



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 07:53 PM EST

PDB ID : 3J9K
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:

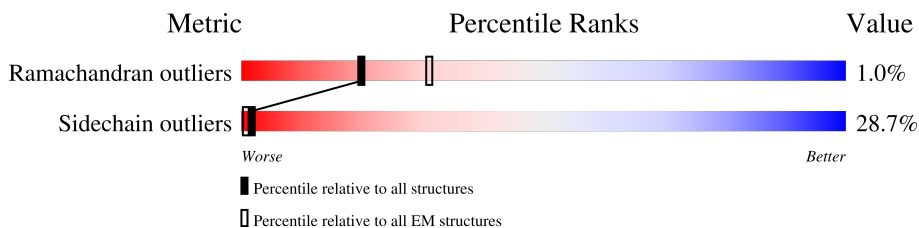
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 4.10 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
1	C	1102	
1	E	1102	
1	G	1102	
1	I	1102	
1	K	1102	
1	M	1102	
1	O	1102	
1	Q	1102	

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Mol	Chain	Length	Quality of chain
1	S	1102	 24% 81% 14% . .
1	U	1102	 25% 81% 14% . .
1	W	1102	 24% 81% 14% . .
1	Y	1102	 25% 81% 14% . .
1	a	1102	 24% 81% 14% . .
1	c	1102	 25% 81% 14% . .
1	e	1102	 24% 81% 14% . .
2	B	450	 15% 7% 77%
2	D	450	 15% 7% 77%
2	F	450	 15% 7% 77%
2	H	450	 15% 7% 77%
2	J	450	 15% 7% 77%
2	L	450	 15% 7% 77%
2	N	450	 15% 7% 77%
2	P	450	 15% 7% 77%
2	R	450	 15% 7% 77%
2	T	450	 15% 7% 77%
2	V	450	 15% 7% 77%
2	X	450	 15% 7% 77%
2	Z	450	 15% 7% 77%
2	b	450	 15% 7% 77%
2	d	450	 15% 7% 77%
2	f	450	 15% 7% 77%

2 Entry composition [i](#)

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.

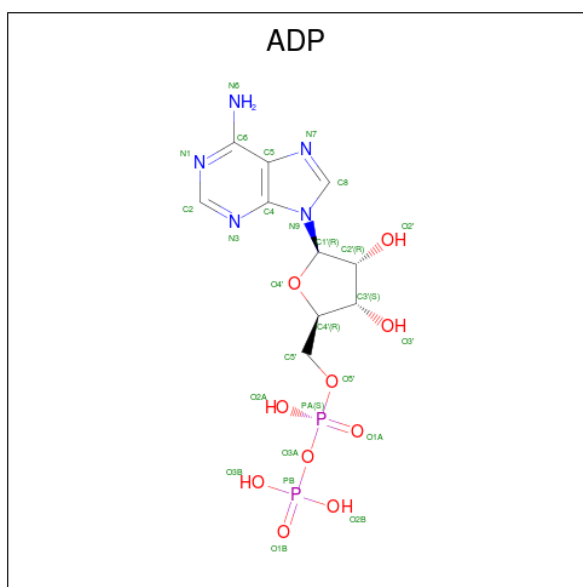
- Molecule 1 is a protein called Apaf-1 related killer DARK.

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

- 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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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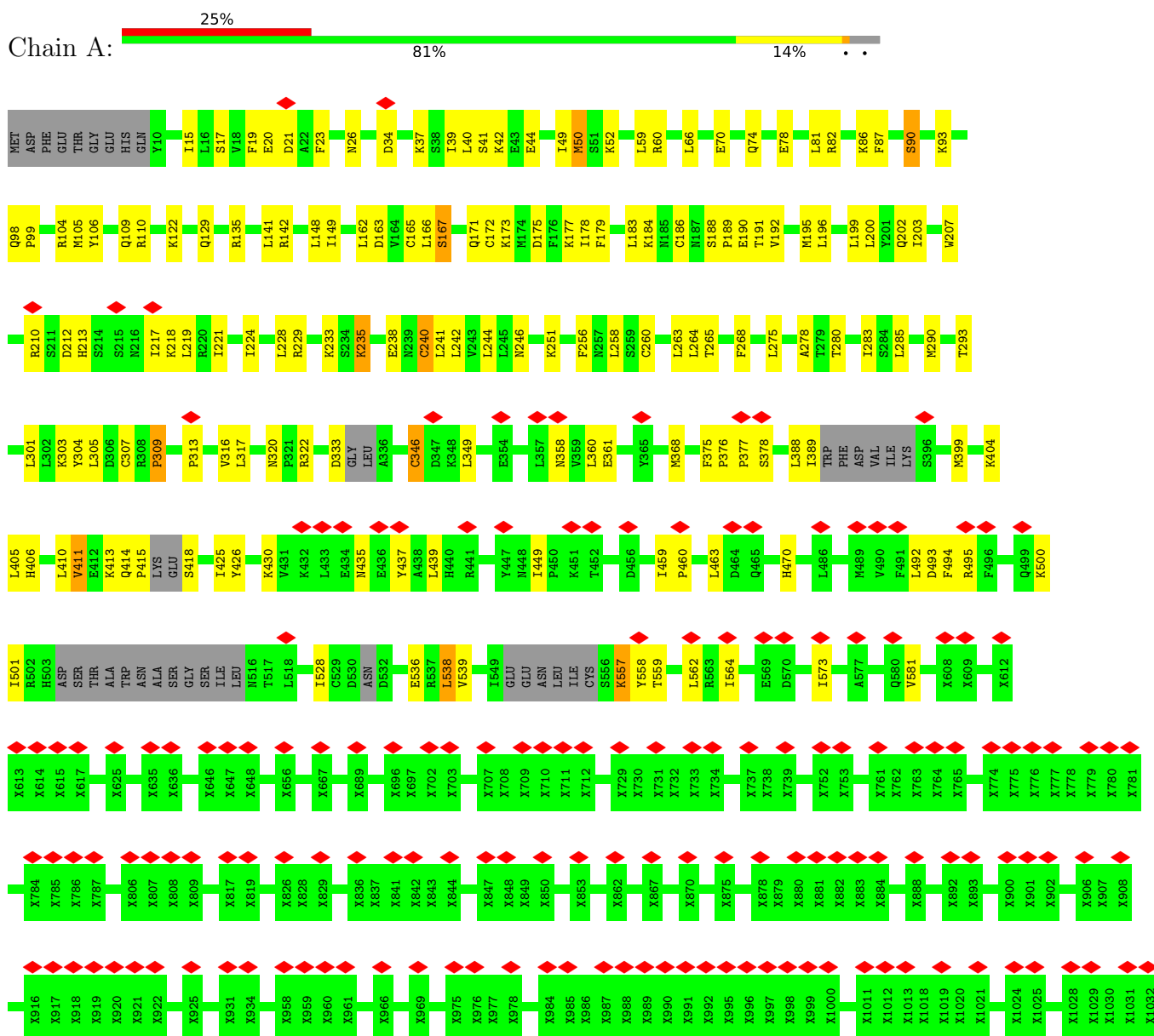
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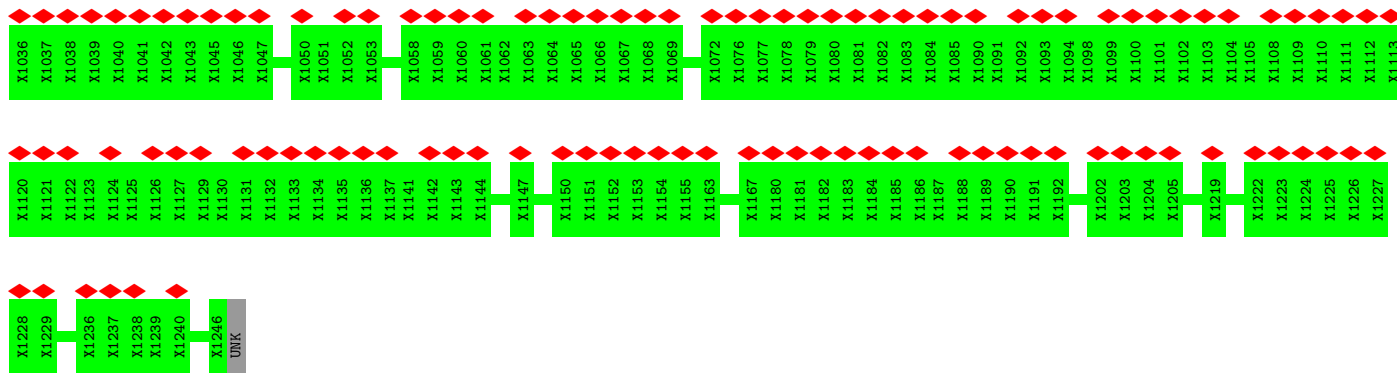
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

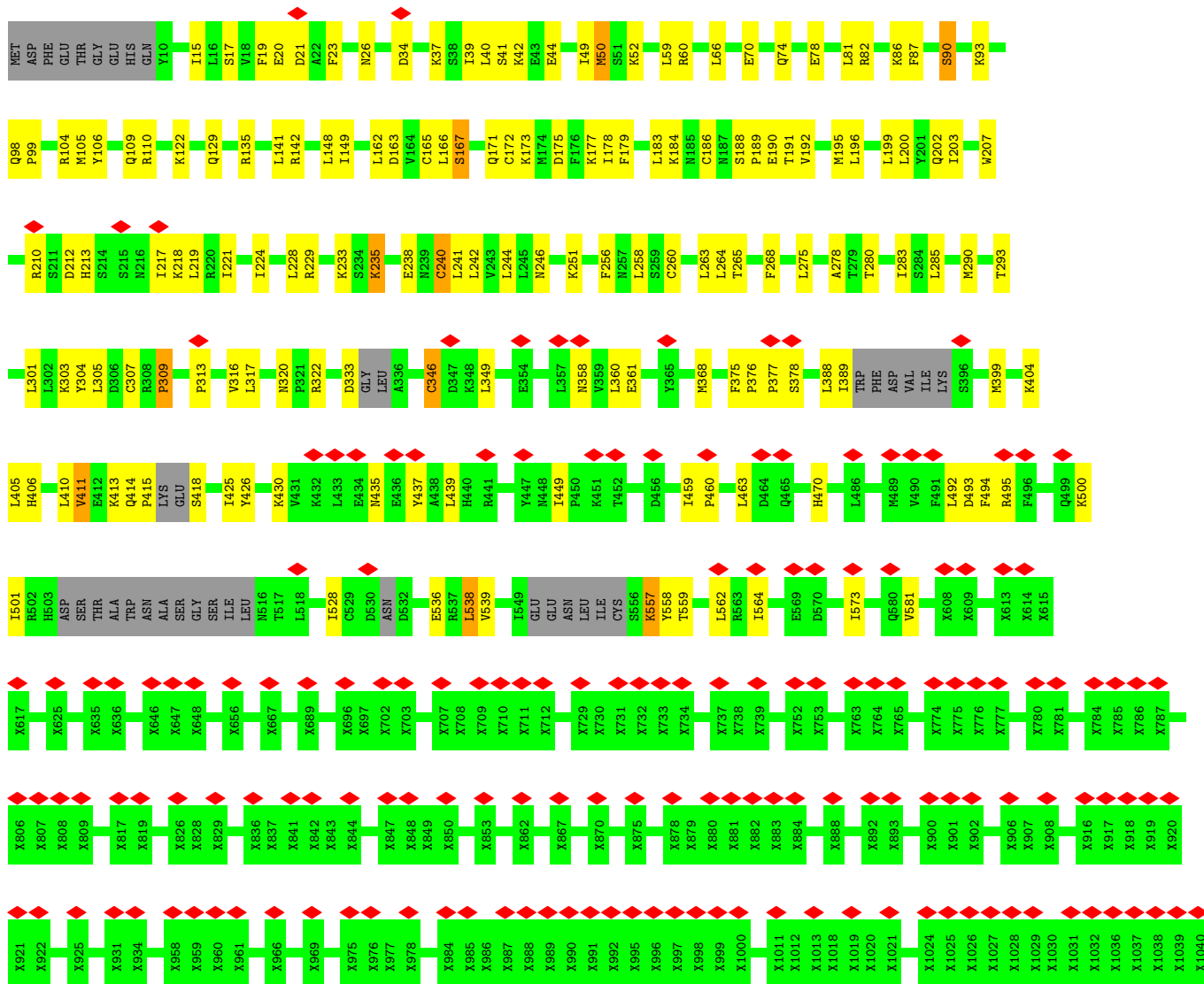
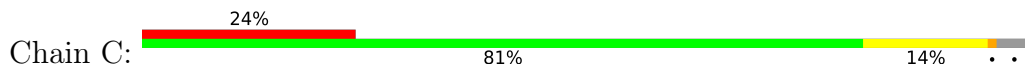
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

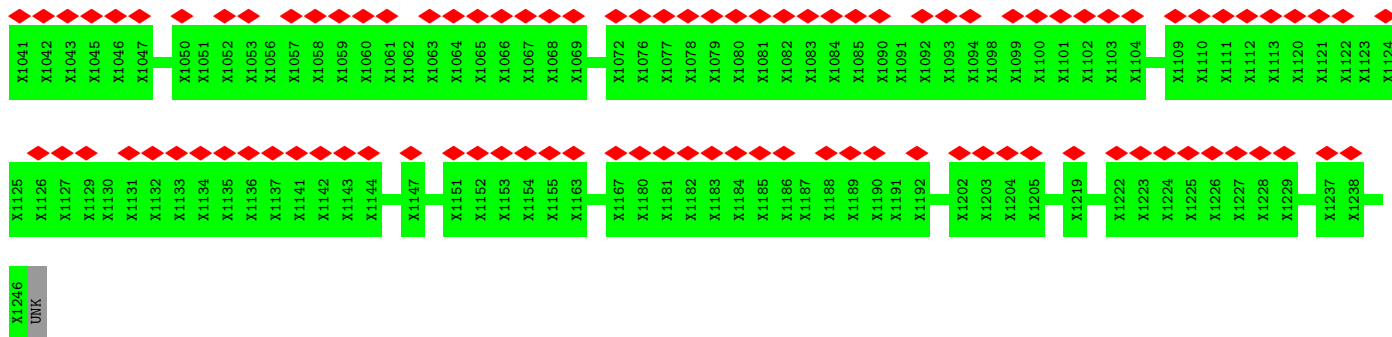
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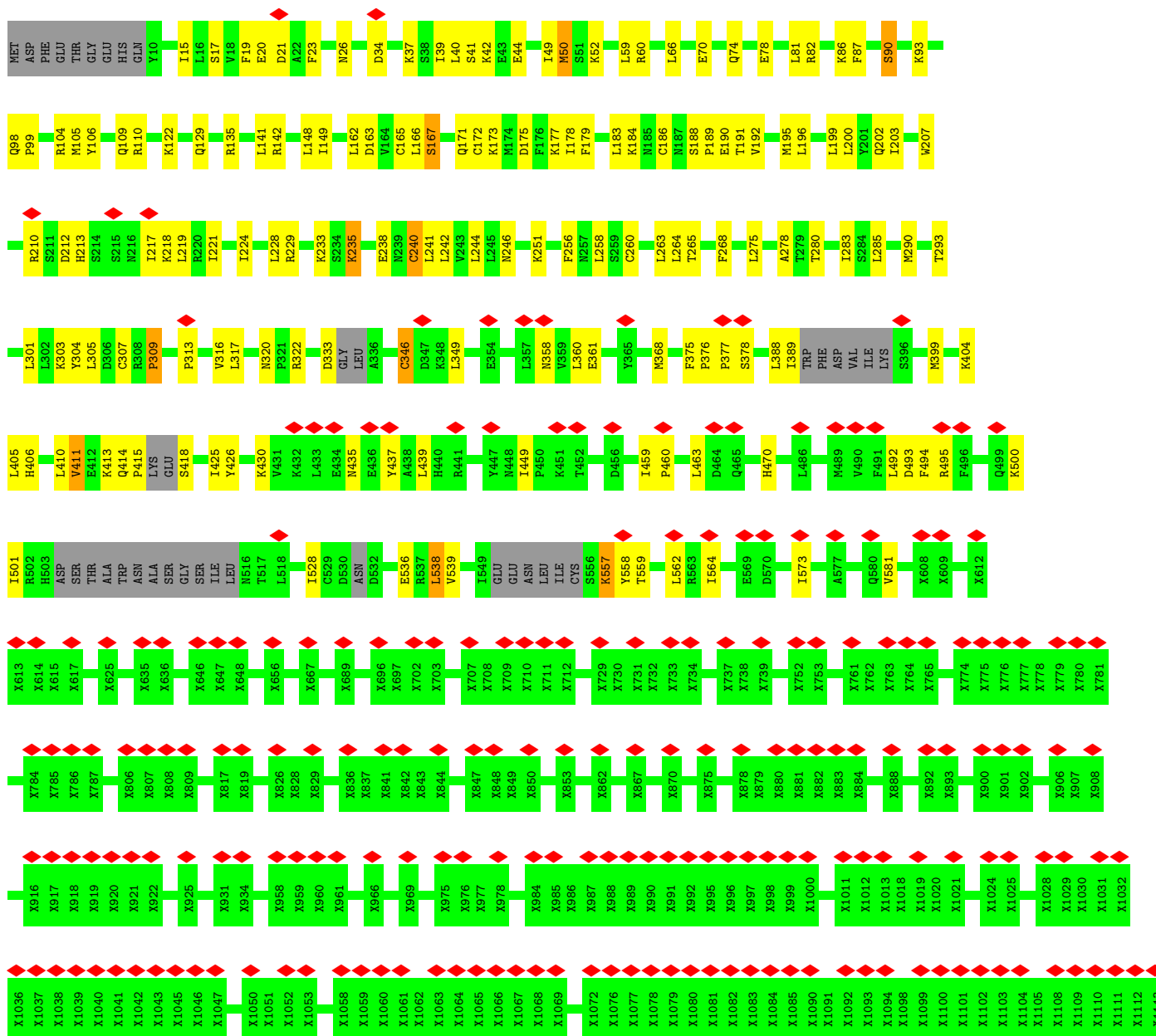
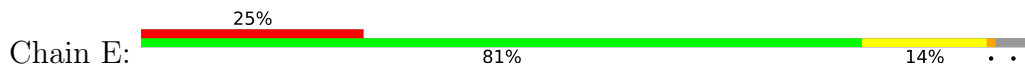


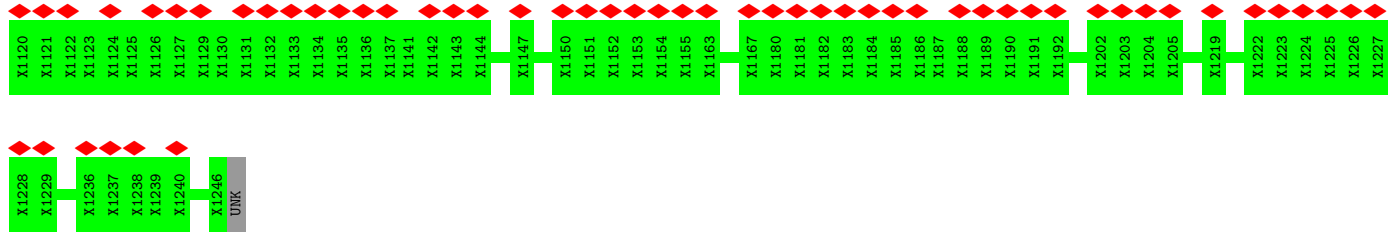
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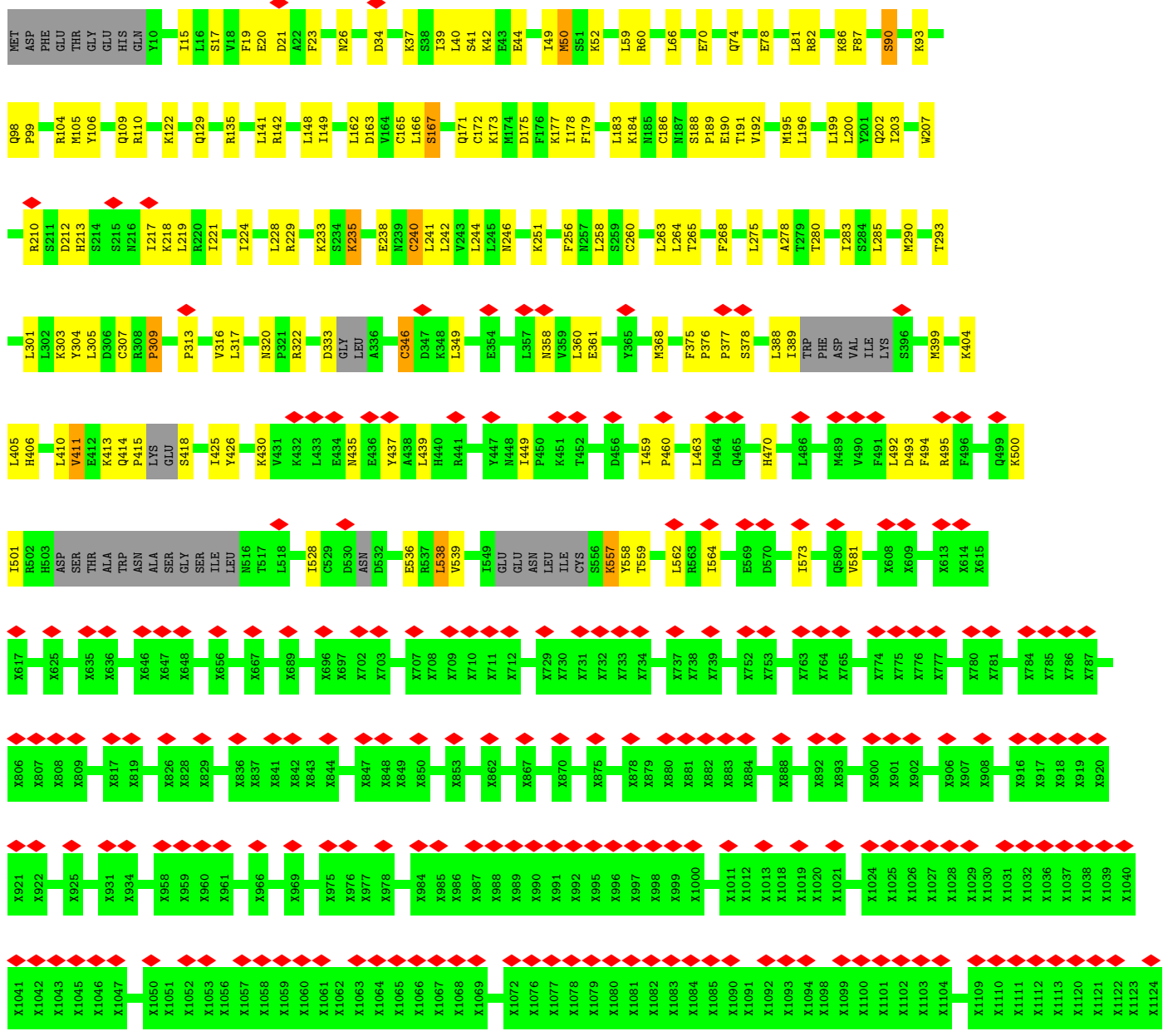
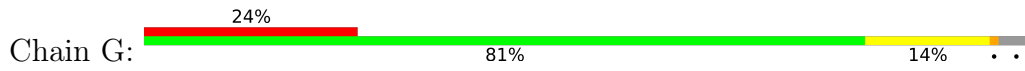


