



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 09:23 AM UTC

PDB ID : 3J9K / pdb_00003j9k
EMDB ID : EMD-2870
Title : Structure of Dark apoptosome in complex with Dronc CARD domain
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 : 4.10 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

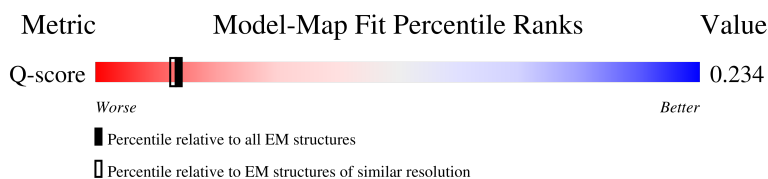
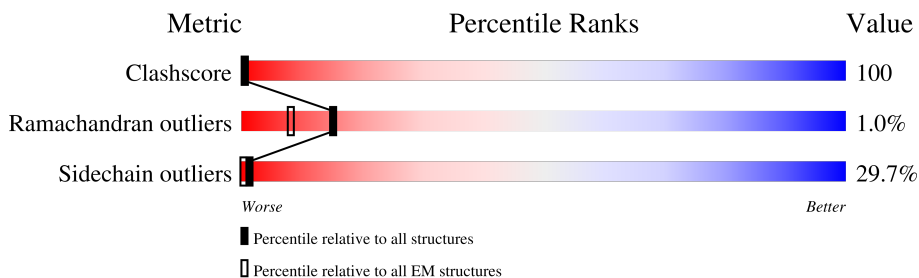
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	1102	25% 49% 30% 14% • •
1	C	1102	24% 49% 30% 14% • •
1	E	1102	25% 49% 30% 14% • •
1	G	1102	24% 49% 30% 14% • •

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Mol	Chain	Length	Quality of chain
1	I	1102	
1	K	1102	
1	M	1102	
1	O	1102	
1	Q	1102	
1	S	1102	
1	U	1102	
1	W	1102	
1	Y	1102	
1	a	1102	
1	c	1102	
1	e	1102	
2	B	450	
2	D	450	
2	F	450	
2	H	450	
2	J	450	
2	L	450	
2	N	450	
2	P	450	
2	R	450	
2	T	450	
2	V	450	
2	X	450	
2	Z	450	

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Mol	Chain	Length	Quality of chain
2	b	450	 14% 5% 77%
2	d	450	 14% 5% 77%
2	f	450	 14% 5% 77%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 126512 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.

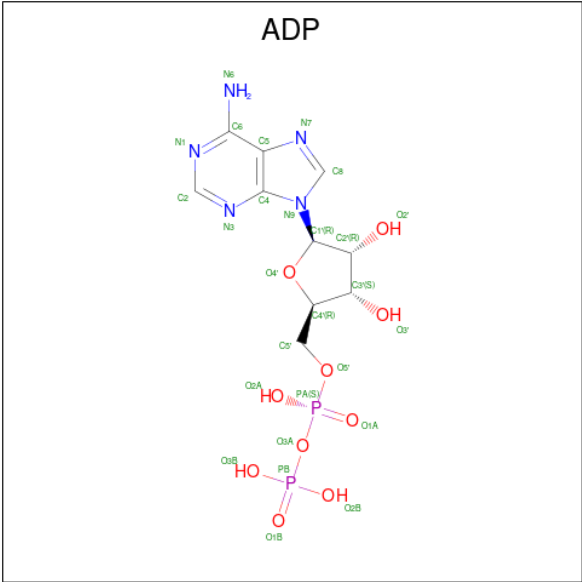
- Molecule 1 is a protein called Apaf-1 related killer DARK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	C	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	E	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	G	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	I	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	K	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	M	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	O	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	Q	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	S	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	U	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	W	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	Y	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	a	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	c	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		
1	e	1063	Total	C	N	O	S	0	0
			7040	4414	1277	1326	23		

- Molecule 2 is a protein called Caspase Nc.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	D	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	F	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	H	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	J	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	L	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	N	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	P	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	R	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	T	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	V	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	X	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	Z	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	b	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	d	102	Total	C	N	O	S	0	0
			840	522	160	152	6		
2	f	102	Total	C	N	O	S	0	0
			840	522	160	152	6		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	S	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	a	1	Total	C	N	O	P	0
			27	10	5	10	2	

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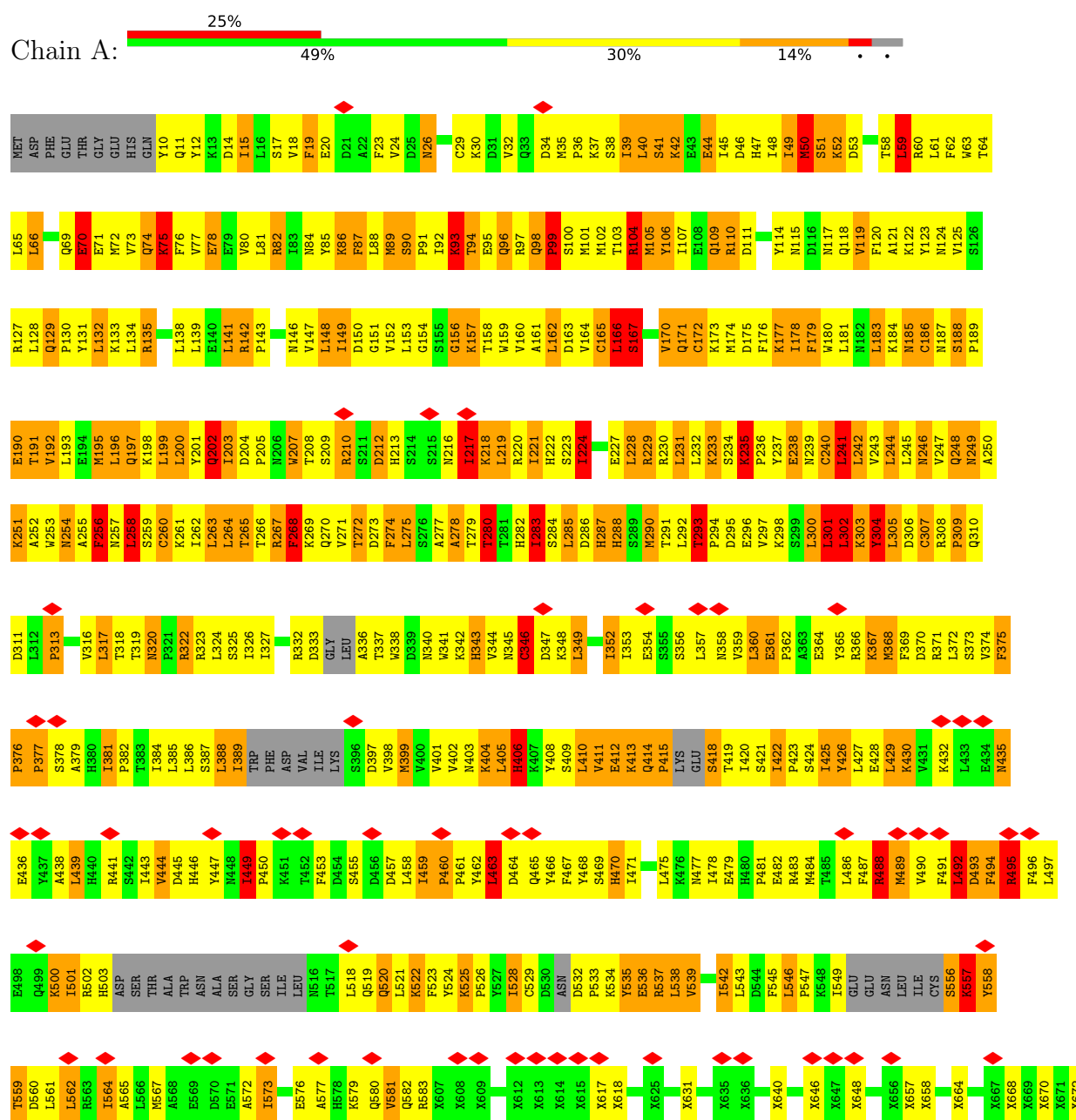
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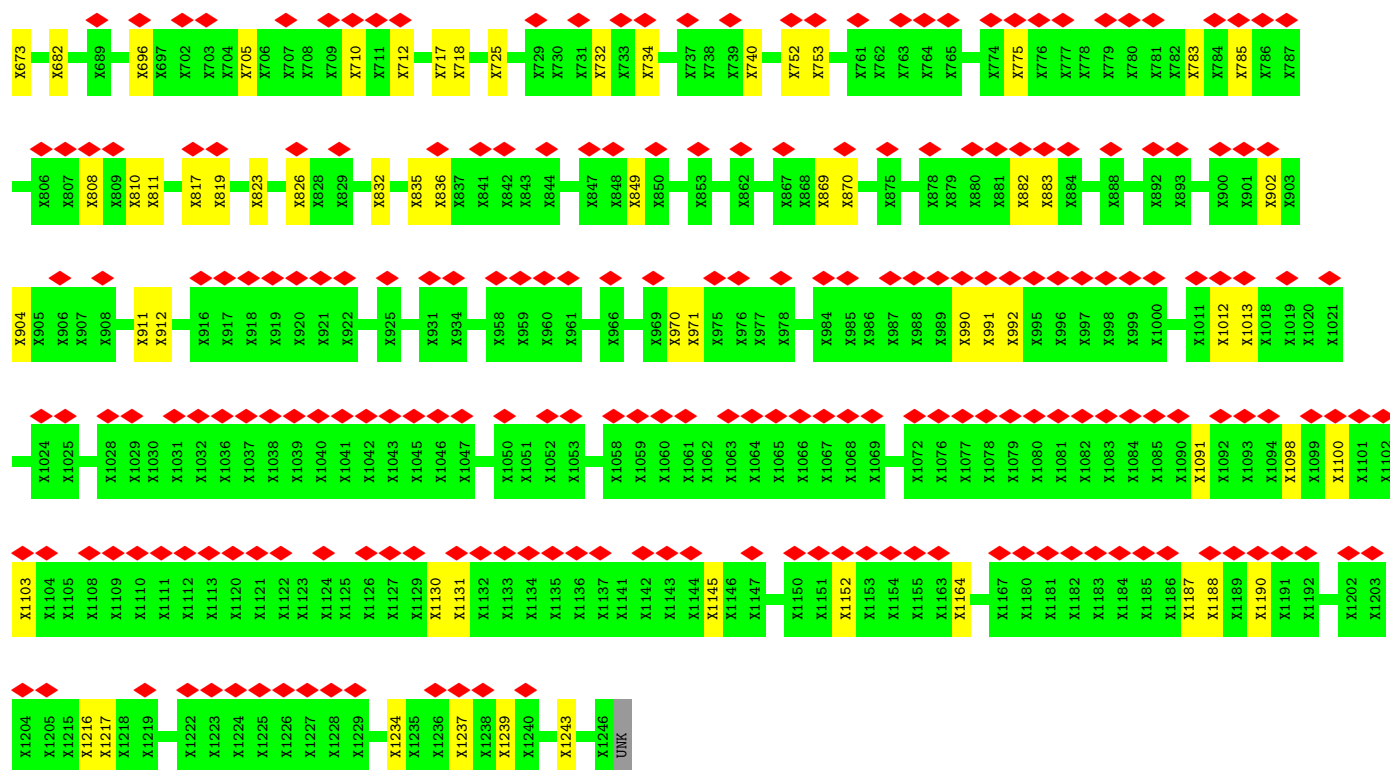
Mol	Chain	Residues	Atoms					AltConf
3	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

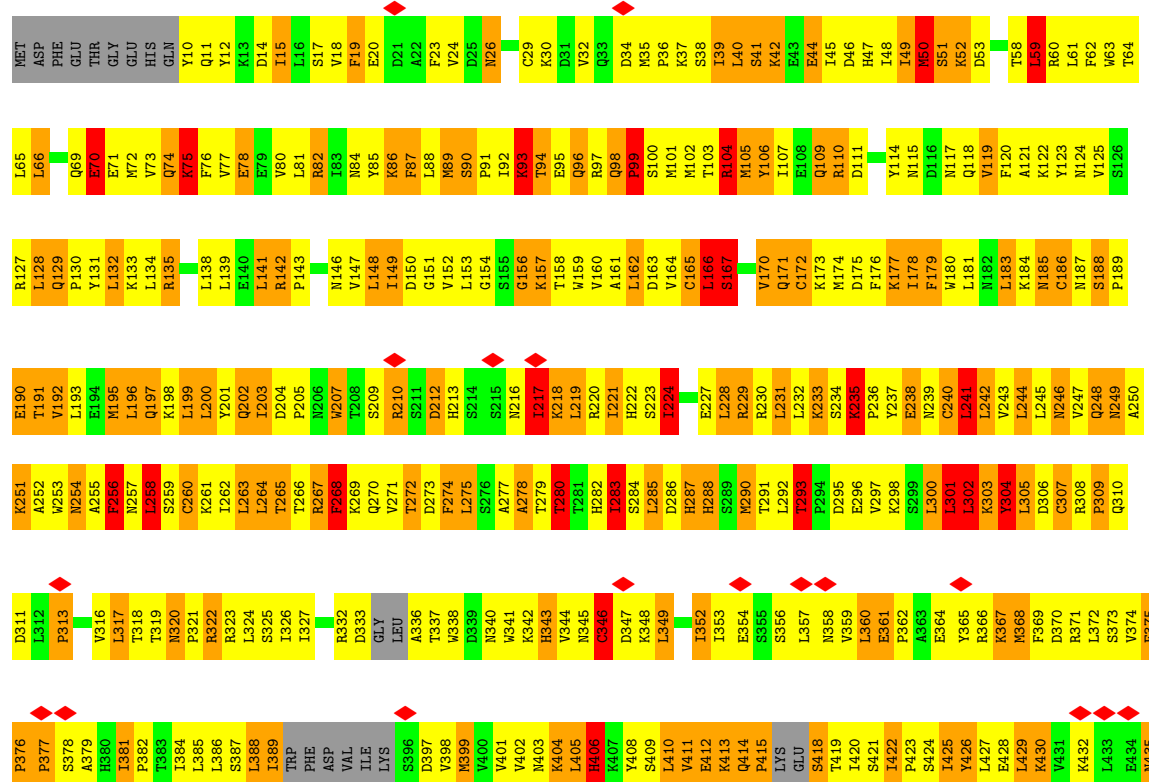
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

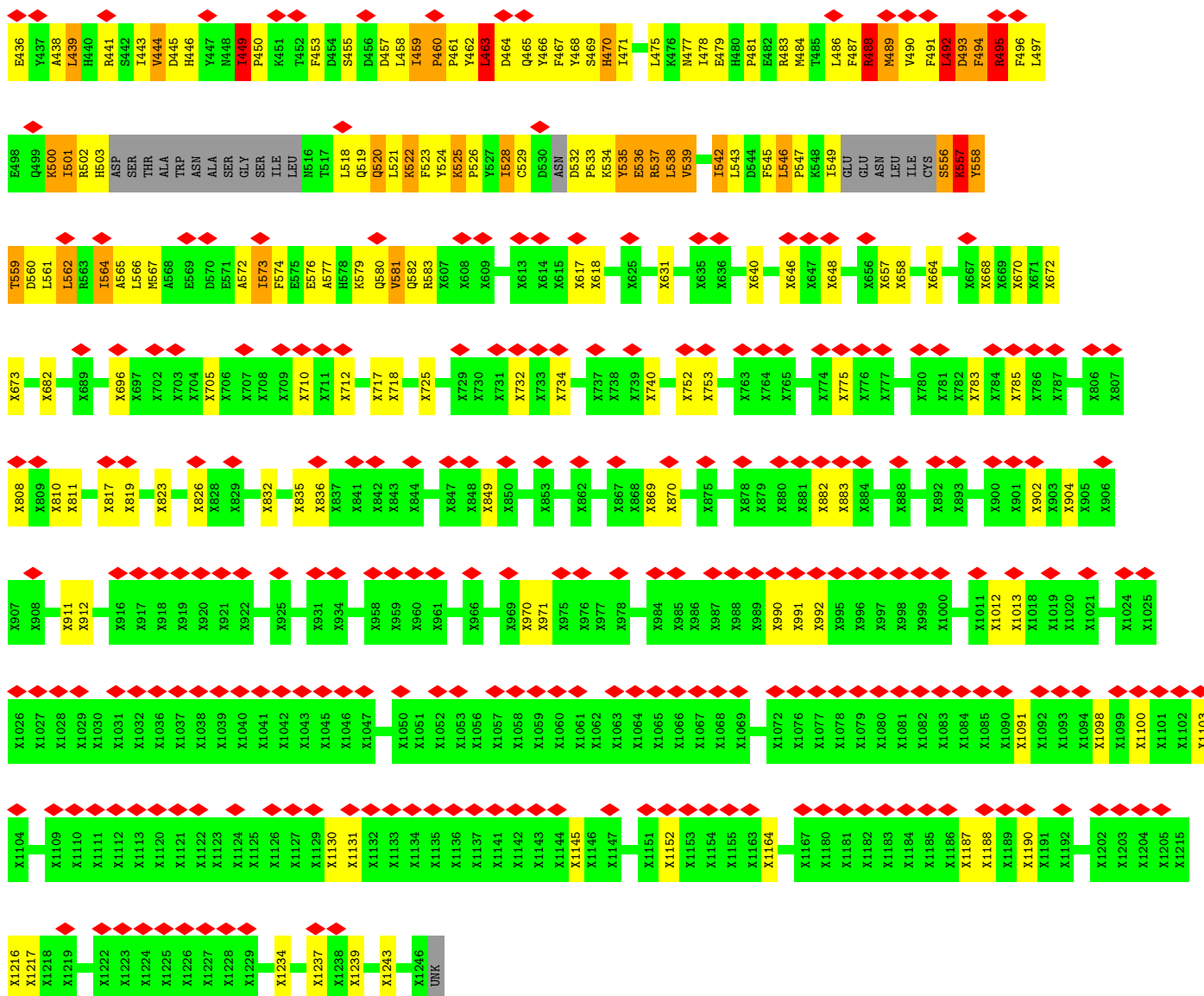
• Molecule 1: Apaf-1 related killer DARK



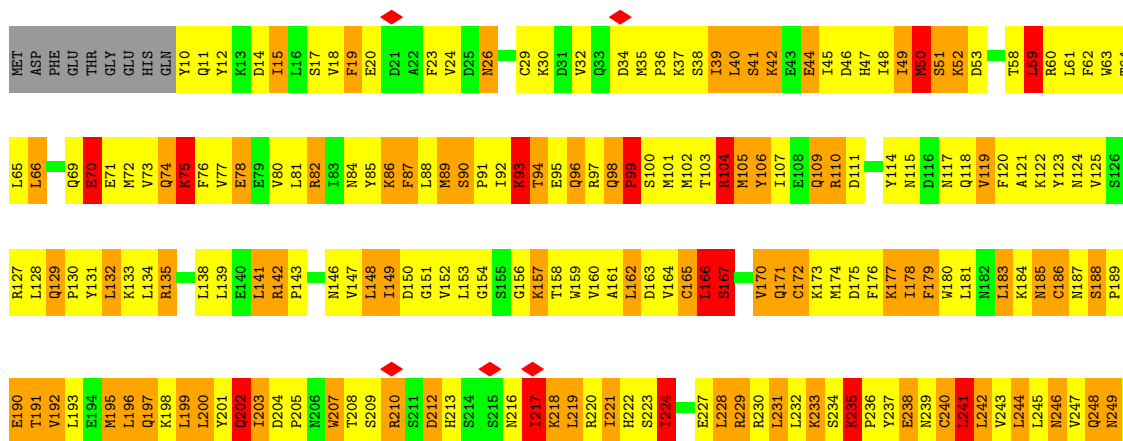


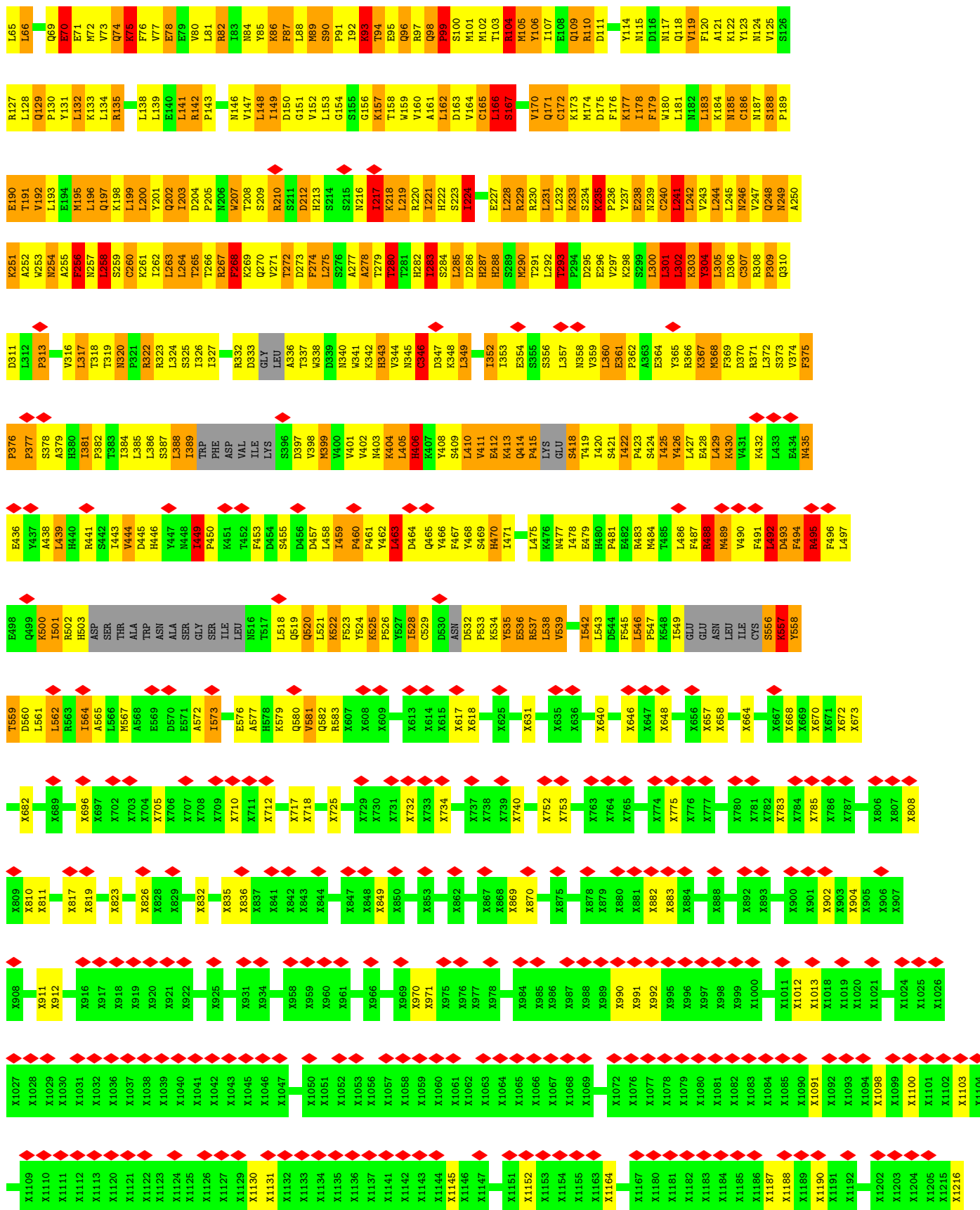
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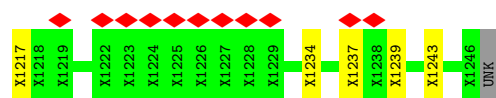




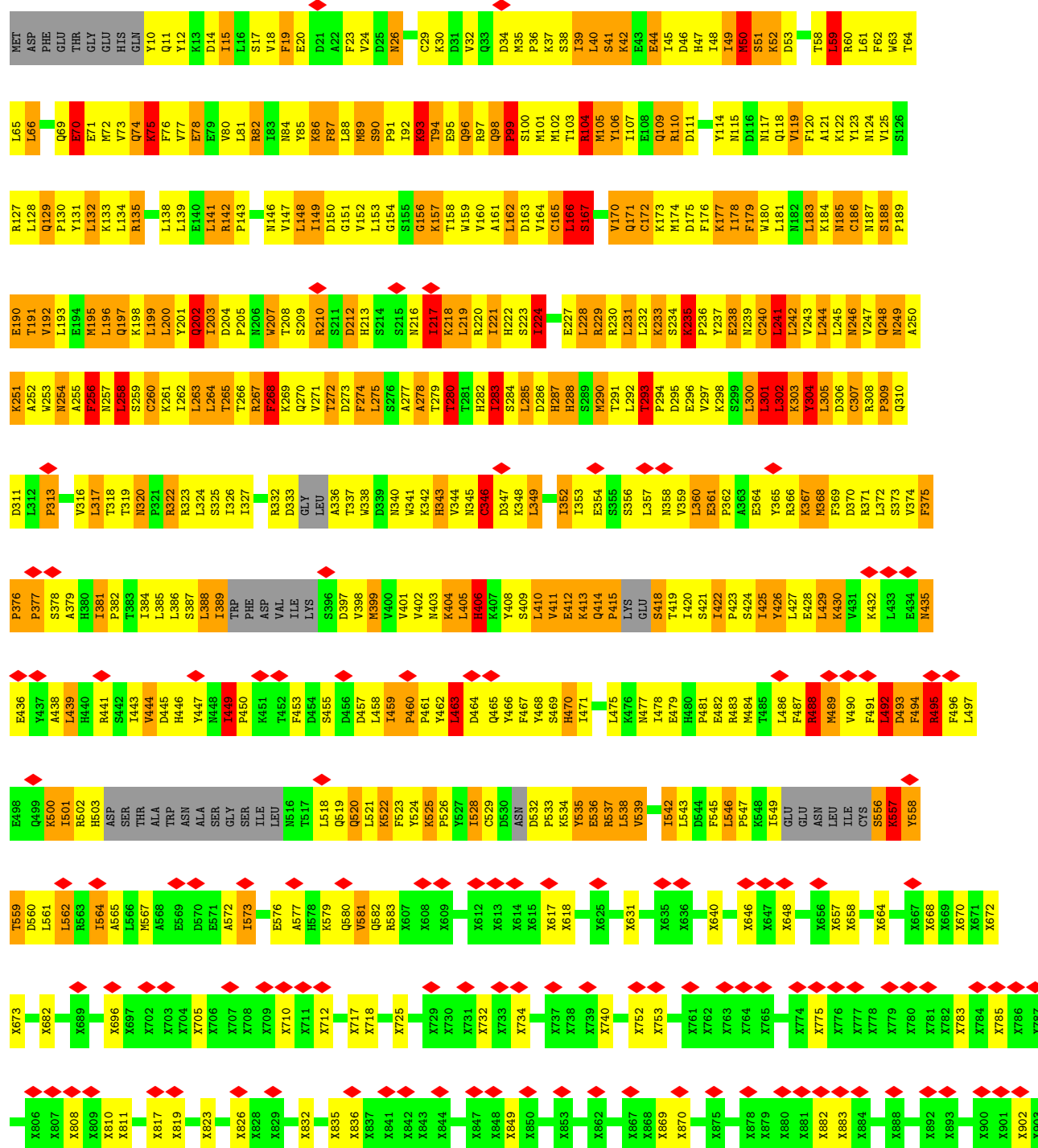
• Molecule 1: Apaf-1 related killer DARK

