 (28%)
2	DTP	F	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.20	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DTP	K	1501	-	31,32,32	3.89	14 (45%)	46,50,50	2.18	12 (26%)
2	DTP	I	1501	-	31,32,32	3.89	14 (45%)	46,50,50	2.18	12 (26%)
2	DTP	H	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.19	13 (28%)
2	DTP	D	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.20	13 (28%)
2	DTP	B	1501	-	31,32,32	3.90	14 (45%)	46,50,50	2.19	13 (28%)
2	DTP	J	1501	-	31,32,32	3.90	15 (48%)	46,50,50	2.18	12 (26%)

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	M	1501	-	-	6/22/34/34	0/3/3/3
2	DTP	A	1501	-	-	5/22/34/34	0/3/3/3
2	DTP	E	1501	-	-	5/22/34/34	0/3/3/3
2	DTP	G	1501	-	-	5/22/34/34	0/3/3/3
2	DTP	L	1501	-	-	6/22/34/34	0/3/3/3
2	DTP	O	1501	-	-	6/22/34/34	0/3/3/3
2	DTP	N	1501	-	-	6/22/34/34	0/3/3/3
2	DTP	P	1501	-	-	6/22/34/34	0/3/3/3
2	DTP	C	1501	-	-	5/22/34/34	0/3/3/3
2	DTP	F	1501	-	-	5/22/34/34	0/3/3/3
2	DTP	K	1501	-	-	6/22/34/34	0/3/3/3
2	DTP	I	1501	-	-	6/22/34/34	0/3/3/3
2	DTP	H	1501	-	-	5/22/34/34	0/3/3/3
2	DTP	D	1501	-	-	5/22/34/34	0/3/3/3
2	DTP	B	1501	-	-	5/22/34/34	0/3/3/3
2	DTP	J	1501	-	-	6/22/34/34	0/3/3/3

The worst 5 of 225 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 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1501	DTP	N6-C6-N1	-5.31	106.55	118.38
2	C	1501	DTP	N6-C6-N1	-5.30	106.56	118.38
2	J	1501	DTP	N6-C6-N1	-5.30	106.57	118.38
2	G	1501	DTP	N6-C6-N1	-5.30	106.58	118.38
2	B	1501	DTP	N6-C6-N1	-5.30	106.58	118.38

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

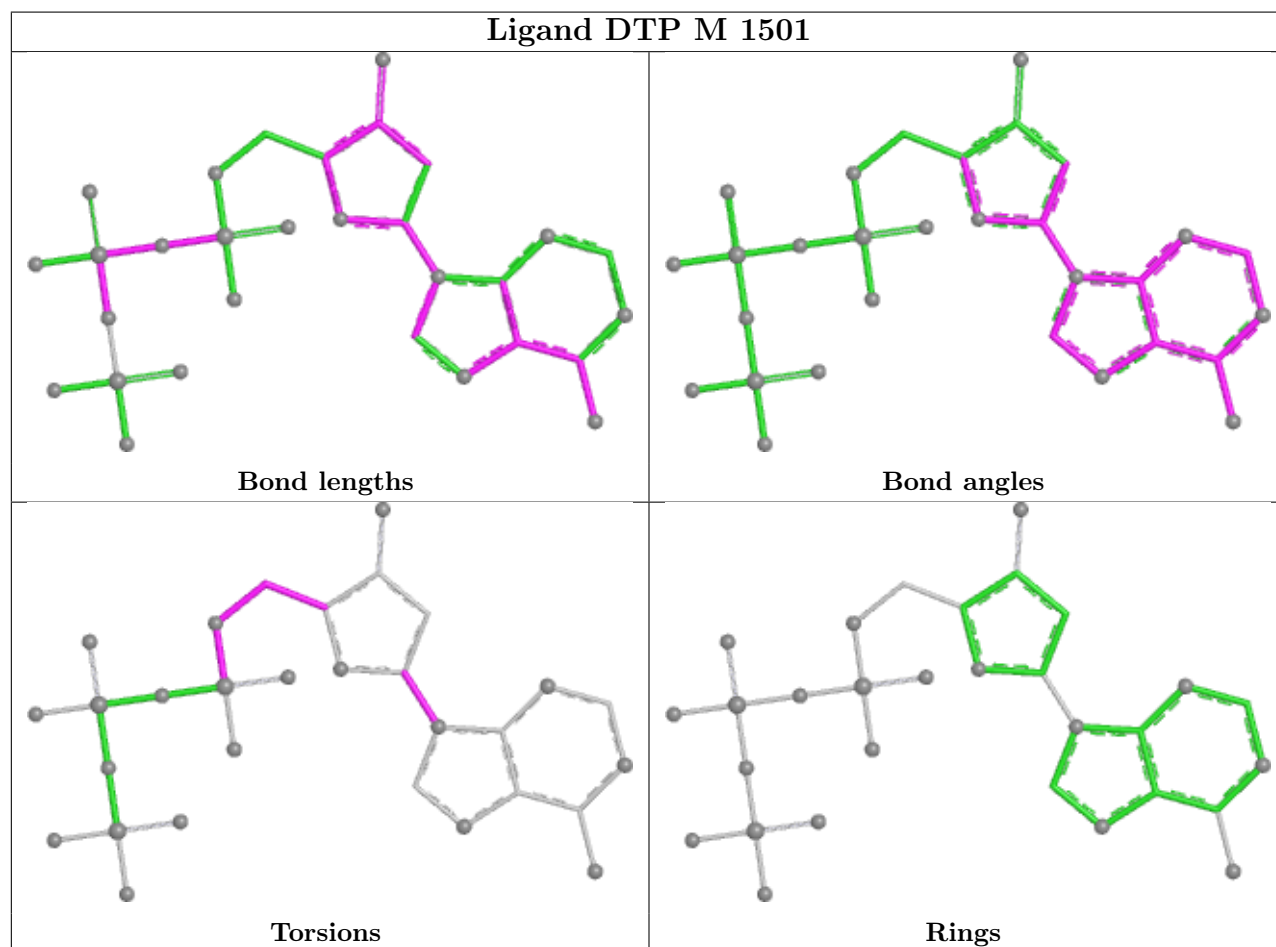
Mol	Chain	Res	Type	Atoms
2	A	1501	DTP	C3'-C4'-C5'-O5'
2	B	1501	DTP	C3'-C4'-C5'-O5'
2	C	1501	DTP	C3'-C4'-C5'-O5'
2	D	1501	DTP	C3'-C4'-C5'-O5'
2	E	1501	DTP	C3'-C4'-C5'-O5'

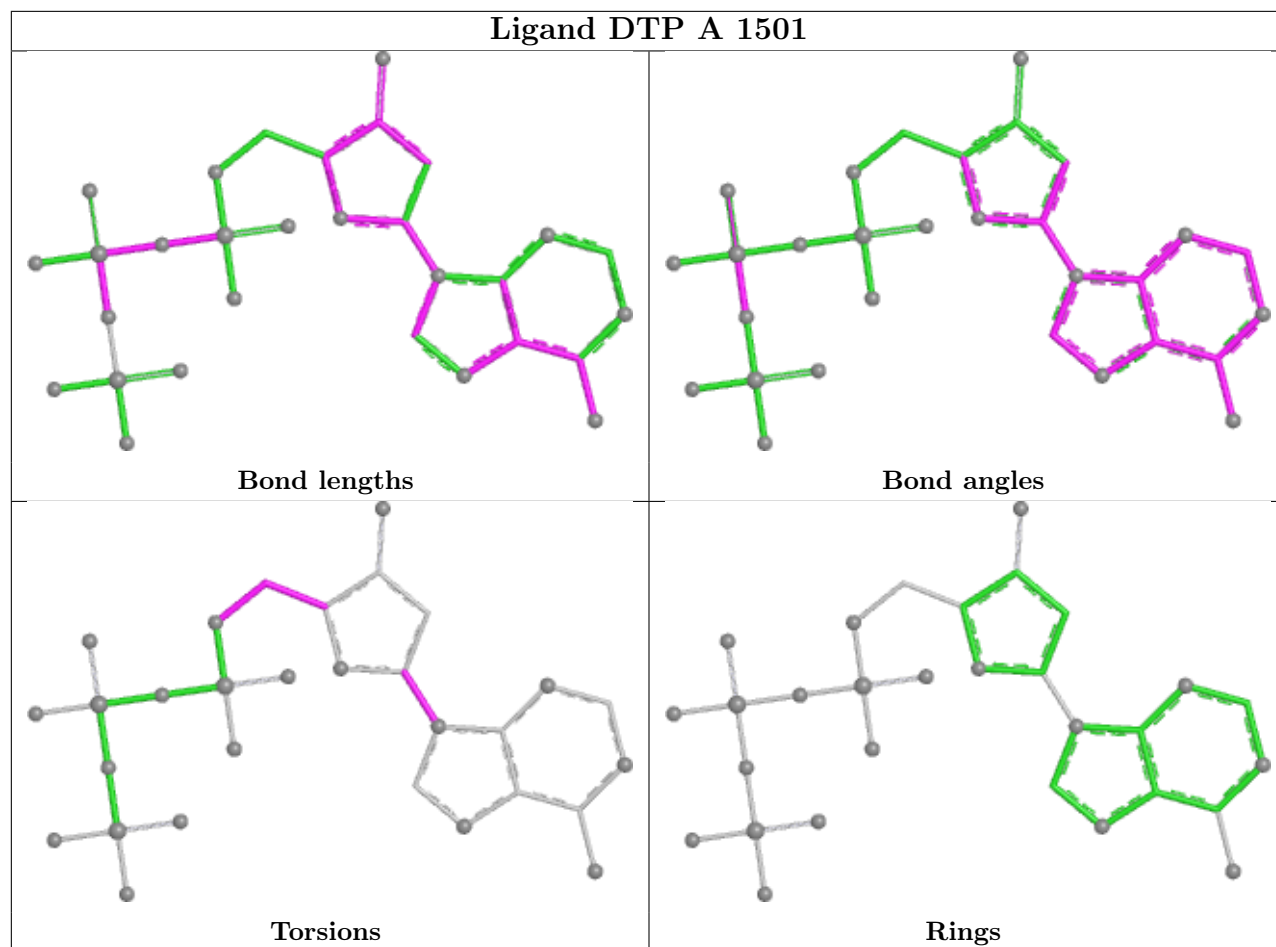
There are no ring outliers.

