



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:07 PM UTC

PDB ID : 3J9L / pdb_00003j9l
EMDB ID : EMD-2871
Title : Structure of Dark apoptosome from *Drosophila melanogaster*
Authors : Pang, Y.; Bai, X.; Yan, C.; Hao, Q.; Chen, Z.; Wang, J.; Scheres, S.H.W.; Shi, Y.
Deposited on : 2015-02-04
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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:

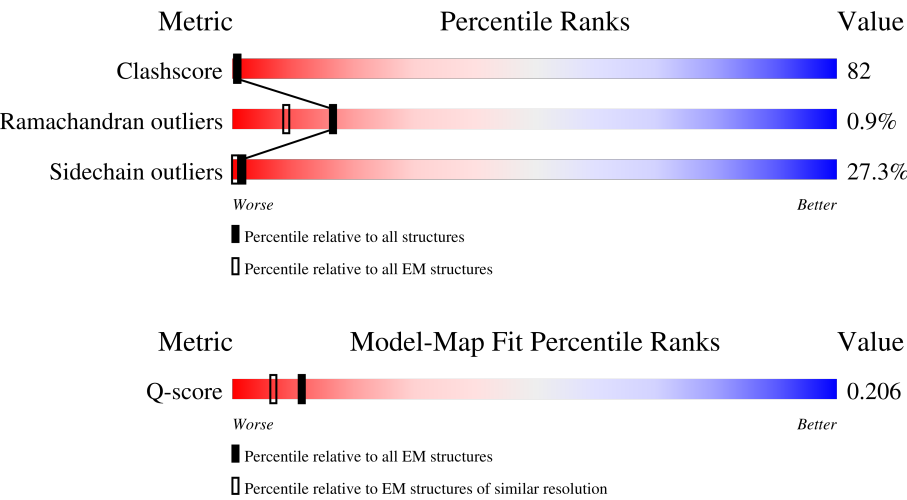
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.00 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.



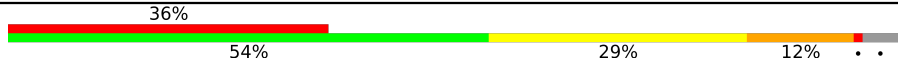
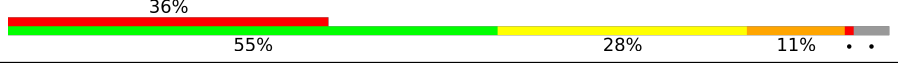
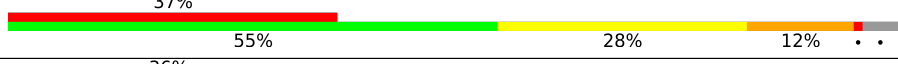
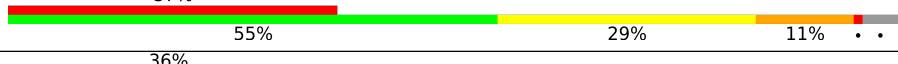
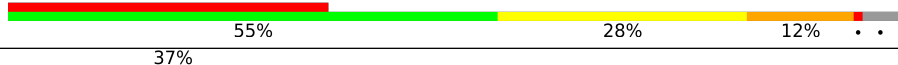
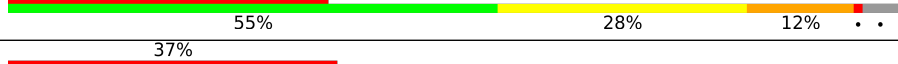
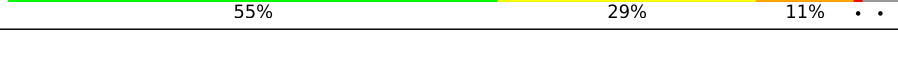
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	1103	
1	C	1103	
1	D	1103	
1	E	1103	

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Mol	Chain	Length	Quality of chain
1	F	1103	
1	G	1103	
1	H	1103	
1	I	1103	
1	J	1103	
1	K	1103	
1	L	1103	
1	M	1103	
1	N	1103	
1	O	1103	
1	P	1103	
1	Q	1103	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTP	C	1301	-	-	X	-
2	DTP	D	1301	-	-	X	-
2	DTP	E	1301	-	-	X	-
2	DTP	F	1301	-	-	X	-
2	DTP	G	1301	-	-	X	-
2	DTP	H	1301	-	-	X	-
2	DTP	I	1301	-	-	X	-
2	DTP	J	1301	-	-	X	-
2	DTP	K	1301	-	-	X	-
2	DTP	L	1301	-	-	X	-
2	DTP	M	1301	-	-	X	-
2	DTP	N	1301	-	-	X	-
2	DTP	O	1301	-	-	X	-
2	DTP	P	1301	-	-	X	-
2	DTP	Q	1301	-	-	X	-

2 Entry composition

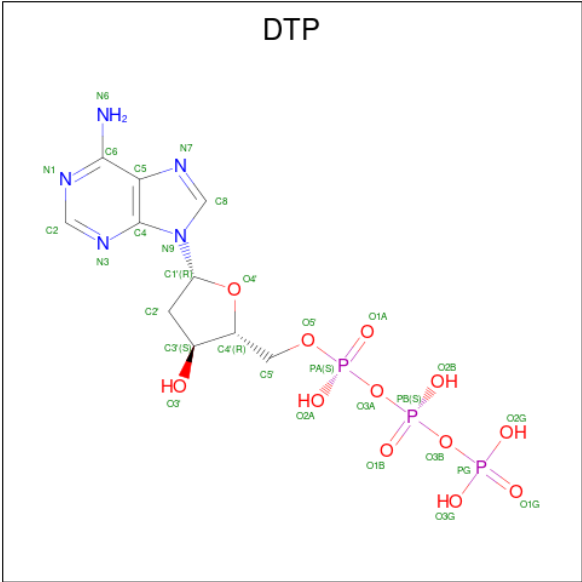
There are 2 unique types of molecules in this entry. The entry contains 112951 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	C	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	D	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	E	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	F	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	G	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	H	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	I	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	J	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	K	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	L	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	M	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	N	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	O	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	P	1062	Total 7031	C 4408	N 1275	O 1325	S 23	0	0
1	Q	1063	Total 7036	C 4411	N 1276	O 1326	S 23	0	0

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



Mol	Chain	Residues	Atoms					AltConf
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	
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	

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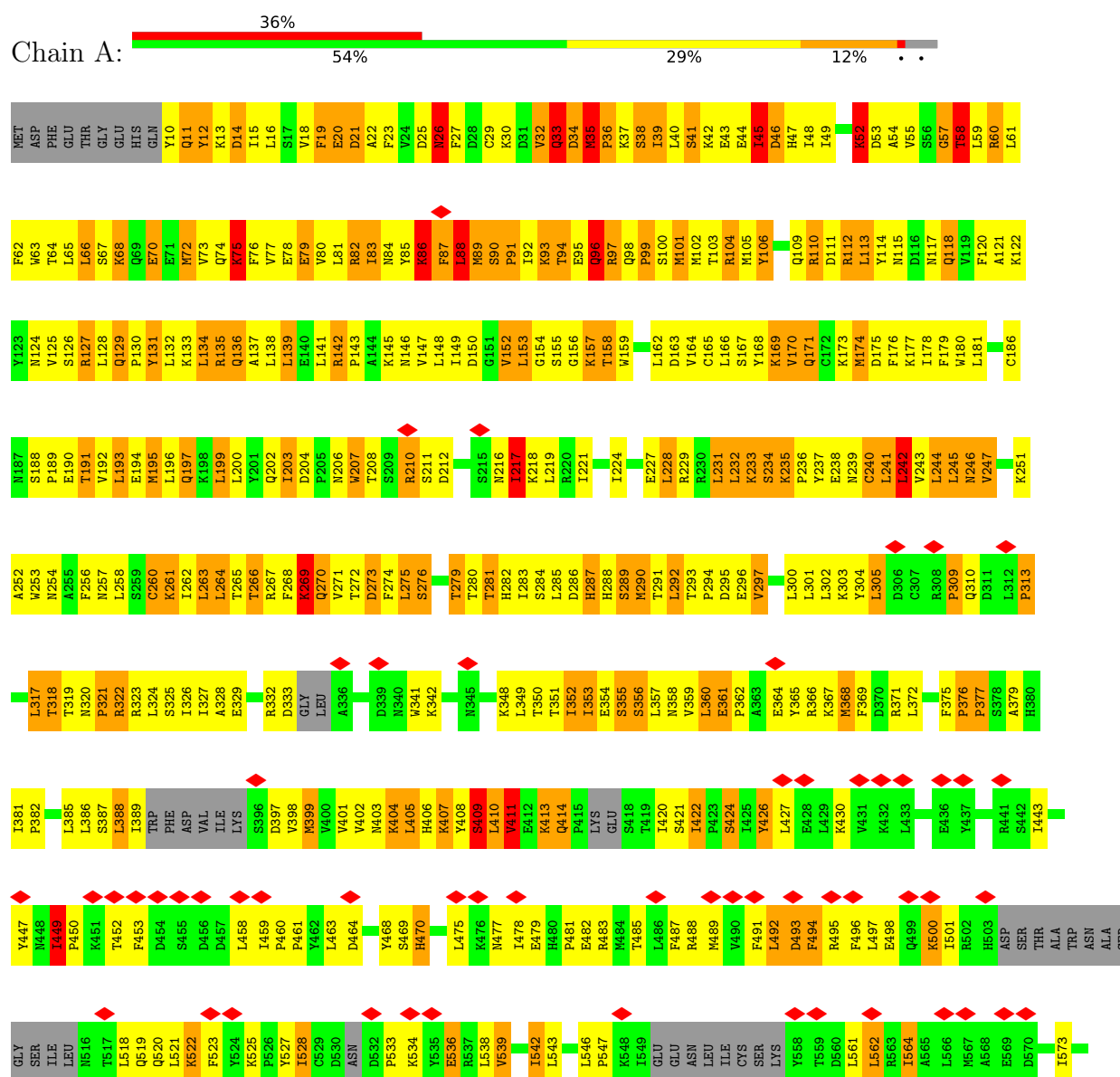
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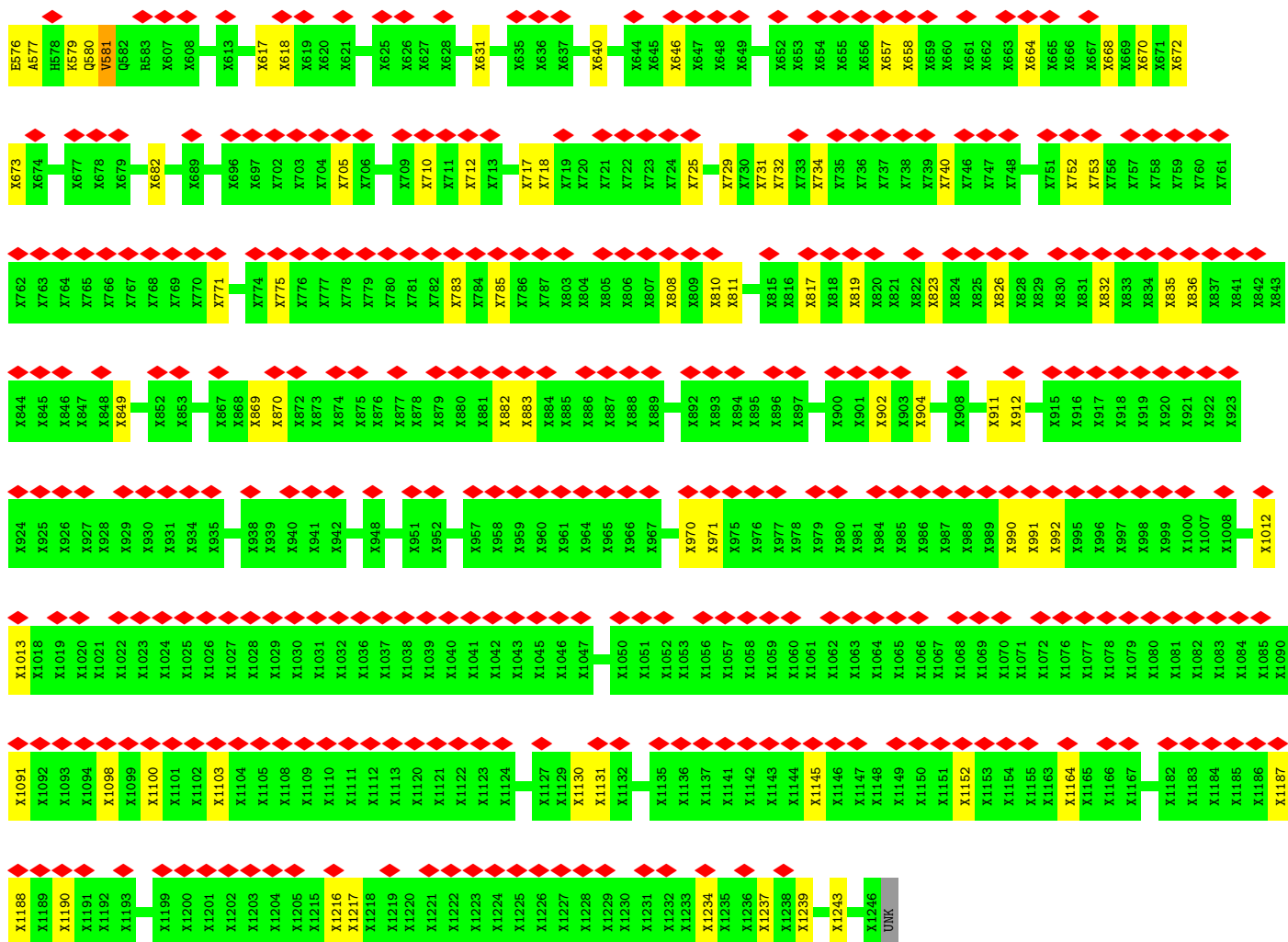
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	Q	1	30	10	5	12	3	0

3 Residue-property plots

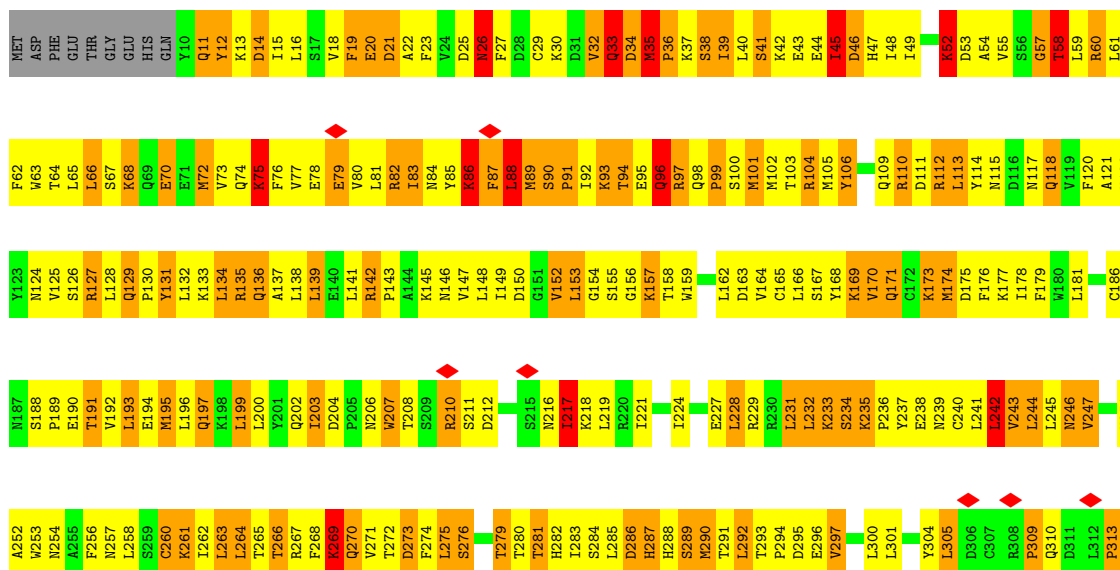
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

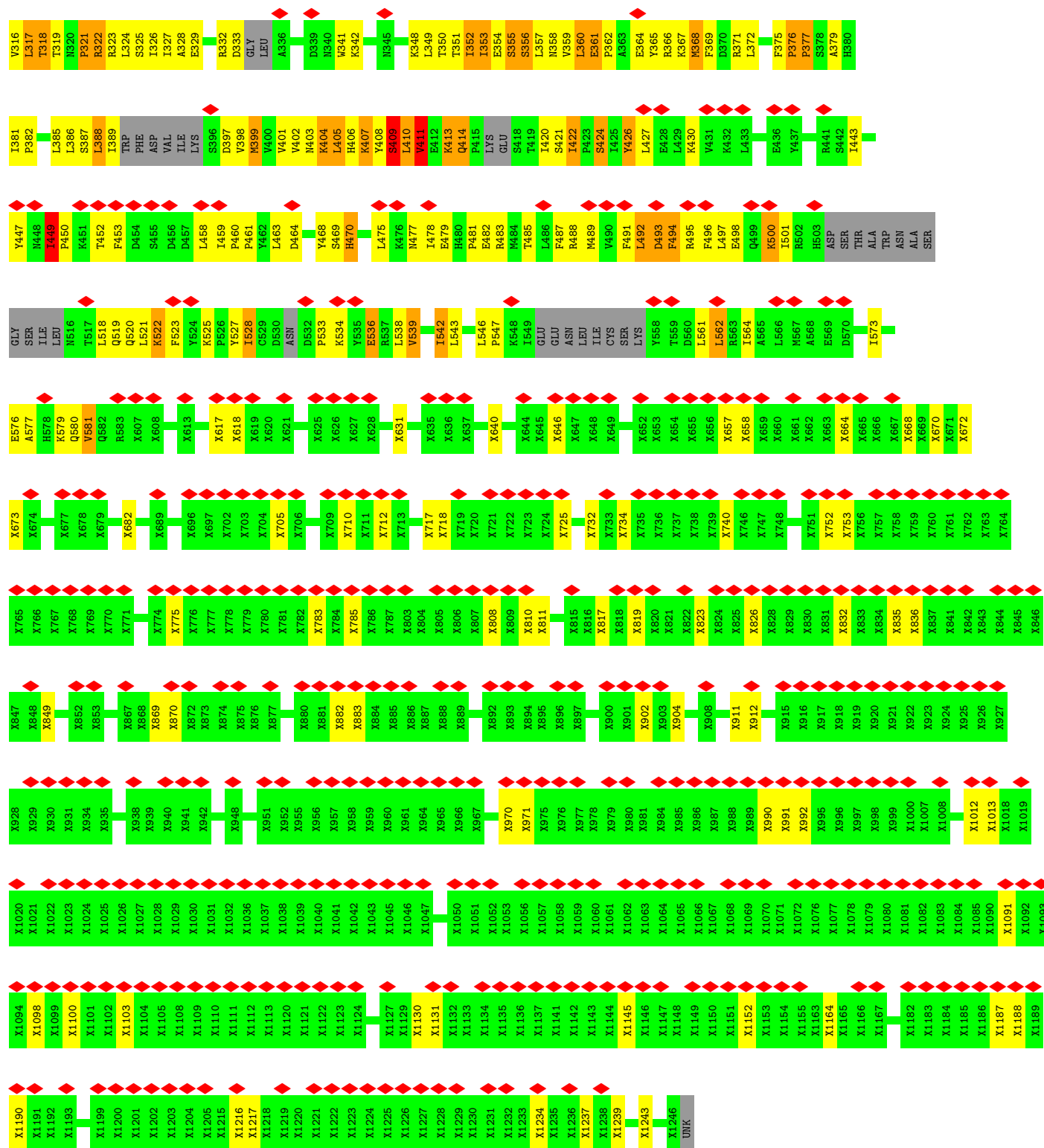
• Molecule 1: Apaf-1 related killer DARK