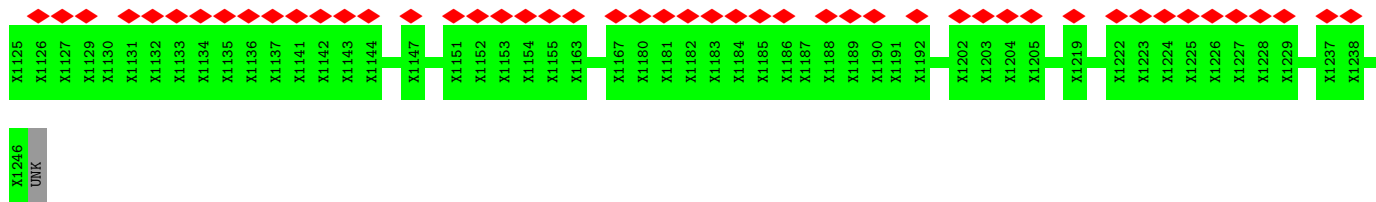
● Molecule 1: Apaf-1 related killer DARK



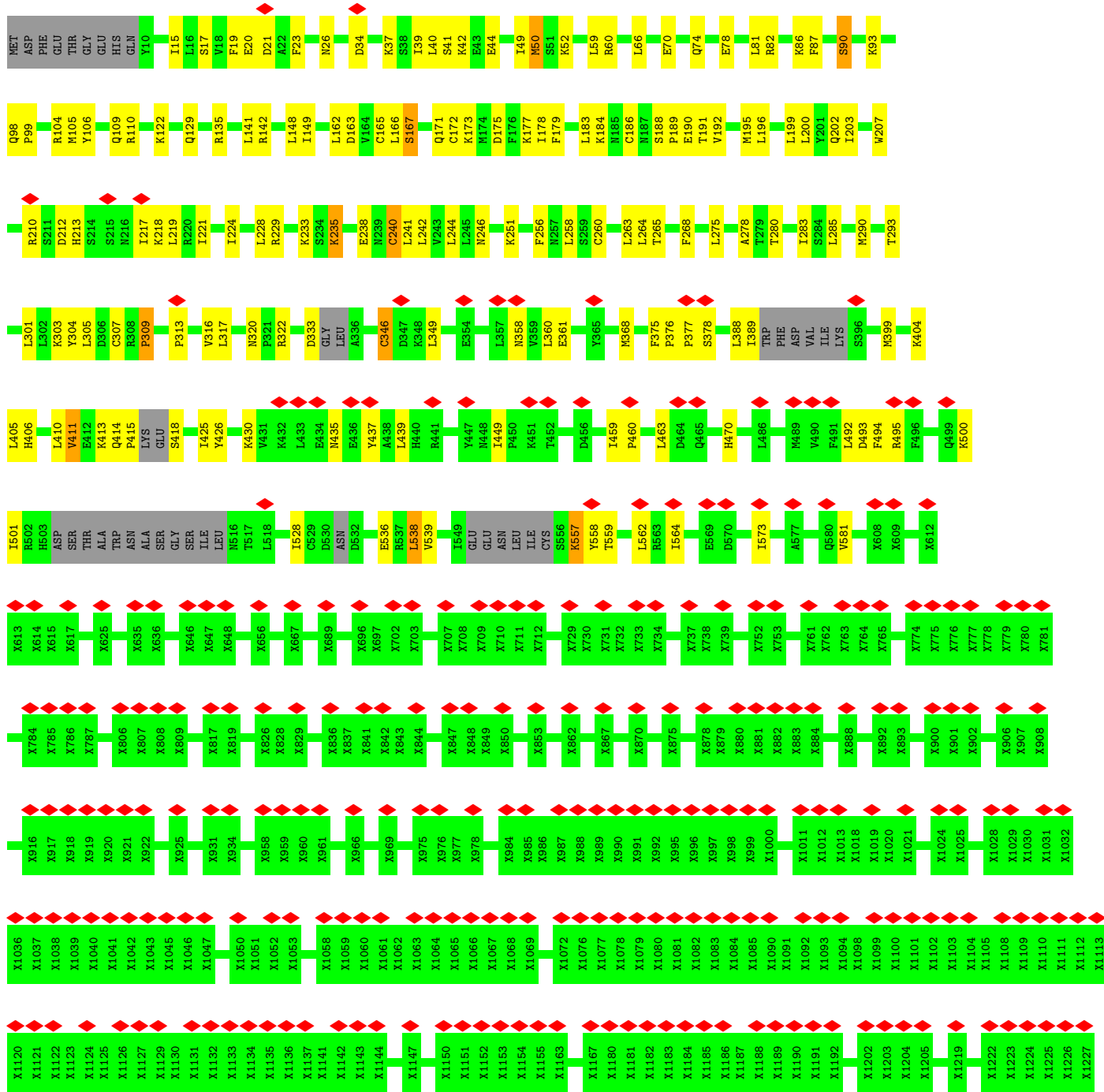
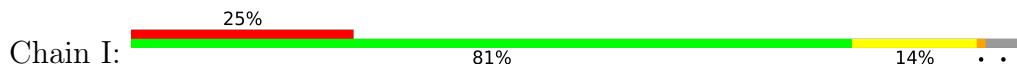


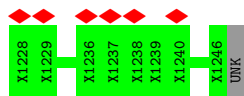
• Molecule 1: Apaf-1 related killer DARK



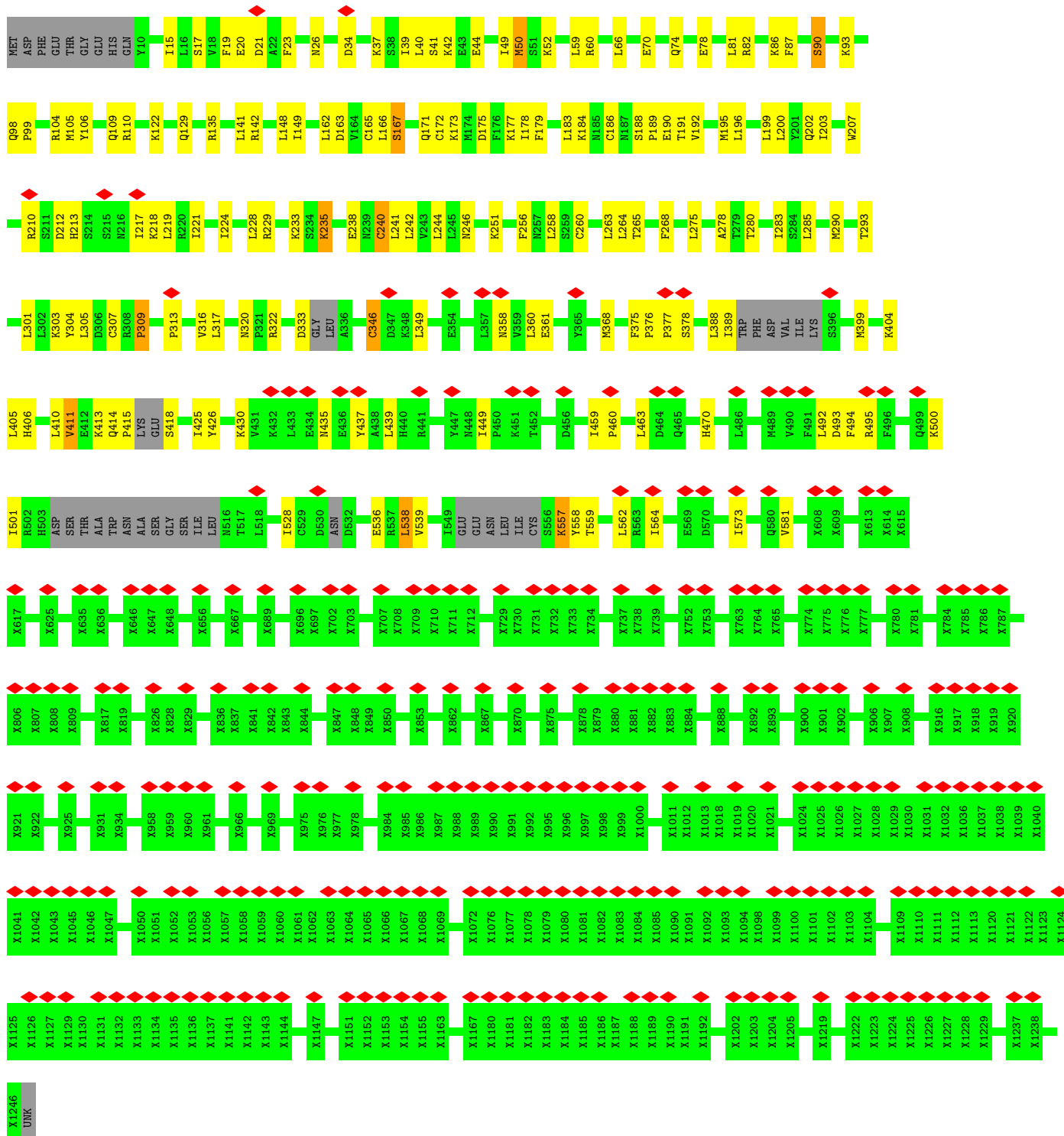
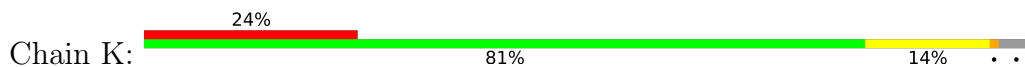


• Molecule 1: Apaf-1 related killer DARK

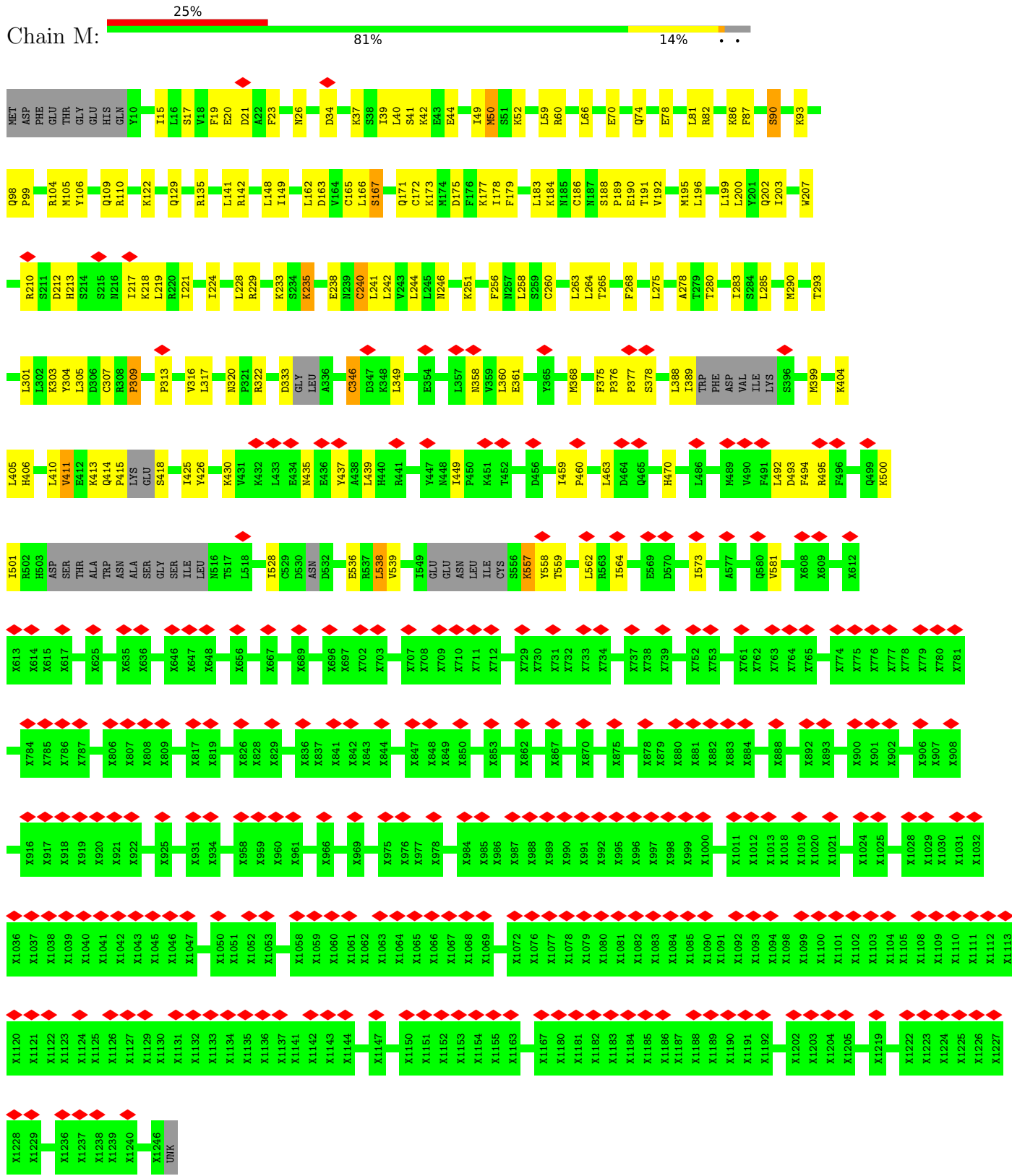




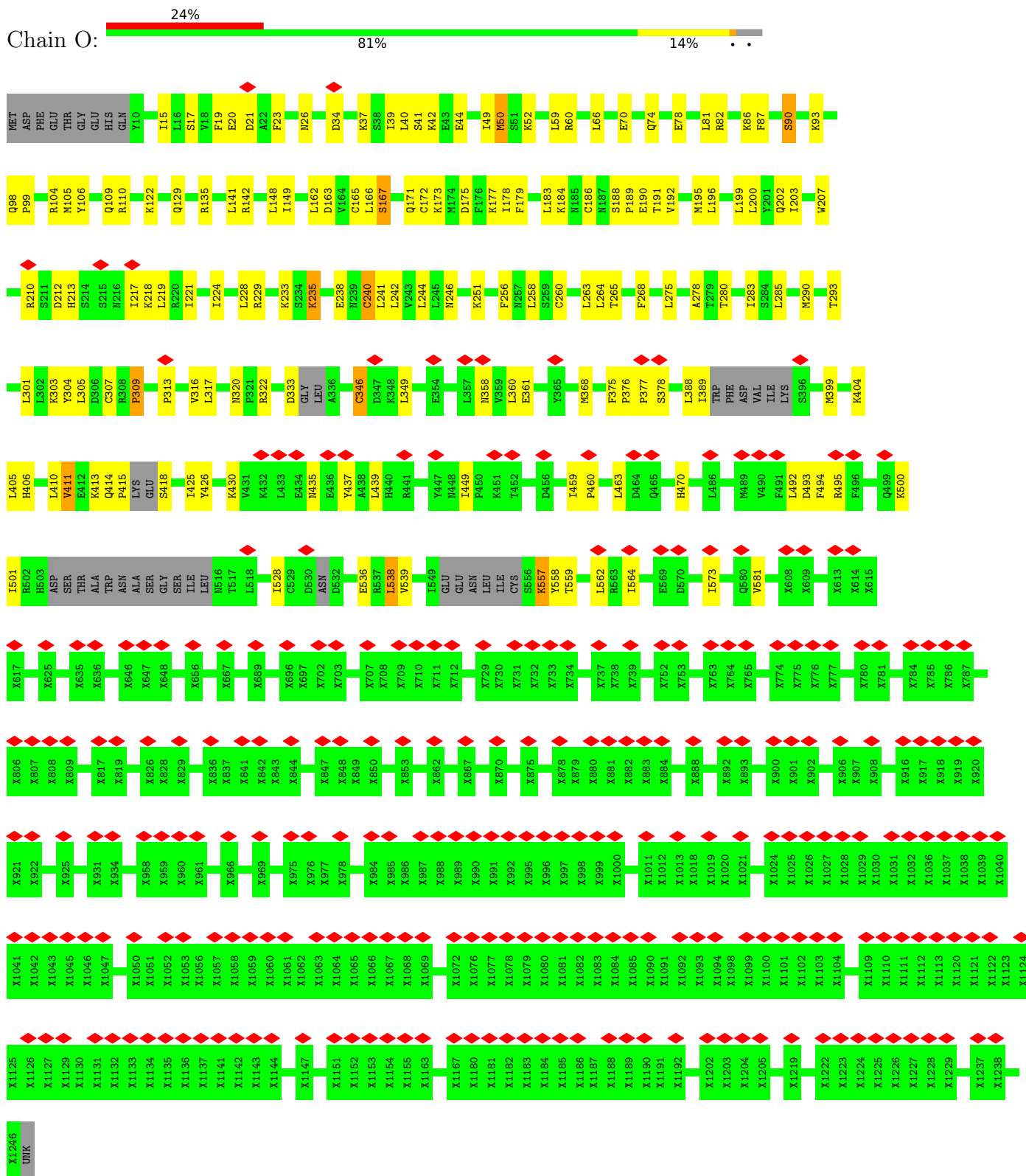
● Molecule 1: Apaf-1 related killer DARK