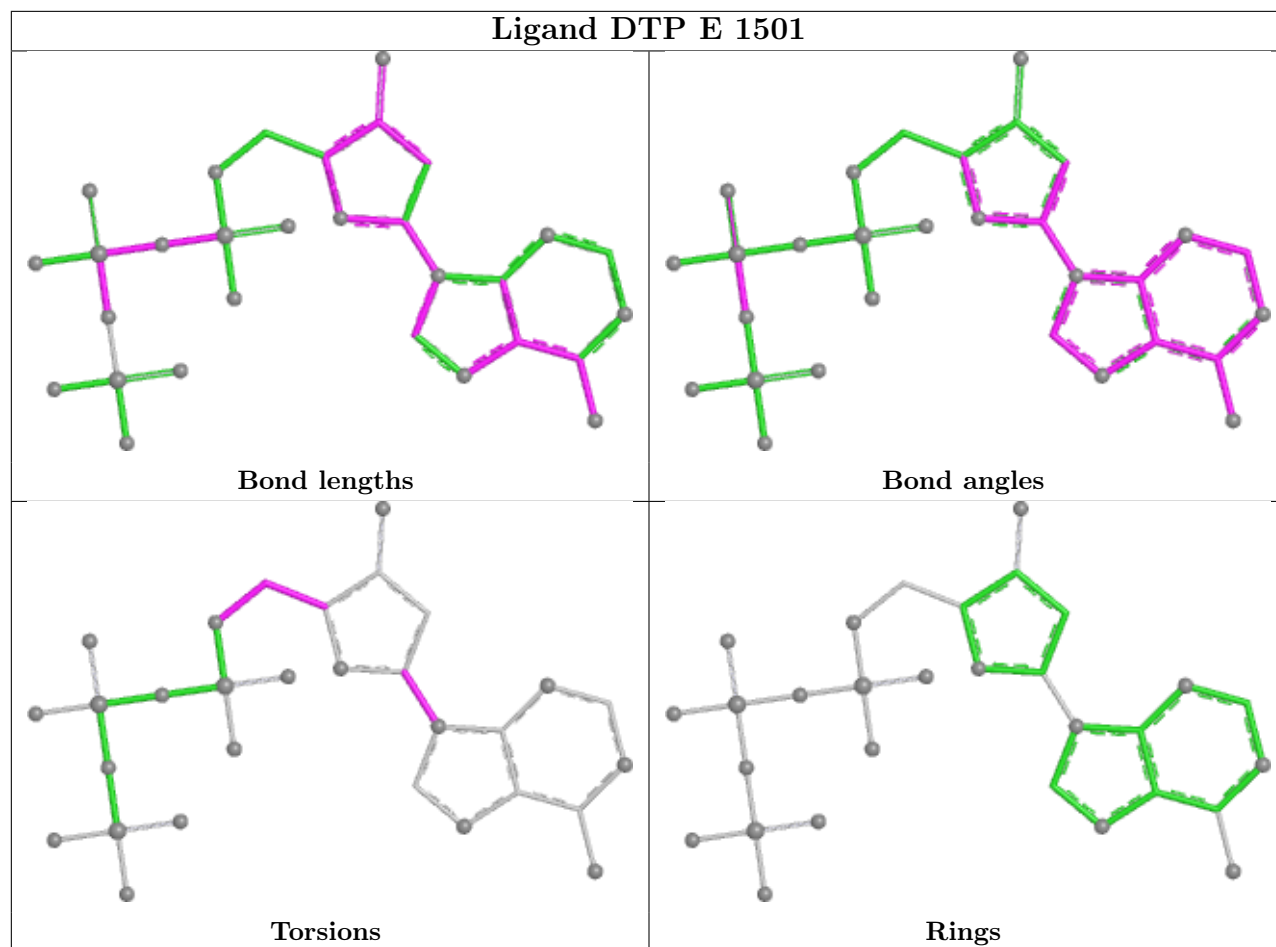
16 monomers are involved in 96 short contacts:

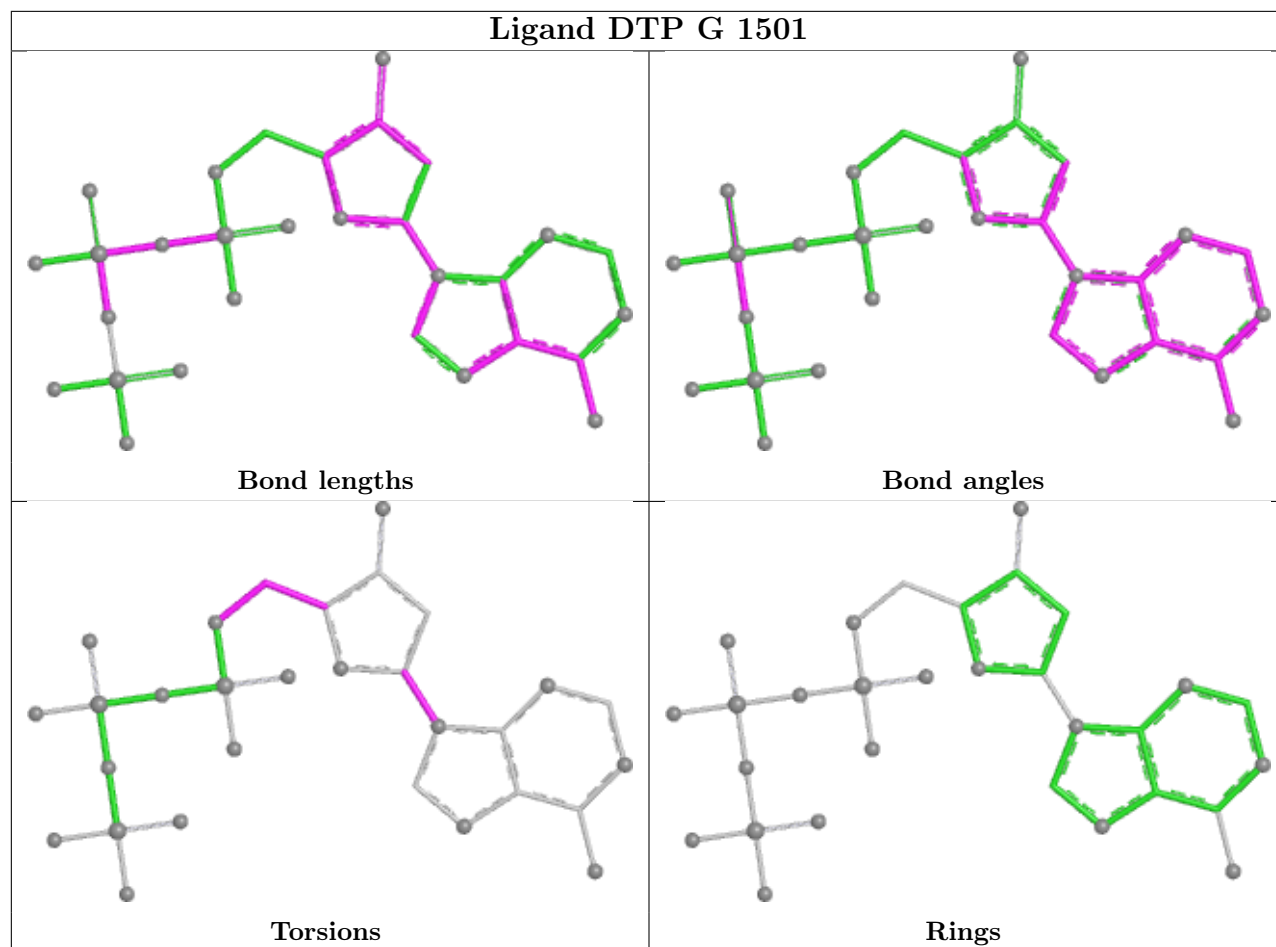
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1501	DTP	6	0
2	A	1501	DTP	6	0
2	E	1501	DTP	6	0
2	G	1501	DTP	6	0
2	L	1501	DTP	6	0
2	O	1501	DTP	6	0
2	N	1501	DTP	6	0
2	P	1501	DTP	6	0
2	C	1501	DTP	6	0
2	F	1501	DTP	6	0
2	K	1501	DTP	6	0
2	I	1501	DTP	6	0
2	H	1501	DTP	6	0
2	D	1501	DTP	6	0
2	B	1501	DTP	6	0
2	J	1501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

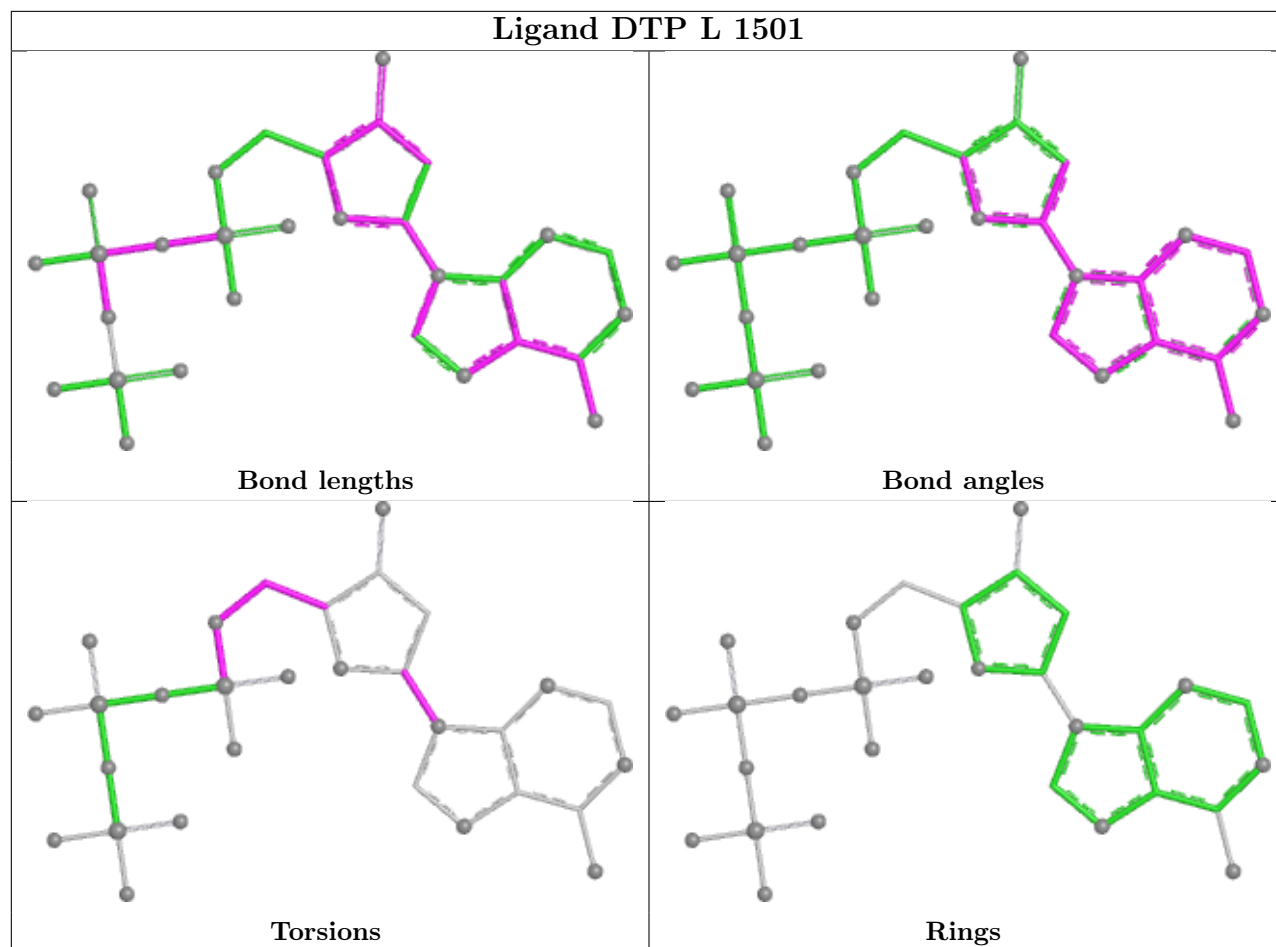
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