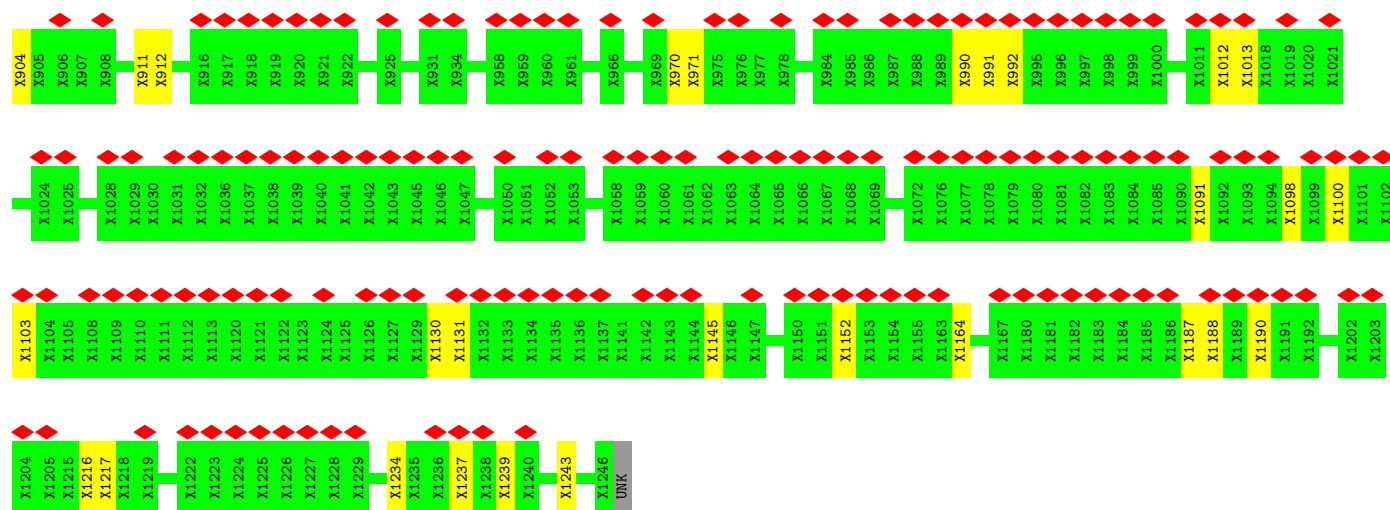




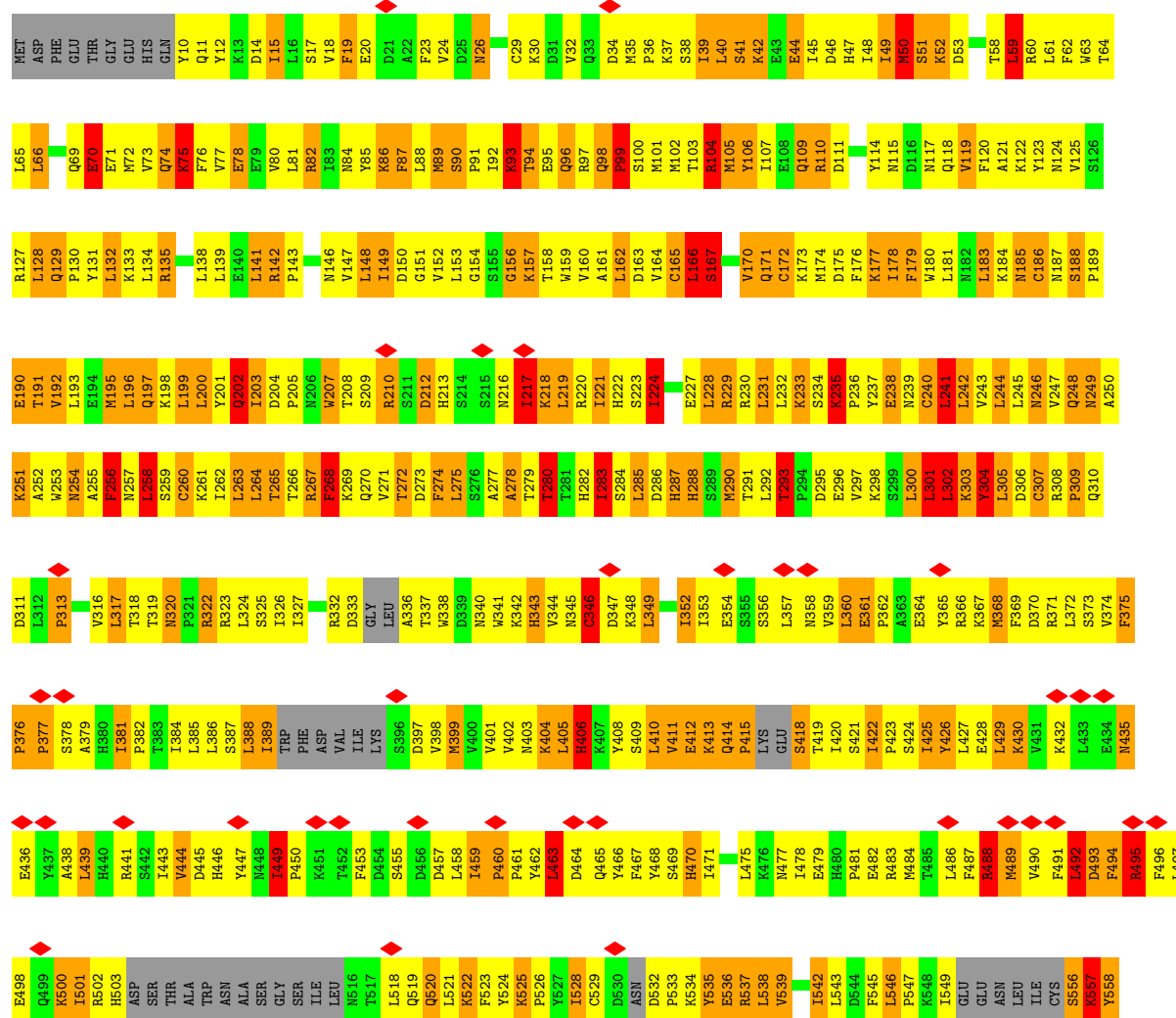


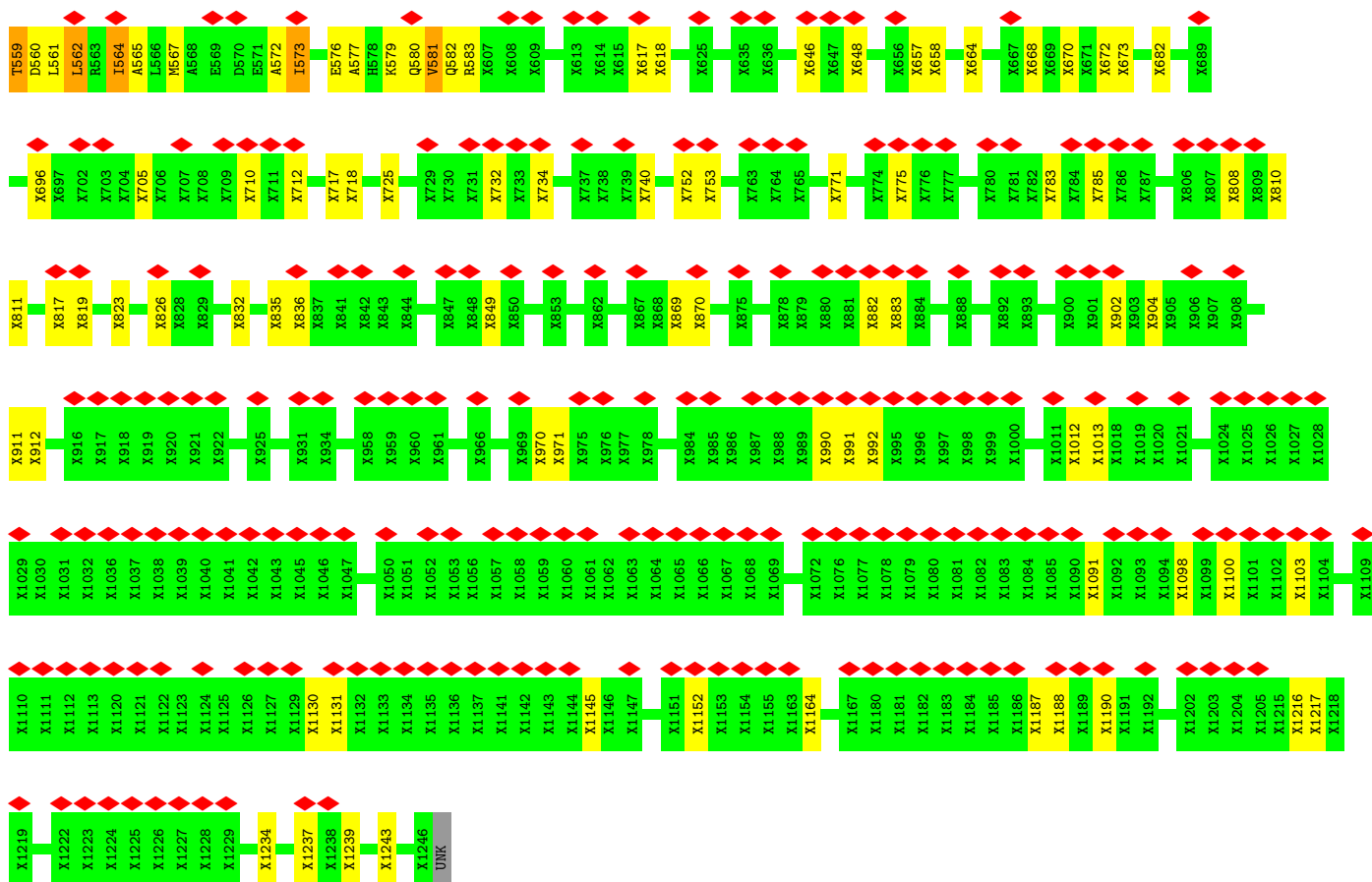
• Molecule 1: Apaf-1 related killer DARK



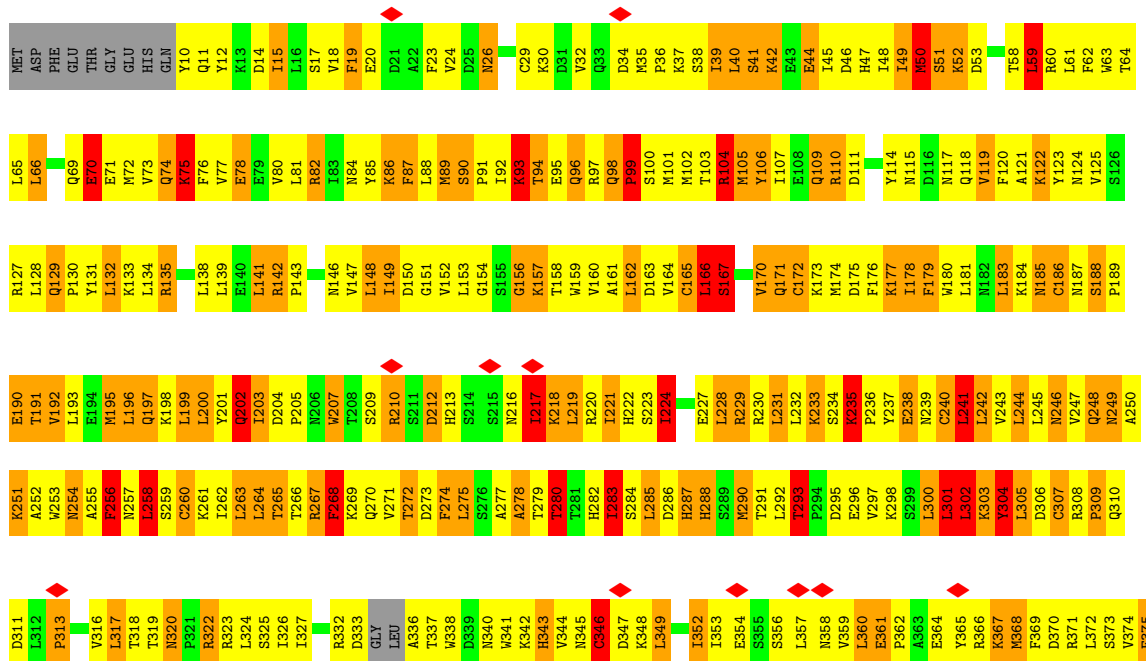


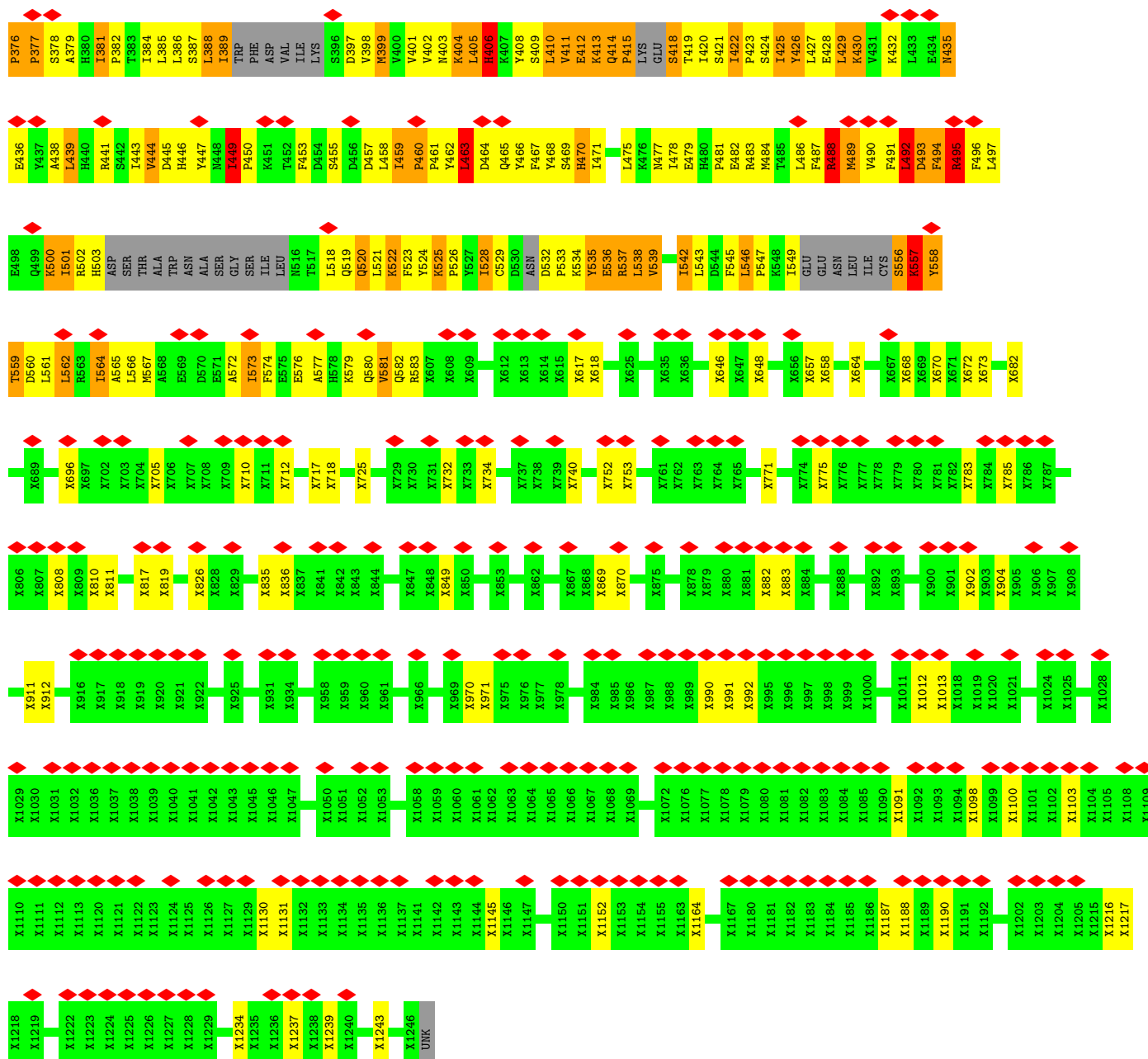
• Molecule 1: Apaf-1 related killer DARK



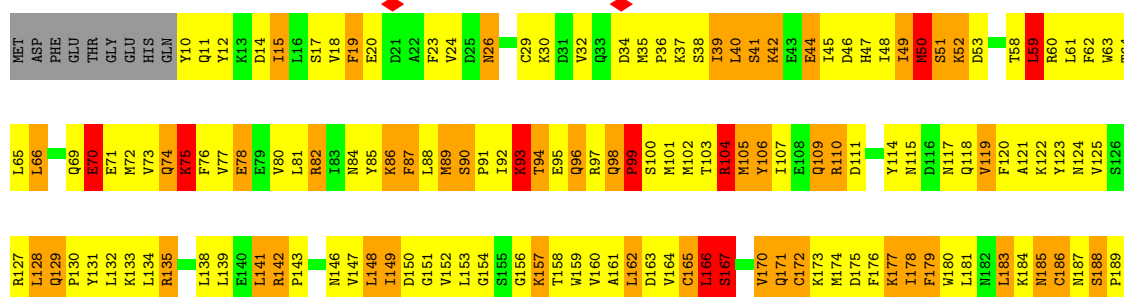


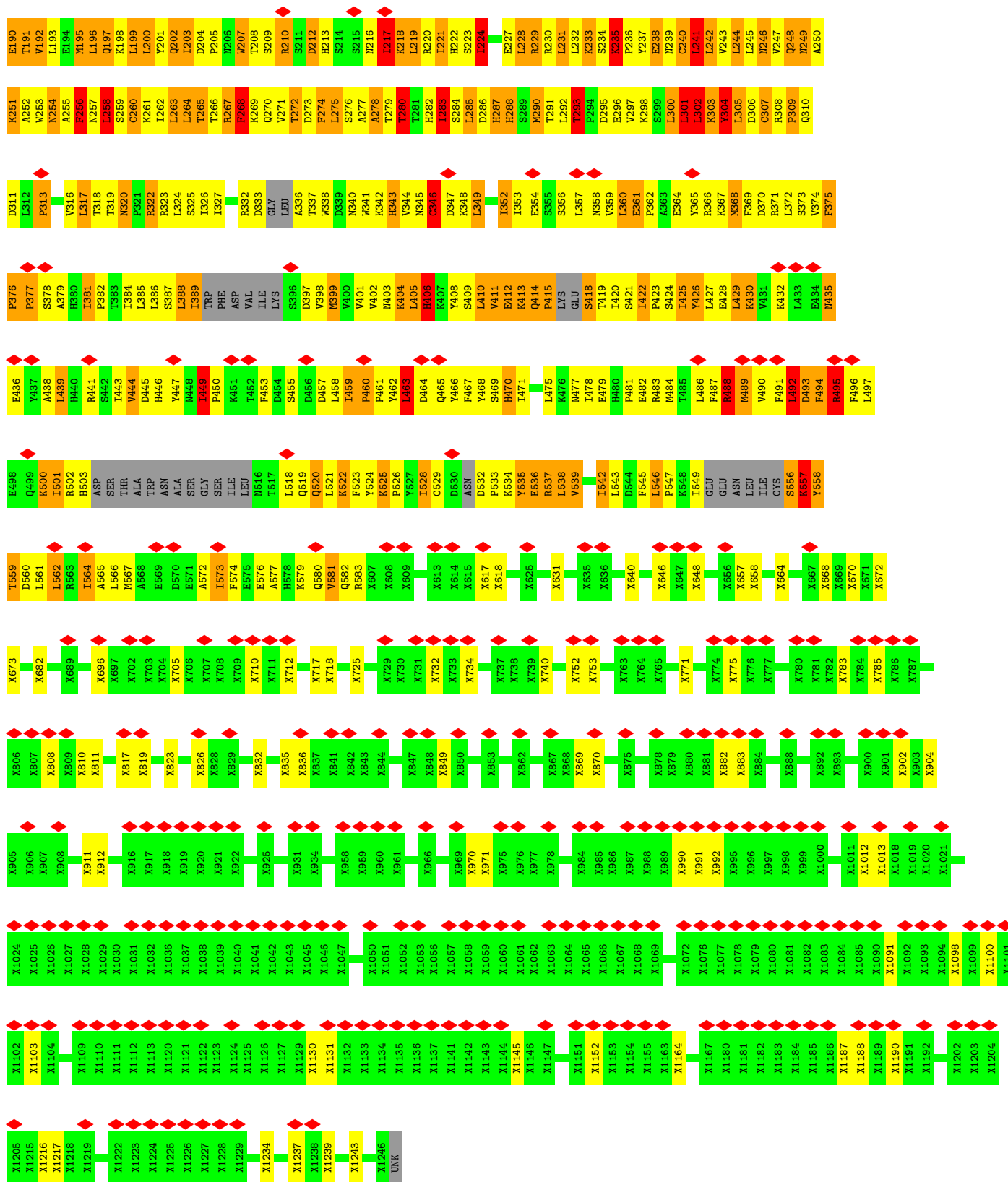
• Molecule 1: Apaf-1 related killer DARK





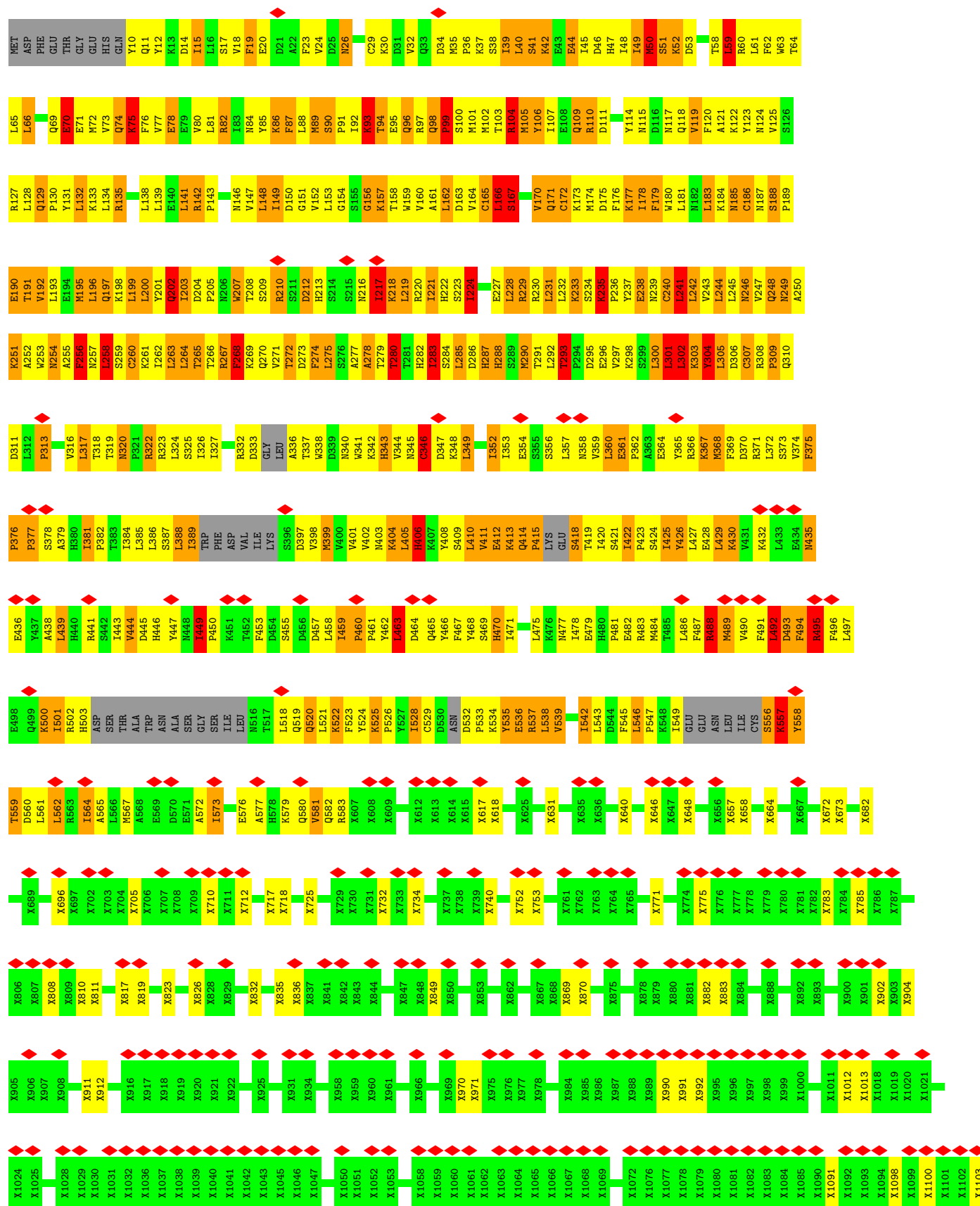
• Molecule 1: Apaf-1 related killer DARK