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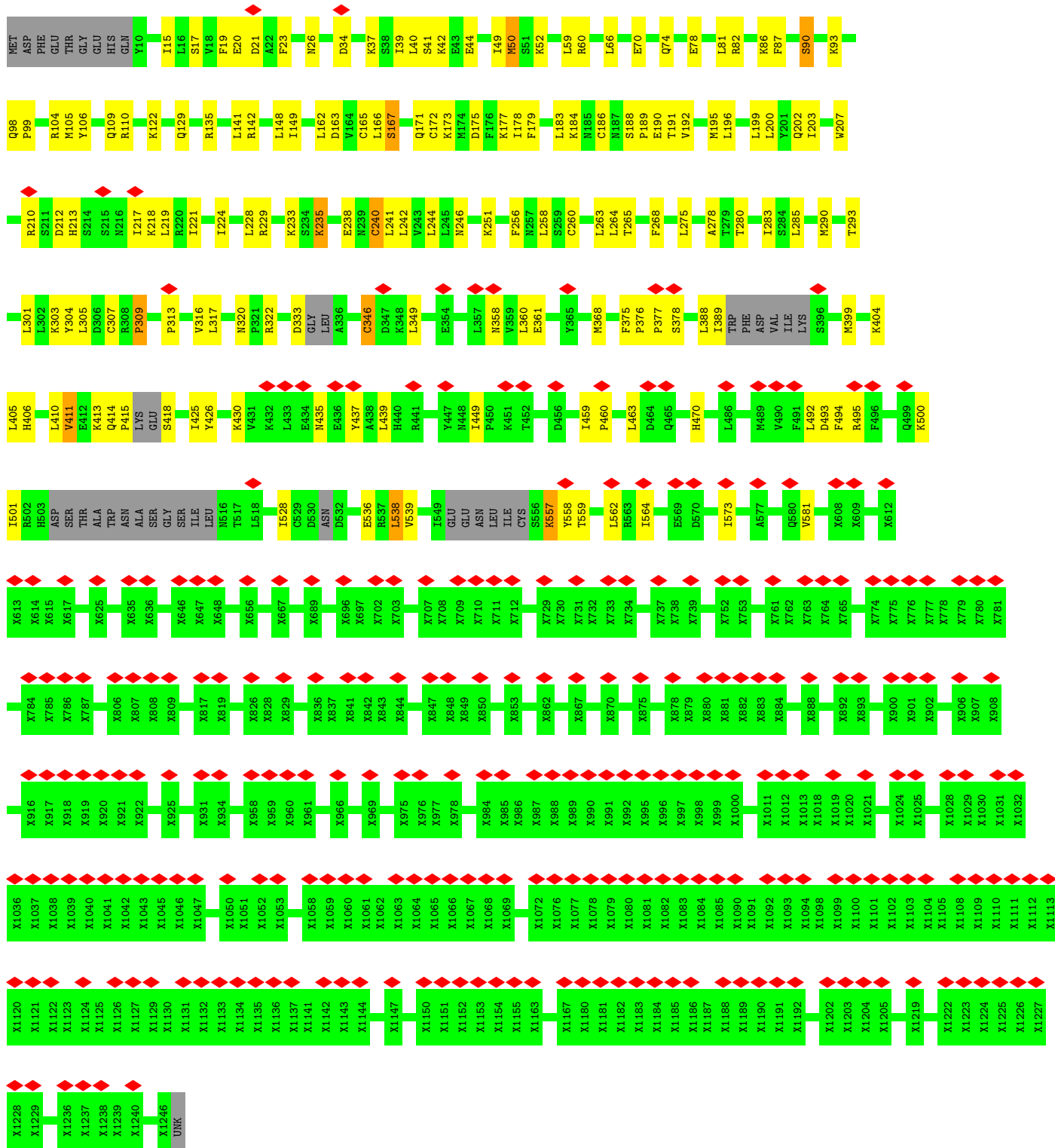


● Molecule 1: Apaf-1 related killer DARK

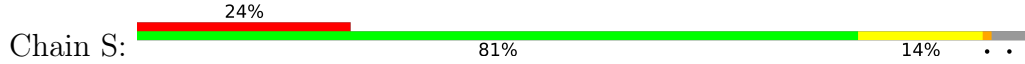


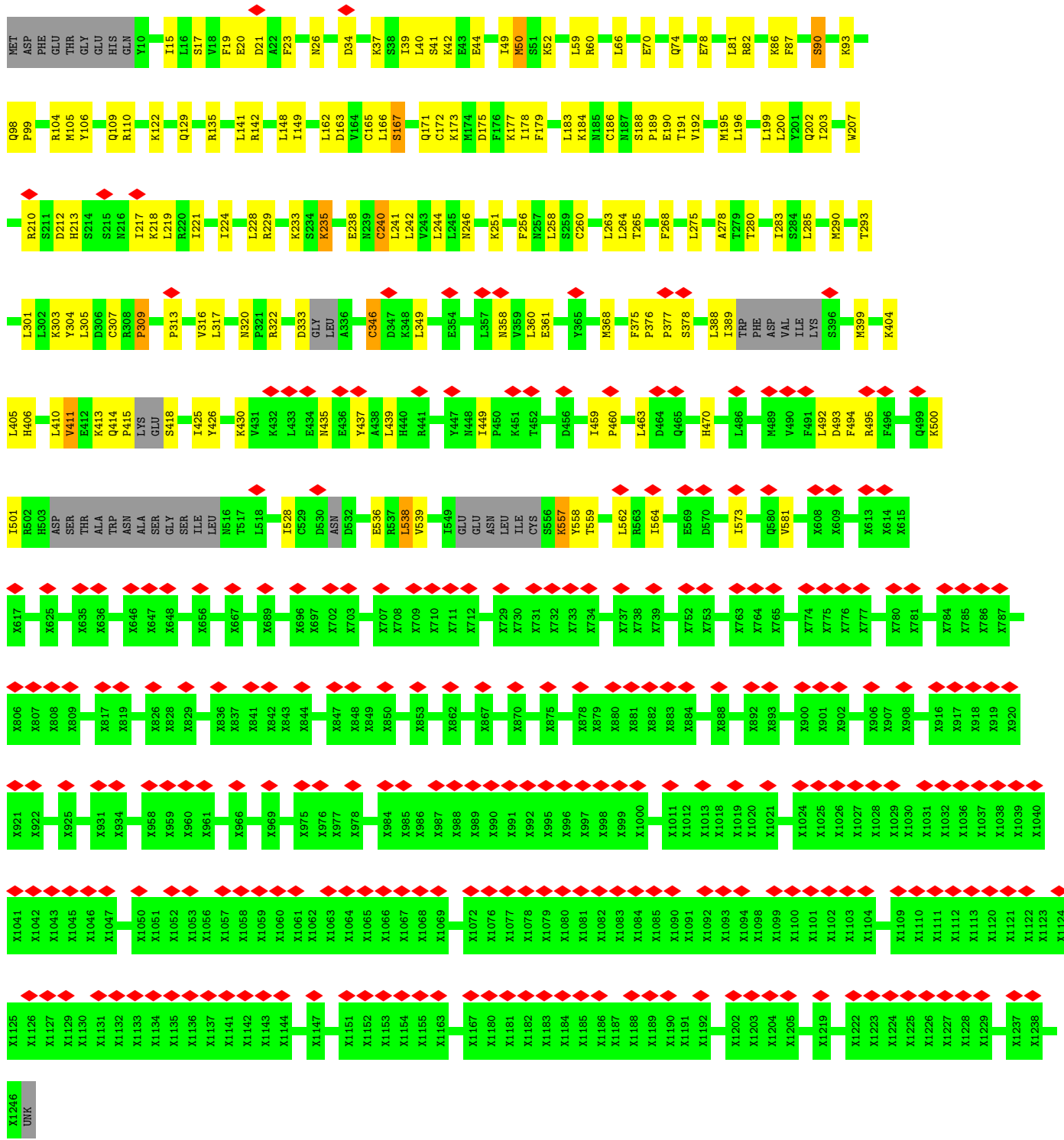
• Molecule 1: Apaf-1 related killer DARK



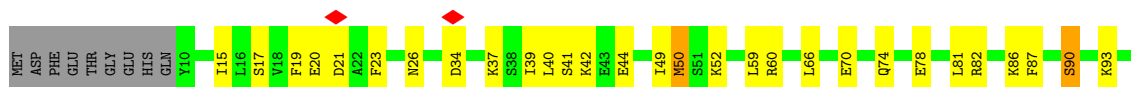
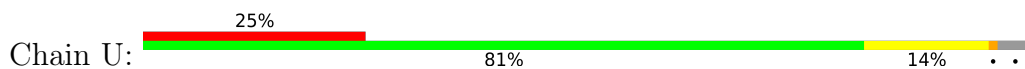


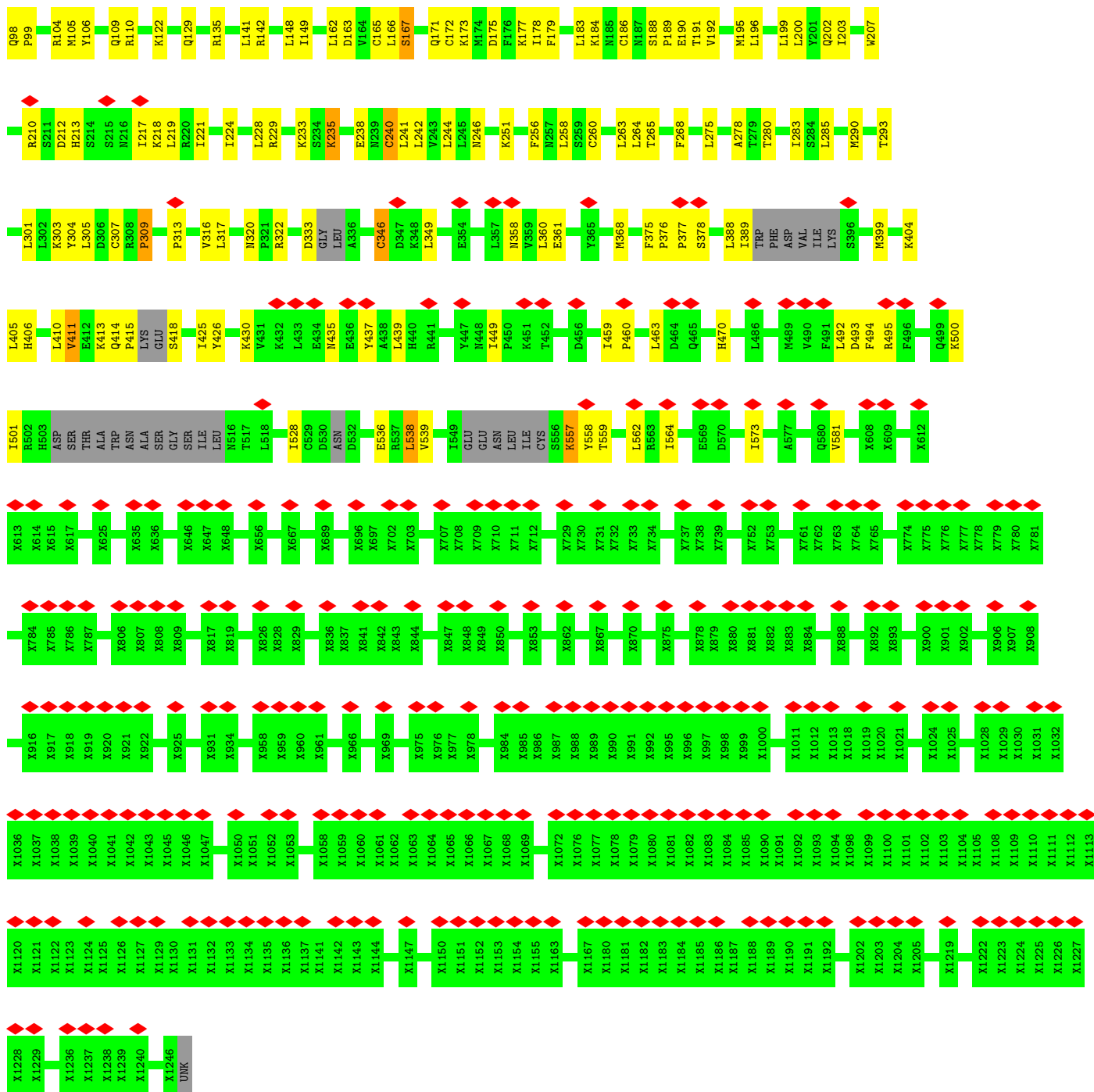
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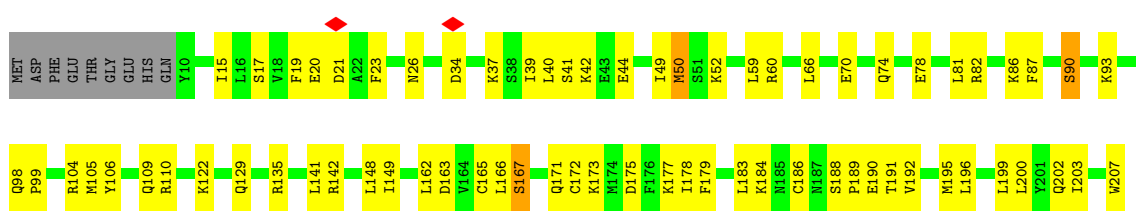
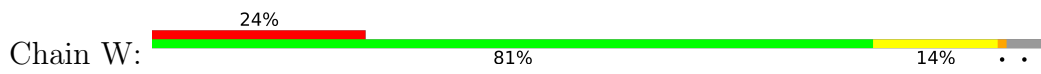


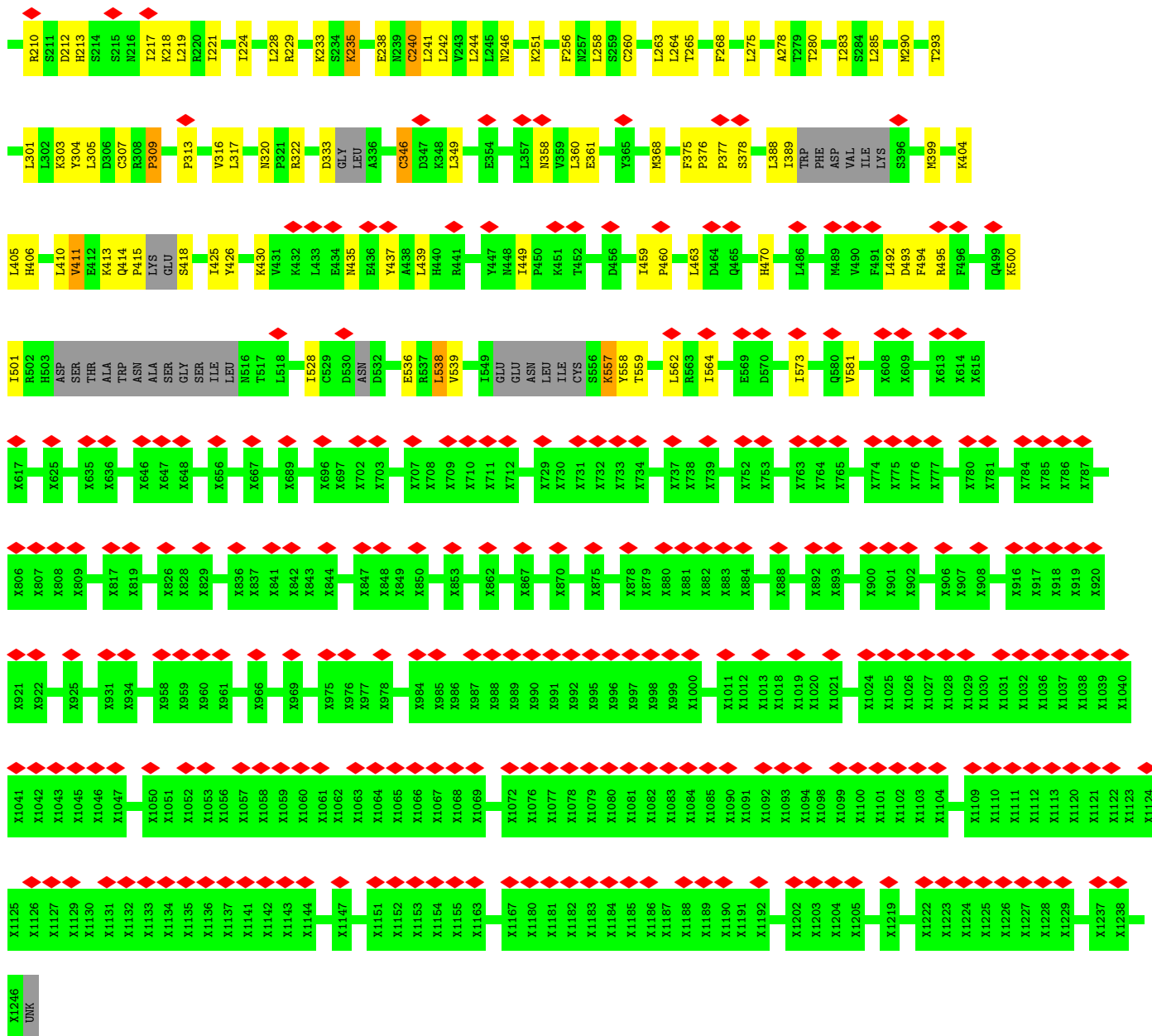
• Molecule 1: Apaf-1 related killer DARK



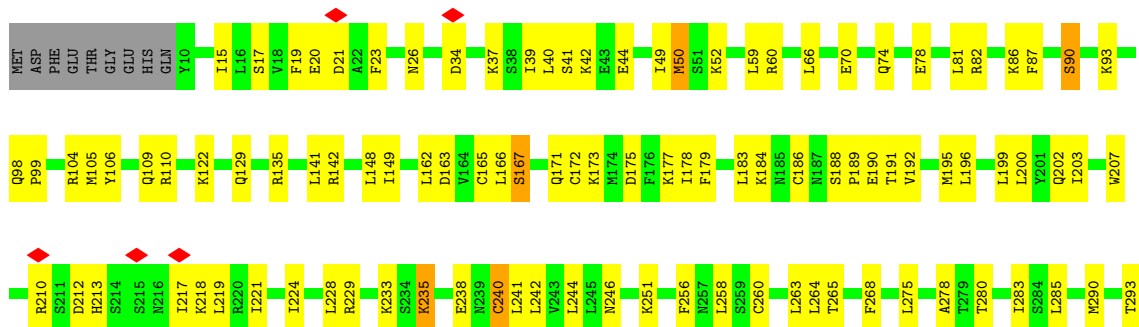
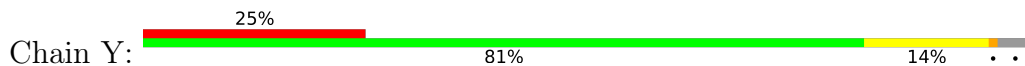


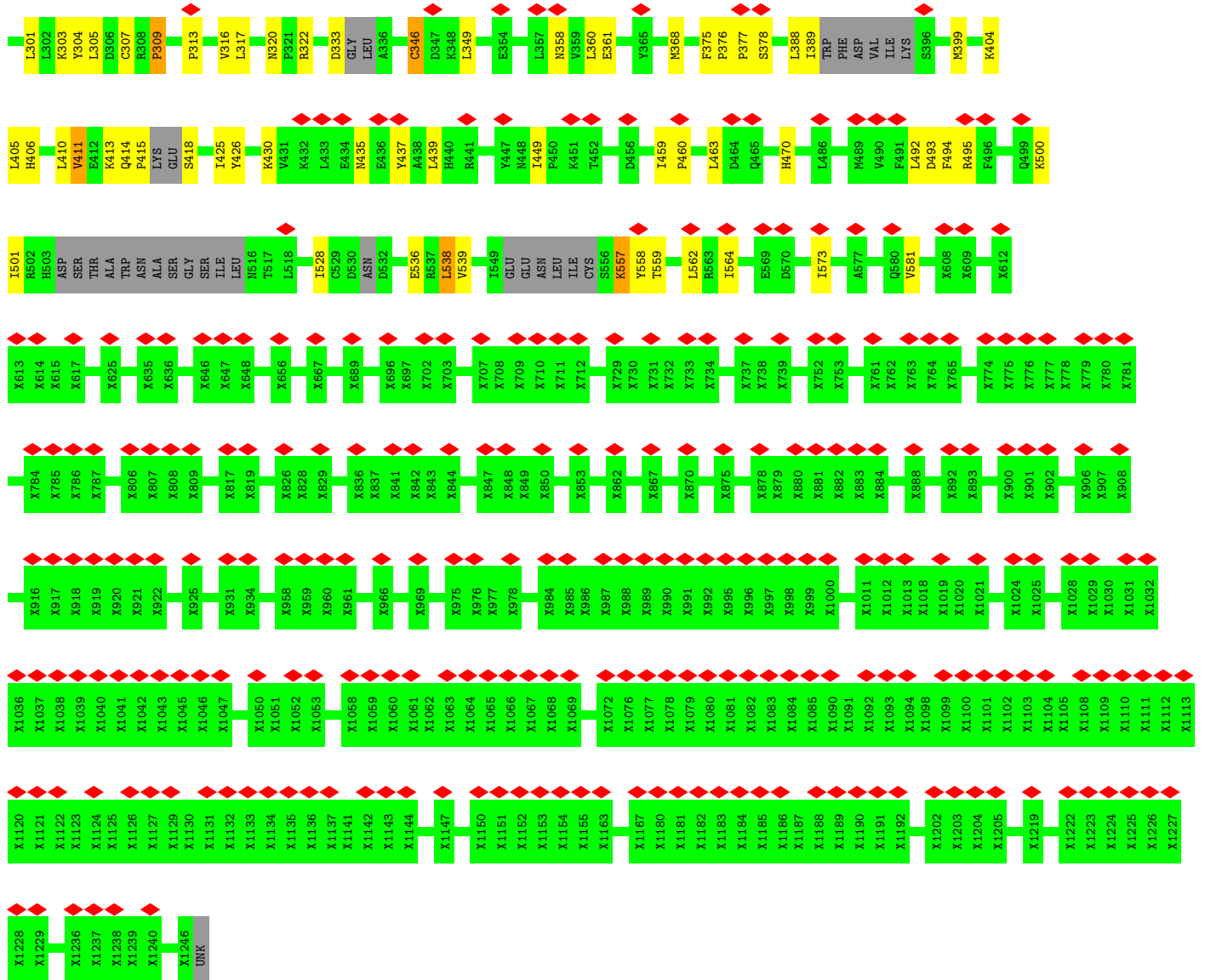
● Molecule 1: Apaf-1 related killer DARK