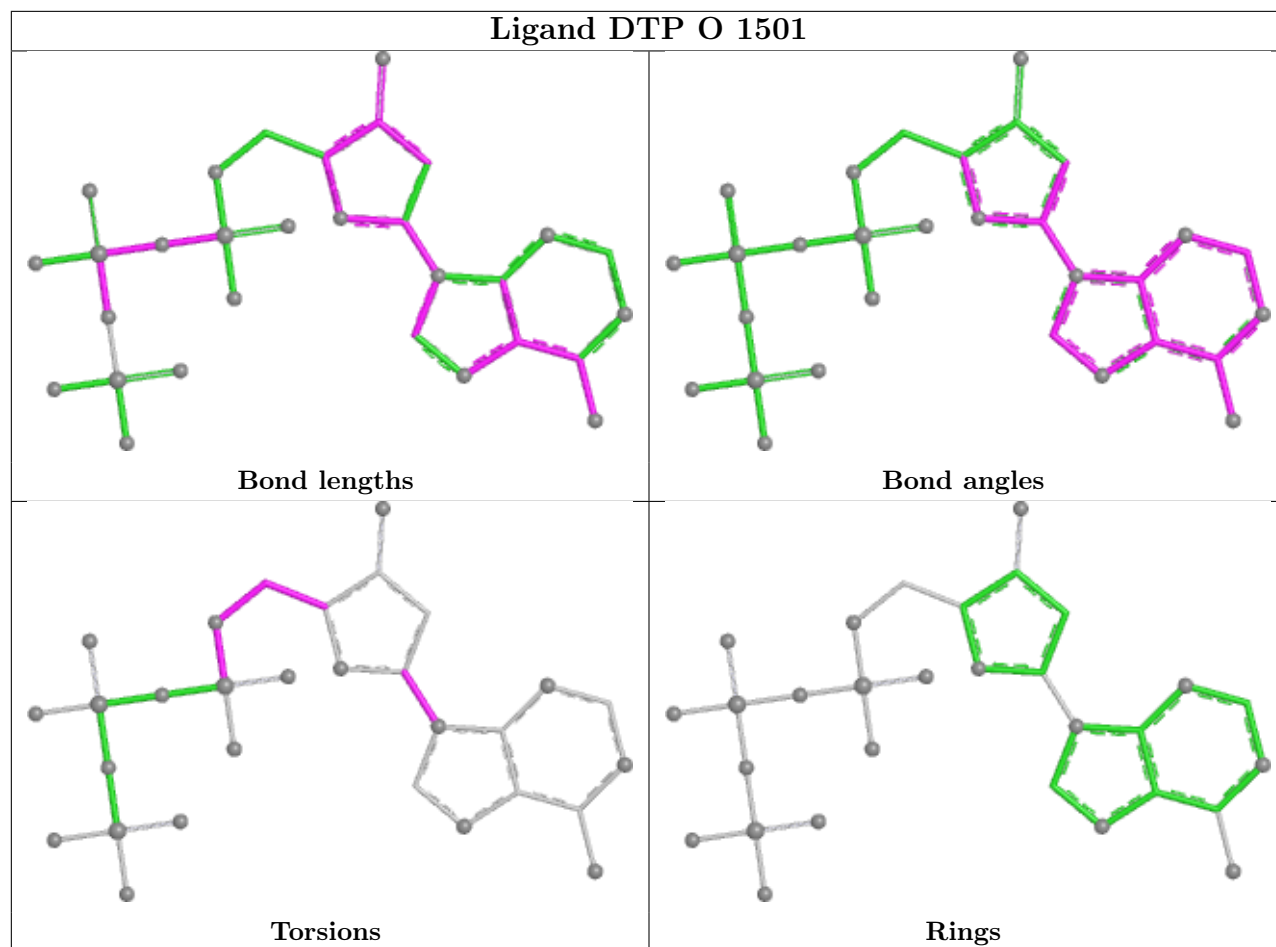


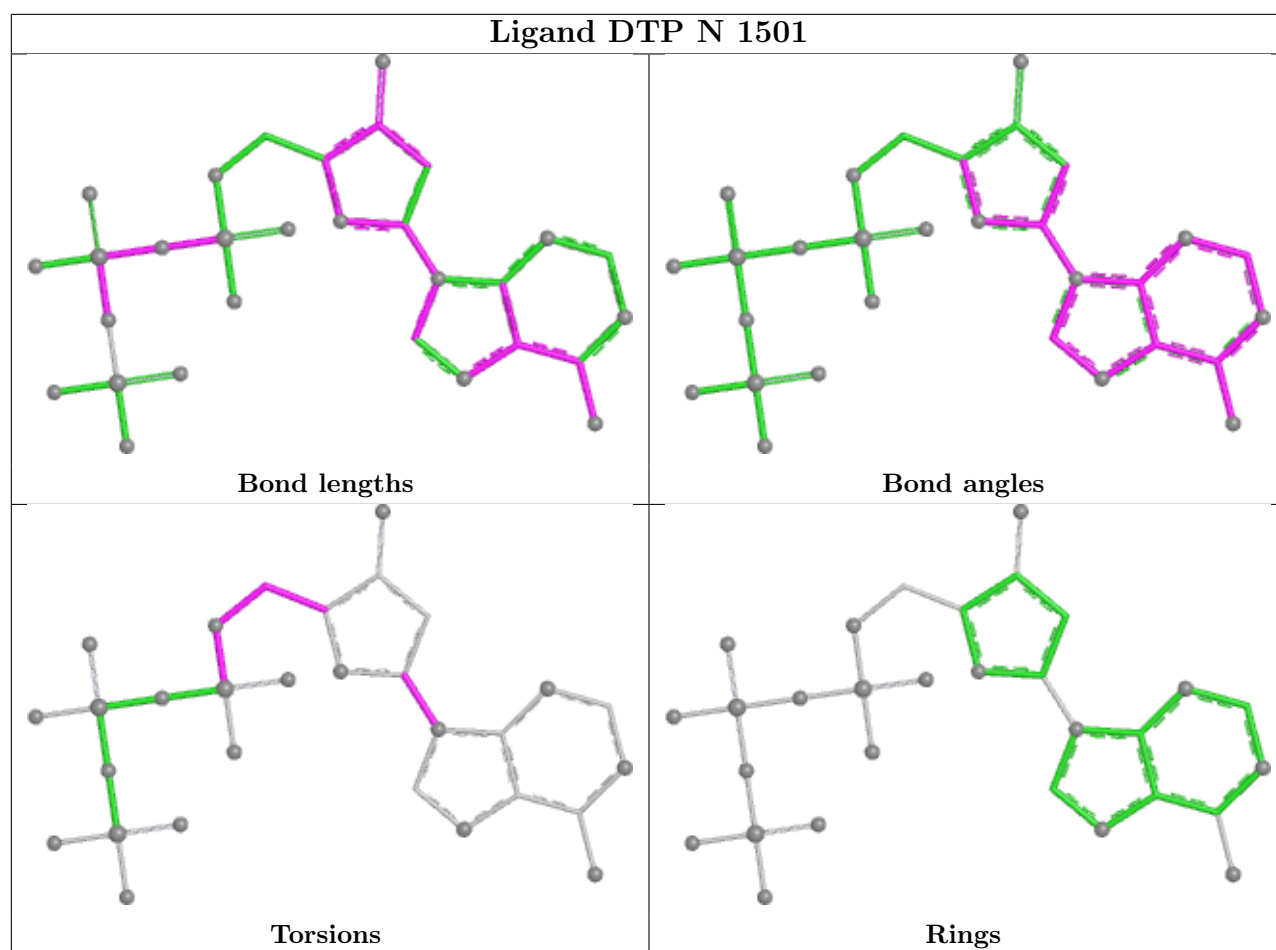


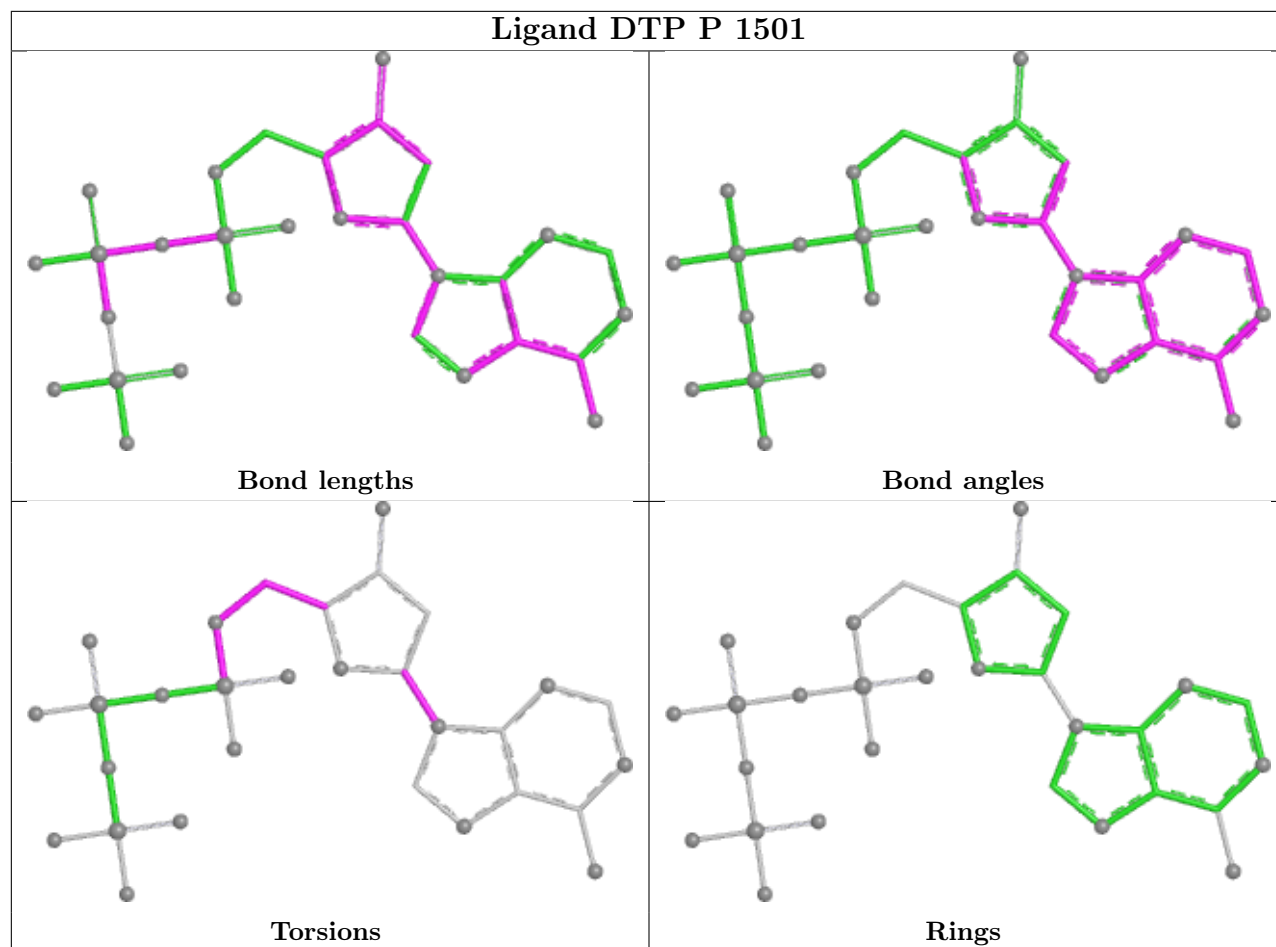


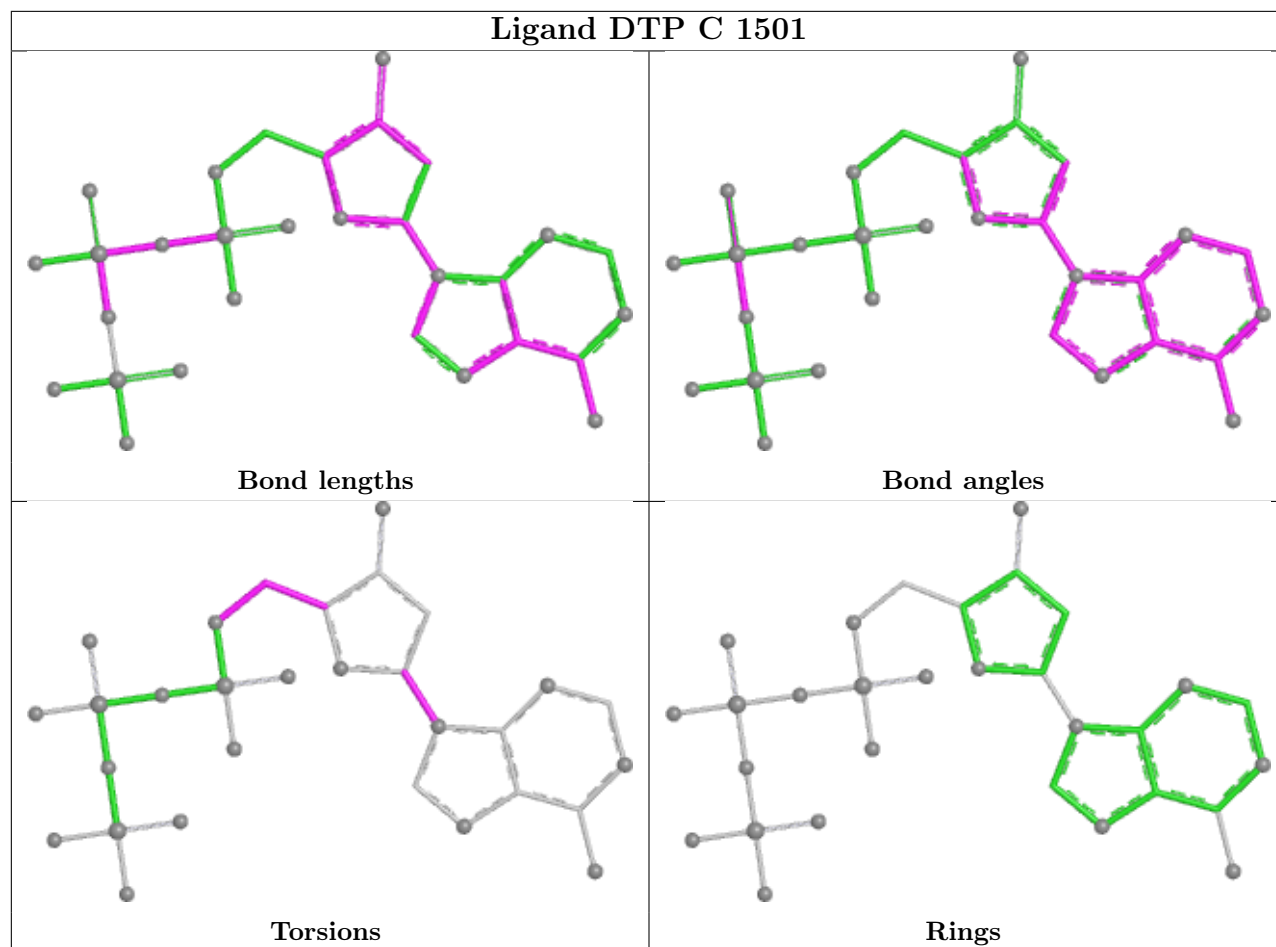


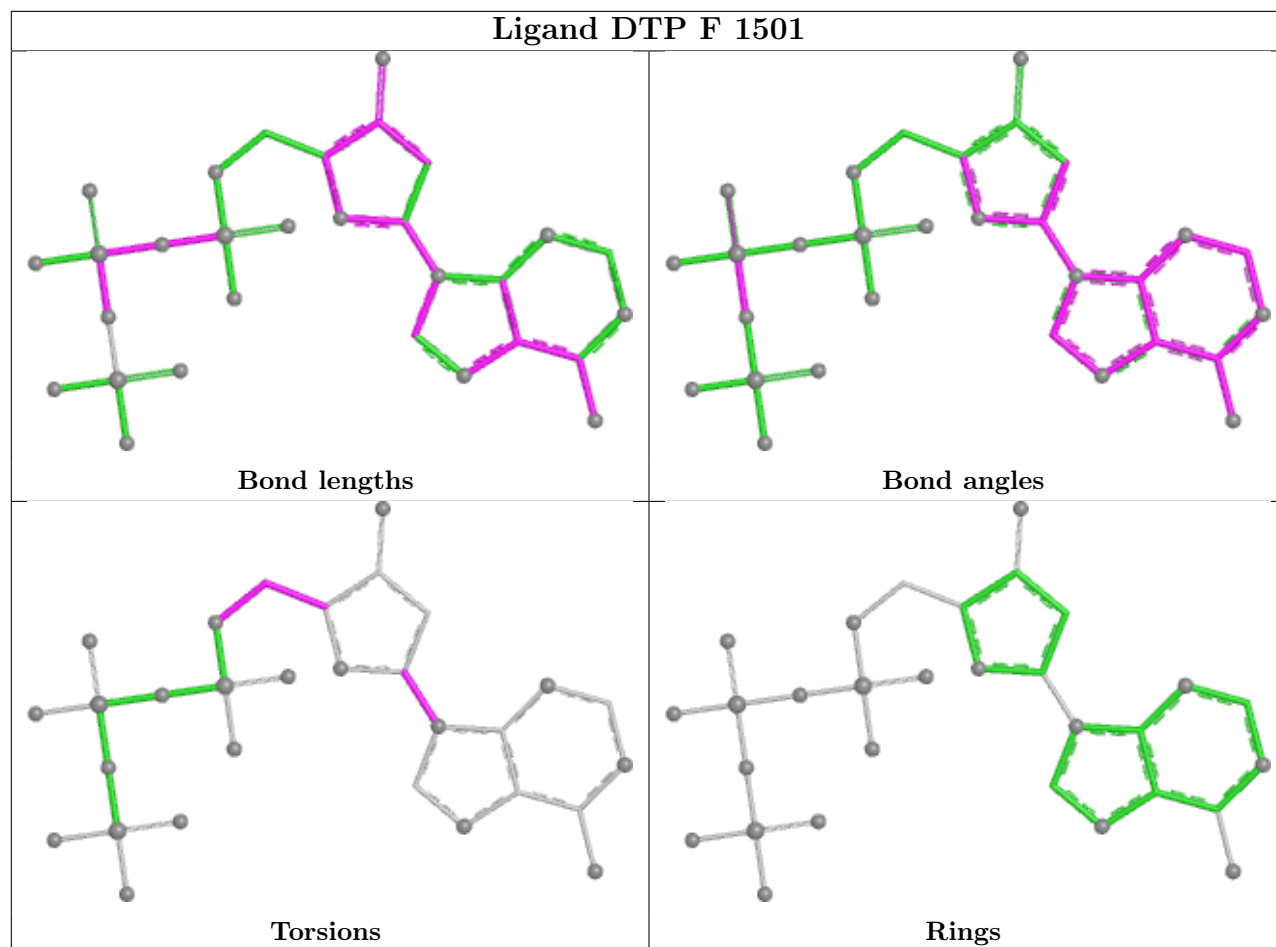


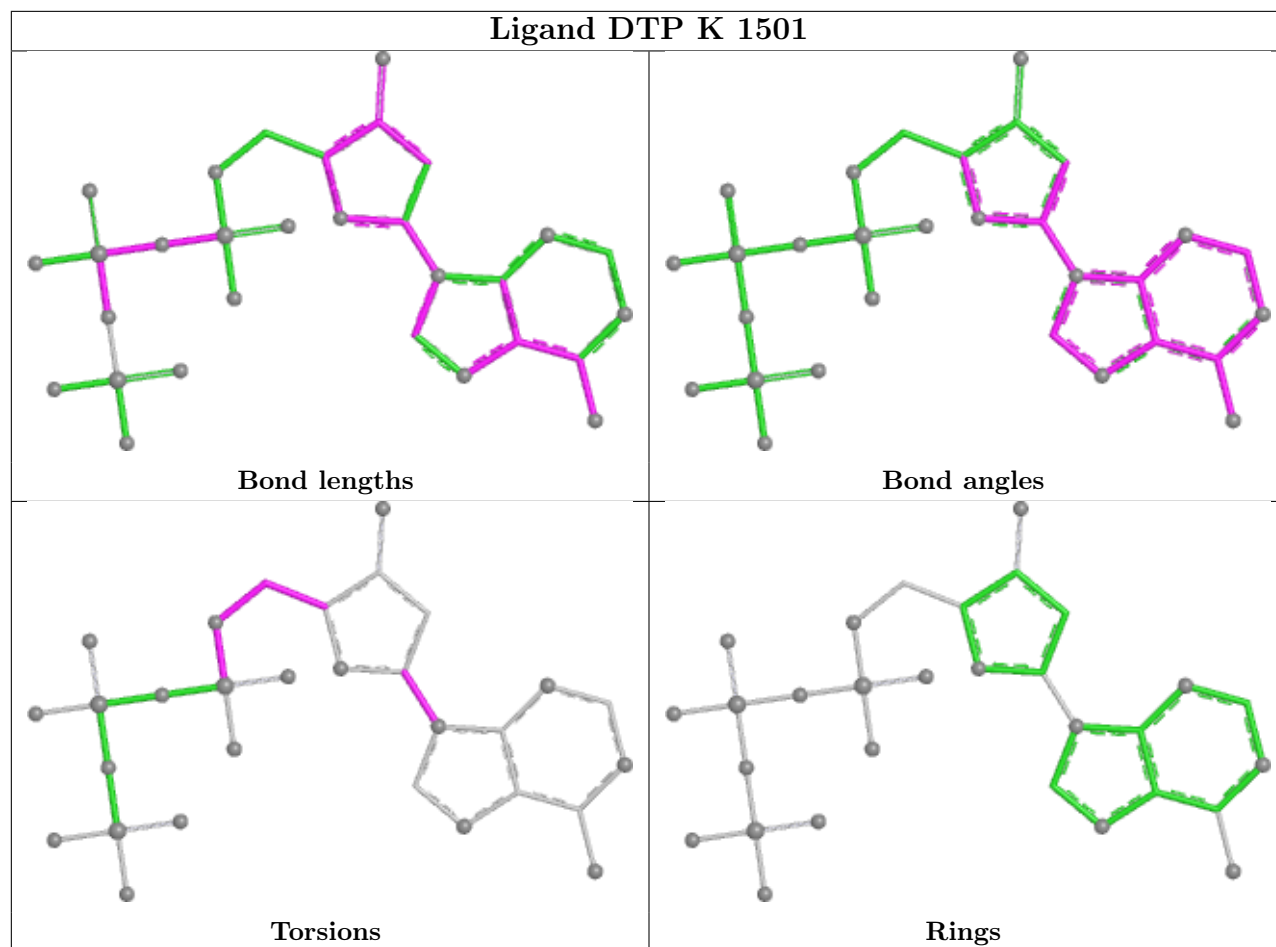


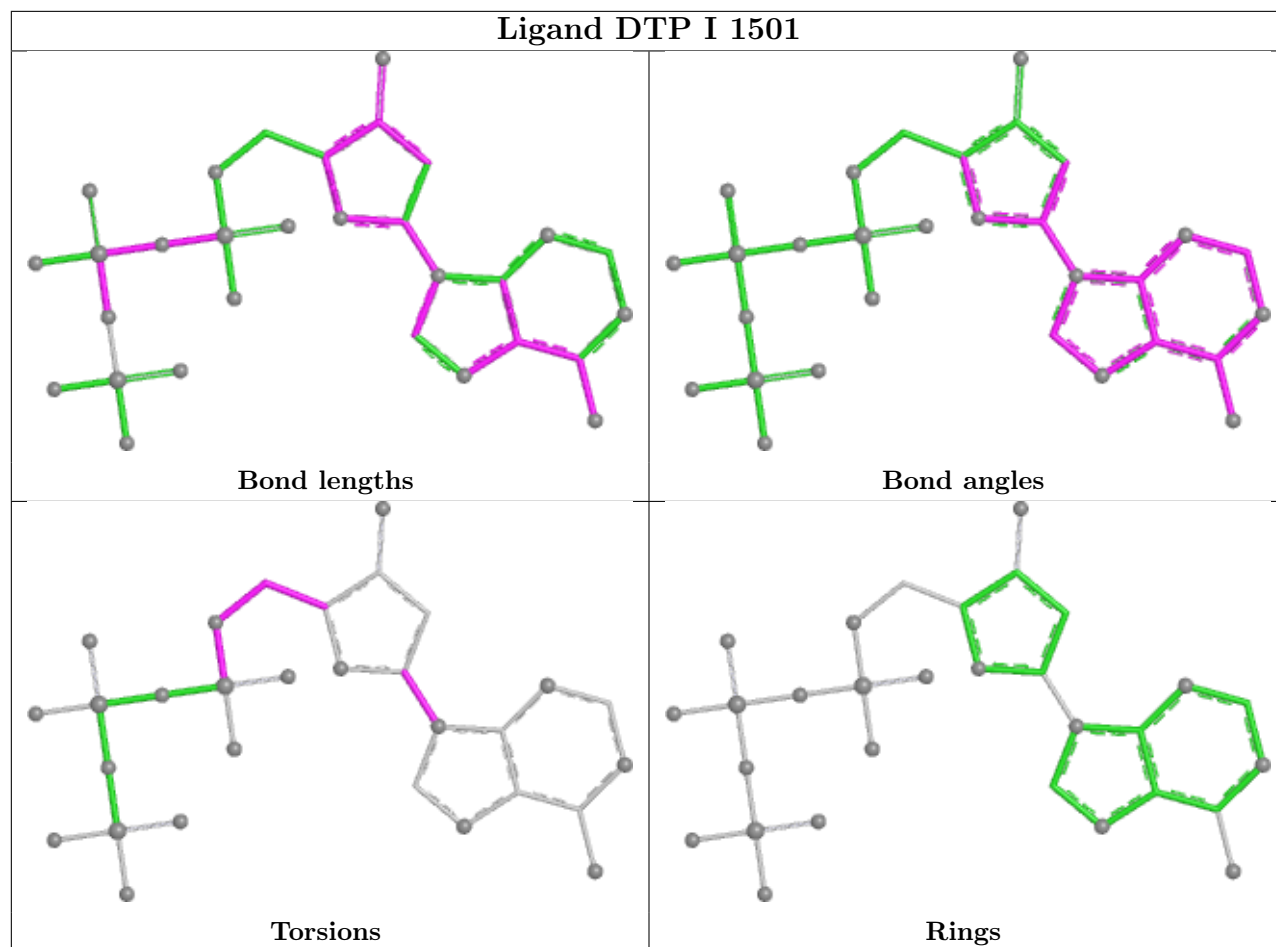


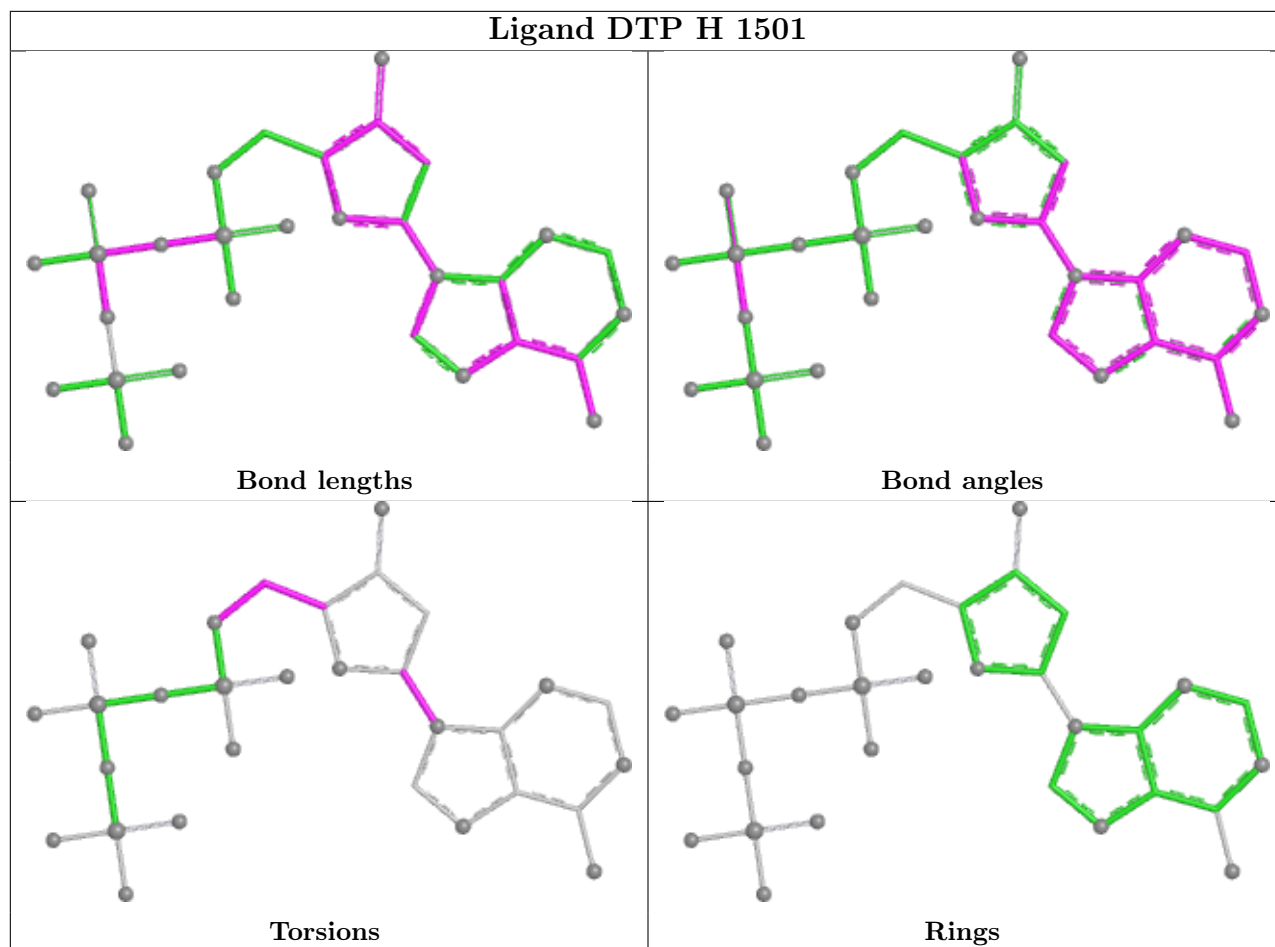


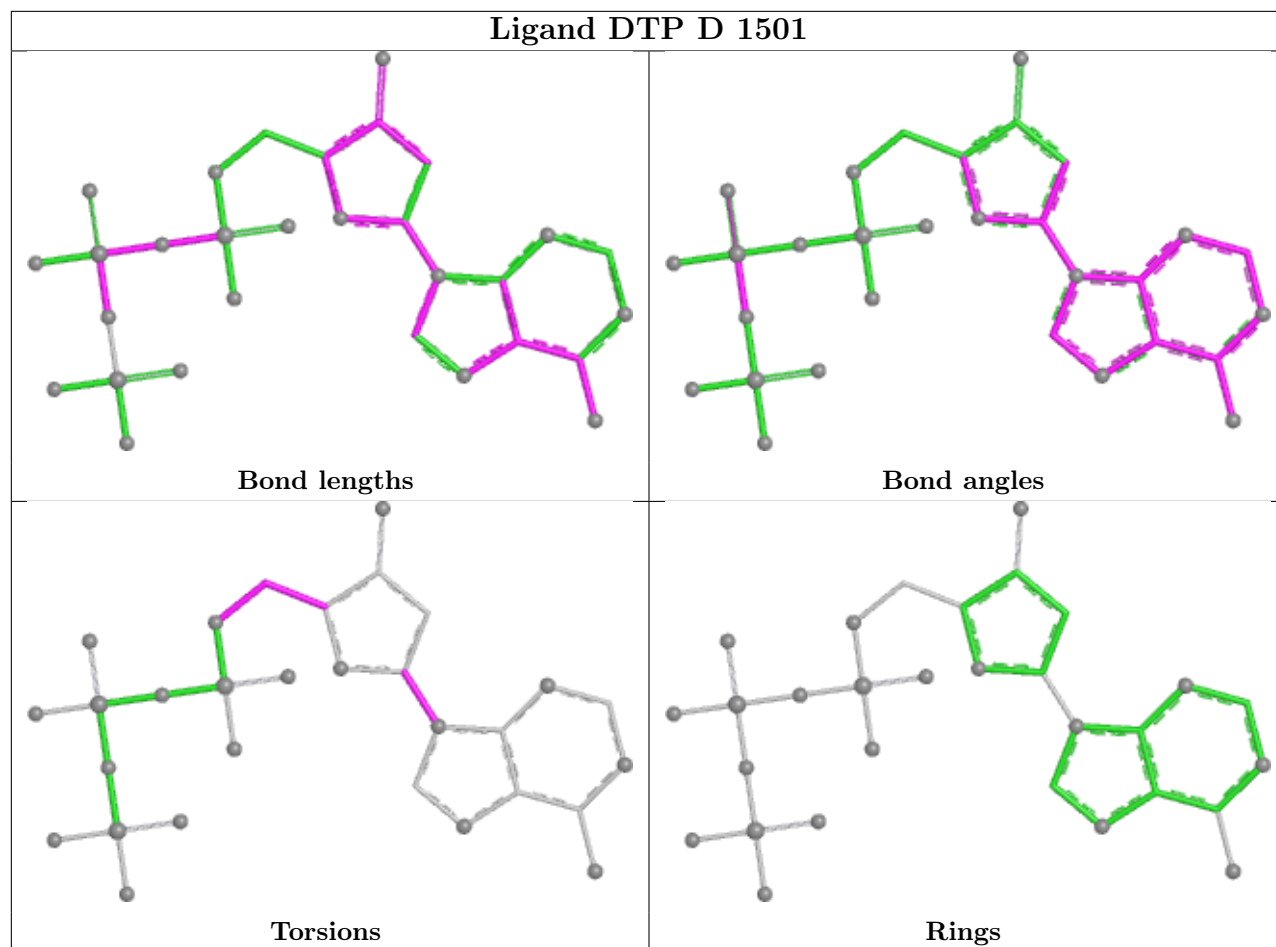