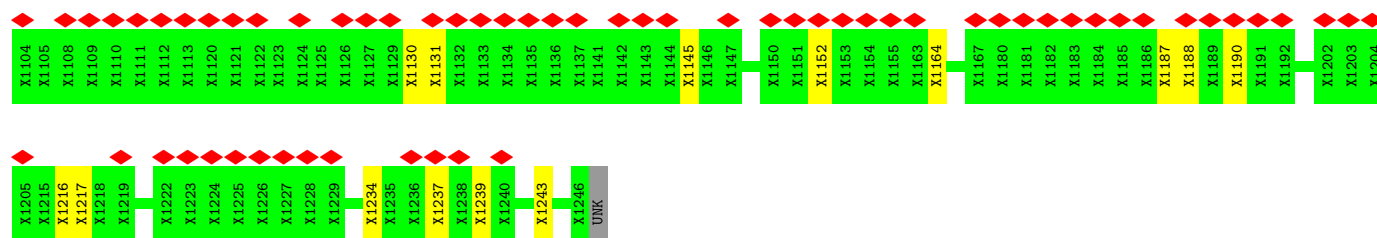




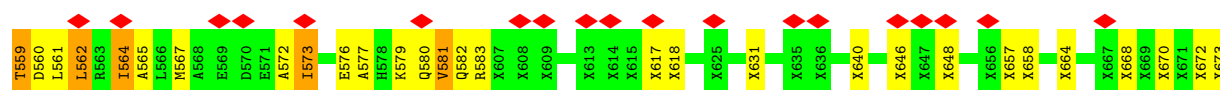
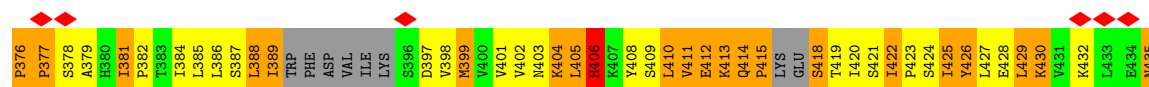
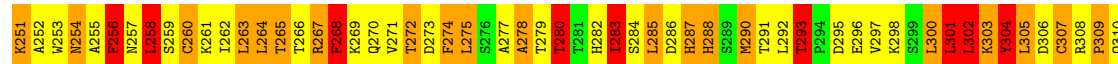
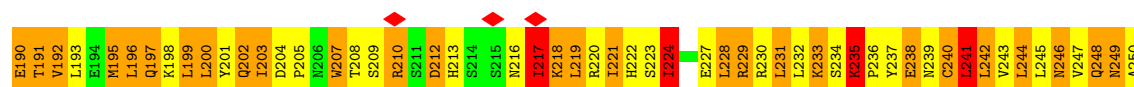
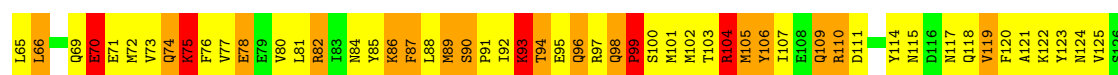
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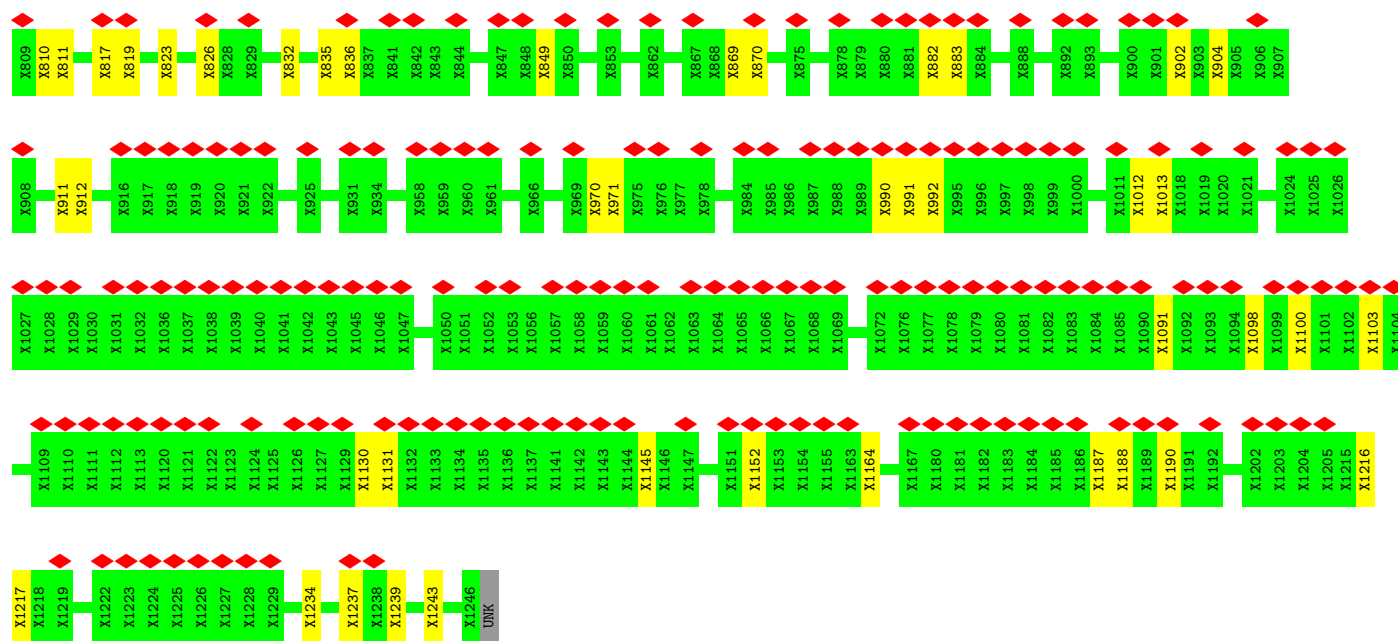




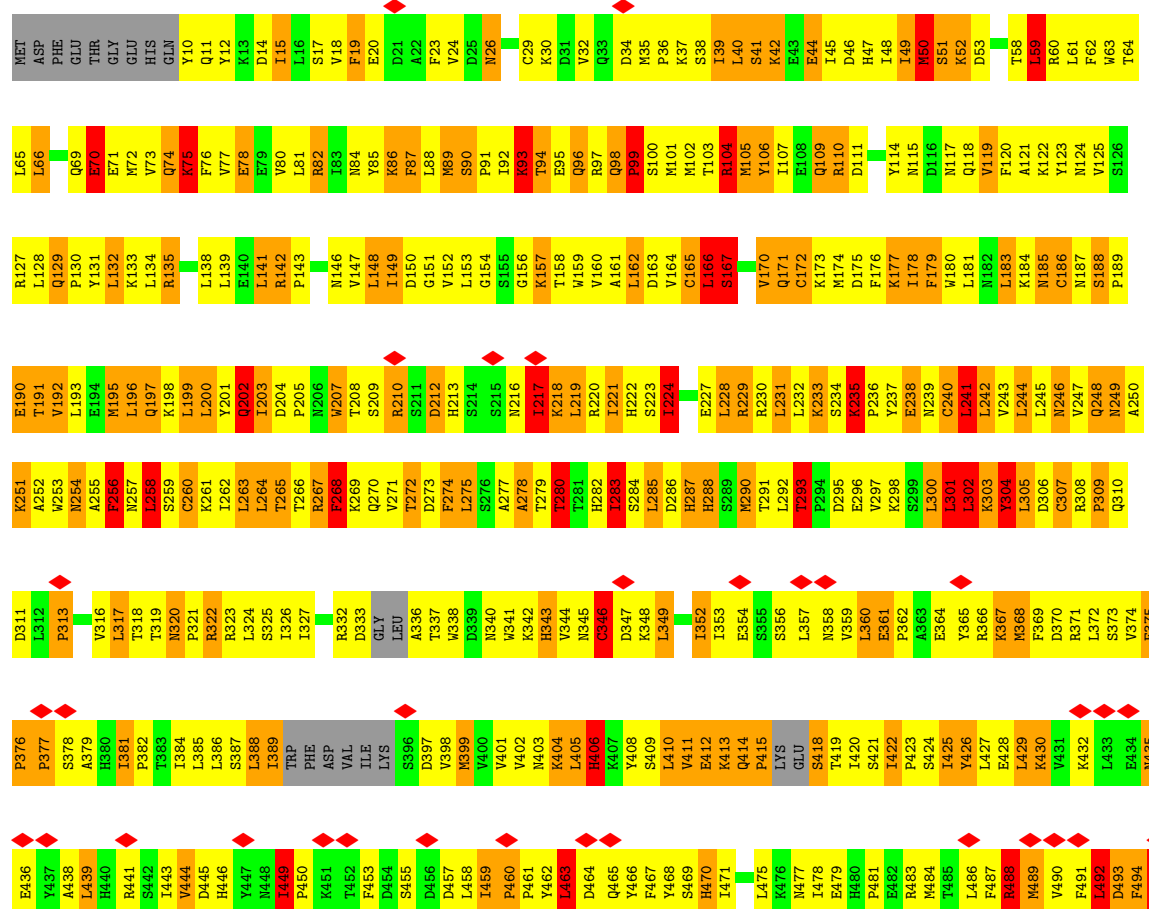


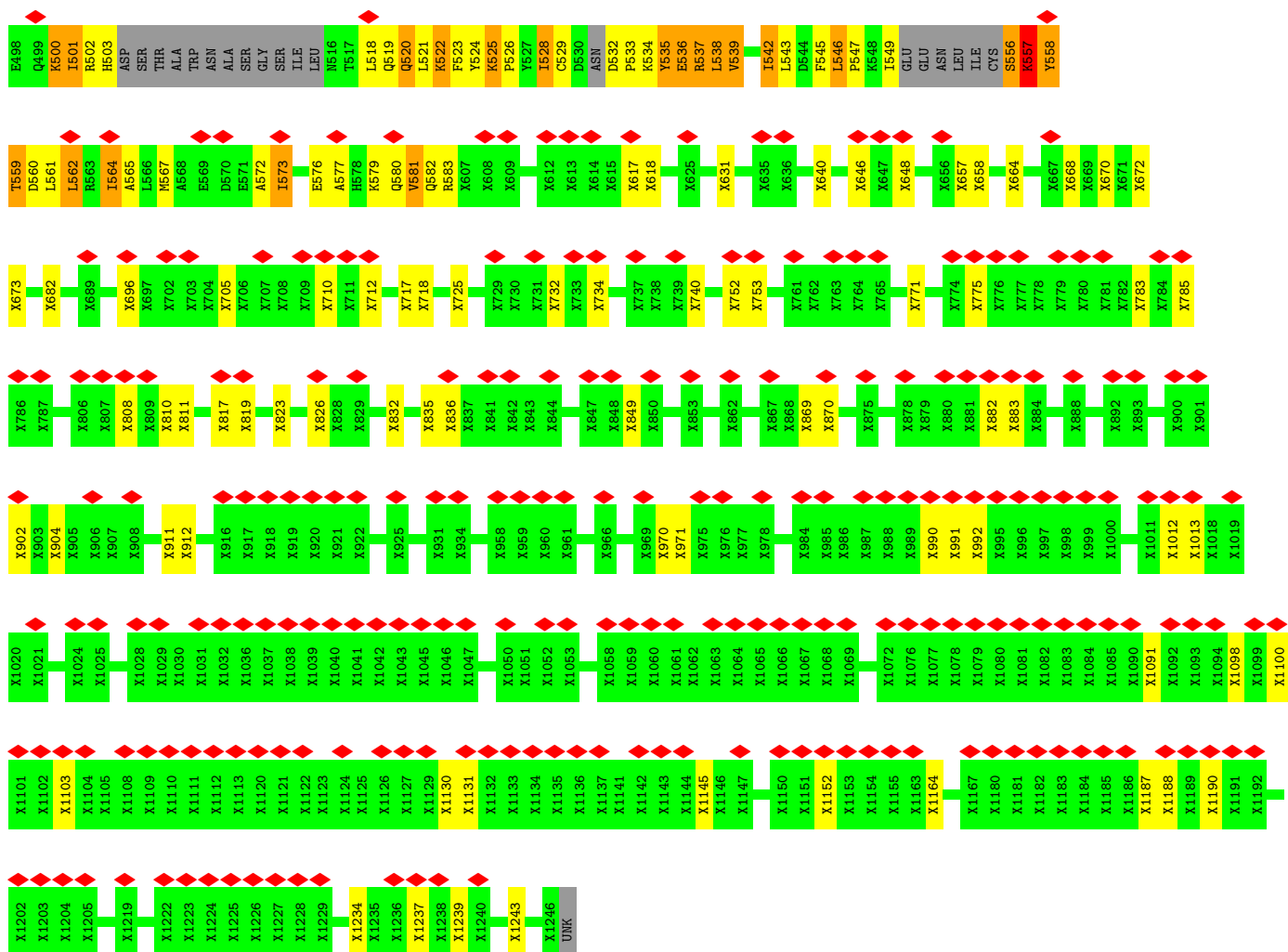
• Molecule 1: Apaf-1 related killer DARK



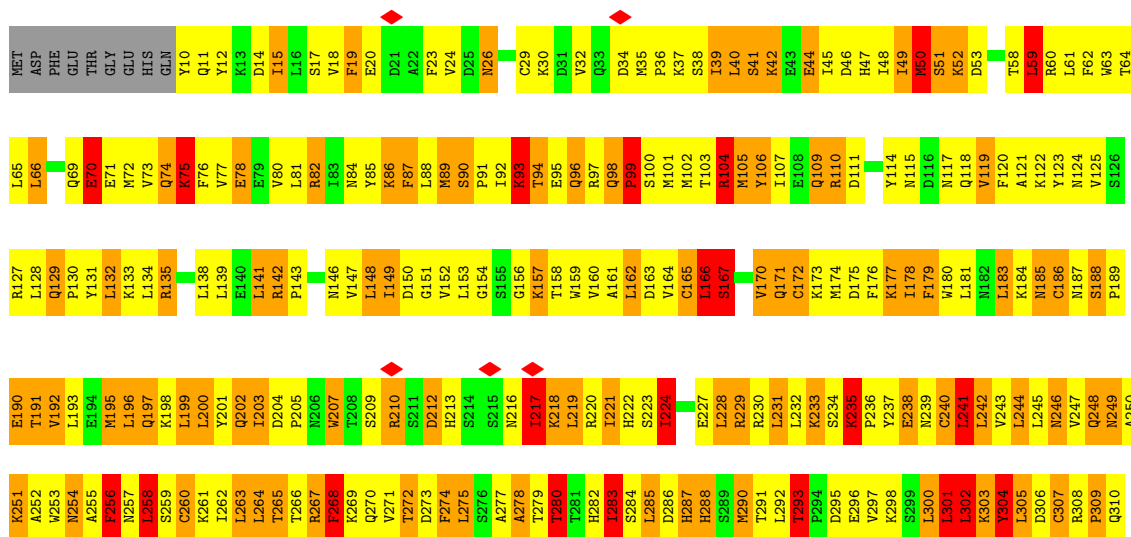


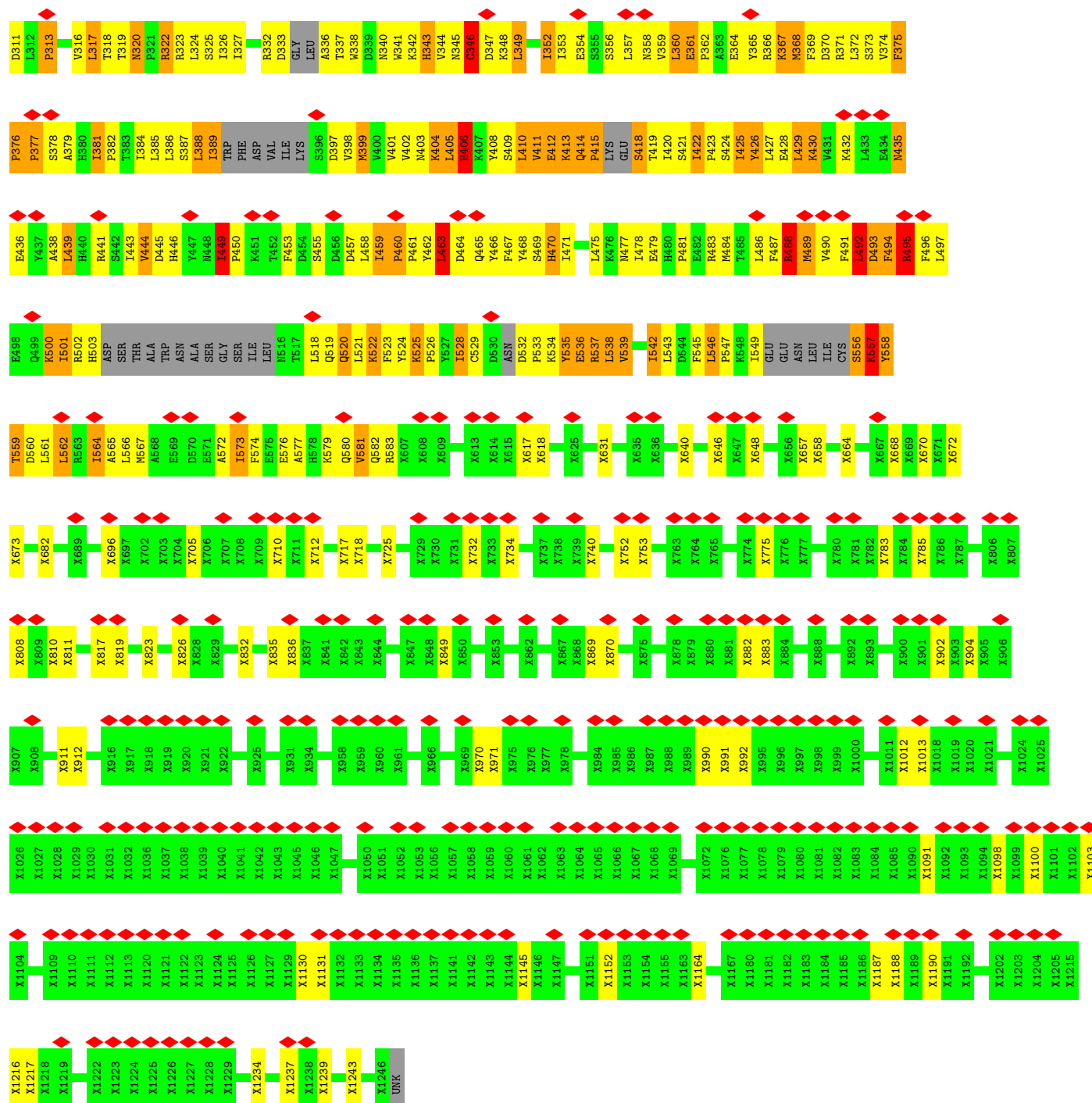
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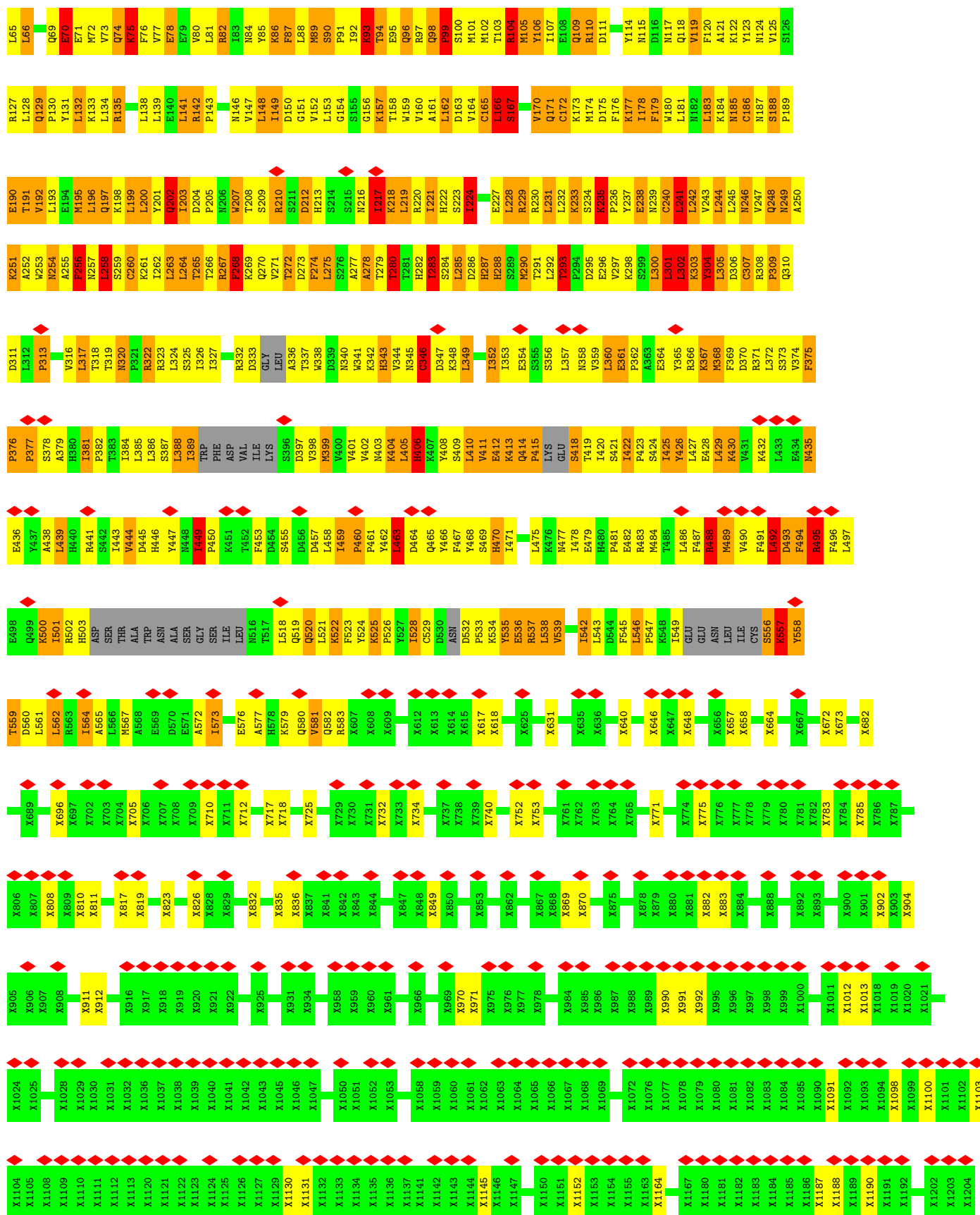