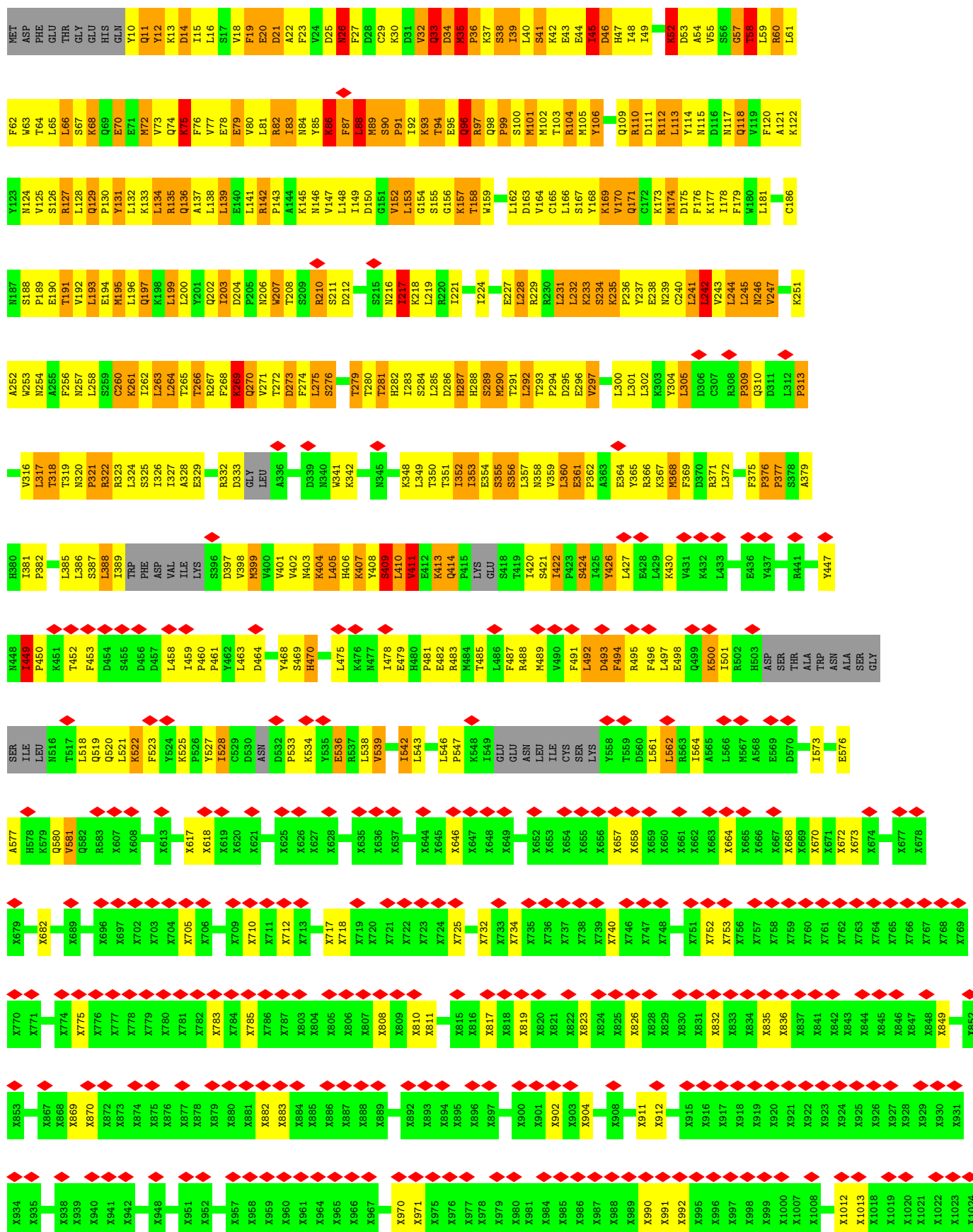
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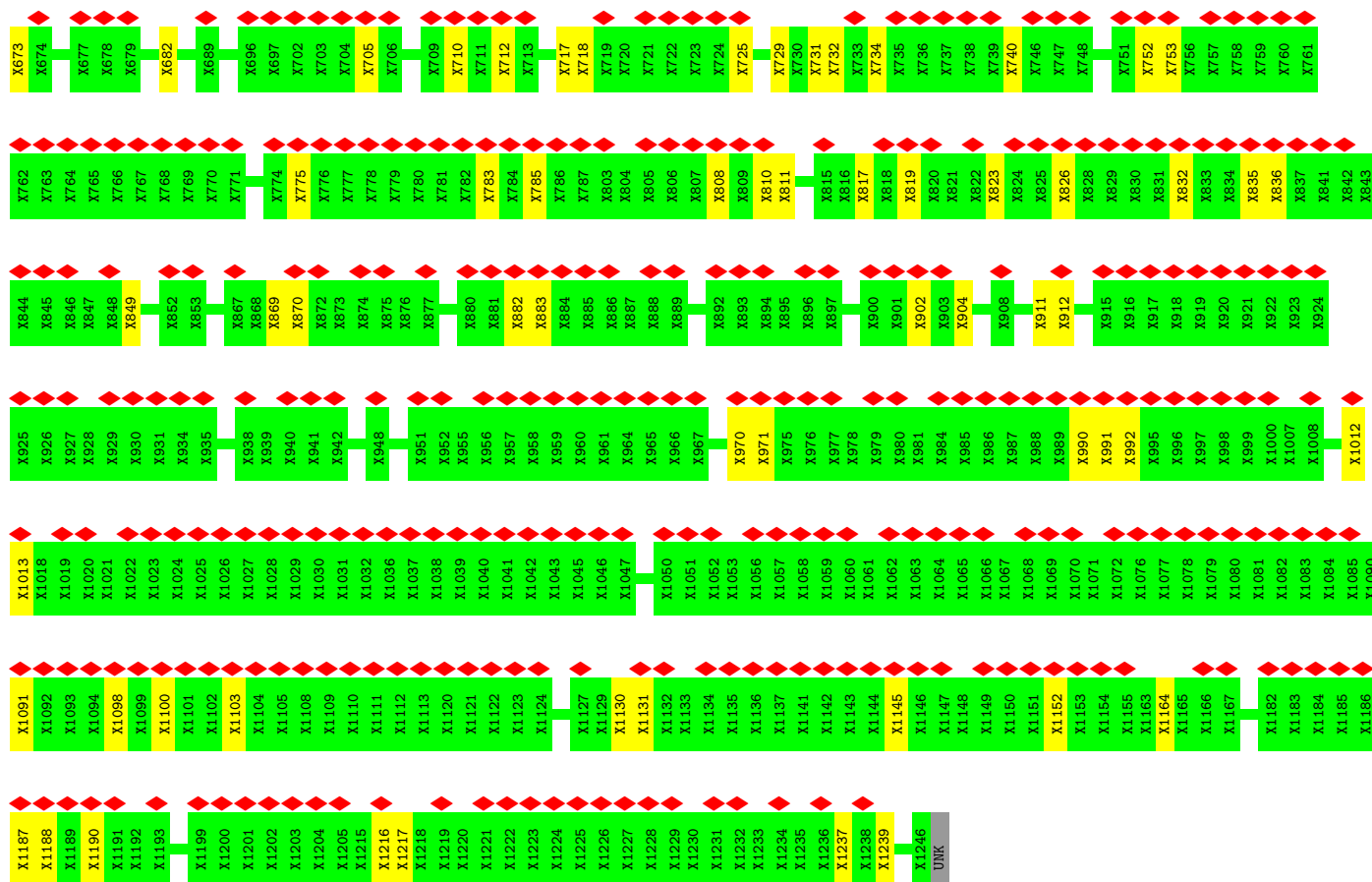


• Molecule 1: Apaf-1 related killer DARK

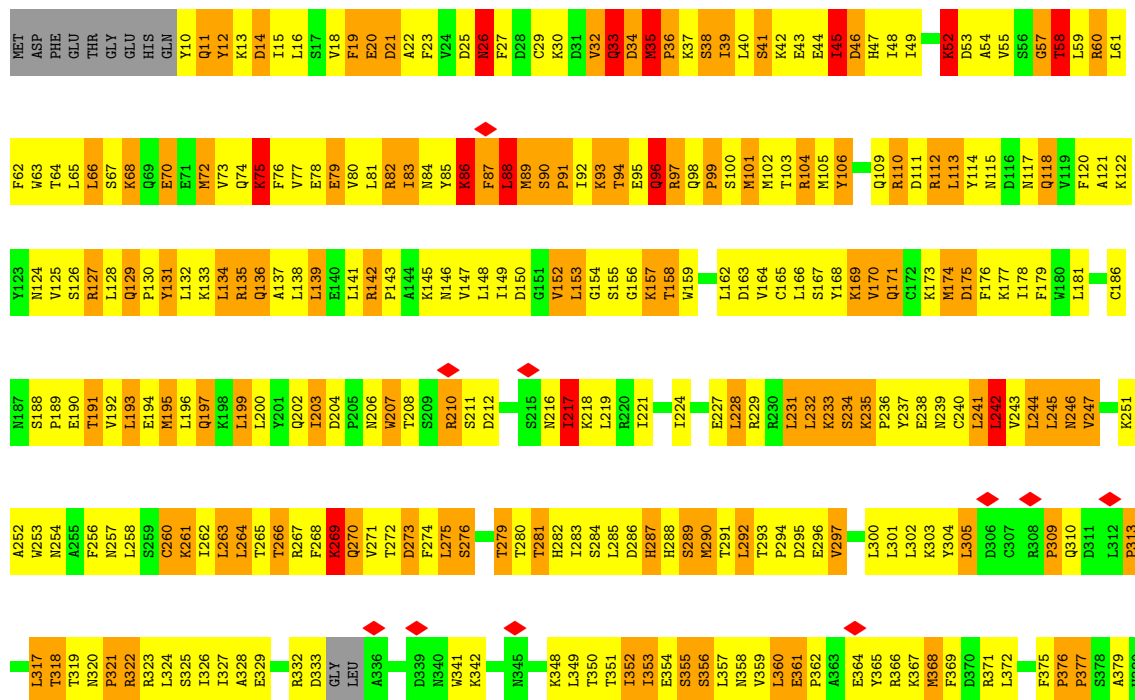


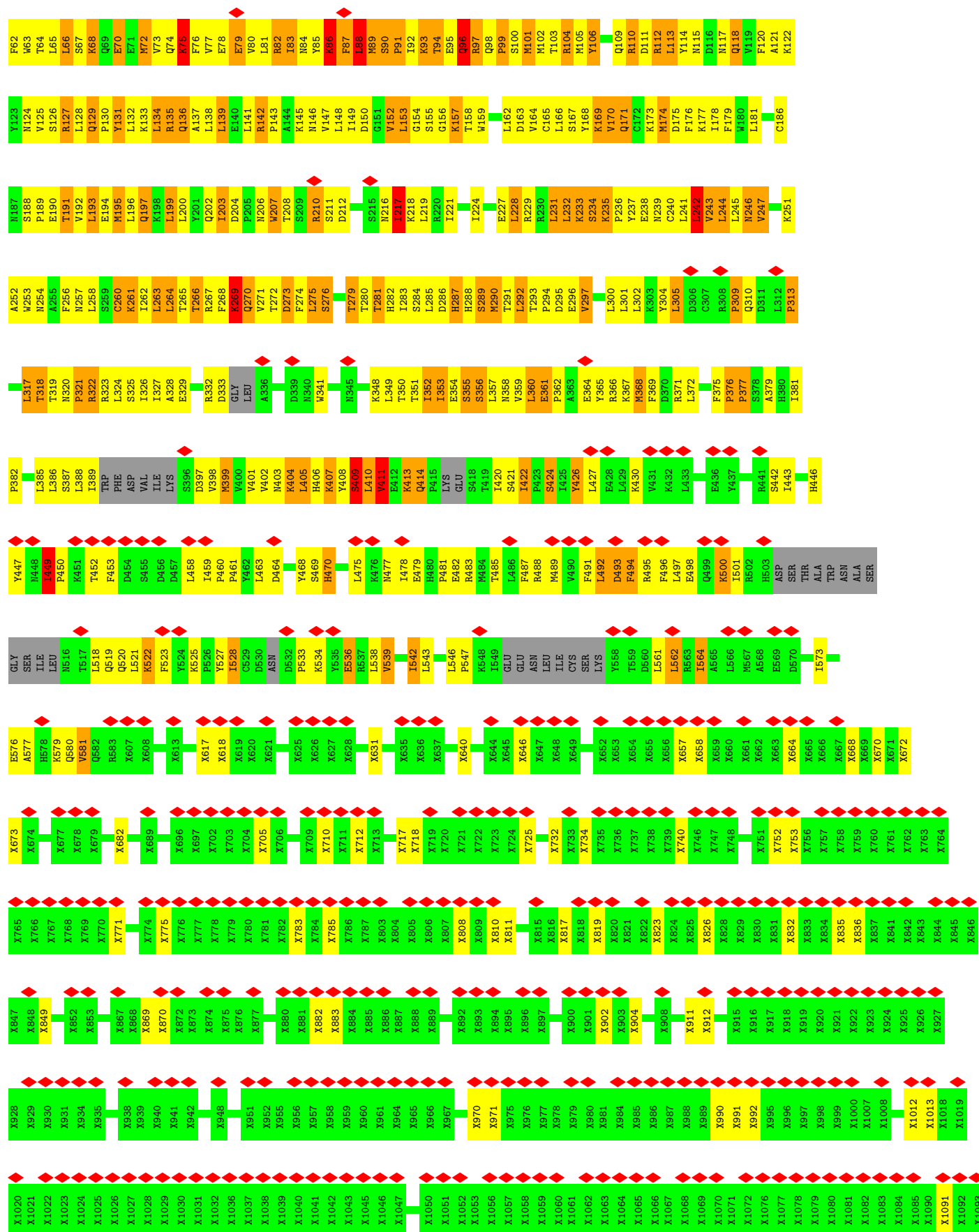


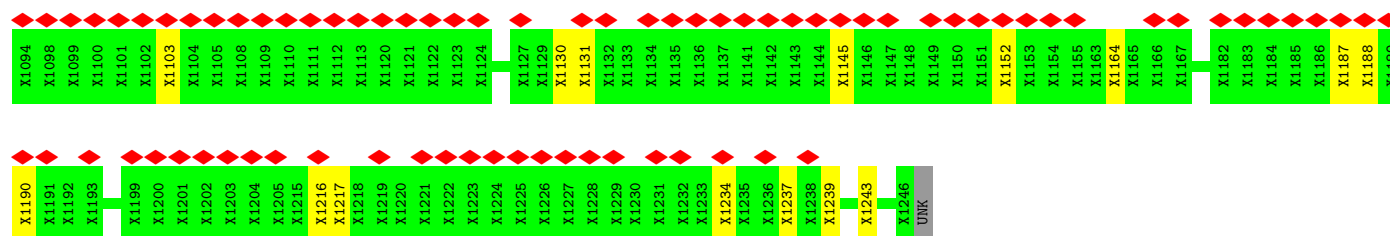




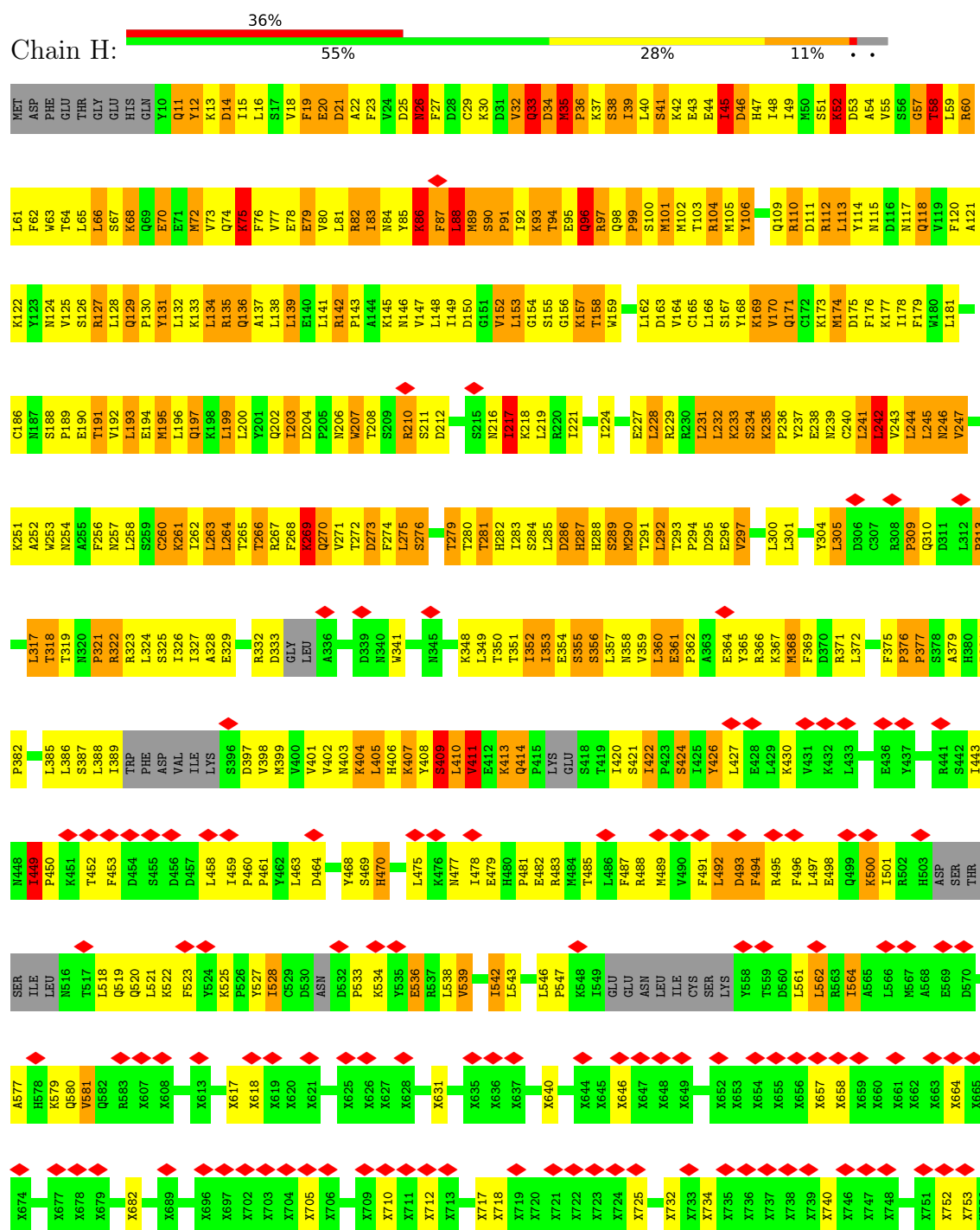
• Molecule 1: Apaf-1 related killer DARK

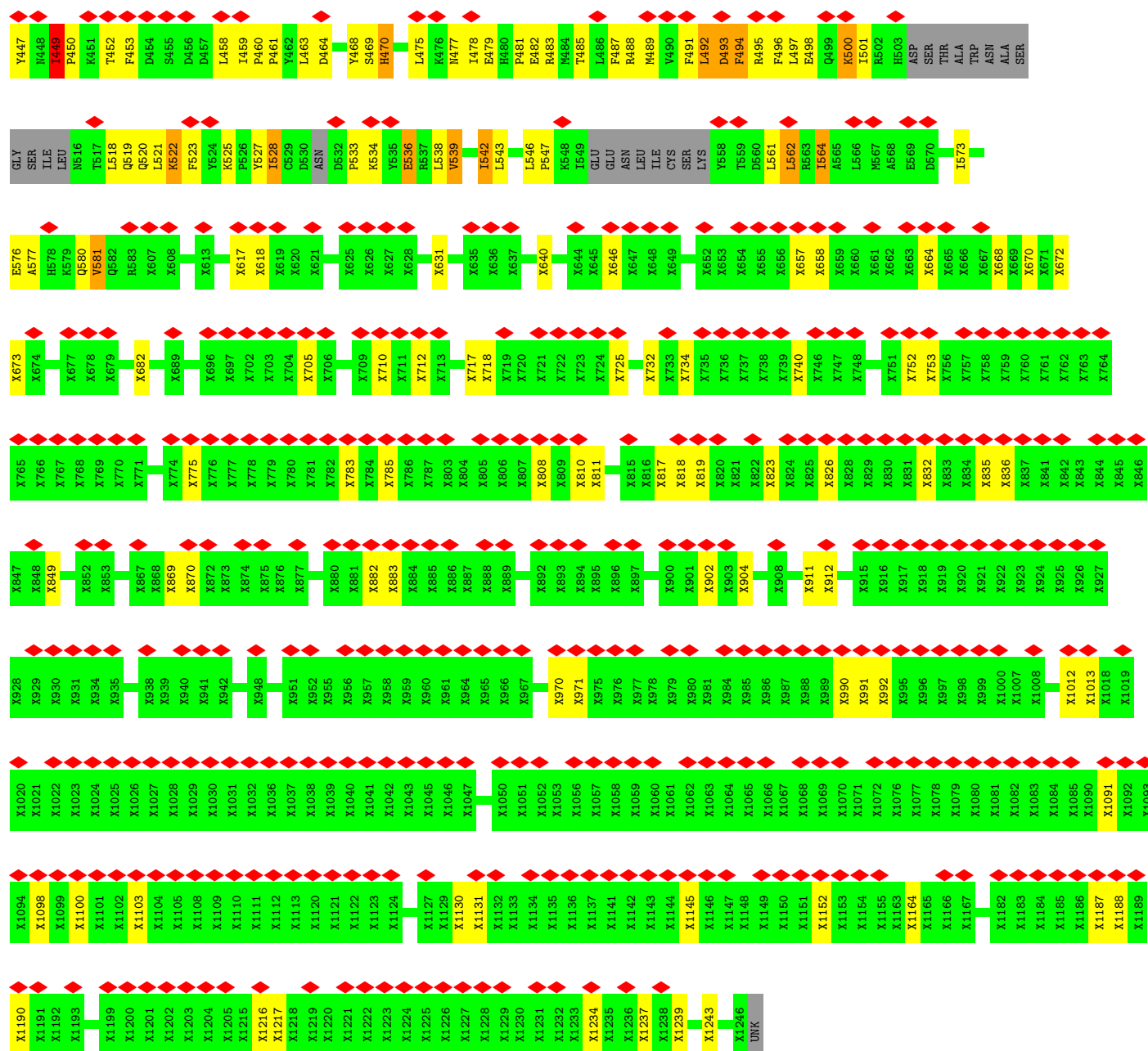




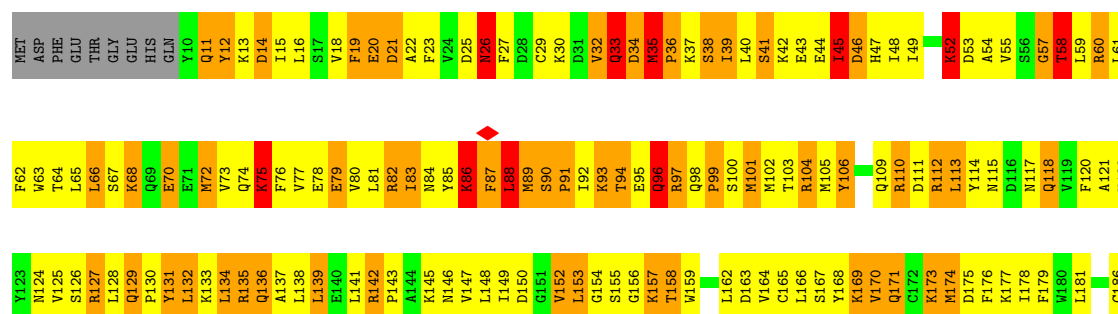


• Molecule 1: Apaf-1 related killer DARK

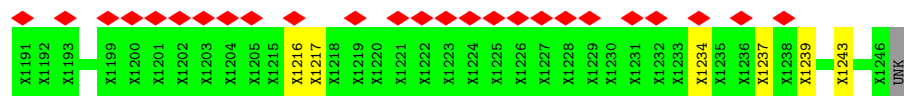




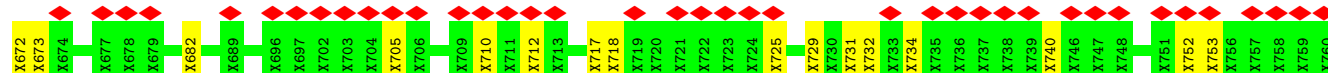
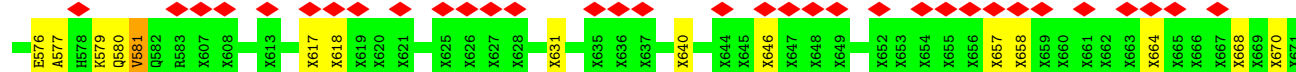
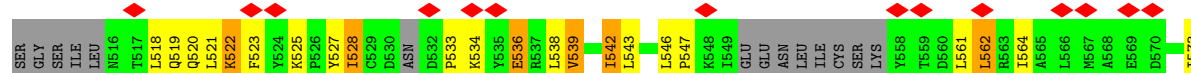
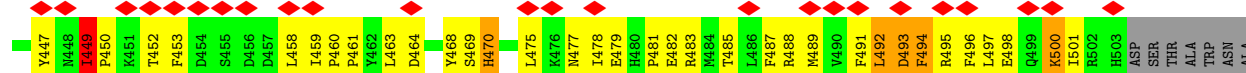
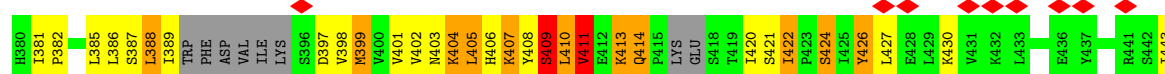
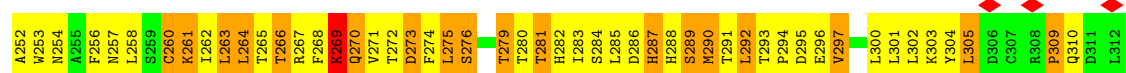
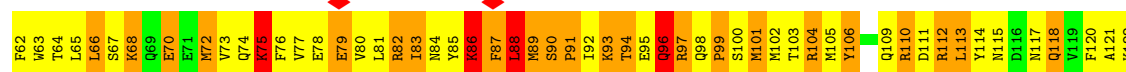
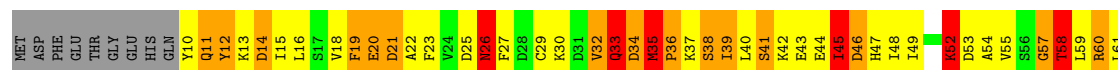
• Molecule 1: Apaf-1 related killer DARK