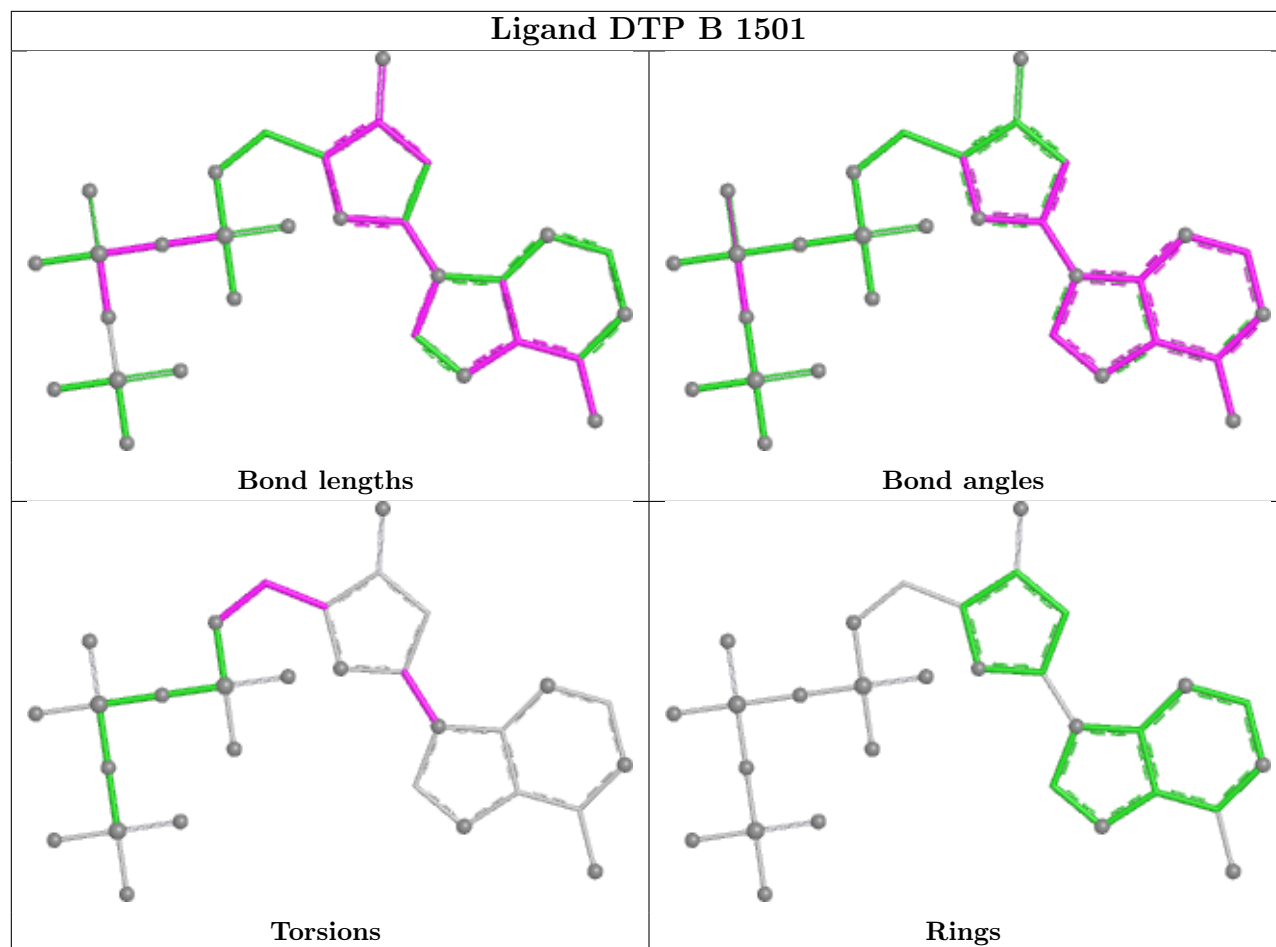


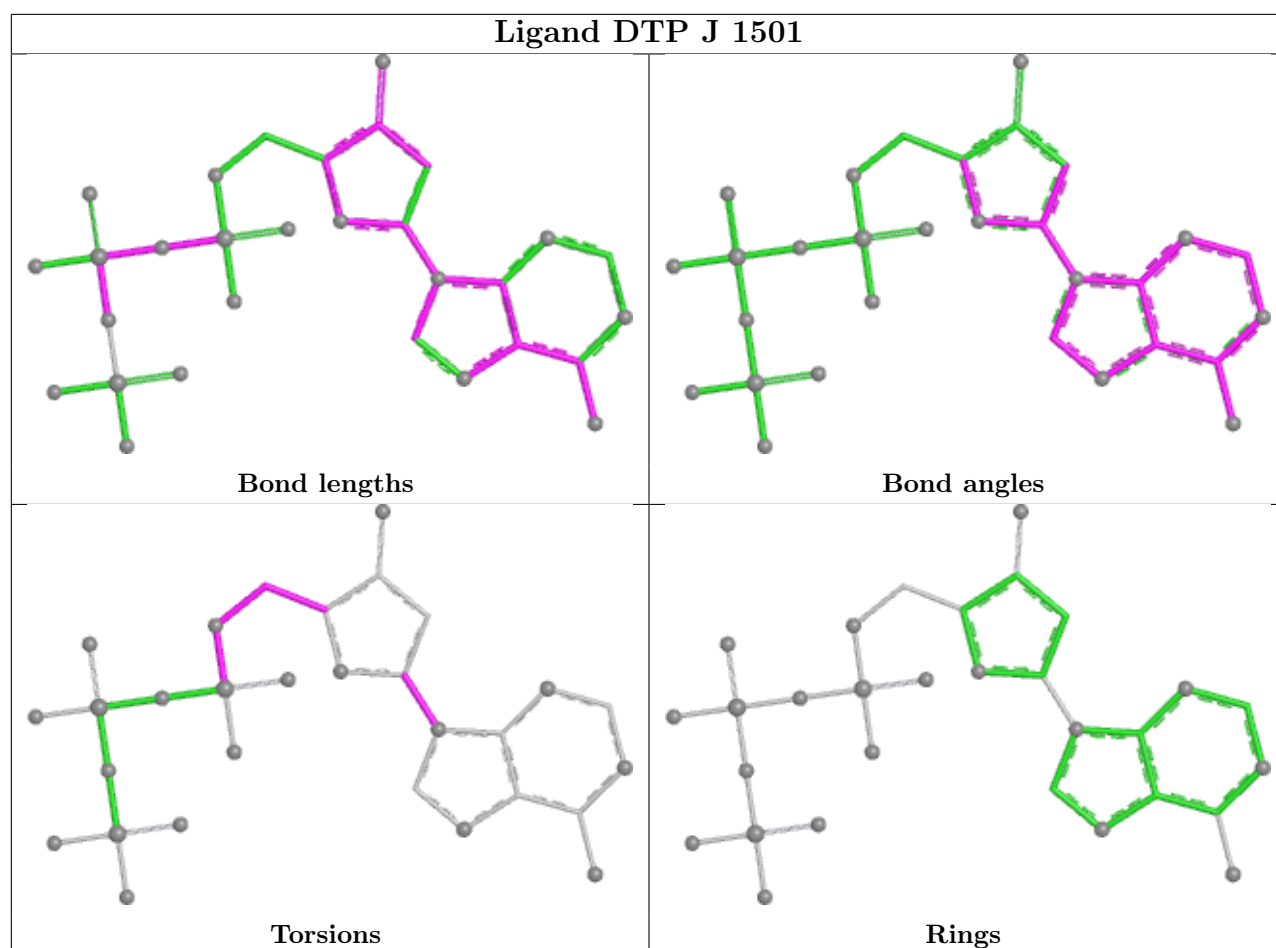












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

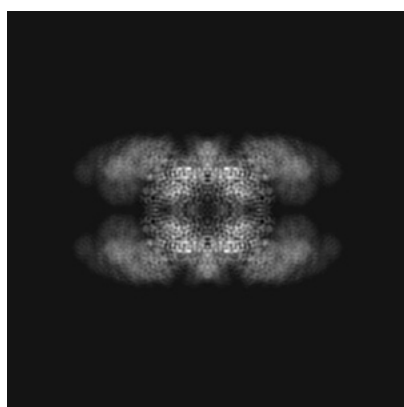
## 6 Map visualisation [i](#)

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.

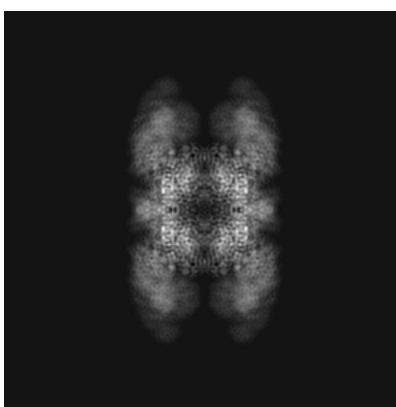
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

