



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 09:42 pm BST

PDB ID : 9T68 / pdb_00009t68
EMDB ID : EMD-55609
Title : Composite structure of the repeat unit of cytoplasmic lattice filament
Authors : Singh, K.; Harasimov, K.; Carter, A.P.
Deposited on : 2025-11-06
Resolution : 8.00 Å(reported)

This is a Full wwPDB EM Validation 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:

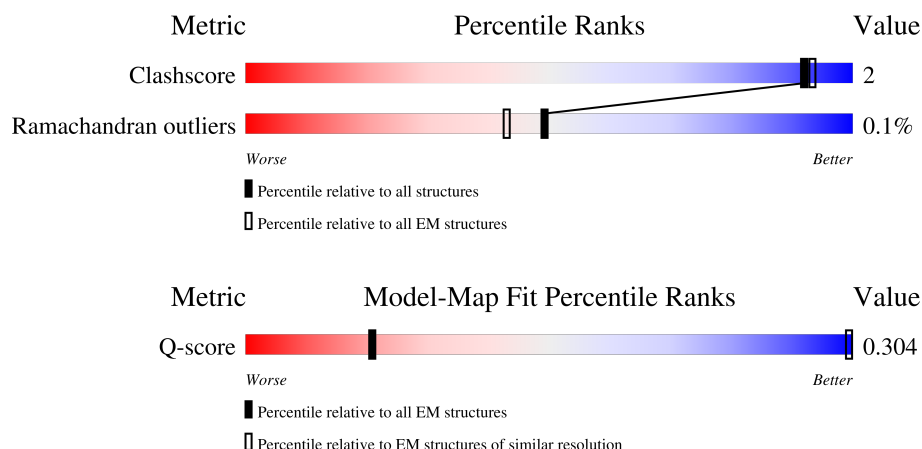
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 8.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	361 (7.50 - 8.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	440	 30% 69%
1	An	440	 30% 69%
1	S	440	 29% 69%
1	j	440	 31% 69%
2	1	682	 12% 98%

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Mol	Chain	Length	Quality of chain
2	2	682	57% 99%
2	3	682	52% 98%
2	A	682	5% 96%
2	AB	682	22% 98%
2	AC	682	66% 98%
2	AD	682	28% 99%
2	Aa	682	15% 99%
2	Ab	682	22% 98%
2	Ac	682	64% 98%
2	Ad	682	28% 99%
2	Az	682	9% 99%
2	B	682	9% 98%
2	C	682	13% 98%
2	D	682	14% 97%
2	E	682	15% 98%
2	F	682	14% 99%
2	G	682	9% 95% 5%
2	H	682	7% 97%
2	I	682	30% 98%
2	J	682	12% 98%
2	K	682	54% 98%
2	L	682	52% 99%
2	l	682	15% 99%
2	m	682	6% 97%
2	t	682	13% 98%

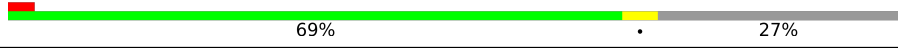
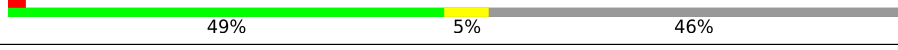
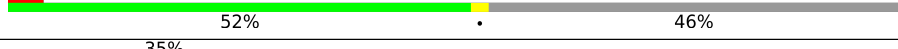
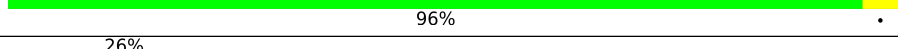
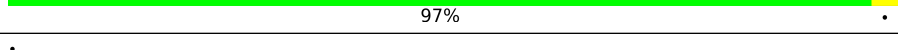
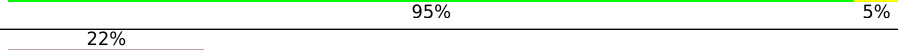
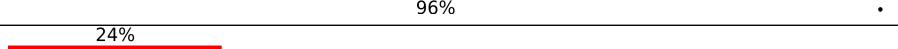
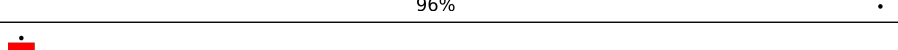
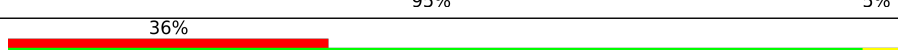
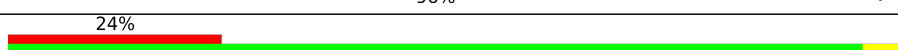
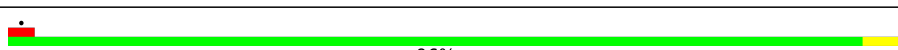
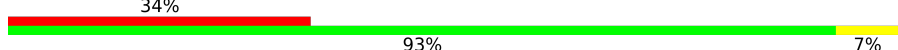
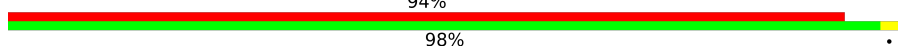
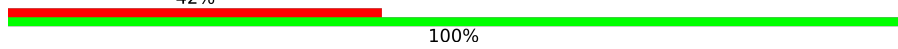
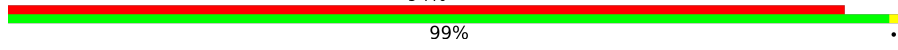
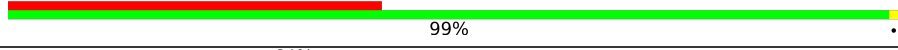
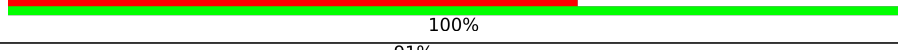
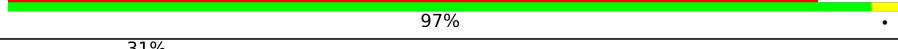
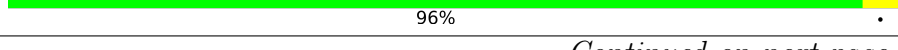
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Mol	Chain	Length	Quality of chain
2	u	682	
2	v	682	
2	w	682	
2	x	682	
2	y	682	
2	z	682	
3	4	1163	
3	7	1163	
3	AF	1163	
3	AR	1163	
3	Af	1163	
3	Ak	1163	
3	M	1163	
3	P	1163	
4	5	581	
4	8	581	
4	AS	581	
4	Ah	581	
4	Al	581	
4	N	581	
4	Q	581	
4	X	581	
5	6	164	
5	9	164	
5	AQ	164	

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Mol	Chain	Length	Quality of chain
5	Aj	164	
5	Am	164	
5	O	164	
5	R	164	
5	i	164	
6	A1	466	
6	AL	466	
6	AN	466	
6	AX	466	
6	At	466	
6	Av	466	
6	Ax	466	
6	e	466	
6	g	466	
6	s	466	
7	A2	163	
7	AM	163	
7	AO	163	
7	AY	163	
7	AZ	163	
7	Au	163	
7	Aw	163	
7	Ay	163	
7	f	163	
7	h	163	

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Mol	Chain	Length	Quality of chain
8	AA	228	
8	AE	228	
8	AP	228	
8	AT	228	
8	Ae	228	
8	Ag	228	
8	Ao	228	
8	Ap	228	
8	T	228	
8	k	228	
9	AG	993	
9	Z	993	
9	n	993	
10	AH	782	
10	a	782	
10	o	782	
11	AI	147	
11	b	147	
11	p	147	
12	AJ	449	
12	AV	449	
12	Ar	449	
12	c	449	
12	q	449	
13	AK	445	

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Mol	Chain	Length	Quality of chain
13	AW	445	 7% 96% . .
13	As	445	 7% 96% .
13	d	445	 5% 95% . .
13	r	445	 90% 96% .
14	AU	937	 17% 98% .
14	Ai	937	 15% 98% .
14	Aq	937	 17% 99% .
14	Y	937	 15% 99% .
15	U	76	 45% 97% .
15	V	76	 88% 97% .
15	W	76	 97% 97% .

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 270782 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 KH domain-containing protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	136	Total	C	N	O	0	0
			673	401	136	136		
1	An	136	Total	C	N	O	0	0
			673	401	136	136		
1	S	136	Total	C	N	O	0	0
			673	401	136	136		
1	j	136	Total	C	N	O	0	0
			673	401	136	136		

- Molecule 2 is a protein called Inactive protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	2	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	3	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	A	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	AB	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	AC	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	AD	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	Aa	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	Ab	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	Ac	682	Total	C	N	O	0	0
			3373	2009	682	682		
2	Ad	682	Total	C	N	O	0	0
			3373	2009	682	682		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	Az	682	Total 3373	C 2009	N 682	O 682	0	0
2	B	682	Total 3373	C 2009	N 682	O 682	0	0
2	C	682	Total 3373	C 2009	N 682	O 682	0	0
2	D	682	Total 3373	C 2009	N 682	O 682	0	0
2	E	682	Total 3373	C 2009	N 682	O 682	0	0
2	F	682	Total 3373	C 2009	N 682	O 682	0	0
2	G	682	Total 3373	C 2009	N 682	O 682	0	0
2	H	682	Total 3373	C 2009	N 682	O 682	0	0
2	I	682	Total 3373	C 2009	N 682	O 682	0	0
2	J	682	Total 3373	C 2009	N 682	O 682	0	0
2	K	682	Total 3373	C 2009	N 682	O 682	0	0
2	L	682	Total 3373	C 2009	N 682	O 682	0	0
2	l	682	Total 3373	C 2009	N 682	O 682	0	0
2	m	682	Total 3373	C 2009	N 682	O 682	0	0
2	t	682	Total 3373	C 2009	N 682	O 682	0	0
2	u	682	Total 3373	C 2009	N 682	O 682	0	0
2	v	682	Total 3373	C 2009	N 682	O 682	0	0
2	w	682	Total 3373	C 2009	N 682	O 682	0	0
2	x	682	Total 3373	C 2009	N 682	O 682	0	0
2	y	682	Total 3373	C 2009	N 682	O 682	0	0
2	z	682	Total 3373	C 2009	N 682	O 682	0	0

- Molecule 3 is a protein called NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	4	949	Total	C	N	O	0	0
			4702	2804	949	949		
3	7	949	Total	C	N	O	0	0
			4702	2804	949	949		
3	AF	949	Total	C	N	O	0	0
			4702	2804	949	949		
3	AR	949	Total	C	N	O	0	0
			4702	2804	949	949		
3	Af	949	Total	C	N	O	0	0
			4702	2804	949	949		
3	Ak	949	Total	C	N	O	0	0
			4702	2804	949	949		
3	M	949	Total	C	N	O	0	0
			4702	2804	949	949		
3	P	949	Total	C	N	O	0	0
			4702	2804	949	949		

- Molecule 4 is a protein called Transducin-like enhancer protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	367	Total	C	N	O	0	0
			1812	1078	367	367		
4	8	367	Total	C	N	O	0	0
			1812	1078	367	367		
4	AS	367	Total	C	N	O	0	0
			1812	1078	367	367		
4	Ah	367	Total	C	N	O	0	0
			1812	1078	367	367		
4	Al	367	Total	C	N	O	0	0
			1812	1078	367	367		
4	N	367	Total	C	N	O	0	0
			1812	1078	367	367		
4	Q	367	Total	C	N	O	0	0
			1812	1078	367	367		
4	X	367	Total	C	N	O	0	0
			1812	1078	367	367		

- Molecule 5 is a protein called Oocyte-expressed protein homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	6	119	Total	C	N	O	0	0
			592	354	119	119		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	9	89	Total 442	C 264	N 89	O 89	0	0
5	AQ	119	Total 592	C 354	N 119	O 119	0	0
5	Aj	119	Total 592	C 354	N 119	O 119	0	0
5	Am	89	Total 442	C 264	N 89	O 89	0	0
5	O	119	Total 592	C 354	N 119	O 119	0	0
5	R	89	Total 442	C 264	N 89	O 89	0	0
5	i	89	Total 442	C 264	N 89	O 89	0	0

- Molecule 6 is a protein called F-box/WD repeat-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A1	466	Total 2312	C 1380	N 466	O 466	0	0
6	AL	466	Total 2312	C 1380	N 466	O 466	0	0
6	AN	466	Total 2312	C 1380	N 466	O 466	0	0
6	AX	466	Total 2312	C 1380	N 466	O 466	0	0
6	At	466	Total 2312	C 1380	N 466	O 466	0	0
6	Av	466	Total 2312	C 1380	N 466	O 466	0	0
6	Ax	466	Total 2312	C 1380	N 466	O 466	0	0
6	e	466	Total 2312	C 1380	N 466	O 466	0	0
6	g	466	Total 2312	C 1380	N 466	O 466	0	0
6	s	466	Total 2312	C 1380	N 466	O 466	0	0

- Molecule 7 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	A2	163	Total	C	N	O	0	0
			809	483	163	163		
7	AM	163	Total	C	N	O	0	0
			809	483	163	163		
7	AO	163	Total	C	N	O	0	0
			809	483	163	163		
7	AY	163	Total	C	N	O	0	0
			809	483	163	163		
7	AZ	163	Total	C	N	O	0	0
			809	483	163	163		
7	Au	163	Total	C	N	O	0	0
			809	483	163	163		
7	Aw	163	Total	C	N	O	0	0
			809	483	163	163		
7	Ay	163	Total	C	N	O	0	0
			809	483	163	163		
7	f	163	Total	C	N	O	0	0
			809	483	163	163		
7	h	163	Total	C	N	O	0	0
			809	483	163	163		

- Molecule 8 is a protein called Zinc finger BED domain-containing protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AA	63	Total	C	N	O	0	0
			311	185	63	63		
8	AE	141	Total	C	N	O	0	0
			698	416	141	141		
8	AP	143	Total	C	N	O	0	0
			708	422	143	143		
8	AT	80	Total	C	N	O	0	0
			397	237	80	80		
8	Ae	141	Total	C	N	O	0	0
			698	416	141	141		
8	Ag	143	Total	C	N	O	0	0
			708	422	143	143		
8	Ao	141	Total	C	N	O	0	0
			698	416	141	141		
8	Ap	80	Total	C	N	O	0	0
			397	237	80	80		
8	T	63	Total	C	N	O	0	0
			311	185	63	63		
8	k	141	Total	C	N	O	0	0
			698	416	141	141		

- Molecule 9 is a protein called NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AG	966	Total	C	N	O	0	0
			4794	2862	966	966		
9	Z	966	Total	C	N	O	0	0
			4794	2862	966	966		
9	n	966	Total	C	N	O	0	0
			4794	2862	966	966		

- Molecule 10 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	AH	635	Total	C	N	O	0	0
			3131	1861	635	635		
10	a	635	Total	C	N	O	0	0
			3131	1861	635	635		
10	o	635	Total	C	N	O	0	0
			3131	1861	635	635		

- Molecule 11 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	AI	147	Total	C	N	O	0	0
			729	435	147	147		
11	b	147	Total	C	N	O	0	0
			729	435	147	147		
11	p	147	Total	C	N	O	0	0
			729	435	147	147		

- Molecule 12 is a protein called Tubulin alpha-1C chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AJ	440	Total	C	N	O	0	0
			2167	1287	440	440		
12	AV	440	Total	C	N	O	0	0
			2167	1287	440	440		
12	Ar	440	Total	C	N	O	0	0
			2167	1287	440	440		
12	c	440	Total	C	N	O	0	0
			2167	1287	440	440		
12	q	440	Total	C	N	O	0	0
			2167	1287	440	440		

- Molecule 13 is a protein called Tubulin beta-4B chain.

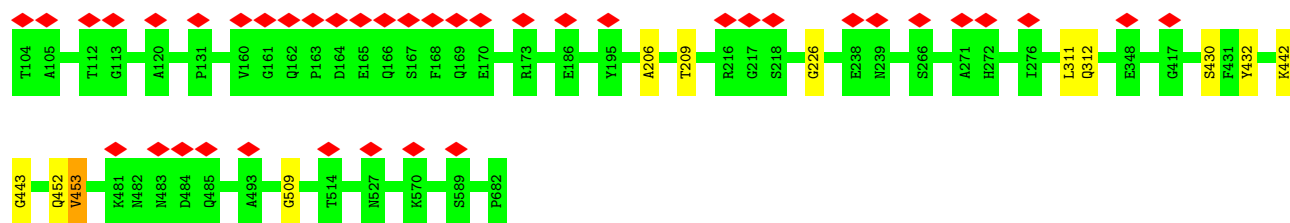
Mol	Chain	Residues	Atoms				AltConf	Trace
13	AK	431	Total	C	N	O	0	0
			2121	1259	431	431		
13	AW	431	Total	C	N	O	0	0
			2121	1259	431	431		
13	As	431	Total	C	N	O	0	0
			2121	1259	431	431		
13	d	431	Total	C	N	O	0	0
			2121	1259	431	431		
13	r	431	Total	C	N	O	0	0
			2121	1259	431	431		

- Molecule 14 is a protein called NLR family, pyrin domain containing 4F.

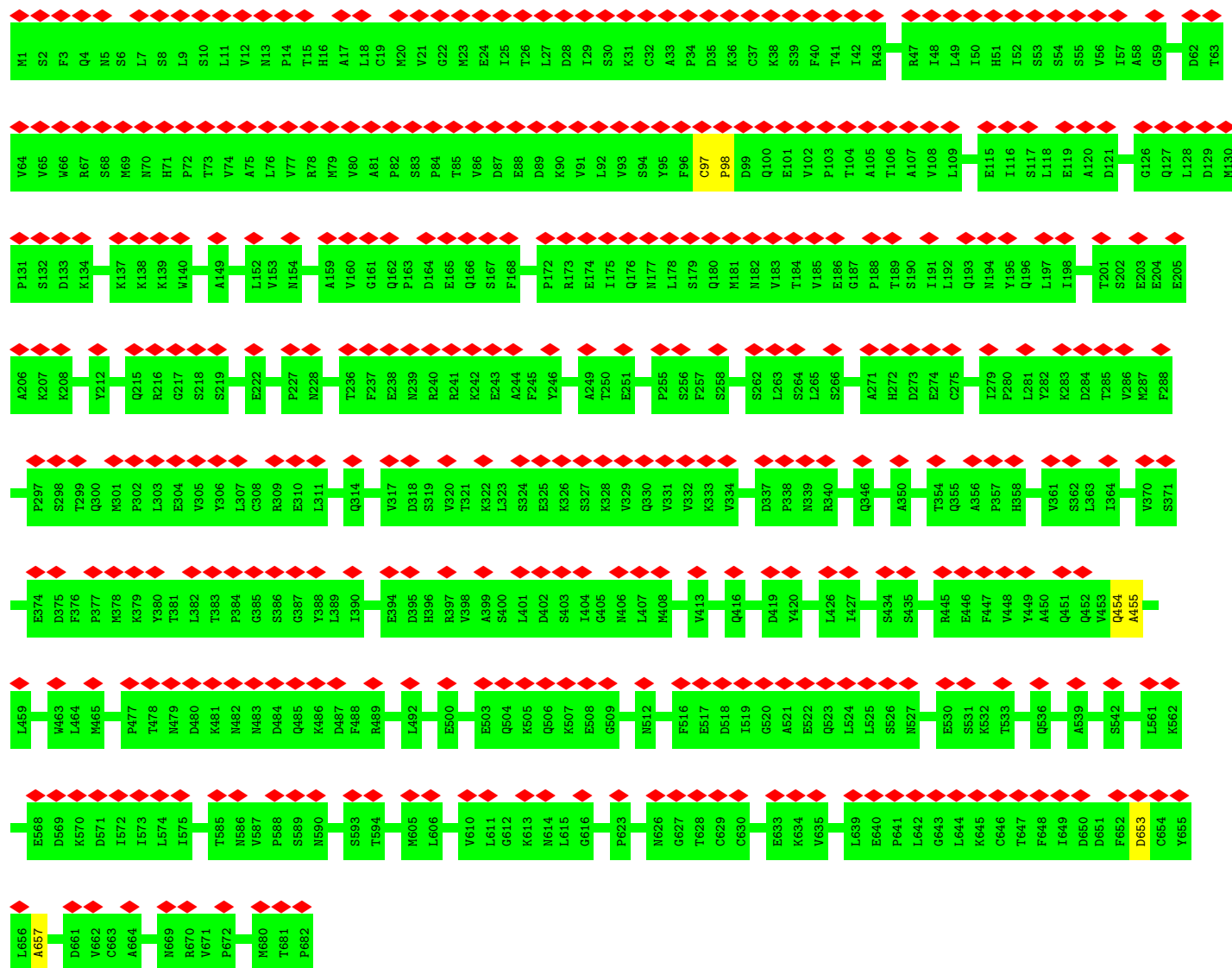
Mol	Chain	Residues	Atoms				AltConf	Trace
14	AU	935	Total	C	N	O	0	0
			4643	2773	935	935		
14	Ai	935	Total	C	N	O	0	0
			4643	2773	935	935		
14	Aq	935	Total	C	N	O	0	0
			4643	2773	935	935		
14	Y	935	Total	C	N	O	0	0
			4643	2773	935	935		

- Molecule 15 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	74	Total	C	N	O	0	0
			366	218	74	74		
15	V	74	Total	C	N	O	0	0
			366	218	74	74		
15	W	74	Total	C	N	O	0	0
			366	218	74	74		