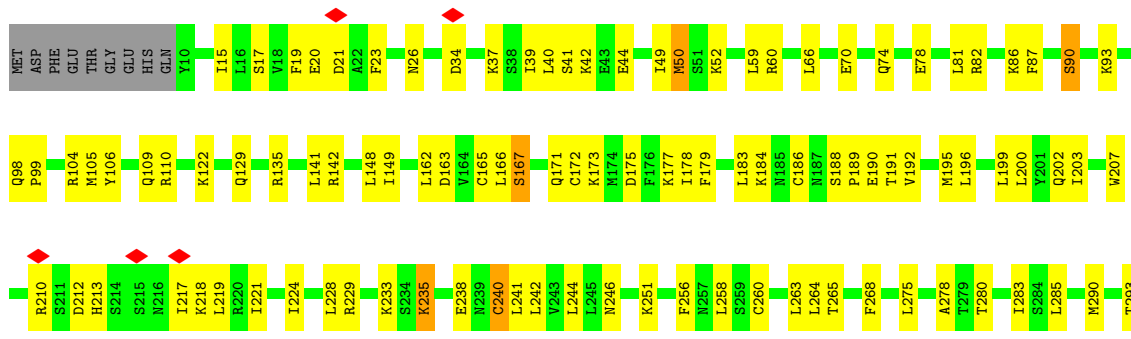
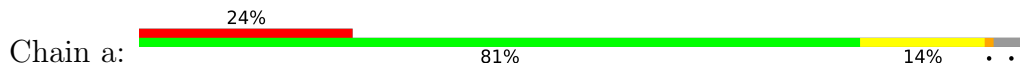


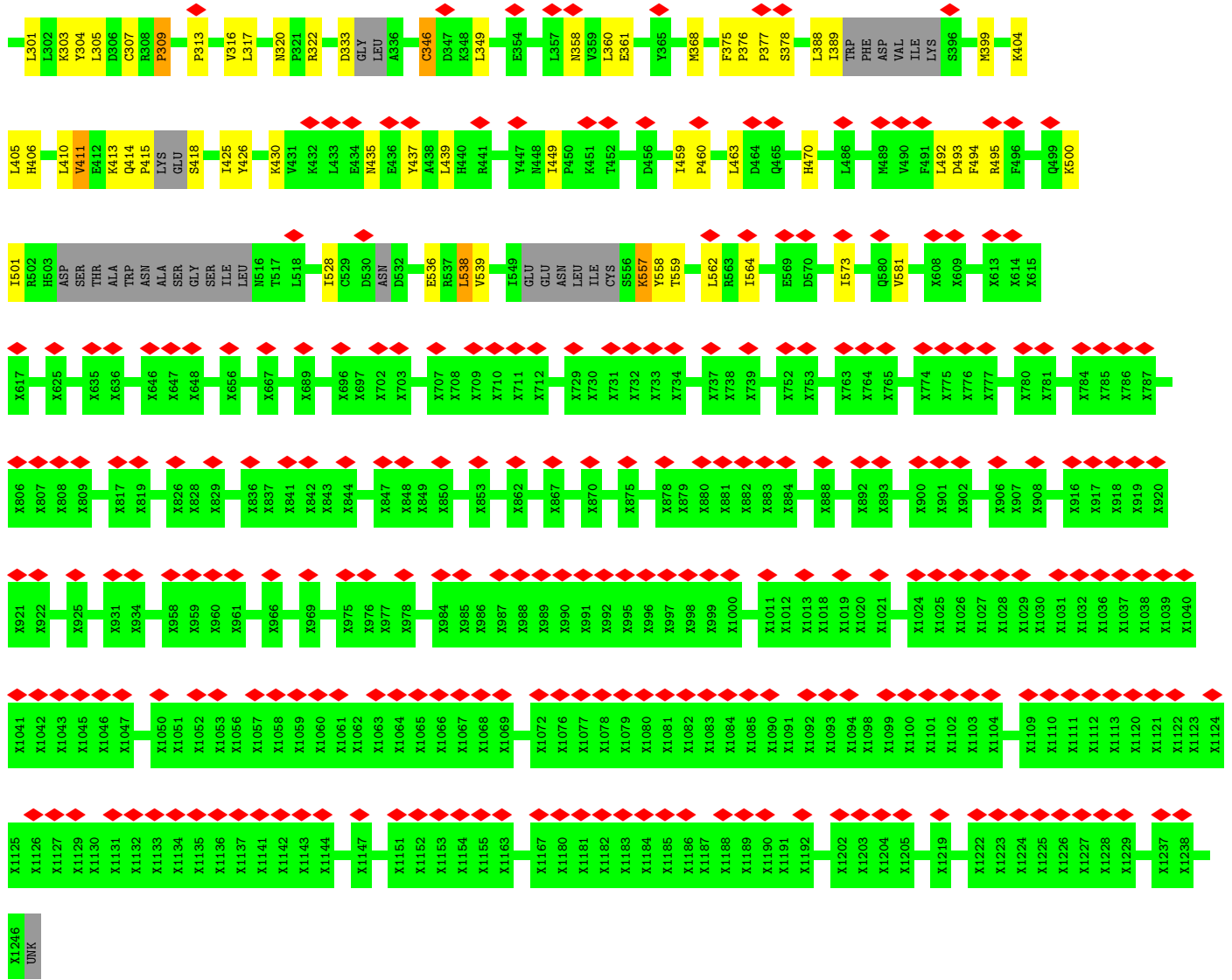
● Molecule 1: Apaf-1 related killer DARK



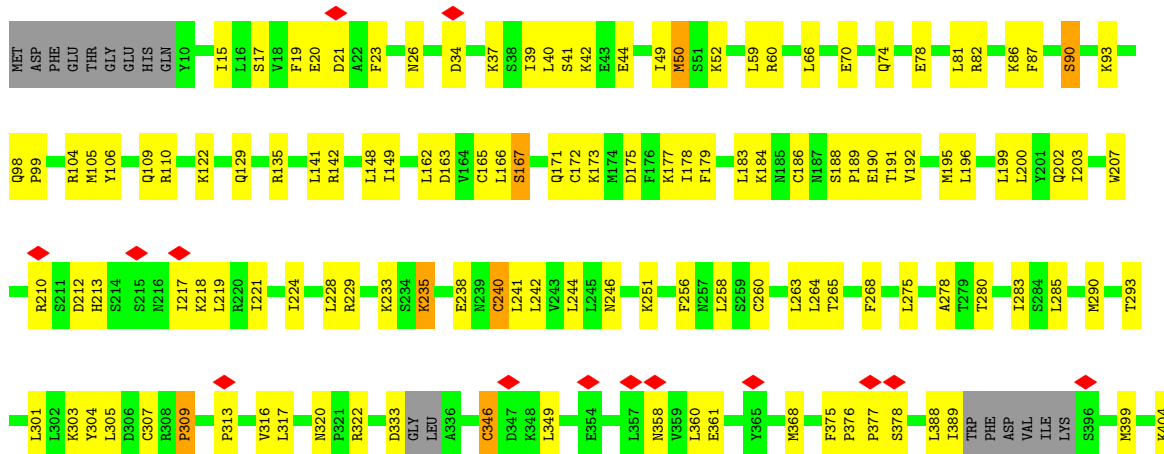
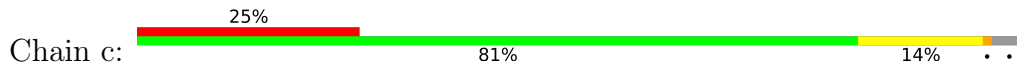


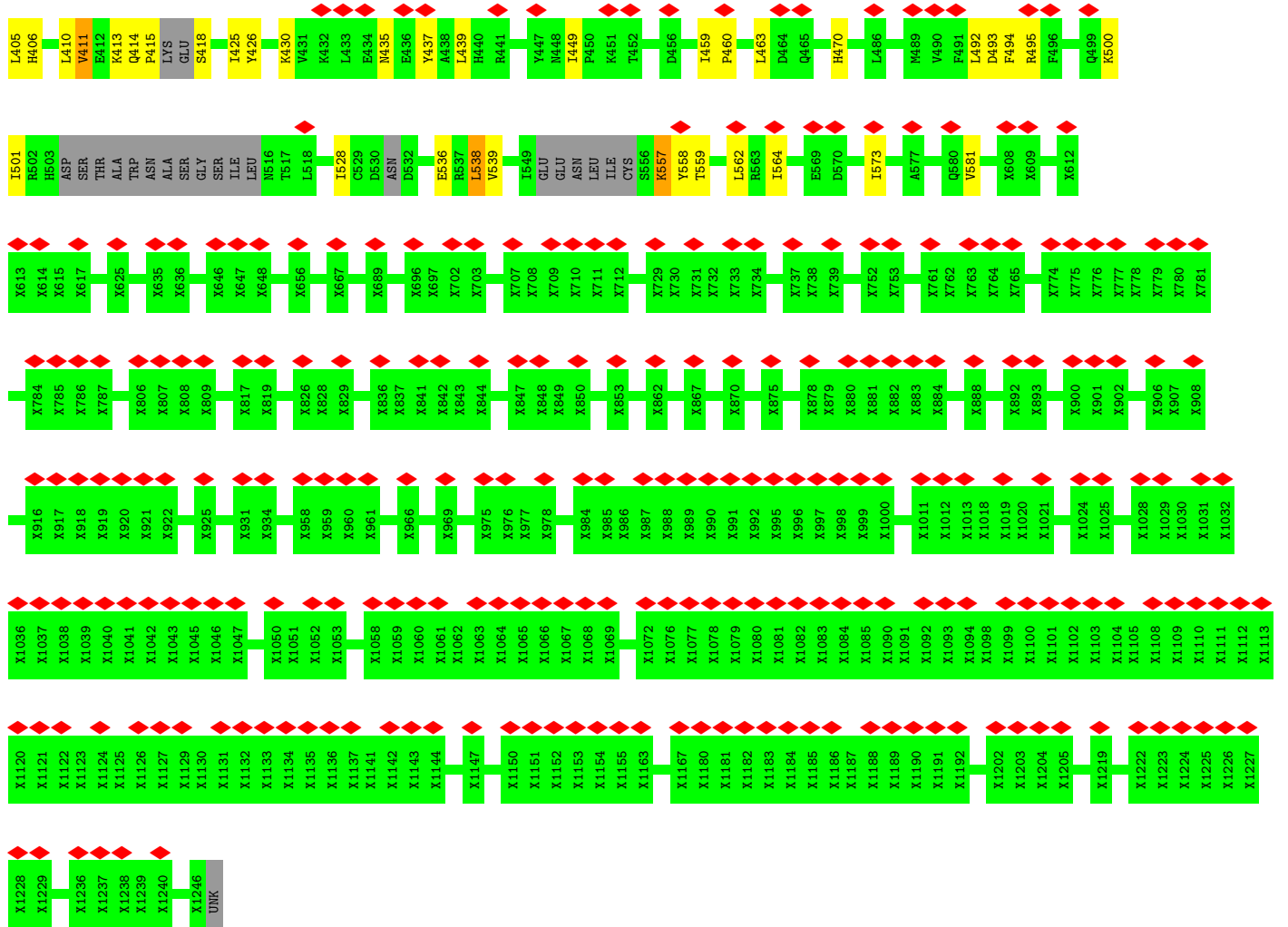
• Molecule 1: Apaf-1 related killer DARK



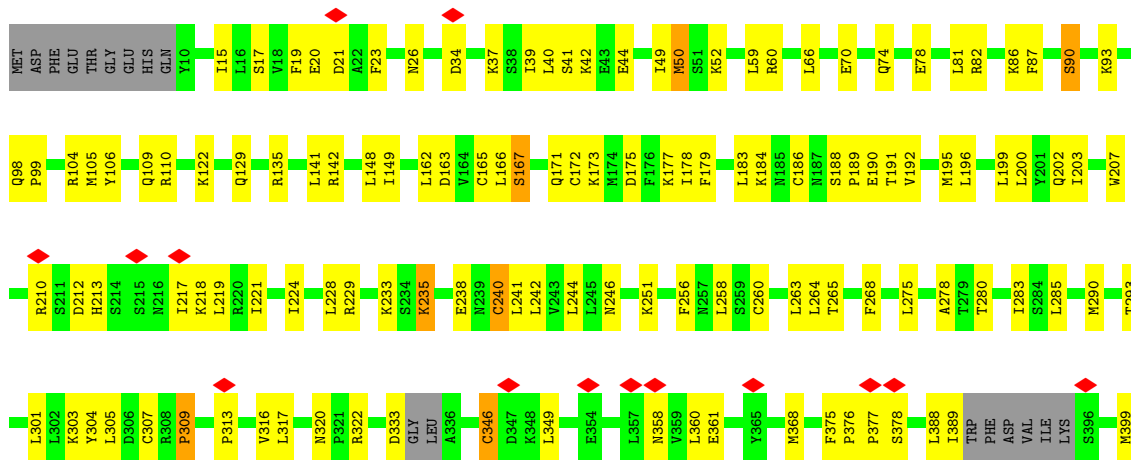
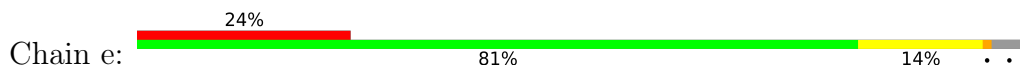


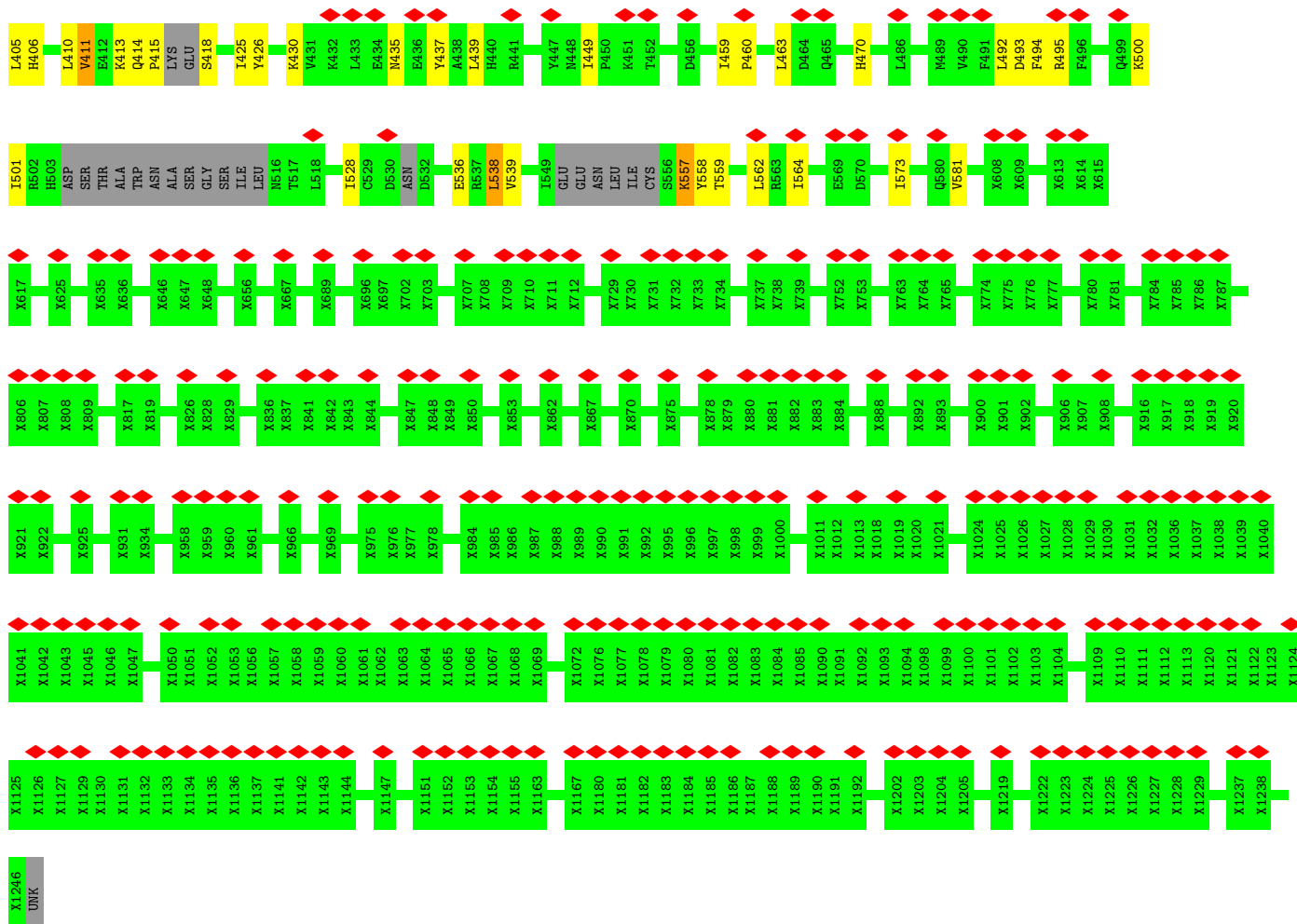
- Molecule 1: Apaf-1 related killer DARK