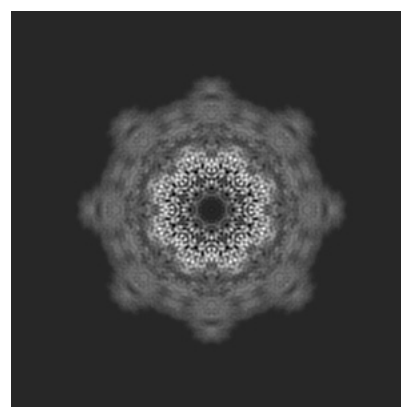
#### 6.1.1 Primary map



X



Y

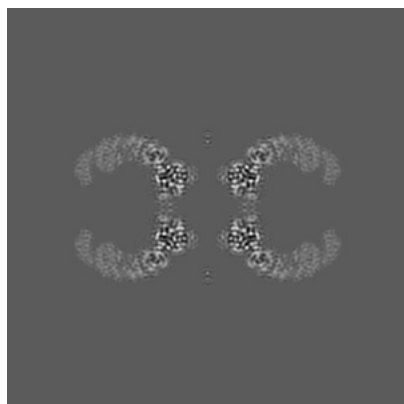


Z

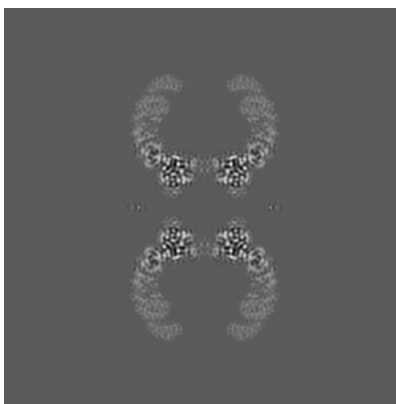
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 160



Y Index: 160

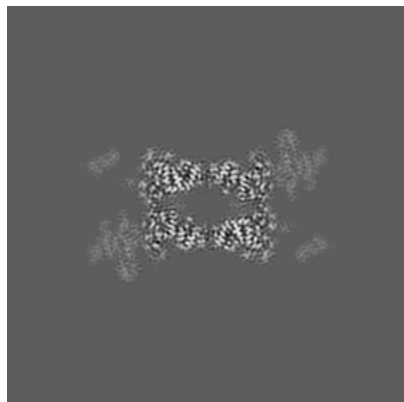


Z Index: 160

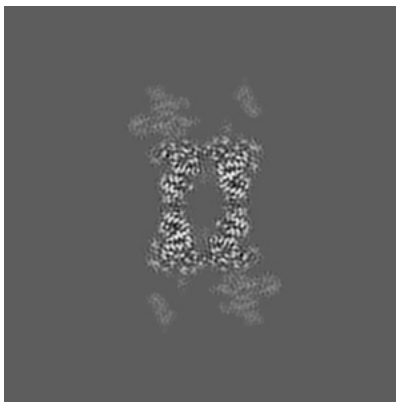
The images above show central slices of the map in three orthogonal directions.