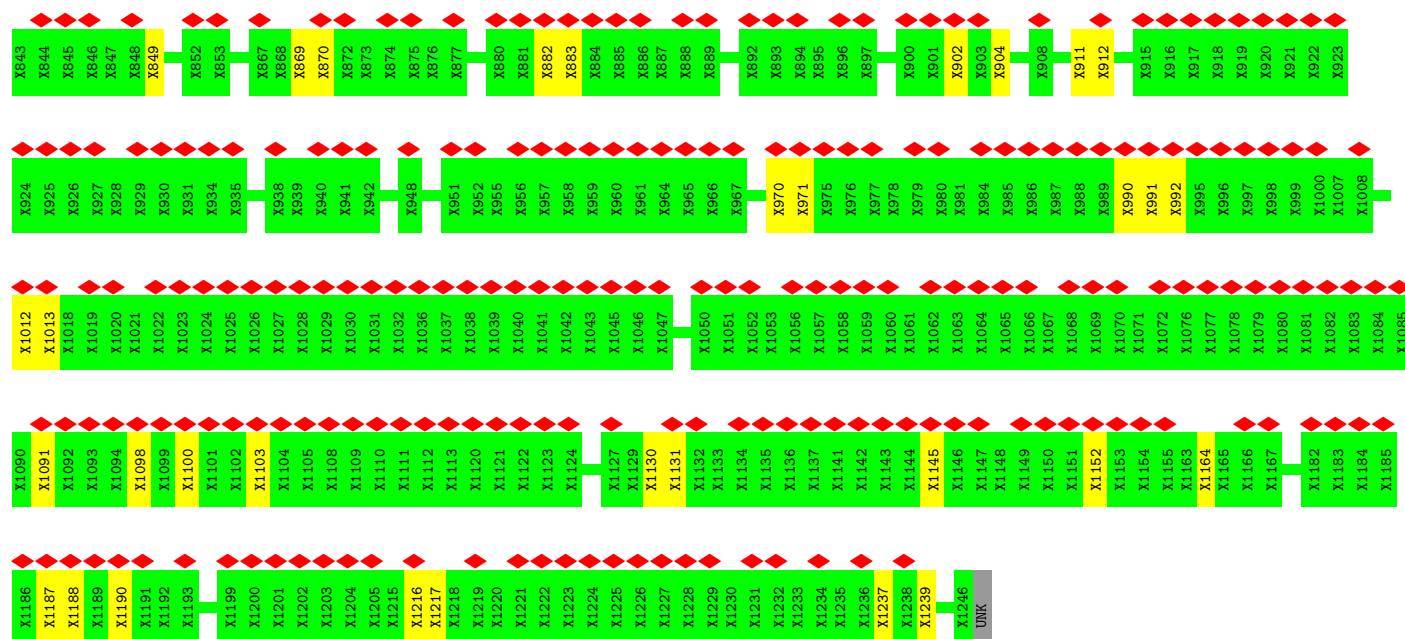




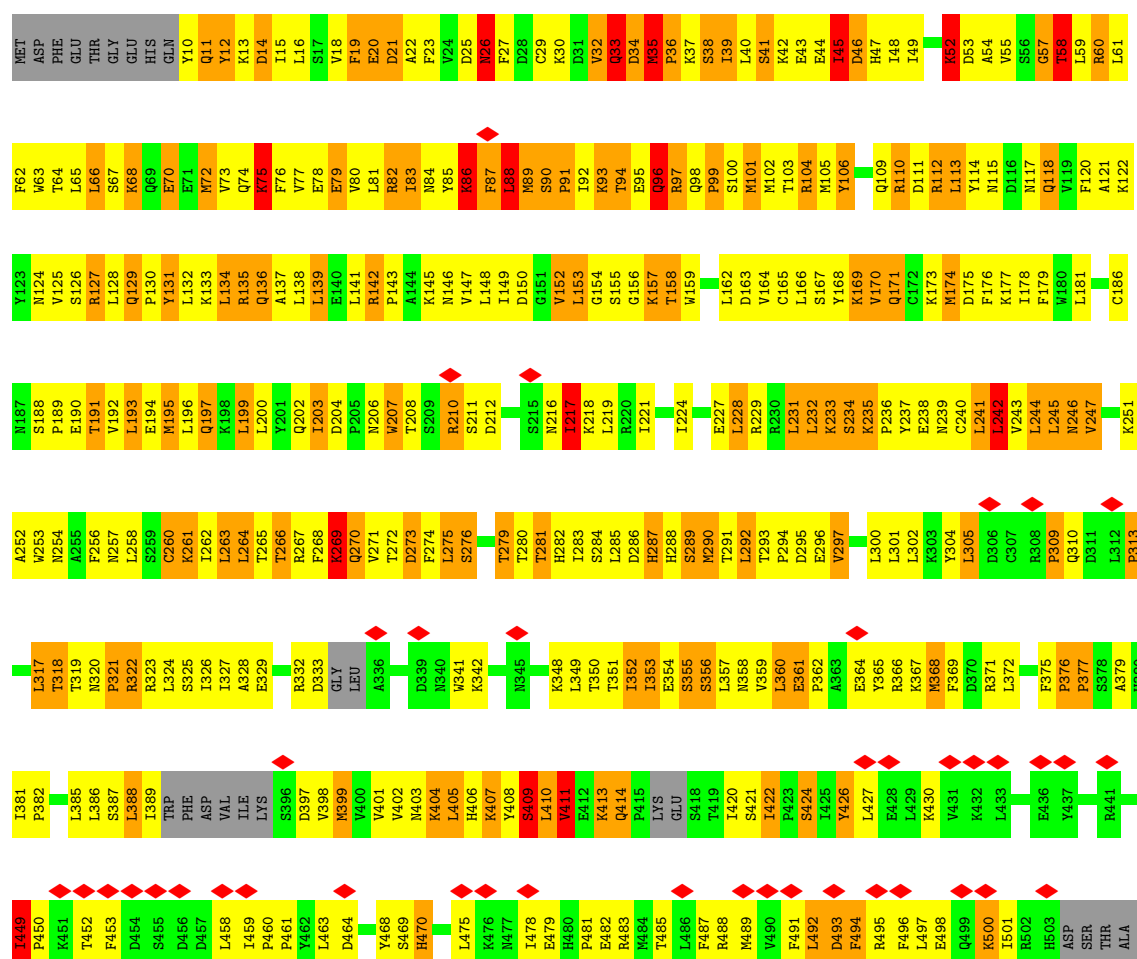


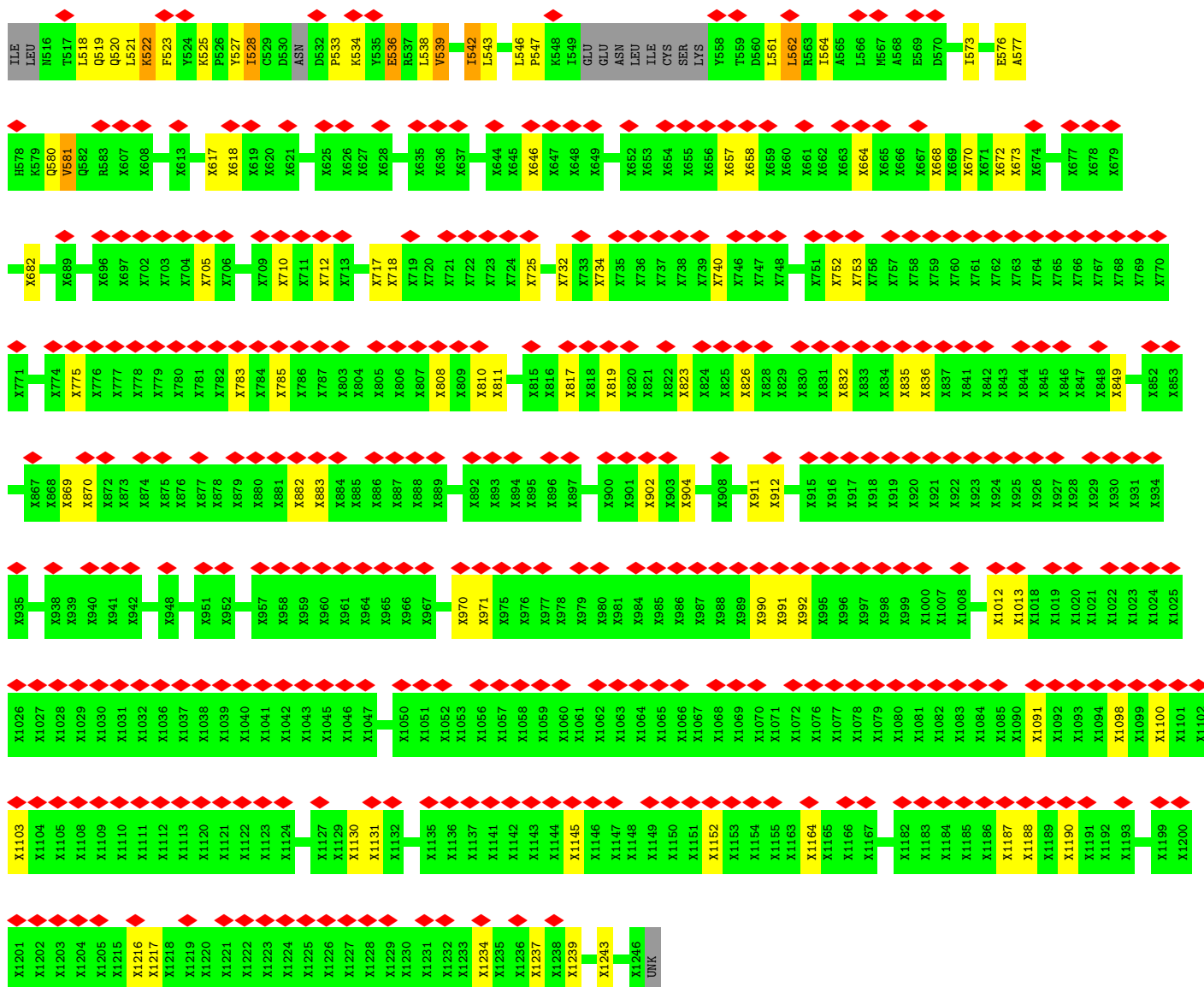
• Molecule 1: Apaf-1 related killer DARK



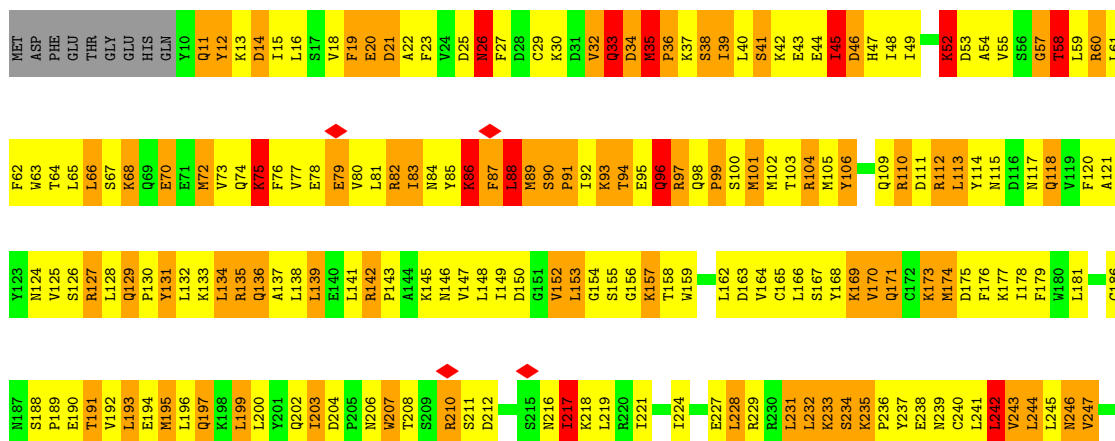


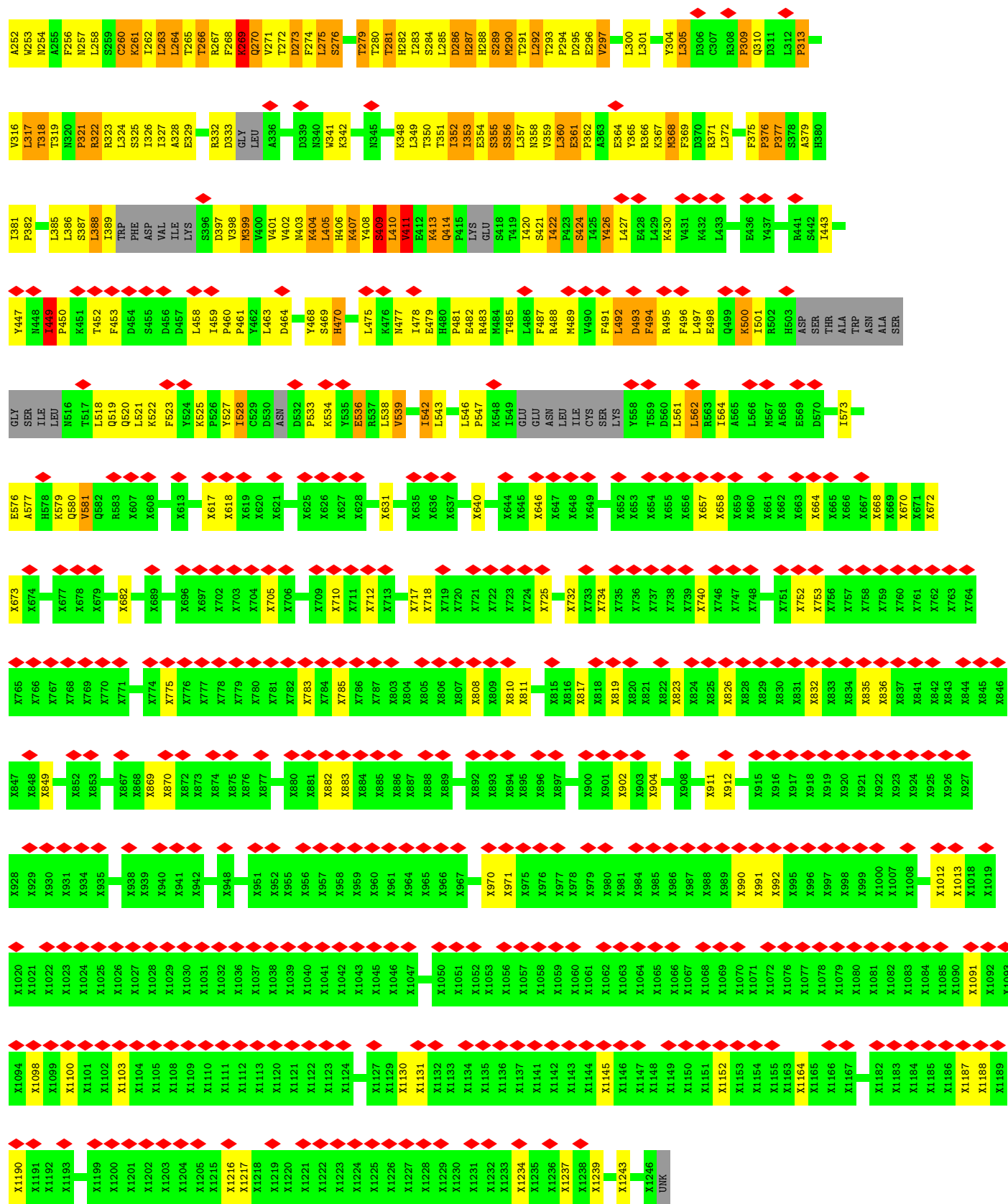
• Molecule 1: Apaf-1 related killer DARK