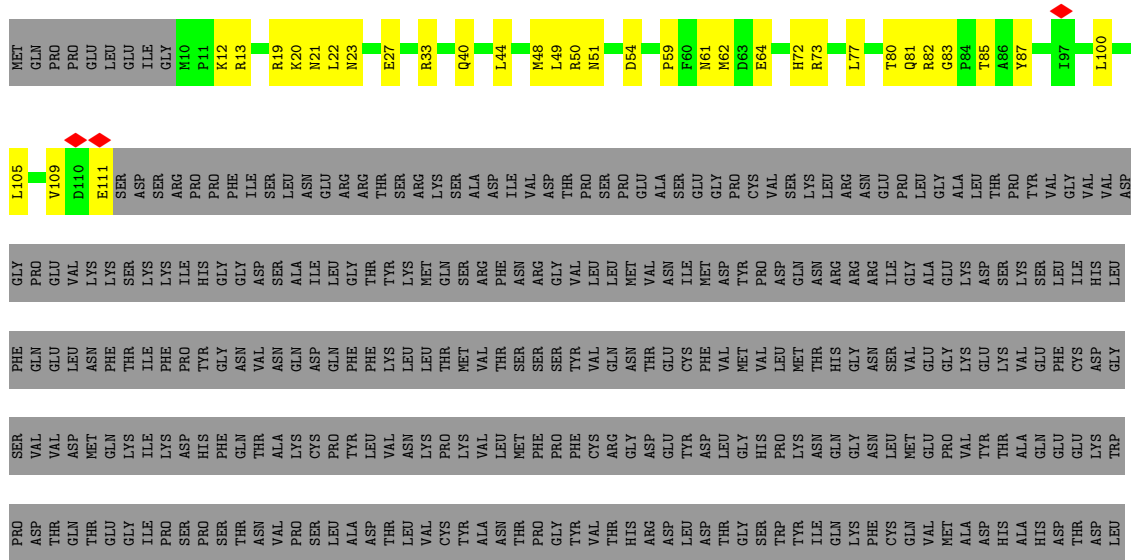


• Molecule 1: Apaf-1 related killer DARK



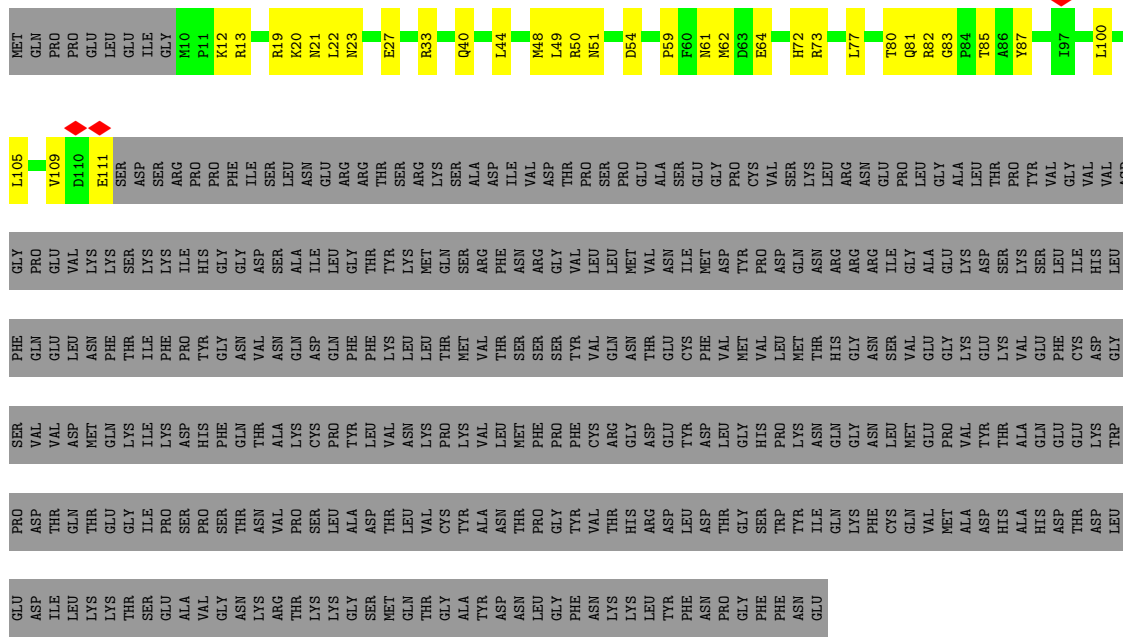


• Molecule 2: Caspase Nc

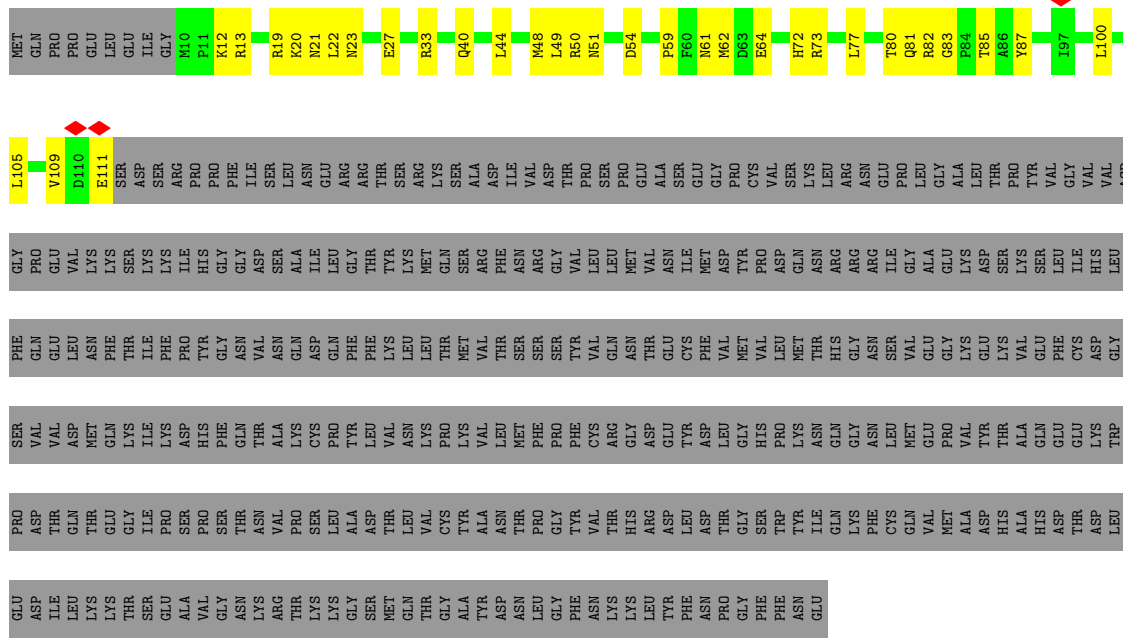


GLU ASP ILE LEU LYS THR SER GLU VAL ALA VAL GLY ASN LYS ARG THR THR LYS LYS ARG GLY MET GLN THR GLY THR LYS ALA TTR ASP ASN LEU GLY PHE ASN LYS LEU LEU LEU TTR PHE ASN PRO GLY PHE ASN GLU

• Molecule 2: Caspase Nc



• Molecule 2: Caspase Nc



• Molecule 2: Caspase Nc



MET	GLN	PRO	PRO	LEU	LEU	GLY	M10	P11	K12	R13	R19	K20	N21	L22	N23	E27	R33	Q40	L44	M48	L49	R50	M51	D54	F60	M61	M62	D63	E64	H72	R73	L77	T80	Q81	R82	G83	P84	T85	Y87	T97	L100										
L105	V109	D110	E111	ASP	ASP	ARG	ARG	PRO	PRO	GLY	LEU	ASN	ASN	GLU	ARG	THR	THR	THR	ALA	ASP	ILE	VAL	THR	THR	PRO	GLU	ALA	GLY	GLY	PRO	CYS	VAL	THR	GLN	LEU	ARG	ASN	GLU	PRO	LEU	LEU	GLY	ALA	LEU	THR	PRO	TYR	VAL	GLY	VAL	ASP
GLY	PRO	GLU	VAL	ASP	LEU	ASN	PHE	THR	ILE	LYS	PHE	PRO	ILE	GLY	HIS	TYR	GLY	GLY	ASP	THR	VAL	ASN	ALA	LEU	ASN	ALA	ILE	GLN	ALA	ILE	LEU	GLY	THR	THR	LEU	LEU	MET	ARG	LYS	THR	THR	LEU	GLN	ALA	GLY	VAL	ASP	LEU			
PHE	GLN	GLU	LEU	ASP	GLN	ASN	PHE	THR	ILE	LYS	PHE	PRO	ILE	GLY	HIS	TYR	GLY	GLY	ASP	THR	VAL	ASN	ALA	LEU	ASN	ALA	ILE	GLN	ALA	ILE	LEU	GLY	THR	THR	LEU	LEU	MET	ARG	LYS	THR	THR	LEU	GLN	ALA	GLY	VAL	ASP	LEU			
SER	VAL	VAL	ASP	THR	GLN	MET	GLM	LYS	THR	ILE	LYS	ASP	ASP	PRO	HIS	PRO	PHE	GLY	THR	THR	VAL	ALA	LEU	ASN	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	TRP		
PRO	ASP	THR	THR	THR	GLY	GLY	THR	GLY	ILE	THR	GLU	ALA	SER	VAL	VAL	VAL	VAL	ASN	THR	THR	VAL	ALA	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU		
GLU	ASP	ILE	LEU	LEU	LYS	THR	THR	SER	THR	SER	GLU	THR	VAL	VAL	ASN	GLY	LYS	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU		

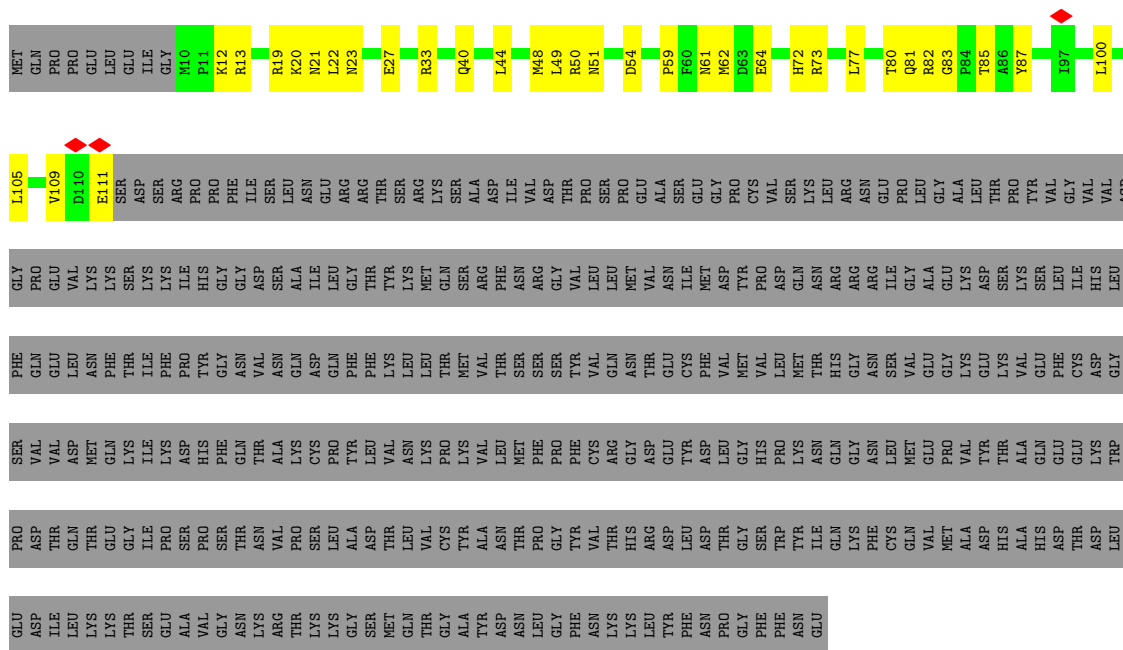
• Molecule 2: Caspase Nc



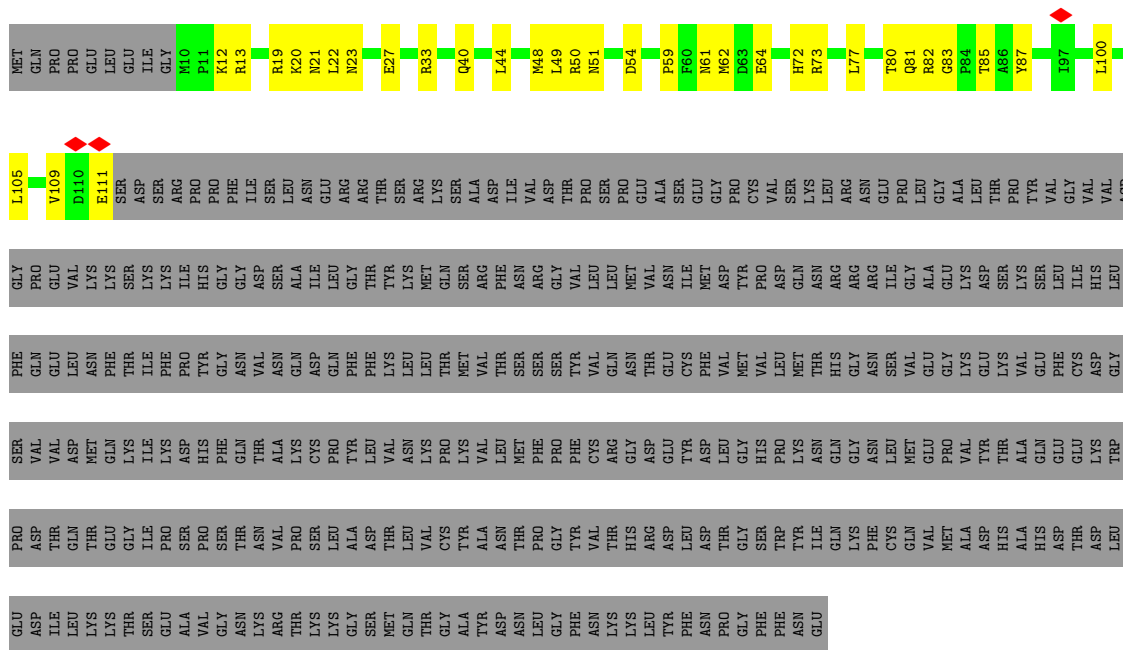
MET	GLN	PRO	PRO	LEU	LEU	GLY	M10	P11	K12	R13	R19	K20	N21	L22	N23	E27	R33	Q40	L44	M48	L49	R50	M51	D54	F60	M61	M62	D63	E64	H72	R73	L77	T80	Q81	R82	G83	P84	T85	Y87	T97	L100										
L105	V109	D110	E111	ASP	ASP	ARG	ARG	PRO	PRO	GLY	LEU	ASN	ASN	GLU	ARG	THR	THR	THR	ALA	ASP	ILE	VAL	THR	THR	PRO	GLU	ALA	GLY	GLY	PRO	CYS	VAL	THR	GLN	LEU	ARG	ASN	GLU	PRO	LEU	LEU	GLY	ALA	LEU	THR	PRO	TYR	VAL	GLY	VAL	ASP
GLY	PRO	GLU	VAL	ASP	LEU	ASN	PHE	THR	ILE	LYS	PHE	PRO	ILE	GLY	HIS	TYR	GLY	GLY	ASP	THR	VAL	ASN	ALA	LEU	ASN	ALA	ILE	GLN	ALA	ILE	LEU	GLY	THR	THR	LEU	LEU	MET	ARG	LYS	THR	THR	LEU	GLN	ALA	GLY	VAL	ASP	LEU			
PHE	GLN	GLU	LEU	ASP	GLN	ASN	PHE	THR	ILE	LYS	PHE	PRO	ILE	GLY	HIS	TYR	GLY	GLY	ASP	THR	VAL	ASN	ALA	LEU	ASN	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	TRP
SER	VAL	VAL	ASP	THR	GLN	MET	GLM	LYS	THR	ILE	LYS	ASP	ASP	PRO	HIS	PRO	PHE	GLY	THR	THR	VAL	ALA	LEU	ASN	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	TRP	
PRO	ASP	THR	THR	THR	GLY	GLY	THR	GLY	ILE	THR	GLU	ALA	SER	VAL	VAL	VAL	VAL	ASN	THR	THR	VAL	ALA	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU	
GLU	ASP	ILE	LEU	LEU	LYS	THR	THR	SER	THR	SER	GLU	THR	VAL	VAL	ASN	GLY	LYS	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU	

• Molecule 2: Caspase Nc





● Molecule 2: Caspase Nc



● Molecule 2: Caspase Nc



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

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

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 (\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 (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	C	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	E	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	G	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	I	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	K	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	M	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	O	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	Q	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	S	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	U	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	W	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	Y	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	a	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	c	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
1	e	0.66	5/4562 (0.1%)	0.96	21/6167 (0.3%)
2	B	0.47	0/850	0.72	1/1146 (0.1%)
2	D	0.47	0/850	0.72	1/1146 (0.1%)
2	F	0.47	0/850	0.72	1/1146 (0.1%)
2	H	0.47	0/850	0.72	1/1146 (0.1%)
2	J	0.47	0/850	0.72	1/1146 (0.1%)
2	L	0.47	0/850	0.72	1/1146 (0.1%)
2	N	0.47	0/850	0.72	1/1146 (0.1%)
2	P	0.47	0/850	0.72	1/1146 (0.1%)
2	R	0.47	0/850	0.72	1/1146 (0.1%)
2	T	0.47	0/850	0.72	1/1146 (0.1%)
2	V	0.47	0/850	0.72	1/1146 (0.1%)
2	X	0.47	0/850	0.72	1/1146 (0.1%)
2	Z	0.47	0/850	0.72	1/1146 (0.1%)
2	b	0.47	0/850	0.72	1/1146 (0.1%)
2	d	0.47	0/850	0.72	1/1146 (0.1%)
2	f	0.47	0/850	0.72	1/1146 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.63	80/86592 (0.1%)	0.93	352/117008 (0.3%)

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 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	PRO	N-CD	5.32	1.55	1.47
1	E	189	PRO	N-CD	5.32	1.55	1.47
1	I	189	PRO	N-CD	5.32	1.55	1.47
1	M	189	PRO	N-CD	5.32	1.55	1.47
1	Q	189	PRO	N-CD	5.32	1.55	1.47

The worst 5 of 352 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	CYS	CA-CB-SG	-9.44	97.02	114.00
1	E	240	CYS	CA-CB-SG	-9.44	97.02	114.00
1	I	240	CYS	CA-CB-SG	-9.44	97.02	114.00
1	M	240	CYS	CA-CB-SG	-9.44	97.02	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	240	CYS	CA-CB-SG	-9.44	97.02	114.00

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	C	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	E	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	G	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	I	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	K	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	M	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	O	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	Q	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	U	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	W	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	Y	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	a	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	c	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
1	e	531/1102 (48%)	466 (88%)	60 (11%)	5 (1%)	17	54
2	B	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	D	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	F	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	H	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	J	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	L	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	N	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	P	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	R	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	T	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	V	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	X	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	Z	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	b	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	d	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
2	f	100/450 (22%)	78 (78%)	21 (21%)	1 (1%)	15	52
All	All	10096/24832 (41%)	8704 (86%)	1296 (13%)	96 (1%)	20	52

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	C	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	E	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	G	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	I	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	K	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	M	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	O	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	Q	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	S	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	U	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	W	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	Y	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	a	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	c	501/551 (91%)	361 (72%)	140 (28%)	0	3
1	e	501/551 (91%)	361 (72%)	140 (28%)	0	3
2	B	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	D	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	F	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	H	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	J	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	L	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	N	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	P	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	R	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	T	94/404 (23%)	63 (67%)	31 (33%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	X	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	Z	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	b	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	d	94/404 (23%)	63 (67%)	31 (33%)	0	2
2	f	94/404 (23%)	63 (67%)	31 (33%)	0	2
All	All	9520/15280 (62%)	6784 (71%)	2736 (29%)	2	2

5 of 2736 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	19	ARG
1	a	224	ILE
1	W	90	SER
2	V	12	LYS
1	Y	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	222	HIS
2	b	51	ASN
1	W	403	ASN
1	Y	435	ASN
1	c	320	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 monosaccharides in this entry.

5.6 Ligand geometry

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	A	2000	-	24,29,29	0.89	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	G	2000	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	E	2000	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	W	2000	-	24,29,29	0.89	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	K	2000	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	C	2000	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	Y	2000	-	24,29,29	0.89	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	U	2000	-	24,29,29	0.89	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	c	2000	-	24,29,29	0.89	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	Q	2000	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	S	2000	-	24,29,29	0.89	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	O	2000	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	e	2000	-	24,29,29	0.89	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	I	2000	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	M	2000	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	5 (17%)
3	ADP	a	2000	-	24,29,29	0.89	1 (4%)	29,45,45	1.49	5 (17%)

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	A	2000	-	-	2/12/32/32	0/3/3/3
3	ADP	G	2000	-	-	3/12/32/32	0/3/3/3
3	ADP	E	2000	-	-	3/12/32/32	0/3/3/3
3	ADP	W	2000	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	K	2000	-	-	3/12/32/32	0/3/3/3
3	ADP	C	2000	-	-	3/12/32/32	0/3/3/3
3	ADP	Y	2000	-	-	2/12/32/32	0/3/3/3
3	ADP	U	2000	-	-	2/12/32/32	0/3/3/3
3	ADP	c	2000	-	-	2/12/32/32	0/3/3/3
3	ADP	Q	2000	-	-	3/12/32/32	0/3/3/3
3	ADP	S	2000	-	-	2/12/32/32	0/3/3/3
3	ADP	O	2000	-	-	3/12/32/32	0/3/3/3
3	ADP	e	2000	-	-	2/12/32/32	0/3/3/3
3	ADP	I	2000	-	-	3/12/32/32	0/3/3/3
3	ADP	M	2000	-	-	3/12/32/32	0/3/3/3
3	ADP	a	2000	-	-	2/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2000	ADP	C5-C4	2.37	1.47	1.40
3	G	2000	ADP	C5-C4	2.37	1.47	1.40
3	K	2000	ADP	C5-C4	2.37	1.47	1.40
3	O	2000	ADP	C5-C4	2.37	1.47	1.40
3	S	2000	ADP	C5-C4	2.37	1.47	1.40

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2000	ADP	C3'-C2'-C1'	4.07	107.11	100.98
3	G	2000	ADP	C3'-C2'-C1'	4.07	107.11	100.98
3	K	2000	ADP	C3'-C2'-C1'	4.07	107.11	100.98
3	O	2000	ADP	C3'-C2'-C1'	4.07	107.11	100.98
3	S	2000	ADP	C3'-C2'-C1'	4.07	107.11	100.98

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	A	2000	ADP	C3'-C4'-C5'-O5'
3	C	2000	ADP	O4'-C4'-C5'-O5'
3	C	2000	ADP	C3'-C4'-C5'-O5'

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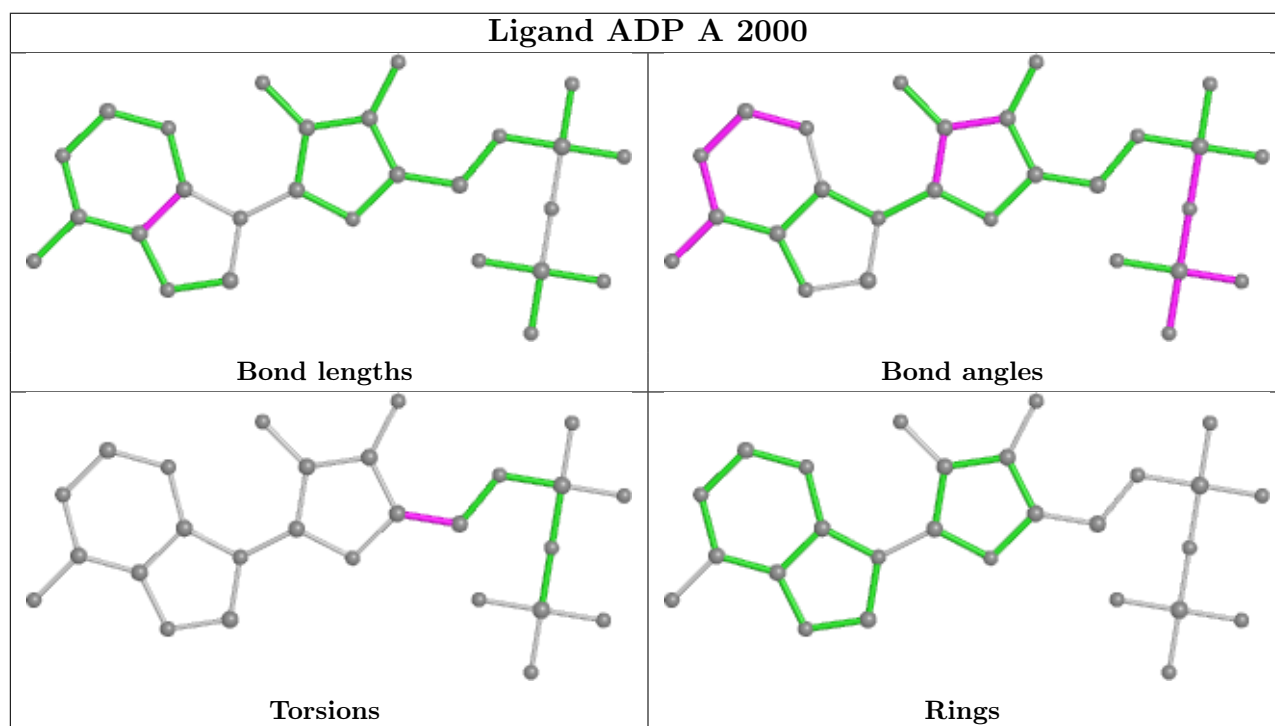
Continued from previous page...