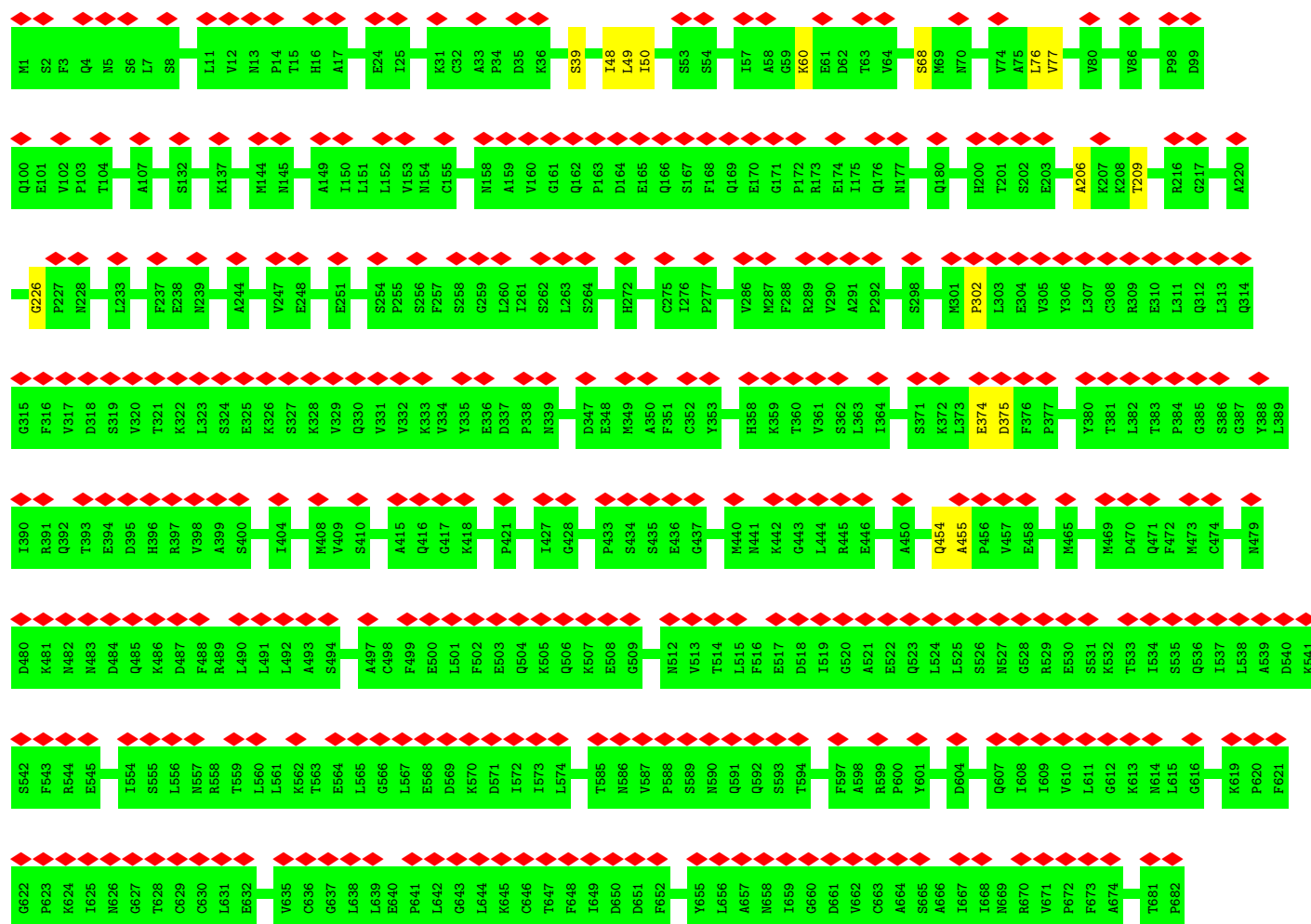


- Molecule 2: Inactive protein-arginine deiminase type-6

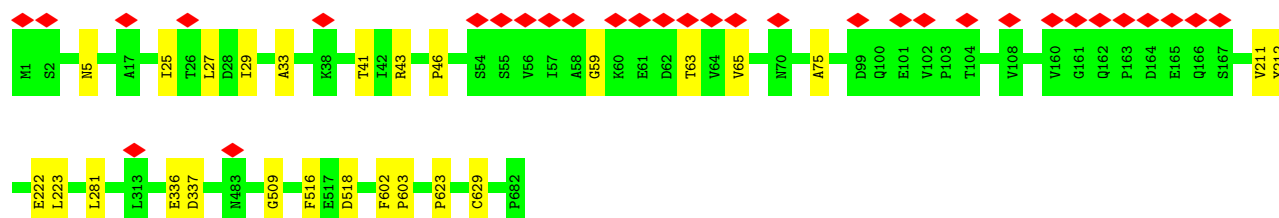


- Molecule 2: Inactive protein-arginine deiminase type-6

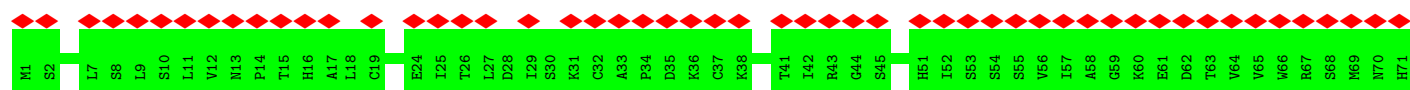


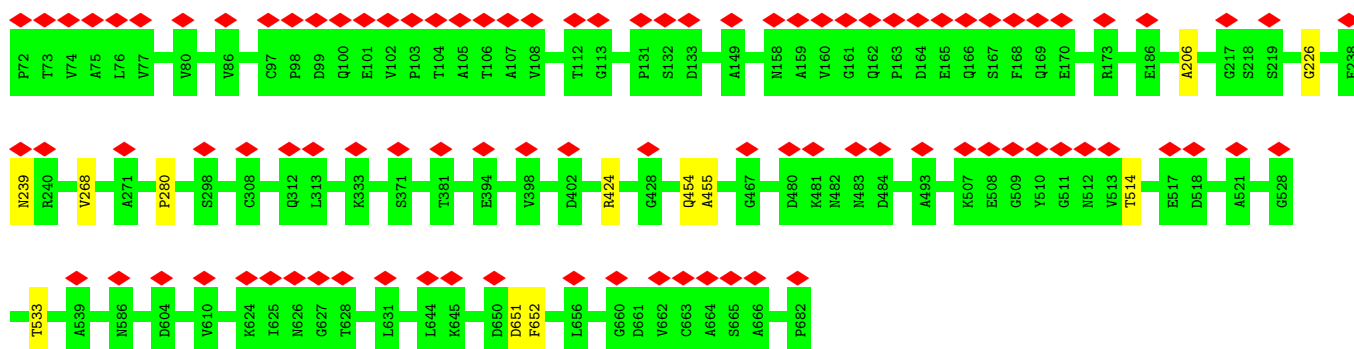


• Molecule 2: Inactive protein-arginine deiminase type-6

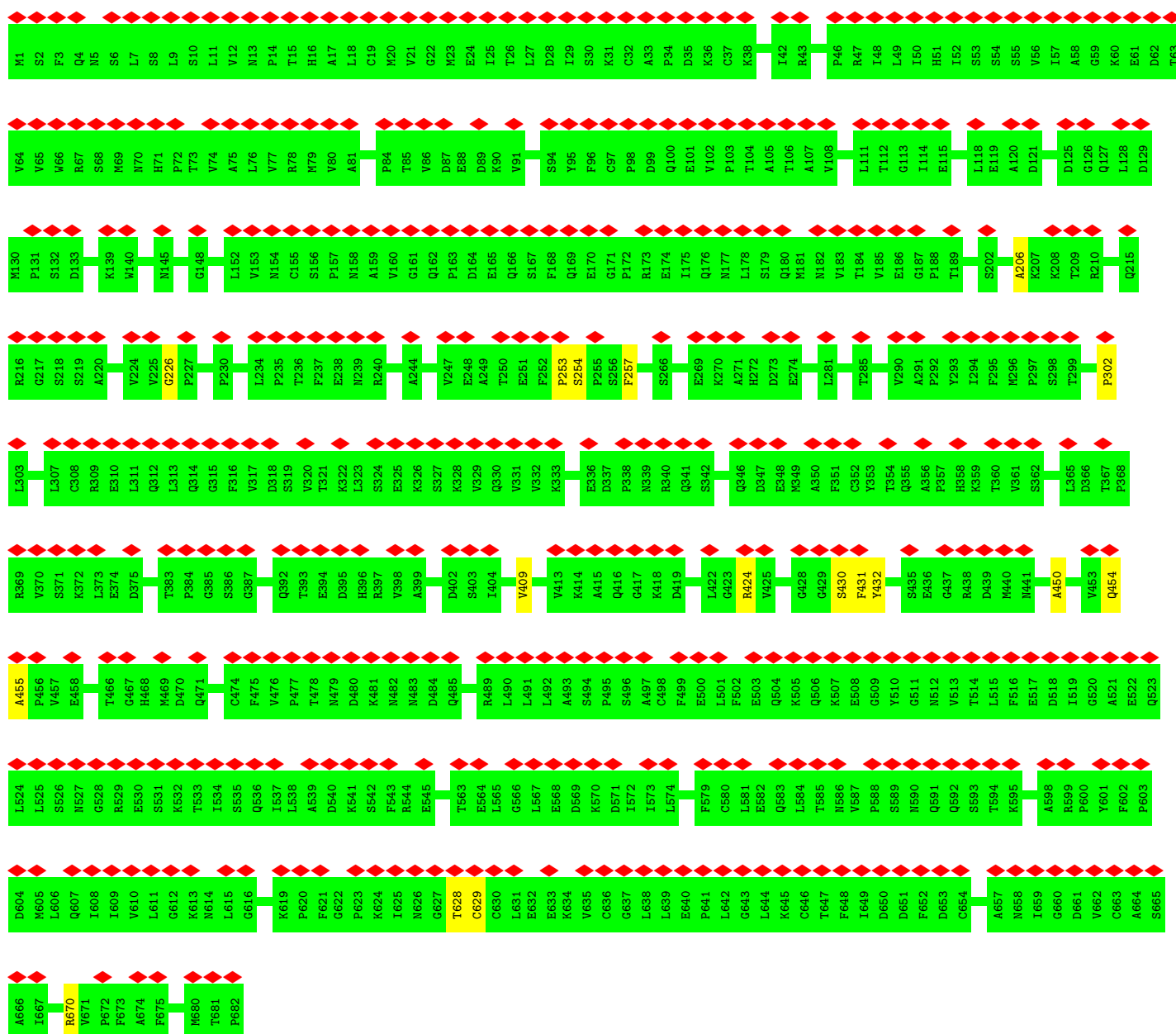


• Molecule 2: Inactive protein-arginine deiminase type-6

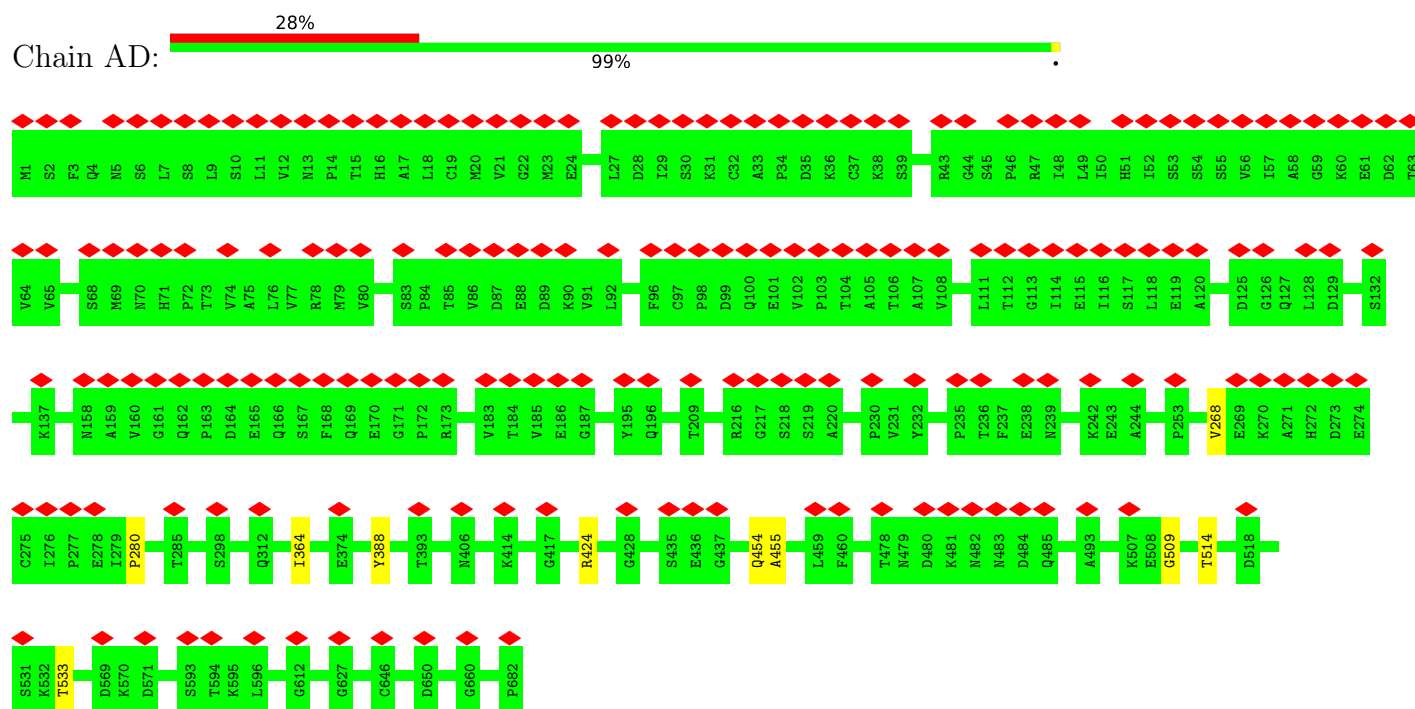




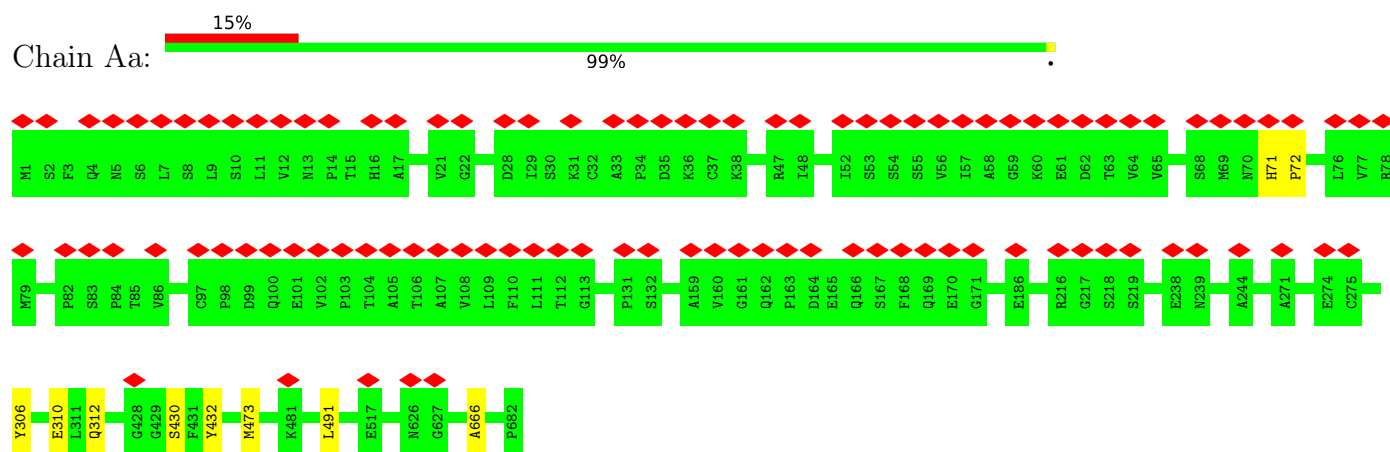
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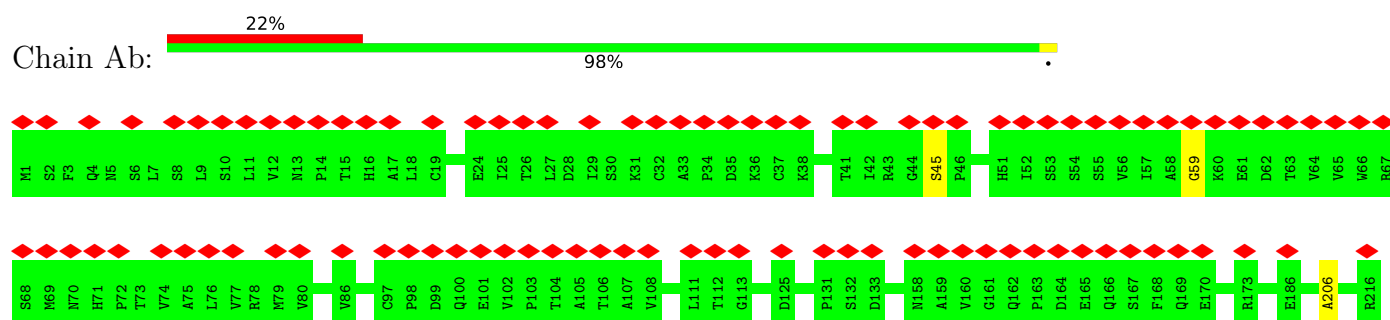
- Molecule 2: Inactive protein-arginine deiminase type-6

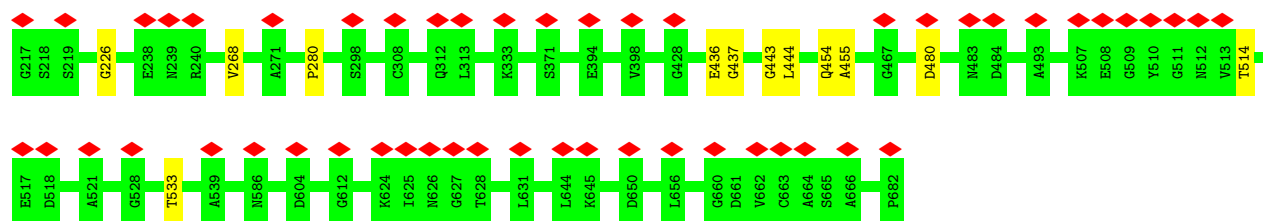


- Molecule 2: Inactive protein-arginine deiminase type-6

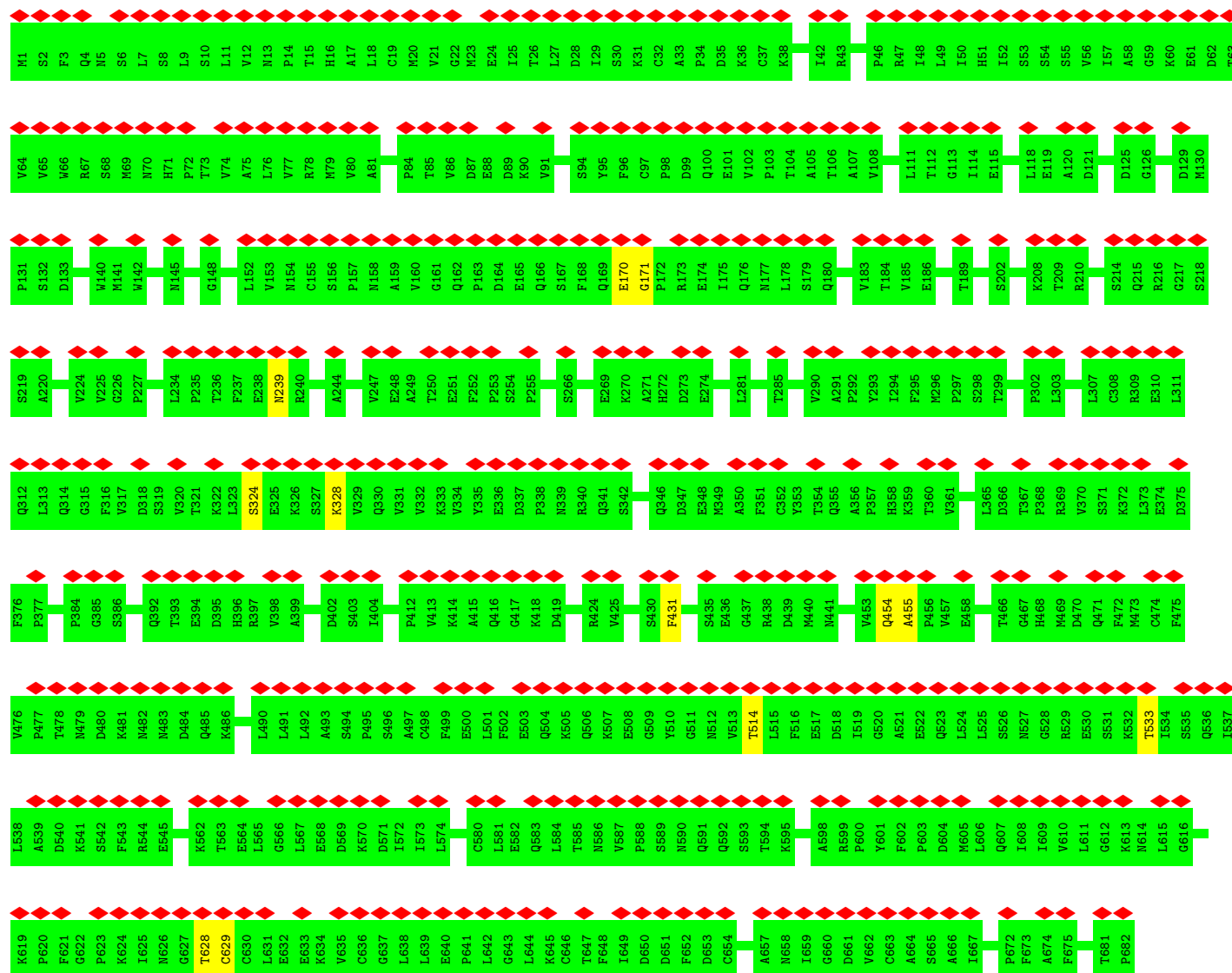


- Molecule 2: Inactive protein-arginine deiminase type-6



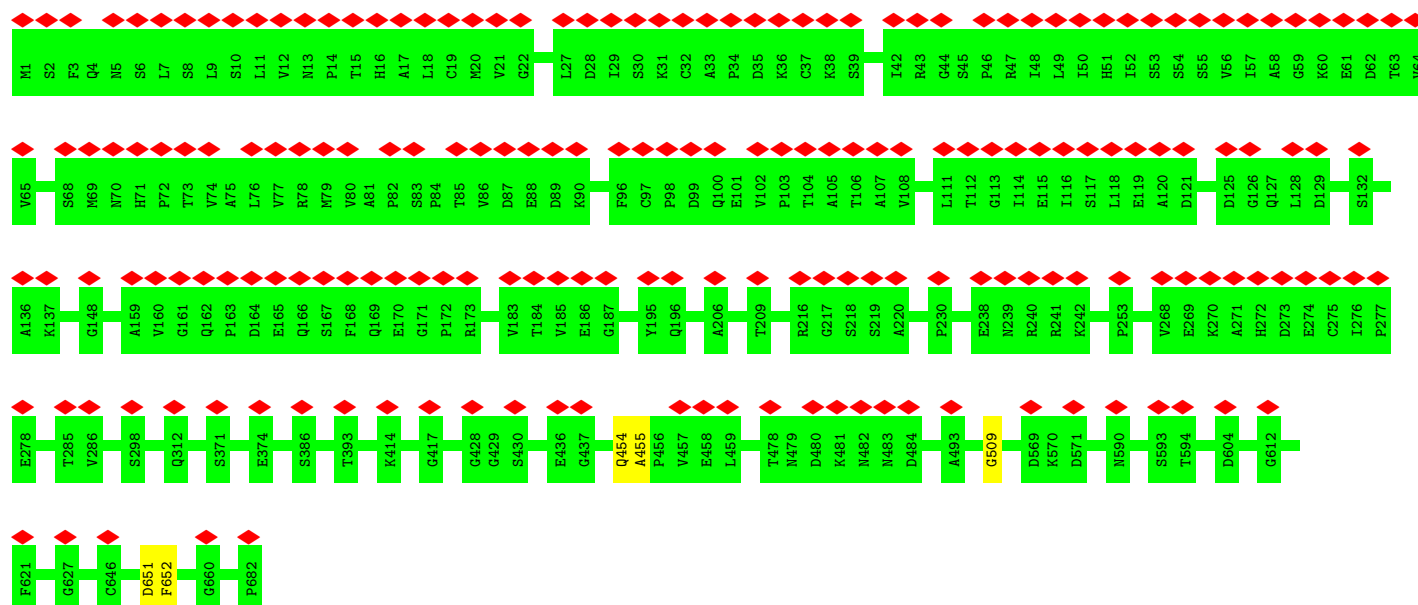


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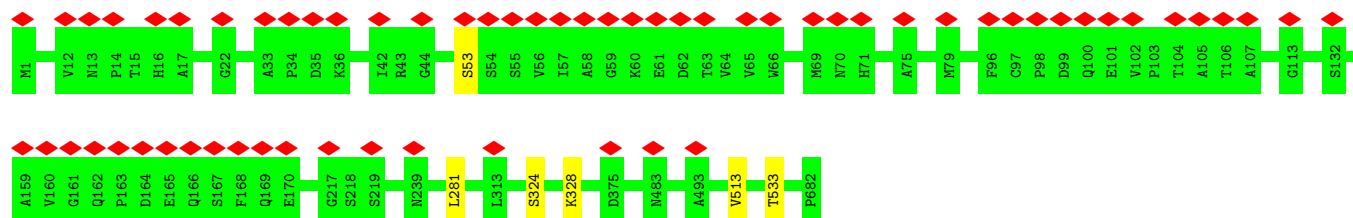


• Molecule 2: Inactive protein-arginine deiminase type-6

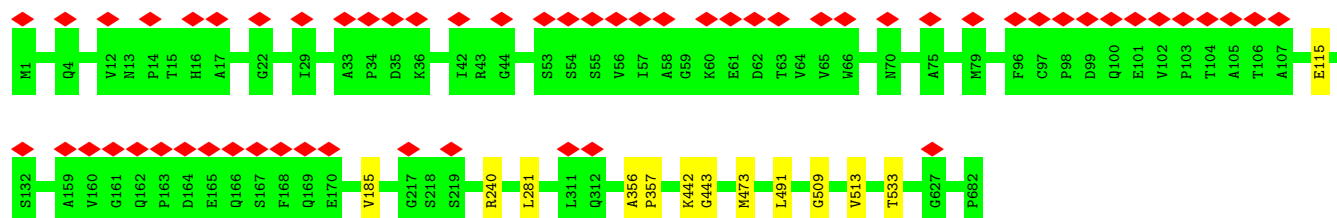




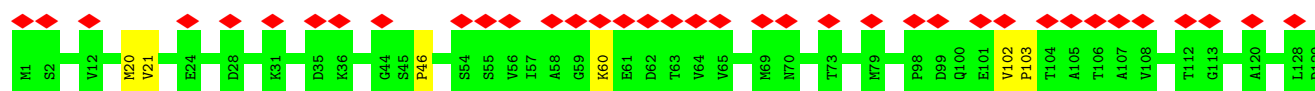
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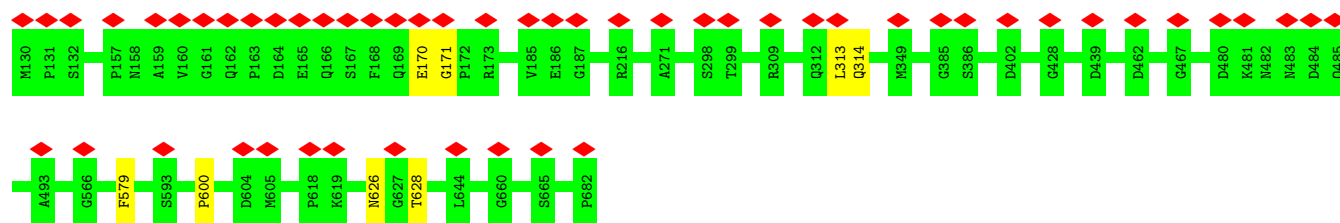


- Molecule 2: Inactive protein-arginine deiminase type-6

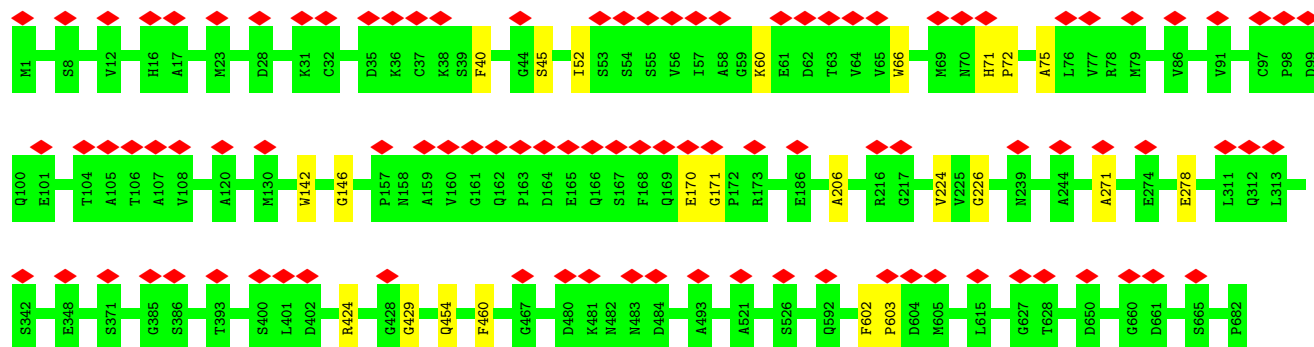


- Molecule 2: Inactive protein-arginine deiminase type-6

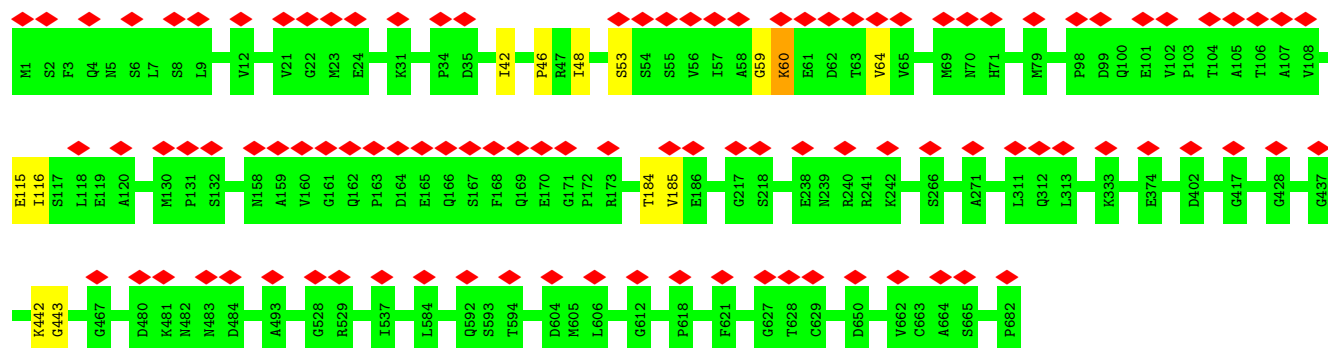




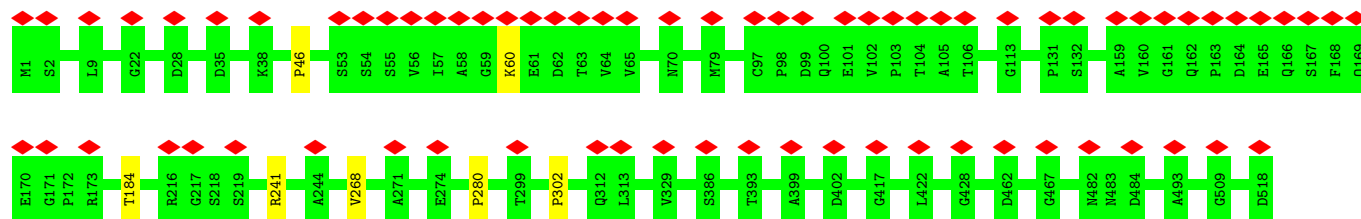
• Molecule 2: Inactive protein-arginine deiminase type-6

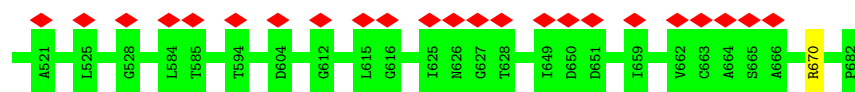


• Molecule 2: Inactive protein-arginine deiminase type-6

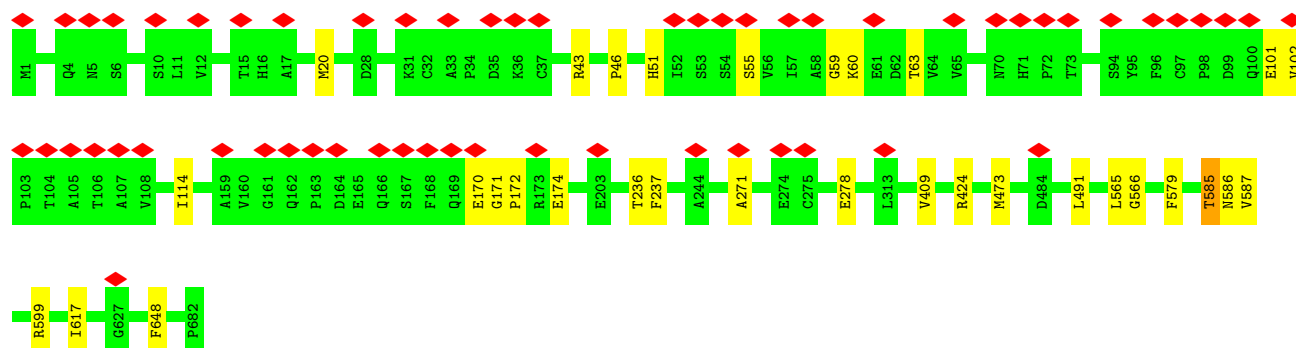


• Molecule 2: Inactive protein-arginine deiminase type-6

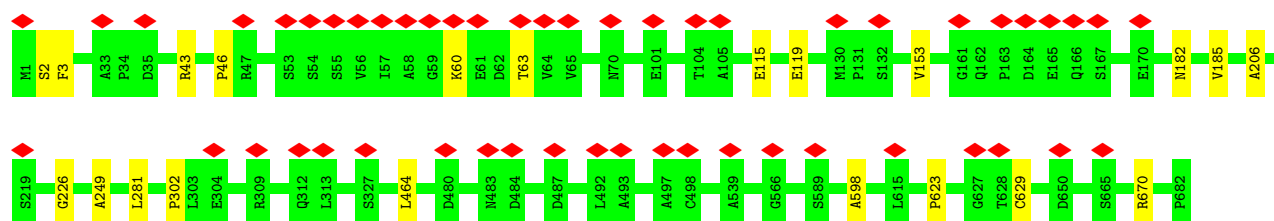




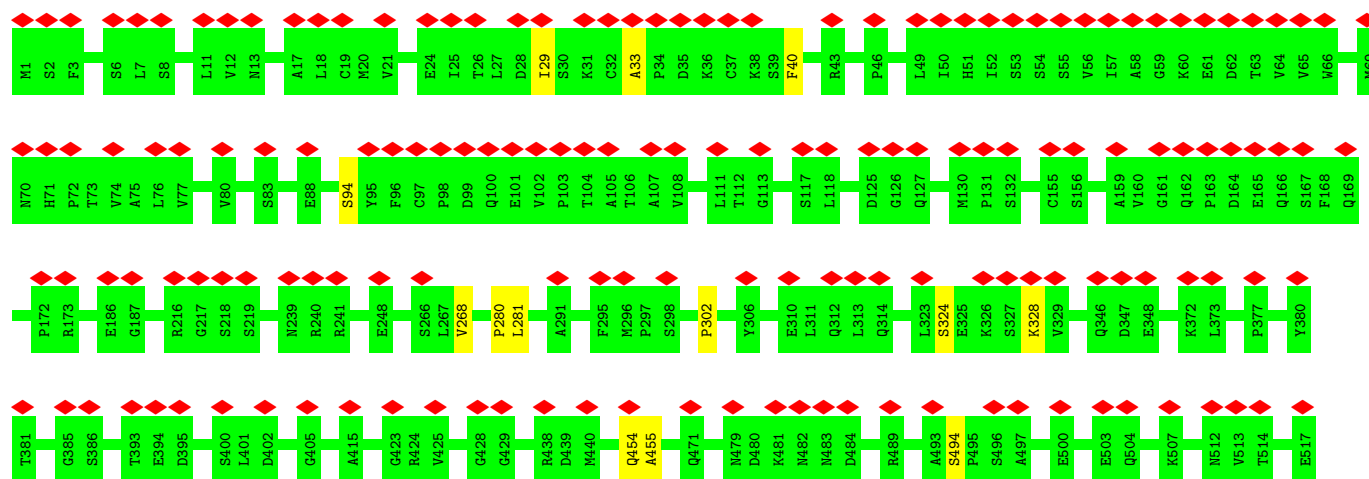
- Molecule 2: Inactive protein-arginine deiminase type-6