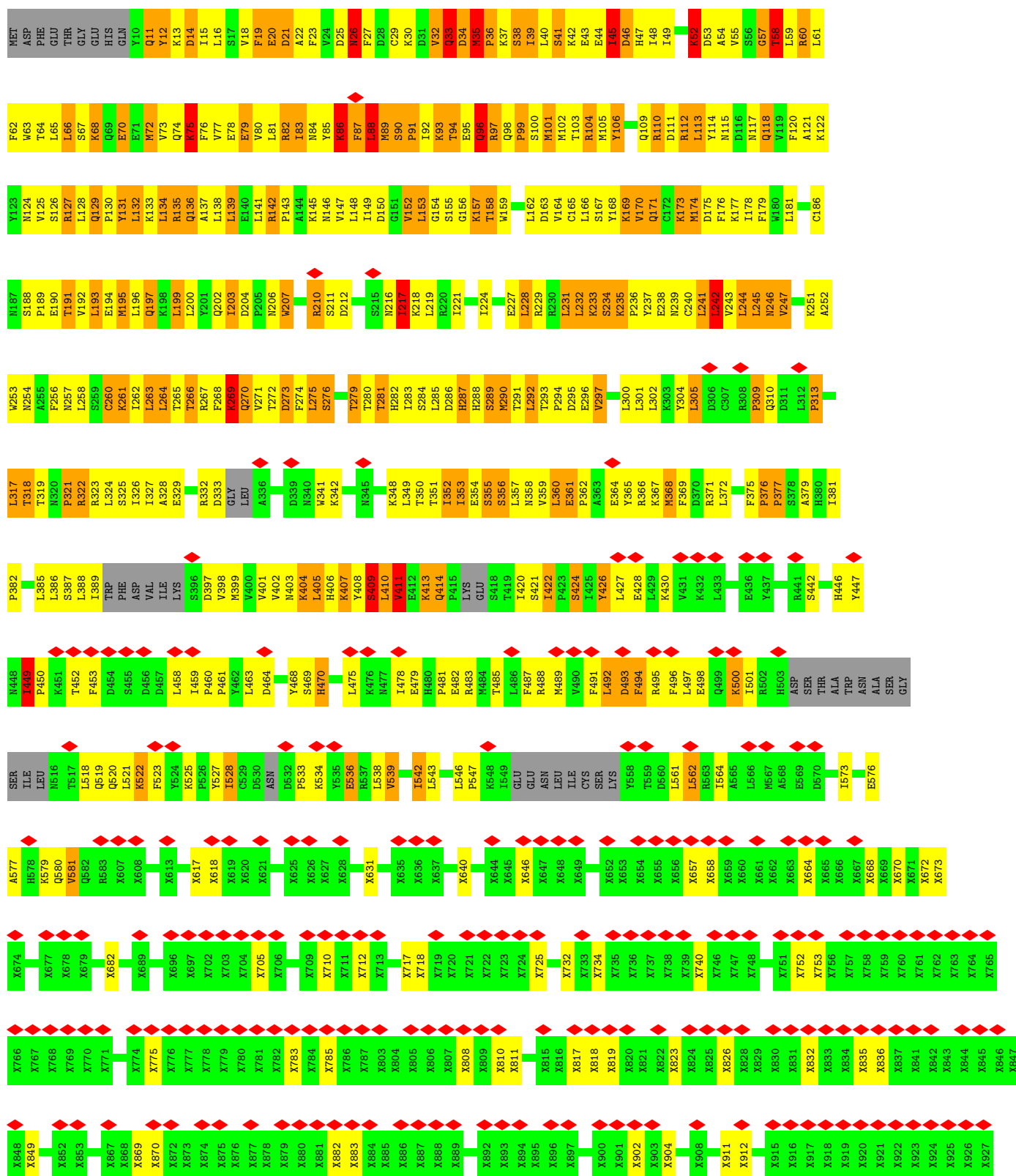


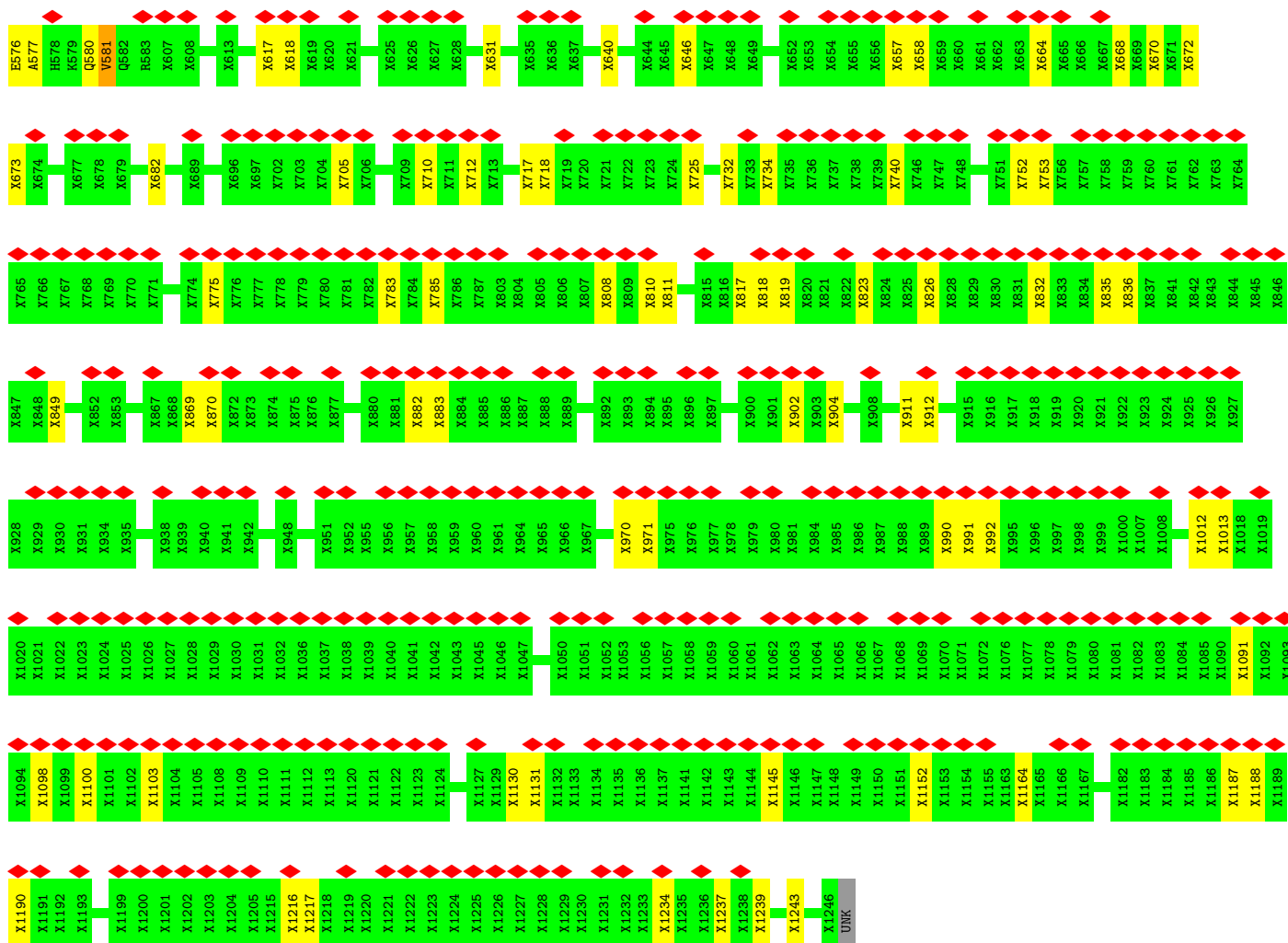


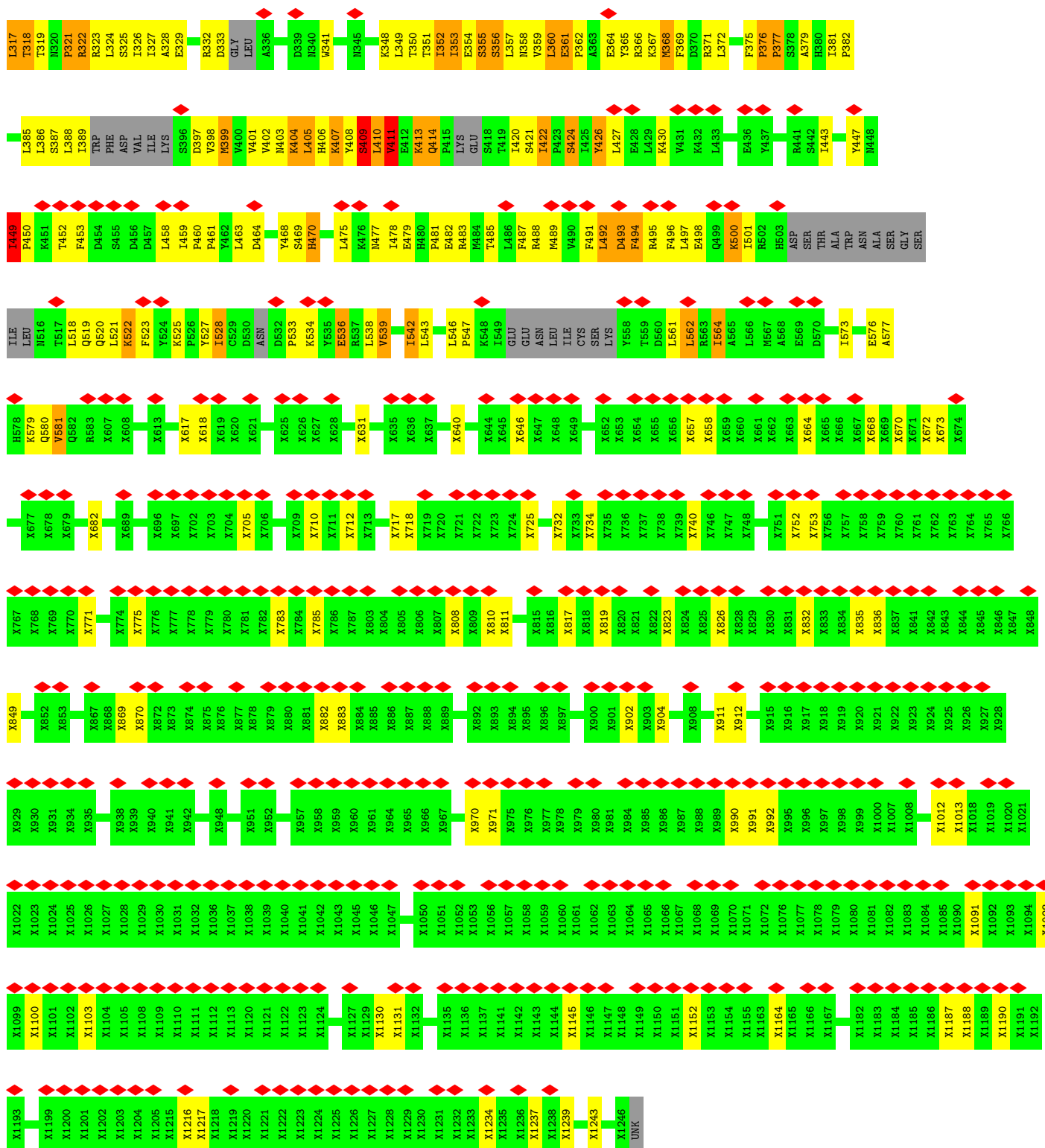
• Molecule 1: Apaf-1 related killer DARK





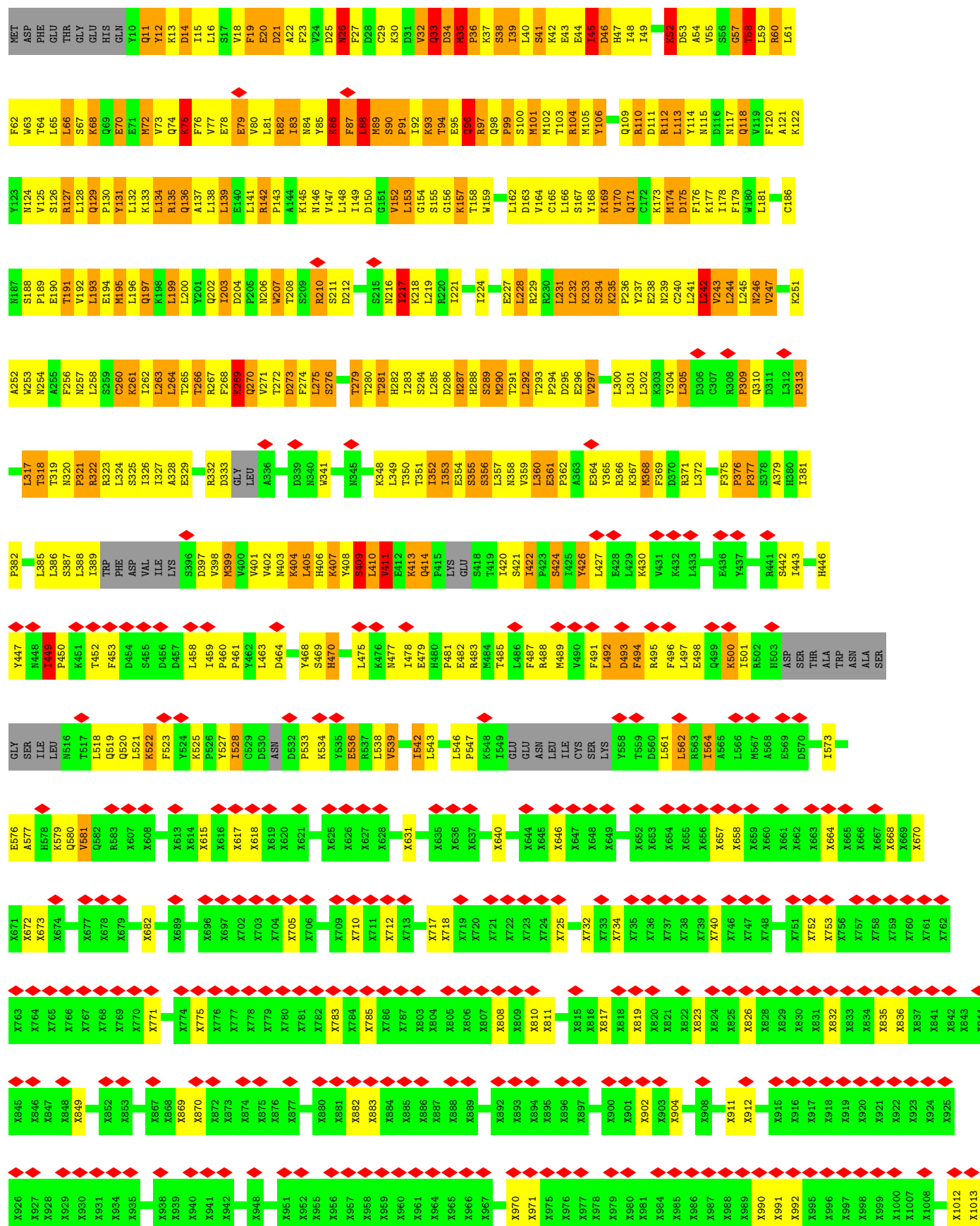






• Molecule 1: Apaf-1 related killer DARK





X1018	X1019	X1020	X1021	X1022	X1023	X1024	X1025	X1026	X1027	X1028	X1029	X1030	X1031	X1032	X1036	X1037	X1038	X1039	X1040	X1041	X1042	X1043	X1045	X1046	X1047	X1050	X1051	X1052	X1053	X1056	X1057	X1058	X1059	X1060	X1061	X1062	X1063	X1064	X1065	X1066	X1067	X1068	X1069	X1070	X1071	X1072	X1076	X1077	X1078	X1079	X1080	X1081	X1082	X1083	X1084	X1085	X1090	X1091
X1092	X1093	X1094	X1098	X1099	X1100	X1101	X1102	X1103	X1104	X1105	X1108	X1109	X1110	X1111	X1112	X1113	X1120	X1121	X1122	X1123	X1124	X1127	X1129	X1130	X1131	X1132	X1133	X1134	X1135	X1136	X1137	X1141	X1142	X1143	X1144	X1145	X1146	X1147	X1148	X1149	X1150	X1151	X1152	X1153	X1154	X1155	X1156	X1157	X1158	X1159	X1160	X1167	X1182	X1183	X1184	X1185	X1186	X1187
X1188	X1189	X1190	X1191	X1192	X1193	X1199	X1200	X1201	X1202	X1203	X1204	X1205	X1215	X1216	X1217	X1218	X1219	X1220	X1221	X1222	X1223	X1224	X1225	X1226	X1227	X1228	X1229	X1230	X1231	X1232	X1233	X1234	X1235	X1236	X1237	X1238	X1239	X1243	X1246																			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D8	Depositor
Number of particles used	9354	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	6600	Depositor
Magnification	104748	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.230	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0643	Depositor
Map size ($\text{\AA}$)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	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

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	0.83	8/4548 (0.2%)	1.22	48/6149 (0.8%)
1	C	0.80	5/4548 (0.1%)	1.22	49/6149 (0.8%)
1	D	0.80	5/4548 (0.1%)	1.22	50/6149 (0.8%)
1	E	0.80	5/4548 (0.1%)	1.22	49/6149 (0.8%)
1	F	0.80	5/4548 (0.1%)	1.22	50/6149 (0.8%)
1	G	0.80	5/4548 (0.1%)	1.22	49/6149 (0.8%)
1	H	0.80	5/4548 (0.1%)	1.22	50/6149 (0.8%)
1	I	0.80	5/4548 (0.1%)	1.22	49/6149 (0.8%)
1	J	0.80	5/4548 (0.1%)	1.22	50/6149 (0.8%)
1	K	0.80	5/4548 (0.1%)	1.22	49/6149 (0.8%)
1	L	0.80	5/4548 (0.1%)	1.22	50/6149 (0.8%)
1	M	0.80	5/4548 (0.1%)	1.22	49/6149 (0.8%)
1	N	0.80	5/4548 (0.1%)	1.22	50/6149 (0.8%)
1	O	0.80	5/4548 (0.1%)	1.22	49/6149 (0.8%)
1	P	0.80	5/4548 (0.1%)	1.22	50/6149 (0.8%)
1	Q	0.80	5/4548 (0.1%)	1.22	49/6149 (0.8%)
All	All	0.81	83/72768 (0.1%)	1.22	790/98384 (0.8%)

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	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
1	G	0	5
1	H	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	5
1	J	0	5
1	K	0	5
1	L	0	5
1	M	0	5
1	N	0	5
1	O	0	5
1	P	0	5
1	Q	0	6
All	All	0	81

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	86	LYS	CA-CB	-17.11	1.27	1.53
1	E	86	LYS	CA-CB	-17.11	1.27	1.53
1	G	86	LYS	CA-CB	-17.11	1.27	1.53
1	I	86	LYS	CA-CB	-17.11	1.27	1.53
1	K	86	LYS	CA-CB	-17.11	1.27	1.53

The worst 5 of 790 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	VAL	N-CA-CB	-20.45	88.48	112.40
1	E	411	VAL	N-CA-CB	-20.45	88.48	112.40
1	G	411	VAL	N-CA-CB	-20.45	88.48	112.40
1	I	411	VAL	N-CA-CB	-20.45	88.48	112.40
1	K	411	VAL	N-CA-CB	-20.45	88.48	112.40

There are no chirality outliers.

5 of 81 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	SER	Peptide
1	A	281	THR	Mainchain
1	A	33	GLN	Peptide
1	A	36	PRO	Peptide
1	A	75	LYS	Mainchain

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	7031	0	5108	1009	0
1	C	7031	0	5108	1023	0
1	D	7031	0	5108	1023	0
1	E	7031	0	5108	1023	0
1	F	7031	0	5108	1035	0
1	G	7031	0	5108	1019	0
1	H	7031	0	5108	1034	0
1	I	7031	0	5108	1023	0
1	J	7031	0	5108	1026	0
1	K	7031	0	5108	1024	0
1	L	7031	0	5108	1021	0
1	M	7031	0	5108	1019	0
1	N	7031	0	5108	1026	0
1	O	7031	0	5108	1020	0
1	P	7031	0	5108	1031	0
1	Q	7036	0	5106	1018	0
2	C	30	0	12	19	0
2	D	30	0	12	20	0
2	E	30	0	12	19	0
2	F	30	0	12	19	0
2	G	30	0	12	19	0
2	H	30	0	12	20	0
2	I	30	0	12	18	0
2	J	30	0	12	19	0
2	K	30	0	12	20	0
2	L	30	0	12	20	0
2	M	30	0	12	19	0
2	N	30	0	12	18	0
2	O	30	0	12	18	0
2	P	30	0	12	18	0
2	Q	30	0	12	19	0
All	All	112951	0	81906	15884	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 82.

The worst 5 of 15884 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:J:174:MET:CE	1:J:241:LEU:HB2	1.26	1.66
1:N:174:MET:CE	1:N:241:LEU:HB2	1.26	1.66
1:M:174:MET:CE	1:M:241:LEU:HB2	1.26	1.64
1:C:174:MET:CE	1:C:241:LEU:HB2	1.26	1.64
1:I:174:MET:CE	1:I:241:LEU:HB2	1.26	1.64

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	14	48
1	C	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	14	48
1	D	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	14	48
1	E	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	14	48
1	F	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	14	48
1	G	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	14	48
1	H	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	14	48
1	I	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	14	48
1	J	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	14	48
1	K	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	14	48
1	L	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	14	48
1	M	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	14	48
1	N	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	14	48
1	O	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	14	48
1	P	529/1103 (48%)	468 (88%)	56 (11%)	5 (1%)	14	48
1	Q	529/1103 (48%)	469 (89%)	55 (10%)	5 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8464/17648 (48%)	7496 (89%)	888 (10%)	80 (1%)	16	48

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	A	409	SER
1	C	99	PRO
1	C	409	SER
1	D	99	PRO

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	500/551 (91%)	363 (73%)	137 (27%)	0	3
1	C	500/551 (91%)	364 (73%)	136 (27%)	0	3
1	D	500/551 (91%)	363 (73%)	137 (27%)	0	3
1	E	500/551 (91%)	364 (73%)	136 (27%)	0	3
1	F	500/551 (91%)	363 (73%)	137 (27%)	0	3
1	G	500/551 (91%)	364 (73%)	136 (27%)	0	3
1	H	500/551 (91%)	363 (73%)	137 (27%)	0	3
1	I	500/551 (91%)	364 (73%)	136 (27%)	0	3
1	J	500/551 (91%)	363 (73%)	137 (27%)	0	3
1	K	500/551 (91%)	364 (73%)	136 (27%)	0	3
1	L	500/551 (91%)	363 (73%)	137 (27%)	0	3
1	M	500/551 (91%)	364 (73%)	136 (27%)	0	3
1	N	500/551 (91%)	363 (73%)	137 (27%)	0	3
1	O	500/551 (91%)	364 (73%)	136 (27%)	0	3
1	P	500/551 (91%)	363 (73%)	137 (27%)	0	3
1	Q	500/551 (91%)	364 (73%)	136 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8000/8816 (91%)	5816 (73%)	2184 (27%)	1 3

5 of 2184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	235	LYS
1	O	562	LEU
1	O	233	LYS
1	Q	93	LYS
1	G	297	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 251 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	129	GLN
1	P	117	ASN
1	K	47	HIS
1	P	26	ASN
1	Q	117	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	G	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	D	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	C	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	I	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	J	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	L	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	M	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	Q	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	E	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	H	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	N	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	F	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	P	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	K	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)
2	DTP	O	1301	-	31,32,32	1.43	4 (12%)	46,50,50	1.79	9 (19%)

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	G	1301	-	-	6/22/34/34	0/3/3/3
2	DTP	D	1301	-	-	6/22/34/34	0/3/3/3
2	DTP	C	1301	-	-	6/22/34/34	0/3/3/3
2	DTP	I	1301	-	-	6/22/34/34	0/3/3/3
2	DTP	J	1301	-	-	6/22/34/34	0/3/3/3
2	DTP	L	1301	-	-	8/22/34/34	0/3/3/3
2	DTP	M	1301	-	-	8/22/34/34	0/3/3/3
2	DTP	Q	1301	-	-	8/22/34/34	0/3/3/3
2	DTP	E	1301	-	-	6/22/34/34	0/3/3/3
2	DTP	H	1301	-	-	6/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	N	1301	-	-	8/22/34/34	0/3/3/3
2	DTP	F	1301	-	-	6/22/34/34	0/3/3/3
2	DTP	P	1301	-	-	8/22/34/34	0/3/3/3
2	DTP	K	1301	-	-	8/22/34/34	0/3/3/3
2	DTP	O	1301	-	-	8/22/34/34	0/3/3/3

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	DTP	C5-C4	4.74	1.47	1.39
2	F	1301	DTP	C5-C4	4.74	1.47	1.39
2	H	1301	DTP	C5-C4	4.74	1.47	1.39
2	J	1301	DTP	C5-C4	4.74	1.47	1.39
2	L	1301	DTP	C5-C4	4.74	1.47	1.39

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1301	DTP	C5-C4-N3	-5.86	118.65	126.72
2	F	1301	DTP	C5-C4-N3	-5.86	118.65	126.72
2	H	1301	DTP	C5-C4-N3	-5.86	118.65	126.72
2	J	1301	DTP	C5-C4-N3	-5.86	118.65	126.72
2	L	1301	DTP	C5-C4-N3	-5.86	118.65	126.72

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1301	DTP	C5'-O5'-PA-O2A
2	C	1301	DTP	C5'-O5'-PA-O3A
2	C	1301	DTP	C4'-C5'-O5'-PA
2	C	1301	DTP	O4'-C1'-N9-C4
2	D	1301	DTP	C5'-O5'-PA-O2A

There are no ring outliers.