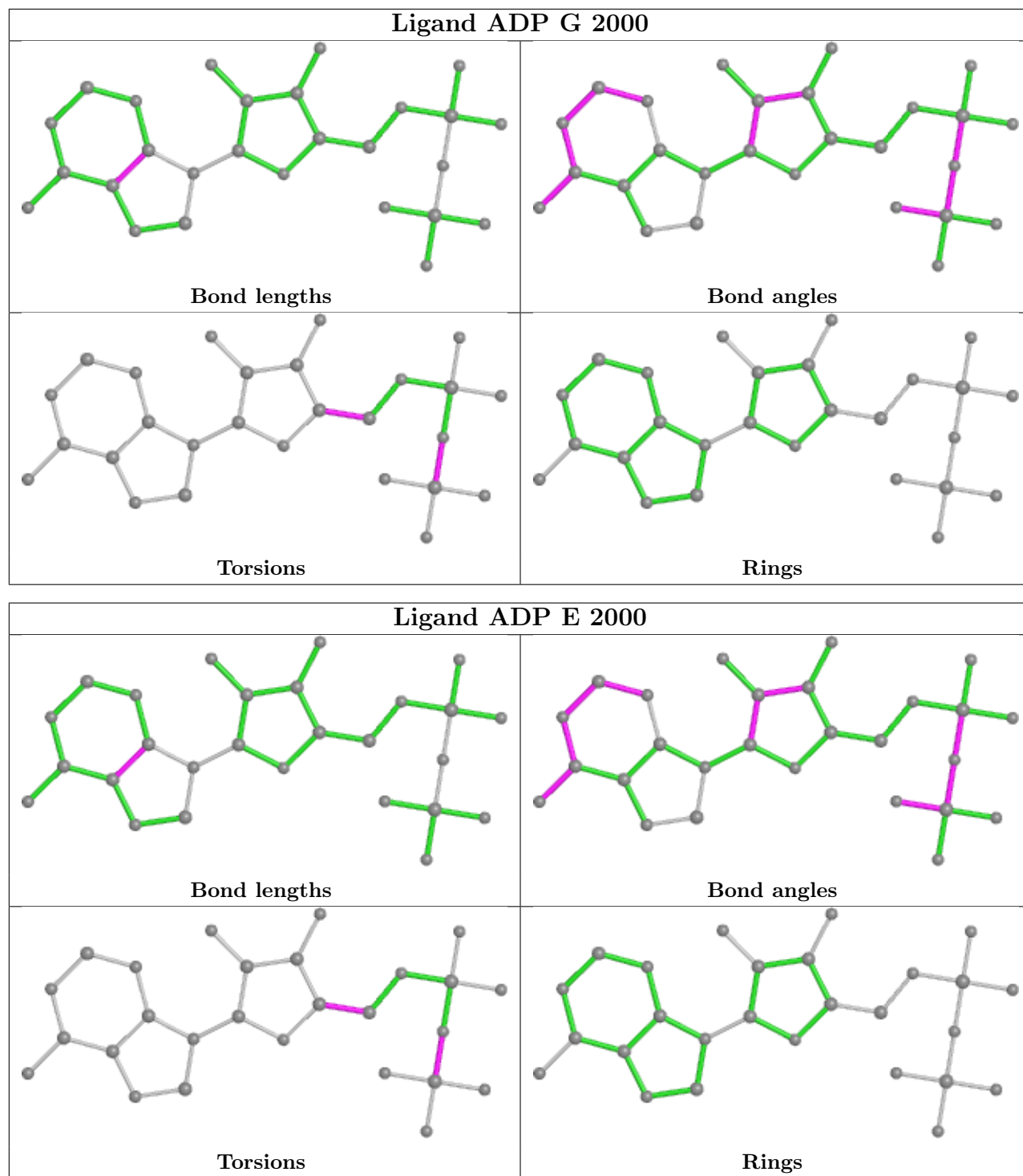
Mol	Chain	Res	Type	Atoms
3	E	2000	ADP	O4'-C4'-C5'-O5'

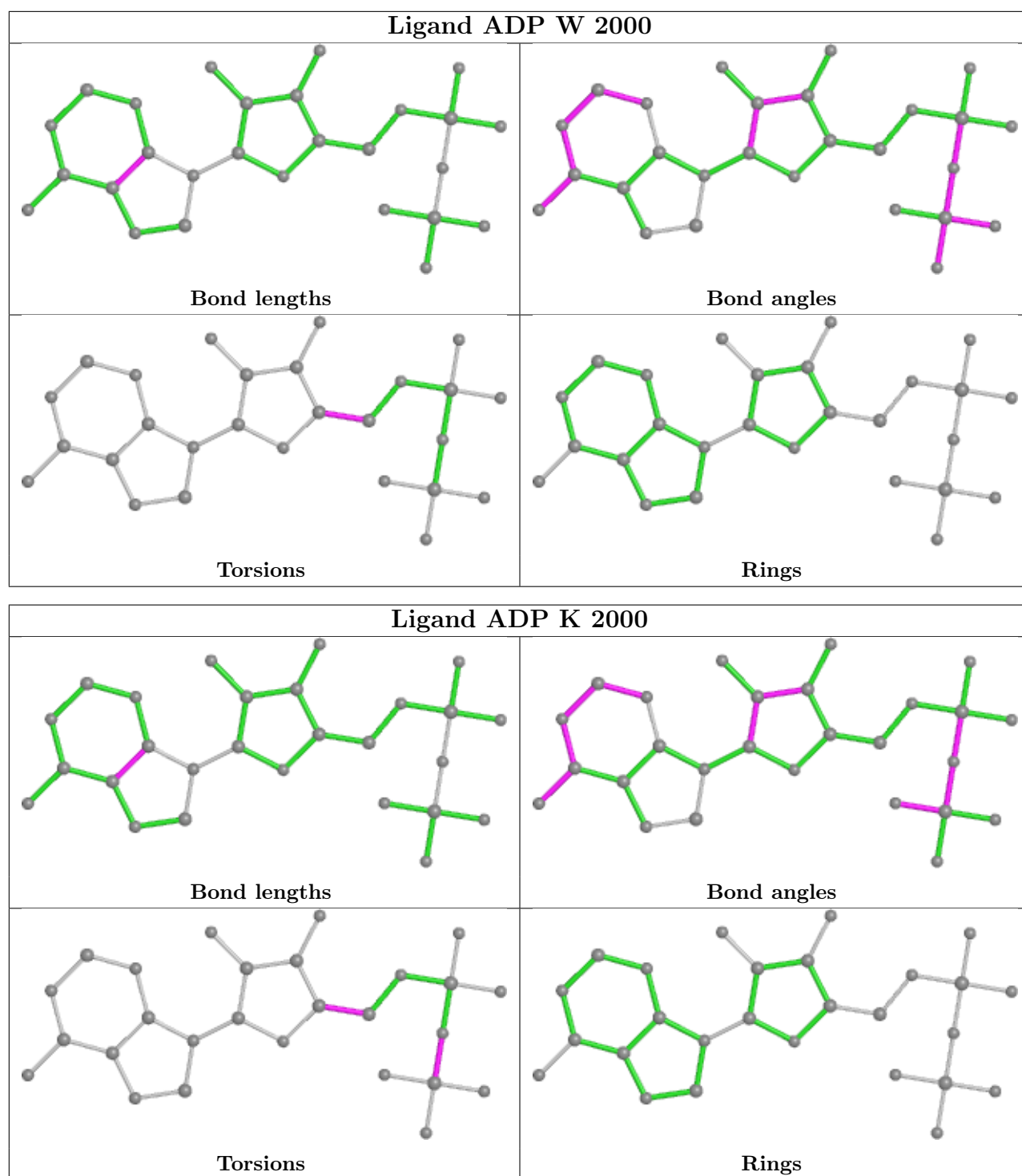
There are no ring outliers.

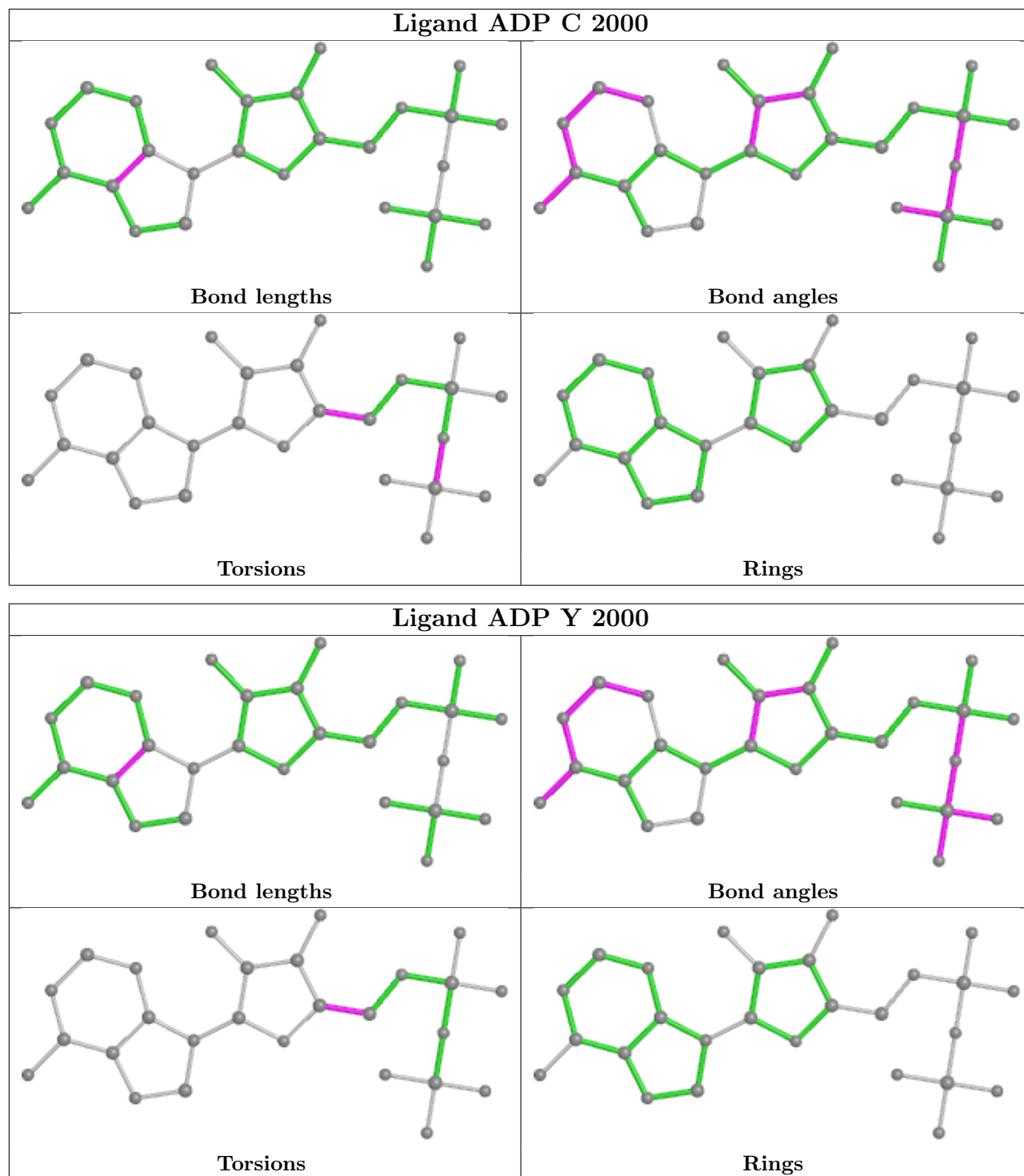
No monomer is involved in short contacts.

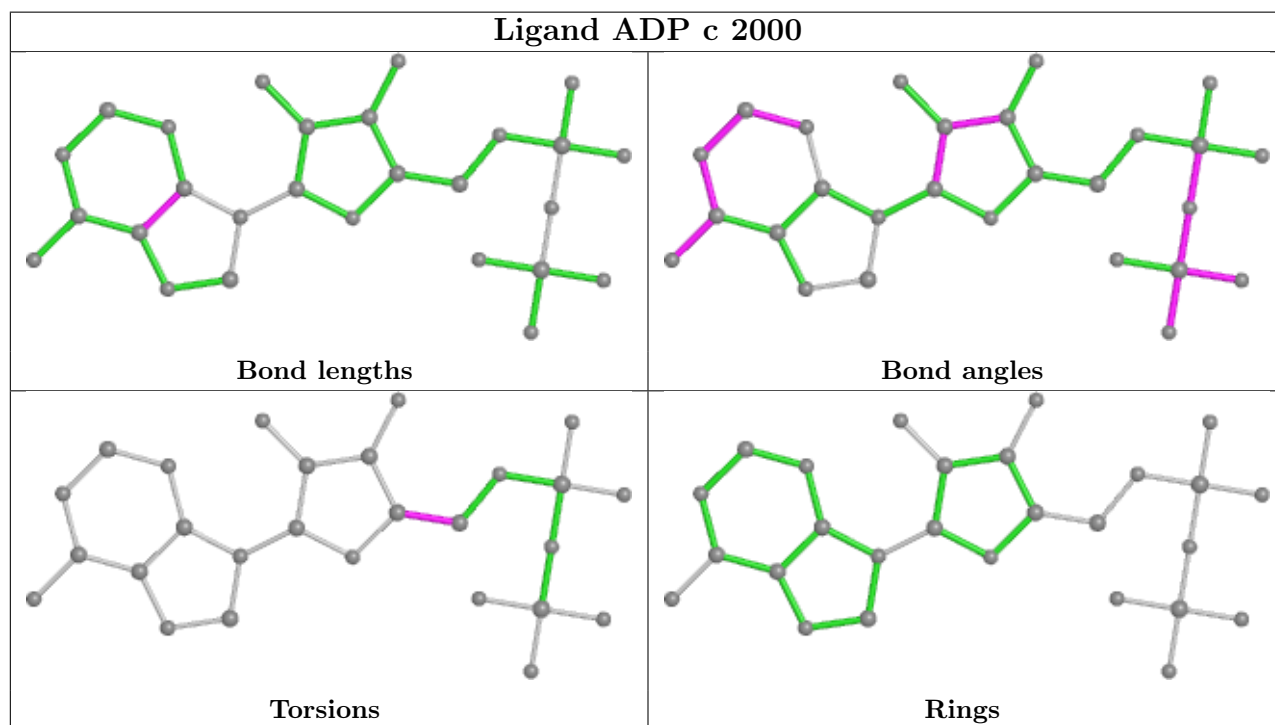
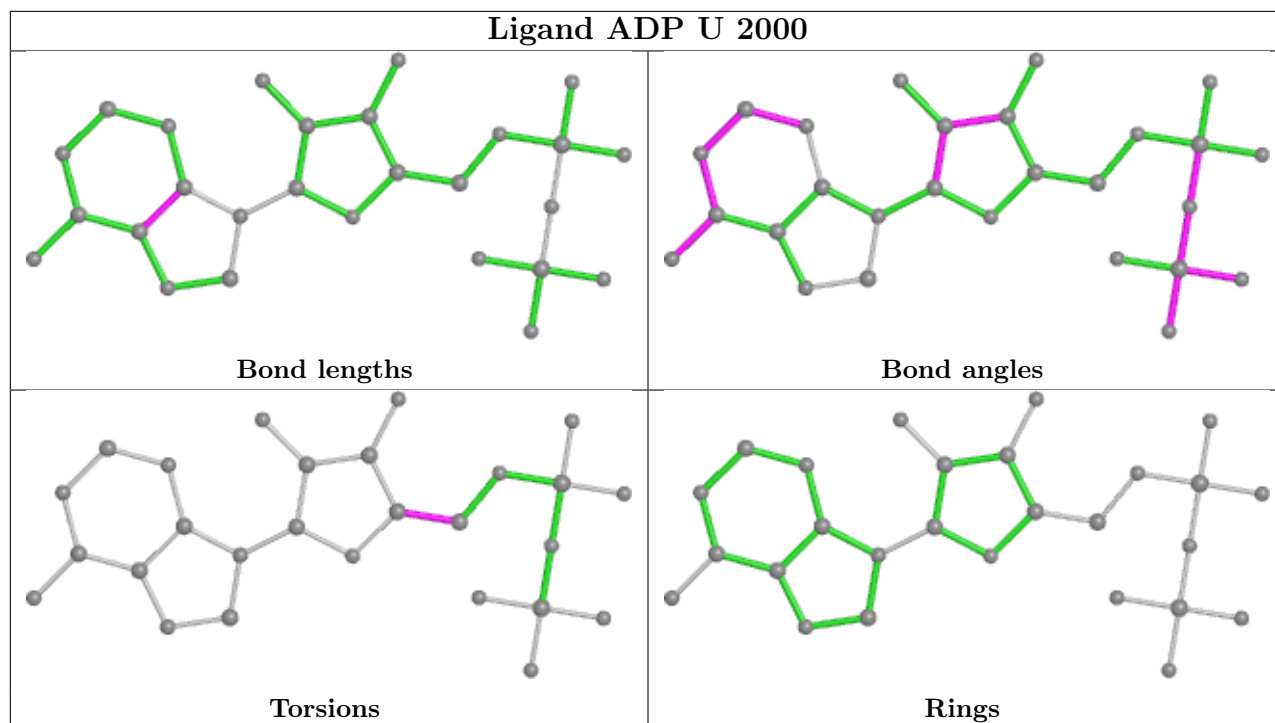
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