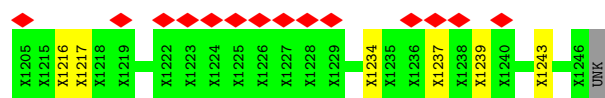


• Molecule 1: Apaf-1 related killer DARK

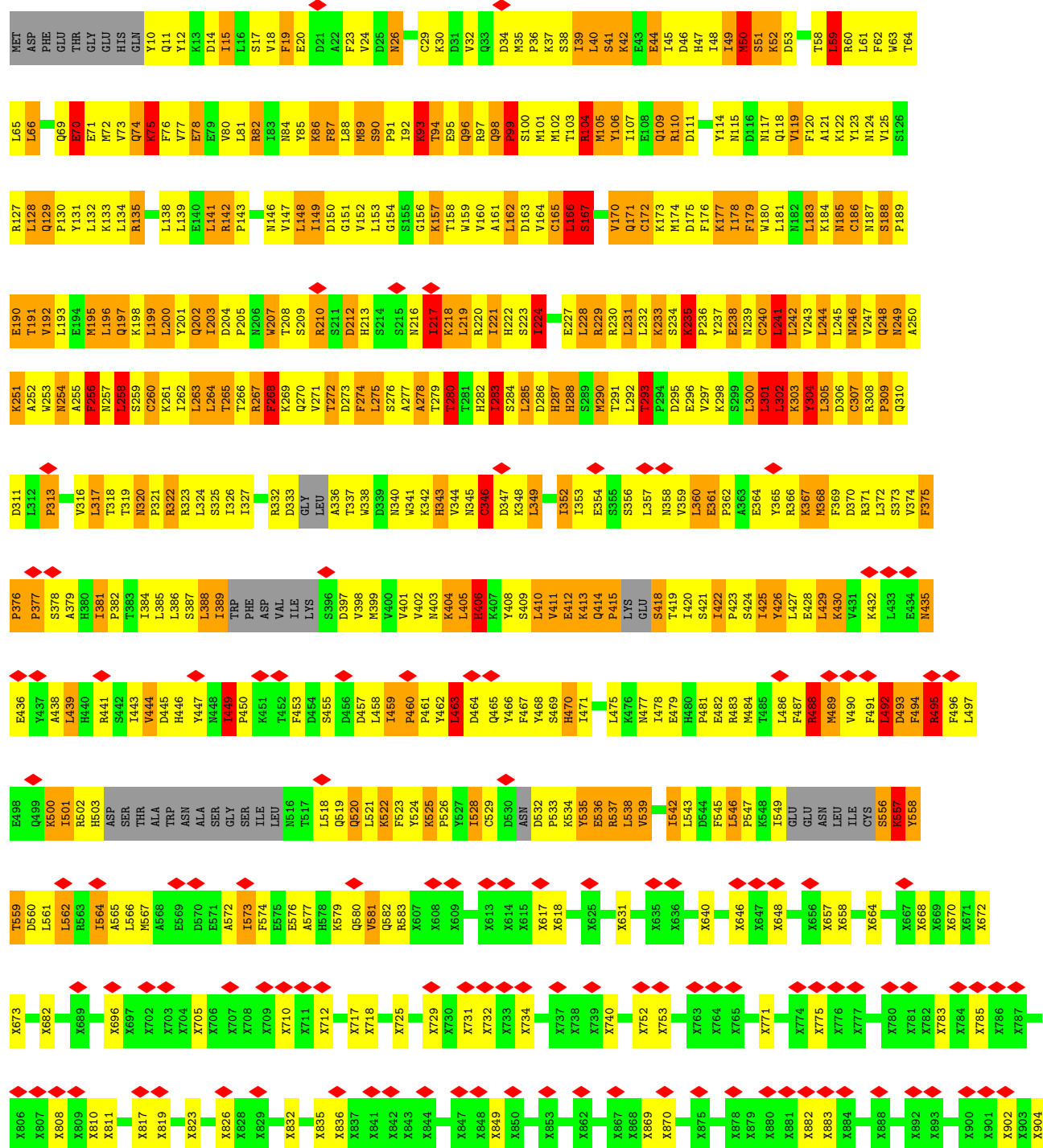


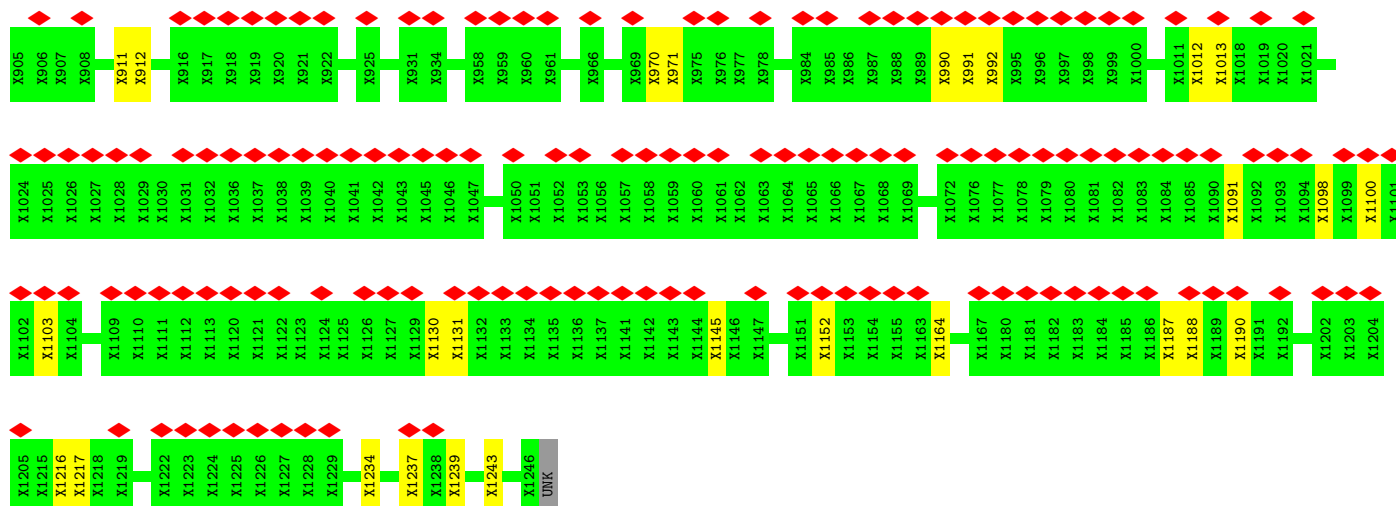




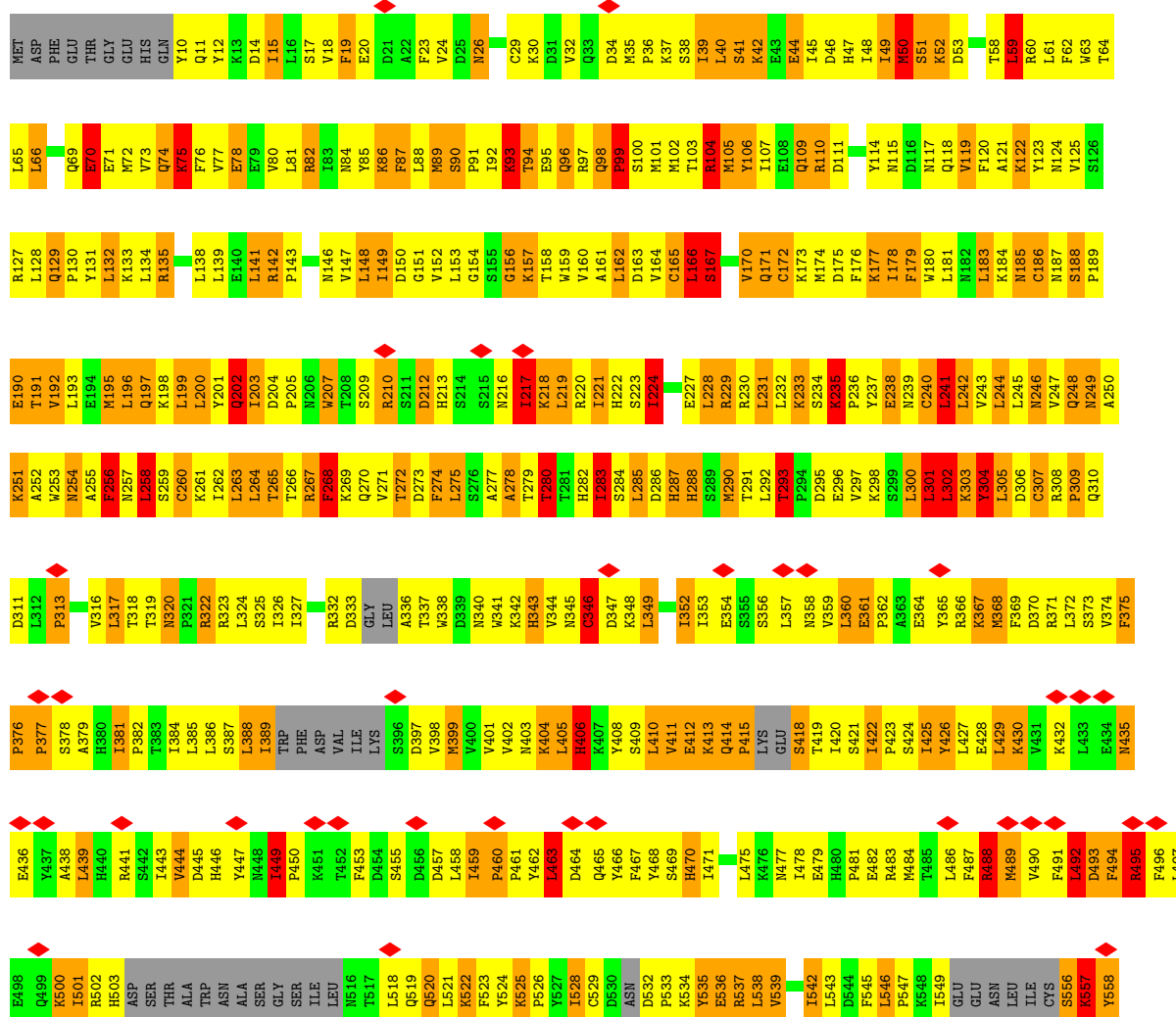


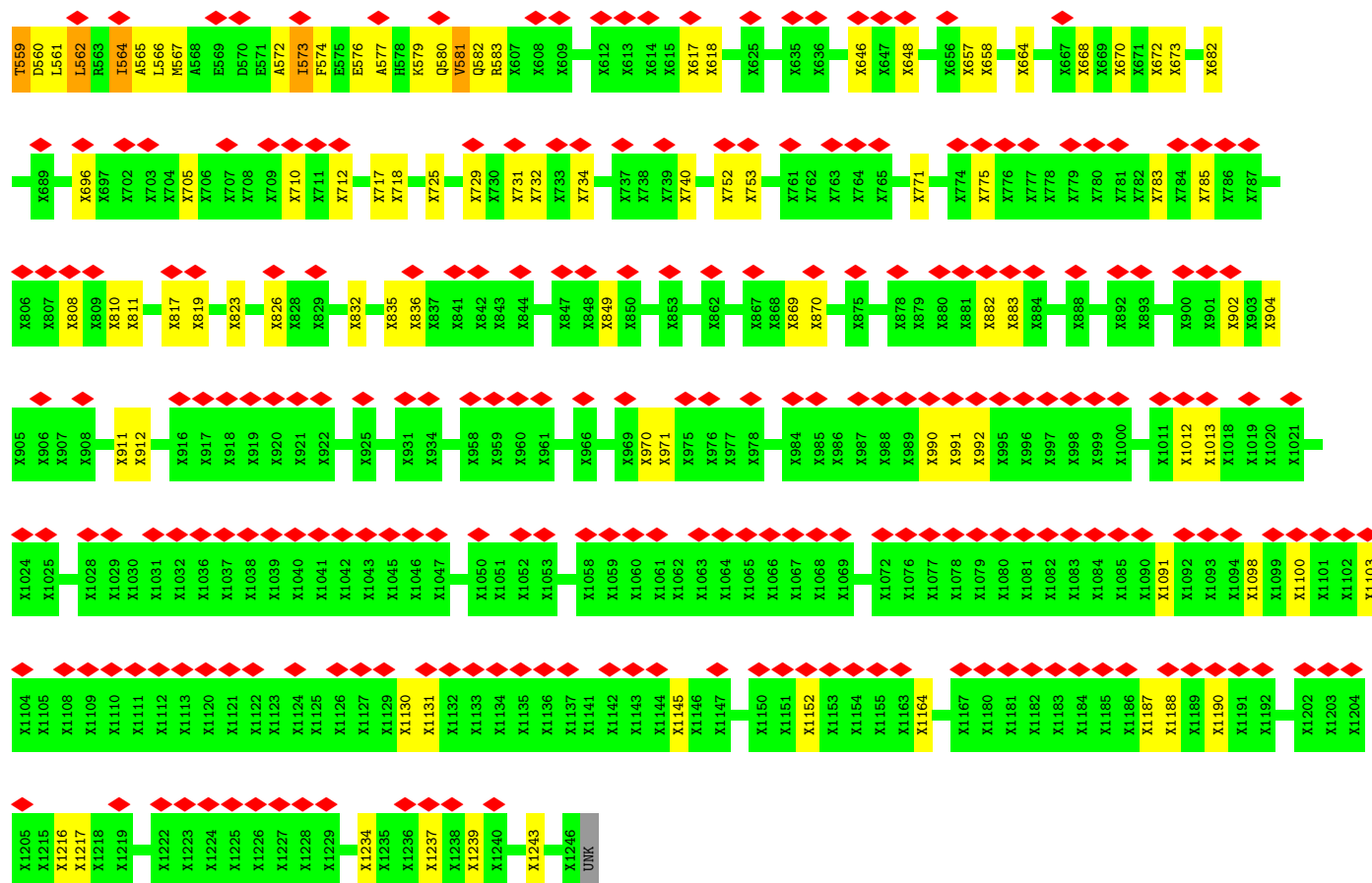
● Molecule 1: Apaf-1 related killer DARK



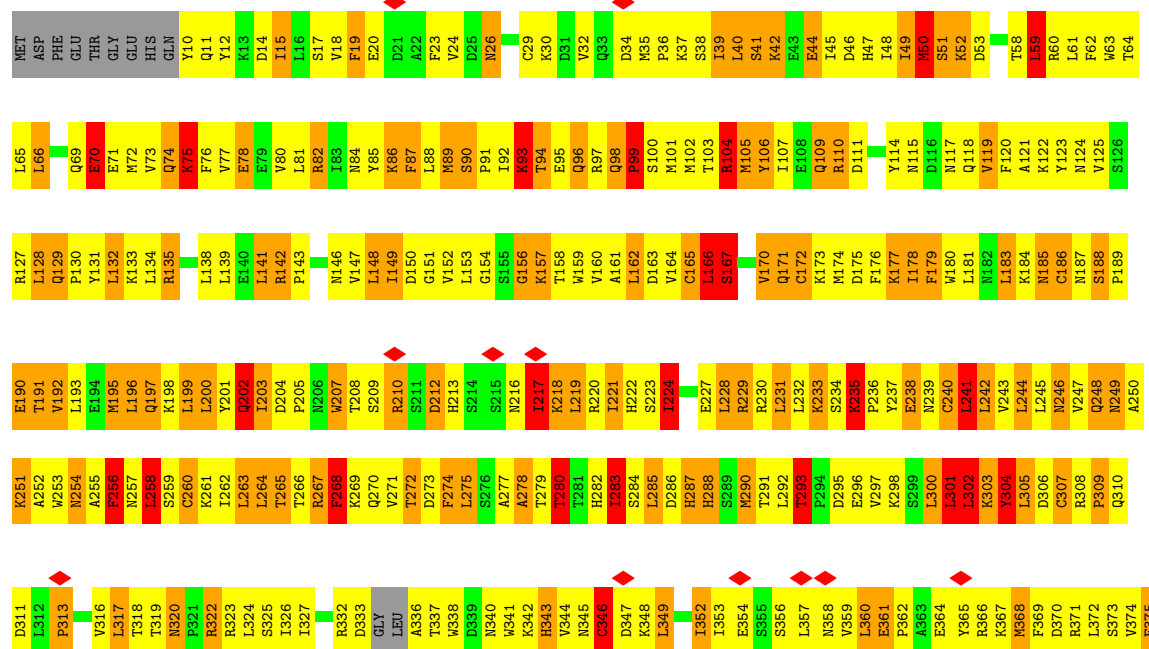


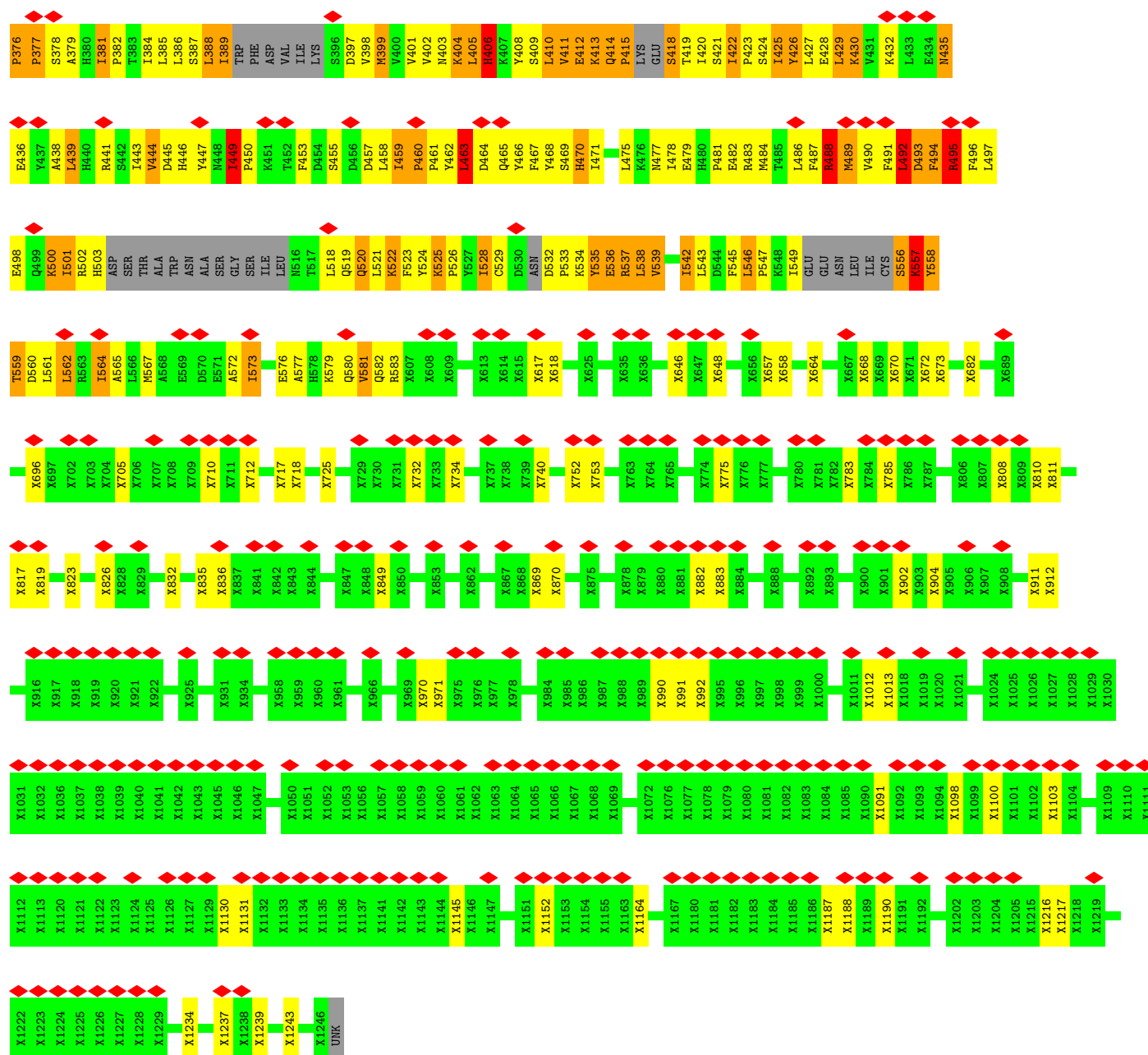
• Molecule 1: Apaf-1 related killer DARK



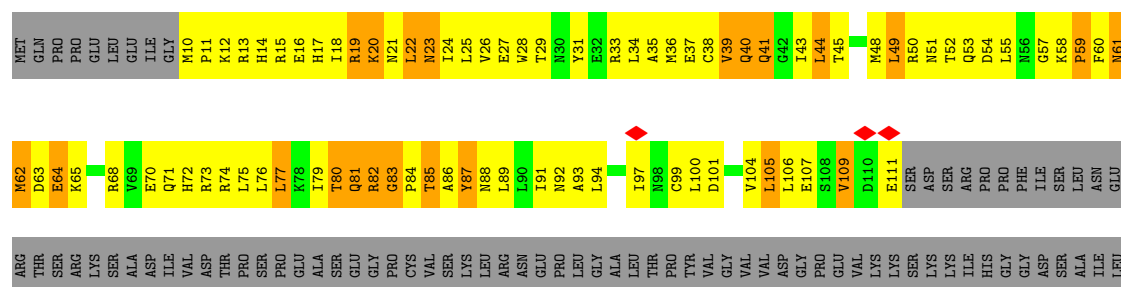


• Molecule 1: Apaf-1 related killer DARK





● Molecule 2: Caspase Nc



[illegible]

- Molecule 2: Caspase Nc



MET	GLN	THR	VAL	LYS	TYR	SER	M62
THR	LEU	LEU	ASN	LEU	LYS	ARG	D63
GLY	CVS	THR	LYS	MET	LYS	ARG	E64
ALA	TYR	MET	PRO	GLN	SER	SER	R65
TYR	ALA	VAL	LYS	MET	ALA	ASP	R68
ASN	ASN	THR	LEU	THR	ARG	ASP	V69
ASP	THR	ASN	LEU	PHE	PHE	ILE	E70
ASN	THR	THR	MET	ASN	ASN	VAL	R71
LEU	PRO	PRO	PHE	SER	ARG	ASP	H72
GLY	GLY	GLY	PRO	SER	GLY	THR	R73
PHE	PHE	THR	PHE	TYR	VAL	VAL	R74
ASN	ASN	VAL	CYS	VAL	LEU	SER	L75
LYS	LYS	THR	ARG	GLN	LEU	PRO	L76
LYS	ASN	HIS	GLY	ASN	MET	GLU	L77
LEU	LEU	THR	ASP	THR	VAL	ALA	R78
THR	PHE	GLU	GLU	GLU	ASN	SER	G79
PHE	GLY	TYR	TYR	CYS	ILE	GLU	E80
ASN	ASN	ASP	ASP	PHE	MET	GLY	T80
PRO	PRO	THR	LEU	VAL	ASP	PRO	Q81
GLY	GLY	GLY	LEU	VAL	TYR	CYS	R82
PHE	PHE	THR	HIS	VAL	PRO	ASP	G83
PHE	THR	ASP	PRO	LEU	ASP	SER	F84
ASN	ASN	TYR	LYS	MET	GLN	LYS	T85
GLU	GLU	ILE	ASN	THR	ASN	LEU	A86
	GLN	GLN	GLN	HIS	ARG	ARG	Y87
	LYS	LYS	GLY	GLY	ARG	ASN	N88
	PHE	PHE	ASN	ASN	ARG	GLU	L89
	CYS	CYS	LEU	SER	ILE	PRO	L90
	GLN	GLN	MET	VAL	GLY	LYS	I91
	VAL	VAL	GLU	GLU	ALA	GLY	N92
	MET	PRO	VAL	GLY	GLU	ALA	A93
	VAL	THR	PRO	LYS	LYS	THR	L94
	ALA	ALA	TYR	GLU	ASP	PRO	I97
	HIS	HIS	THR	LYS	LYS	TYR	R98
	ALA	ALA	ALA	VAL	LYS	TYR	C99
	HIS	ASP	GLN	GLU	SER	VAL	L100
	ASP	THR	GLU	PHE	GLY	GLY	
	THR	THR	GLU	CYS	ILE	VAL	
	ASP	LYS	LYS	ASP	HIS	VAL	
	LYS	TRP	PRO	GLY	LEU	VAL	L105
	GLU	PRO	PRO	SER	PHE	GLY	L106
	ASP	ASP	ASP	VAL	GLN	PRO	E107
	ILE	ILE	THR	VAL	LEU	VAL	G108
	LEU	THR	GLN	ASP	GLU	VAL	V109
	LYS	LYS	THR	MET	ASN	GLY	D110
	GLY	GLY	GLU	GLN	PHE	LYS	E111
	THR	THR	GLY	LYS	THR	SER	
	SER	SER	ILE	ILE	ILE	SER	M48
	GLU	GLU	PRO	LYS	PHE	LYS	L49
	ALA	ALA	SER	ASP	PRO	ILE	R50
	VAL	VAL	PRO	HIS	TYR	HIS	N51
	GLY	GLY	SER	PHE	GLY	GLY	T52
	ASN	THR	THR	GLN	ASN	GLY	Q53
	LYS	LYS	ASN	THR	VAL	ASP	D54
	ARG	ARG	VAL	ALA	THR	ILE	L55
	THR	THR	PRO	ALA	ASN	SER	N56
	GLY	GLY	VAL	LYS	ASN	GLU	G57
	LYS	LYS	SER	CYS	ILE	ASN	K58
	LYS	LYS	LEU	LYS	GLU	GLY	P59
	GLY	GLY	ALA	THR	ARG	ARG	F60
	ASP	ASP	ASP	THR	THR	THR	N61

- Molecule 2: Caspase Nc



ARG	THR	SER	ARG	LVS	SER	ALA	ASP	ILE	VAL	ASP	THR	PRO	PRO	GLY	VAL	VAL	VAL	ASP	PRO	GLY	VAL	LVS	LVS	SER	LVS	THR	PRO	THR	PRO	GLY	ALA	THR	LEU	LEU	ALA	LEU	GLY	LEU	GLY	THR	PRO	PRO	GLN	GLM	MET																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
R62	D63	E64	K65	R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	I79	T80	Q81	R82	PRO	G83	P84	T85	T86	A86	T87	N88	R89	ASN	L90	I91	N92	A93	L94	I97	A98	C99	L100	D101	V104	L105	L106	E107	S108	V109	D110	E111	SER	ASP	N11	T52	Q63	PRO	D54	PRO	PHE	ILE	LEU	ASN	GLU	M43	L49	R50	N51	T52	Q63	D54	L55	N56	G57	K58	P59	A60	N61	R62	D63	E64	K65	R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	I79	T80	Q81	R82	PRO	G83	P84	T85	T86	A86	T87	N88	R89	ASN	L90	I91	N92	A93	L94	I97	A98	C99	L100	D101	V104	L105	L106	E107	S108	V109	D110	E111	SER	ASP	N11	T52	Q63	PRO	D54	PRO	PHE	ILE	LEU	ASN	GLU	M43	L49	R50	N51	T52	Q63	D54	L55	N56	G57	K58	P59	A60	N61	R62	D63	E64	K65	R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	I79	T80	Q81	R82	PRO	G83	P84	T85	T86	A86	T87	N88	R89	ASN	L90	I91	N92	A93	L94	I97	A98	C99	L100	D101	V104	L105	L106	E107	S108	V109	D110	E111	SER	ASP	N11	T52	Q63	PRO	D54	PRO	PHE	ILE	LEU	ASN	GLU	M43	L49	R50	N51	T52	Q63	D54	L55	N56	G57	K58	P59	A60	N61	R62	D63	E64	K65	R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	I79	T80	Q81	R82	PRO	G83	P84	T85	T86	A86	T87	N88	R89	ASN	L90	I91	N92	A93	L94	I97	A98	C99	L100	D101	V104	L105	L106	E107	S108	V109	D110	E111	SER	ASP	N11	T52	Q63	PRO	D54	PRO	PHE	ILE	LEU	ASN	GLU	M43	L49	R50	N51	T52	Q63	D54	L55	N56	G57	K58	P59	A60	N61	R62	D63	E64	K65	R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	I79	T80	Q81	R82	PRO	G83	P84	T85	T86	A86	T87	N88	R89	ASN	L90	I91	N92	A93	L94	I97	A98	C99	L100	D101	V104	L105	L106	E107	S108	V109	D110	E111	SER	ASP	N11	T52	Q63	PRO	D54	PRO	PHE	ILE	LEU	ASN	GLU	M43	L49	R50	N51	T52	Q63	D54	L55	N56	G57	K58	P59	A60	N61	R62	D63	E64	K65	R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	I79	T80	Q81	R82	PRO	G83	P84	T85	T86	A86	T87	N88	R89	ASN	L90	I91	N92	A93	L94	I97	A98	C99	L100	D101	V104	L105	L106	E107	S108	V109	D110	E111	SER	ASP	N11	T52	Q63	PRO	D54	PRO	PHE	ILE	LEU	ASN	GLU	M43	L49	R50	N51	T52	Q63	D54	L55	N56	G57	K58	P59	A60	N61	R62	D63	E64	K65	R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	I79	T80	Q81	R82	PRO	G83	P84	T85	T86	A86	T87	N88	R89	ASN	L90	I91	N92	A93	L94	I97	A98	C99	L100	D101	V104	L105	L106	E107	S108	V109	D110	E111	SER	ASP	N11	T52	Q63	PRO	D54	PRO	PHE	ILE	LEU	ASN	GLU	M43	L49	R50	N51	T52	Q63	D54	L55	N56	G57	K58	P59	A60	N61	R62	D63	E64	K65	R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	I79	T80	Q81	R82	PRO