15 monomers are involved in 285 short contacts:

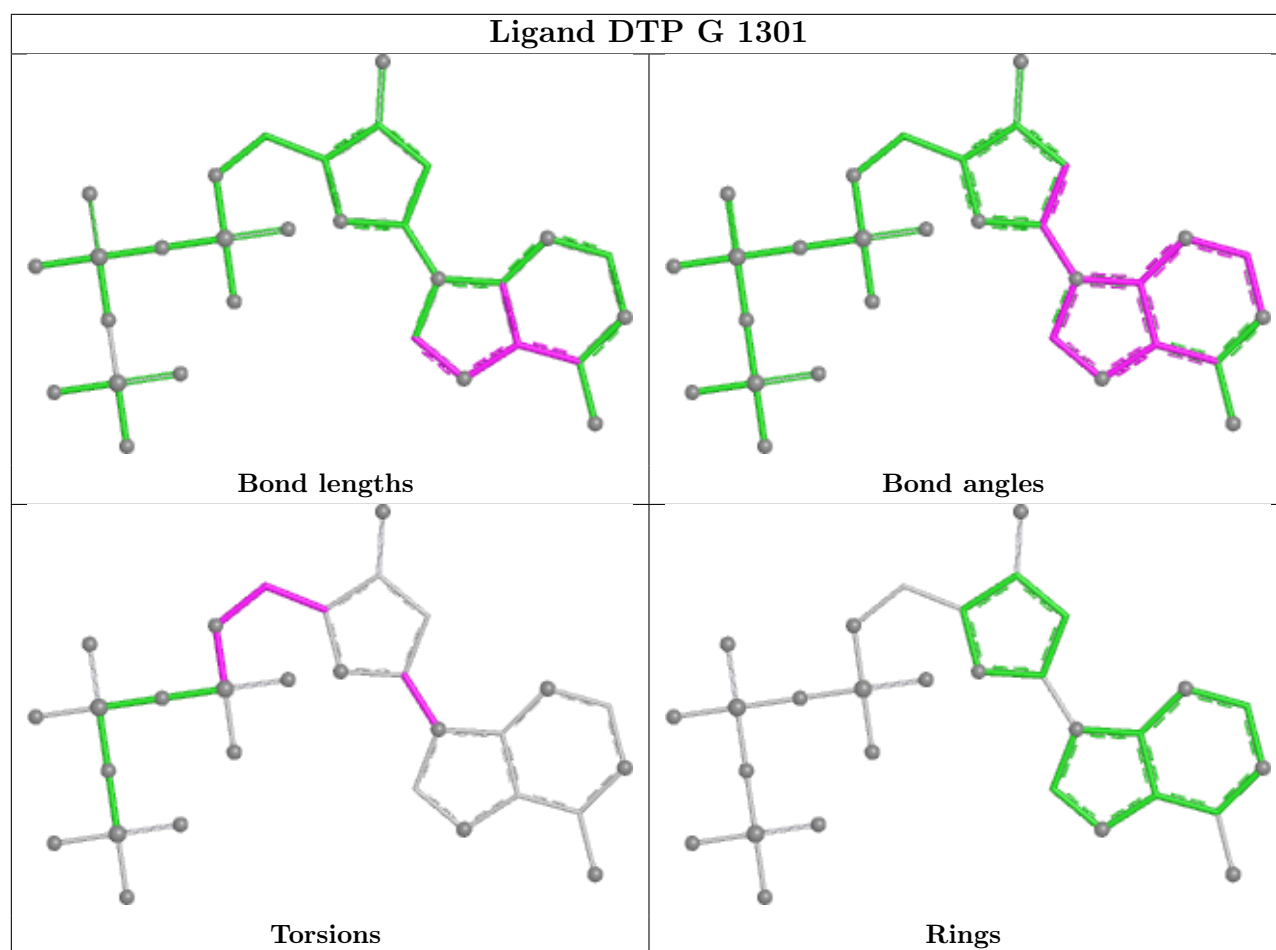
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1301	DTP	19	0
2	D	1301	DTP	20	0

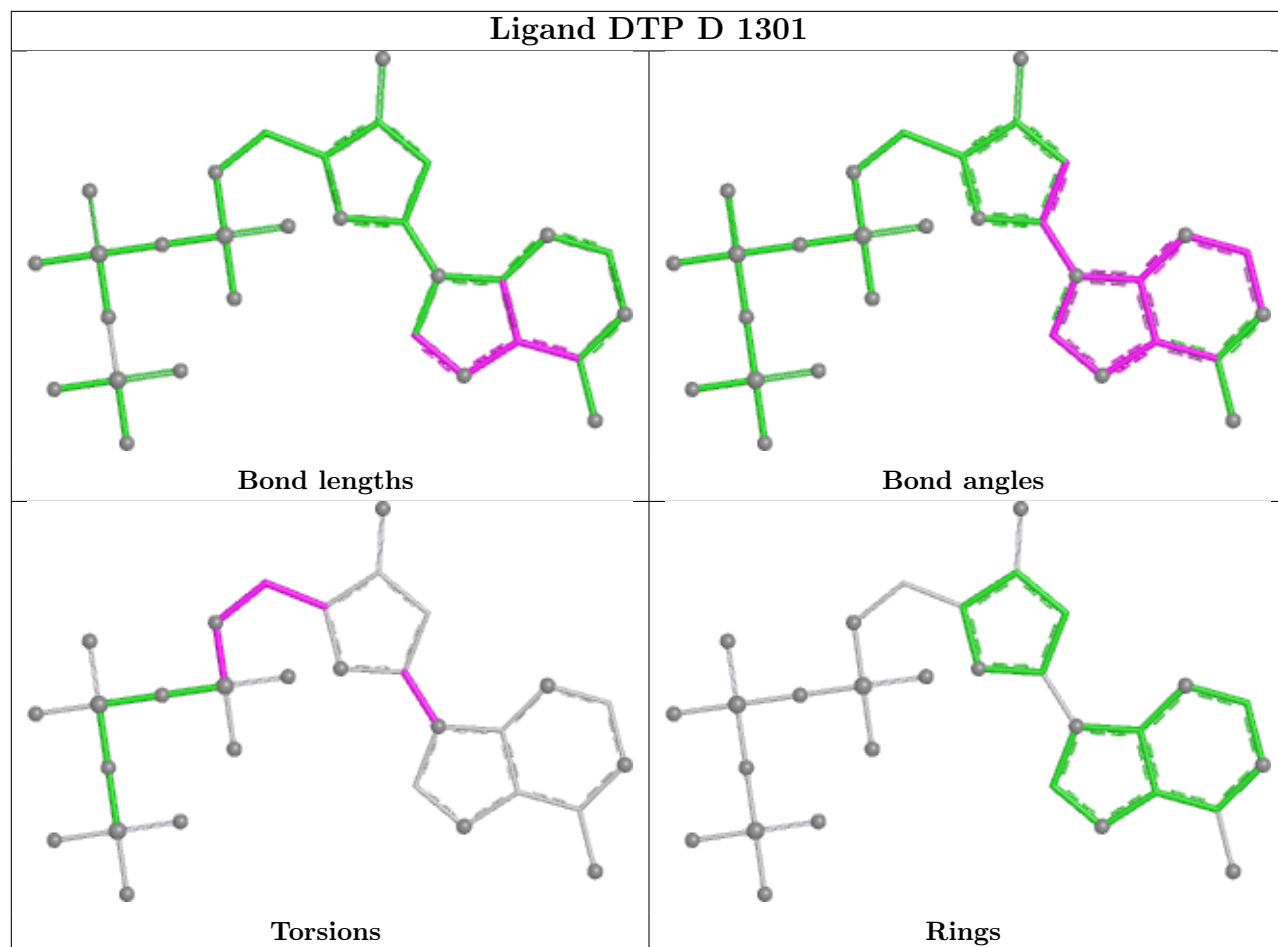
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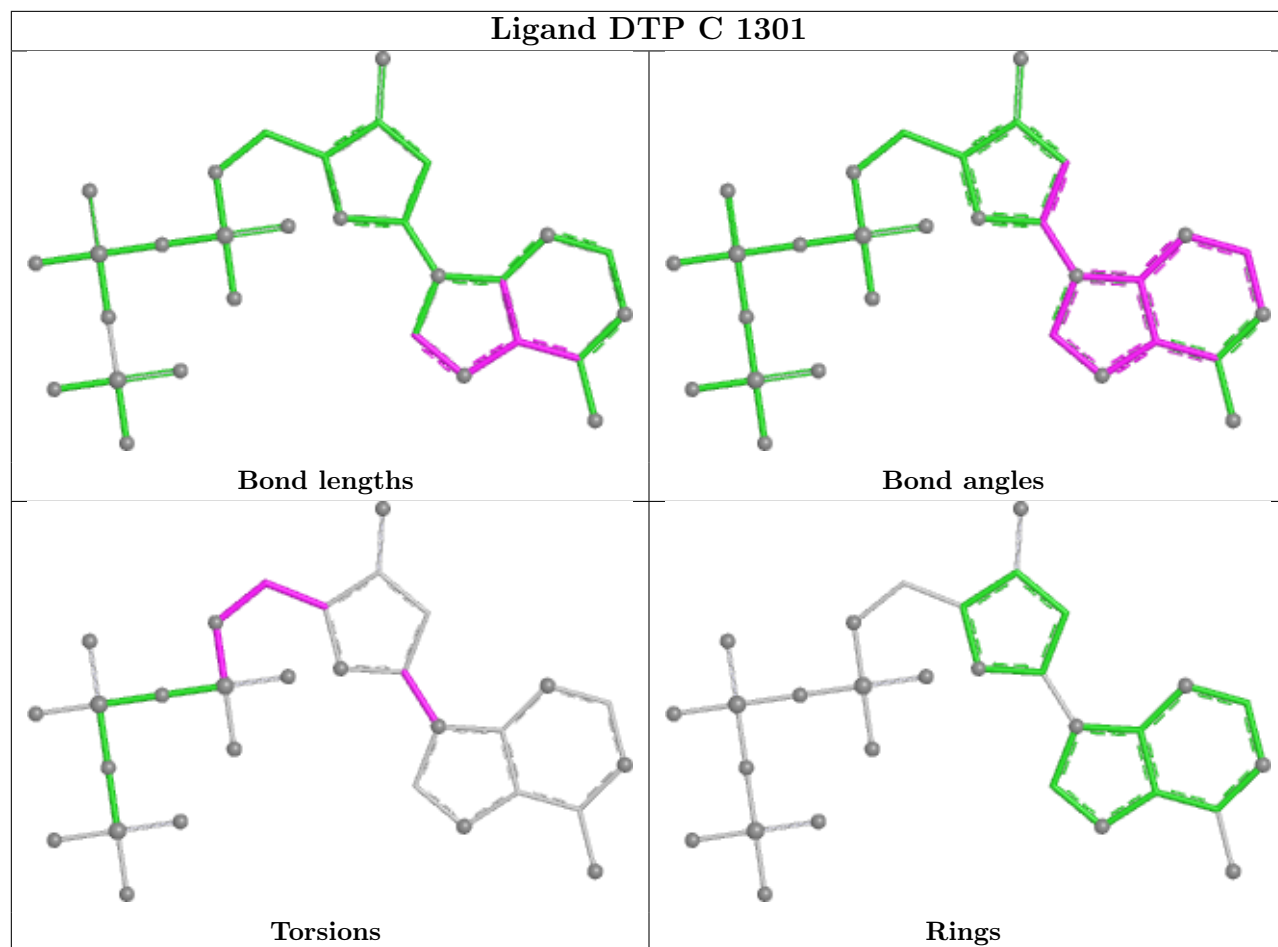
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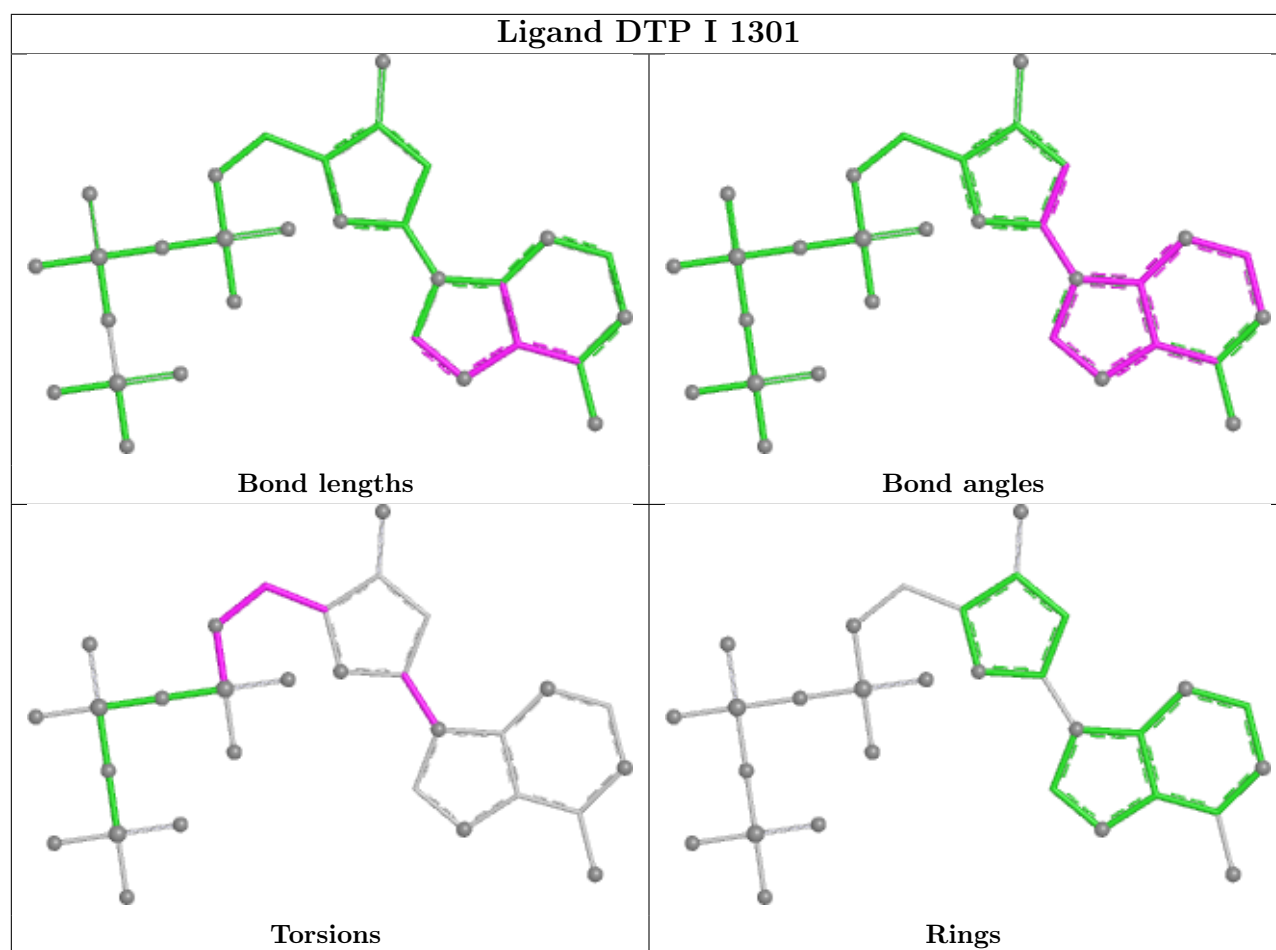
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	DTP	19	0
2	I	1301	DTP	18	0
2	J	1301	DTP	19	0
2	L	1301	DTP	20	0
2	M	1301	DTP	19	0
2	Q	1301	DTP	19	0
2	E	1301	DTP	19	0
2	H	1301	DTP	20	0
2	N	1301	DTP	18	0
2	F	1301	DTP	19	0
2	P	1301	DTP	18	0
2	K	1301	DTP	20	0
2	O	1301	DTP	18	0

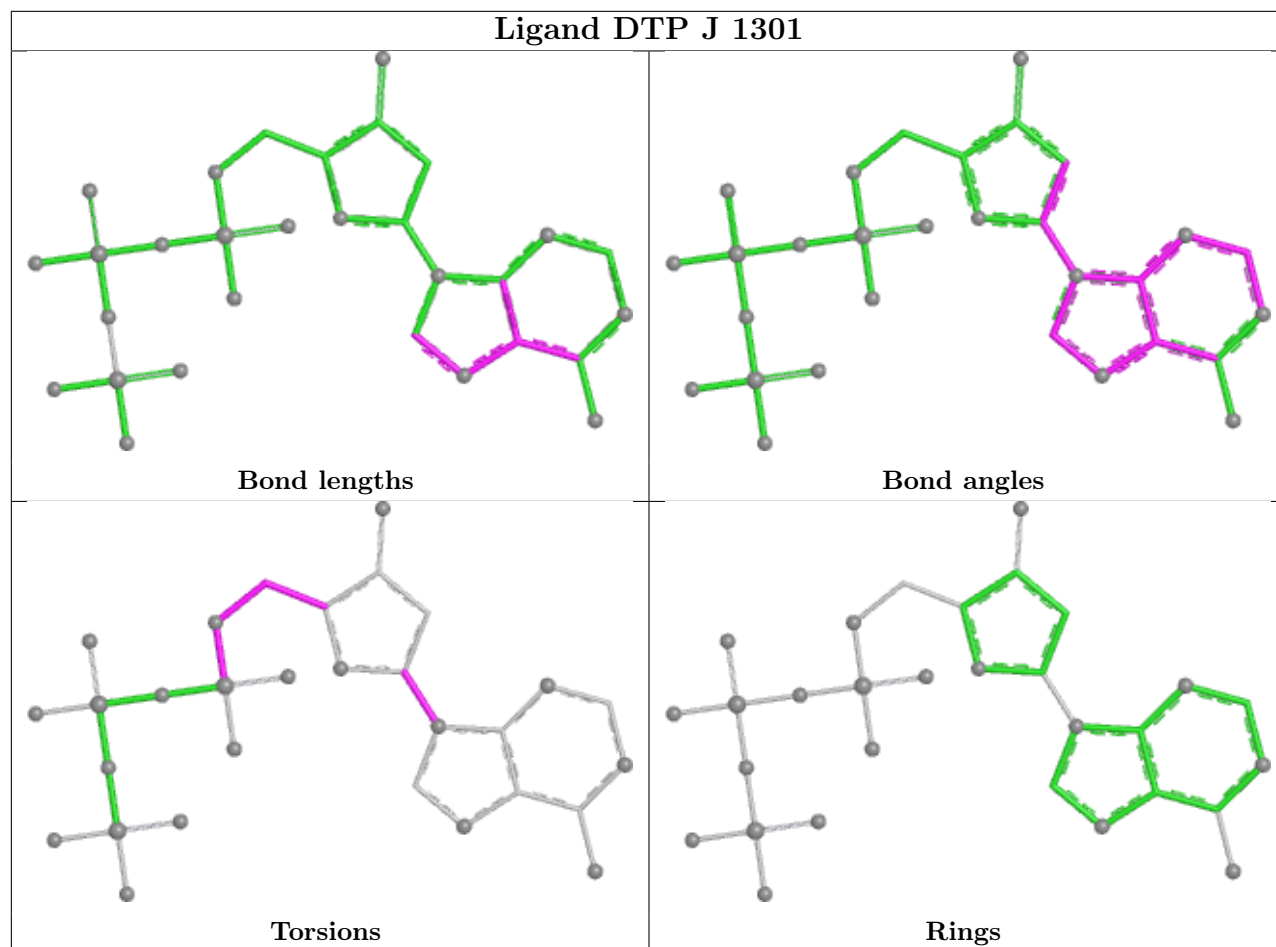
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