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

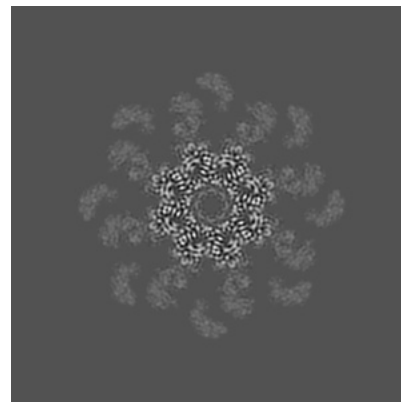
### 6.3.1 Primary map



X Index: 143



Y Index: 143

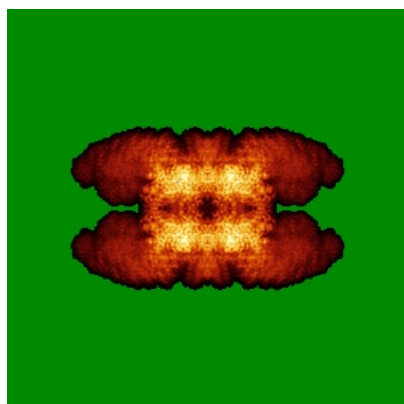


Z Index: 185

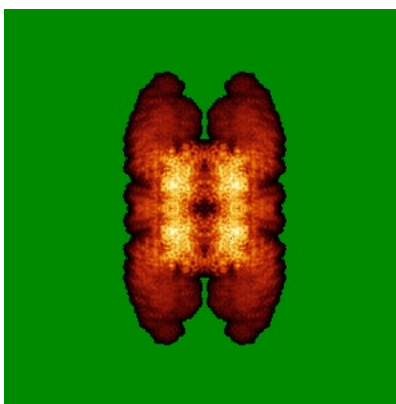
The images above show the largest variance slices of the map in three orthogonal directions.