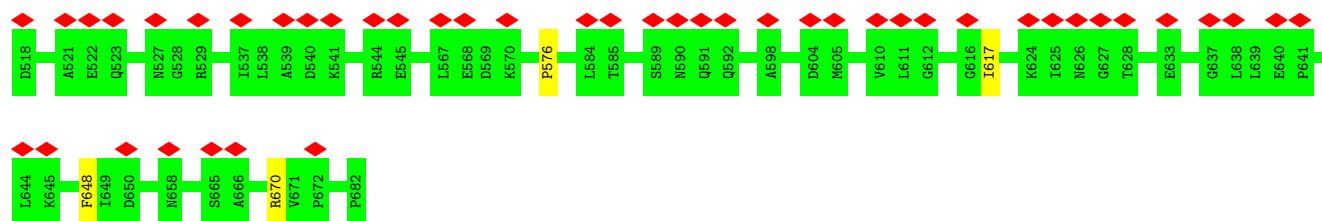


- Molecule 2: Inactive protein-arginine deiminase type-6

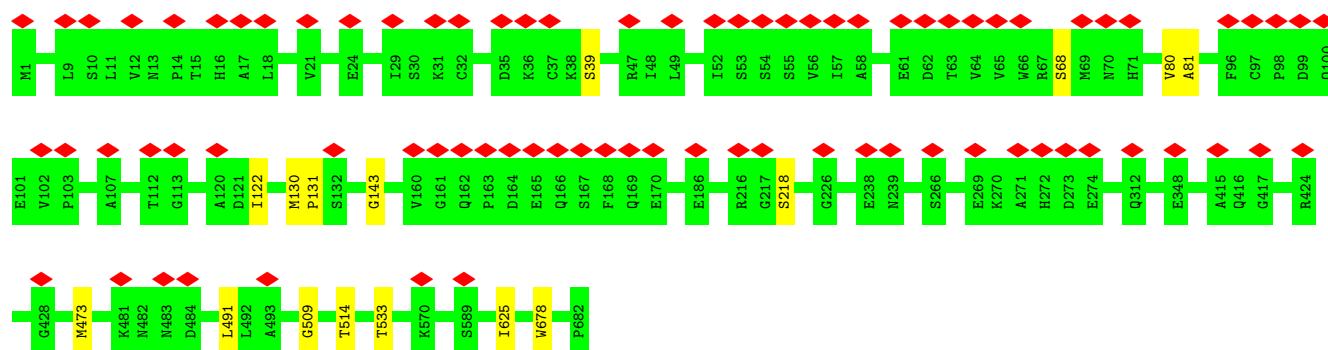


- Molecule 2: Inactive protein-arginine deiminase type-6

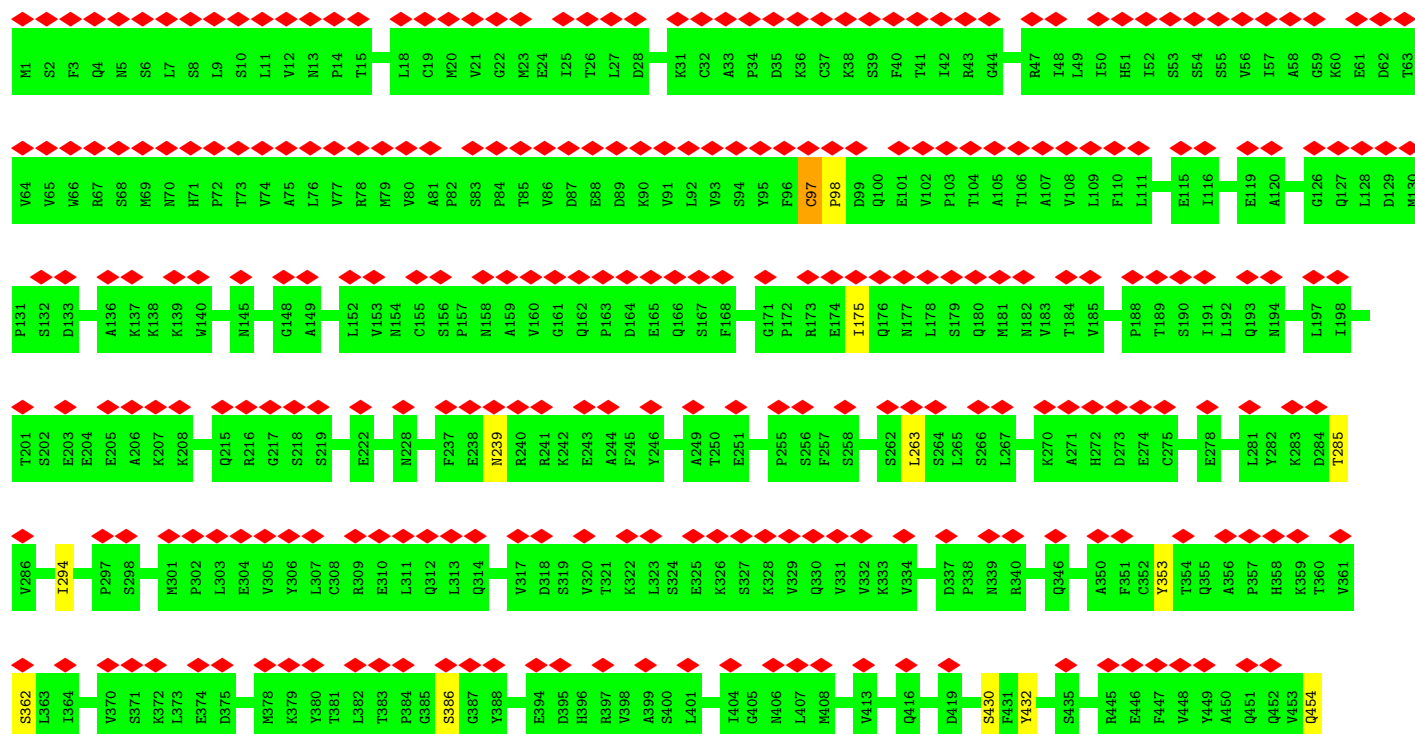


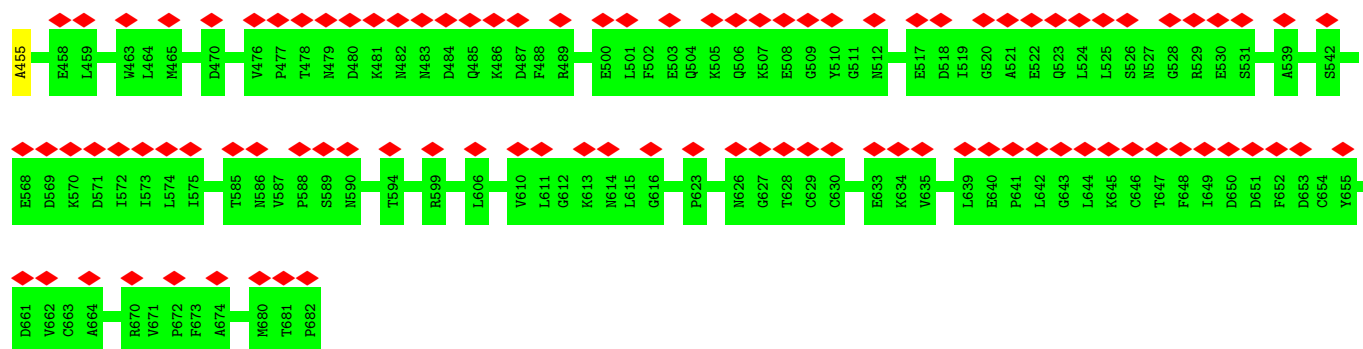


• Molecule 2: Inactive protein-arginine deiminase type-6

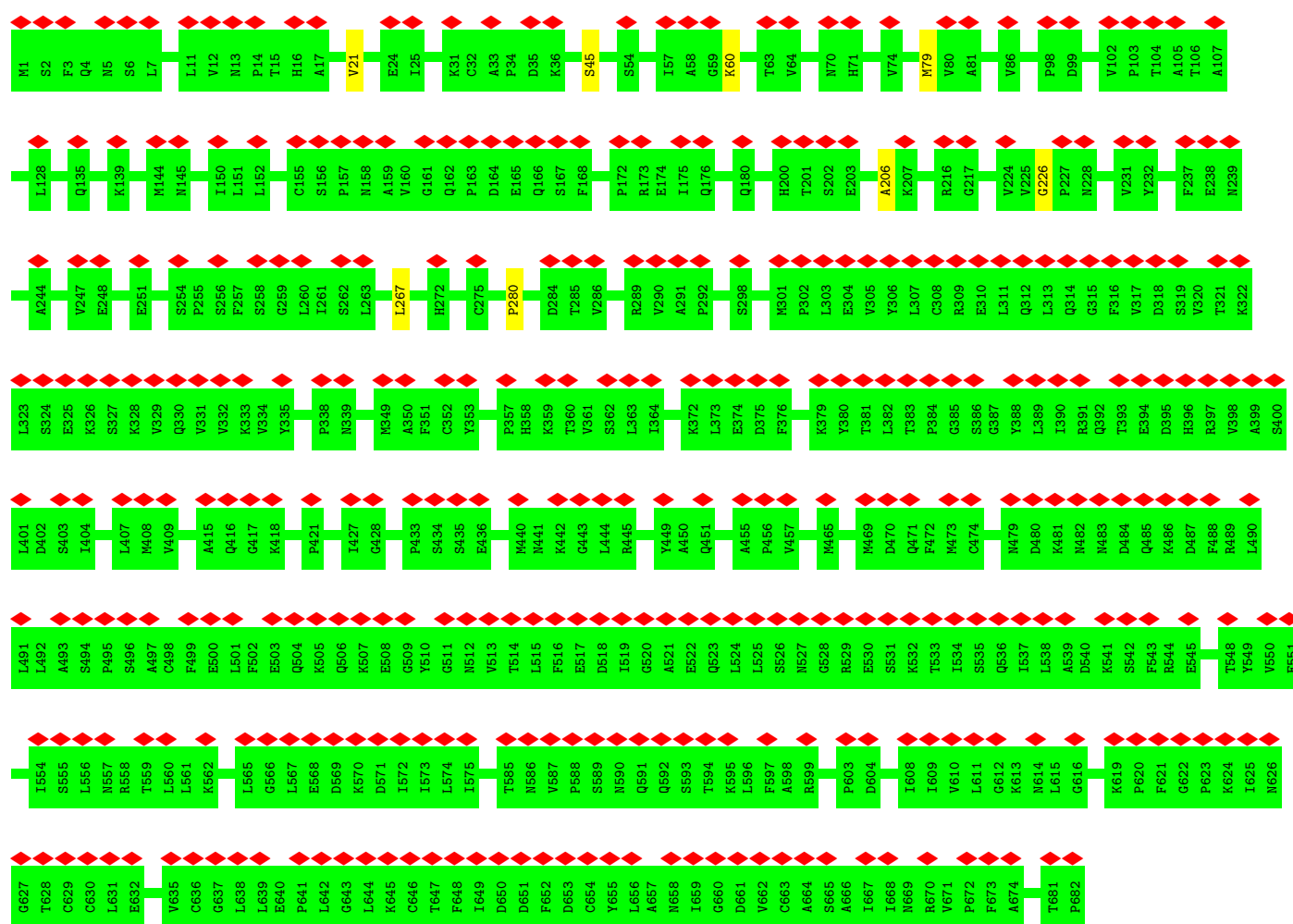


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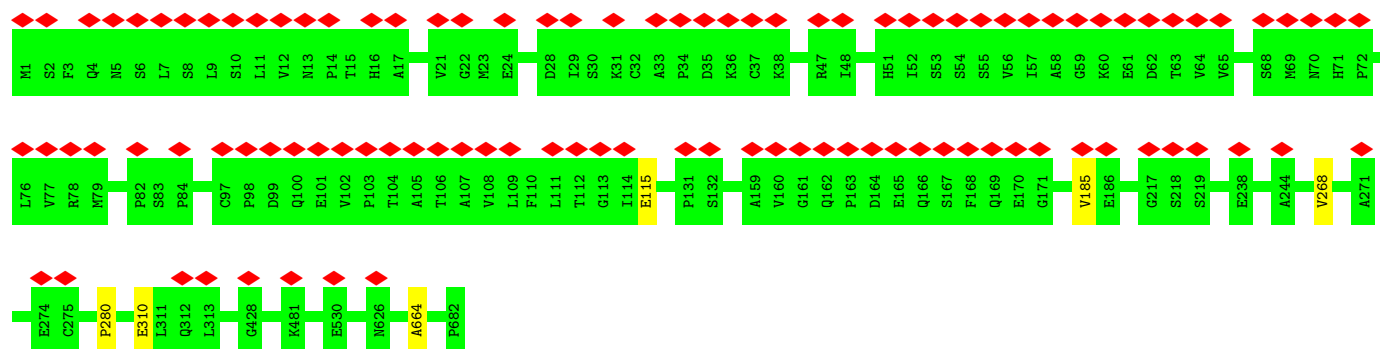


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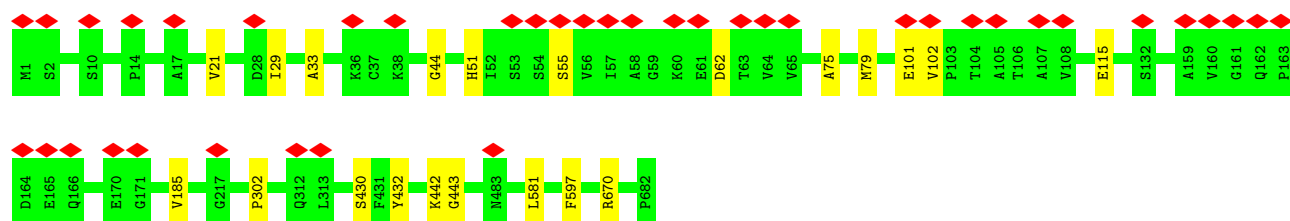


• Molecule 2: Inactive protein-arginine deiminase type-6

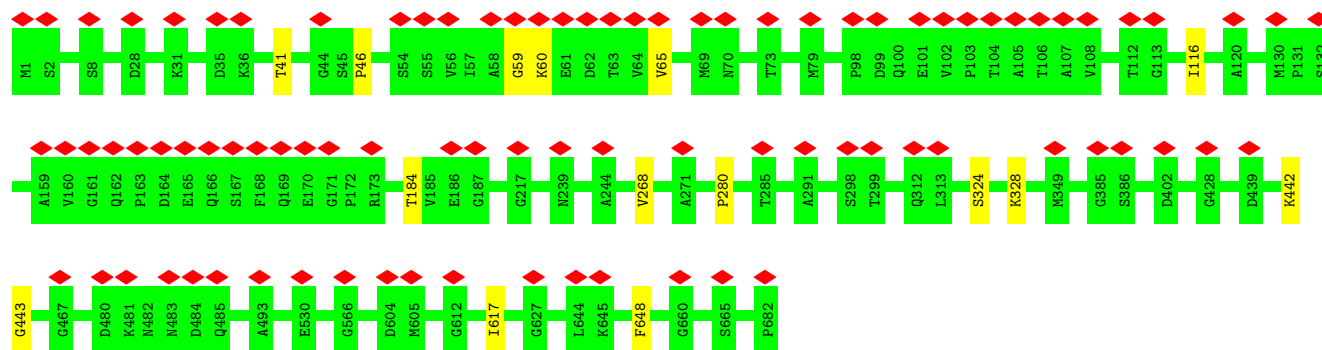




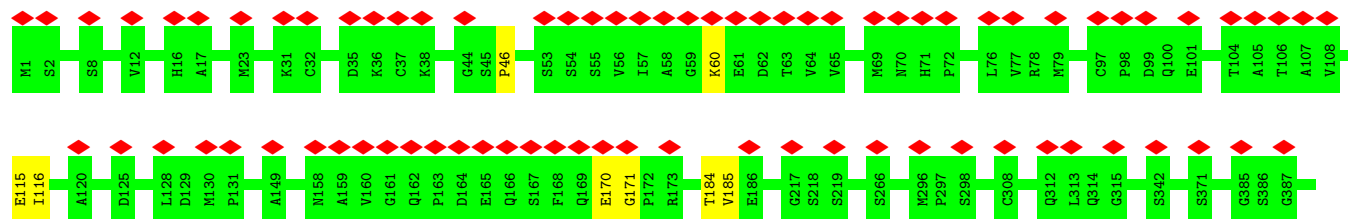
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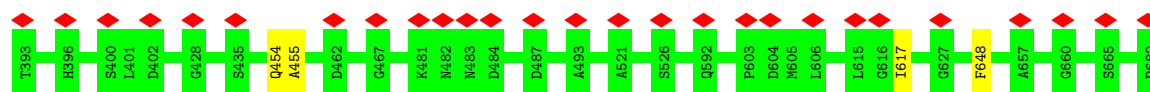


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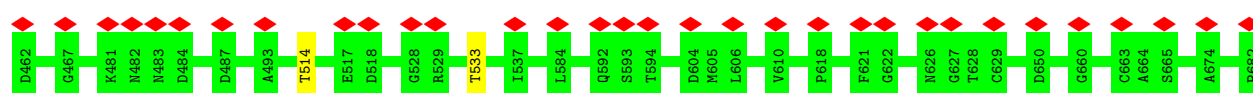
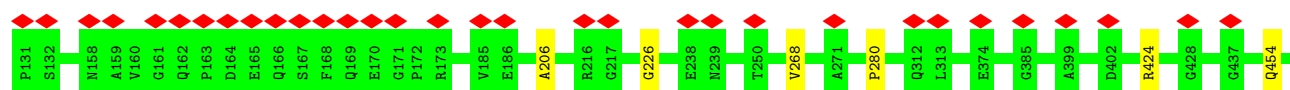
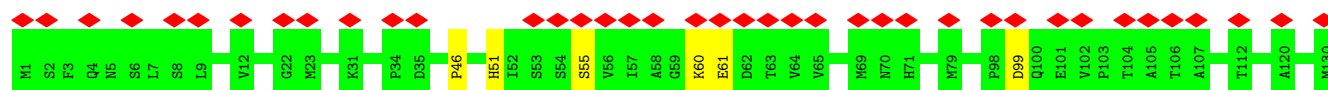


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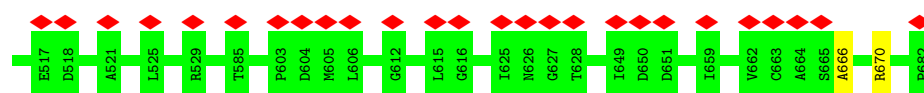
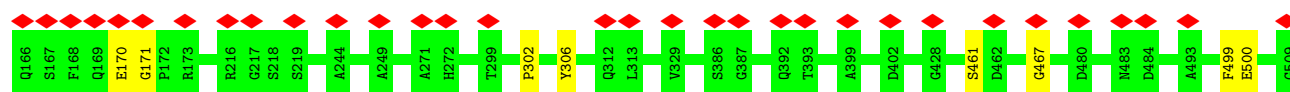
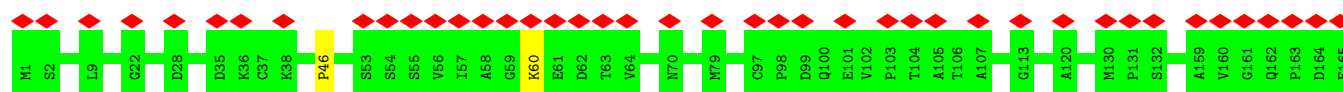




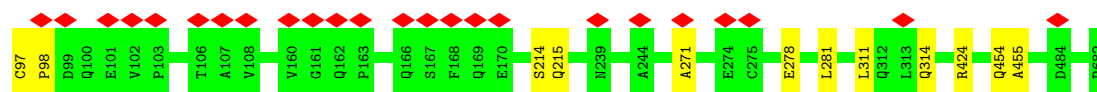
• Molecule 2: Inactive protein-arginine deiminase type-6



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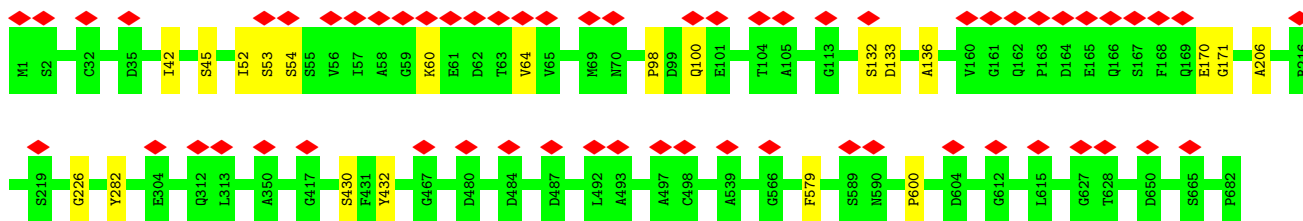


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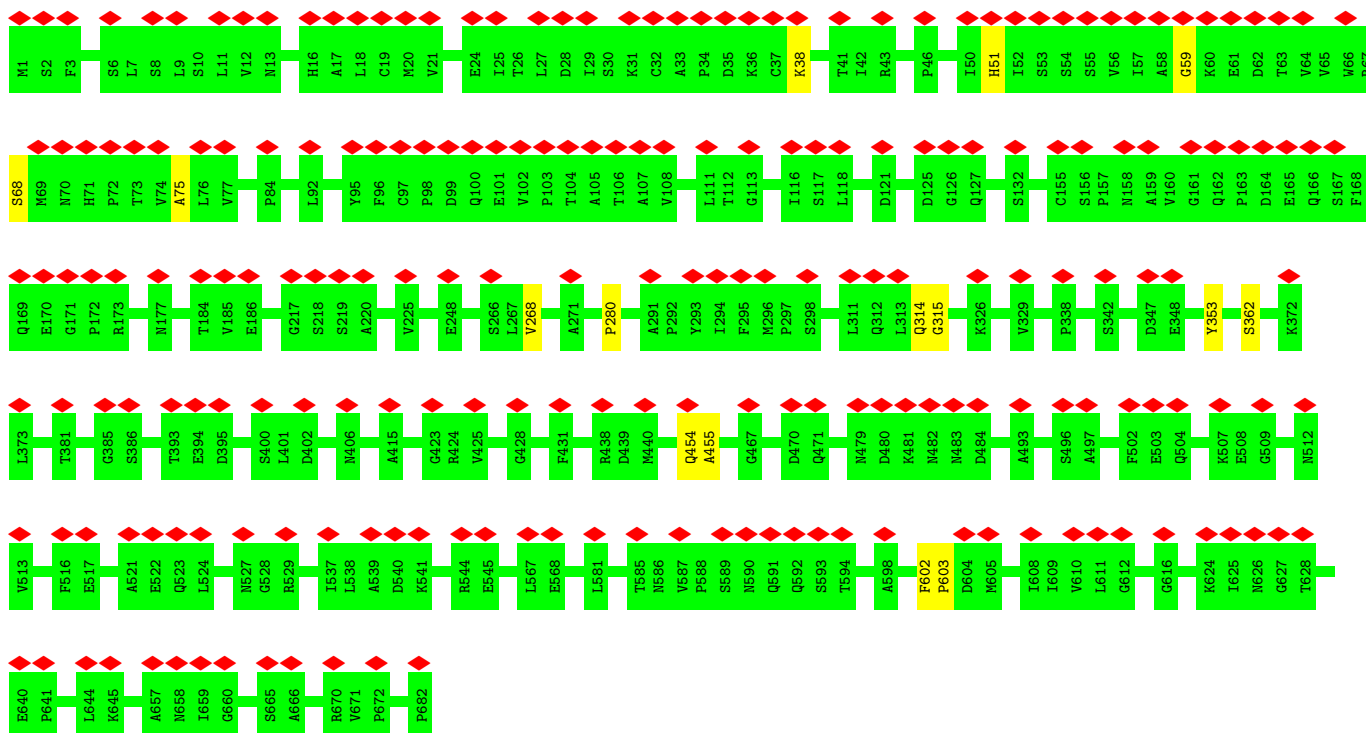


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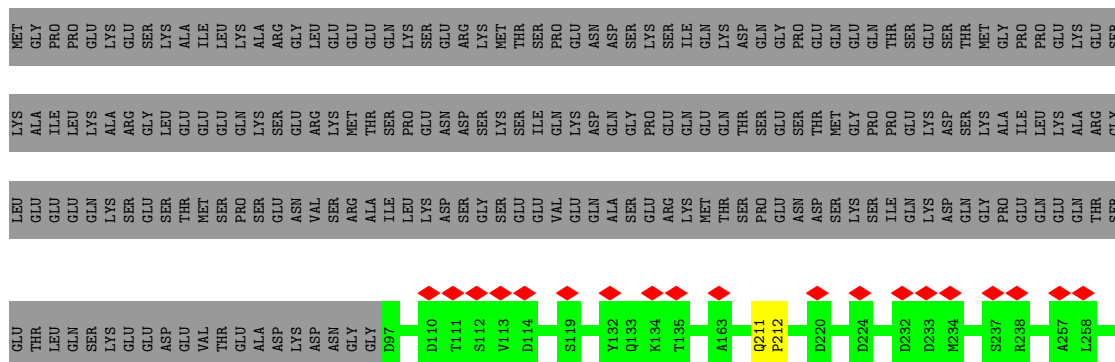
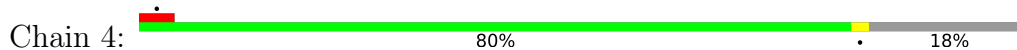




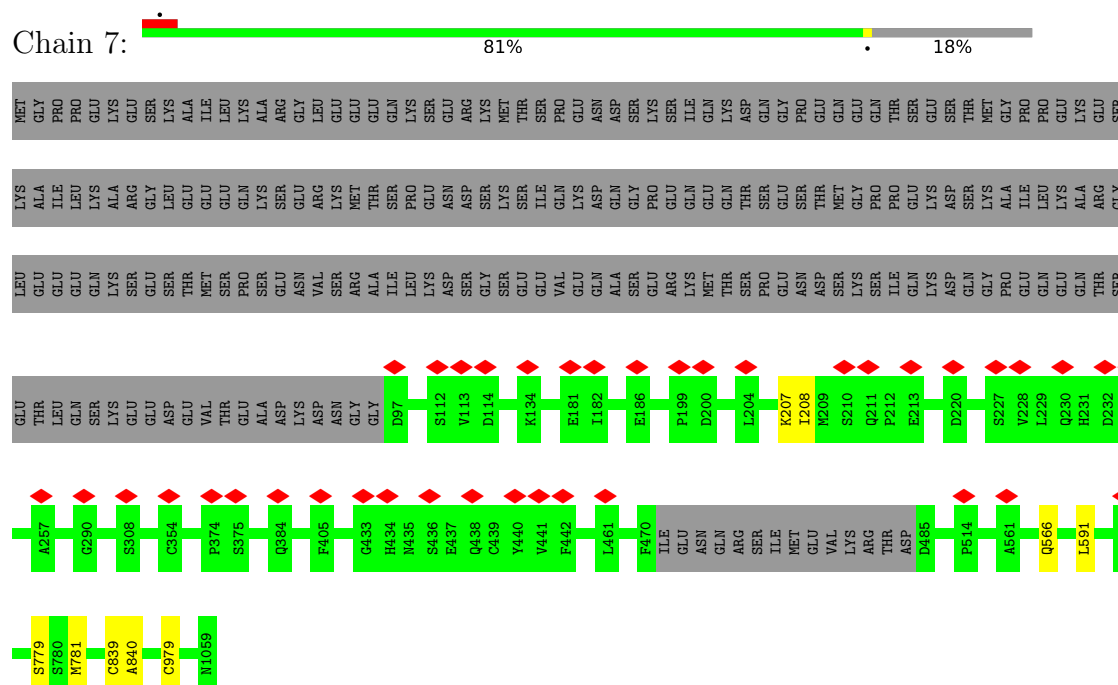
- Molecule 2: Inactive protein-arginine deiminase type-6



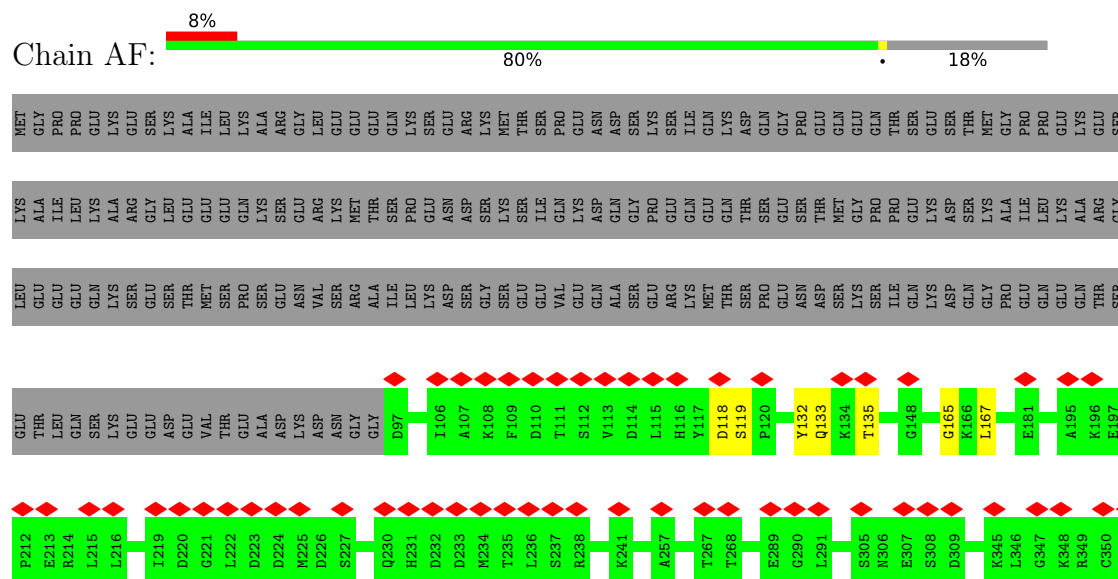
- Molecule 3: NACHT, LRR and PYD domains-containing protein 5

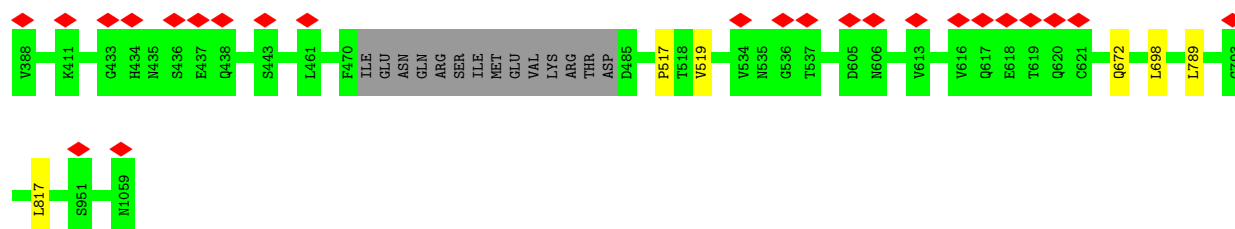


- Molecule 3: NACHT, LRR and PYD domains-containing protein 5

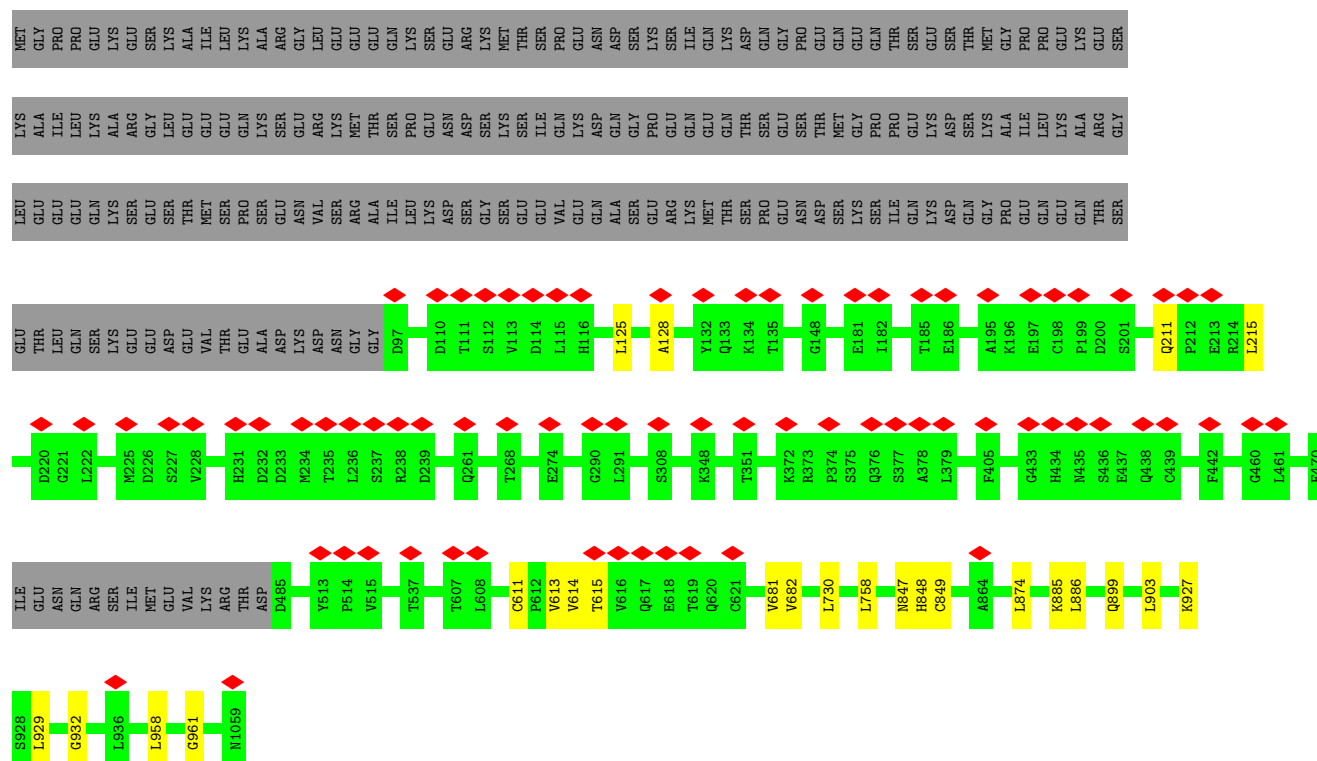
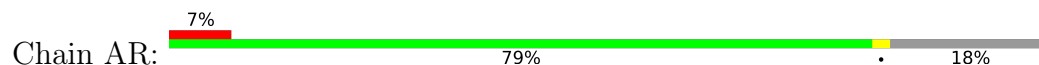