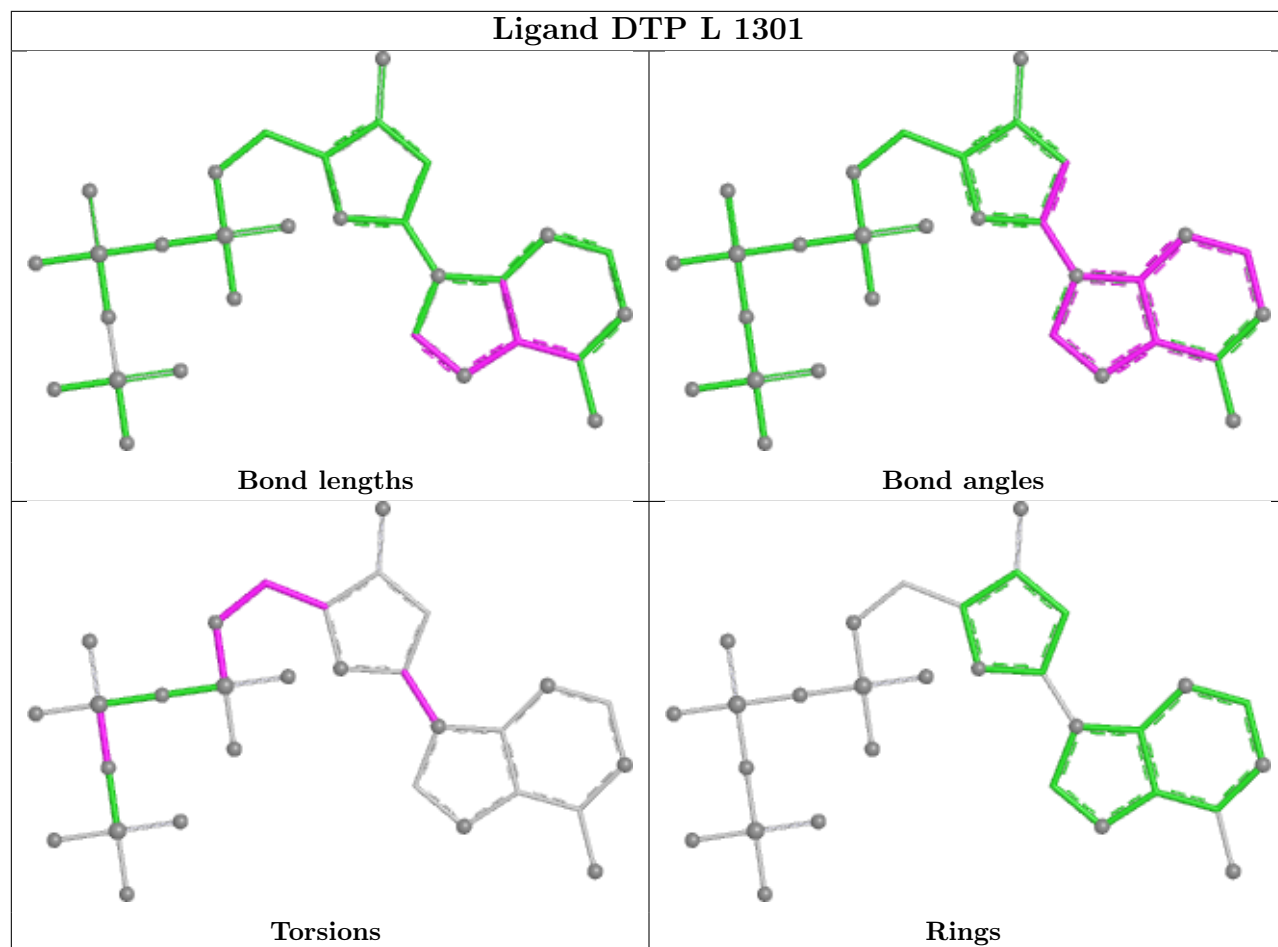


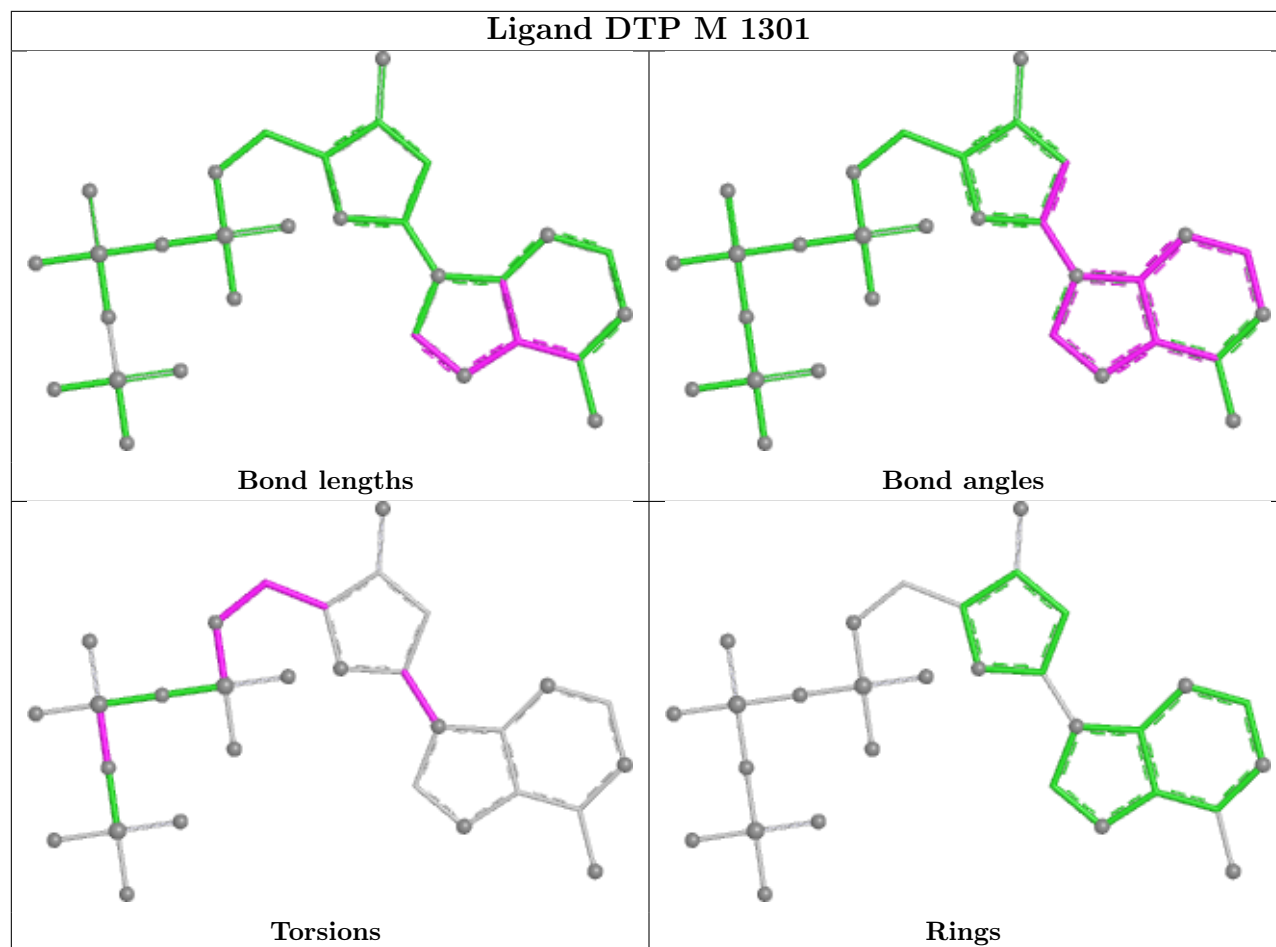


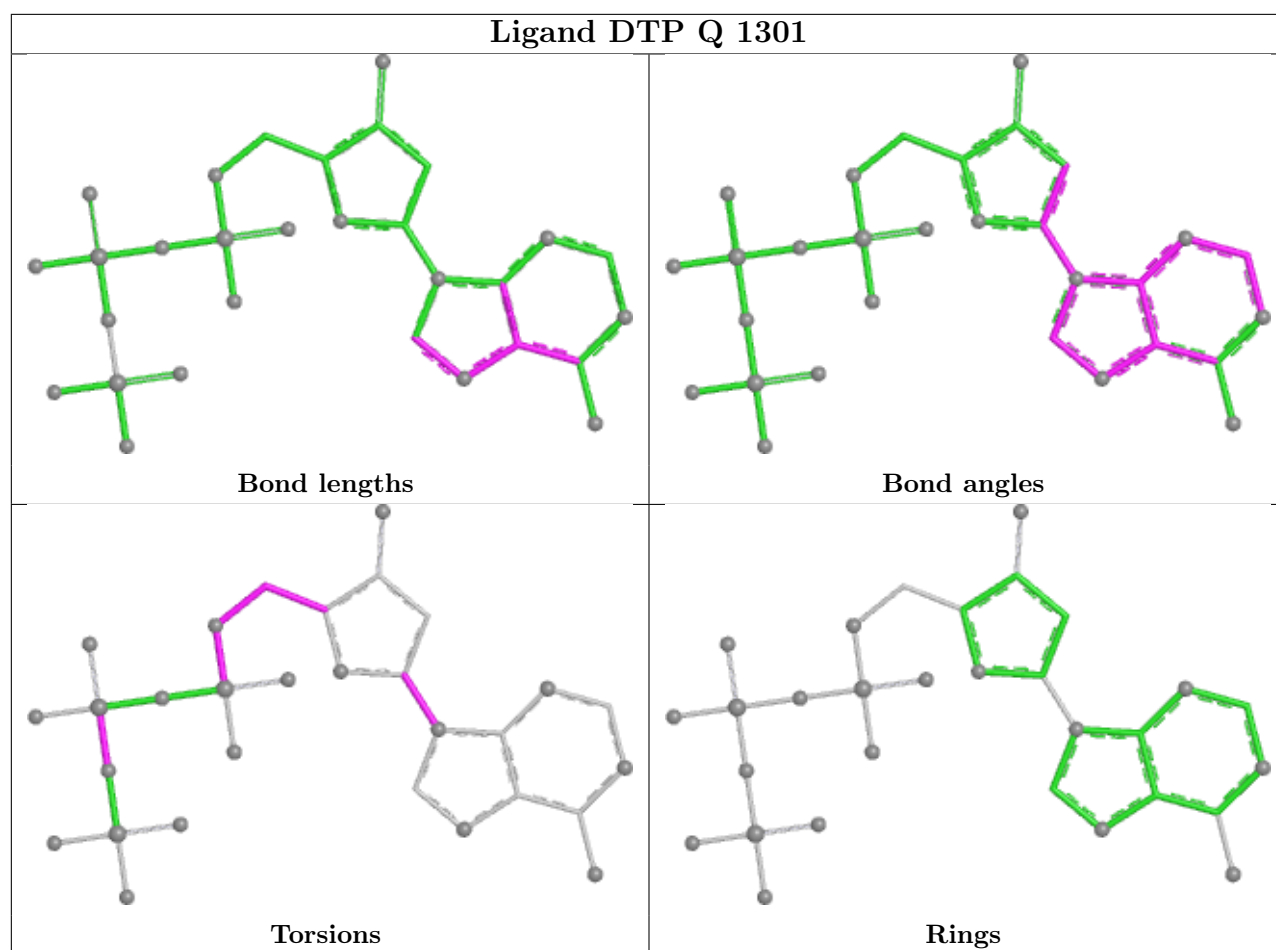


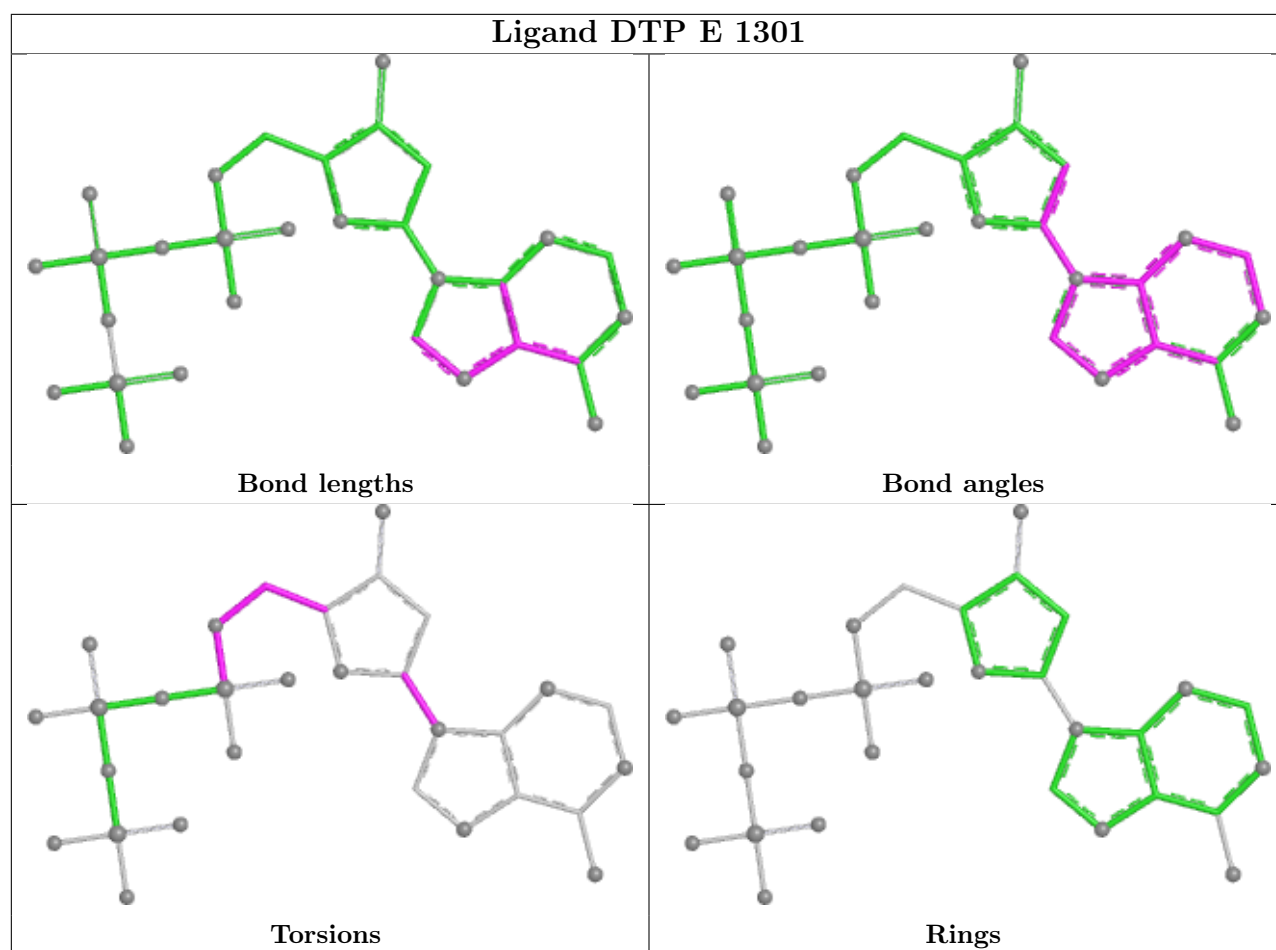


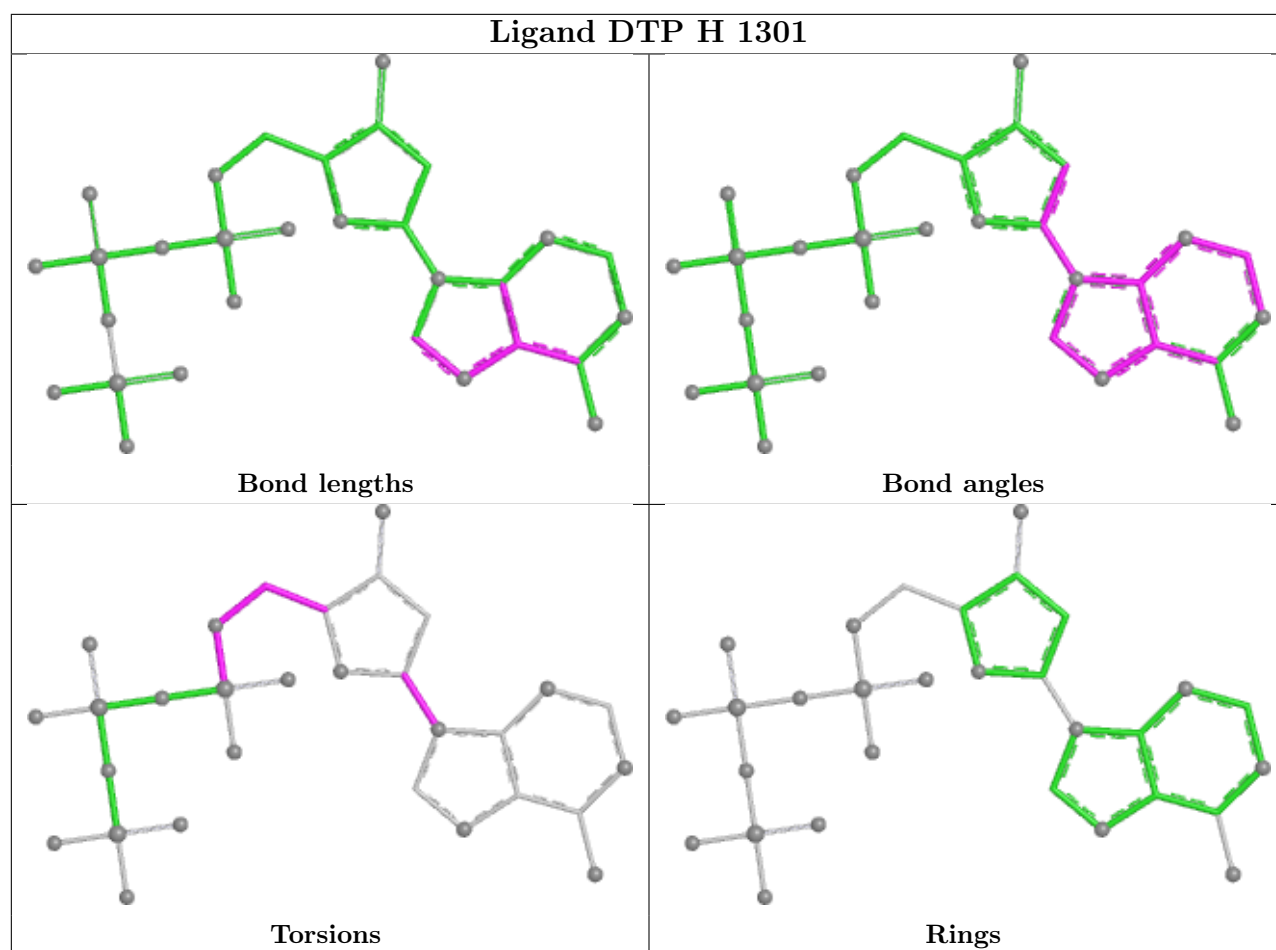


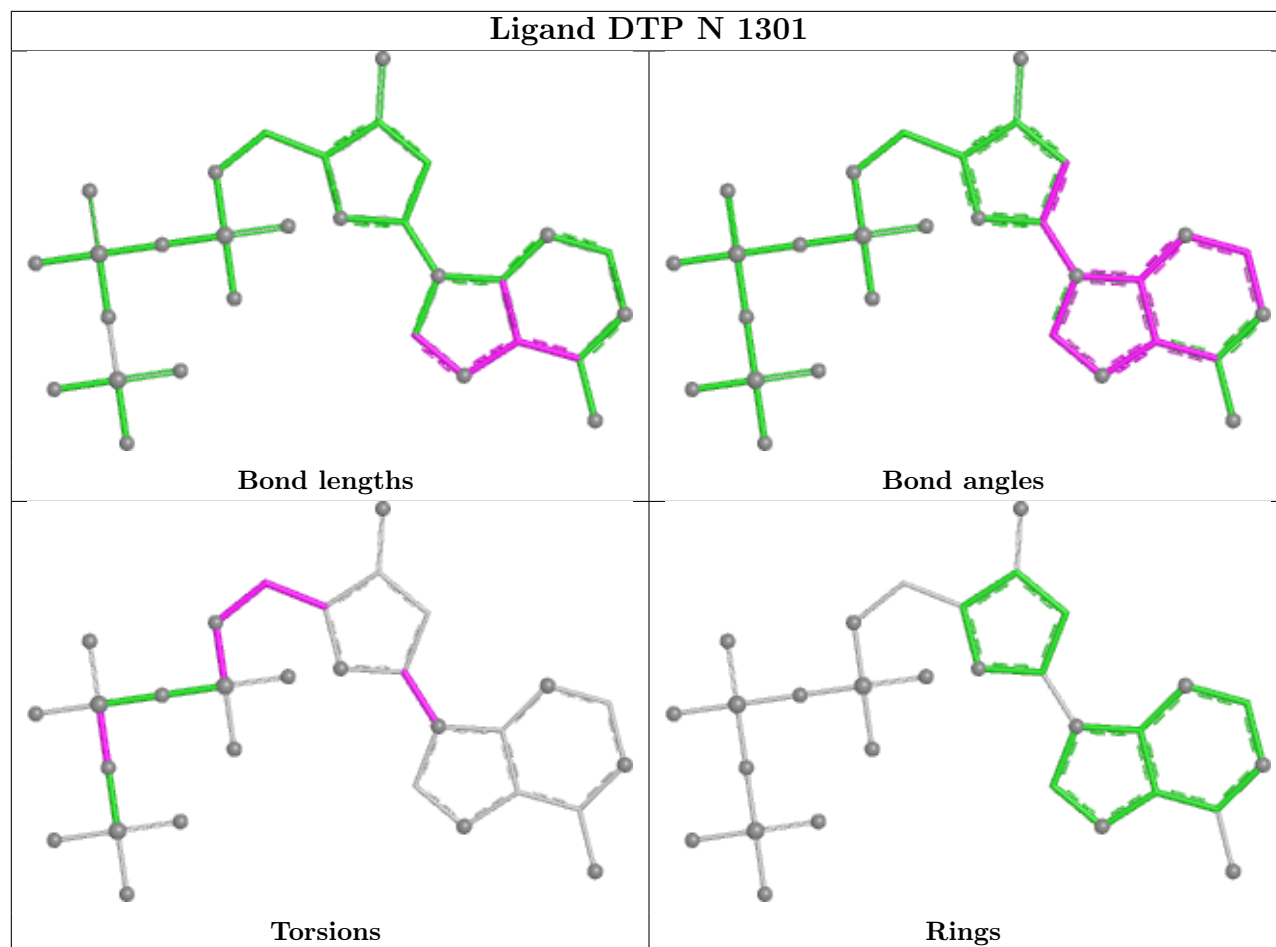


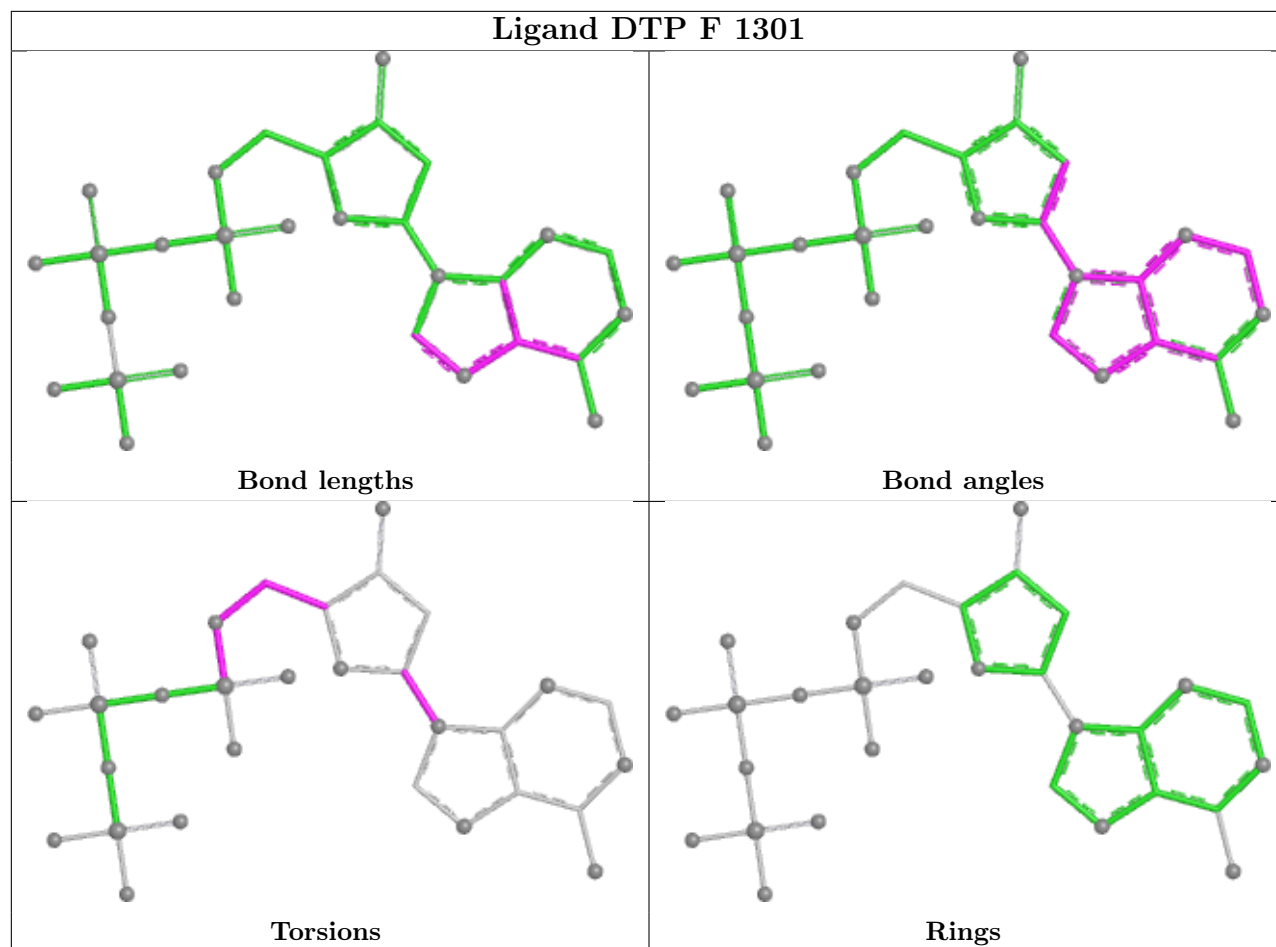


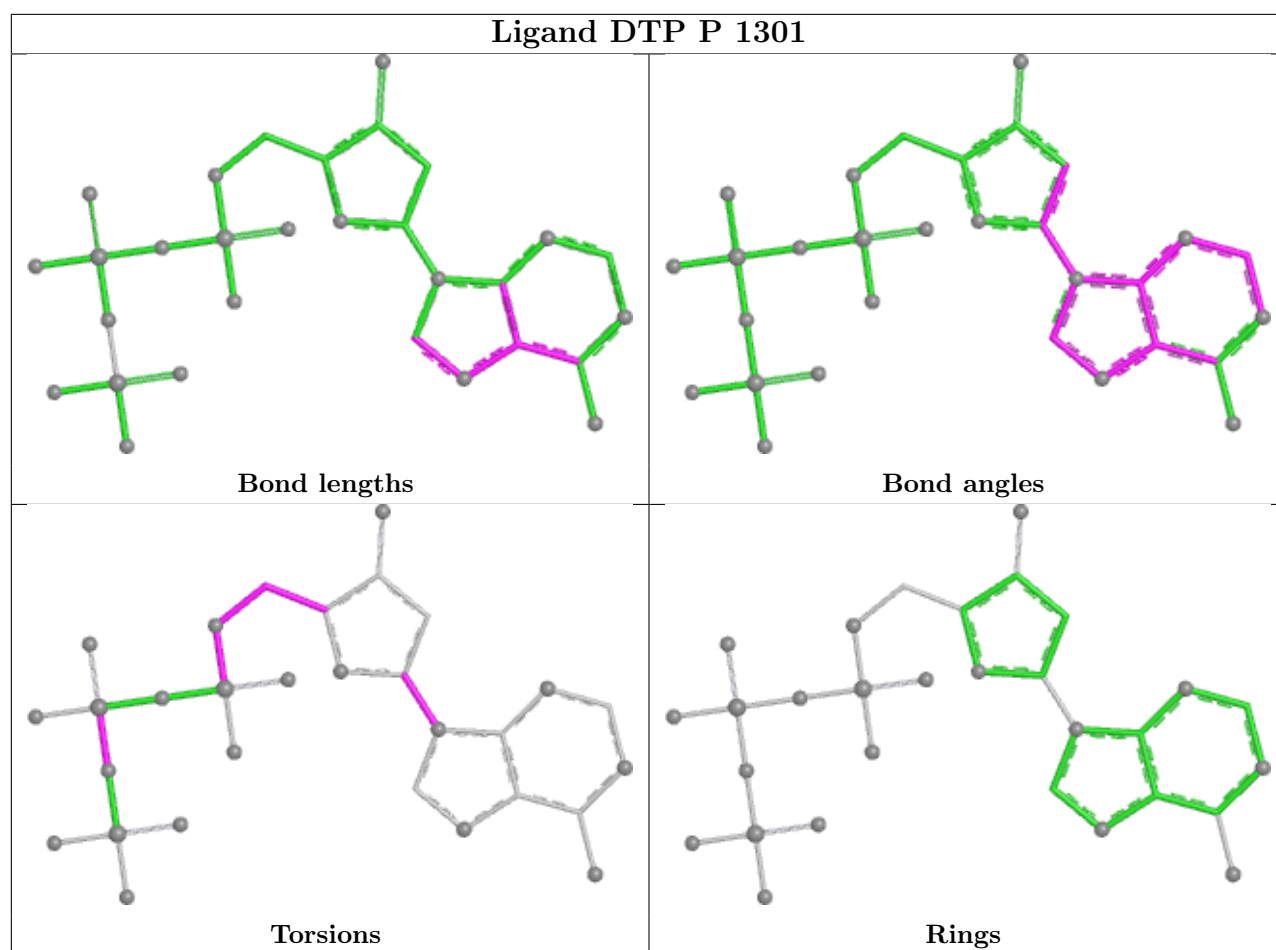


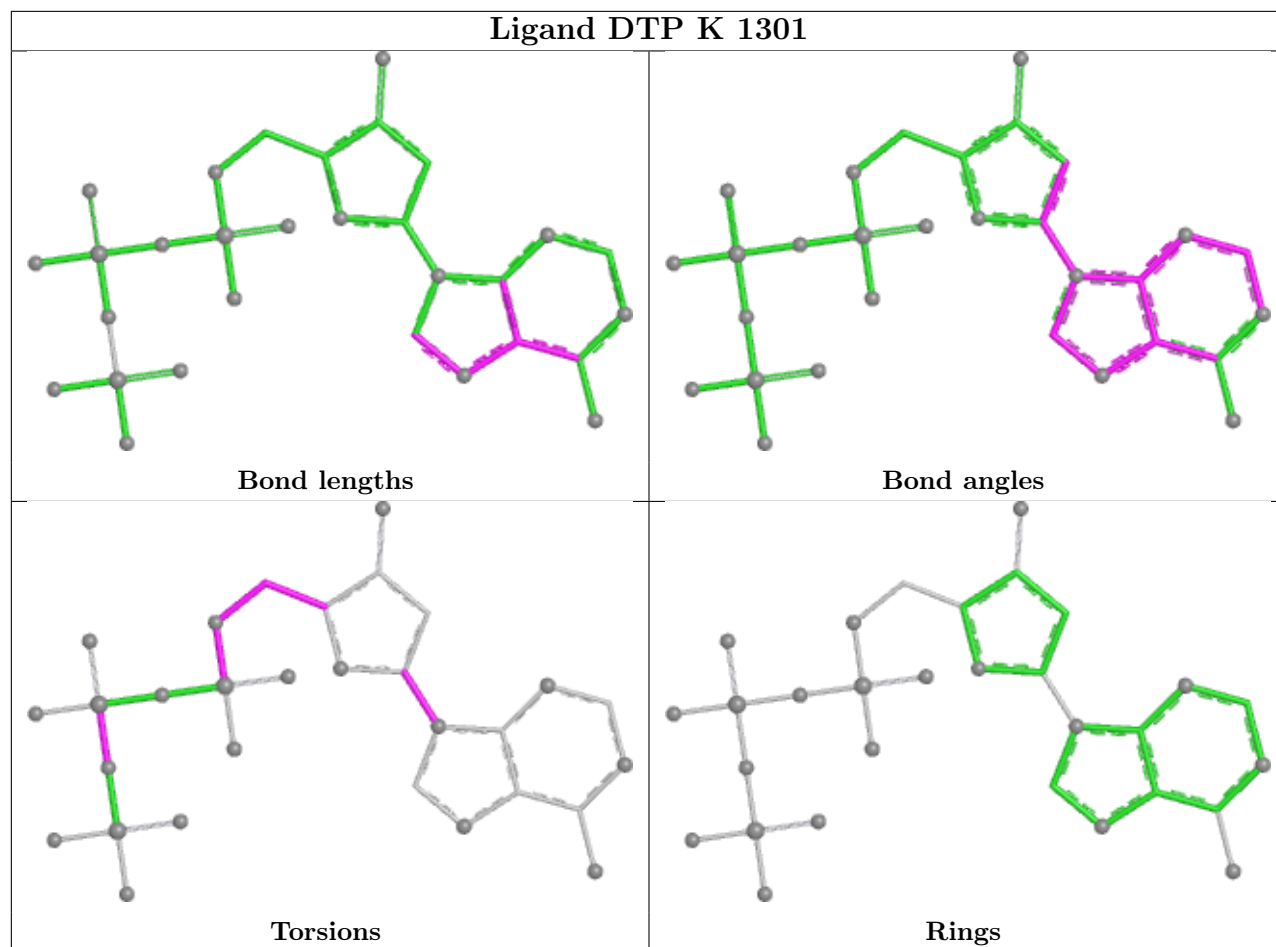


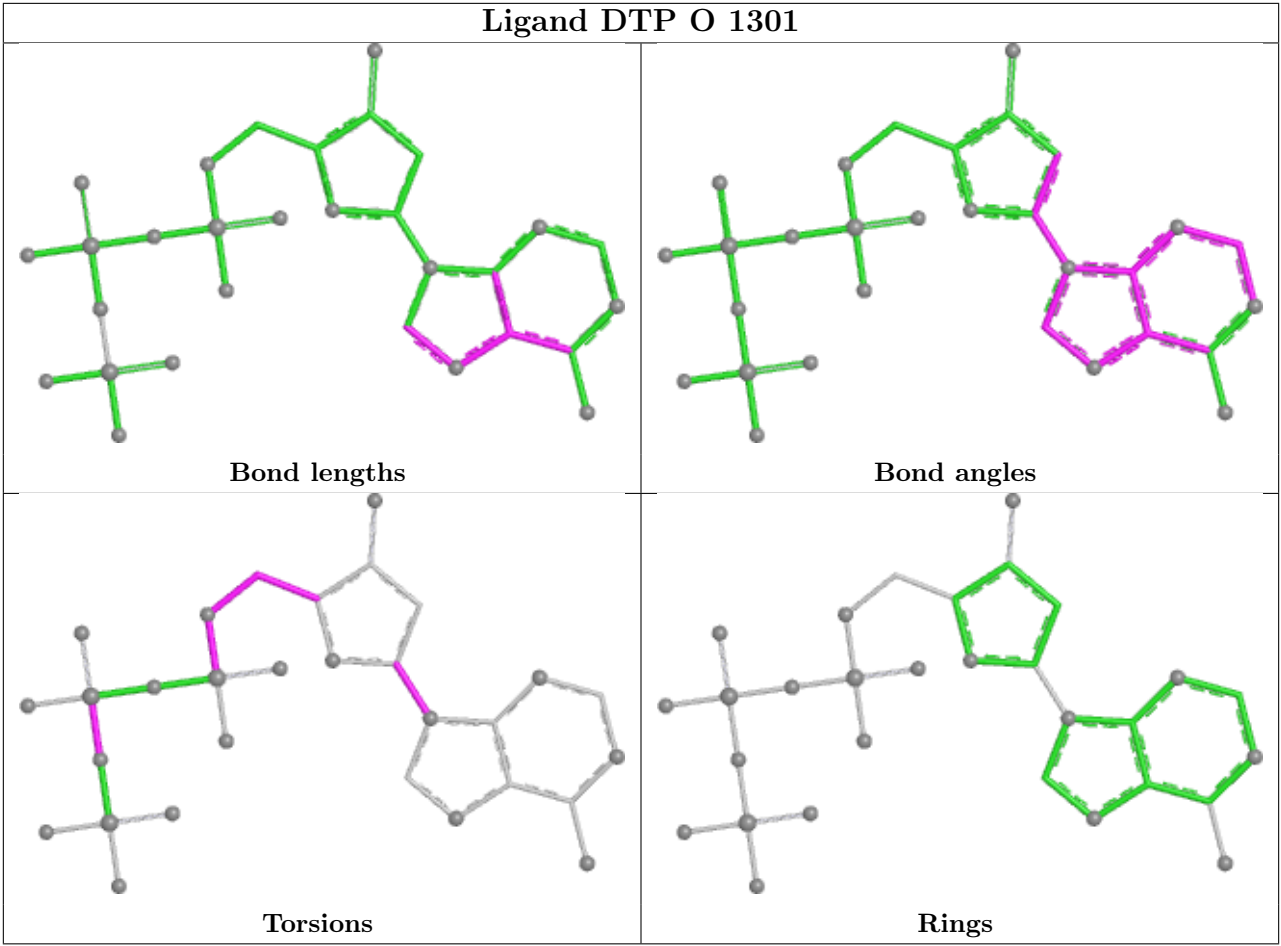












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	39
1	C	39
1	D	39
1	E	39
1	F	39
1	G	39
1	H	39
1	I	39
1	J	39
1	K	39

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Mol	Chain	Number of breaks
1	L	39
1	M	39
1	N	39
1	O	39
1	P	39
1	Q	39

The worst 5 of 624 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	583:ARG	C	607:UNK	N	28.65
1	C	583:ARG	C	607:UNK	N	28.65
1	D	583:ARG	C	607:UNK	N	28.65
1	E	583:ARG	C	607:UNK	N	28.65
1	F	583:ARG	C	607:UNK	N	28.65

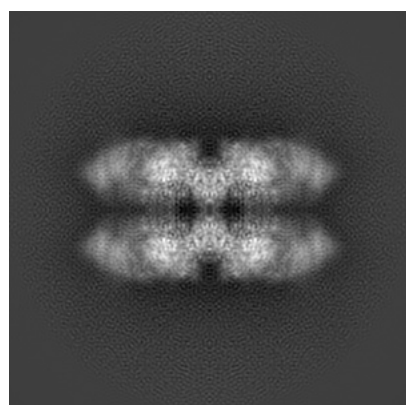