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

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LYS	LEU	PRO	GLN	LEU	ARG	M62	MET
GLY	ALA	TYR	PHE	GLY	ARG	D63	GLN
SER	LEU	LEU	PHE	THR	THR	E64	PRO
MET	THR	VAL	LYS	TYR	SER	K65	PRO
GLN	LEU	ASN	LEU	LYS	ARG	D66	GLU
THR	VAL	LYS	LEU	MET	LYS	V67	LEU
GLY	CYS	PRO	THR	GLN	SER	R68	GLU
ALA	TYR	LYS	MET	SER	ALA	V69	ILE
TYR	ALA	VAL	VAL	ARG	ASP	E70	ASP
ASP	ASN	LEU	THR	PHE	ILE	Q71	GLY
ASN	THR	MET	SER	ASN	VAL	H72	P11
PRO	PRO	PHE	SER	ARG	ASP	R73	K12
GLY	GLY	PRO	SER	GLY	THR	R74	R13
PHE	TYR	PHE	TYR	VAL	THR	L75	H14
ASN	VAL	CYS	VAL	LEU	SER	L76	R15
LYS	THR	ARG	GLN	LEU	PRO	L77	E16
LYS	HIS	GLY	ASN	MET	GLU	K78	H17
LEU	ARG	ASP	THR	VAL	ALA	L79	I18
TYR	ASP	GLU	GLU	ASN	SER	T80	R19
PHE	LEU	TYR	CYS	ILE	GLU	Q81	K20
ASN	ASN	ASP	PHE	MET	GLY	R82	N21
PRO	THR	LEU	VAL	ASP	PRO	G83	L22
GLY	THR	GLY	MET	TYR	CYS	P84	N23
SER	GLY	HIS	VAL	PRO	VAL	T85	T24
PHE	THR	PRO	LEU	ASP	SER	A86	L25
PHE	ASN	LYS	MET	GLN	LYS	V87	V26
GLU	ILE	ASN	THR	ASN	LEU	N88	E27
	GLN	GLN	HIS	ARG	LEU	L89	N28
LYS	LYS	GLY	GLY	ARG	ASN	L90	T29
PHE	PHE	ASN	ASN	ARG	GLU	L91	R30
CYS	CYS	LEU	SER	ILE	PRO	N92	E31
VAL	VAL	MET	VAL	GLN	GLY	A93	E32
THR	GLU	GLU	GLY	ALA	GLY	L94	R33
MET	MET	PRO	GLY	GLU	ALA		L34
ALA	ALA	VAL	LYS	LYS	LEU		A35
ASP	ASP	TYR	GLU	ASP	THR	I97	R36
HIS	HIS	THR	LYS	SER	THR	N98	E37
ALA	ALA	ALA	VAL	LYS	TYR	C99	C38
HIS	HIS	GLN	GLU	SER	VAL	L100	V39
GLY	GLY	GLU	PHE	LEU	GLY	D101	
THR	THR	GLU	CYS	ILE	VAL		Q40
ASP	ASP	LYS	ASP	HIS	VAL	V104	Q41
LEU	LEU	PRO	GLY	LEU	ASP	L105	G42
PRO	GLU	TYR	PRO	PHE	GLY	L106	L43
ASP	ASP	ASP	VAL	GLN	PRO	E107	L44
THR	ILE	THR	VAL	GLU	GLU	S108	T45
GLN	LEU	GLN	MET	LEU	VAL	V109	
LYS	LYS	THR	ASP	ASN	LYS	D110	M48
THR	THR	GLU	GLN	PHE	LYS	E111	L49
THR	THR	ILE	LYS	THR	SER		R50
GLU	GLU	ILE	ILE	ILE	ASP		N51
GLU	GLU	PRO	LYS	PHE	SER		O53
ALA	ALA	SER	ASN	PRO	ARG		D54
VAL	VAL	PRO	HIS	TYR	ILE		L55
GLY	GLY	THR	PHE	GLY	HIS		R56
ASN	ASN	SER	GLN	GLY	ASP		O57
LYS	LYS	THR	THR	ASN	ILE		K58
ARG	ARG	VAL	ALA	VAL	SER		P59
THR	THR	PRO	LYS	GLN	LEU		F60
LYS	LYS	SER	CYS	ASP	ALA		N61

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ARG	THR	SER	ARG	LVS	SER	ALA	ASP	ILE	VAL	ASP	THR	PRO	PRO	PRO	PRO	GLU	ALA	SER	GLY	GLU	GLN	PRO	PRO	PRO	GLU	LEU	GLU	ILE	GLY	MET																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
M62	D63	E64	K65		R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	L79	T80	Q81	R82	Q83	P84	T85	R86	R87	N88	R89	L90	I91	N92	A93	L94		I97	R98	C99	L100	D101		V104	L105	L106	E107	S108	I109	D110	E111	SER	ASP	SER	LYS	LYS	ARG	ILE	PRO	PRO	GLY	GLY	ASP	SER	ALA	LEU	ASN	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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GLY	SER	GLY	ALA	TYR	PHE	GLY
SER	THR	ASP	ASP	VAL	PHE	THR
THR	MET	THR	THR	VAL	LEU	TYR
GLN	GLN	LEU	LEU	ASN	LYS	LYS
THR	THR	VAL	VAL	LYS	LEU	MET
GLY	ALA	CYS	CYS	PRO	THR	GLN
ALA	TYR	TYR	TYR	LYS	MET	SER
THR	TYR	ALA	ALA	VAL	VAL	ARG
ASP	ASP	ASN	ASN	LEU	THR	PHE
ASN	ASN	THR	THR	MET	SER	ASN
LEU	LEU	PRO	PRO	PHE	SER	ARG
GLY	GLY	GLY	GLY	PRO	SER	GLY
PHE	PHE	TYR	TYR	PHE	TYR	VAL
ASN	ASN	VAL	VAL	CYS	GLN	LEU
GLU	PRO	THR	THR	ARG	VAL	LEU
	GLY	GLY	GLY	GLY	ASN	MET
	PHE	SER	SER	HIS	VAL	VAL
	PHE	THR	THR	PRO	LEU	PRO
ASN	ASN	TYR	TYR	LYS	MET	ASP
GLU	GLU	ILE	ILE	ASN	THR	GLN
		LYS	LYS	GLN	HIS	ARG
		LYS	LYS	GLY	GLY	ARG
		CYS	CYS	LEU	SER	ILE
		PHE	PHE	LEU	VAL	GLY
		GLN	GLN	MET	VAL	ALA
		THR	THR	THR	GLY	LYS
		ASP	ASP	GLN	ASP	GLU
		GLU	GLU	THR	VAL	GLN
		TRP	TRP	LYS	GLY	PHE
		LEU	LEU	LYS	THR	LEU
		GLU	GLU	THR	SER	PHE
		ASP	ASP	PRO	GLN	ASN
		ILE	ILE	ASN	VAL	GLN
		THR	THR	GLN	VAL	LEU
		LYS	LYS	THR	MET	ASN
		ASP	ASP	THR	GLY	THR
		THR	THR	GLY	LYS	PHE
		ASP	ASP	PRO	ILE	ASN
		GLY	GLY	THR	LYS	GLY
		ALA	ALA	SER	THR	ASN
		VAL	VAL	PRO	HIS	TYR
		GLY	GLY	SER	PHE	GLY
		ASN	ASN	THR	GLN	ASN
		THR	THR	ASN	THR	VAL
		THR	THR	VAL	ALA	ASN
		THR	THR	PRO	VAL	GLN
		LYS	LYS	SER	LYS	ASN
		THR	THR	LEU	CYS	GLN
		LYS	LYS	THR	THR	ASN

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- Molecule 2: Caspase Nc

[illegible]

[illegible]

- Molecule 2: Caspase Nc

[illegible]

- Molecule 2: Caspase Nc



SER	ARG	LYS	SER	ALA	ASP	ILE	VAL	ASP	THR	PRO	SER	PRO	GLU	ALA	GLY	SER	GLU	GLY	PRO	CYS	GLU	GLY	LEU	ARG	ASN	GLU	GLY	LEU	GLY	ALA	LEU	THR	TYR	GLY	VAL	VAL	ASP	GLY	PRO	GLU	VAL	LYS	LYS	SER	LYS	LYS	ASP	ARG	N61	T62	Q63	P64	ILE	SER	LEU	ASN	GLU	ARG	
M62	D63	E64	K65		R68	V69	E70	Q71	H72	R73	R74	L75	L76	L77	K78	T79	T80	Q81	R82	G83	P84	T85	A86	Y87	N88	L89	L90	L91	N92	A93	L94		I97	R98	C99	L100		L105	L106	E107	S108	V109	D110	E111	SER	ASP	SER	LYS	ARG	N61	T62	Q63	P64	ILE	SER	LEU	ASN	GLU	ARG
MET	GLN	PRO	PRO	GLU	LEU	ILE	ILE	GLY	M10	P11	K12	R13	H14	H15	E16	H17	I18	R19	K20	N21	L22	N23	I24	L25	V26	E27	W28	T29	N30	Y31	E32	R33	L34	A35	M36	E37	C38	V39	Q40	Q41	G42	I43	L44	T45		M43	L49	R50		T52	Q53	P54	L55	H56	G57	K58	P59	F60	N61

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Lys	Leu	Pro	Gln	Leu	Arg	M62
Gly	Ala	Tyr	Phe	Gly	Arg	D63
Ser	Asp	Leu	Phe	Thr	Thr	E64
Met	Thr	Val	Lys	Tyr	Ser	R65
Gln	Thr	Asn	Leu	Lys	Arg	D66
Thr	Val	Lys	Leu	Met	Lys	M67
Gly	Cys	Pro	Thr	Gln	Ser	R68
Ala	Tyr	Lys	Met	Ser	Ala	M69
Tyr	Val	Val	Val	Arg	Arg	E70
Asp	Asn	Leu	Thr	Phe	Ile	Q71
Asn	Thr	Met	Ser	Asn	Val	R72
Leu	Pro	Phe	Ser	Arg	Asp	K73
Gly	Gly	Pro	Ser	Gly	Thr	R74
Phe	Tyr	Phe	Tyr	Val	Pro	L75
Asn	Val	Cys	Val	Leu	Ser	R15
Lys	Thr	Arg	Gln	Leu	Pro	L77
Lys	His	Gly	Asn	Met	Glu	K78
Leu	Arg	Asp	Thr	Val	Ala	L79
Leu	Asp	Glu	Glu	Asn	Ser	T80
Tyr	Asp	Tyr	Leu	Cys	Glu	Q81
Phe	Asn	Asp	Phe	Met	Arg	R82
Asn	Thr	Leu	Val	Asp	Pro	G83
Pro	Thr	Gly	Val	Met	Cys	P84
Gly	Gly	Gly	Met	Tyr	Val	T24
Phe	Ser	His	Val	Pro	Cys	T85
Phe	Trp	Pro	Val	Asp	Ser	A86
Asn	Tyr	Lys	Met	Gln	Leu	R87
Asn	Gln	Gln	His	Arg	Leu	N88
Lys	Lys	Leu	Gly	Arg	Asn	L90
Phe	Phe	Asn	Asn	Arg	Glu	I91
Cys	Gly	Met	Ser	Ile	Pro	N92
Val	Met	Leu	Val	Gly	Gly	A93
Met	Val	Glu	Glu	Ala	Gly	L94
Ala	Val	Pro	Gly	Glu	Ala	
Asp	Ala	Val	Lys	Lys	Leu	I97
Asp	Asp	Tyr	Glu	Asp	Thr	M98
His	His	Thr	Lys	Pro	Pro	C99
Ala	Ala	Ala	Val	Lys	Tyr	L100
His	His	Gln	Glu	Ser	Val	D101
Glu	Glu	Glu	Phe	Leu	Gly	
Thr	Thr	Glu	Cys	Ile	Val	V104
Asp	Asp	Lys	Asp	His	Val	L105
Leu	Leu	Trp	Gly	Leu	Val	L106
Pro	Pro	Pro	Ser	Phe	Gly	E107
Asp	Asp	Val	Val	Gln	Pro	M108
Thr	Thr	Thr	Val	Glu	Glu	V109
Gln	Gln	Leu	Asp	Leu	Val	D110
Lys	Lys	Thr	Met	Asn	Lys	M111
Thr	Glu	Glu	Gln	Phe	Ser	E111
Thr	Thr	Ile	Lys	Thr	Lys	Ser
Ser	Ser	Ile	Ile	Ile	Asp	T52
Pro	Glu	Pro	Lys	Phe	Ser	Q53
Ala	Ala	Ser	Asp	Arg	Arg	D54
Val	Val	Pro	His	Tyr	Pro	L55
Gly	Gly	Thr	Phe	Gly	Pro	M56
Asn	Asn	Thr	Gln	Asn	Phe	G57
Lys	Lys	Ser	Thr	Val	Ile	K58
Arg	Arg	Val	Ala	Asn	Ser	P59
Thr	Thr	Pro	Lys	Asn	Ser	F60
Lys	Lys	Ser	Lys	Gln	Leu	M61
Trp	Trp	Pro	Cys	Arg	Asn	N62

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MET	GLN	THR	VAL	LYS	TYR	SER	M62
THR	LEU	LEU	ASN	LEU	LYS	ARG	D63
GLY	CVS	THR	LYS	THR	MET	LYS	E64
ALA	TYR	MET	PRO	MET	GLN	SER	R65
TYR	ALA	VAL	LYS	VAL	ARG	ASP	R68
ASN	ASN	THR	LEU	THR	PHE	ILE	V69
ASP	THR	ASN	LEU	THR	ASN	VAL	E70
ASN	THR	THR	MET	SER	ASN	VAL	Q71
LEU	PRO	GLY	PHE	SER	ARG	THR	R72
GLY	GLY	PRO	PRO	SER	GLY	THR	R73
PHE	PHE	THR	PHE	TYR	VAL	VAL	R74
ASN	ASN	VAL	CYS	VAL	LEU	SER	L75
LYS	LYS	THR	ARG	GLN	LEU	PRO	L76
LYS	ASN	HIS	GLY	ASN	MET	GLU	L77
LEU	LEU	THR	ASP	THR	VAL	ALA	R78
THR	PHE	GLU	GLU	GLU	ASN	SER	R79
PHE	TYR	LEU	TYR	CYS	ILE	GLU	T80
ASN	ASN	ASP	ASP	PHE	MET	GLY	Q81
PRO	PRO	THR	LEU	VAL	ASP	PRO	R82
GLY	GLY	GLY	LEU	VAL	TYR	CYS	R83
PHE	PHE	THR	HIS	VAL	PRO	ASN	R84
ASN	ASN	TYR	LYS	LEU	ASP	SER	T85
GLU	GLU	ILE	ASN	MET	GLN	LEU	A86
		GLN	GLN	HIS	ARG	ARG	Y87
		LYS	GLY	GLY	ARG	ASN	N88
		PHE	ASN	ASN	ARG	GLU	L89
		CYS	ASN	SER	ILE	PRO	L90
		GLN	MET	VAL	GLY	LEU	I91
		VAL	GLU	GLY	ALA	GLY	N92
		MET	PRO	GLY	GLU	ALA	A93
		ALA	VAL	LYS	LYS	THR	I94
		THR	THR	GLU	ASP	THR	I97
		HIS	ALA	LYS	LYS	TYR	R98
		ASP	GLN	GLU	SER	VAL	C99
		HIS	GLU	GLU	GLY	GLY	L100
		THR	GLU	PHE	ILE	VAL	
		ASP	GLU	CYS	ILE	VAL	
		LYS	LYS	ASP	HIS	VAL	L105
		TRP	PRO	GLY	LEU	VAL	L106
		GLU	PRO	SER	PHE	GLY	E107
		ASP	ASP	VAL	GLN	PRO	Q108
		ILE	THR	VAL	LEU	VAL	G109
		LEU	GLN	ASP	GLU	VAL	D110
		LYS	THR	MET	ASN	LYS	E111
		GLY	GLU	GLN	PHE	LYS	SER
		THR	GLY	LYS	THR	SER	ASP
		SER	ILE	ILE	ILE	LYS	R48
		GLU	PRO	LYS	PHE	LYS	L49
		ALA	SER	ASP	PRO	ILE	R50
		VAL	PRO	HIS	TYR	PRO	N51
		GLY	SER	THR	GLY	HIS	T52
		ASN	THR	PHE	GLY	PRO	Q53
		LYS	ASN	GLN	ASN	GLY	D54
		THR	ASN	THR	VAL	ASP	L55
		ARG	VAL	ALA	ASN	SER	R56
		THR	PRO	GLN	GLN	ASN	G57
		LYS	SER	CYS	ASP	ILE	K58
		LYS	LEU	LYS	GLY	GLU	P59
		GLY	LEU	PRO	GLN	ARG	F60
		ASP	ALA	THR	PHE	THR	R61
		ASP	ASP	LEU	THR	ARG	N62

- Molecule 2: Caspase Nc

[illegible]

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

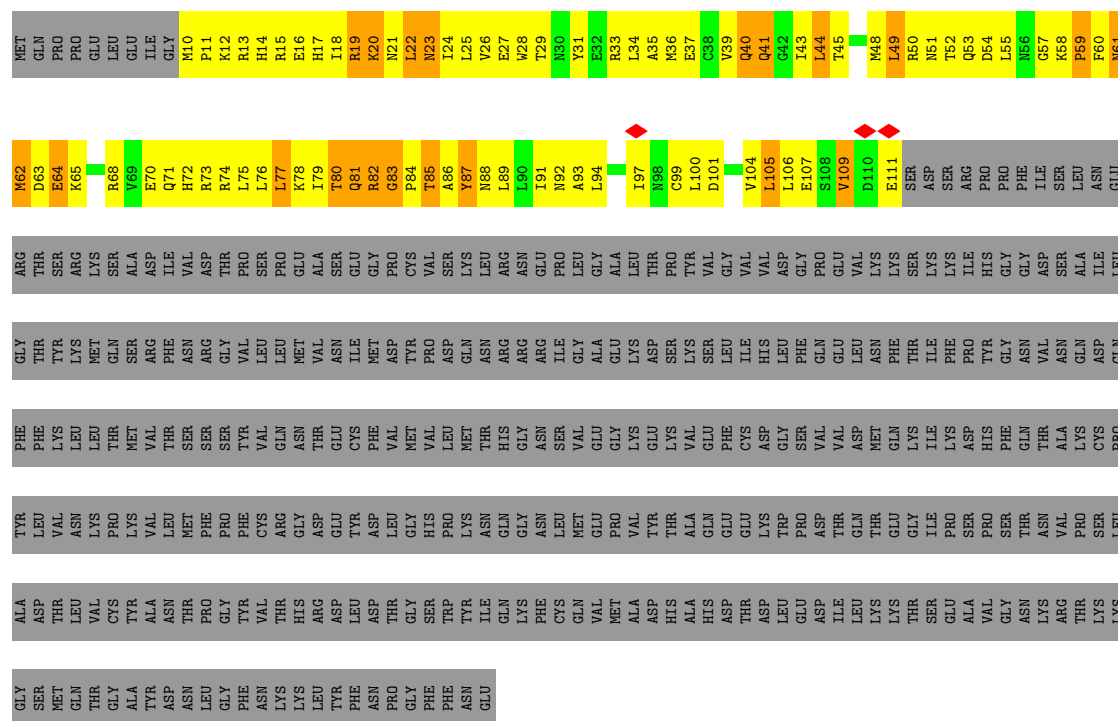
- Molecule 2: Caspase Nc

[illegible]

- Molecule 2: Caspase Nc

[illegible]

- Molecule 2: Caspase Nc



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D8	Depositor
Number of particles used	11359	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)	1400	Depositor
Maximum defocus (nm)	6400	Depositor
Magnification	104748	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.384	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0642	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: ADP

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	0.92	12/4562 (0.3%)	1.50	113/6167 (1.8%)
1	C	0.92	12/4562 (0.3%)	1.50	111/6167 (1.8%)
1	E	0.92	12/4562 (0.3%)	1.50	113/6167 (1.8%)
1	G	0.92	12/4562 (0.3%)	1.50	111/6167 (1.8%)
1	I	0.92	12/4562 (0.3%)	1.50	113/6167 (1.8%)
1	K	0.92	12/4562 (0.3%)	1.50	111/6167 (1.8%)
1	M	0.92	12/4562 (0.3%)	1.50	113/6167 (1.8%)
1	O	0.92	12/4562 (0.3%)	1.50	111/6167 (1.8%)
1	Q	0.92	12/4562 (0.3%)	1.50	113/6167 (1.8%)
1	S	0.92	12/4562 (0.3%)	1.50	111/6167 (1.8%)
1	U	0.92	12/4562 (0.3%)	1.50	113/6167 (1.8%)
1	W	0.92	12/4562 (0.3%)	1.50	111/6167 (1.8%)
1	Y	0.92	12/4562 (0.3%)	1.50	113/6167 (1.8%)
1	a	0.92	12/4562 (0.3%)	1.50	111/6167 (1.8%)
1	c	0.92	12/4562 (0.3%)	1.50	113/6167 (1.8%)
1	e	0.92	12/4562 (0.3%)	1.50	111/6167 (1.8%)
2	B	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	D	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	F	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	H	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	J	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	L	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	N	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	P	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	R	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	T	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	V	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	X	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	Z	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	b	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	d	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)
2	f	0.65	1/850 (0.1%)	1.08	5/1146 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.88	208/86592 (0.2%)	1.44	1872/117008 (1.6%)

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	7
1	C	0	7
1	E	0	7
1	G	0	7
1	I	0	7
1	K	0	7
1	M	0	7
1	O	0	7
1	Q	0	7
1	S	0	7
1	U	0	7
1	W	0	7
1	Y	0	7
1	a	0	7
1	c	0	7
1	e	0	7
All	All	0	112

The worst 5 of 208 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	449	ILE	CA-CB	8.66	1.59	1.54
1	E	449	ILE	CA-CB	8.66	1.59	1.54
1	I	449	ILE	CA-CB	8.66	1.59	1.54
1	M	449	ILE	CA-CB	8.66	1.59	1.54
1	Q	449	ILE	CA-CB	8.66	1.59	1.54

The worst 5 of 1872 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	244	LEU	N-CA-C	-11.36	95.53	110.53
1	G	244	LEU	N-CA-C	-11.36	95.53	110.53
1	K	244	LEU	N-CA-C	-11.36	95.53	110.53
1	O	244	LEU	N-CA-C	-11.36	95.53	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	S	244	LEU	N-CA-C	-11.36	95.53	110.53

There are no chirality outliers.

5 of 112 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	ALA	Peptide
1	A	346	CYS	Mainchain
1	A	410	LEU	Peptide
1	A	50	MET	Peptide
1	A	66	LEU	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	7040	0	5126	1296	0
1	C	7040	0	5126	1295	0
1	E	7040	0	5126	1290	0
1	G	7040	0	5126	1277	0
1	I	7040	0	5126	1299	0
1	K	7040	0	5126	1292	0
1	M	7040	0	5126	1295	0
1	O	7040	0	5126	1280	0
1	Q	7040	0	5126	1285	0
1	S	7040	0	5126	1276	0
1	U	7040	0	5126	1286	0
1	W	7040	0	5126	1291	0
1	Y	7040	0	5126	1281	0
1	a	7040	0	5126	1283	0
1	c	7040	0	5126	1295	0
1	e	7040	0	5126	1291	0
2	B	840	0	863	128	0
2	D	840	0	863	125	0
2	F	840	0	863	129	0
2	H	840	0	863	129	0
2	J	840	0	863	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	840	0	863	125	0
2	N	840	0	863	126	0
2	P	840	0	863	129	0
2	R	840	0	863	126	0
2	T	840	0	863	129	0
2	V	840	0	863	129	0
2	X	840	0	863	125	0
2	Z	840	0	863	126	0
2	b	840	0	863	128	0
2	d	840	0	863	127	0
2	f	840	0	863	123	0
3	A	27	0	12	4	0
3	C	27	0	12	4	0
3	E	27	0	12	4	0
3	G	27	0	12	4	0
3	I	27	0	12	4	0
3	K	27	0	12	4	0
3	M	27	0	12	4	0
3	O	27	0	12	4	0
3	Q	27	0	12	4	0
3	S	27	0	12	4	0
3	U	27	0	12	4	0
3	W	27	0	12	4	0
3	Y	27	0	12	4	0
3	a	27	0	12	4	0
3	c	27	0	12	4	0
3	e	27	0	12	4	0
All	All	126512	0	96016	22156	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 100.