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

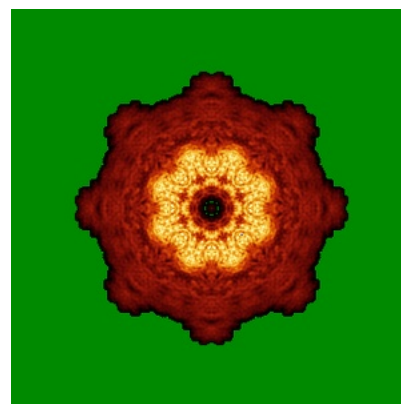
### 6.4.1 Primary map



X



Y

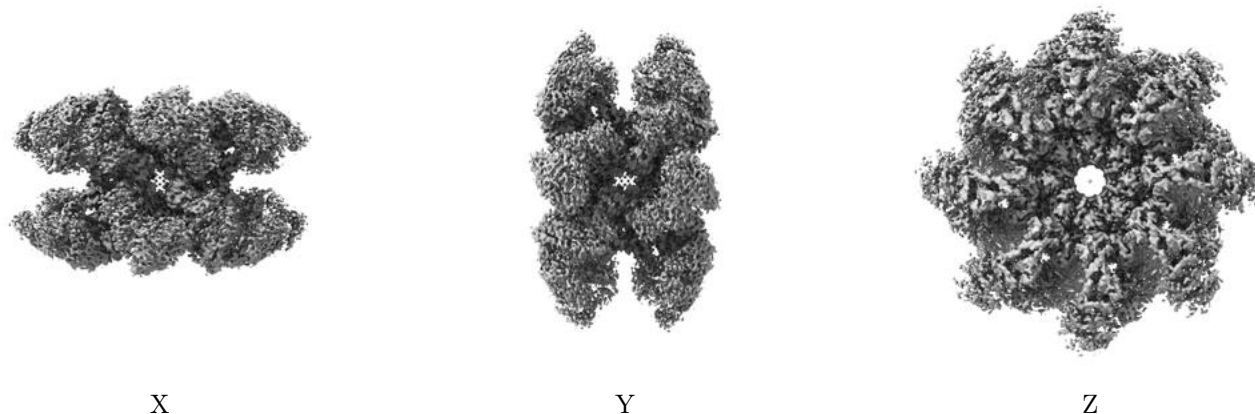


Z

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.

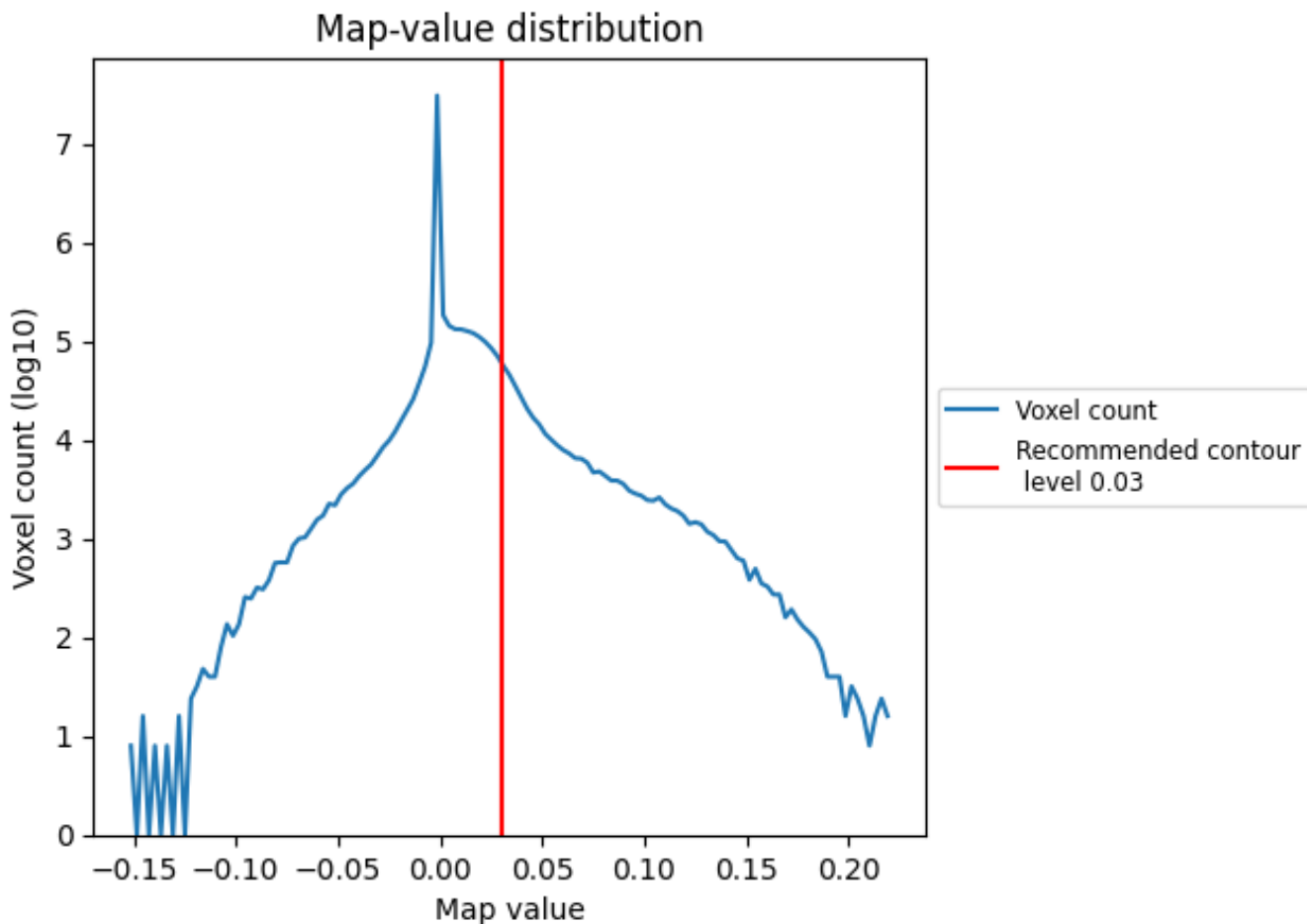
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

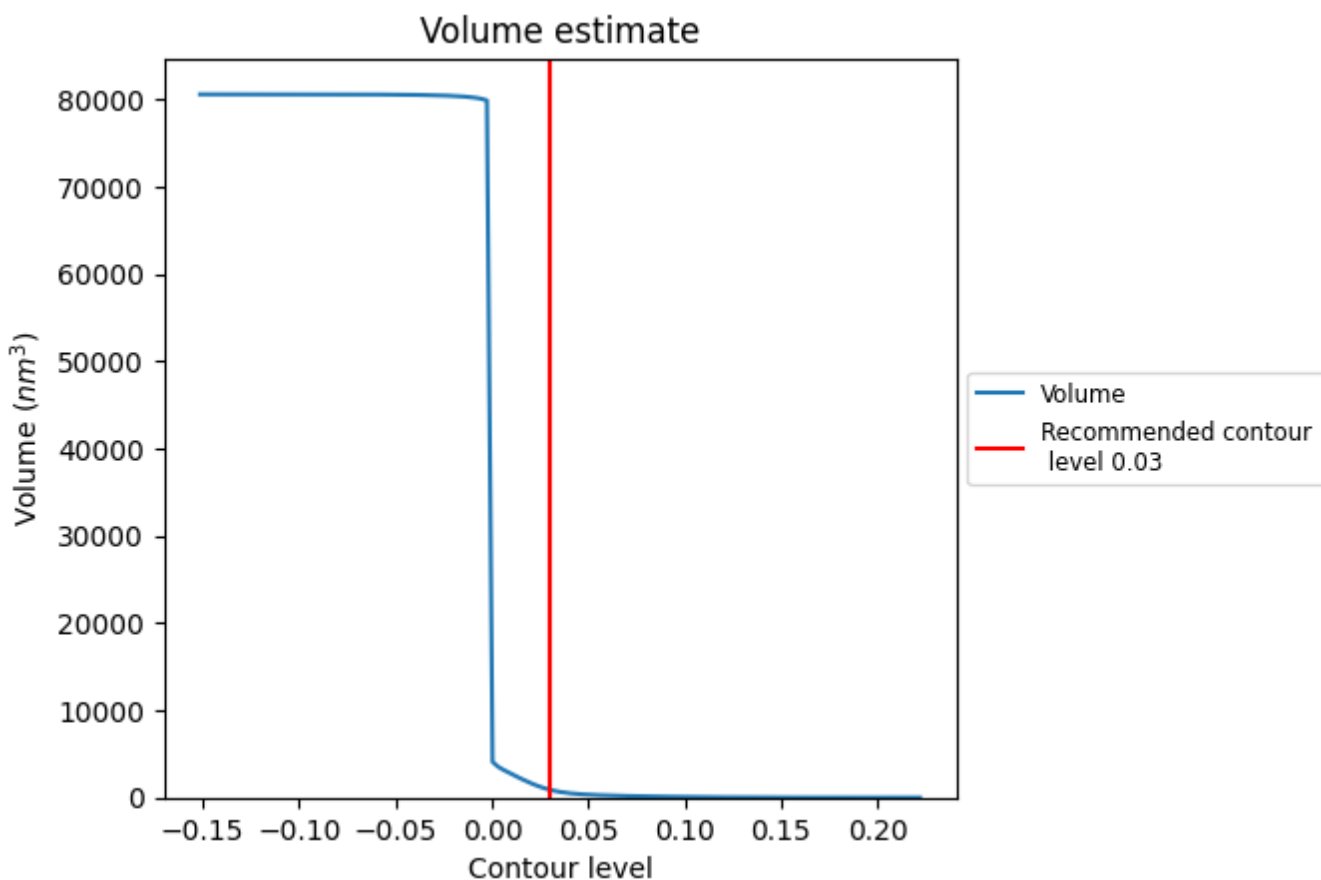
This section contains the results of statistical analysis of the map.