- Molecule 3: NACHT, LRR and PYD domains-containing protein 5

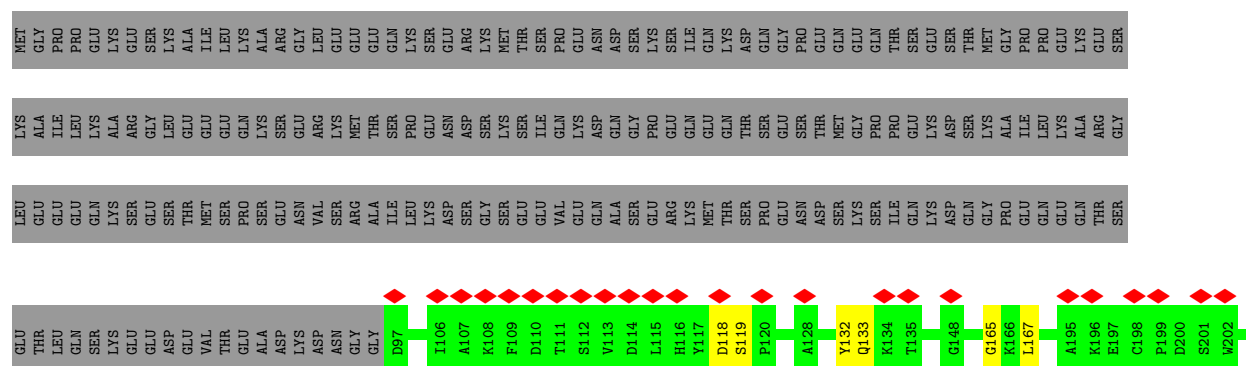
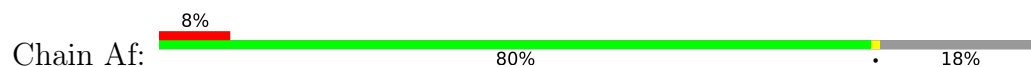


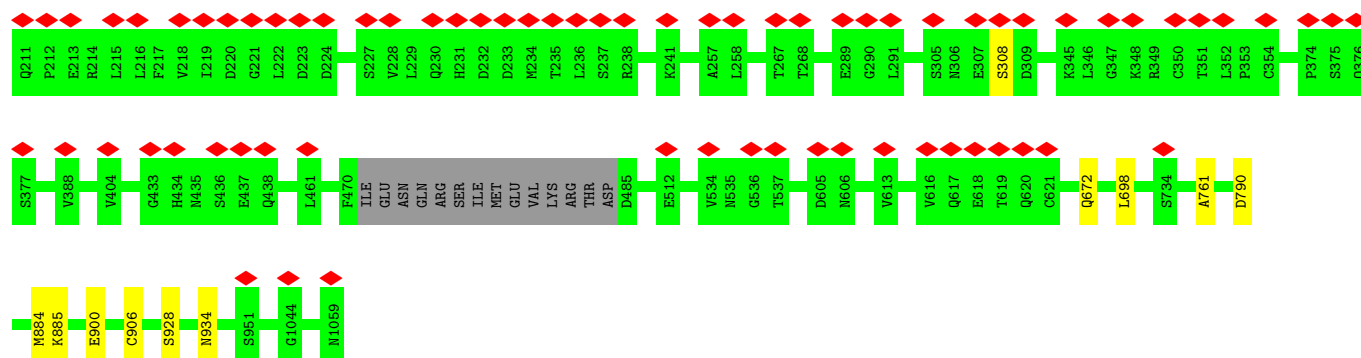


• Molecule 3: NACHT, LRR and PYD domains-containing protein 5



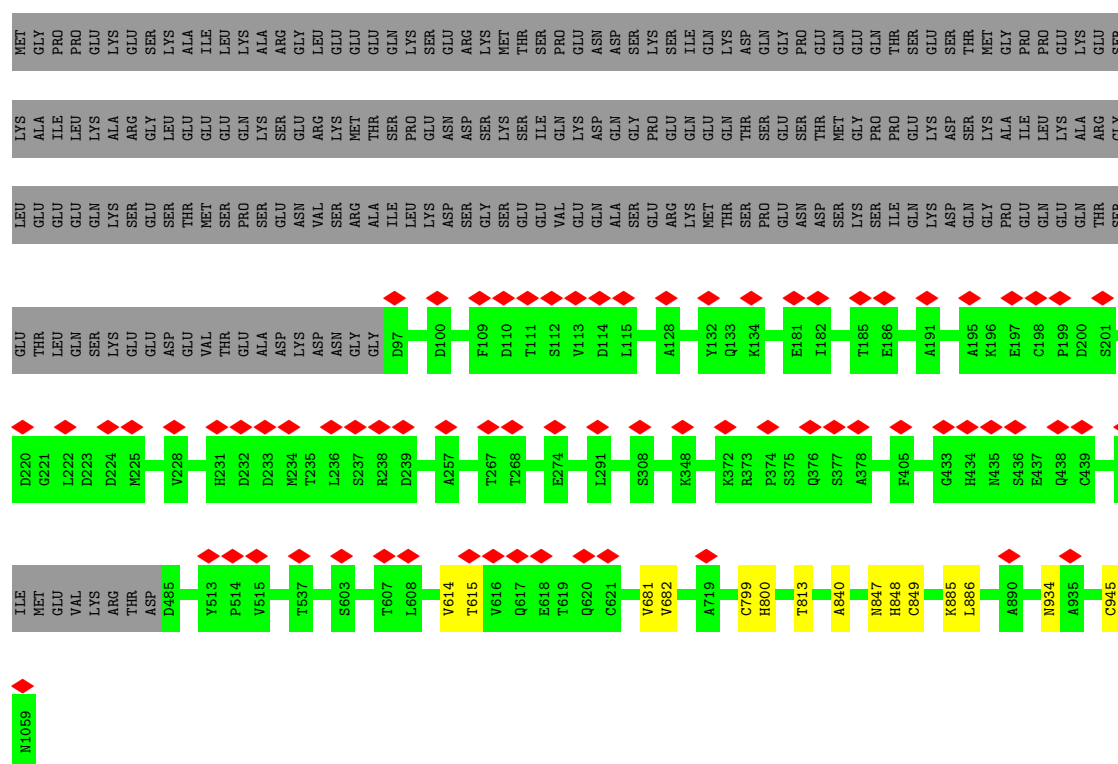
• Molecule 3: NACHT, LRR and PYD domains-containing protein 5





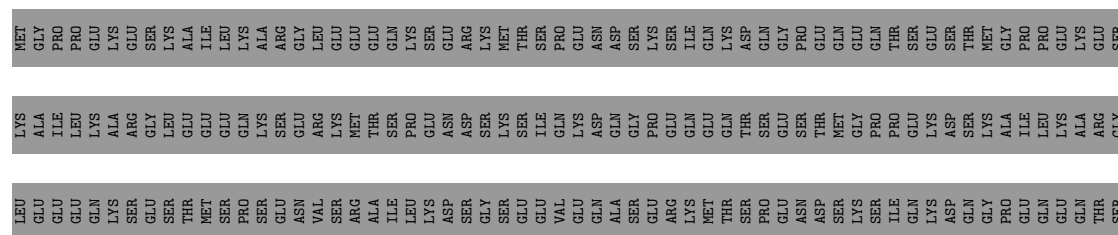
• Molecule 3: NACHT, LRR and PYD domains-containing protein 5

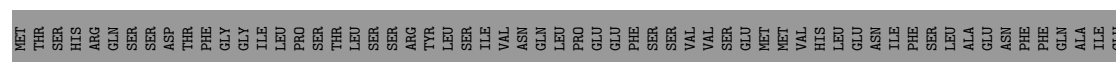
Chain Ak: 7% 80% 18%

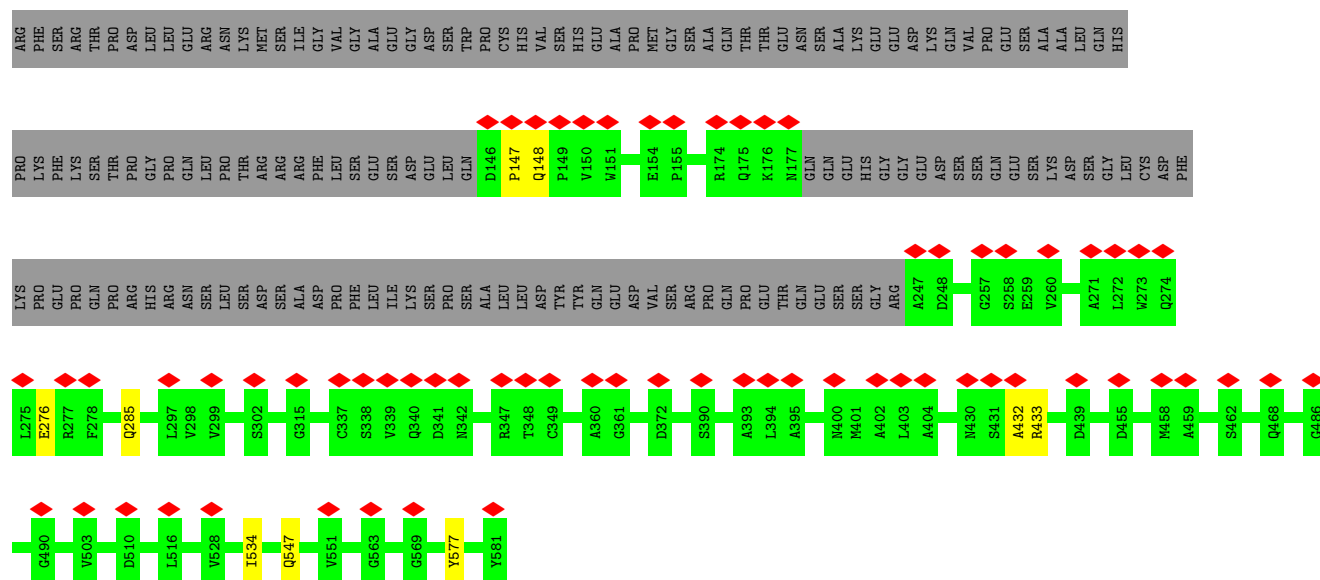


• Molecule 3: NACHT, LRR and PYD domains-containing protein 5

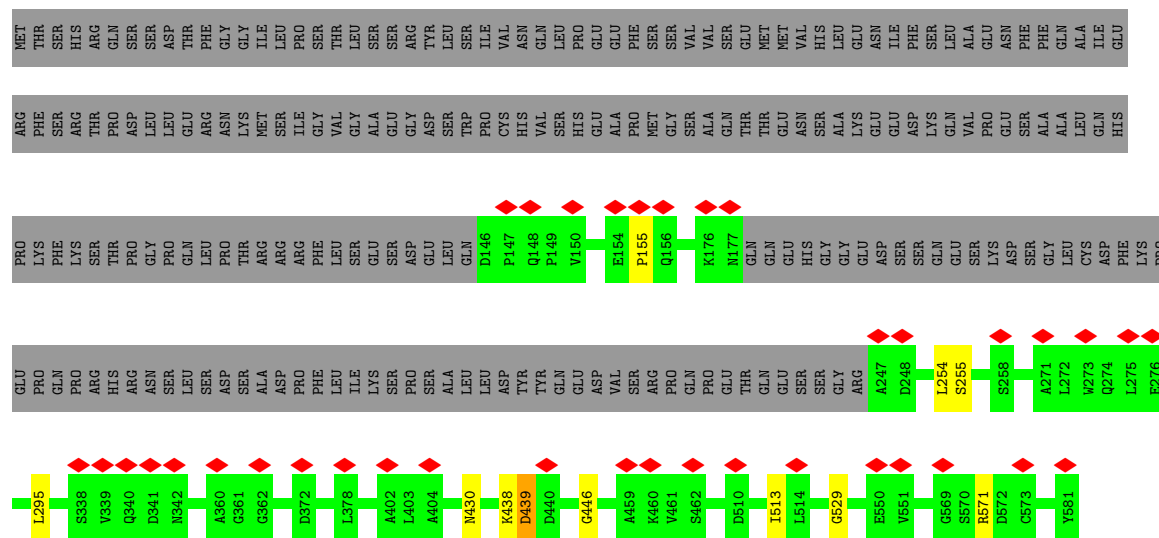
Chain M: 80% 18%



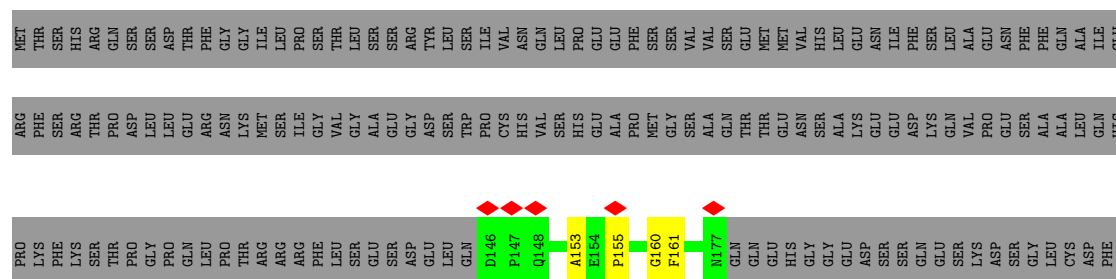


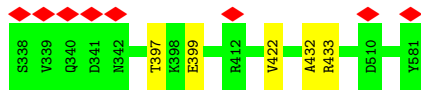


• Molecule 4: Transducin-like enhancer protein 6

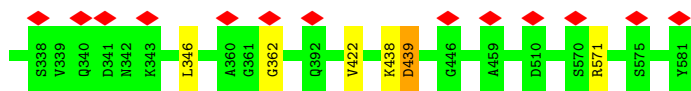


• Molecule 4: Transducin-like enhancer protein 6

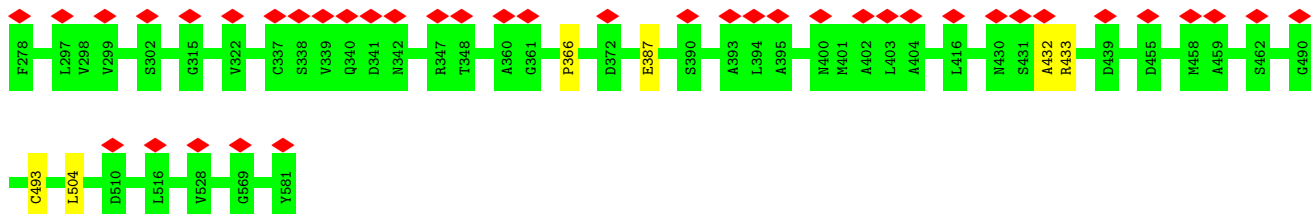




Chain Q: 61% . 37%



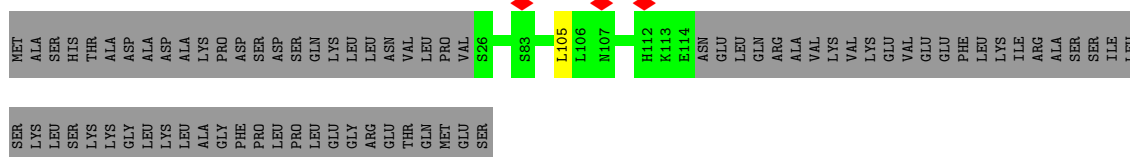
Chain X:



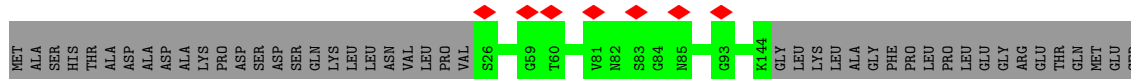
• Molecule 5: Oocyte-expressed protein homolog

Chain 6:  71% 27%

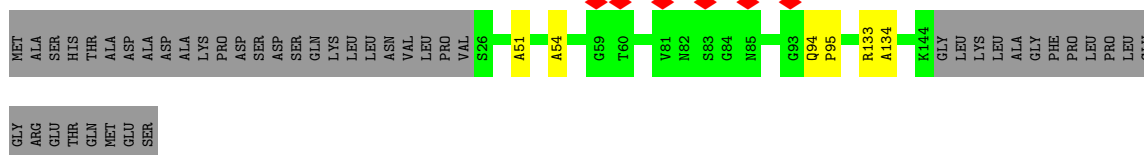
• Molecule 5: Oocyte-expressed protein homolog

Chain 9:  54% 46%

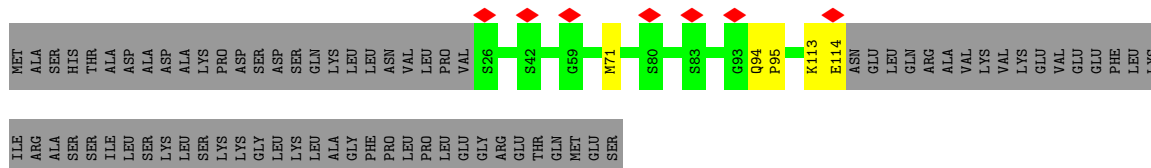
• Molecule 5: Oocyte-expressed protein homolog

Chain AQ:  73% 27%

• Molecule 5: Oocyte-expressed protein homolog

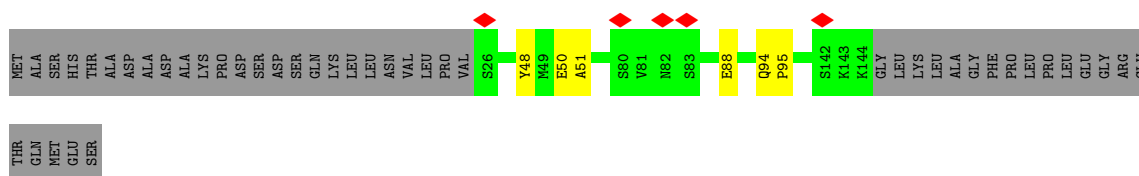
Chain Aj:  69% 27%

• Molecule 5: Oocyte-expressed protein homolog

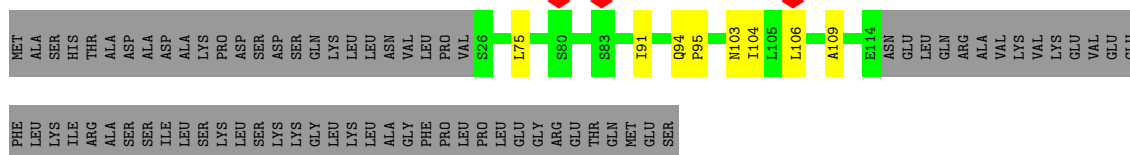
Chain Am:  51% 46%

• Molecule 5: Oocyte-expressed protein homolog

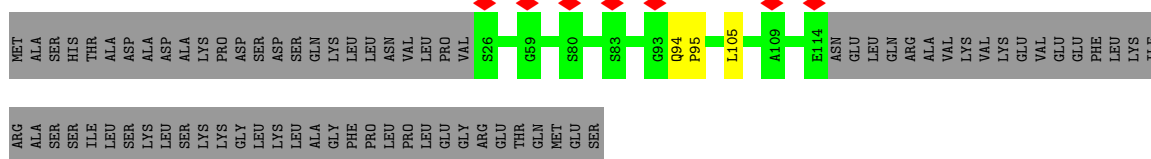
Chain O:  69% 27%



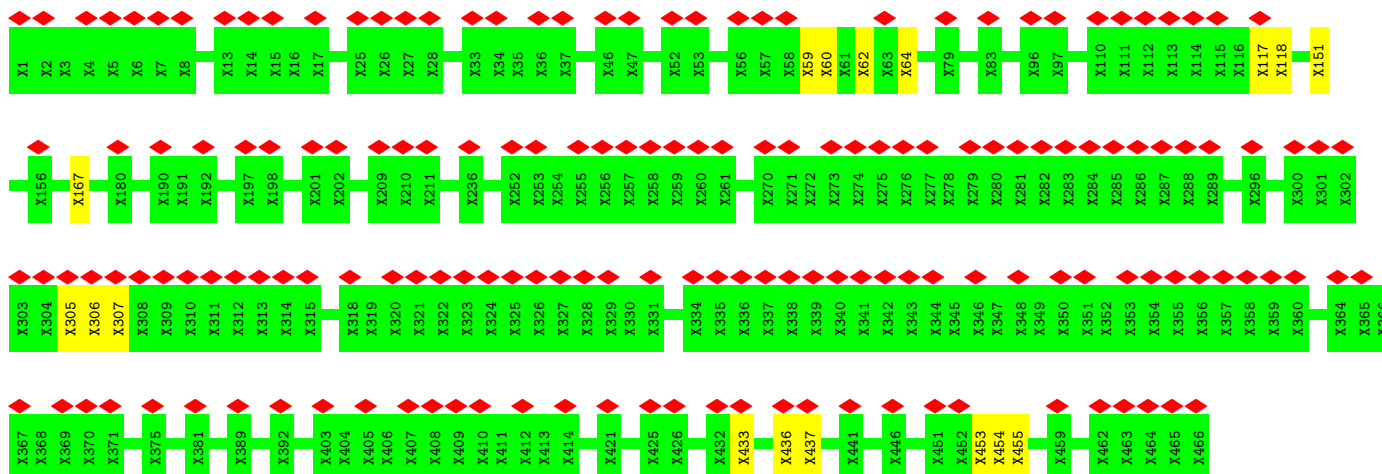
- Molecule 5: Oocyte-expressed protein homolog



- Molecule 5: Oocyte-expressed protein homolog

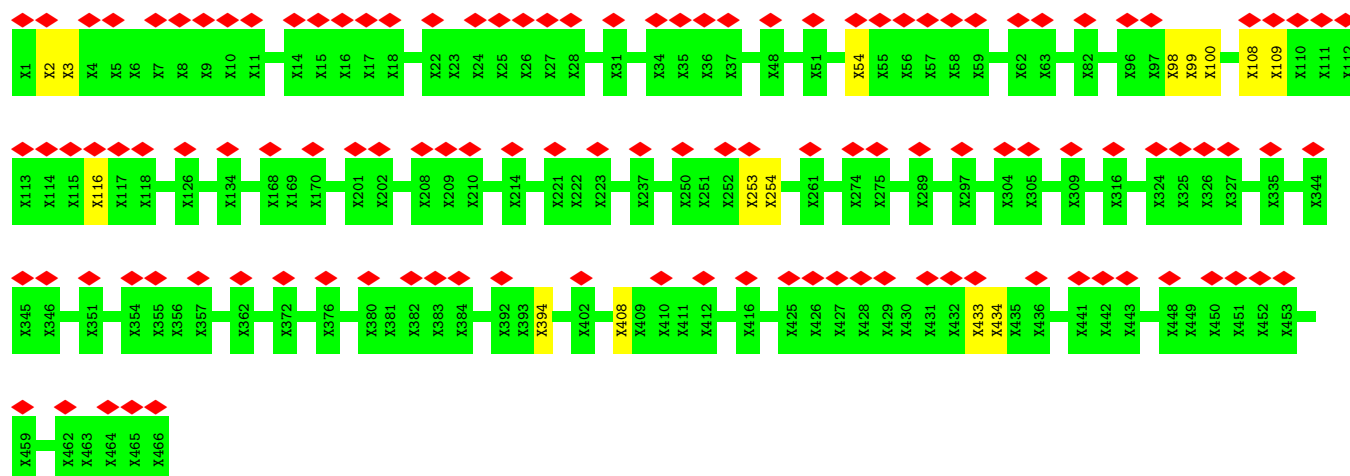


- Molecule 6: F-box/WD repeat-containing protein



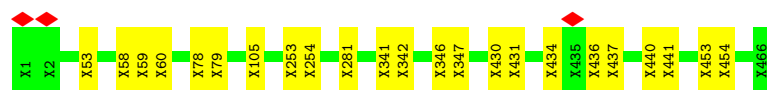
- Molecule 6: F-box/WD repeat-containing protein





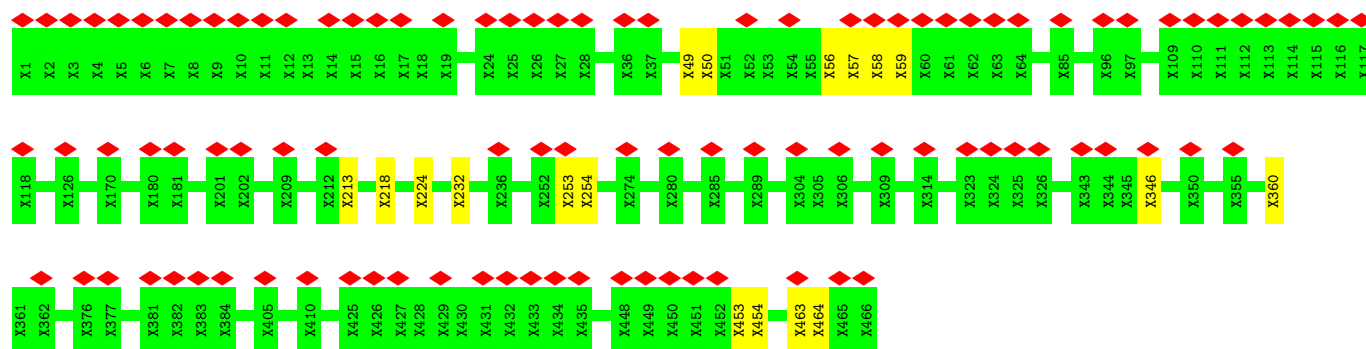
- Molecule 6: F-box/WD repeat-containing protein

Chain AN: 95% 5%



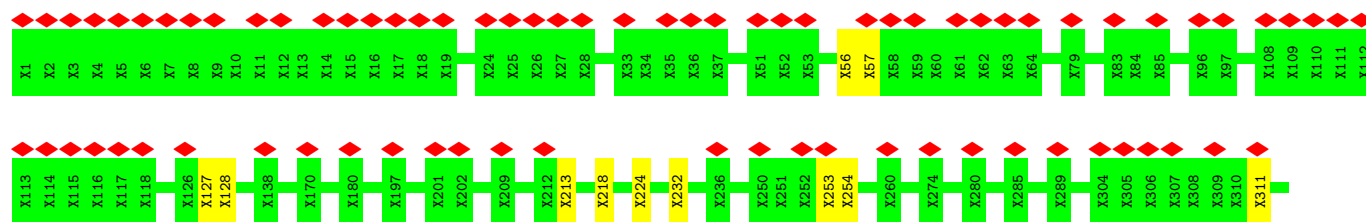
- Molecule 6: F-box/WD repeat-containing protein

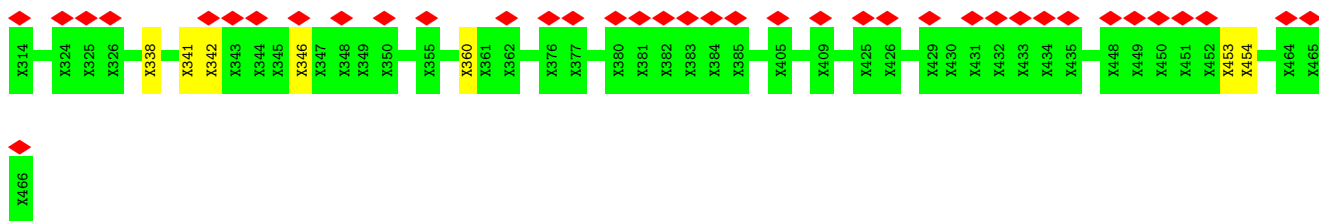
Chain AX: 22% 96% .



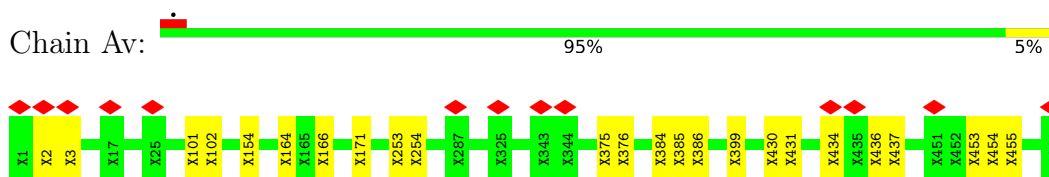
- Molecule 6: F-box/WD repeat-containing protein

Chain At: 24% 96% .