The worst 5 of 22156 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:U:410:LEU:HB3	1:U:426:TYR:CE1	1.29	1.68
1:E:410:LEU:HB3	1:E:426:TYR:CE1	1.29	1.67
1:C:410:LEU:HB3	1:C:426:TYR:CE1	1.29	1.67
1:W:410:LEU:HB3	1:W:426:TYR:CE1	1.29	1.66
1:W:183:LEU:HD22	1:W:186:CYS:SG	1.35	1.66

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	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	C	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	E	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	G	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	I	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	K	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	M	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	O	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	Q	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	S	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	U	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	W	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	Y	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	a	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	c	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
1	e	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	14	49
2	B	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	D	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	F	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	H	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	J	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	L	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	P	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	R	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	T	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	V	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	X	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	Z	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	b	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	d	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
2	f	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	12	46
All	All	10096/24832 (41%)	8704 (86%)	1296 (13%)	96 (1%)	15	46

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	VAL
1	A	346	CYS
1	C	316	VAL
1	C	346	CYS
1	E	316	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	C	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	E	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	G	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	I	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	K	501/551 (91%)	353 (70%)	148 (30%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	O	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	Q	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	S	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	U	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	W	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	Y	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	a	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	c	501/551 (91%)	353 (70%)	148 (30%)	0	3
1	e	501/551 (91%)	353 (70%)	148 (30%)	0	3
2	B	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	D	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	F	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	H	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	J	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	L	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	N	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	P	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	R	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	T	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	V	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	X	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	Z	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	b	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	d	94/404 (23%)	65 (69%)	29 (31%)	0	2
2	f	94/404 (23%)	65 (69%)	29 (31%)	0	2
All	All	9520/15280 (62%)	6688 (70%)	2832 (30%)	1	3

5 of 2832 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	256	PHE
2	Z	80	THR

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Mol	Chain	Res	Type
1	U	522	LYS
1	U	246	ASN
1	W	494	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 334 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	98	GLN
1	a	520	GLN
1	W	282	HIS
1	Y	288	HIS
1	c	249	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](#)

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	$\# Z > 2$
3	ADP	C	2000	-	28,29,29	1.33	3 (10%)	43,45,45	1.89	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	G	2000	-	28,29,29	1.33	3 (10%)	43,45,45	1.89	10 (23%)
3	ADP	S	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.91	10 (23%)
3	ADP	K	2000	-	28,29,29	1.33	3 (10%)	43,45,45	1.89	10 (23%)
3	ADP	O	2000	-	28,29,29	1.33	3 (10%)	43,45,45	1.89	10 (23%)
3	ADP	c	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.90	10 (23%)
3	ADP	A	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.90	10 (23%)
3	ADP	a	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.91	10 (23%)
3	ADP	e	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.91	10 (23%)
3	ADP	E	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.89	10 (23%)
3	ADP	Q	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.89	10 (23%)
3	ADP	W	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.91	10 (23%)
3	ADP	Y	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.90	10 (23%)
3	ADP	I	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.89	10 (23%)
3	ADP	U	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.90	10 (23%)
3	ADP	M	2000	-	28,29,29	1.32	3 (10%)	43,45,45	1.89	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	2000	-	-	3/16/32/32	0/3/3/3
3	ADP	G	2000	-	-	3/16/32/32	0/3/3/3
3	ADP	S	2000	-	-	2/16/32/32	0/3/3/3
3	ADP	K	2000	-	-	3/16/32/32	0/3/3/3
3	ADP	O	2000	-	-	3/16/32/32	0/3/3/3
3	ADP	c	2000	-	-	2/16/32/32	0/3/3/3
3	ADP	A	2000	-	-	2/16/32/32	0/3/3/3
3	ADP	a	2000	-	-	2/16/32/32	0/3/3/3
3	ADP	e	2000	-	-	2/16/32/32	0/3/3/3
3	ADP	E	2000	-	-	3/16/32/32	0/3/3/3
3	ADP	Q	2000	-	-	3/16/32/32	0/3/3/3
3	ADP	W	2000	-	-	2/16/32/32	0/3/3/3
3	ADP	Y	2000	-	-	2/16/32/32	0/3/3/3
3	ADP	I	2000	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	U	2000	-	-	2/16/32/32	0/3/3/3
3	ADP	M	2000	-	-	3/16/32/32	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2000	ADP	C5-C4	4.55	1.47	1.39
3	G	2000	ADP	C5-C4	4.55	1.47	1.39
3	K	2000	ADP	C5-C4	4.55	1.47	1.39
3	O	2000	ADP	C5-C4	4.55	1.47	1.39
3	S	2000	ADP	C5-C4	4.55	1.47	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	ADP	C5-C4-N3	-6.12	118.28	126.72
3	E	2000	ADP	C5-C4-N3	-6.12	118.28	126.72
3	I	2000	ADP	C5-C4-N3	-6.12	118.28	126.72
3	M	2000	ADP	C5-C4-N3	-6.12	118.28	126.72
3	Q	2000	ADP	C5-C4-N3	-6.12	118.28	126.72

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	ADP	O4'-C4'-C5'-O5'
3	C	2000	ADP	O4'-C4'-C5'-O5'
3	E	2000	ADP	O4'-C4'-C5'-O5'
3	G	2000	ADP	O4'-C4'-C5'-O5'
3	I	2000	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 64 short contacts:

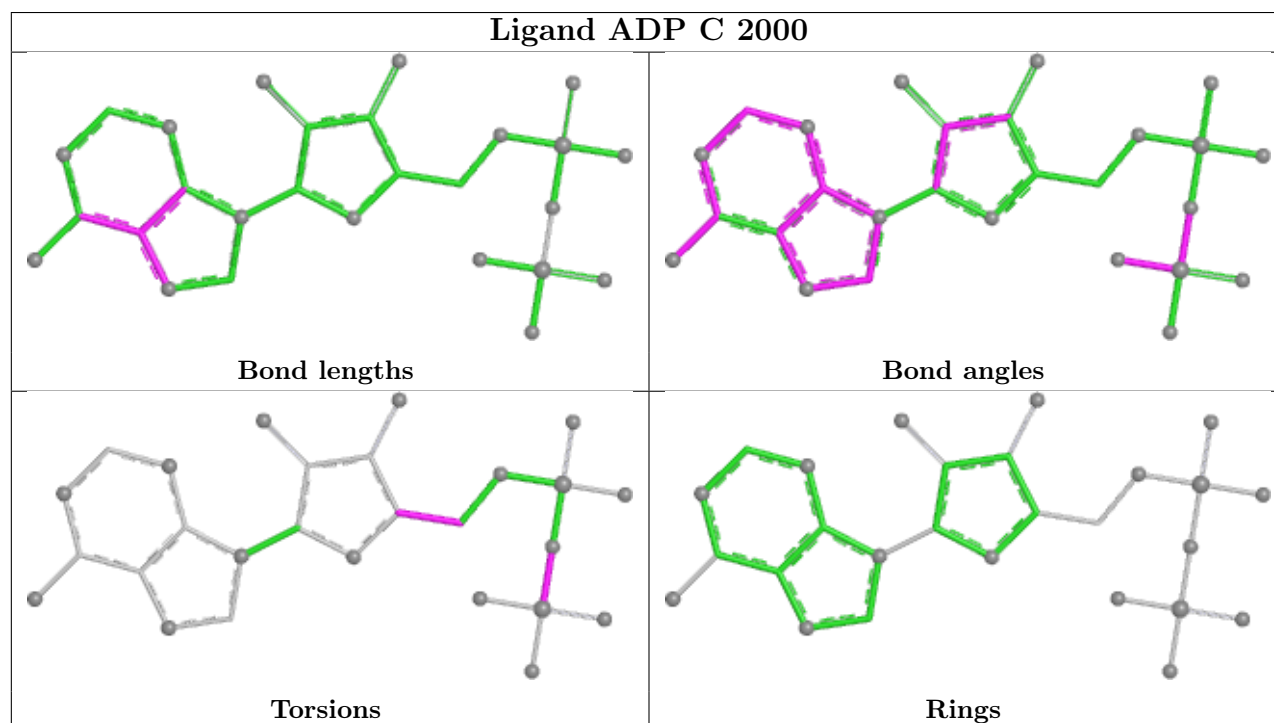
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2000	ADP	4	0
3	G	2000	ADP	4	0
3	S	2000	ADP	4	0
3	K	2000	ADP	4	0
3	O	2000	ADP	4	0

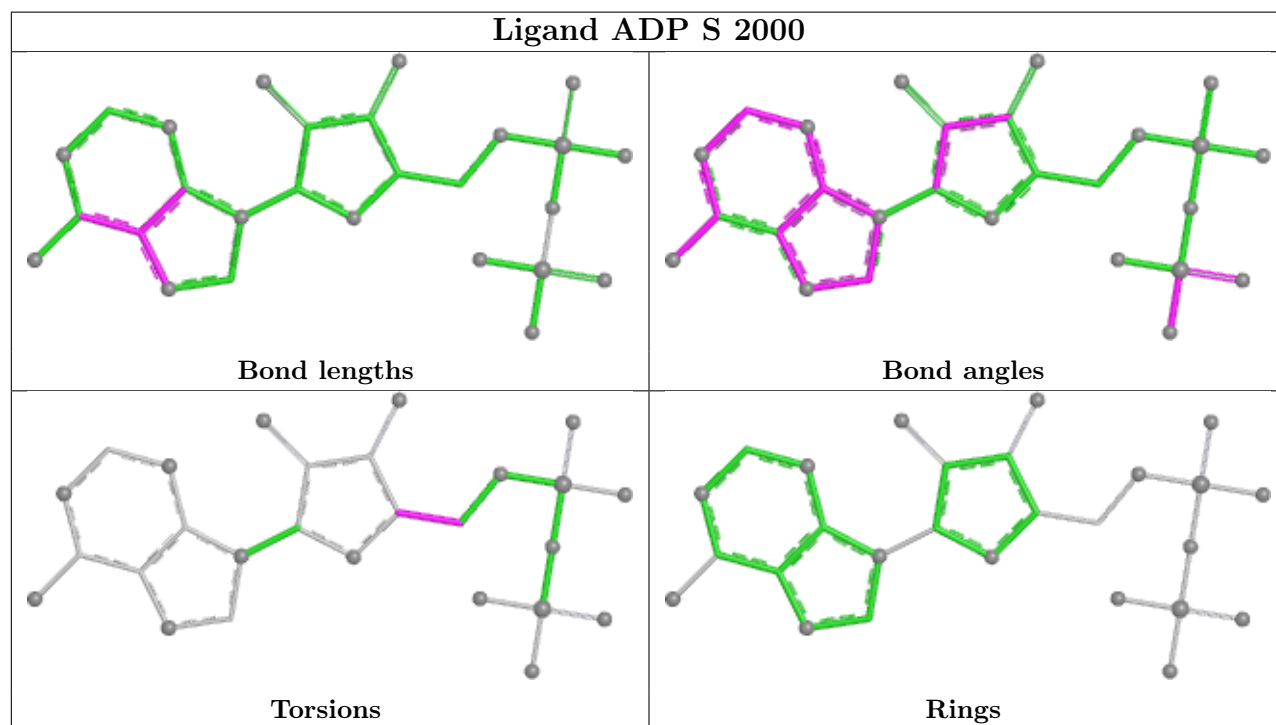
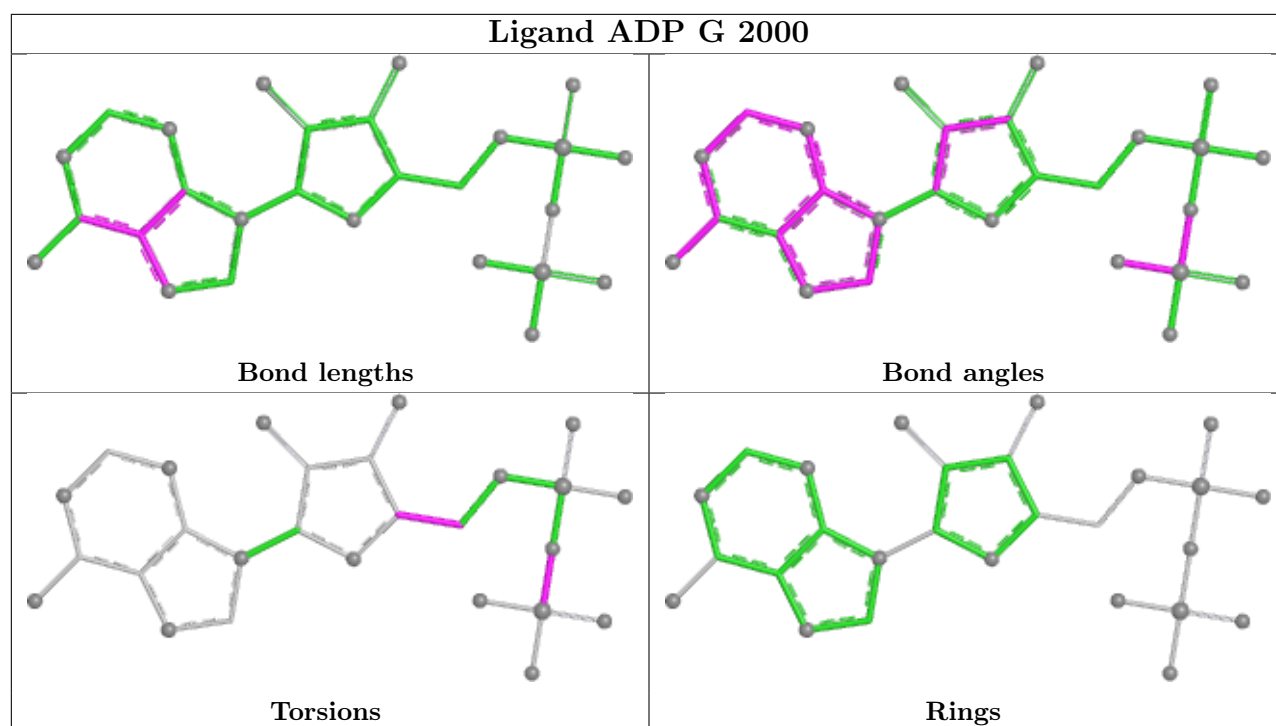
Continued on next page...

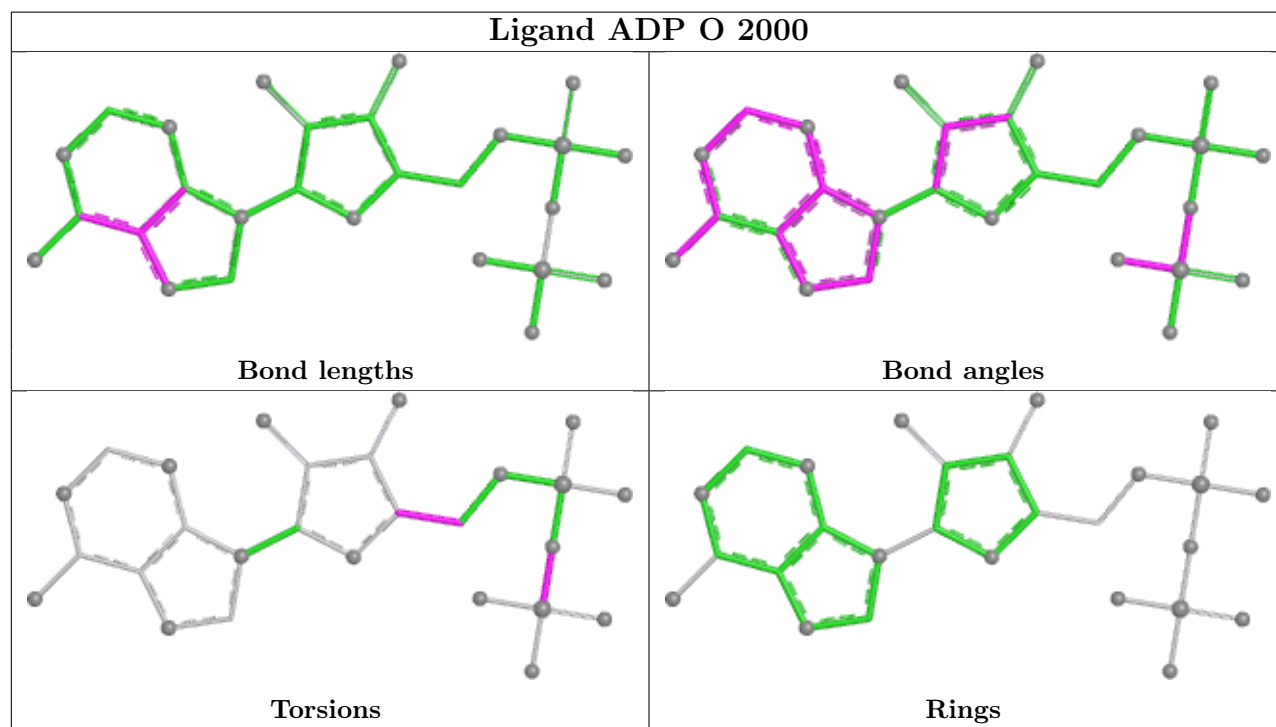
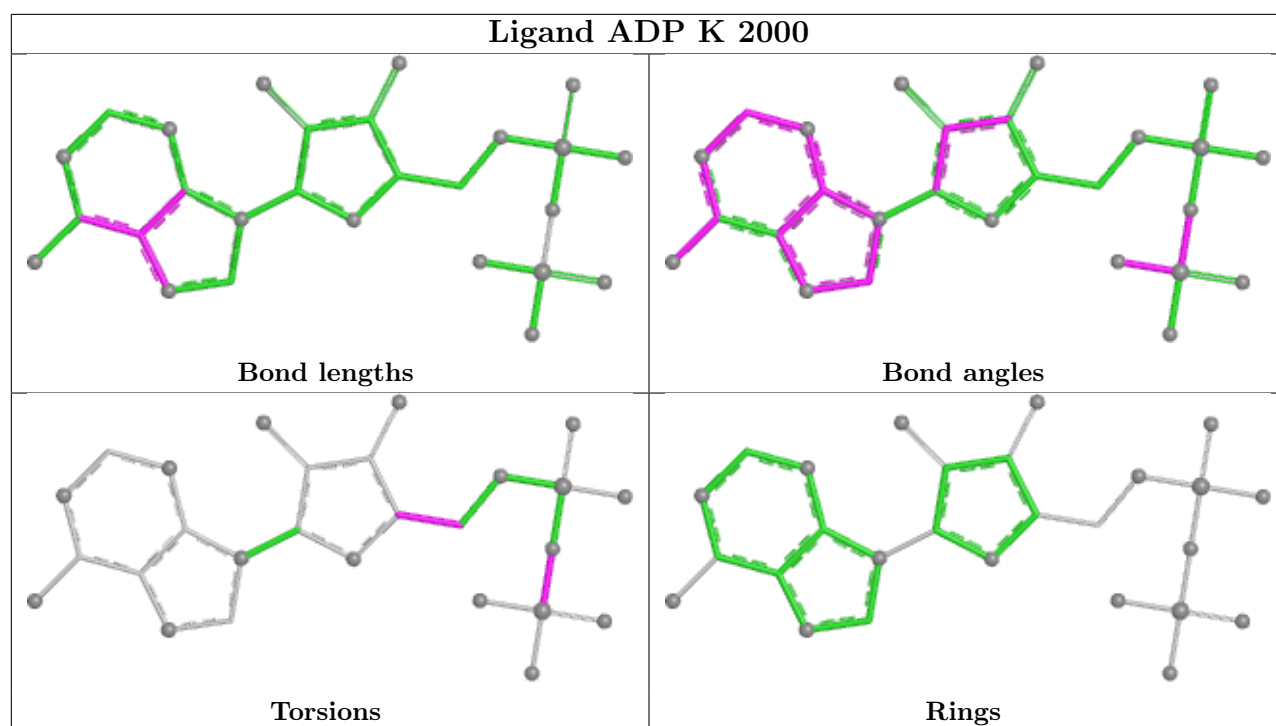
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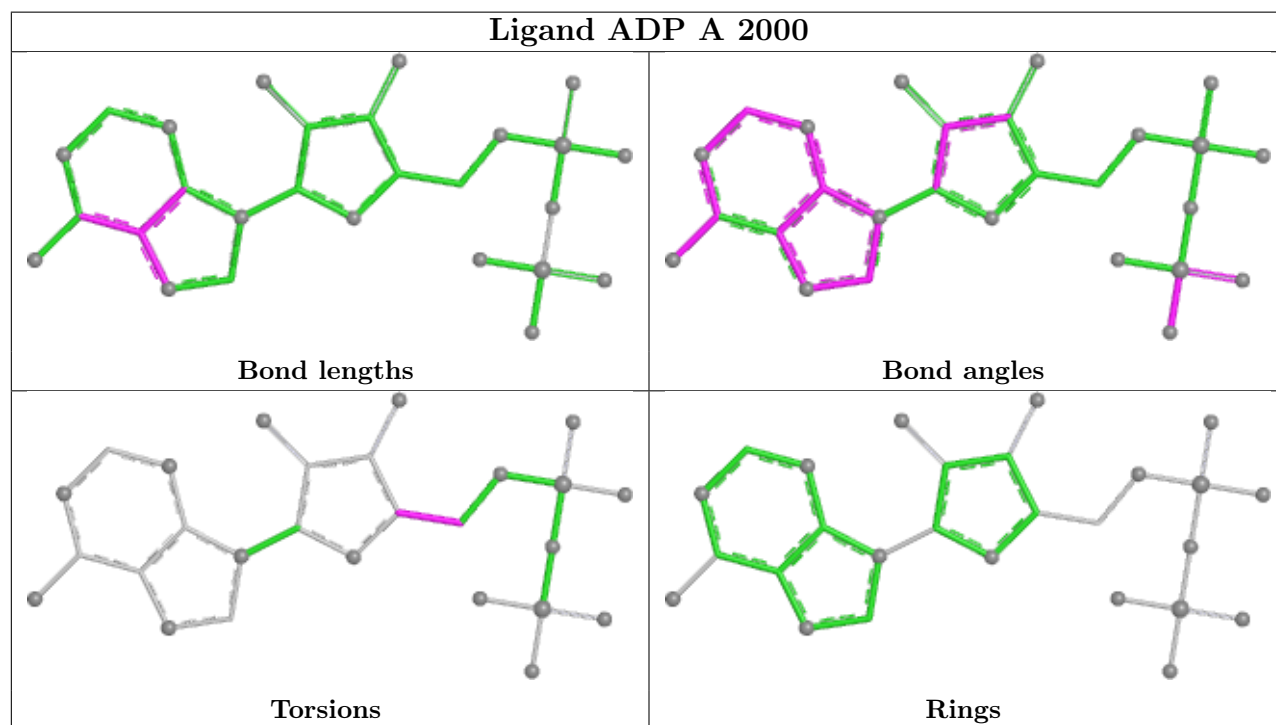
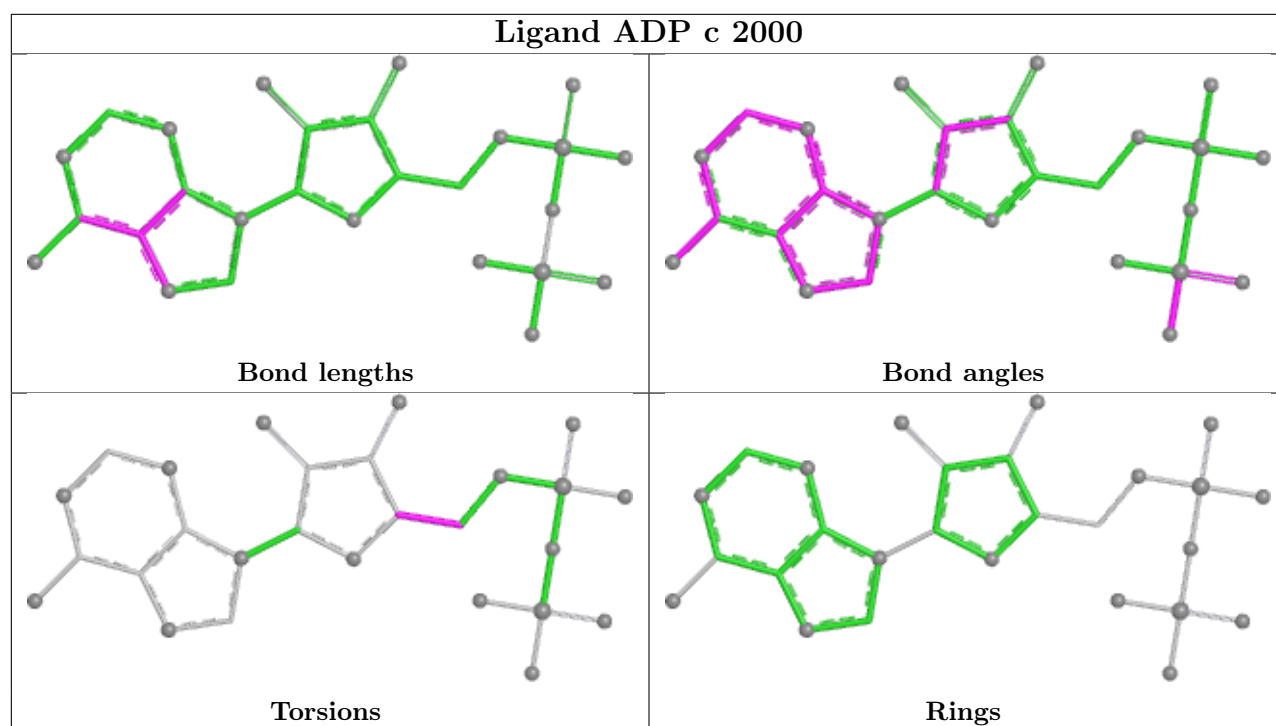
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	c	2000	ADP	4	0
3	A	2000	ADP	4	0
3	a	2000	ADP	4	0
3	e	2000	ADP	4	0
3	E	2000	ADP	4	0
3	Q	2000	ADP	4	0
3	W	2000	ADP	4	0
3	Y	2000	ADP	4	0
3	I	2000	ADP	4	0
3	U	2000	ADP	4	0
3	M	2000	ADP	4	0

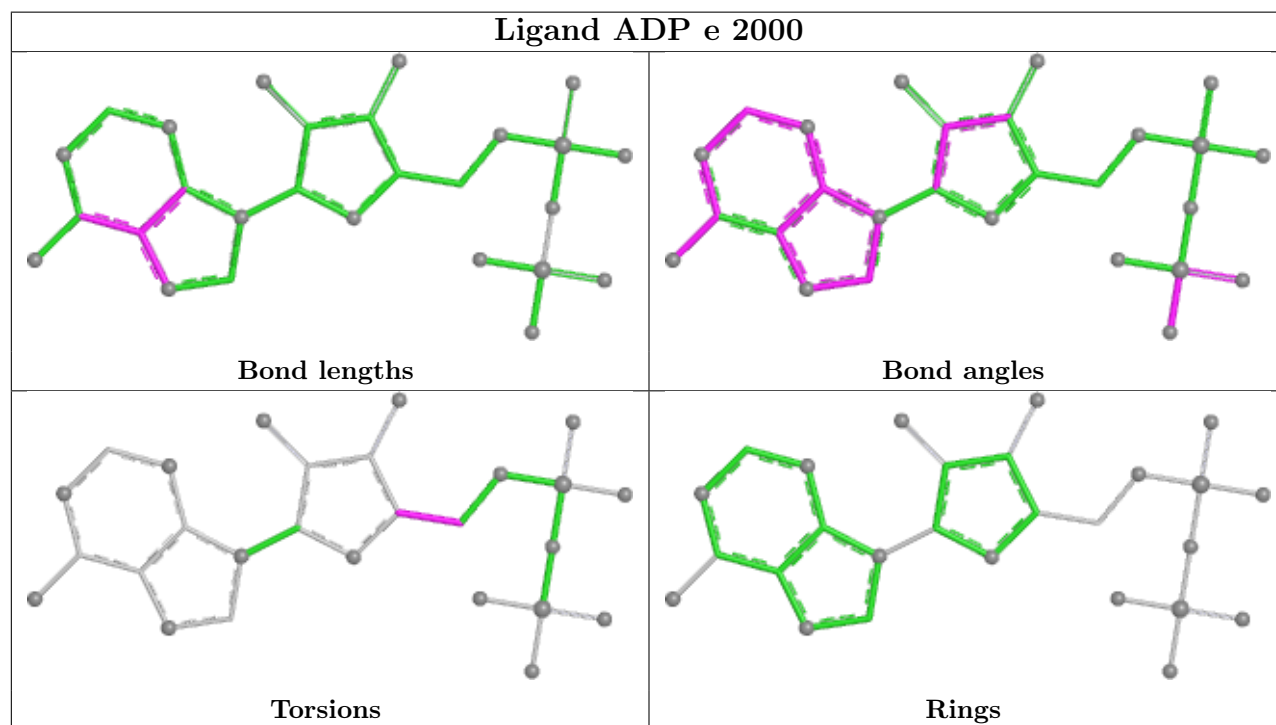
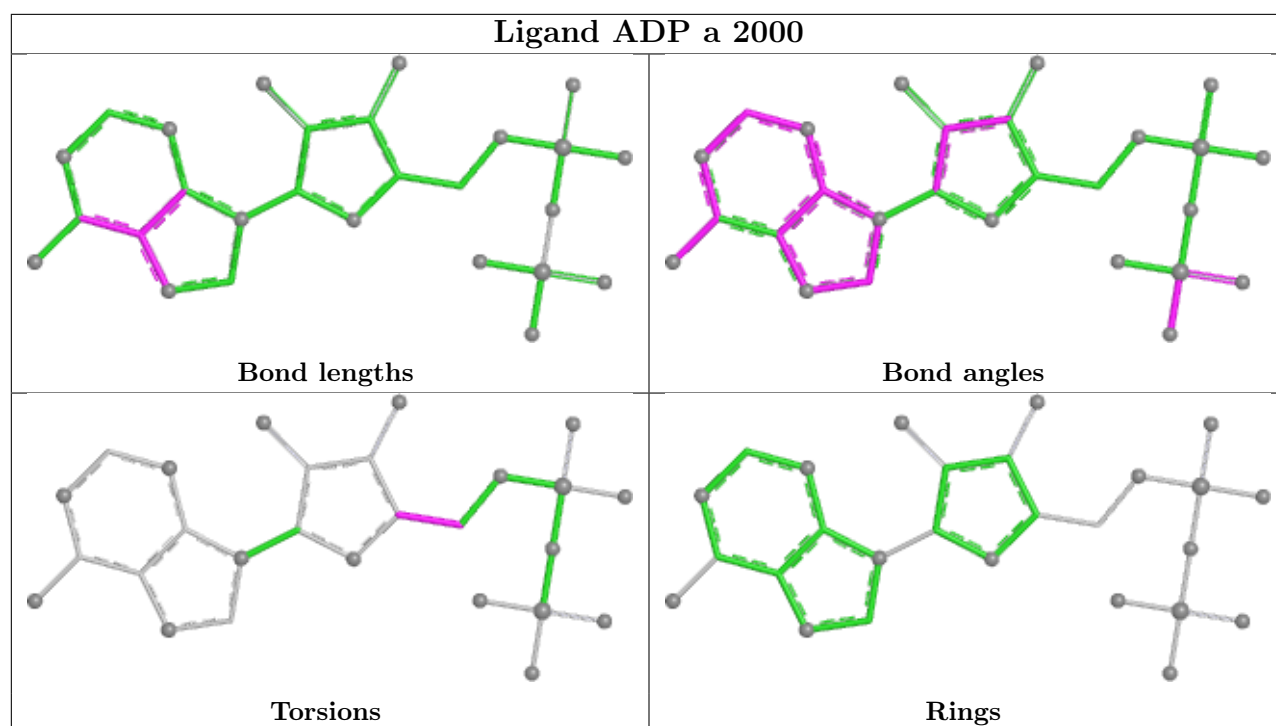
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