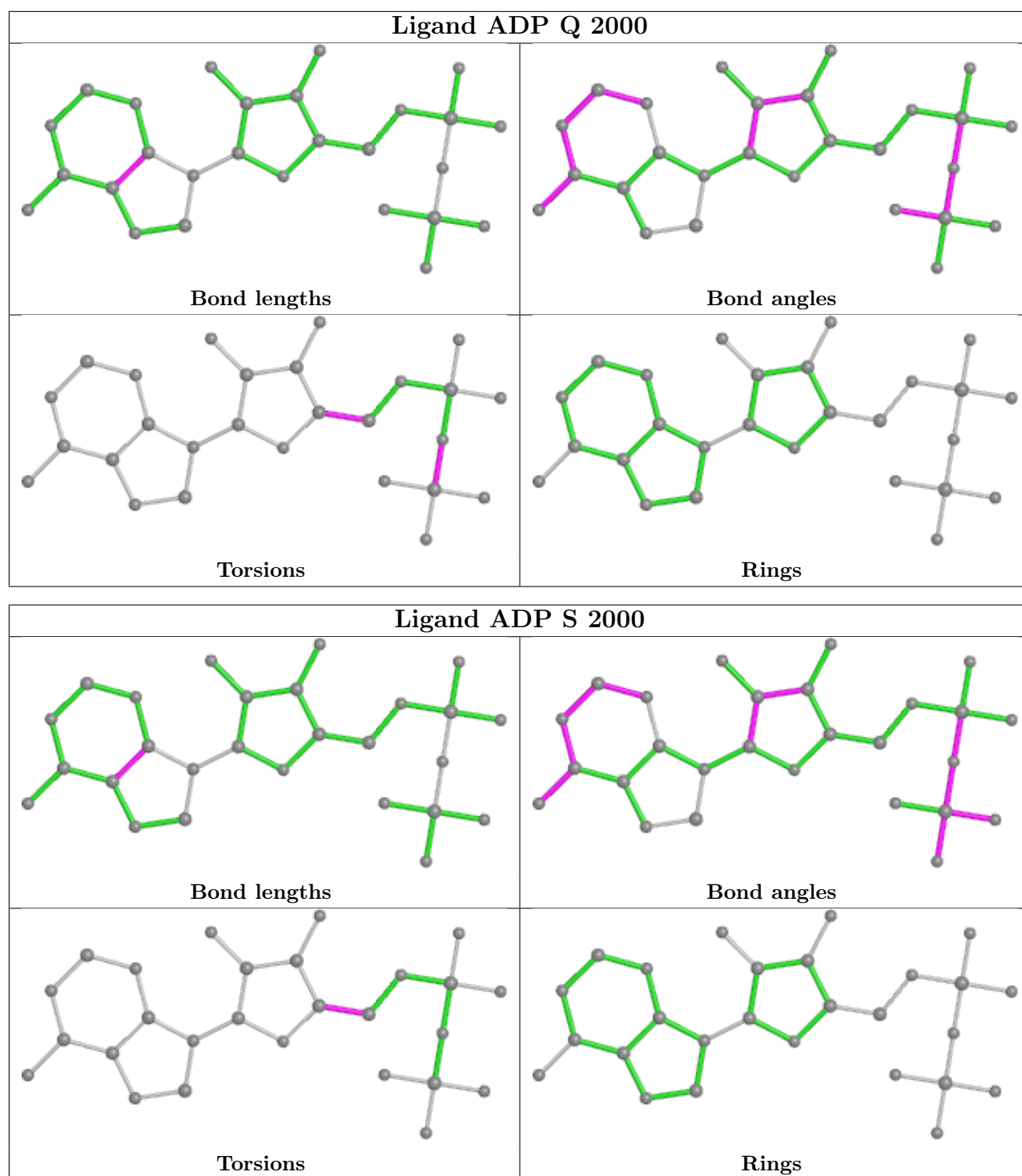


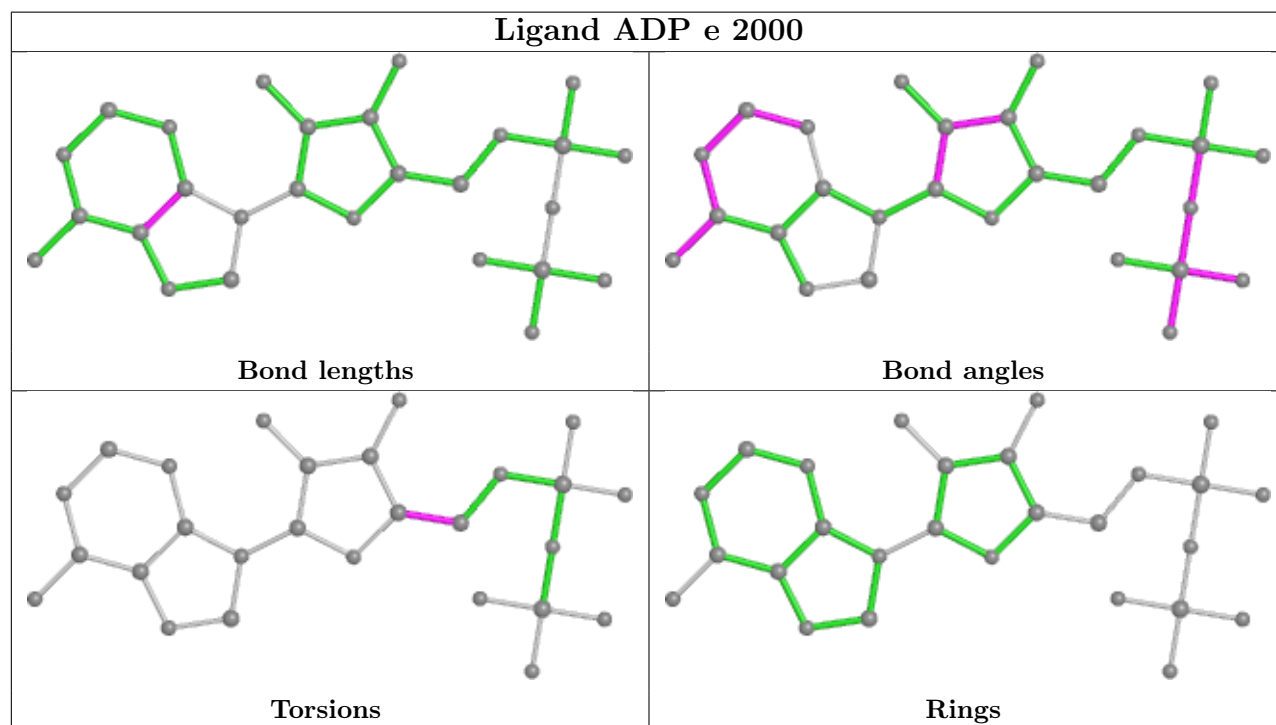
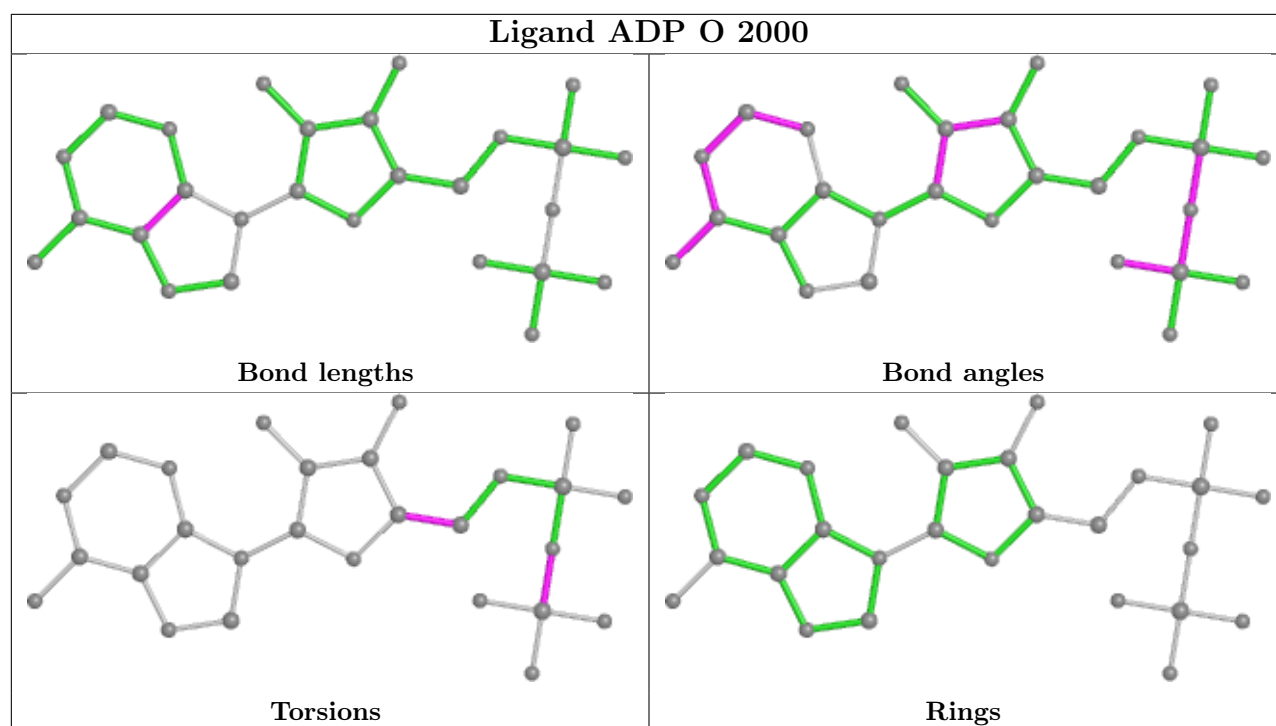


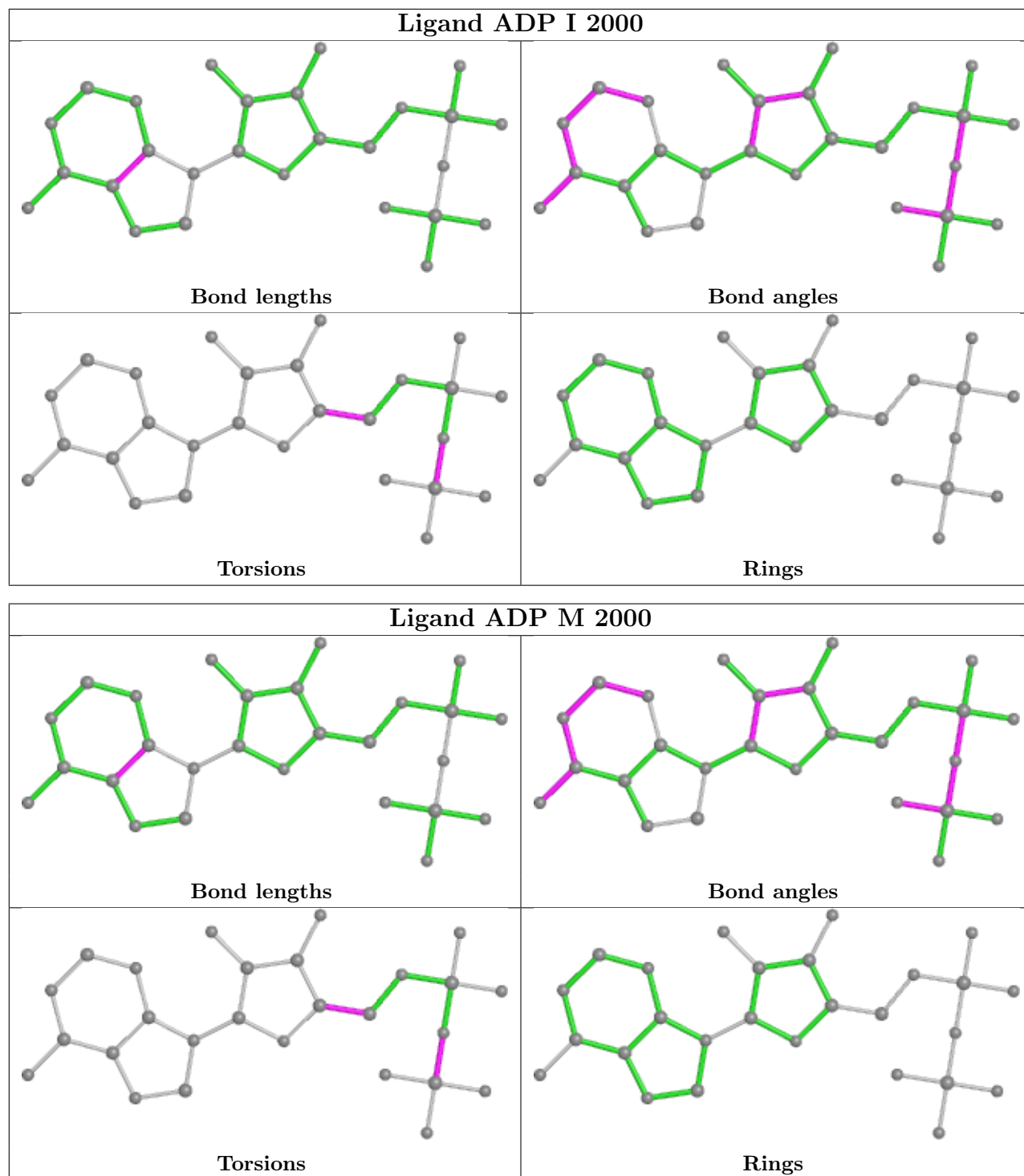


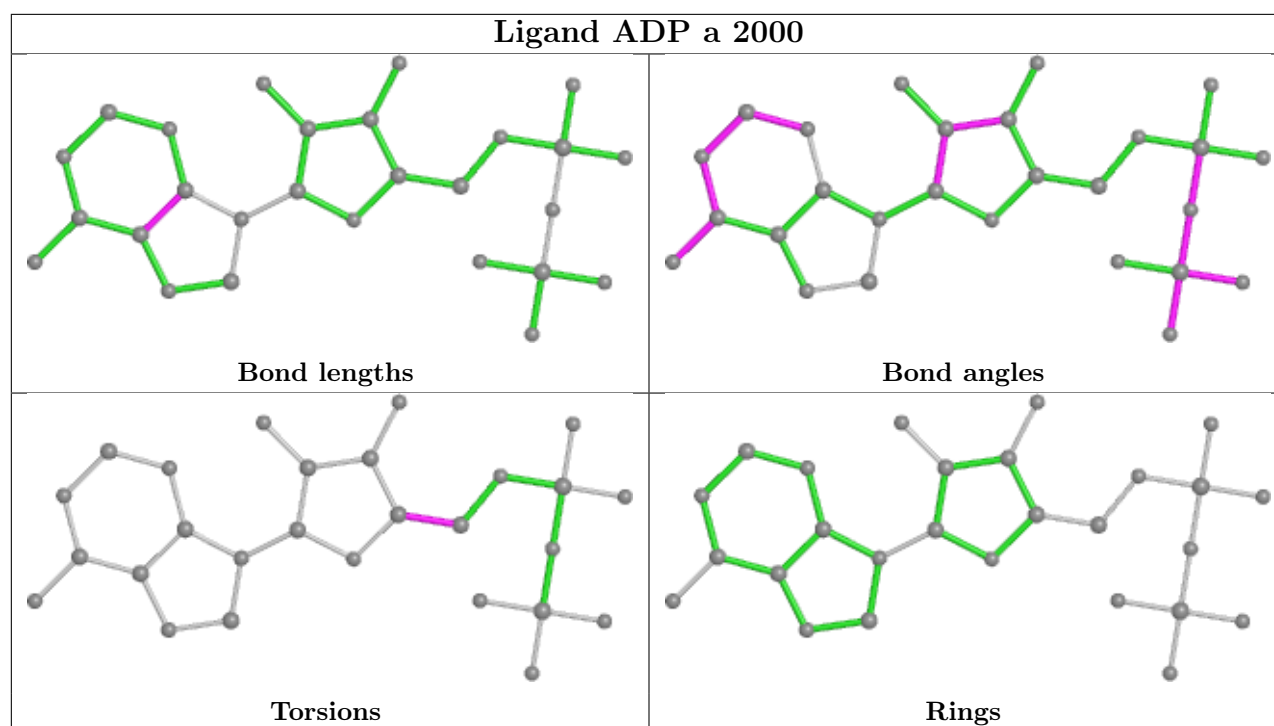












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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

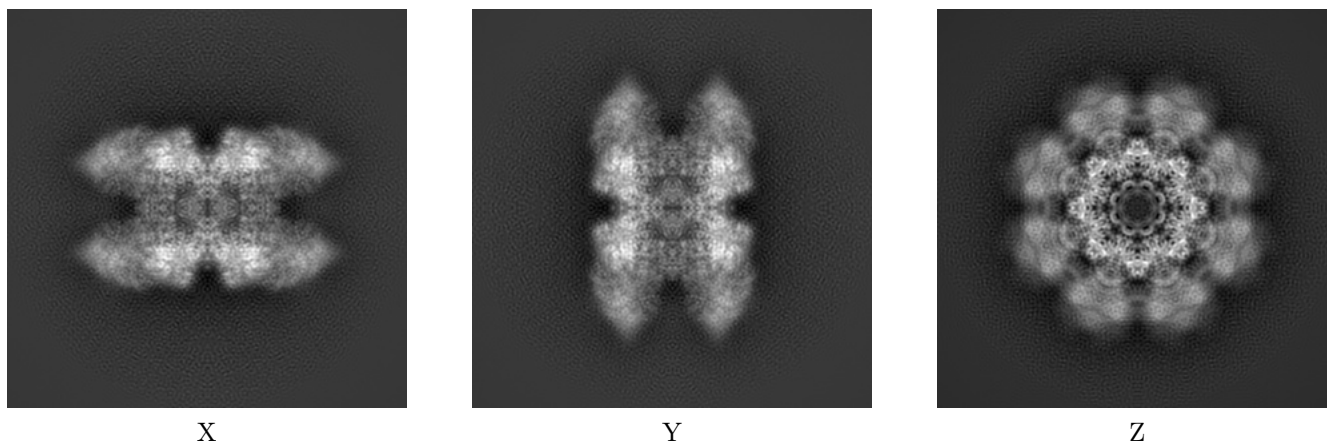
6 Map visualisation [i](#)

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](#)

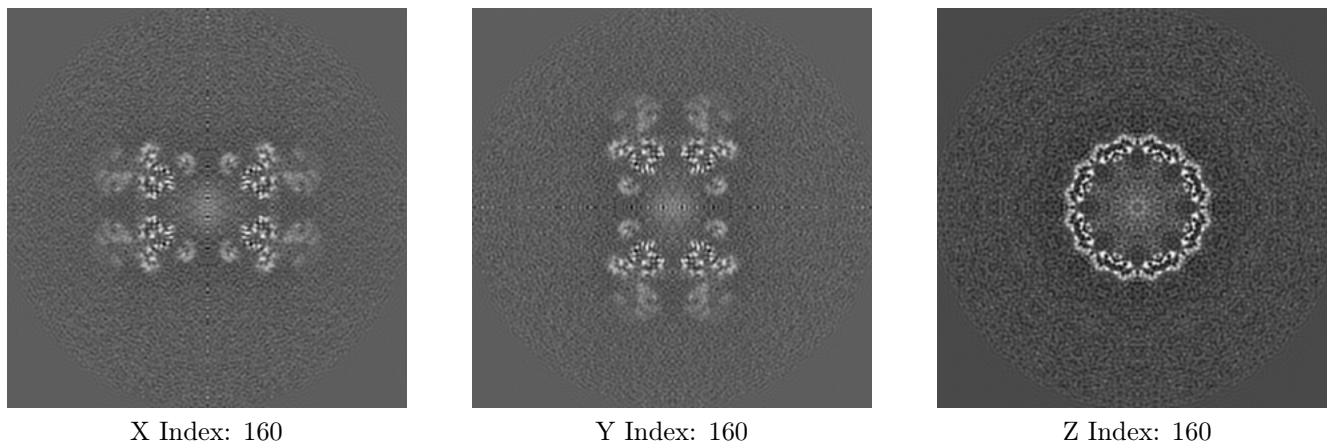
6.1.1 Primary map



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

6.2 Central slices [i](#)

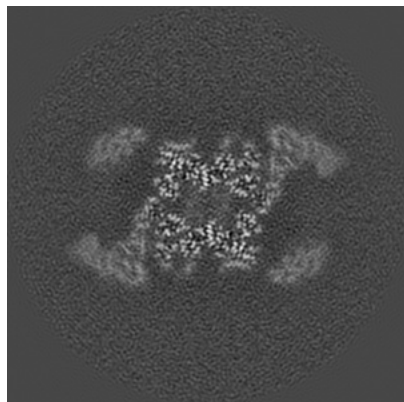
6.2.1 Primary map



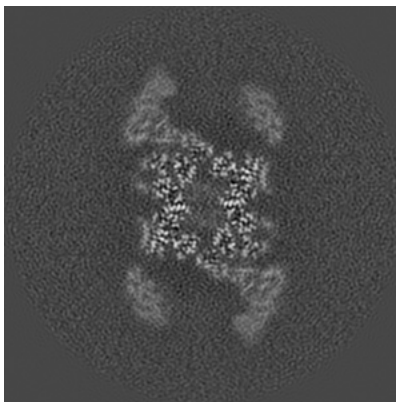
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

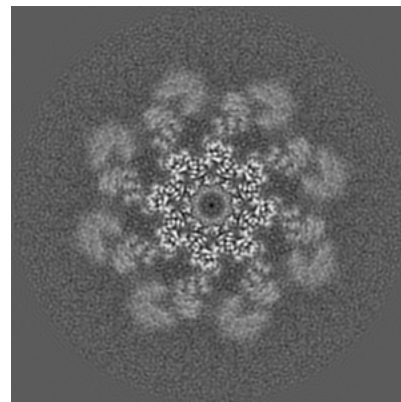
6.3.1 Primary map



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 surface views [i](#)