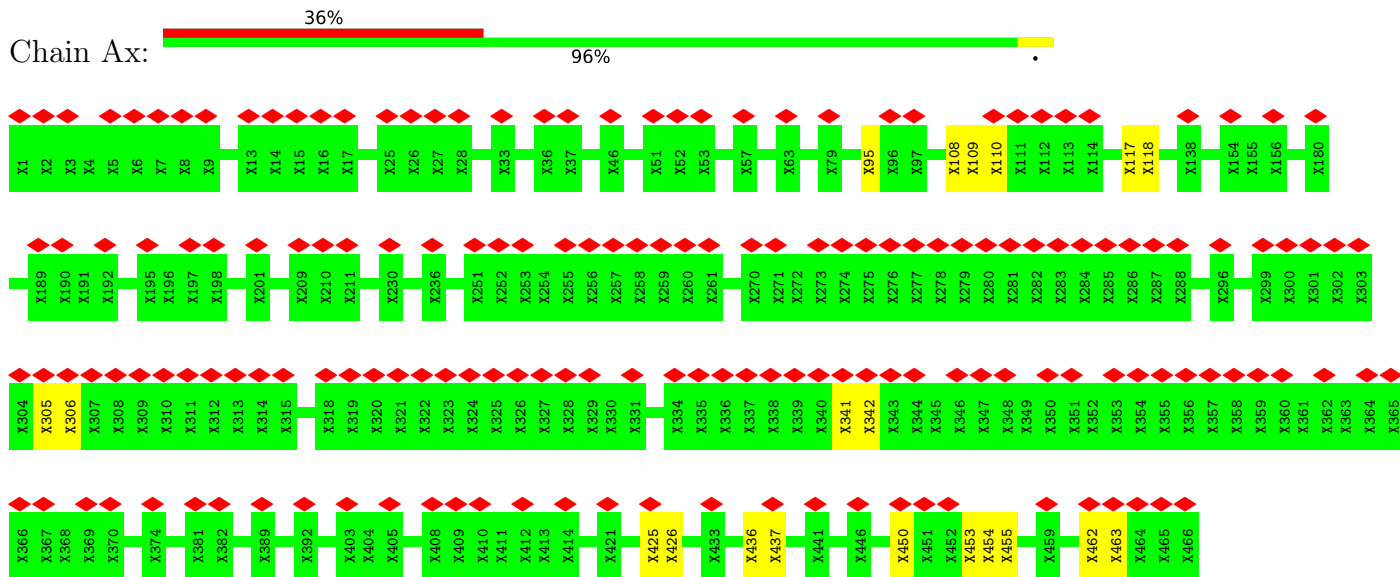




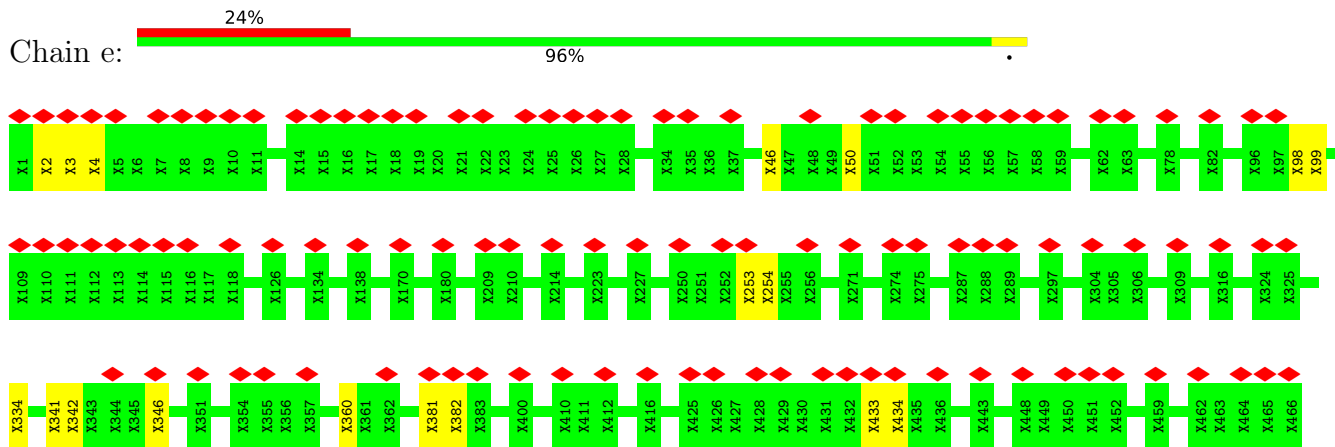
- Molecule 6: F-box/WD repeat-containing protein



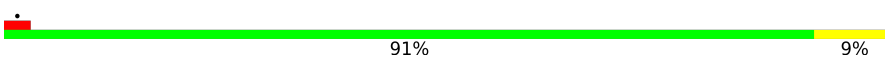
- Molecule 6: F-box/WD repeat-containing protein

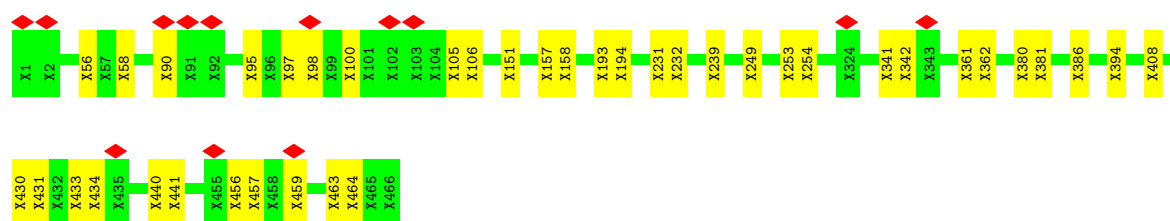


- Molecule 6: F-box/WD repeat-containing protein

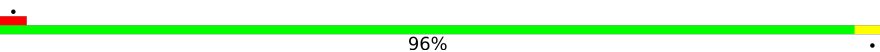


- Molecule 6: F-box/WD repeat-containing protein

Chain g: 

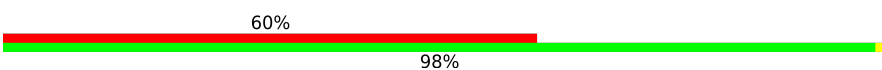


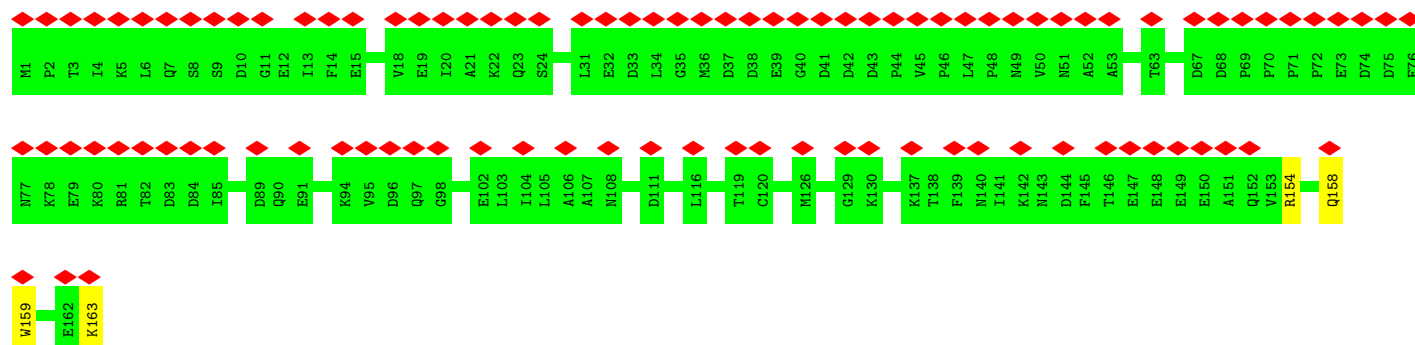
- Molecule 6: F-box/WD repeat-containing protein

Chain s: 

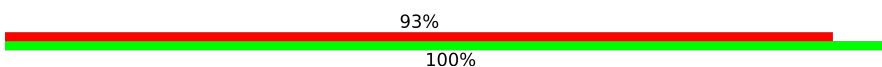


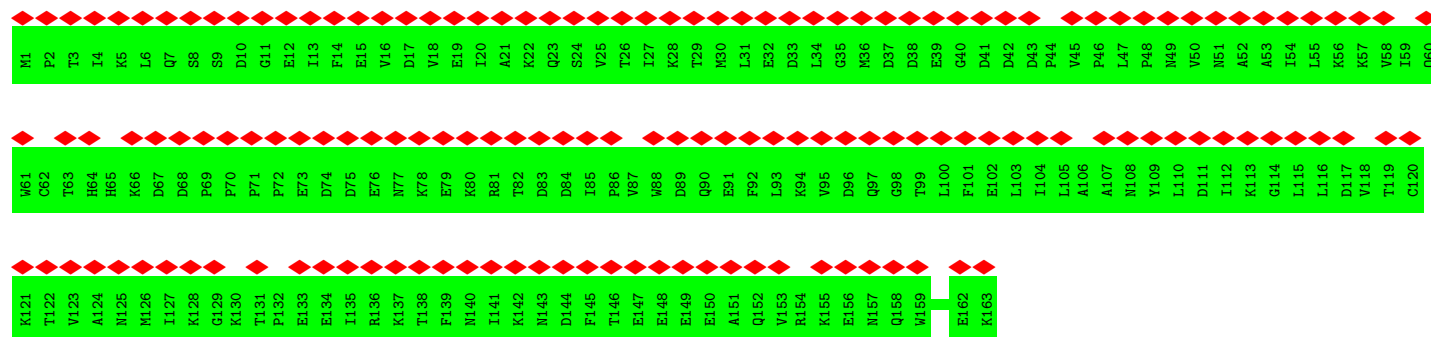
- Molecule 7: S-phase kinase-associated protein 1

Chain A2: 



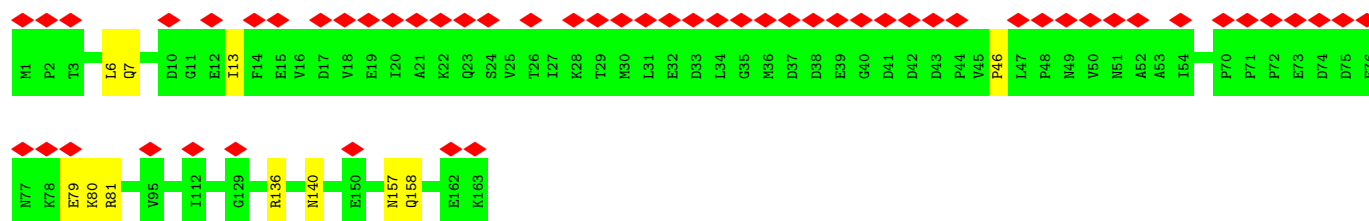
- Molecule 7: S-phase kinase-associated protein 1

Chain AM: 

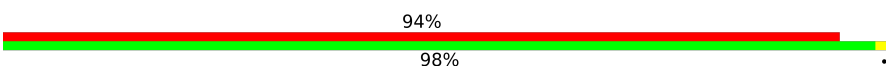


- Molecule 7: S-phase kinase-associated protein 1

Chain AO: 

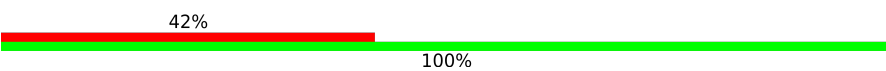


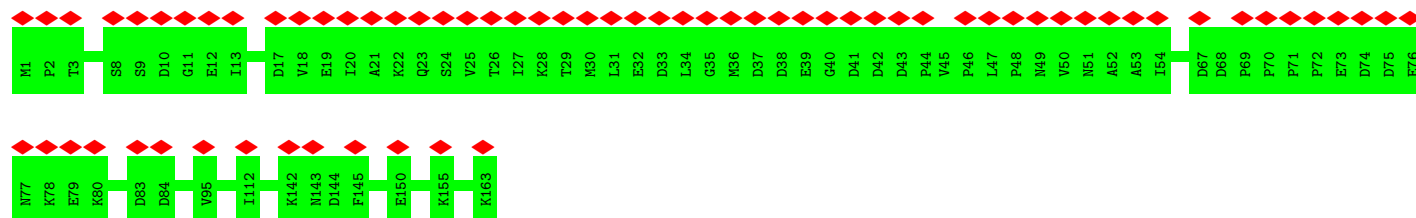
- Molecule 7: S-phase kinase-associated protein 1

Chain AY: 

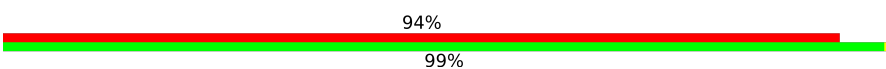


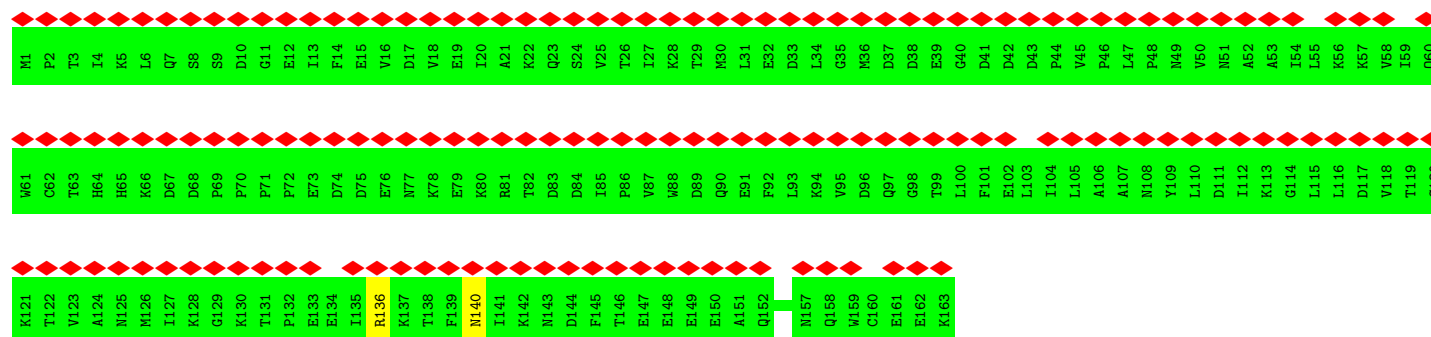
- Molecule 7: S-phase kinase-associated protein 1

Chain AZ: 

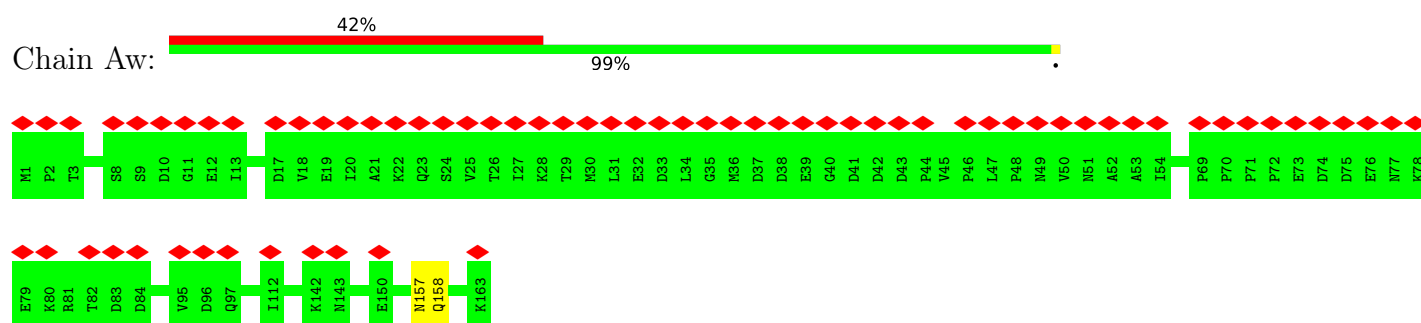


- Molecule 7: S-phase kinase-associated protein 1

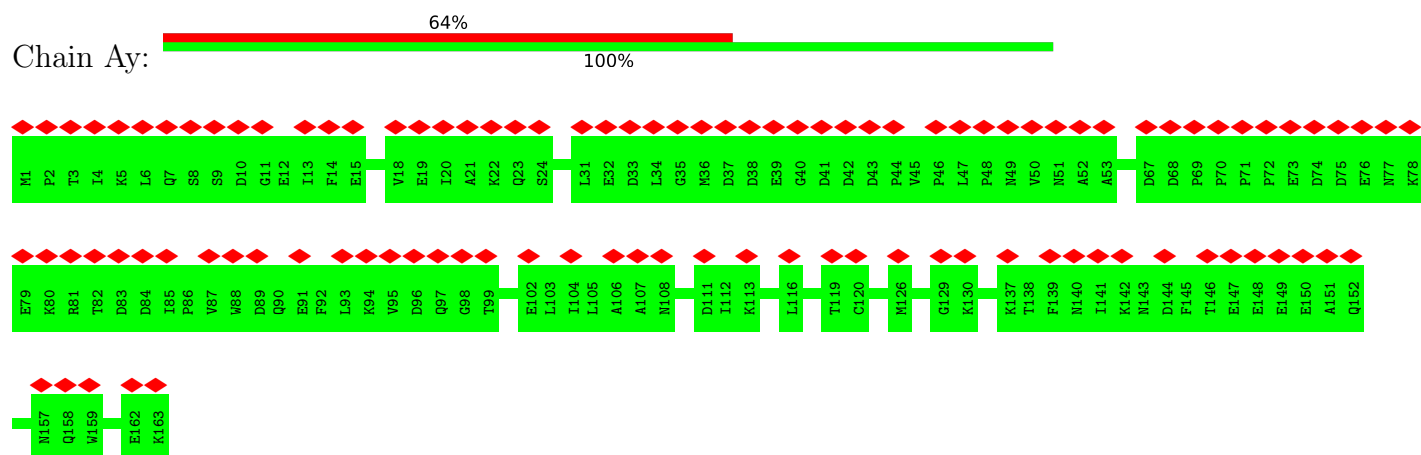
Chain Au: 



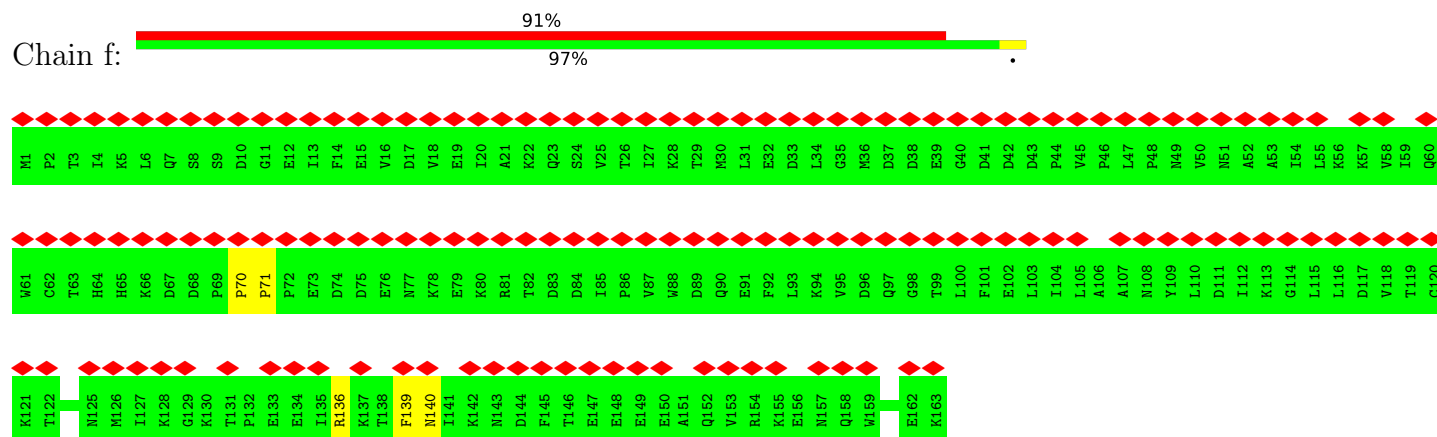
- Molecule 7: S-phase kinase-associated protein 1



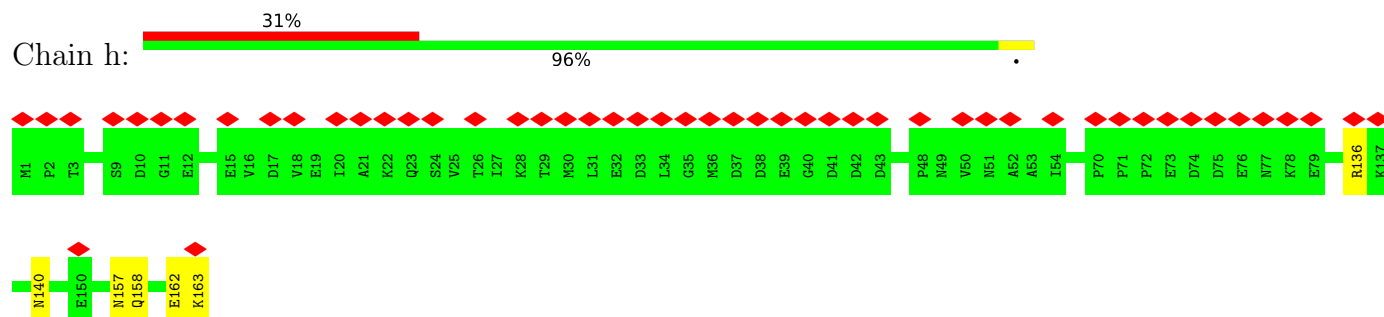
• Molecule 7: S-phase kinase-associated protein 1



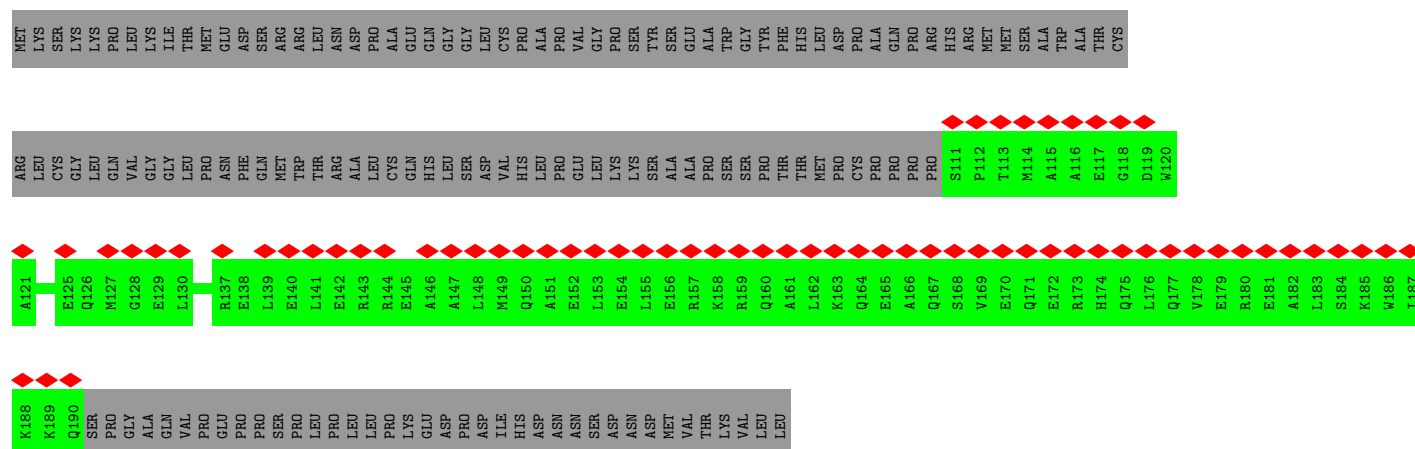
• Molecule 7: S-phase kinase-associated protein 1



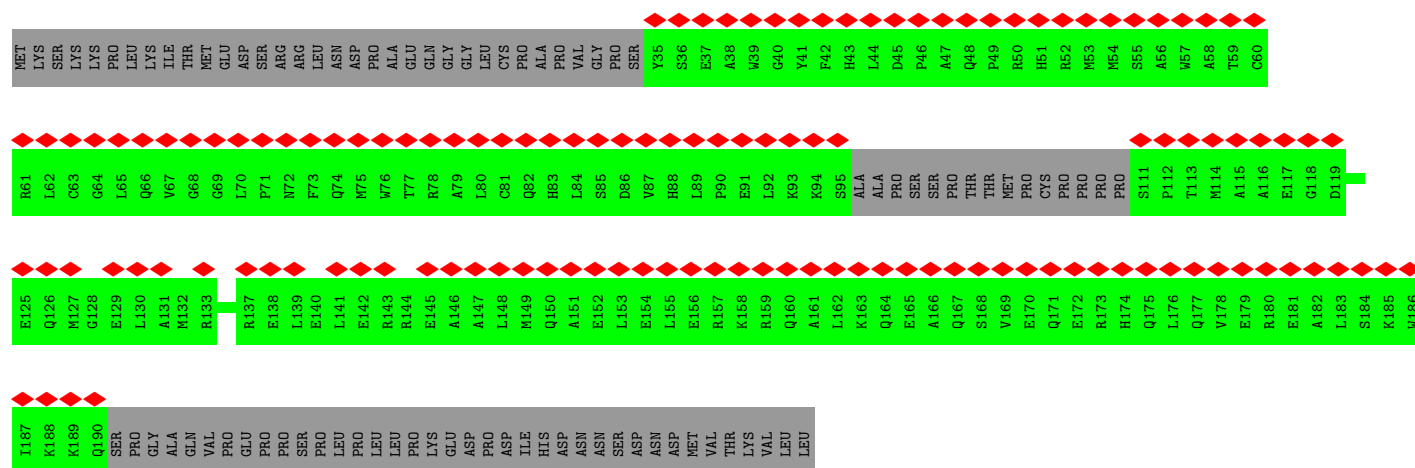
• Molecule 7: S-phase kinase-associated protein 1



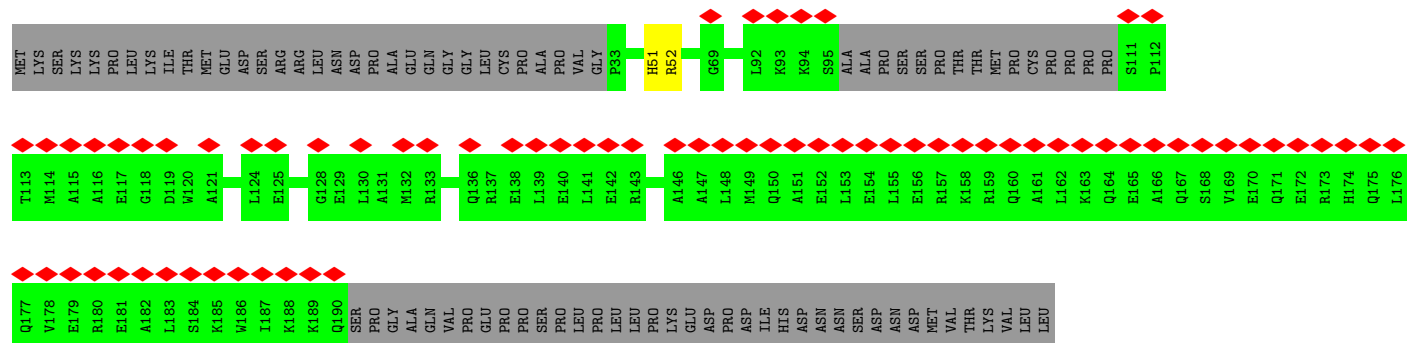




• Molecule 8: Zinc finger BED domain-containing protein 3

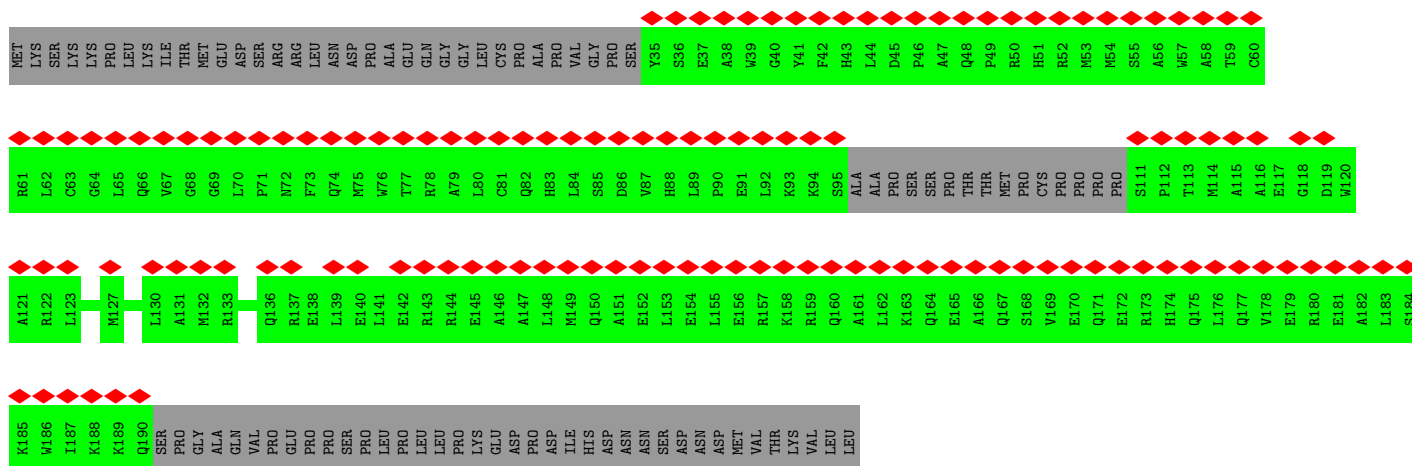


• Molecule 8: Zinc finger BED domain-containing protein 3

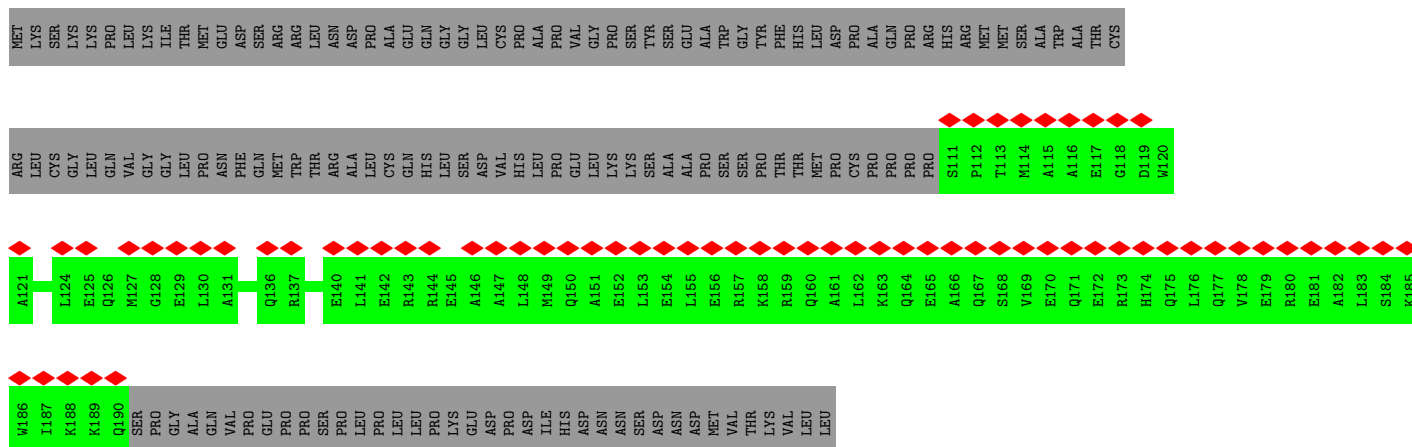


• Molecule 8: Zinc finger BED domain-containing protein 3

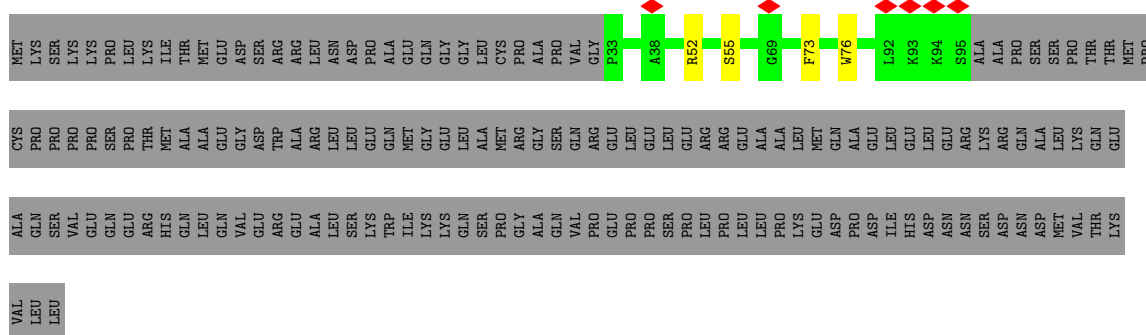




- Molecule 8: Zinc finger BED domain-containing protein 3

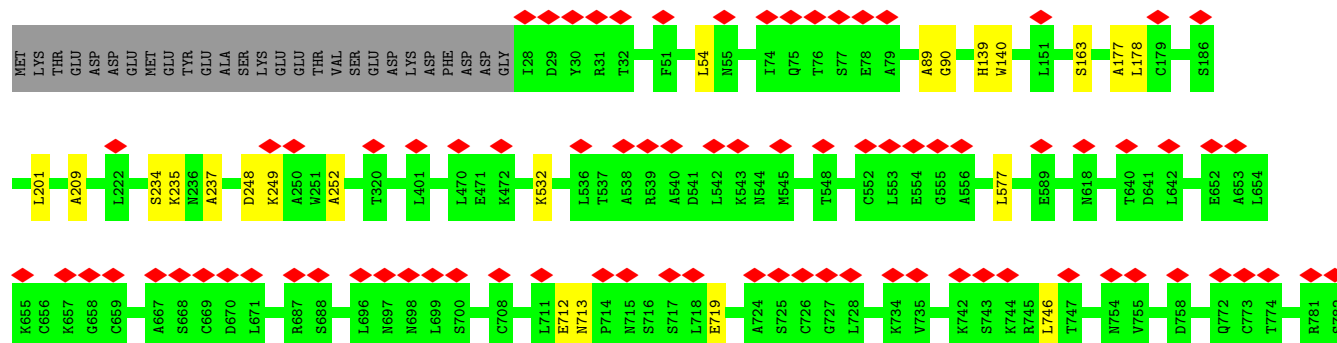


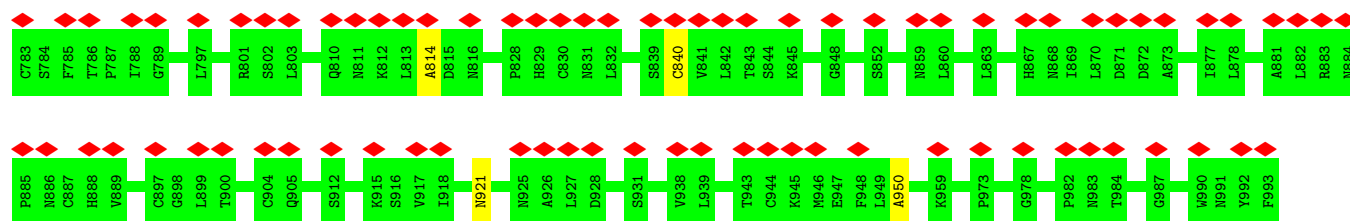
- Molecule 8: Zinc finger BED domain-containing protein 3