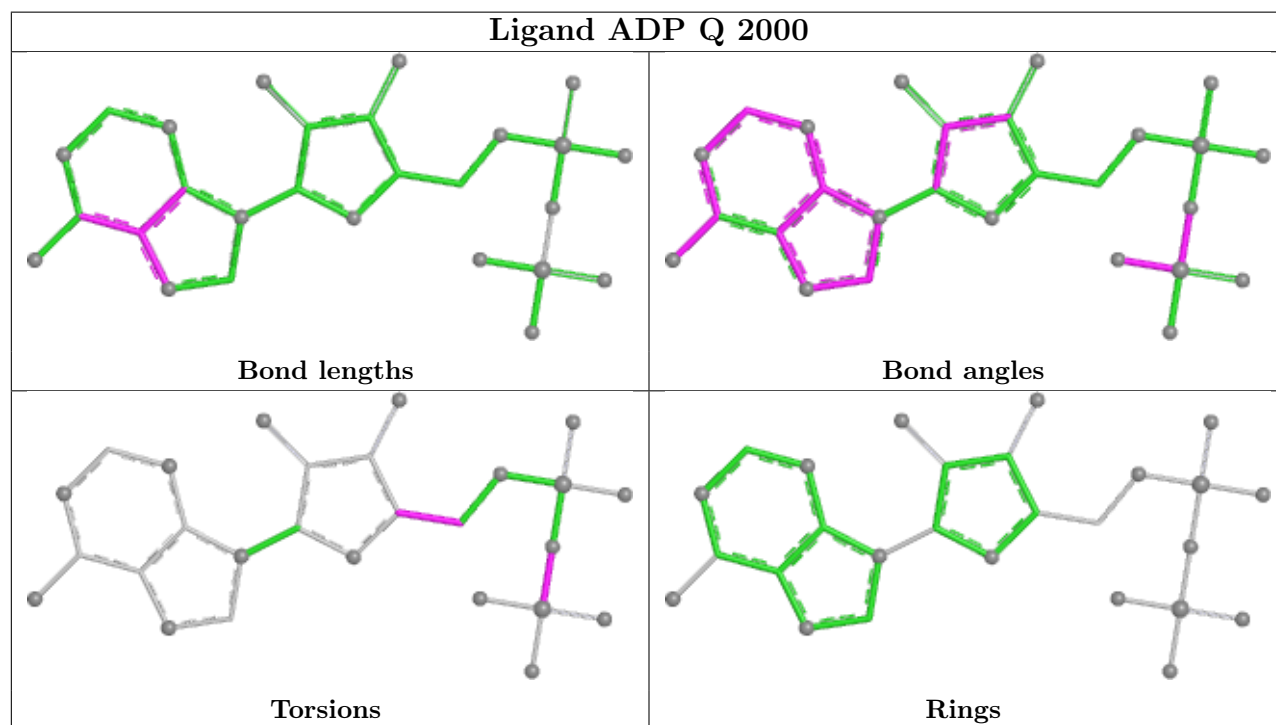
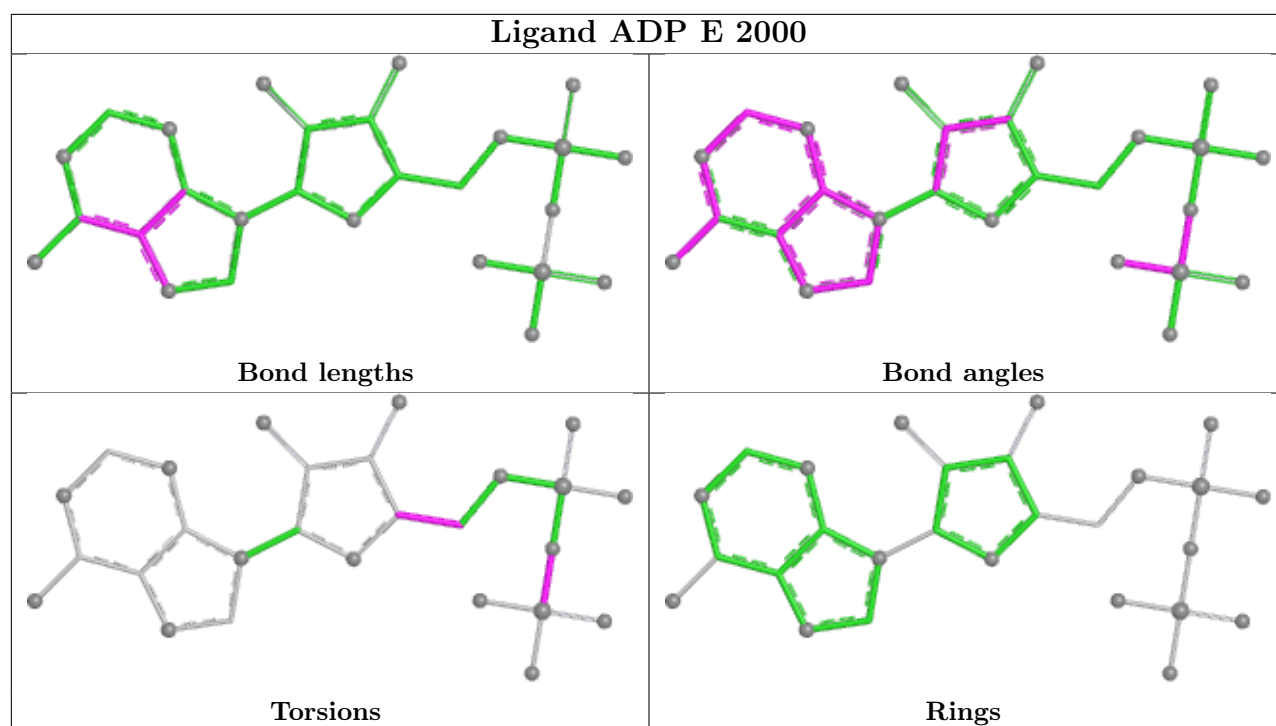


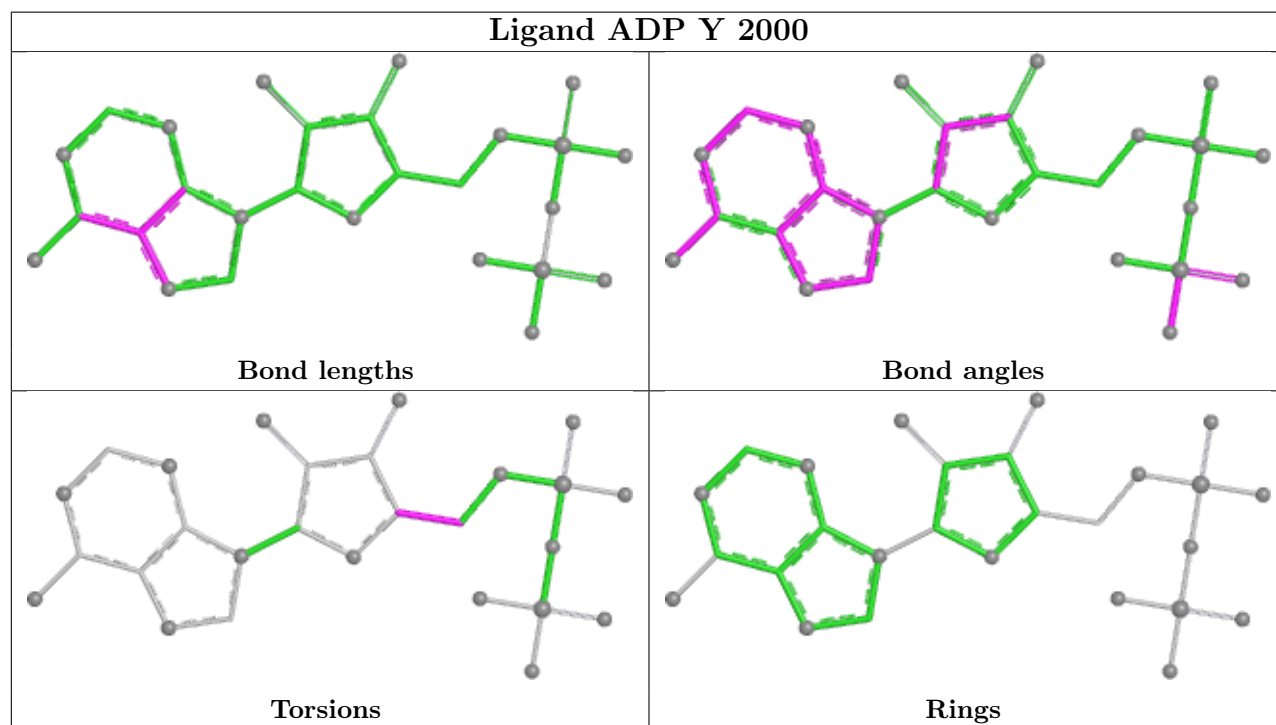
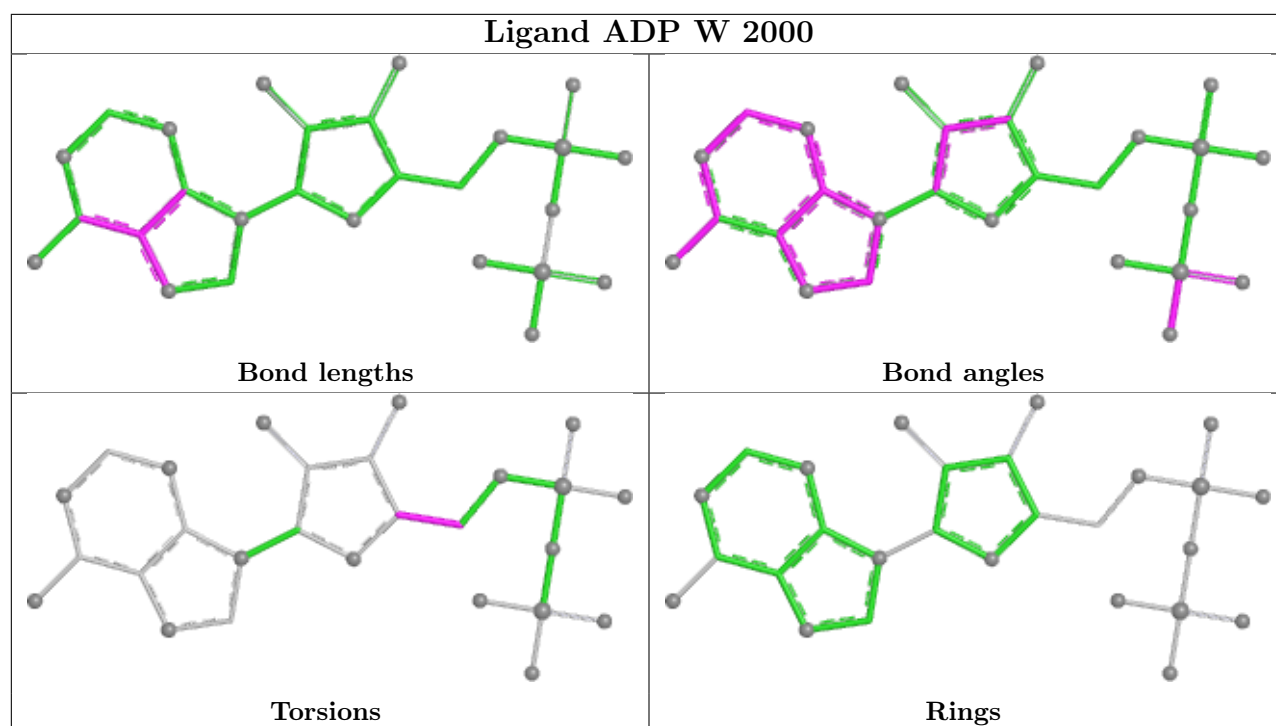


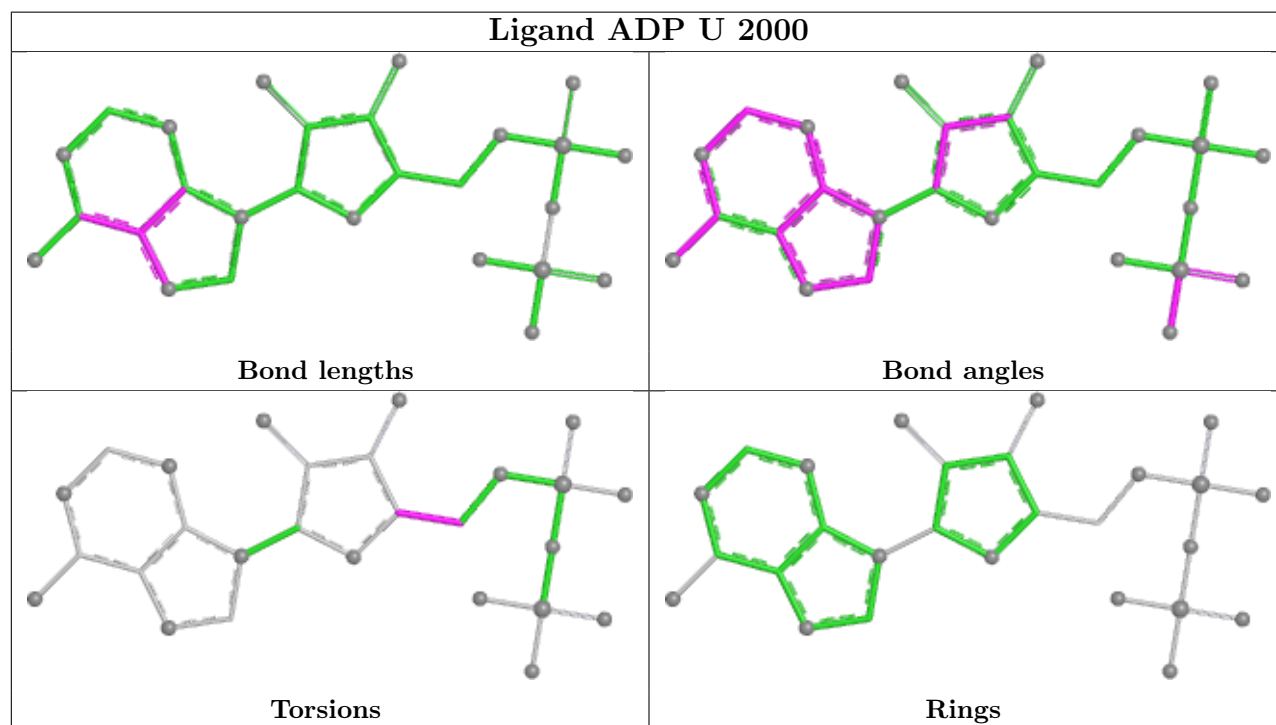
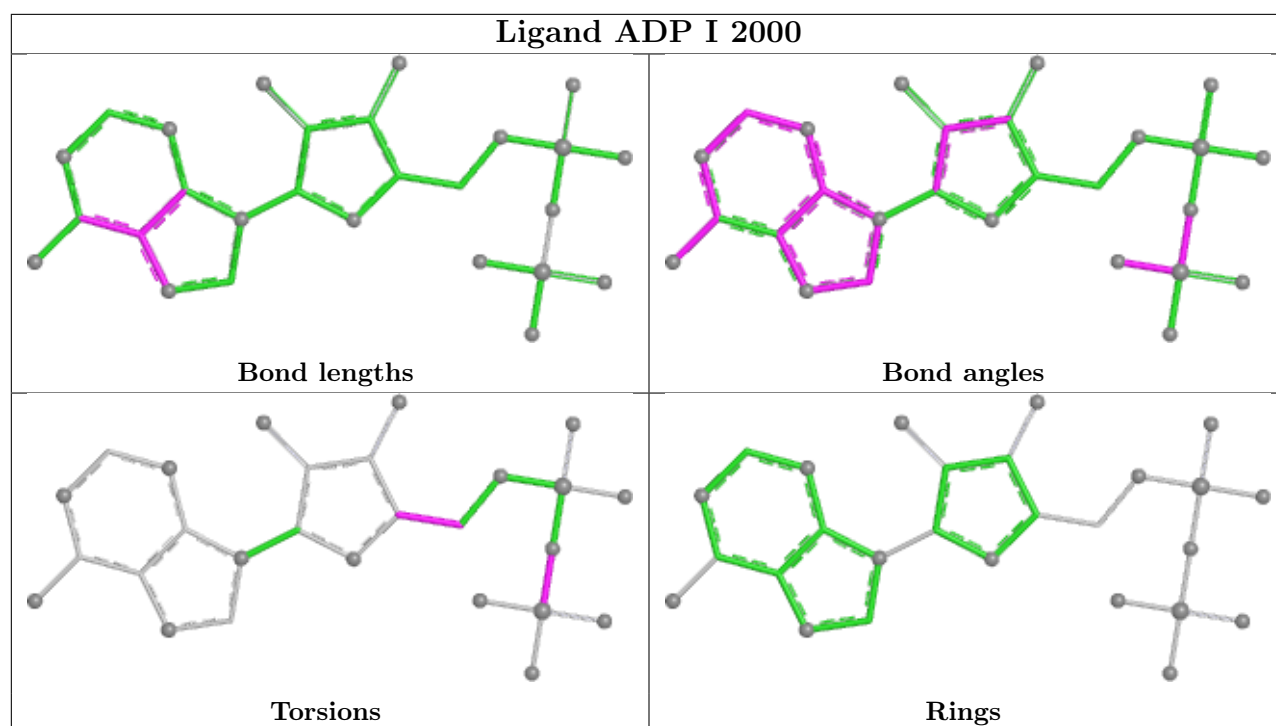


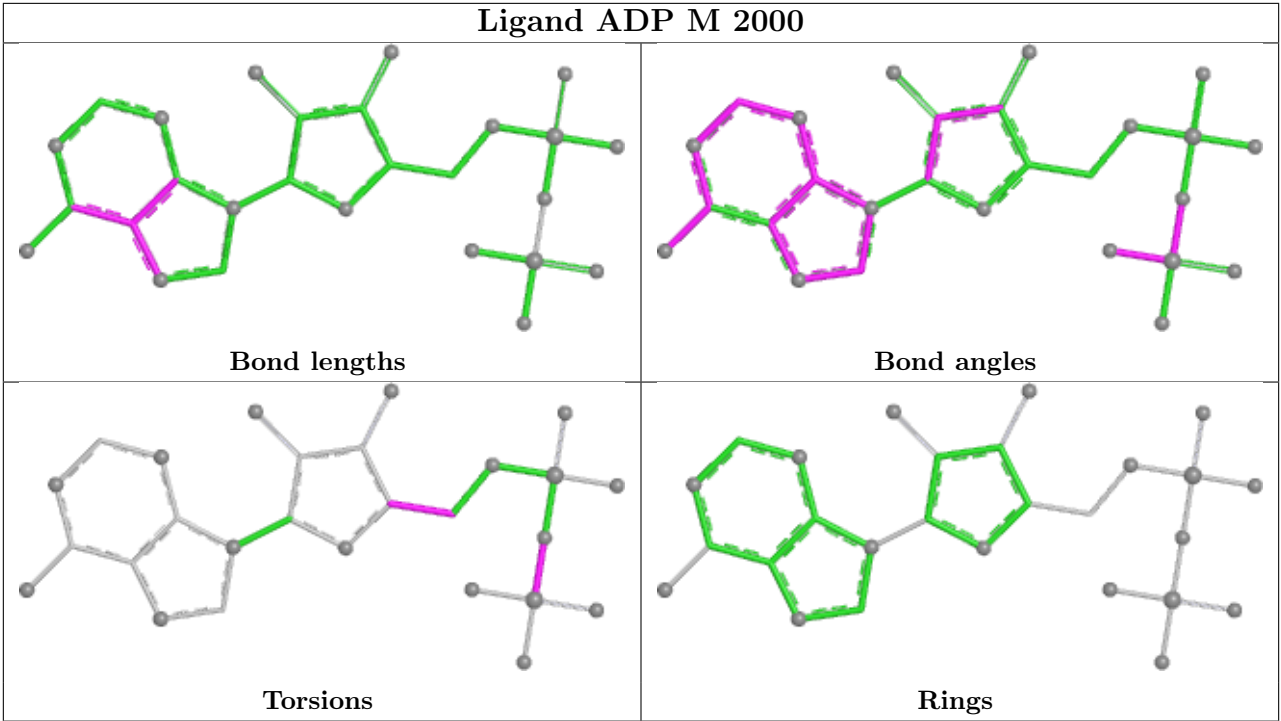












5.7 Other polymers ⓘ

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	40
1	C	40
1	E	40
1	G	40
1	I	40
1	K	40
1	M	40
1	O	40
1	Q	40
1	S	40
1	U	40
1	W	40
1	Y	40
1	a	40
1	c	40

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Mol	Chain	Number of breaks
1	e	40

The worst 5 of 640 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	28.52
1	C	583:ARG	C	607:UNK	N	28.52
1	E	583:ARG	C	607:UNK	N	28.52
1	G	583:ARG	C	607:UNK	N	28.52
1	I	583:ARG	C	607:UNK	N	28.52

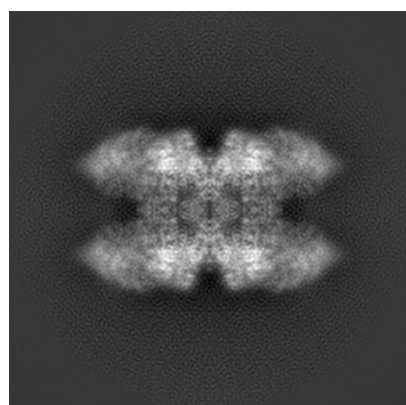
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2870. These allow visual inspection of the internal detail of the map and identification of artifacts.