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2871. These allow visual inspection of the internal detail of the map and identification of artifacts.

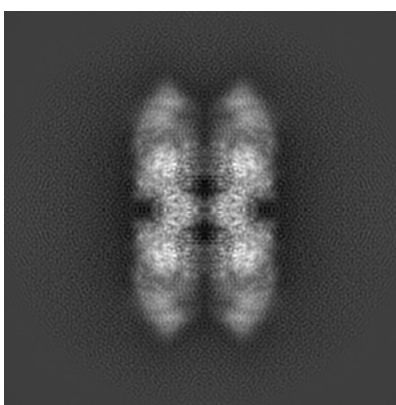
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

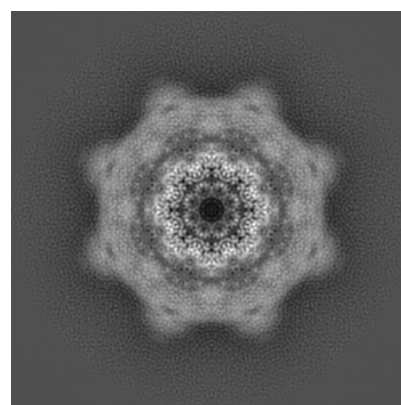
6.1.1 Primary map



X



Y

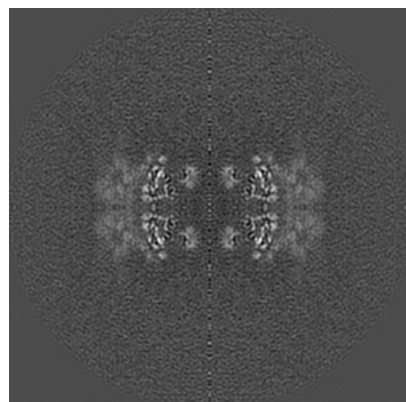


Z

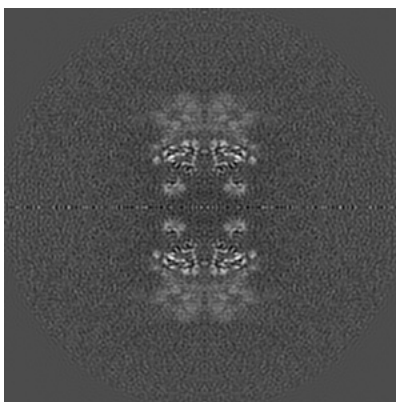
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

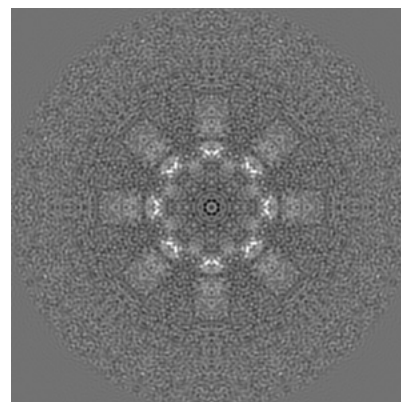
6.2.1 Primary map



X Index: 160



Y Index: 160

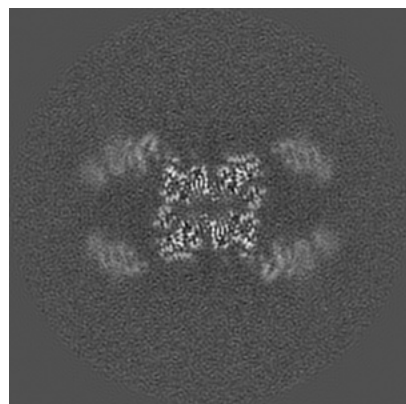


Z Index: 160

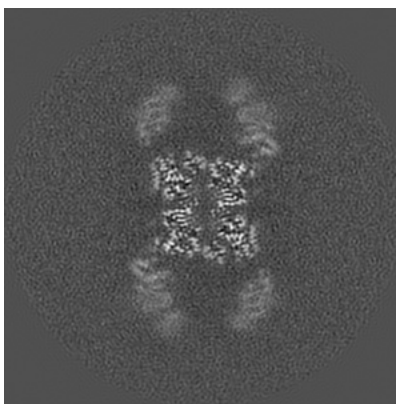
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

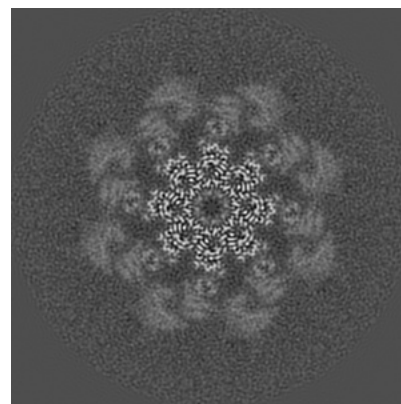
6.3.1 Primary map



X Index: 188



Y Index: 188

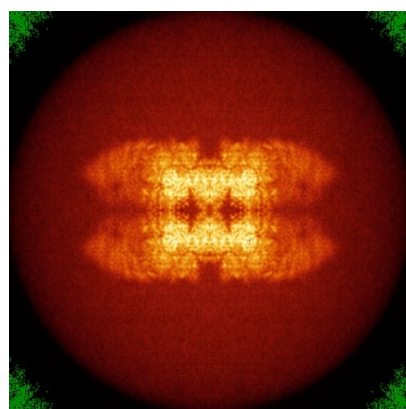


Z Index: 185

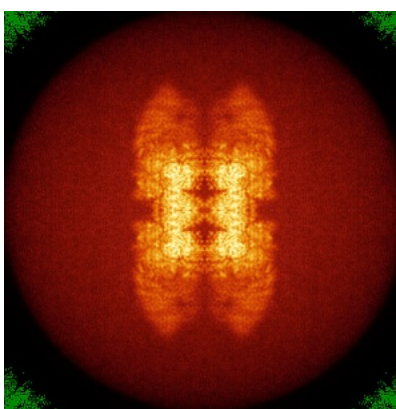
The images above show the largest variance slices of the map in three orthogonal directions.