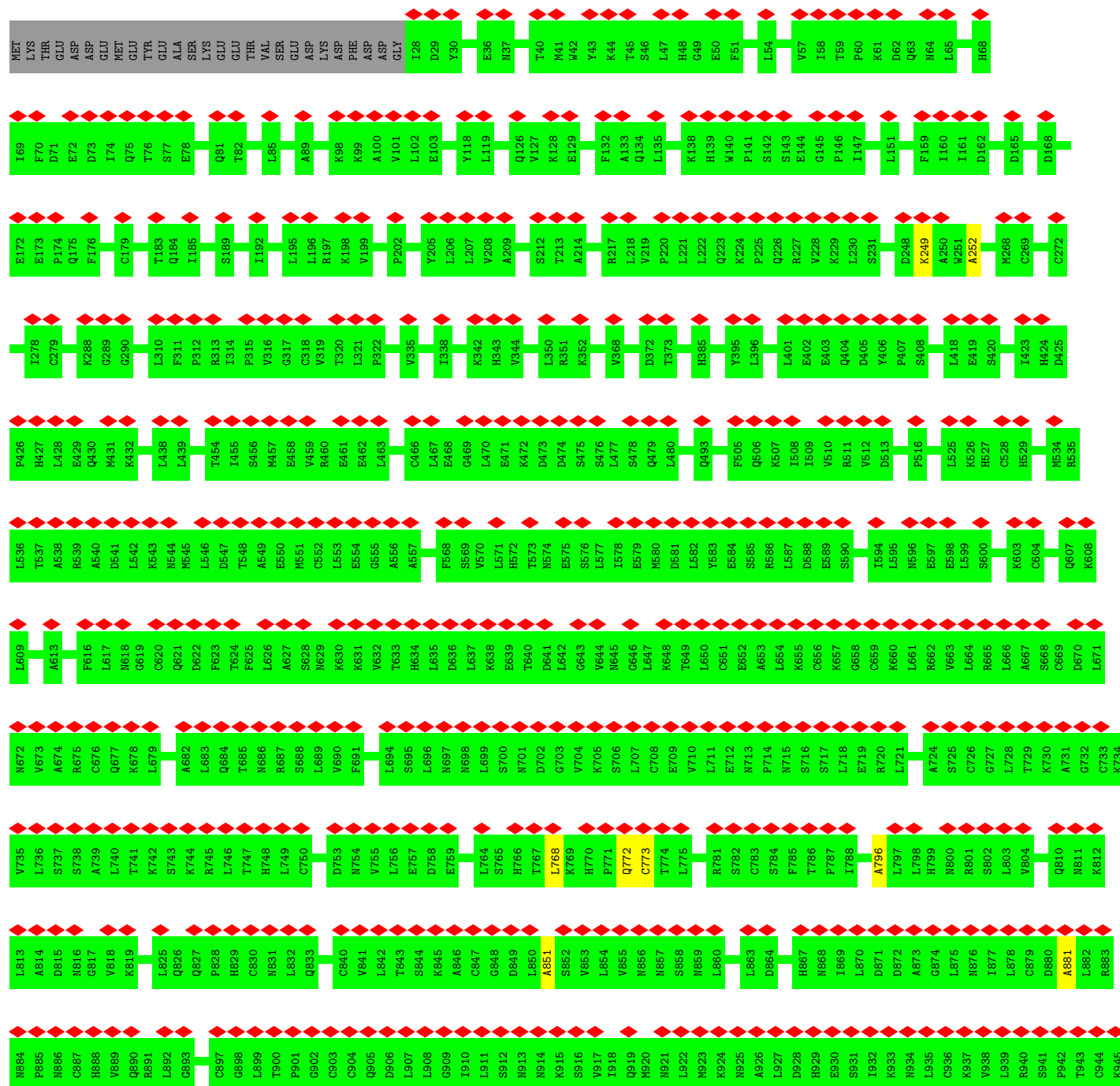
- Molecule 8: Zinc finger BED domain-containing protein 3

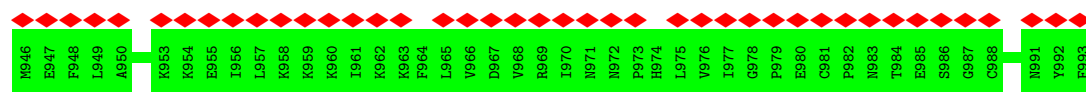




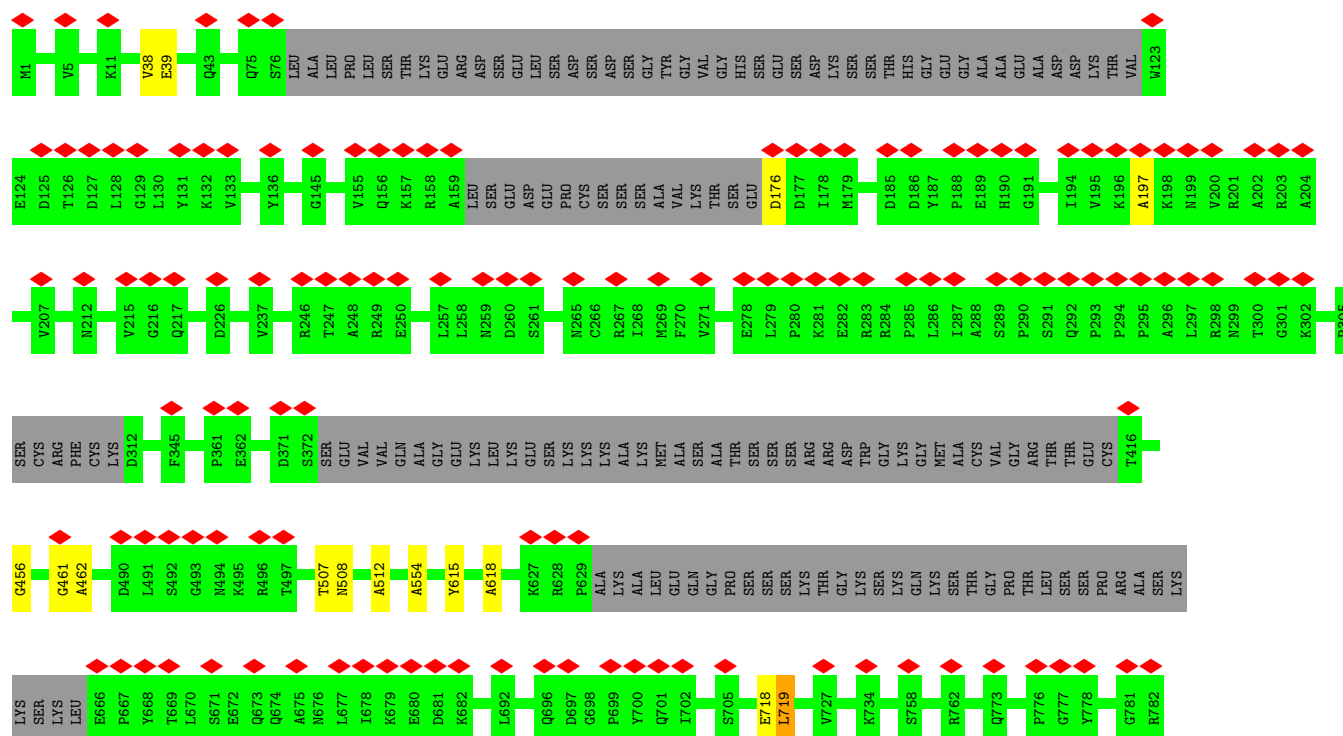
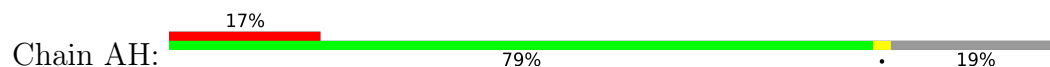


• Molecule 9: NACHT, LRR and PYD domains-containing protein 14

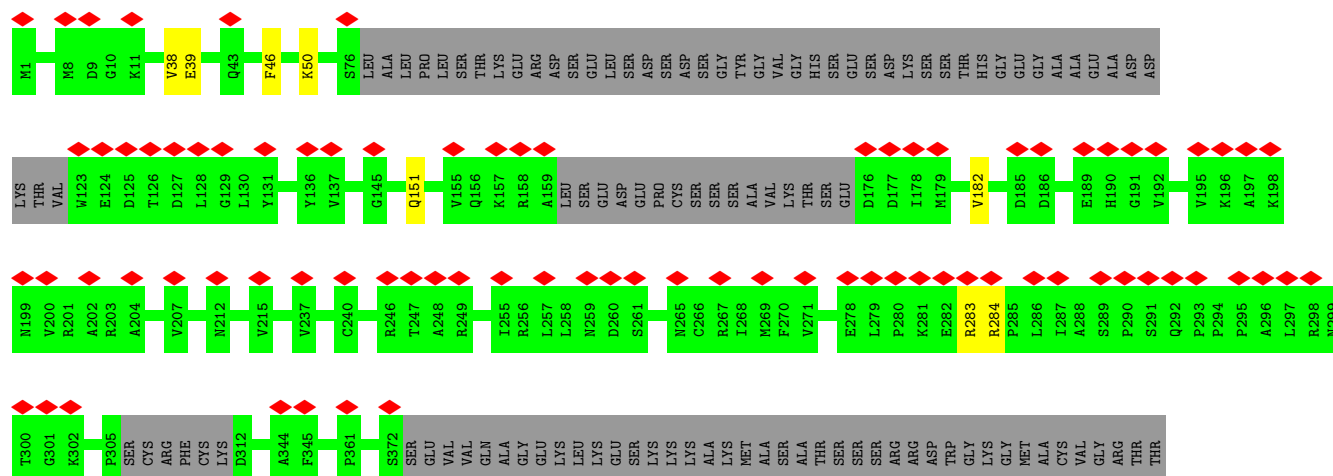
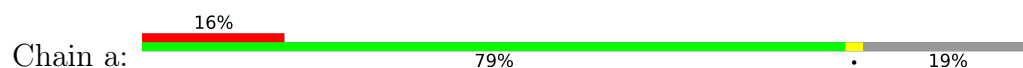


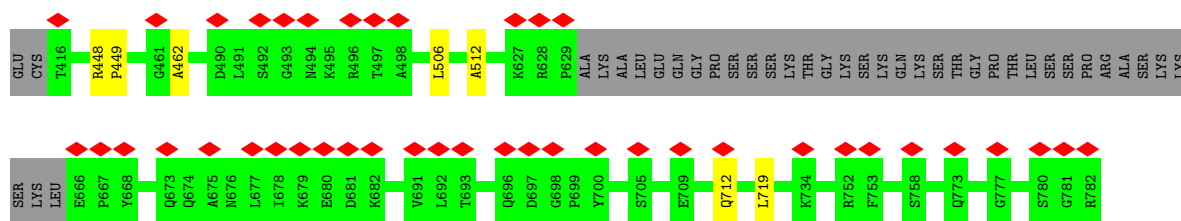


• Molecule 10: E3 ubiquitin-protein ligase UHRF1

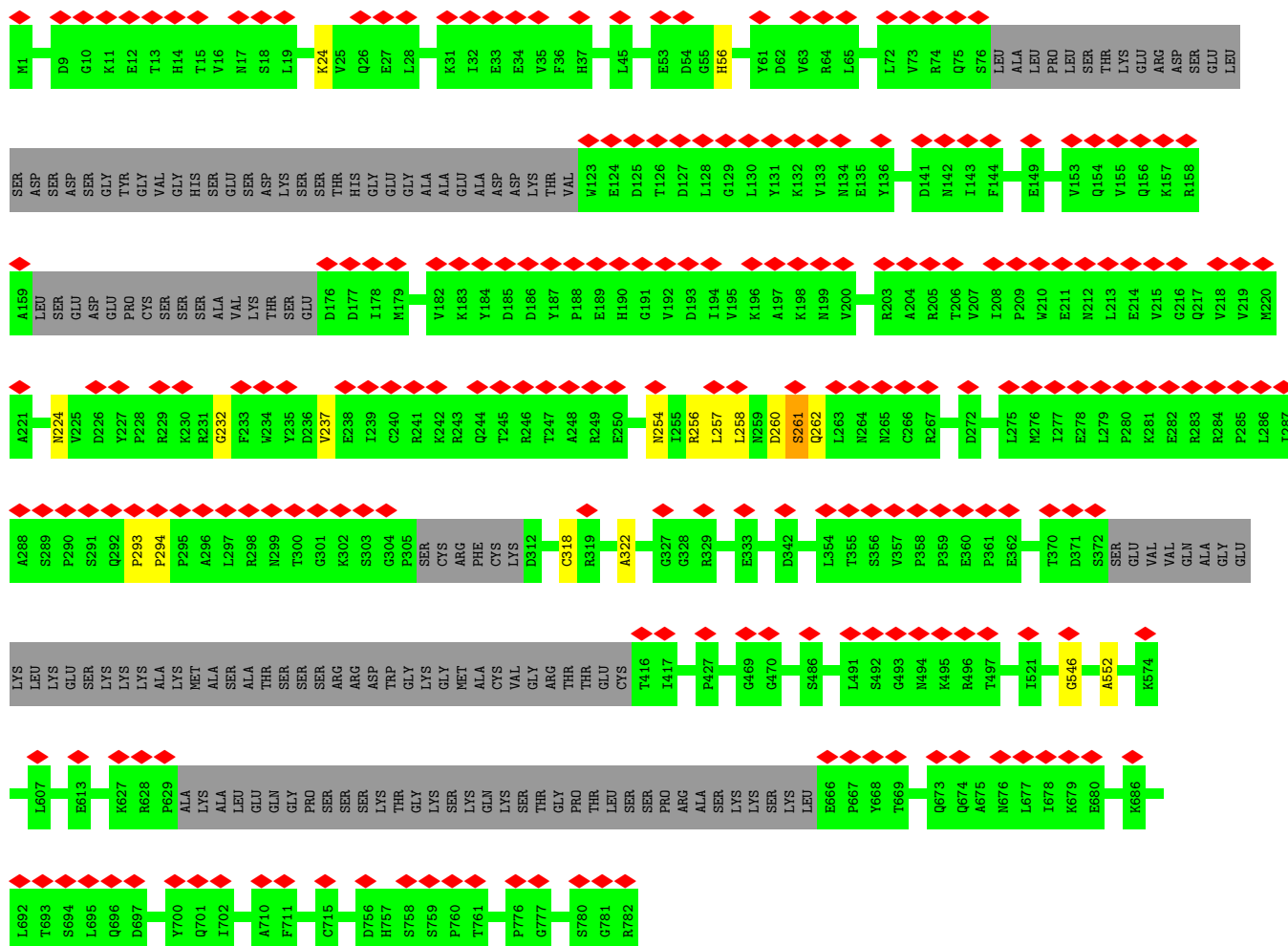
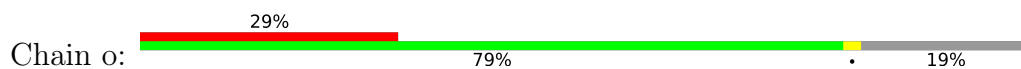


• Molecule 10: E3 ubiquitin-protein ligase UHRF1

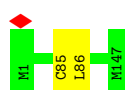




• Molecule 10: E3 ubiquitin-protein ligase UHRF1



• Molecule 11: Ubiquitin-conjugating enzyme E2 D3

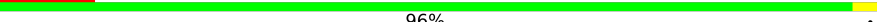


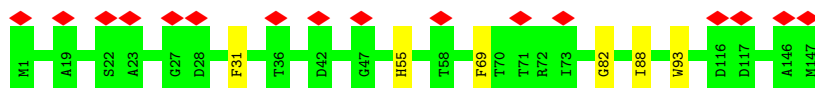
• Molecule 11: Ubiquitin-conjugating enzyme E2 D3

Chain b:  100%

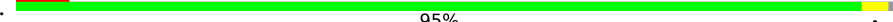


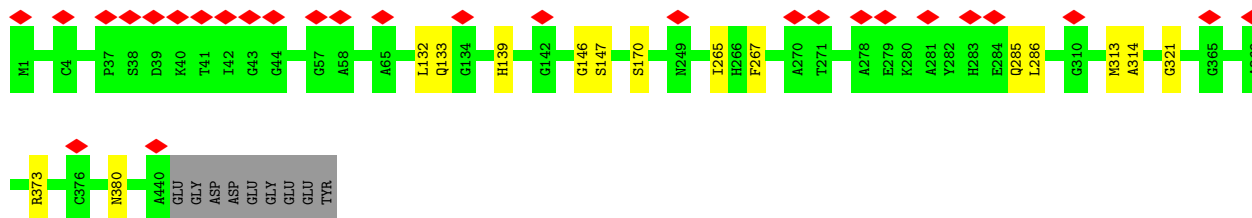
- Molecule 11: Ubiquitin-conjugating enzyme E2 D3

Chain p:  11%  96%  1%



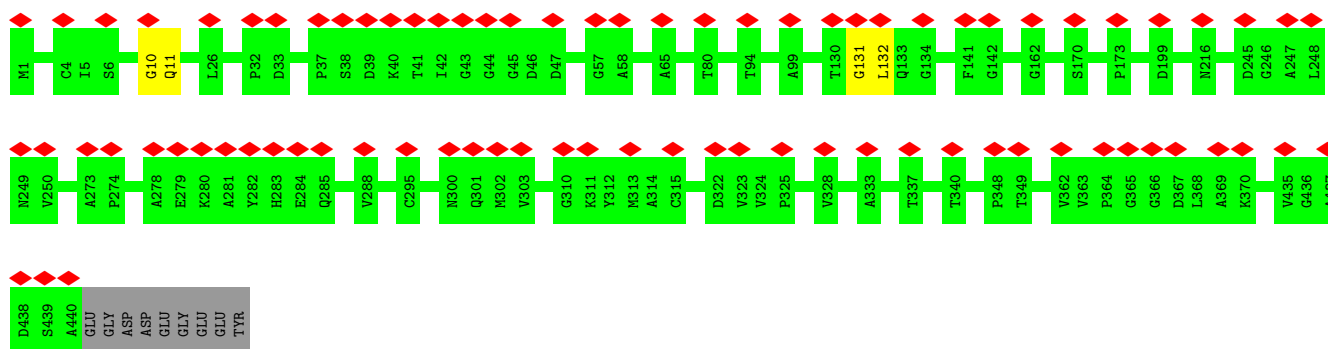
- Molecule 12: Tubulin alpha-1C chain

Chain AJ:  6%  95%  1%

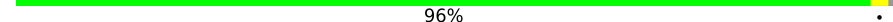


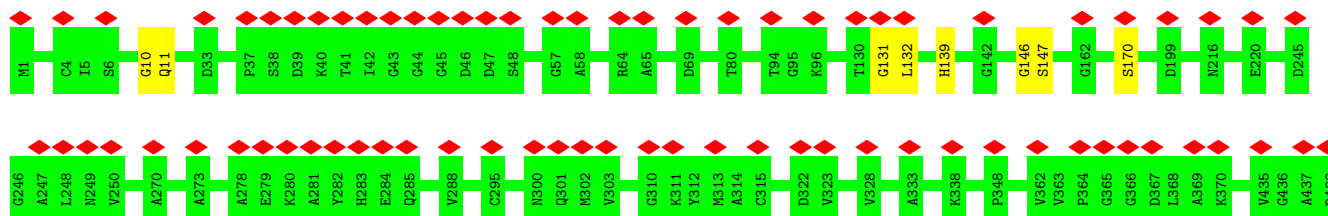
- Molecule 12: Tubulin alpha-1C chain

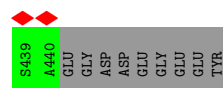
Chain AV:  18%  97%  1%



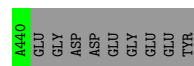
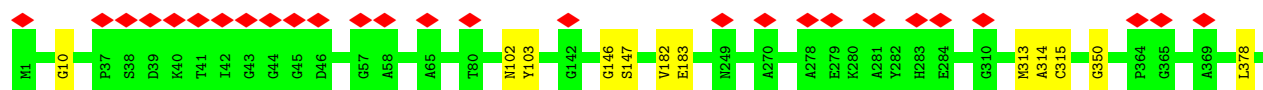
- Molecule 12: Tubulin alpha-1C chain

Chain Ar:  17%  96%  1%

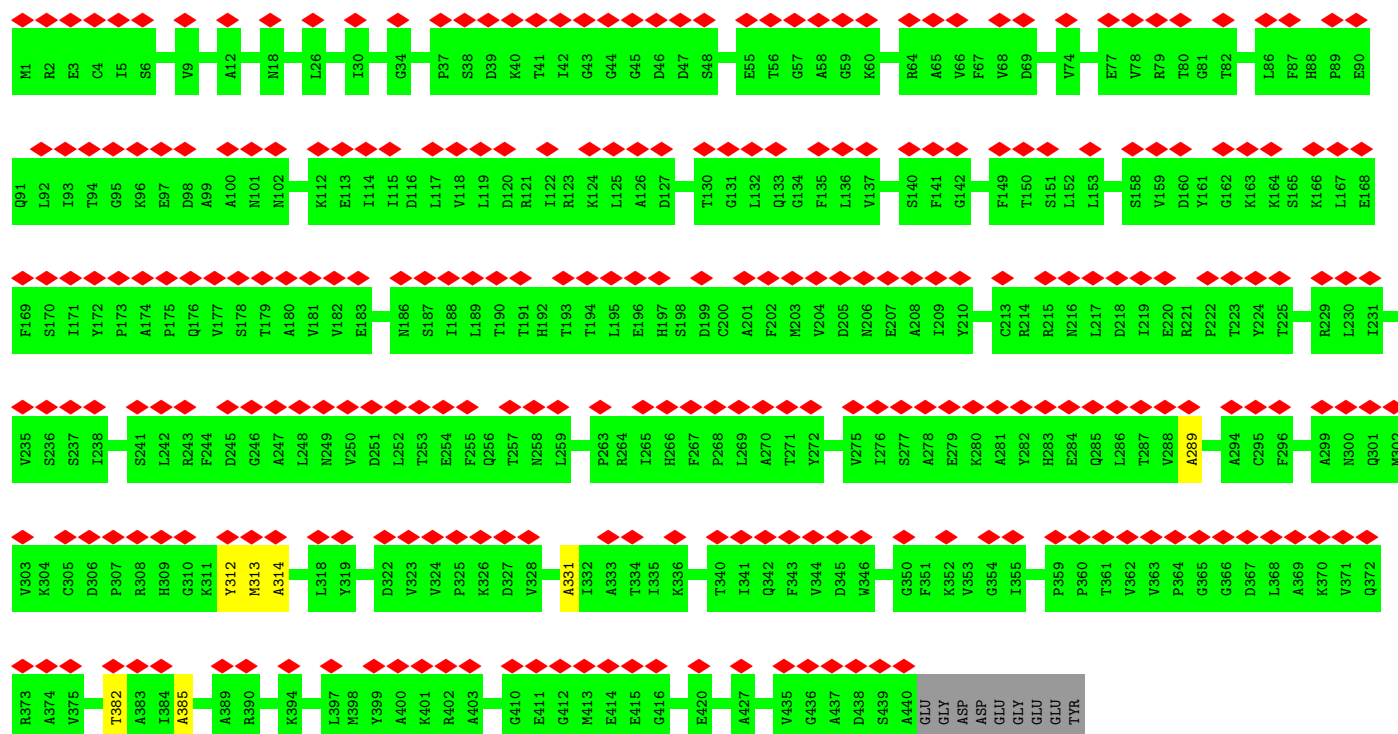




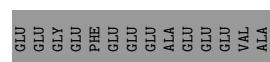
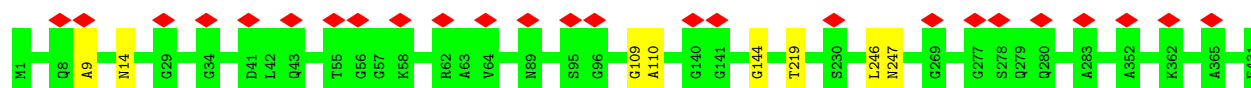
- Molecule 12: Tubulin alpha-1C chain