### 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.

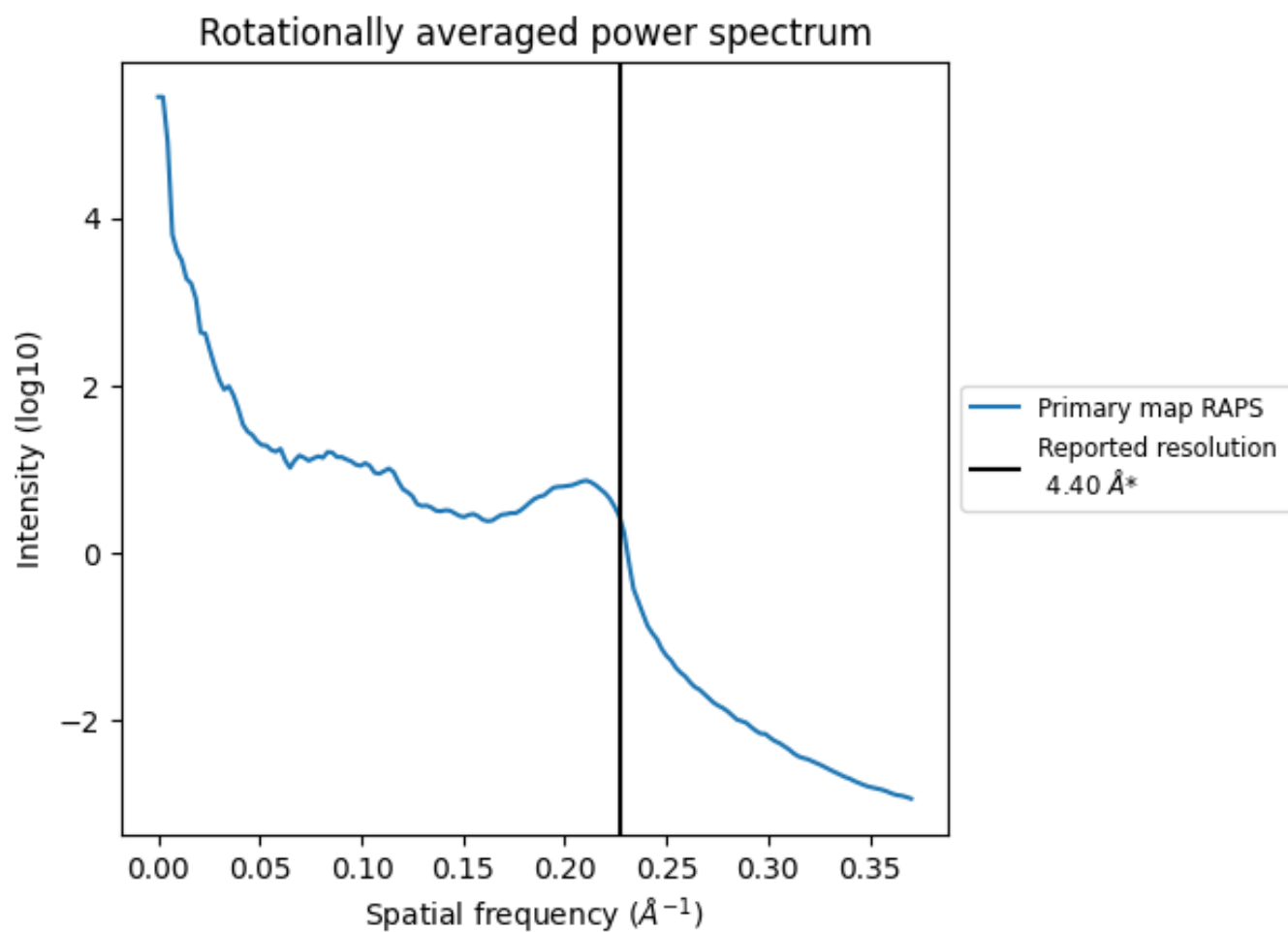
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 904 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  $0.227 \text{\AA}^{-1}$

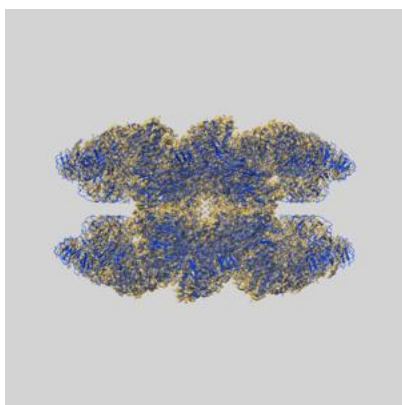
## 8 Fourier-Shell correlation

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

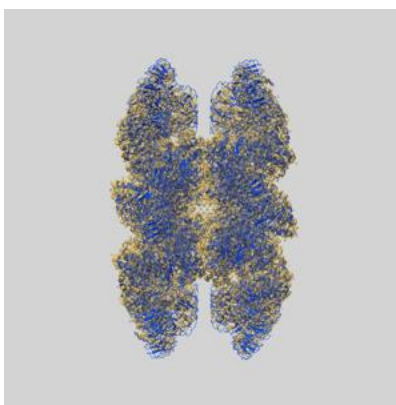
## 9 Map-model fit [i](#)

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.

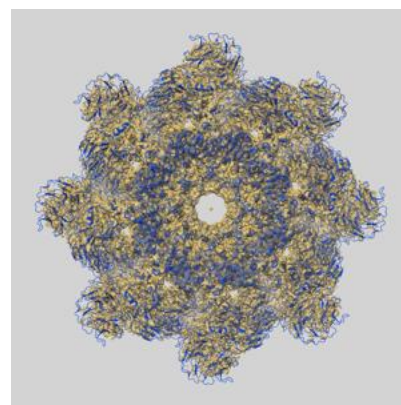
### 9.1 Map-model overlay [i](#)



X



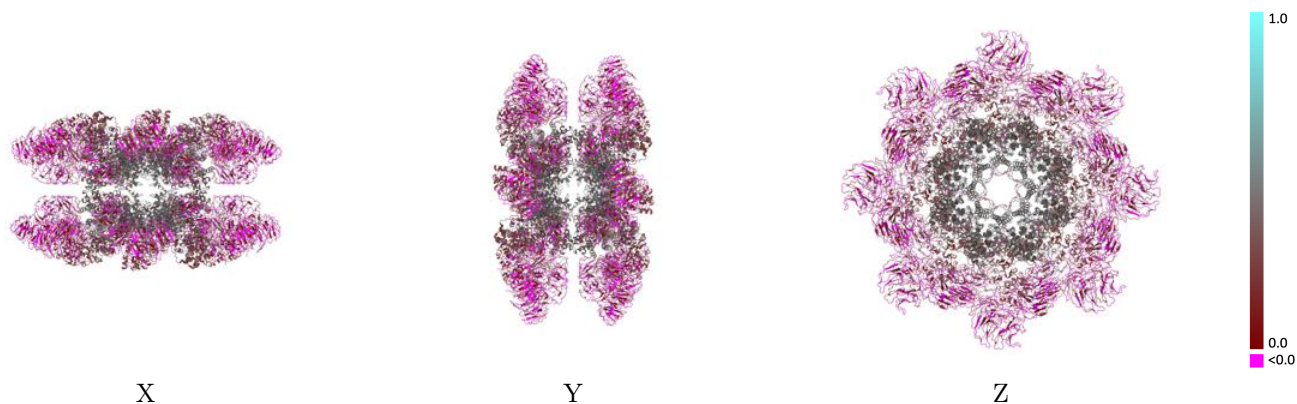
Y



Z

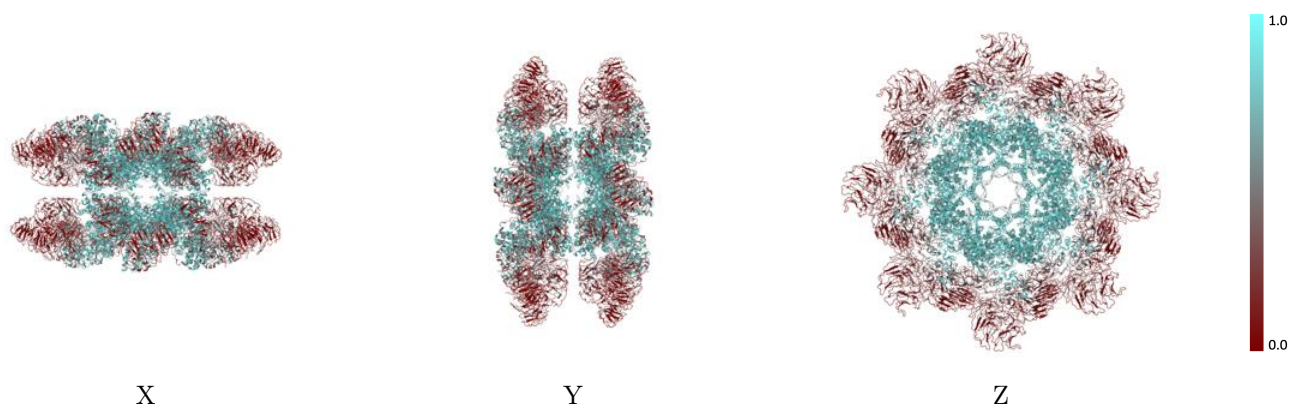
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



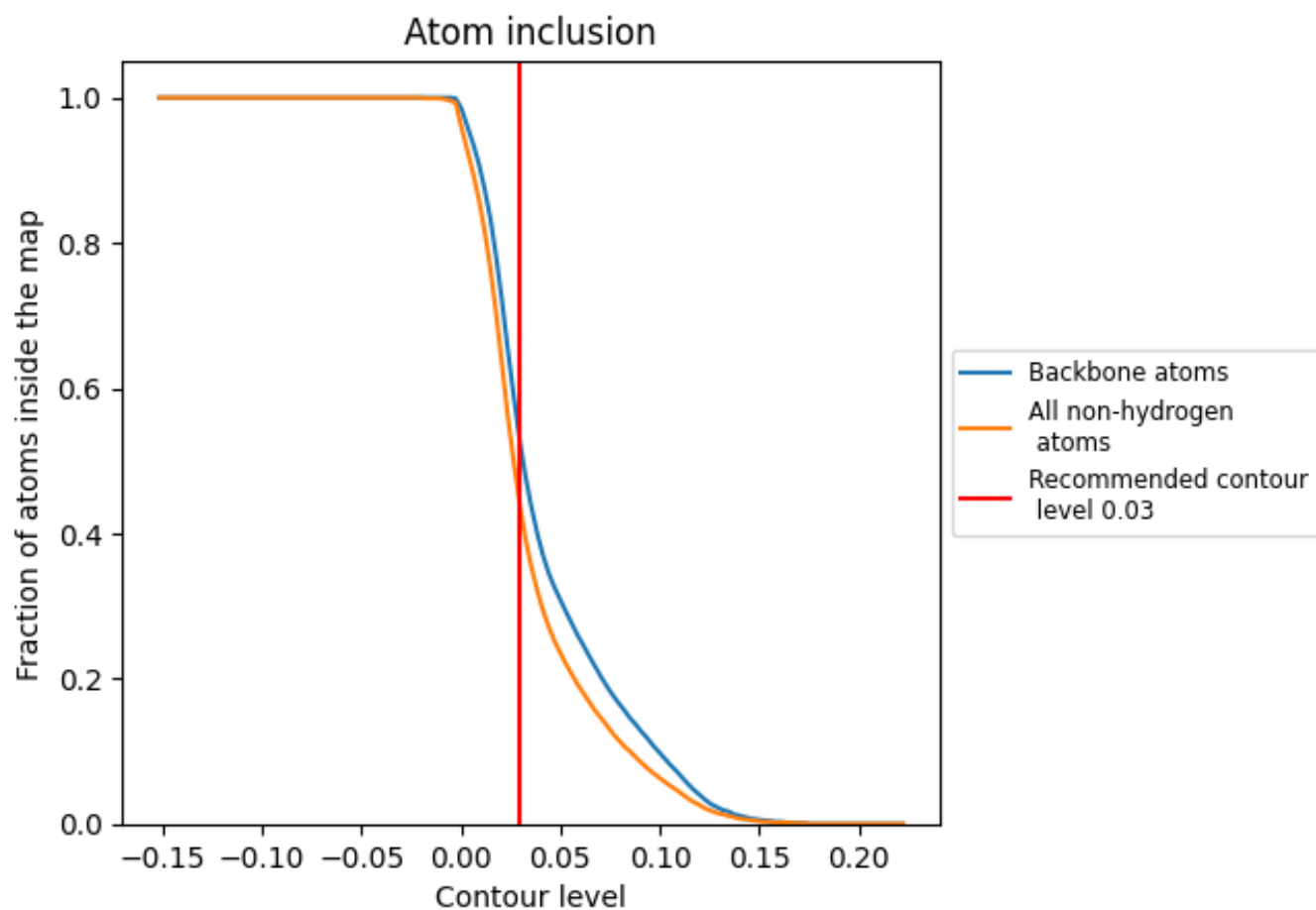
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.4300	0.1890
C	0.4310	0.1890
D	0.4330	0.1960
E	0.4370	0.1950
F	0.4280	0.1900
G	0.4360	0.1940
H	0.4360	0.1950
I	0.4350	0.1950
J	0.4370	0.1950
K	0.4340	0.1960
L	0.4280	0.1880
M	0.4350	0.1950
N	0.4370	0.1950
O	0.4350	0.1950
P	0.4330	0.1960