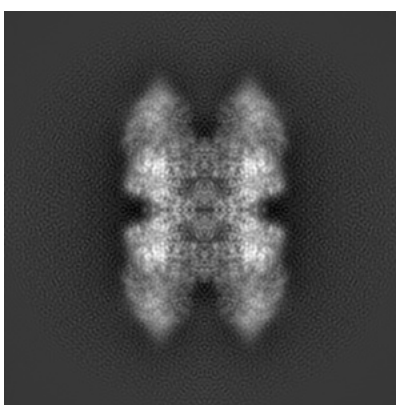
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

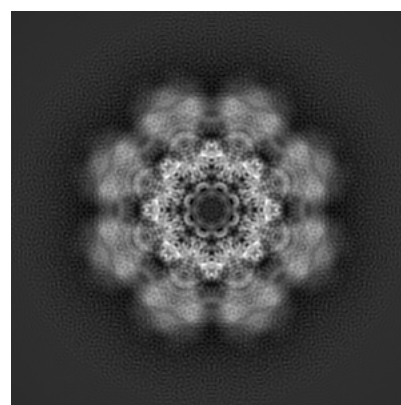
6.1.1 Primary map



X



Y

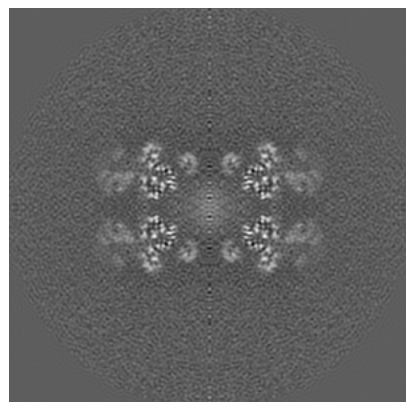


Z

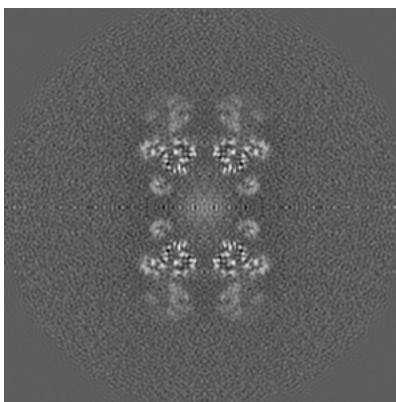
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

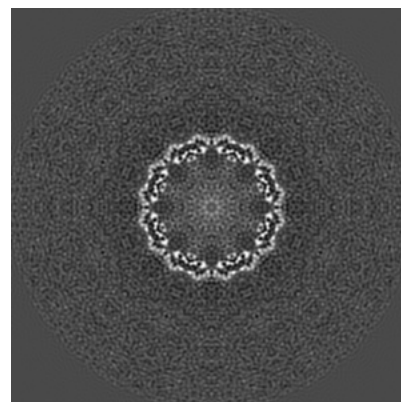
6.2.1 Primary map



X Index: 160



Y Index: 160

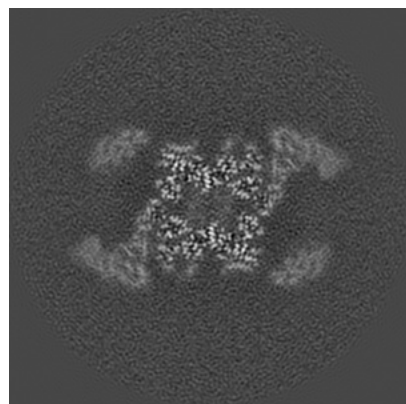


Z Index: 160

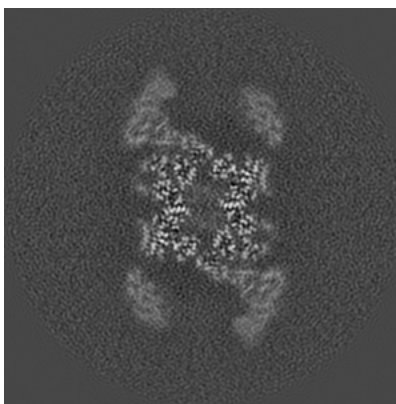
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

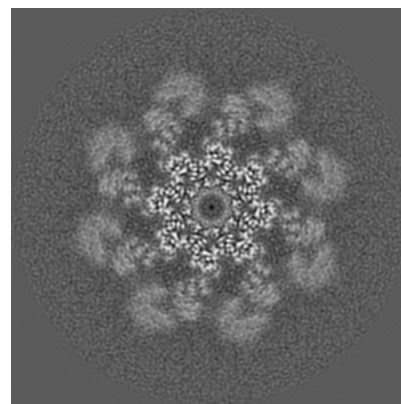
6.3.1 Primary map



X Index: 129



Y Index: 129

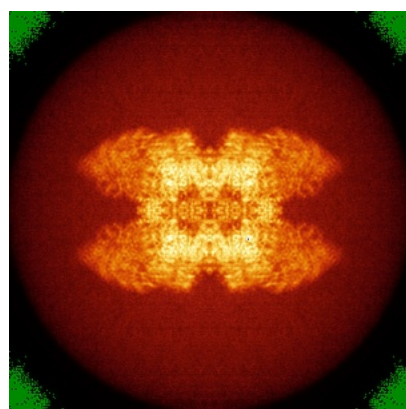


Z Index: 193

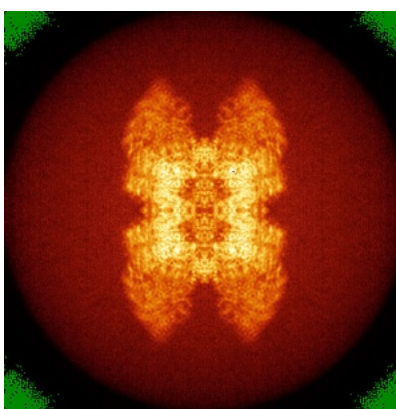
The images above show the largest variance slices of the map in three orthogonal directions.

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

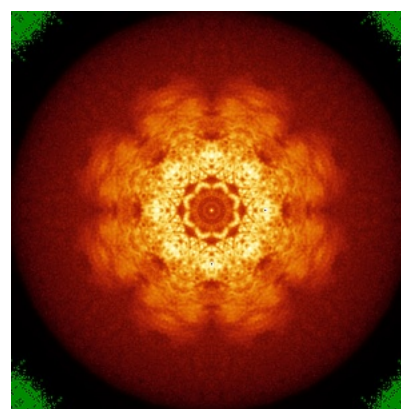
6.4.1 Primary map



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](#)

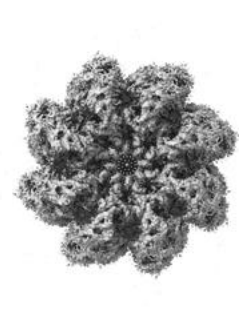
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0642. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

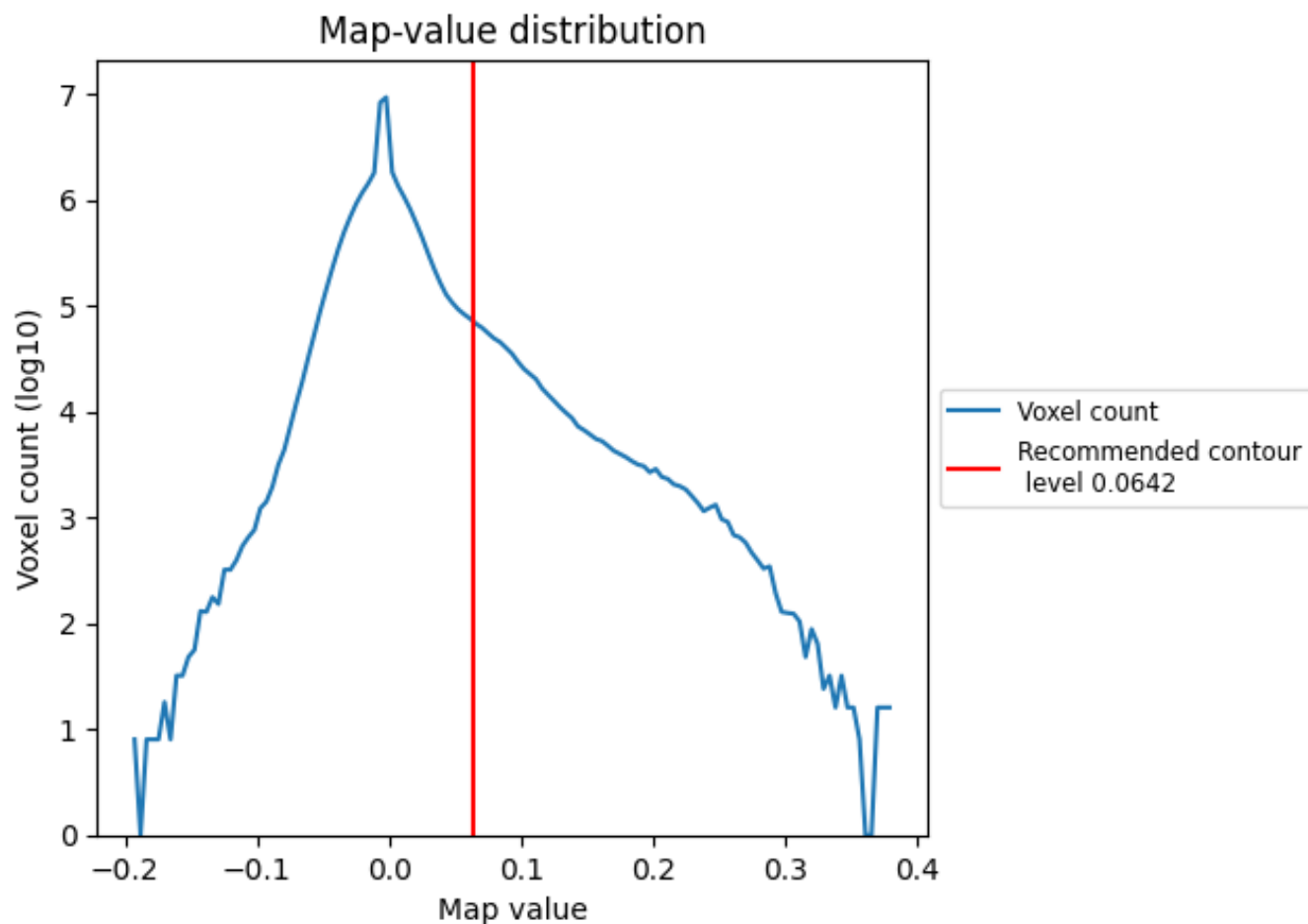
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

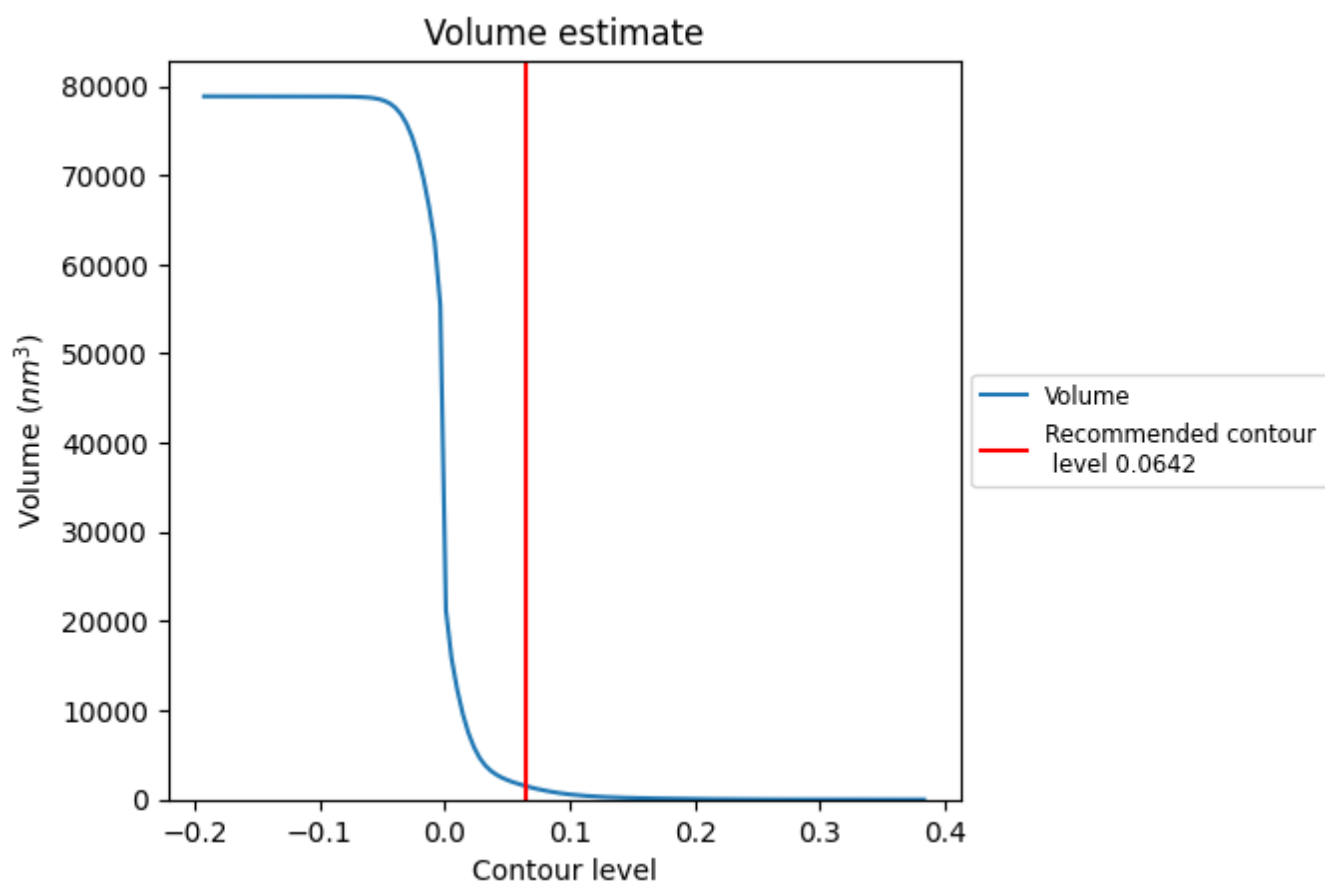
This section contains the results of statistical analysis of the map.

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.

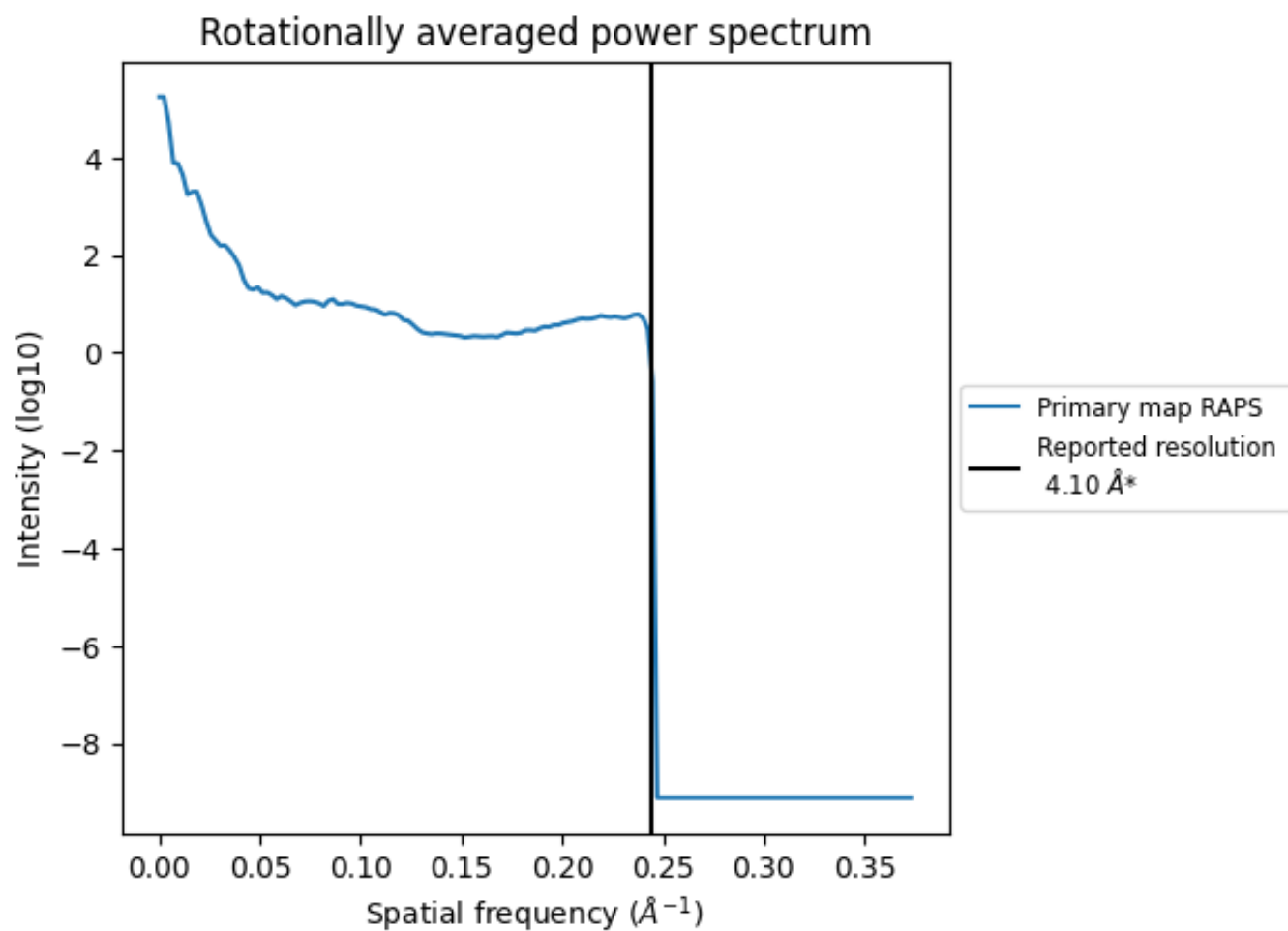
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1533 nm³; this corresponds to an approximate mass of 1385 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 0.244 Å⁻¹

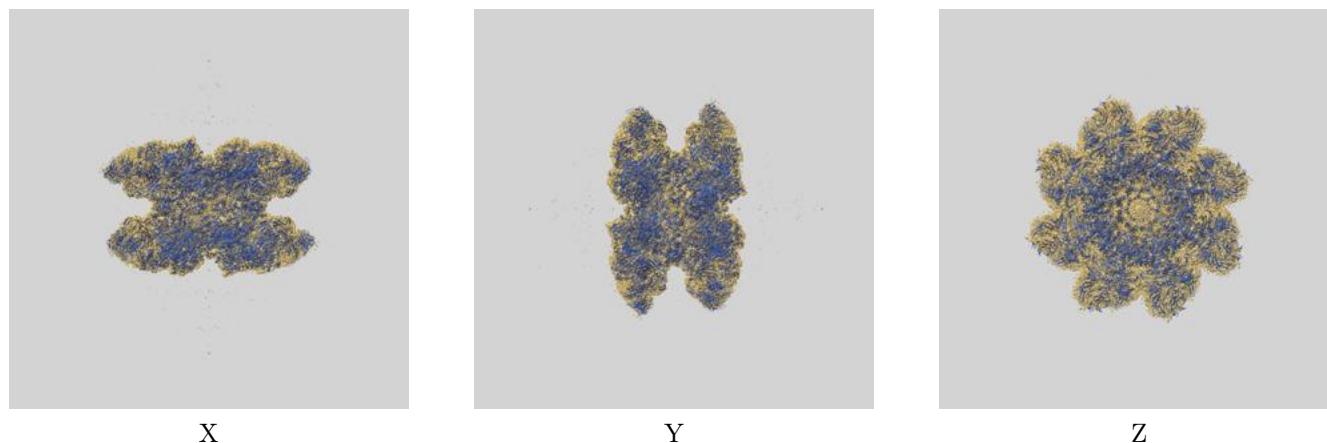
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

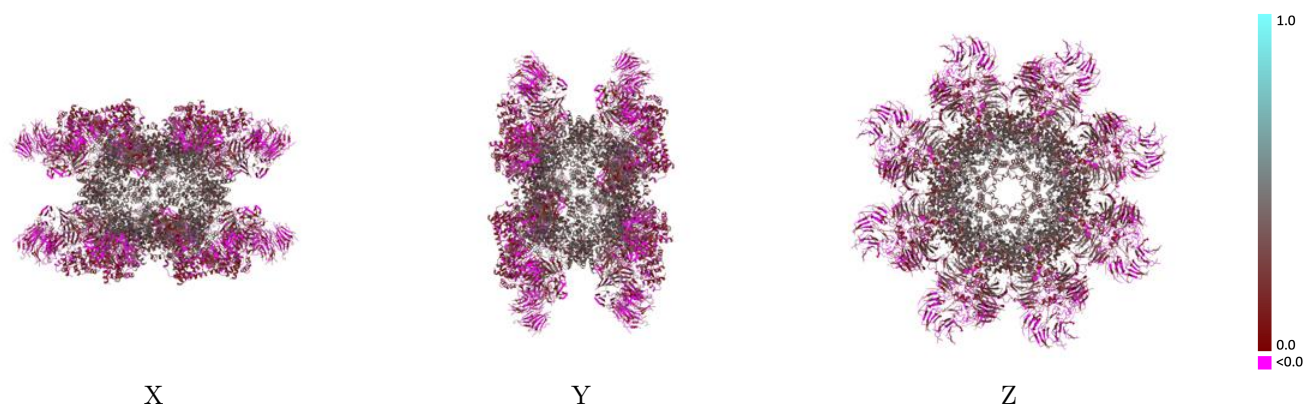
This section contains information regarding the fit between EMDB map EMD-2870 and PDB model 3J9K. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



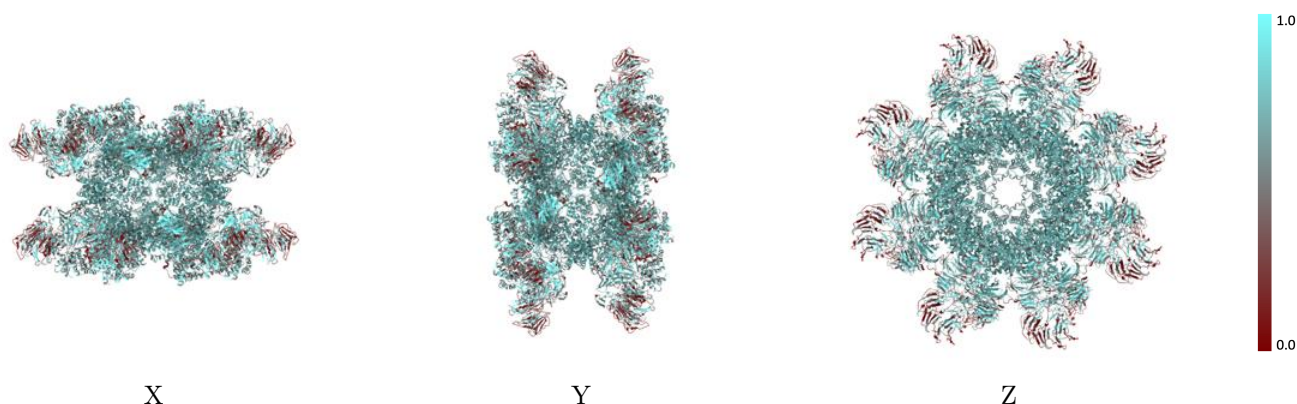
The images above show the 3D surface view of the map at the recommended contour level 0.0642 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



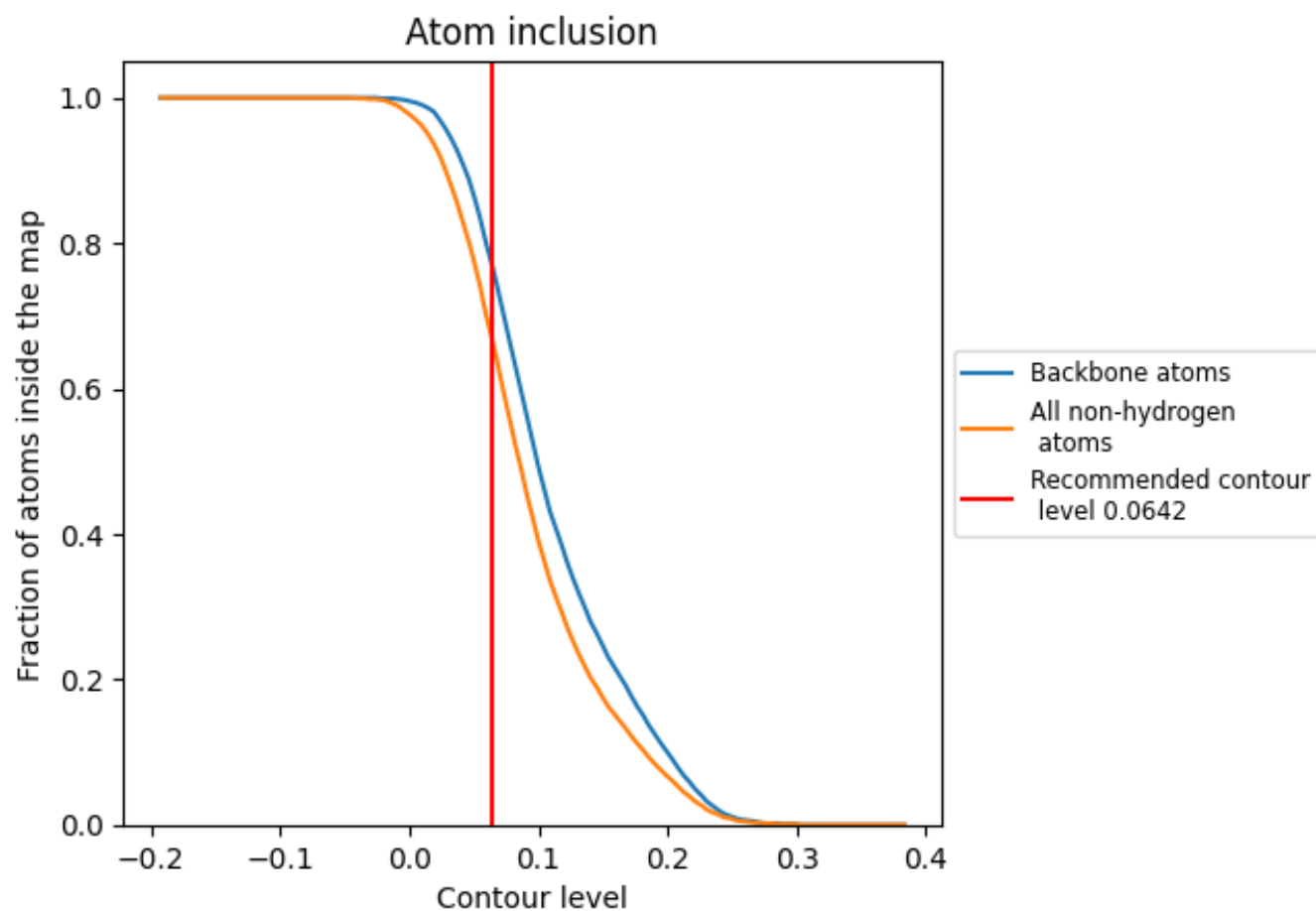
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0642).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.0642) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.2340
A	 0.6560	 0.2210
B	 0.7540	 0.3470
C	 0.6580	 0.2220
D	 0.7480	 0.3460
E	 0.6560	 0.2210
F	 0.7540	 0.3480
G	 0.6570	 0.2210
H	 0.7480	 0.3470
I	 0.6560	 0.2200
J	 0.7540	 0.3480
K	 0.6570	 0.2200
L	 0.7480	 0.3460
M	 0.6560	 0.2200
N	 0.7540	 0.3430
O	 0.6580	 0.2200
P	 0.7480	 0.3440
Q	 0.6560	 0.2210
R	 0.7540	 0.3440
S	 0.6570	 0.2210
T	 0.7480	 0.3460
U	 0.6560	 0.2200
V	 0.7540	 0.3440
W	 0.6570	 0.2200
X	 0.7480	 0.3460
Y	 0.6560	 0.2190
Z	 0.7540	 0.3450
a	 0.6570	 0.2190
b	 0.7480	 0.3450
c	 0.6560	 0.2200
d	 0.7540	 0.3460
e	 0.6570	 0.2200
f	 0.7480	 0.3440