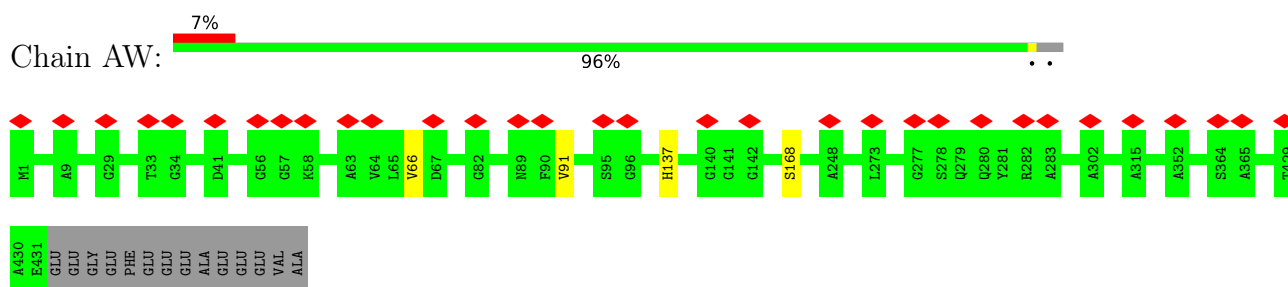
- Molecule 12: Tubulin alpha-1C chain



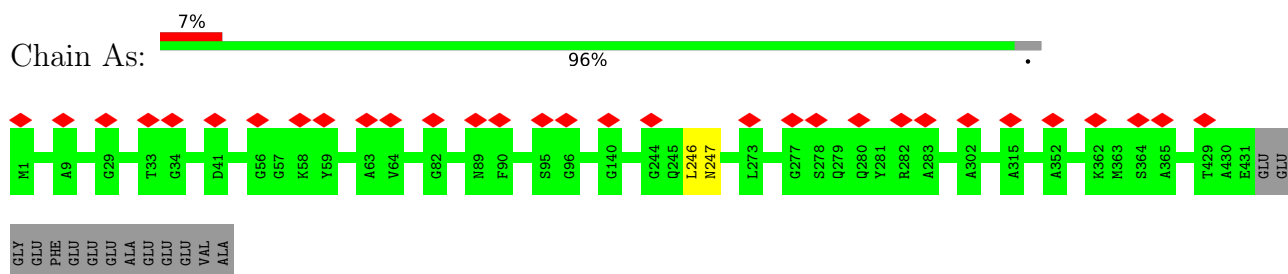
- Molecule 13: Tubulin beta-4B chain



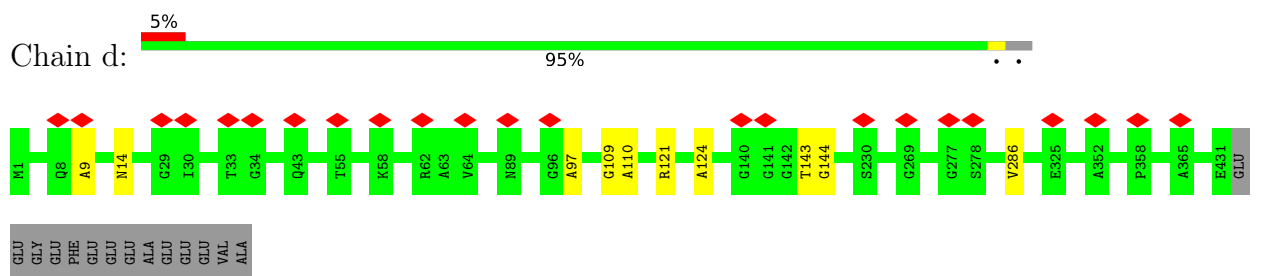
- Molecule 13: Tubulin beta-4B chain



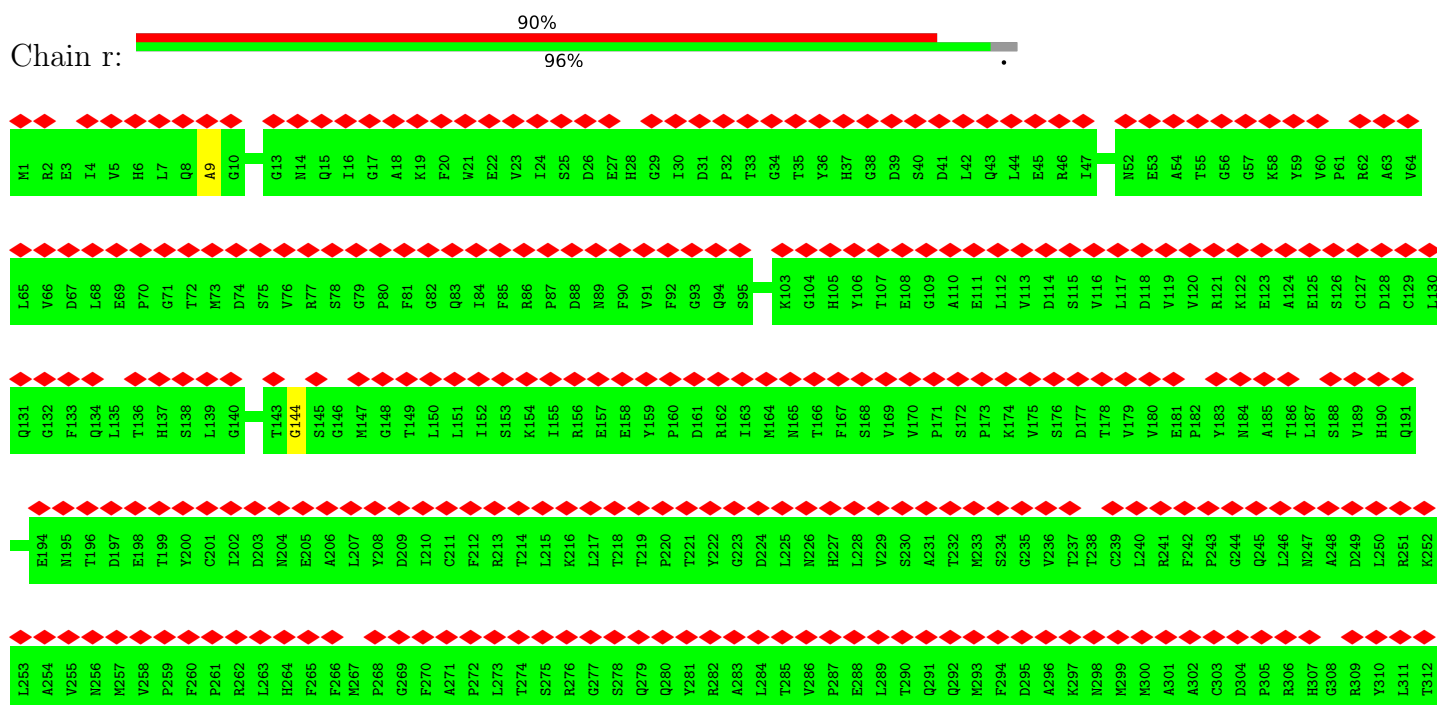
- Molecule 13: Tubulin beta-4B chain

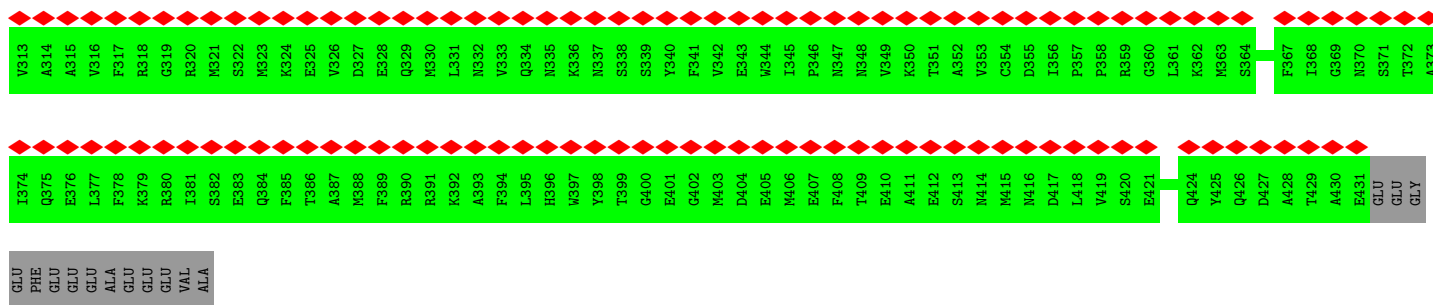


- Molecule 13: Tubulin beta-4B chain

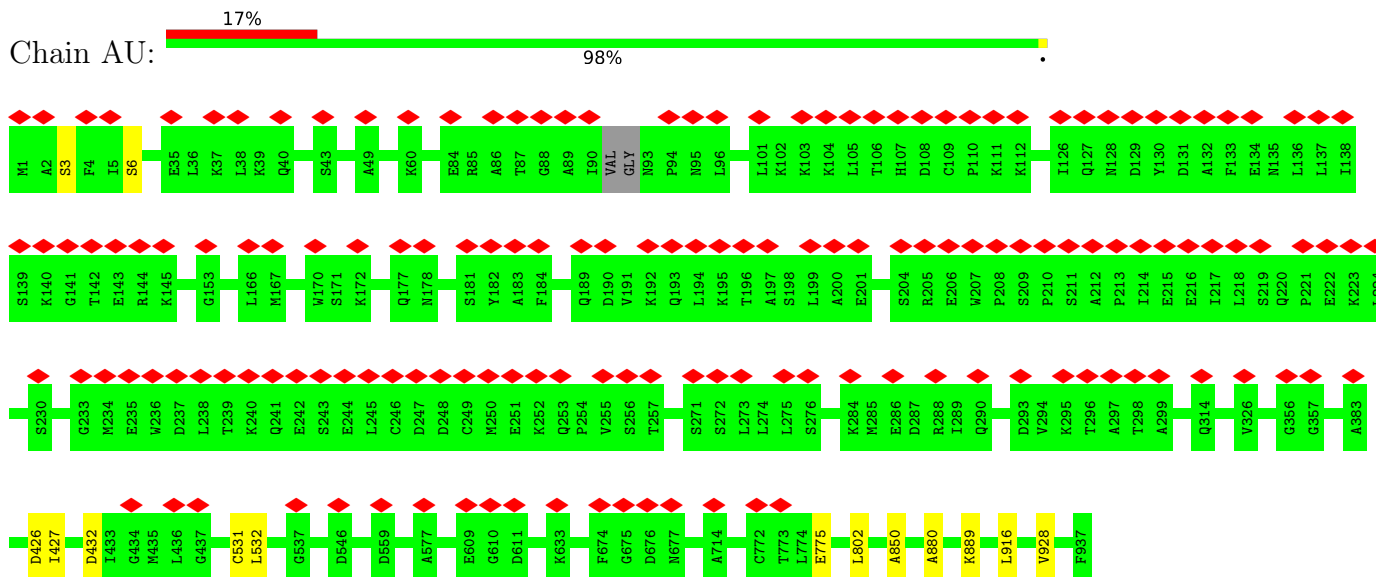


- Molecule 13: Tubulin beta-4B chain

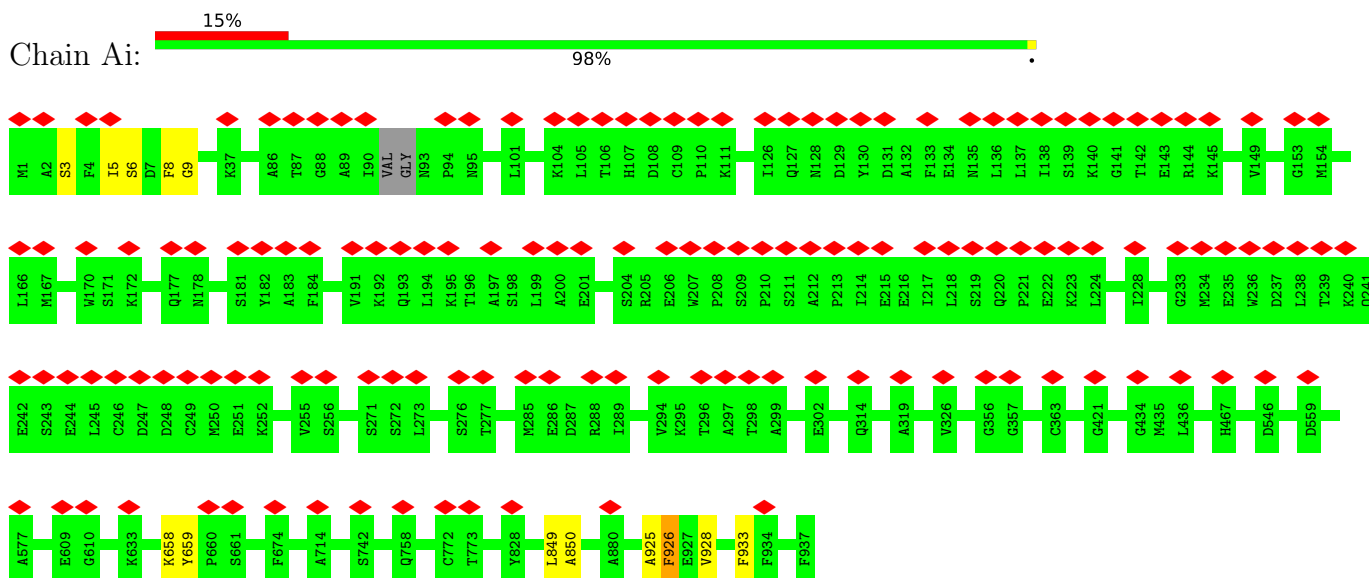




- Molecule 14: NLR family, pyrin domain containing 4F

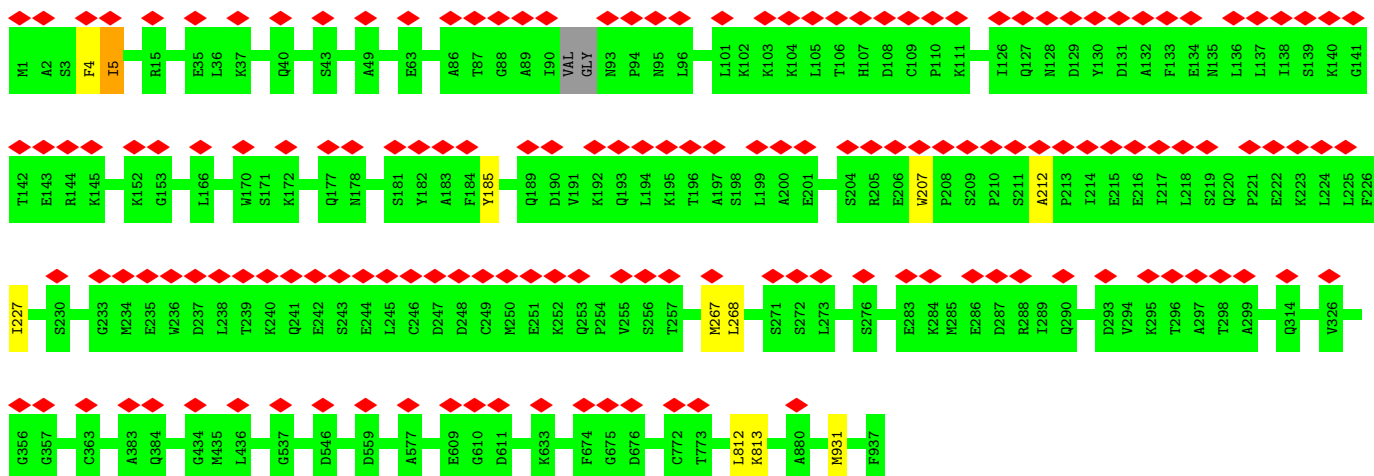


- Molecule 14: NLR family, pyrin domain containing 4F



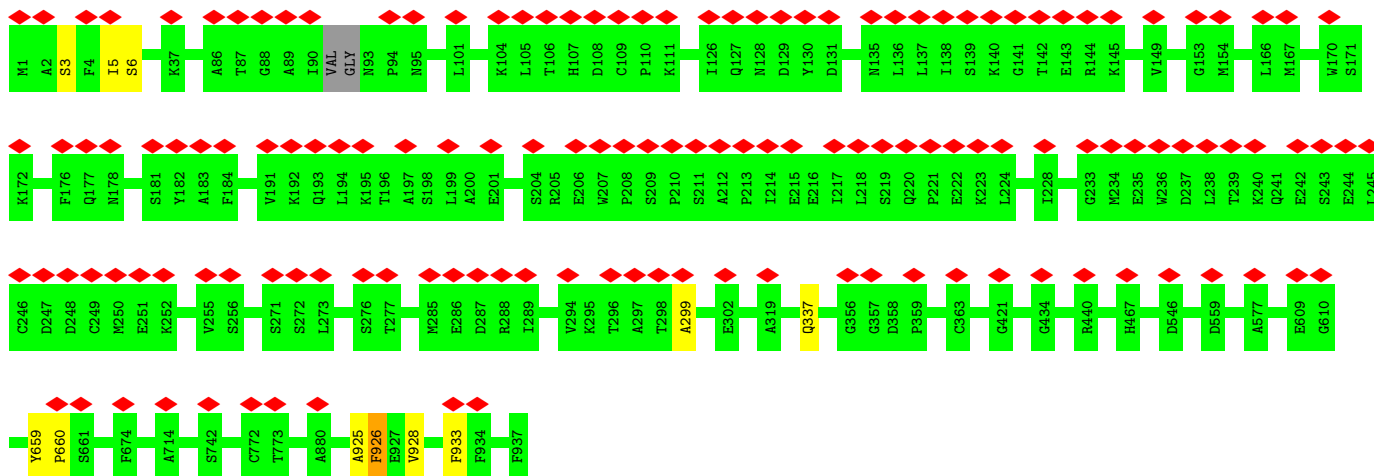
- Molecule 14: NLR family, pyrin domain containing 4F





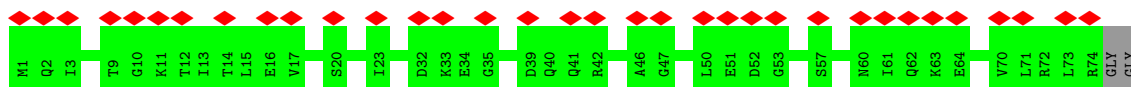
- Molecule 14: NLR family, pyrin domain containing 4F

Chain Y: 15% 99%



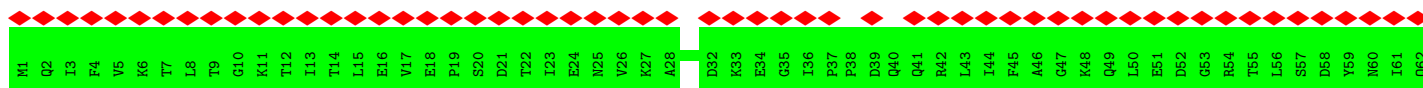
- Molecule 15: Polyubiquitin-C

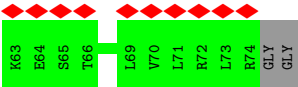
Chain U: 45% 97%



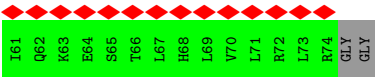
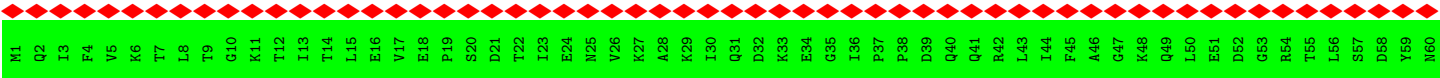
- Molecule 15: Polyubiquitin-C

Chain V: 88% 97%





● Molecule 15: Polyubiquitin-C



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	134387	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	115.5	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.202	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	916.8, 916.8, 916.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.91, 1.91, 1.91	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0	0.22	0/672	0.51	0/935
1	An	0.22	0/672	0.45	0/935
1	S	0.20	0/672	0.46	0/935
1	j	0.19	0/672	0.48	0/935
2	1	0.17	0/3372	0.50	0/4697
2	2	0.16	0/3372	0.48	0/4697
2	3	0.17	0/3372	0.49	0/4697
2	A	0.18	0/3372	0.49	0/4697
2	AB	0.16	0/3372	0.47	0/4697
2	AC	0.19	1/3372 (0.0%)	0.46	0/4697
2	AD	0.15	0/3372	0.45	0/4697
2	Aa	0.17	0/3372	0.48	0/4697
2	Ab	0.16	0/3372	0.48	0/4697
2	Ac	0.15	0/3372	0.44	0/4697
2	Ad	0.18	0/3372	0.45	0/4697
2	Az	0.17	0/3372	0.46	0/4697
2	B	0.18	0/3372	0.48	0/4697
2	C	0.16	0/3372	0.46	0/4697
2	D	0.15	0/3372	0.46	0/4697
2	E	0.16	0/3372	0.45	0/4697
2	F	0.15	0/3372	0.44	0/4697
2	G	0.20	0/3372	0.52	0/4697
2	H	0.17	0/3372	0.50	0/4697
2	I	0.16	0/3372	0.48	0/4697
2	J	0.17	0/3372	0.49	1/4697 (0.0%)
2	K	0.16	0/3372	0.47	0/4697
2	L	0.16	0/3372	0.47	0/4697
2	l	0.16	0/3372	0.47	0/4697
2	m	0.19	0/3372	0.50	0/4697
2	t	0.16	0/3372	0.45	0/4697
2	u	0.17	0/3372	0.47	0/4697
2	v	0.15	0/3372	0.44	0/4697
2	w	0.16	0/3372	0.48	0/4697
2	x	0.19	0/3372	0.50	0/4697

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	y	0.17	0/3372	0.50	0/4697
2	z	0.17	0/3372	0.48	1/4697 (0.0%)
3	4	0.18	0/4700	0.48	0/6551
3	7	0.18	0/4700	0.48	0/6551
3	AF	0.17	0/4700	0.47	0/6551
3	AR	0.18	0/4700	0.47	0/6551
3	Af	0.17	0/4700	0.48	0/6551
3	Ak	0.17	0/4700	0.46	0/6551
3	M	0.18	0/4700	0.50	0/6551
3	P	0.18	0/4700	0.50	0/6551
4	5	0.19	0/1810	0.58	0/2517
4	8	0.17	0/1810	0.52	0/2517
4	AS	0.17	0/1810	0.50	0/2517
4	Ah	0.18	0/1810	0.50	0/2517
4	Al	0.18	0/1810	0.54	0/2517
4	N	0.19	0/1810	0.58	0/2517
4	Q	0.18	0/1810	0.57	0/2517
4	X	0.18	0/1810	0.51	0/2517
5	6	0.19	0/591	0.46	0/824
5	9	0.21	0/441	0.61	0/614
5	AQ	0.18	0/591	0.45	0/824
5	Aj	0.19	0/591	0.51	0/824
5	Am	0.20	0/441	0.55	0/614
5	O	0.20	0/591	0.48	0/824
5	R	0.23	0/441	0.69	0/614
5	i	0.20	0/441	0.55	0/614
7	A2	0.17	0/808	0.41	0/1126
7	AM	0.16	0/808	0.43	0/1126
7	AO	0.26	0/808	0.47	0/1126
7	AY	0.15	0/808	0.43	0/1126
7	AZ	0.15	0/808	0.39	0/1126
7	Au	0.16	0/808	0.42	0/1126
7	Aw	0.16	0/808	0.39	0/1126
7	Ay	0.16	0/808	0.39	0/1126
7	f	0.20	0/808	0.42	0/1126
7	h	0.16	0/808	0.43	0/1126
8	AA	0.31	0/310	0.58	0/430
8	AE	0.16	0/696	0.42	0/967
8	AP	0.21	0/706	0.55	0/981
8	AT	0.15	0/396	0.37	0/551
8	Ae	0.18	0/696	0.41	0/967
8	Ag	0.20	0/706	0.54	0/981
8	Ao	0.16	0/696	0.42	0/967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	Ap	0.18	0/396	0.38	0/551
8	T	0.17	0/310	0.53	0/430
8	k	0.16	0/696	0.42	0/967
9	AG	0.17	0/4793	0.47	1/6687 (0.0%)
9	Z	0.19	1/4793 (0.0%)	0.45	0/6687
9	n	0.14	0/4793	0.40	0/6687
10	AH	0.16	0/3125	0.47	0/4339
10	a	0.19	0/3125	0.48	1/4339 (0.0%)
10	o	0.15	0/3125	0.47	0/4339
11	AI	0.23	0/728	0.46	0/1014
11	b	0.23	0/728	0.45	0/1014
11	p	0.21	0/728	0.48	0/1014
12	AJ	0.18	0/2166	0.47	0/3011
12	AV	0.16	0/2166	0.44	0/3011
12	Ar	0.17	0/2166	0.46	0/3011
12	c	0.19	0/2166	0.50	1/3011 (0.0%)
12	q	0.15	0/2166	0.40	0/3011
13	AK	0.18	0/2120	0.48	0/2946
13	AW	0.17	0/2120	0.43	0/2946
13	As	0.18	0/2120	0.45	0/2946
13	d	0.22	1/2120 (0.0%)	0.49	0/2946
13	r	0.14	0/2120	0.40	0/2946
14	AU	0.17	0/4641	0.44	0/6475
14	Ai	0.17	0/4641	0.44	0/6475
14	Aq	0.16	0/4641	0.46	1/6475 (0.0%)
14	Y	0.16	0/4641	0.45	0/6475
15	U	0.17	0/365	0.42	0/507
15	V	0.31	0/365	0.53	0/507
15	W	0.17	0/365	0.44	0/507
All	All	0.17	3/247515 (0.0%)	0.47	6/344718 (0.0%)

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
2	1	0	3
2	3	0	1
2	A	0	2
2	AD	0	1
2	Ab	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Ad	0	1
2	Az	0	1
2	B	0	3
2	D	0	1
2	E	0	1
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	2
2	K	0	1
2	x	0	2
3	7	0	1
3	M	0	1
4	5	0	1
4	8	0	1
4	N	0	2
4	Q	0	2
5	9	0	1
5	R	0	2
6	A1	0	2
6	AL	0	1
6	AN	0	3
6	Av	0	1
6	e	0	1
6	g	0	5
6	s	0	1
8	AA	0	1
9	AG	0	4
9	Z	0	1
10	AH	0	1
12	q	0	1
13	AK	0	1
14	AU	0	1
14	Ai	0	2
14	Aq	0	1
14	Y	0	2
All	All	0	63

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AC	409	VAL	C-N	7.16	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	201	LEU	C-O	-5.47	1.21	1.23
13	d	286	VAL	CA-CB	5.27	1.56	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Aq	931	MET	N-CA-C	6.00	120.18	112.26
10	a	506	LEU	N-CA-C	-5.78	106.84	112.97
9	AG	199	VAL	N-CA-C	-5.51	108.47	113.71
2	z	59	GLY	N-CA-C	-5.44	106.34	112.33
2	J	122	ILE	N-CA-C	-5.05	108.92	113.71
12	c	10	GLY	N-CA-C	5.05	120.41	111.02

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	103	PRO	Peptide
2	1	509	GLY	Peptide
2	1	59	GLY	Peptide
2	3	302	PRO	Peptide
4	5	545	LEU	Peptide
3	7	979	CYS	Peptide
4	8	174	ARG	Peptide
5	9	105	LEU	Peptide
2	A	281	LEU	Peptide
2	A	509	GLY	Peptide
6	A1	307	UNK	Peptide
6	A1	433	UNK	Peptide
8	AA	71	PRO	Peptide
2	AD	509	GLY	Peptide
9	AG	248	ASP	Peptide
9	AG	315	PRO	Peptide
9	AG	50	GLU	Peptide
9	AG	757	GLU	Peptide
10	AH	719	LEU	Peptide
13	AK	219	THR	Peptide
6	AL	54	UNK	Peptide
6	AN	105	UNK	Peptide
6	AN	281	UNK	Peptide
6	AN	53	UNK	Peptide
14	AU	432	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	Ab	480	ASP	Peptide
2	Ad	509	GLY	Peptide
14	Ai	5	ILE	Peptide
14	Ai	933	PHE	Peptide
14	Aq	5	ILE	Peptide
6	Av	386	UNK	Peptide
2	Az	281	LEU	Peptide
2	B	240	ARG	Peptide
2	B	281	LEU	Peptide
2	B	509	GLY	Peptide
2	D	224	VAL	Peptide
2	E	60	LYS	Peptide
2	G	585	THR	Peptide
2	H	281	LEU	Peptide
2	I	281	LEU	Peptide
2	J	218	SER	Peptide
2	J	509	GLY	Peptide
2	K	97	CYS	Peptide
3	M	132	TYR	Peptide
4	N	153	ALA	Peptide
4	N	422	VAL	Peptide
4	Q	287	VAL	Peptide
4	Q	422	VAL	Peptide
5	R	103	ASN	Peptide
5	R	104	ILE	Peptide
14	Y	5	ILE	Peptide
14	Y	933	PHE	Peptide
9	Z	248	ASP	Peptide
6	e	334	UNK	Peptide
6	g	105	UNK	Peptide
6	g	106	UNK	Peptide
6	g	151	UNK	Peptide
6	g	386	UNK	Peptide
6	g	98	UNK	Peptide
12	q	312	TYR	Peptide
6	s	386	UNK	Peptide
2	x	281	LEU	Peptide
2	x	96	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	673	0	298	2	0
1	An	673	0	298	1	0
1	S	673	0	298	4	0
1	j	673	0	298	0	0
2	1	3373	0	1454	8	0
2	2	3373	0	1454	3	0
2	3	3373	0	1454	8	0
2	A	3373	0	1454	12	0
2	AB	3373	0	1454	6	0
2	AC	3373	0	1454	9	0
2	AD	3373	0	1454	5	0
2	Aa	3373	0	1454	5	0
2	Ab	3373	0	1454	7	0
2	Ac	3373	0	1454	5	0
2	Ad	3373	0	1454	2	0
2	Az	3373	0	1454	2	0
2	B	3373	0	1454	5	0
2	C	3373	0	1454	7	0
2	D	3373	0	1454	11	0
2	E	3373	0	1454	6	0
2	F	3373	0	1454	4	0
2	G	3373	0	1454	16	0
2	H	3373	0	1454	10	0
2	I	3373	0	1454	8	0
2	J	3373	0	1454	7	0
2	K	3373	0	1454	6	0
2	L	3373	0	1454	4	0
2	l	3373	0	1454	3	0
2	m	3373	0	1454	11	0
2	t	3373	0	1454	9	0
2	u	3373	0	1454	6	0
2	v	3373	0	1454	7	0
2	w	3373	0	1454	6	0
2	x	3373	0	1454	12	0
2	y	3373	0	1454	10	0
2	z	3373	0	1454	7	0
3	4	4702	0	2048	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7	4702	0	2048	4	0
3	AF	4702	0	2048	7	0
3	AR	4702	0	2048	12	0
3	Af	4702	0	2048	8	0
3	Ak	4702	0	2048	8	0
3	M	4702	0	2048	7	0
3	P	4702	0	2048	9	0
4	5	1812	0	802	4	0
4	8	1812	0	802	9	0
4	AS	1812	0	802	2	0
4	Ah	1812	0	802	4	0
4	Al	1812	0	802	5	0
4	N	1812	0	802	4	0
4	Q	1812	0	802	4	0
4	X	1812	0	802	3	0
5	6	592	0	266	1	0
5	9	442	0	200	0	0
5	AQ	592	0	266	0	0
5	Aj	592	0	266	3	0
5	Am	442	0	200	2	0
5	O	592	0	266	3	0
5	R	442	0	200	3	0
5	i	442	0	200	1	0
6	A1	2312	0	488	8	0
6	AL	2312	0	493	8	0
6	AN	2312	0	497	11	0
6	AX	2312	0	499	9	0
6	At	2312	0	505	9	0
6	Av	2312	0	497	13	0
6	Ax	2312	0	496	12	0
6	e	2312	0	498	9	0
6	g	2312	0	503	19	0
6	s	2312	0	503	9	0
7	A2	809	0	345	2	0
7	AM	809	0	345	0	0
7	AO	809	0	345	5	0
7	AY	809	0	345	2	0
7	AZ	809	0	345	0	0
7	Au	809	0	345	1	0
7	Aw	809	0	345	1	0
7	Ay	809	0	345	0	0
7	f	809	0	345	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	809	0	345	3	0
8	AA	311	0	140	0	0
8	AE	698	0	327	0	0
8	AP	708	0	331	1	0
8	AT	397	0	191	0	0
8	Ae	698	0	327	0	0
8	Ag	708	0	331	1	0
8	Ao	698	0	327	0	0
8	Ap	397	0	191	0	0
8	T	311	0	140	2	0
8	k	698	0	327	0	0
9	AG	4794	0	2077	7	0
9	Z	4794	0	2077	13	0
9	n	4794	0	2077	4	0
10	AH	3131	0	1365	8	0
10	a	3131	0	1365	8	0
10	o	3131	0	1365	11	0
11	AI	729	0	314	1	0
11	b	729	0	314	0	0
11	p	729	0	314	3	0
12	AJ	2167	0	1009	8	0
12	AV	2167	0	1009	2	0
12	Ar	2167	0	1009	4	0
12	c	2167	0	1009	6	0
12	q	2167	0	1009	3	0
13	AK	2121	0	962	4	0
13	AW	2121	0	962	2	0
13	As	2121	0	962	1	0
13	d	2121	0	962	7	0
13	r	2121	0	962	1	0
14	AU	4643	0	2005	6	0
14	Ai	4643	0	2005	5	0
14	Aq	4643	0	2005	5	0
14	Y	4643	0	2005	4	0
15	U	366	0	157	0	0
15	V	366	0	157	0	0
15	W	366	0	157	0	0
All	All	270782	0	113059	584	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 2.