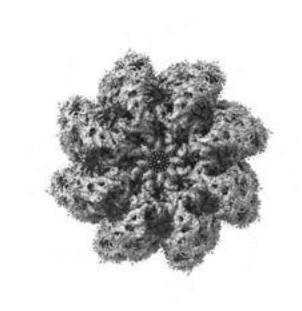
6.4.1 Primary map



X



Y



Z

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

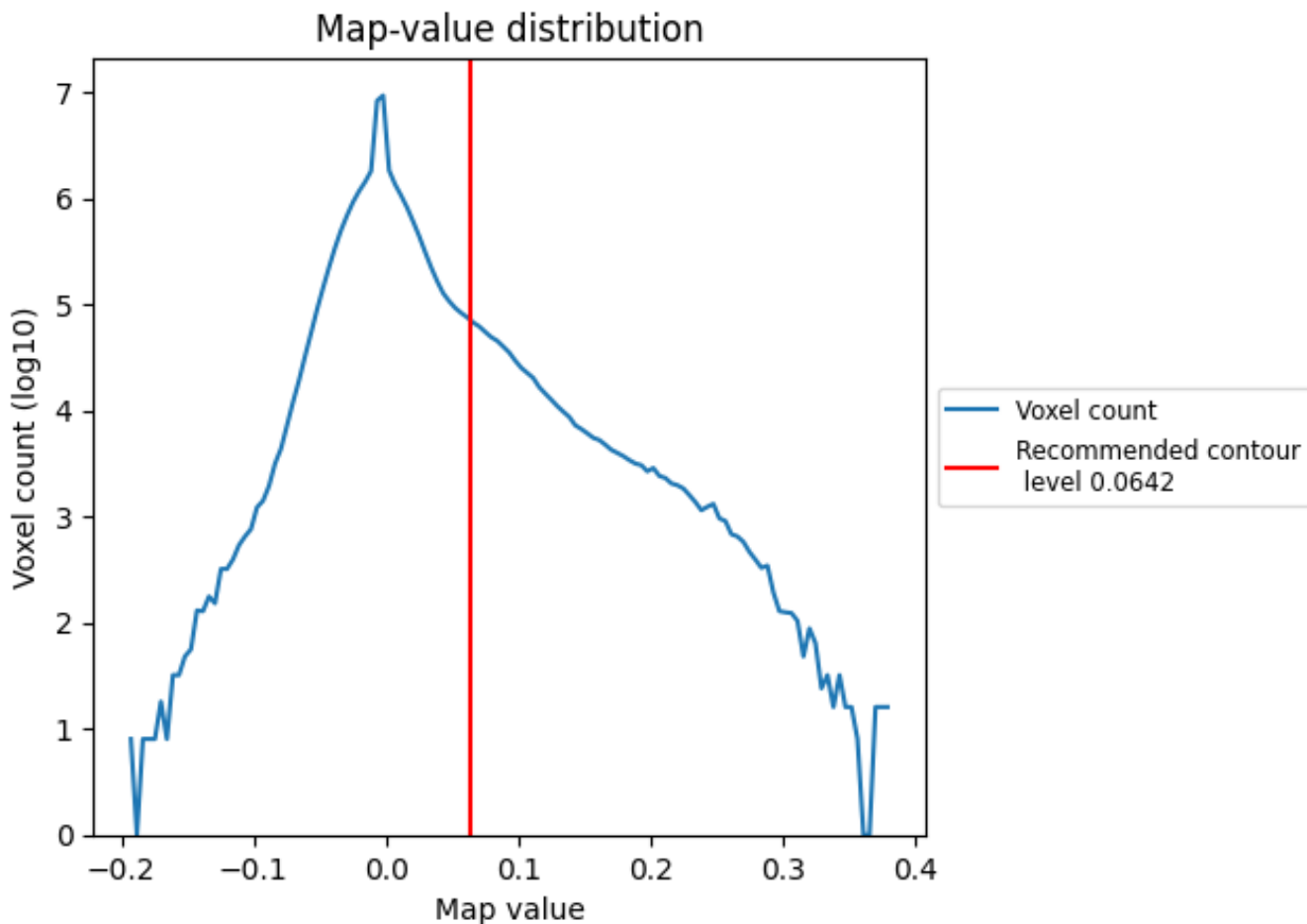
6.5 Mask visualisation

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

7 Map analysis [i](#)

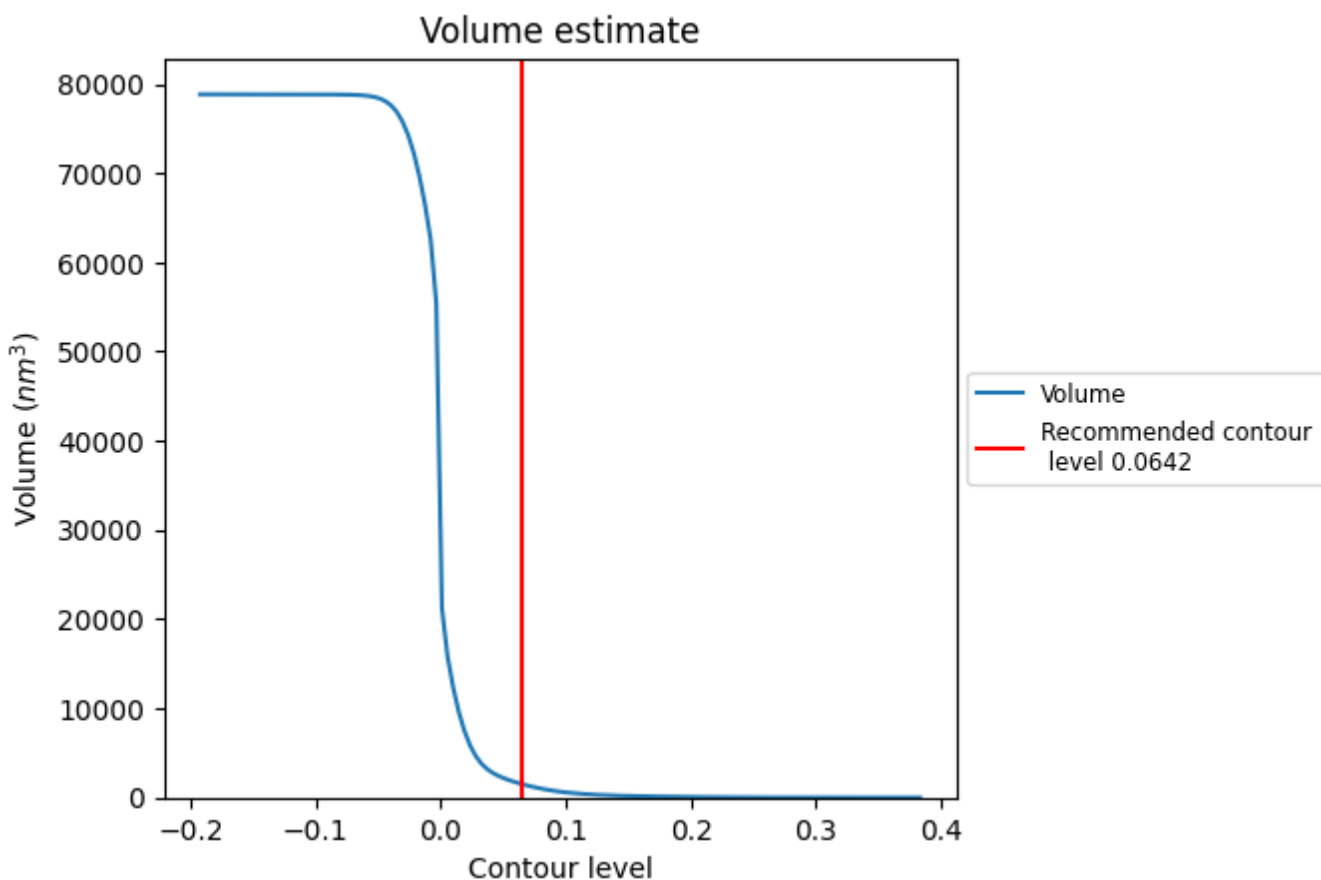
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

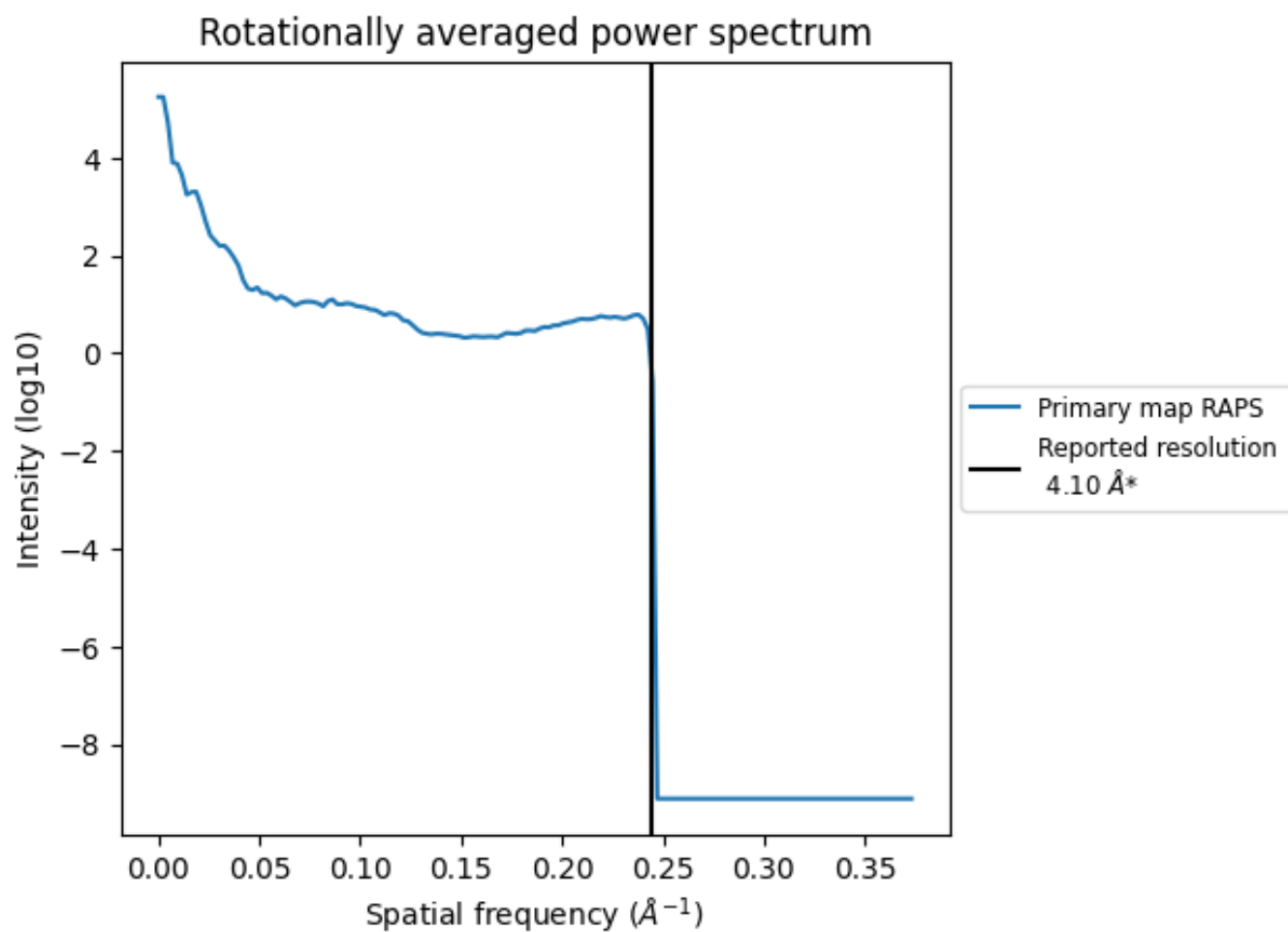
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 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 i



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

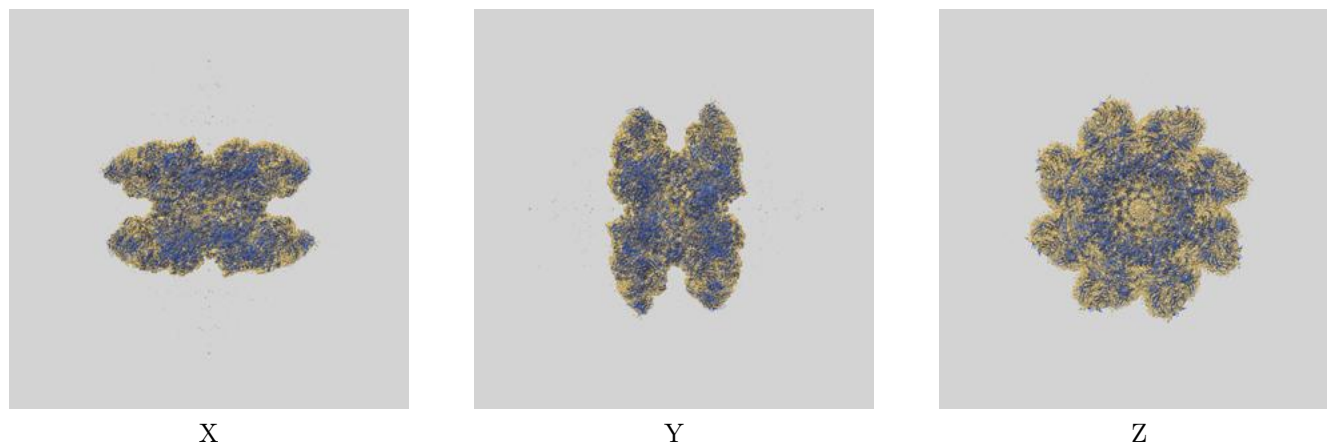
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

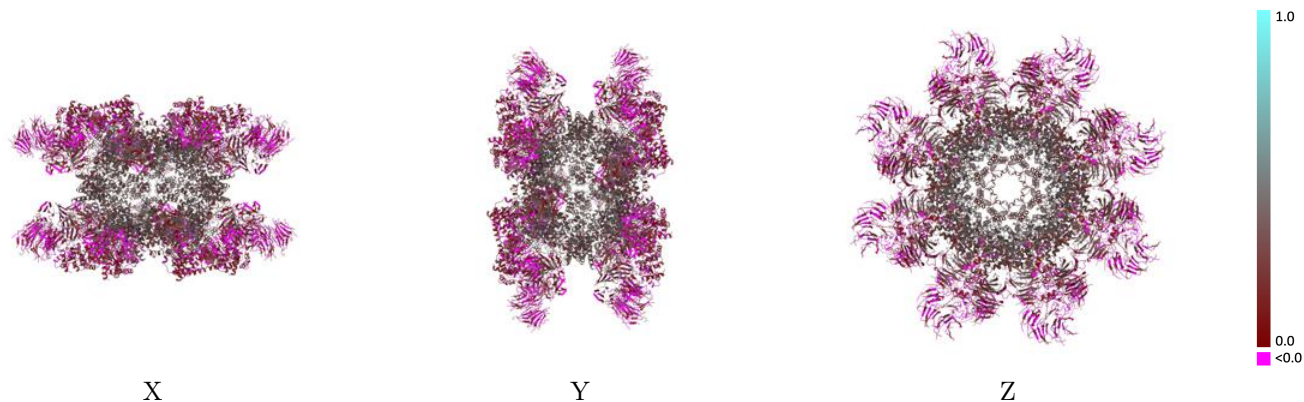
This section contains information regarding the fit between EMDB map EMD-2870 and PDB model 3J9K. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



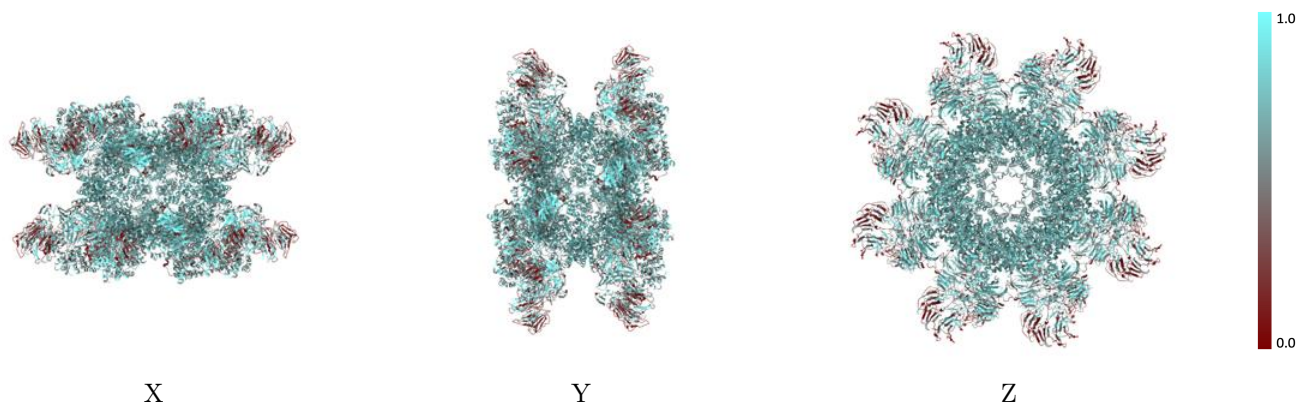
The images above show the 3D surface view of the map at the recommended contour level 0.0642 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



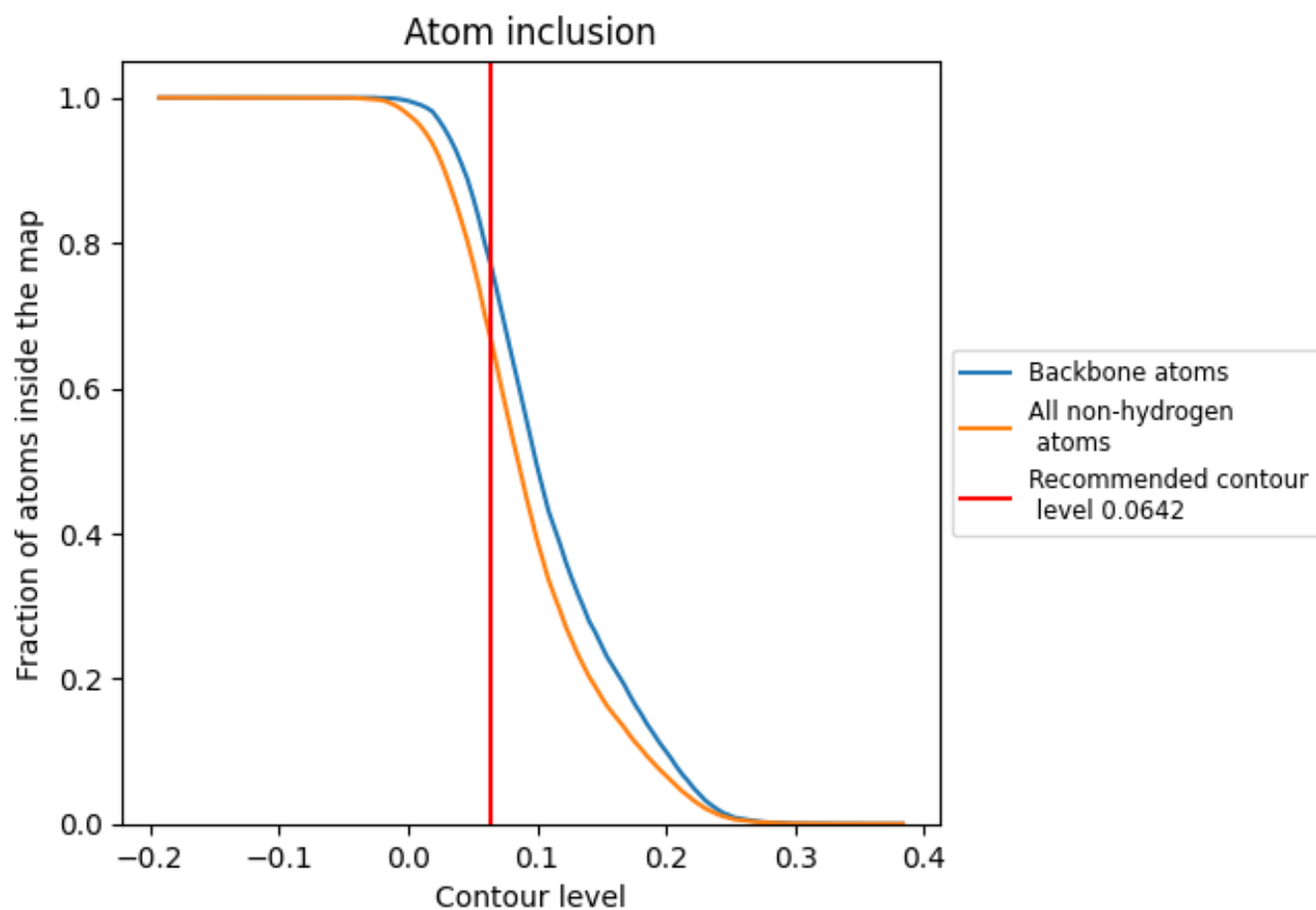
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6667	 0.2340
A	 0.6560	 0.2210
B	 0.7540	 0.3470
C	 0.6576	 0.2220
D	 0.7479	 0.3460
E	 0.6562	 0.2210
F	 0.7540	 0.3480
G	 0.6575	 0.2210
H	 0.7479	 0.3470
I	 0.6562	 0.2200
J	 0.7540	 0.3480
K	 0.6575	 0.2200
L	 0.7479	 0.3460
M	 0.6562	 0.2200
N	 0.7540	 0.3430
O	 0.6576	 0.2200
P	 0.7479	 0.3440
Q	 0.6562	 0.2210
R	 0.7540	 0.3440
S	 0.6575	 0.2210
T	 0.7479	 0.3460
U	 0.6562	 0.2200
V	 0.7540	 0.3440
W	 0.6575	 0.2200
X	 0.7479	 0.3460
Y	 0.6562	 0.2190
Z	 0.7540	 0.3450
a	 0.6573	 0.2190
b	 0.7479	 0.3450
c	 0.6562	 0.2200
d	 0.7540	 0.3460
e	 0.6573	 0.2200
f	 0.7479	 0.3440