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

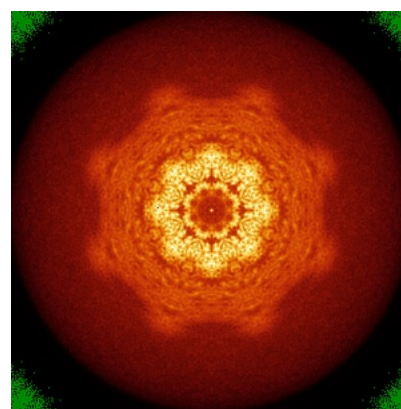
6.4.1 Primary map



X



Y

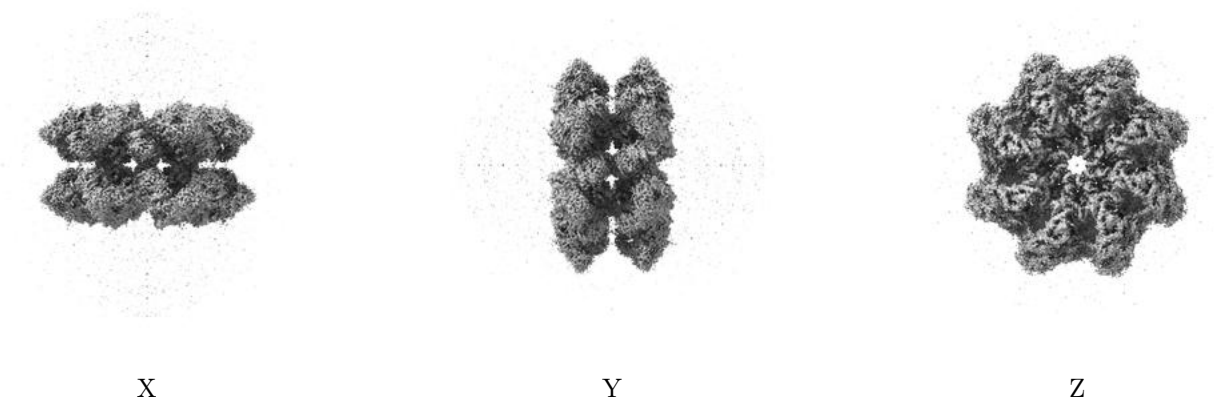


Z

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 0.0643. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

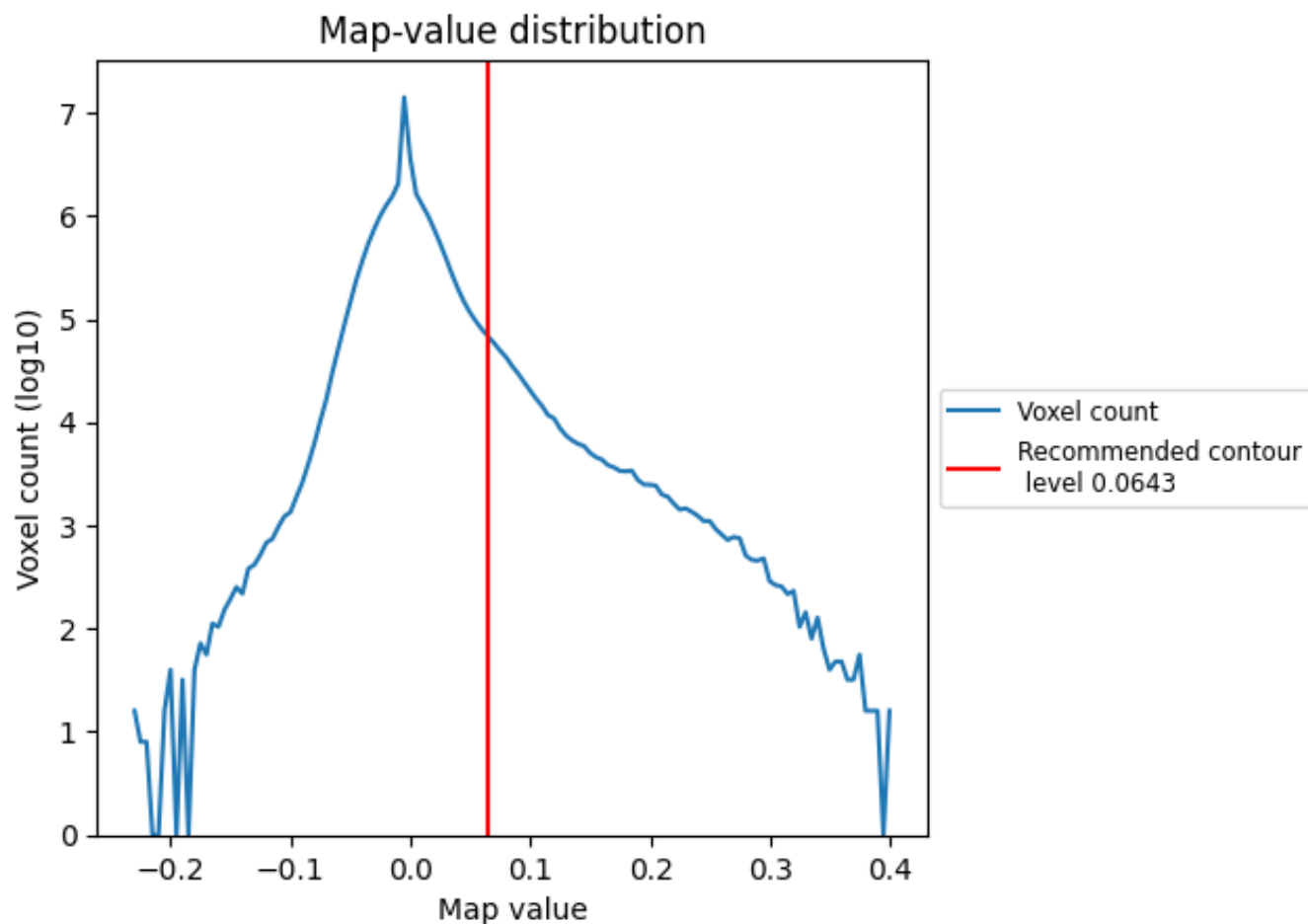
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

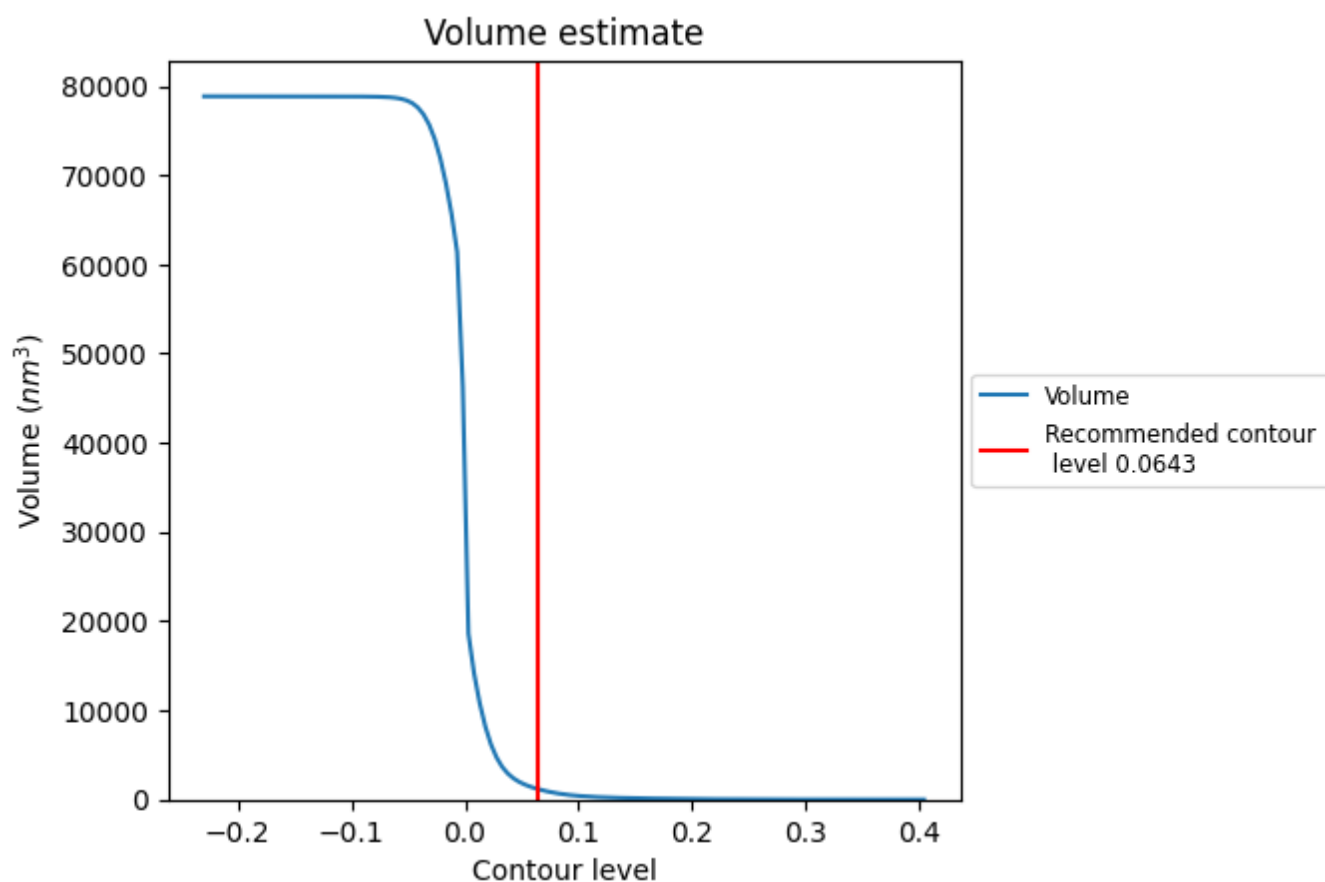
This section contains the results of statistical analysis of the map.

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.

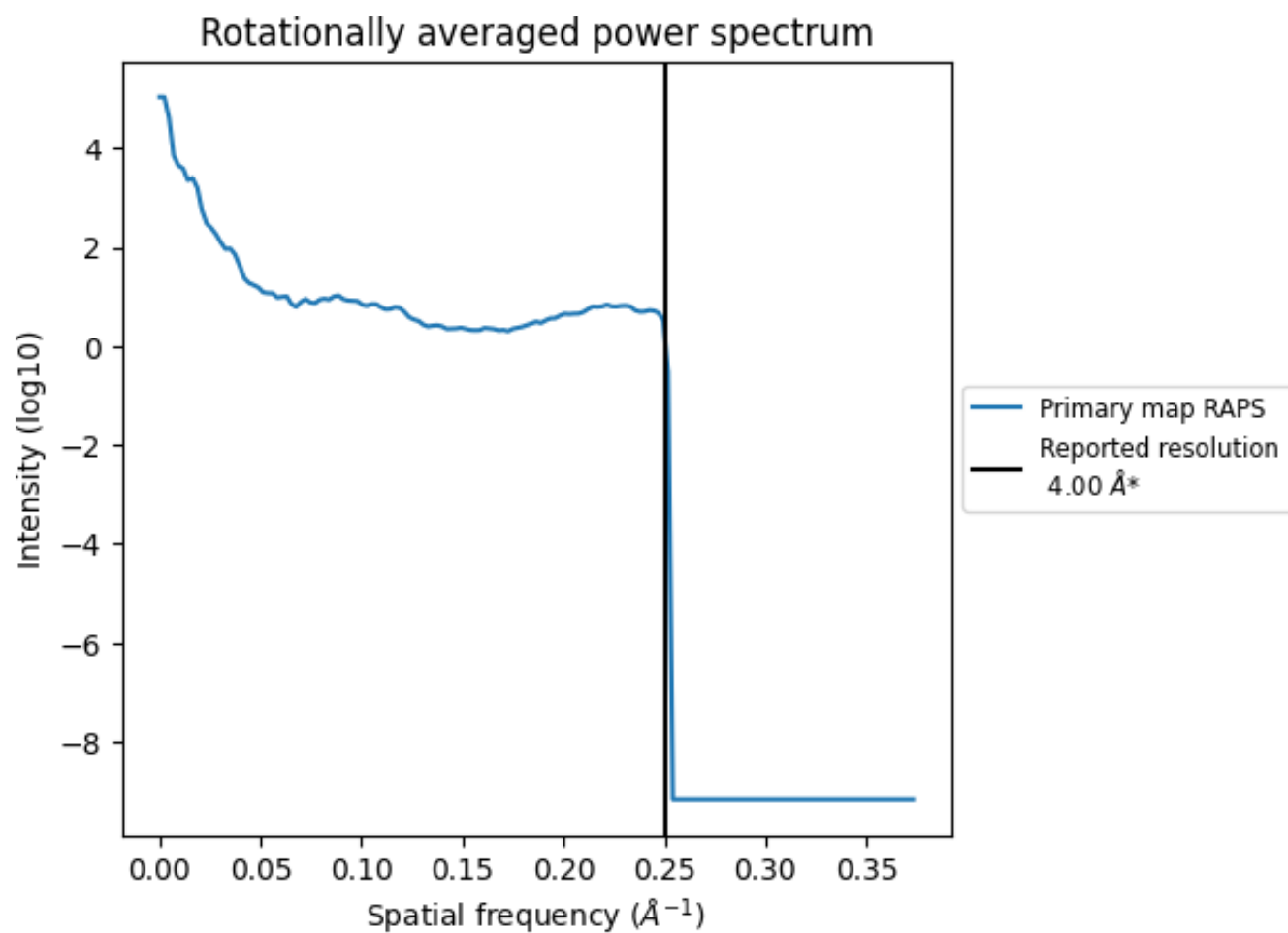
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1179 nm³; this corresponds to an approximate mass of 1065 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 0.250 Å⁻¹

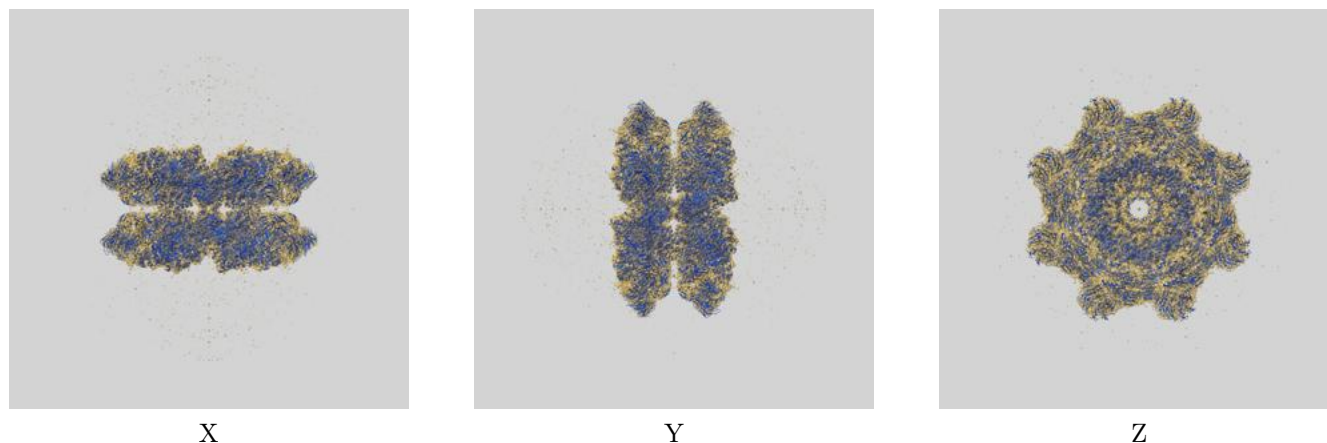
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

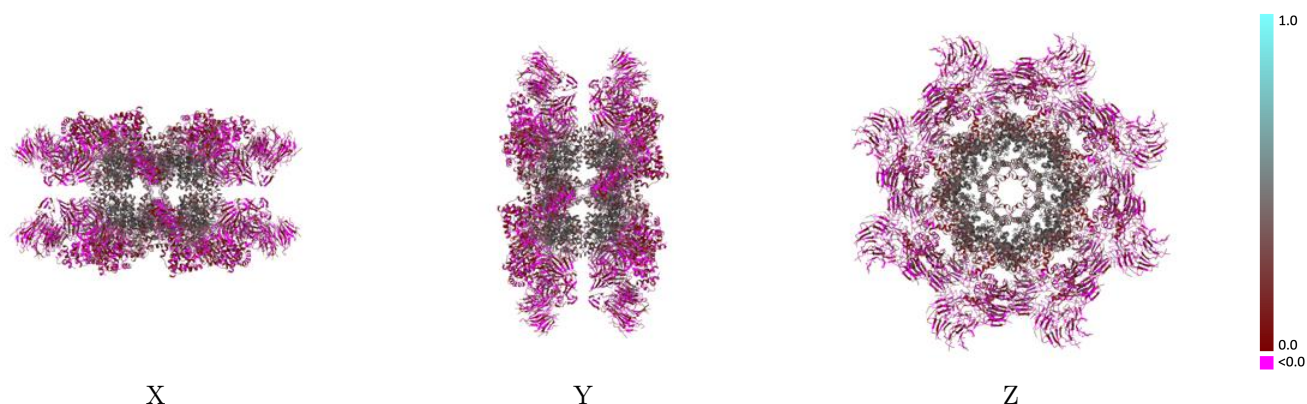
This section contains information regarding the fit between EMDB map EMD-2871 and PDB model 3J9L. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



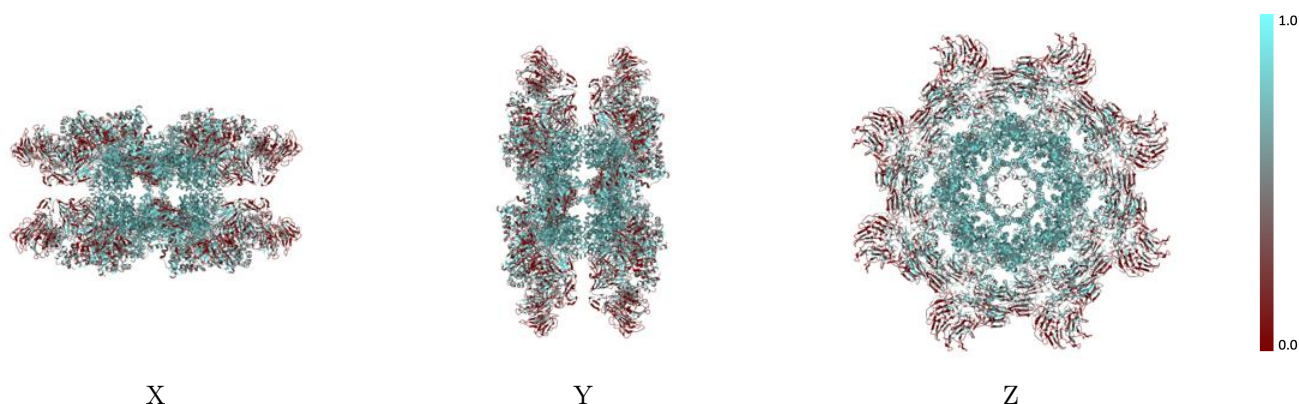
The images above show the 3D surface view of the map at the recommended contour level 0.0643 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



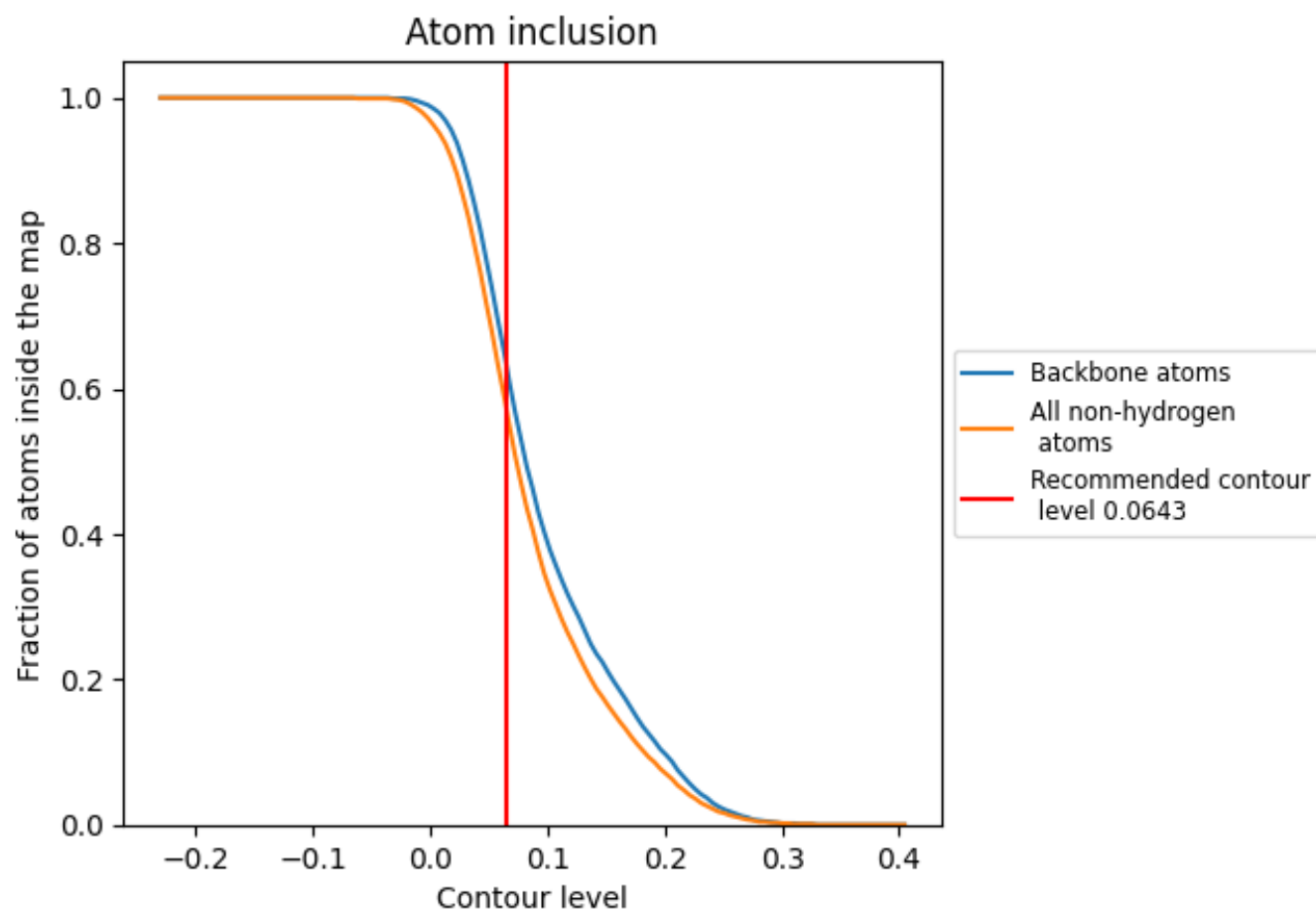
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0643).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 58% 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 (0.0643) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5790	0.2060
A	0.5770	0.2050
C	0.5790	0.2050
D	0.5790	0.2070
E	0.5790	0.2040
F	0.5790	0.2060
G	0.5790	0.2050
H	0.5790	0.2060
I	0.5790	0.2050
J	0.5790	0.2070
K	0.5790	0.2050
L	0.5790	0.2070
M	0.5790	0.2050
N	0.5790	0.2060
O	0.5790	0.2050
P	0.5790	0.2070
Q	0.5790	0.2050

1.0

0.0

<0.0