All (584) 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)
13:d:9:ALA:HB1	13:d:144:GLY:HA2	1.73	0.70
2:H:464:LEU:HA	2:H:598:ALA:HB3	1.74	0.70
13:AK:9:ALA:HB1	13:AK:144:GLY:HA2	1.73	0.68
13:d:9:ALA:HB1	13:d:144:GLY:CA	2.26	0.65
3:M:672:GLN:HA	3:M:698:LEU:HA	1.81	0.62
2:G:46:PRO:HA	2:G:59:GLY:O	2.01	0.61
10:a:151:GLN:O	10:a:182:VAL:HA	2.01	0.60
13:d:97:ALA:HB2	13:d:143:THR:HA	1.84	0.60
3:4:672:GLN:HA	3:4:698:LEU:HA	1.87	0.56
3:M:933:ASN:HA	3:M:962:ALA:HB3	1.87	0.56
2:v:51:HIS:HA	2:v:55:SER:O	2.06	0.55
6:g:231:UNK:O	6:g:232:UNK:C	2.54	0.55
13:r:9:ALA:HB1	13:r:144:GLY:HA2	1.88	0.55
4:Q:295:LEU:HA	4:Q:571:ARG:O	2.05	0.55
2:D:271:ALA:HB2	2:D:278:GLU:N	2.20	0.55
2:2:653:ASP:O	2:2:657:ALA:HB2	2.07	0.55
5:R:106:LEU:HA	5:R:109:ALA:HB3	1.89	0.55
6:g:95:UNK:O	6:g:456:UNK:C	2.54	0.54
8:AP:51:HIS:O	8:AP:52:ARG:C	2.50	0.54
4:Al:438:LYS:O	4:Al:439:ASP:C	2.51	0.54
6:Ax:454:UNK:O	6:Ax:455:UNK:C	2.56	0.54
2:H:206:ALA:HB1	2:H:226:GLY:O	2.07	0.53
2:x:46:PRO:HA	2:x:59:GLY:O	2.09	0.53
6:At:218:UNK:HA	6:At:224:UNK:O	2.09	0.53
2:A:27:LEU:CB	2:A:75:ALA:HB3	2.39	0.53
6:g:253:UNK:O	6:g:254:UNK:C	2.57	0.53
3:4:1055:ASN:O	3:4:1057:TRP:N	2.41	0.53
2:F:46:PRO:HA	2:F:60:LYS:HA	1.90	0.53
2:m:302:PRO:HA	2:m:670:ARG:HA	1.90	0.53
5:Aj:51:ALA:O	5:Aj:54:ALA:HB3	2.09	0.52
6:AN:453:UNK:O	6:AN:454:UNK:C	2.58	0.52
9:Z:249:LYS:HA	9:Z:252:ALA:HB3	1.90	0.52
4:AS:438:LYS:O	4:AS:439:ASP:C	2.52	0.52
4:Q:438:LYS:O	4:Q:439:ASP:C	2.53	0.52
2:Ab:268:VAL:HA	2:Ab:280:PRO:HA	1.91	0.51
2:u:46:PRO:HA	2:u:60:LYS:O	2.11	0.51
6:g:430:UNK:O	6:g:431:UNK:C	2.58	0.51
2:y:42:ILE:O	2:y:64:VAL:HA	2.10	0.51
6:g:90:UNK:HA	6:g:459:UNK:O	2.11	0.51
2:1:80:VAL:O	2:1:81:ALA:C	2.54	0.51
2:H:623:PRO:O	2:H:629:CYS:HA	2.10	0.51
6:Ax:462:UNK:O	6:Ax:463:UNK:C	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:579:PHE:HA	2:C:600:PRO:HA	1.93	0.50
6:e:3:UNK:O	6:e:4:UNK:C	2.59	0.50
11:p:69:PHE:H	11:p:82:GLY:HA3	1.76	0.50
6:AX:49:UNK:O	6:AX:50:UNK:C	2.59	0.50
6:Av:453:UNK:O	6:Av:454:UNK:C	2.58	0.50
6:Ax:450:UNK:H	6:Ax:453:UNK:HA	1.77	0.50
6:A1:454:UNK:O	6:A1:455:UNK:C	2.58	0.50
2:L:21:VAL:HA	2:L:79:MET:O	2.11	0.50
3:P:1058:LYS:O	3:P:1059:ASN:C	2.55	0.50
2:w:302:PRO:HA	2:w:670:ARG:HA	1.94	0.49
6:g:97:UNK:CB	6:g:457:UNK:HA	2.42	0.49
2:y:579:PHE:HA	2:y:600:PRO:HA	1.94	0.49
2:G:271:ALA:HB2	2:G:278:GLU:N	2.27	0.49
2:t:442:LYS:O	2:t:443:GLY:C	2.54	0.49
2:3:206:ALA:O	2:3:226:GLY:HA2	2.11	0.49
2:Ac:628:THR:O	2:Ac:629:CYS:C	2.55	0.49
2:E:442:LYS:O	2:E:443:GLY:C	2.55	0.49
2:D:45:SER:O	2:D:60:LYS:HA	2.13	0.49
6:s:94:UNK:HA	6:s:456:UNK:HA	1.95	0.49
4:8:438:LYS:O	4:8:439:ASP:C	2.55	0.49
2:t:46:PRO:HA	2:t:60:LYS:HA	1.94	0.49
2:w:46:PRO:HA	2:w:60:LYS:HA	1.95	0.49
5:Aj:133:ARG:O	5:Aj:134:ALA:C	2.56	0.49
3:Ak:799:CYS:O	3:Ak:800:HIS:C	2.56	0.49
6:Av:375:UNK:O	6:Av:376:UNK:C	2.61	0.49
6:s:453:UNK:O	6:s:454:UNK:C	2.61	0.49
6:AN:341:UNK:O	6:AN:342:UNK:C	2.61	0.49
6:At:453:UNK:O	6:At:454:UNK:C	2.60	0.49
2:y:206:ALA:HB1	2:y:226:GLY:O	2.12	0.49
2:AC:628:THR:O	2:AC:629:CYS:C	2.56	0.48
6:A1:62:UNK:O	6:A1:64:UNK:O	2.32	0.48
2:x:97:CYS:O	2:x:98:PRO:C	2.57	0.48
2:A:43:ARG:HA	2:A:63:THR:O	2.13	0.48
4:Al:513:ILE:HA	4:Al:529:GLY:HA2	1.96	0.48
2:z:602:PHE:O	2:z:603:PRO:C	2.57	0.48
10:AH:38:VAL:O	10:AH:39:GLU:C	2.57	0.48
2:G:409:VAL:HA	2:G:424:ARG:O	2.13	0.48
14:Y:3:SER:HA	14:Y:6:SER:HA	1.95	0.48
3:AF:517:PRO:O	3:AF:519:VAL:N	2.47	0.48
14:Ai:3:SER:HA	14:Ai:6:SER:HA	1.96	0.48
2:J:80:VAL:O	2:J:81:ALA:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:98:UNK:O	6:e:99:UNK:C	2.61	0.48
2:m:115:GLU:O	2:m:185:VAL:HA	2.14	0.48
2:H:46:PRO:O	2:H:60:LYS:HA	2.14	0.48
3:P:730:LEU:O	3:P:758:LEU:HA	2.14	0.48
8:T:73:PHE:HA	8:T:76:TRP:CB	2.44	0.48
9:Z:234:SER:O	9:Z:237:ALA:N	2.47	0.48
2:t:268:VAL:HA	2:t:280:PRO:HA	1.95	0.48
2:v:61:GLU:O	2:y:132:SER:HA	2.13	0.48
6:AN:59:UNK:O	6:AN:60:UNK:C	2.60	0.47
3:P:750:ILE:O	3:P:751:SER:O	2.32	0.47
10:a:462:ALA:HB2	10:a:512:ALA:CB	2.44	0.47
2:AB:514:THR:HA	2:AB:533:THR:HA	1.96	0.47
2:m:430:SER:C	2:m:432:TYR:H	2.22	0.47
2:w:170:GLU:O	2:w:171:GLY:C	2.57	0.47
14:Y:925:ALA:O	14:Y:926:PHE:O	2.32	0.47
9:n:851:ALA:HB1	9:n:881:ALA:HB2	1.95	0.47
3:AR:847:ASN:O	3:AR:849:CYS:N	2.47	0.47
3:AK:681:VAL:O	3:AK:682:VAL:C	2.58	0.47
8:Ag:51:HIS:O	8:Ag:52:ARG:C	2.57	0.47
2:J:131:PRO:HA	2:x:61:GLU:O	2.14	0.47
13:d:9:ALA:O	13:d:14:ASN:N	2.48	0.47
6:AL:2:UNK:O	6:AL:3:UNK:C	2.63	0.47
2:Ad:651:ASP:O	2:Ad:652:PHE:C	2.57	0.47
2:E:115:GLU:O	2:E:185:VAL:HA	2.13	0.47
5:i:94:GLN:O	5:i:95:PRO:C	2.58	0.47
9:n:249:LYS:HA	9:n:252:ALA:HB3	1.97	0.47
3:Af:672:GLN:HA	3:Af:698:LEU:HA	1.97	0.47
12:Ar:131:GLY:O	12:Ar:132:LEU:C	2.58	0.47
2:C:46:PRO:HA	2:C:60:LYS:HA	1.97	0.47
2:D:40:PHE:O	2:D:66:TRP:HA	2.15	0.47
2:D:142:TRP:O	2:D:146:GLY:HA3	2.13	0.47
2:H:43:ARG:HA	2:H:63:THR:O	2.14	0.47
2:H:302:PRO:HA	2:H:670:ARG:HA	1.97	0.47
12:c:315:CYS:HA	12:c:378:LEU:O	2.13	0.47
12:q:289:ALA:HB2	12:q:331:ALA:HB2	1.97	0.47
2:A:41:THR:HA	2:A:65:VAL:O	2.14	0.47
12:q:382:THR:O	12:q:385:ALA:HB3	2.15	0.47
2:y:170:GLU:O	2:y:171:GLY:C	2.58	0.47
5:Am:113:LYS:O	5:Am:114:GLU:C	2.58	0.47
6:AX:58:UNK:O	6:AX:59:UNK:C	2.63	0.46
13:AK:9:ALA:O	13:AK:14:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:253:UNK:O	6:e:254:UNK:C	2.63	0.46
3:AF:789:LEU:O	3:AF:817:LEU:HA	2.15	0.46
2:E:116:ILE:HA	2:E:184:THR:O	2.16	0.46
6:g:97:UNK:N	6:g:456:UNK:O	2.48	0.46
13:AK:109:GLY:O	13:AK:110:ALA:C	2.58	0.46
6:AX:218:UNK:HA	6:AX:224:UNK:O	2.16	0.46
6:AX:463:UNK:O	6:AX:464:UNK:C	2.63	0.46
2:Ab:514:THR:HA	2:Ab:533:THR:HA	1.96	0.46
6:At:341:UNK:O	6:At:342:UNK:O	2.32	0.46
2:C:626:ASN:C	2:C:628:THR:H	2.24	0.46
2:v:206:ALA:HB1	2:v:226:GLY:O	2.16	0.46
2:G:46:PRO:O	2:G:60:LYS:HA	2.15	0.46
2:J:39:SER:HA	2:J:68:SER:HA	1.98	0.46
10:a:712:GLN:HA	10:a:719:LEU:HA	1.98	0.46
5:Am:94:GLN:O	5:Am:95:PRO:C	2.59	0.46
7:h:136:ARG:O	7:h:140:ASN:HA	2.15	0.46
3:4:566:GLN:HA	3:4:591:LEU:HA	1.98	0.46
3:7:566:GLN:HA	3:7:591:LEU:HA	1.98	0.46
10:AH:718:GLU:O	10:AH:719:LEU:C	2.58	0.46
7:AO:7:GLN:O	7:AO:46:PRO:HA	2.16	0.46
3:Af:884:MET:O	3:Af:885:LYS:C	2.59	0.46
6:Ax:117:UNK:O	6:Ax:118:UNK:C	2.64	0.46
6:Ax:425:UNK:O	6:Ax:426:UNK:C	2.63	0.46
6:A1:453:UNK:O	6:A1:455:UNK:N	2.49	0.46
14:AU:889:LYS:HA	14:AU:916:LEU:HA	1.97	0.46
9:Z:163:SER:HA	9:Z:209:ALA:O	2.16	0.46
10:a:283:ARG:O	10:a:284:ARG:C	2.59	0.46
6:e:46:UNK:O	6:e:50:UNK:O	2.34	0.46
6:AX:253:UNK:O	6:AX:254:UNK:C	2.64	0.46
2:F:268:VAL:HA	2:F:280:PRO:HA	1.98	0.46
2:K:97:CYS:O	2:K:98:PRO:C	2.58	0.46
2:K:454:GLN:O	2:K:455:ALA:C	2.58	0.46
9:Z:139:HIS:O	9:Z:140:TRP:C	2.59	0.46
12:c:313:MET:O	12:c:314:ALA:HB2	2.16	0.46
9:n:768:LEU:CB	9:n:796:ALA:HB1	2.46	0.46
2:v:46:PRO:O	2:v:60:LYS:N	2.49	0.46
3:Ak:847:ASN:O	3:Ak:849:CYS:N	2.49	0.45
6:e:381:UNK:HA	6:e:382:UNK:C	2.46	0.45
7:f:70:PRO:O	7:f:71:PRO:C	2.59	0.45
2:u:617:ILE:O	2:u:648:PHE:HA	2.16	0.45
2:3:49:LEU:O	2:3:77:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:29:ILE:O	2:I:33:ALA:HB3	2.16	0.45
12:c:146:GLY:O	12:c:147:SER:C	2.59	0.45
2:t:116:ILE:HA	2:t:184:THR:O	2.15	0.45
2:AB:424:ARG:HA	2:AB:454:GLN:O	2.16	0.45
3:AR:125:LEU:O	3:AR:128:ALA:HB3	2.16	0.45
14:Aq:185:TYR:HA	14:Aq:227:ILE:O	2.16	0.45
6:s:430:UNK:O	6:s:431:UNK:C	2.64	0.45
2:3:39:SER:HA	2:3:68:SER:HA	1.99	0.45
4:8:301:VAL:O	4:8:302:SER:C	2.58	0.45
12:AJ:321:GLY:HA3	12:AJ:373:ARG:HA	1.99	0.45
6:AN:430:UNK:O	6:AN:431:UNK:C	2.64	0.45
6:At:311:UNK:O	6:At:338:UNK:HA	2.17	0.45
13:d:97:ALA:HB2	13:d:143:THR:CA	2.46	0.45
10:o:224:ASN:HA	10:o:232:GLY:HA3	1.98	0.45
2:AB:454:GLN:O	2:AB:455:ALA:C	2.59	0.45
6:g:463:UNK:O	6:g:464:UNK:C	2.65	0.45
4:8:346:LEU:HA	4:8:362:GLY:HA2	1.98	0.45
12:AJ:313:MET:O	12:AJ:314:ALA:HB2	2.17	0.45
3:AR:681:VAL:O	3:AR:682:VAL:C	2.60	0.45
14:Ai:925:ALA:O	14:Ai:926:PHE:O	2.33	0.45
12:Ar:146:GLY:O	12:Ar:147:SER:C	2.59	0.45
2:l:115:GLU:O	2:l:185:VAL:HA	2.16	0.45
2:E:46:PRO:HA	2:E:60:LYS:N	2.32	0.45
2:F:302:PRO:HA	2:F:670:ARG:HA	1.99	0.45
7:h:157:ASN:O	7:h:158:GLN:C	2.57	0.45
2:m:51:HIS:HA	2:m:55:SER:O	2.16	0.45
2:z:314:GLN:O	2:z:315:GLY:C	2.59	0.45
3:AF:672:GLN:HA	3:AF:698:LEU:HA	1.98	0.45
2:C:170:GLU:O	2:C:171:GLY:C	2.59	0.45
7:AO:136:ARG:O	7:AO:140:ASN:N	2.50	0.45
2:Ab:454:GLN:O	2:Ab:455:ALA:C	2.60	0.45
14:Ai:849:LEU:O	14:Ai:850:ALA:C	2.58	0.45
12:Ar:139:HIS:O	12:Ar:170:SER:HA	2.17	0.45
10:o:260:ASP:O	10:o:261:SER:C	2.59	0.45
2:2:454:GLN:O	2:2:455:ALA:C	2.60	0.45
3:7:779:SER:C	3:7:781:MET:H	2.25	0.45
3:AR:611:CYS:O	3:AR:613:VAL:N	2.50	0.44
2:Ab:443:GLY:O	2:Ab:444:LEU:C	2.60	0.44
14:Aq:207:TRP:CB	14:Aq:212:ALA:HB2	2.47	0.44
6:g:394:UNK:HA	6:g:408:UNK:HA	1.98	0.44
2:t:46:PRO:O	2:t:60:LYS:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:29:ILE:O	2:m:33:ALA:HB2	2.18	0.44
2:3:454:GLN:O	2:3:455:ALA:C	2.59	0.44
2:B:115:GLU:O	2:B:185:VAL:HA	2.18	0.44
8:T:52:ARG:HA	8:T:55:SER:O	2.18	0.44
2:x:44:GLY:O	2:x:62:ASP:HA	2.18	0.44
2:A:602:PHE:O	2:A:603:PRO:C	2.60	0.44
3:Ak:885:LYS:O	3:Ak:886:LEU:C	2.61	0.44
2:J:143:GLY:HA2	2:J:678:TRP:O	2.17	0.44
9:Z:54:LEU:HA	12:c:350:GLY:CA	2.48	0.44
10:a:462:ALA:HB2	10:a:512:ALA:HB3	1.99	0.44
2:A:29:ILE:O	2:A:33:ALA:HB3	2.18	0.44
14:Au:426:ASP:O	14:Au:427:ILE:C	2.60	0.44
6:Ax:436:UNK:O	6:Ax:437:UNK:C	2.65	0.44
2:1:452:GLN:O	2:1:453:VAL:C	2.60	0.44
2:A:516:PHE:C	2:A:518:ASP:N	2.75	0.44
10:AH:456:GLY:HA3	10:AH:462:ALA:HA	2.00	0.44
6:AL:433:UNK:O	6:AL:434:UNK:C	2.65	0.44
6:At:127:UNK:O	6:At:128:UNK:C	2.66	0.44
6:g:97:UNK:HA	6:g:100:UNK:O	2.17	0.44
2:m:21:VAL:HA	2:m:79:MET:O	2.17	0.44
2:AB:268:VAL:HA	2:AB:280:PRO:HA	2.00	0.44
2:G:51:HIS:HA	2:G:55:SER:O	2.17	0.44
2:t:617:ILE:O	2:t:648:PHE:HA	2.18	0.44
3:AR:211:GLN:O	3:AR:215:LEU:N	2.51	0.44
6:Av:2:UNK:O	6:Av:3:UNK:C	2.64	0.44
9:Z:921:ASN:HA	9:Z:950:ALA:HB3	2.00	0.44
2:x:424:ARG:HA	2:x:454:GLN:O	2.18	0.44
3:4:699:LYS:HA	3:4:727:VAL:HA	1.99	0.44
4:8:155:PRO:O	4:8:156:GLN:C	2.60	0.44
2:x:271:ALA:HB2	2:x:278:GLU:N	2.32	0.44
6:Av:101:UNK:O	6:Av:102:UNK:C	2.65	0.43
2:I:454:GLN:O	2:I:455:ALA:C	2.61	0.43
10:o:237:VAL:HA	10:o:254:ASN:O	2.18	0.43
6:s:375:UNK:O	6:s:376:UNK:C	2.66	0.43
2:t:46:PRO:HA	2:t:59:GLY:O	2.18	0.43
2:z:454:GLN:O	2:z:455:ALA:C	2.61	0.43
2:A:336:GLU:O	2:A:337:ASP:C	2.61	0.43
2:AC:424:ARG:HA	2:AC:454:GLN:O	2.18	0.43
6:AN:346:UNK:O	6:AN:347:UNK:C	2.66	0.43
7:AO:6:LEU:O	7:AO:13:ILE:HA	2.19	0.43
7:Aw:157:ASN:O	7:Aw:158:GLN:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:HIS:O	2:D:72:PRO:C	2.60	0.43
2:H:153:VAL:HA	2:H:249:ALA:O	2.18	0.43
3:4:211:GLN:O	3:4:212:PRO:C	2.60	0.43
6:A1:59:UNK:O	6:A1:60:UNK:C	2.66	0.43
6:AX:453:UNK:O	6:AX:454:UNK:C	2.67	0.43
6:Ax:341:UNK:O	6:Ax:342:UNK:C	2.67	0.43
10:o:257:LEU:H	10:o:260:ASP:HA	1.83	0.43
2:3:48:ILE:O	2:3:60:LYS:N	2.52	0.43
6:AX:56:UNK:O	6:AX:57:UNK:C	2.66	0.43
2:C:102:VAL:O	2:C:103:PRO:C	2.61	0.43
9:Z:234:SER:O	9:Z:235:LYS:C	2.60	0.43
2:x:42:ILE:HA	2:x:92:LEU:O	2.19	0.43
2:x:311:LEU:O	2:x:314:GLN:CB	2.67	0.43
2:3:209:THR:O	2:3:226:GLY:HA2	2.18	0.43
4:8:370:VAL:O	4:8:380:GLU:HA	2.18	0.43
2:AC:454:GLN:O	2:AC:455:ALA:C	2.61	0.43
6:AN:434:UNK:C	6:AN:436:UNK:N	2.80	0.43
7:AO:79:GLU:C	7:AO:81:ARG:H	2.25	0.43
12:Ar:10:GLY:O	12:Ar:11:GLN:C	2.61	0.43
2:m:51:HIS:O	2:m:75:ALA:HA	2.18	0.43
12:AJ:132:LEU:O	12:AJ:133:GLN:C	2.62	0.43
12:AJ:314:ALA:HB3	12:AJ:380:ASN:N	2.33	0.43
7:AO:157:ASN:O	7:AO:158:GLN:C	2.60	0.43
5:R:94:GLN:O	5:R:95:PRO:C	2.61	0.43
6:e:433:UNK:O	6:e:434:UNK:C	2.66	0.43
2:Aa:310:GLU:O	2:Aa:312:GLN:N	2.51	0.43
14:Ai:658:LYS:O	14:Ai:659:TYR:C	2.62	0.43
6:Ax:95:UNK:N	6:Ax:455:UNK:O	2.52	0.43
2:D:170:GLU:O	2:D:171:GLY:C	2.62	0.43
2:D:206:ALA:HB1	2:D:226:GLY:O	2.18	0.43
1:S:55:PHE:O	1:S:58:ASP:O	2.37	0.43
6:s:2:UNK:O	6:s:3:UNK:C	2.67	0.43
7:A2:159:TRP:O	7:A2:163:LYS:N	2.51	0.43
6:AL:98:UNK:O	6:AL:99:UNK:C	2.66	0.43
6:AN:436:UNK:O	6:AN:437:UNK:C	2.67	0.43
3:Ak:614:VAL:O	3:Ak:615:THR:C	2.60	0.43
2:E:48:ILE:H	2:E:59:GLY:HA3	1.84	0.43
2:F:184:THR:HA	2:F:241:ARG:O	2.19	0.43
2:G:101:GLU:O	2:G:102:VAL:C	2.61	0.43
3:M:1055:ASN:O	3:M:1056:TRP:C	2.61	0.43
4:Q:346:LEU:HA	4:Q:362:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:432:ALA:O	4:X:433:ARG:C	2.61	0.43
10:o:318:CYS:O	10:o:322:ALA:HB3	2.18	0.43
13:d:109:GLY:O	13:d:110:ALA:C	2.62	0.43
6:g:239:UNK:HA	6:g:249:UNK:O	2.19	0.43
3:4:735:CYS:O	3:4:736:GLU:C	2.60	0.43
12:Aj:285:GLN:O	12:Aj:286:LEU:C	2.61	0.43
6:AN:440:UNK:O	6:AN:441:UNK:C	2.66	0.43
6:Av:253:UNK:O	6:Av:254:UNK:C	2.67	0.43
6:Av:434:UNK:C	6:Av:436:UNK:N	2.82	0.43
2:G:236:THR:O	2:G:237:PHE:C	2.62	0.43
2:H:115:GLU:O	2:H:185:VAL:HA	2.19	0.43
4:Q:155:PRO:O	4:Q:156:GLN:C	2.61	0.43
14:Y:299:ALA:HB1	14:Y:337:GLN:O	2.19	0.43
1:0:2:ALA:HB1	1:0:77:VAL:H	1.84	0.42
2:A:46:PRO:HA	2:A:59:GLY:O	2.18	0.42
2:Ac:514:THR:HA	2:Ac:533:THR:HA	2.01	0.42
2:B:356:ALA:O	2:B:357:PRO:C	2.61	0.42
2:L:267:LEU:O	2:L:280:PRO:HA	2.19	0.42
4:N:397:THR:O	4:N:399:GLU:O	2.36	0.42
6:g:56:UNK:O	6:g:58:UNK:N	2.52	0.42
6:A1:436:UNK:O	6:A1:437:UNK:C	2.66	0.42
9:AG:116:VAL:HA	9:AG:158:LEU:O	2.19	0.42
6:Av:454:UNK:O	6:Av:455:UNK:C	2.67	0.42
2:I:302:PRO:HA	2:I:670:ARG:HA	2.01	0.42
2:K:294:ILE:N	2:K:353:TYR:O	2.53	0.42
4:N:256:TRP:C	4:N:258:SER:H	2.28	0.42
6:g:341:UNK:O	6:g:342:UNK:C	2.67	0.42
6:g:361:UNK:O	6:g:362:UNK:C	2.66	0.42
2:m:442:LYS:O	2:m:443:GLY:C	2.62	0.42
2:v:424:ARG:HA	2:v:454:GLN:O	2.20	0.42
2:y:430:SER:C	2:y:432:TYR:H	2.27	0.42
2:AC:430:SER:O	2:AC:432:TYR:N	2.53	0.42
2:AD:454:GLN:O	2:AD:455:ALA:C	2.61	0.42
9:AG:532:LYS:HA	9:AG:577:LEU:HA	2.01	0.42
2:Ac:454:GLN:O	2:Ac:455:ALA:C	2.61	0.42
2:H:2:SER:O	2:H:3:PHE:C	2.61	0.42
2:J:130:MET:O	2:x:61:GLU:O	2.37	0.42
2:l:268:VAL:HA	2:l:280:PRO:HA	2.01	0.42
2:u:115:GLU:O	2:u:185:VAL:HA	2.18	0.42
2:AC:254:SER:O	2:AC:257:PHE:O	2.38	0.42
10:AH:461:GLY:HA2	10:AH:512:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Af:118:ASP:O	3:Af:119:SER:C	2.63	0.42
6:Av:384:UNK:O	6:Av:399:UNK:HA	2.19	0.42
3:M:903:LEU:C	3:M:905:ASP:H	2.27	0.42
5:O:48:TYR:HA	5:O:88:GLU:HA	2.00	0.42
3:P:211:GLN:O	3:P:212:PRO:C	2.62	0.42
2:w:461:SER:O	2:w:467:GLY:HA2	2.20	0.42
2:1:442:LYS:O	2:1:443:GLY:C	2.61	0.42
6:A1:117:UNK:O	6:A1:118:UNK:C	2.67	0.42
2:AC:206:ALA:HB1	2:AC:226:GLY:C	2.43	0.42
13:As:246:LEU:O	13:As:247:ASN:C	2.63	0.42
1:S:2:ALA:HB1	1:S:77:VAL:H	1.84	0.42
9:Z:814:ALA:HB2	9:Z:840:CYS:O	2.19	0.42
2:1:311:LEU:O	2:1:312:GLN:C	2.63	0.42
2:3:374:GLU:O	2:3:375:ASP:C	2.62	0.42
3:4:903:LEU:O	3:4:905:ASP:N	2.53	0.42
2:A:5:ASN:O	2:A:25:ILE:HA	2.20	0.42
2:A:211:VAL:O	2:A:223:LEU:HA	2.20	0.42
2:AD:424:ARG:HA	2:AD:454:GLN:O	2.20	0.42
6:AL:99:UNK:O	6:AL:100:UNK:C	2.65	0.42
3:AR:929:LEU:O	3:AR:958:LEU:HA	2.20	0.42
5:Aj:94:GLN:O	5:Aj:95:PRO:C	2.62	0.42
6:Av:436:UNK:O	6:Av:437:UNK:C	2.67	0.42
2:E:42:ILE:O	2:E:64:VAL:HA	2.19	0.42
3:P:397:GLY:O	3:P:401:MET:N	2.53	0.42
6:s:436:UNK:O	6:s:437:UNK:C	2.68	0.42
2:t:41:THR:HA	2:t:65:VAL:O	2.20	0.42
2:z:51:HIS:O	2:z:75:ALA:HA	2.19	0.42
14:AU:3:SER:HA	14:AU:6:SER:HA	2.01	0.42
6:AX:346:UNK:HA	6:AX:360:UNK:C	2.50	0.42
7:AY:136:ARG:O	7:AY:140:ASN:HA	2.19	0.42
4:Al:295:LEU:HA	4:Al:571:ARG:O	2.20	0.42
6:Av:166:UNK:HA	6:Av:171:UNK:O	2.20	0.42
2:G:20:MET:HA	2:G:114:ILE:O	2.20	0.42
2:G:172:PRO:O	2:G:174:GLU:N	2.53	0.42
2:I:268:VAL:HA	2:I:280:PRO:HA	2.02	0.42
6:s:434:UNK:C	6:s:436:UNK:N	2.82	0.42
2:2:97:CYS:O	2:2:98:PRO:C	2.62	0.42
2:3:50:ILE:HA	2:3:76:LEU:O	2.20	0.42
2:AC:253:PRO:O	2:AC:450:ALA:HB1	2.20	0.42
3:AF:165:GLY:C	3:AF:167:LEU:H	2.27	0.42
9:AG:883:ARG:O	9:AG:884:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AV:131:GLY:O	12:AV:132:LEU:C	2.63	0.42
2:D:424:ARG:HA	2:D:454:GLN:O	2.20	0.42
10:a:46:PHE:HA	10:a:50:LYS:O	2.20	0.42
10:o:256:ARG:HA	10:o:260:ASP:O	2.19	0.42
2:x:46:PRO:O	2:x:60:LYS:HA	2.20	0.42
1:0:2:ALA:HB1	1:0:77:VAL:N	2.34	0.42
3:AR:730:LEU:O	3:AR:758:LEU:HA	2.20	0.42
3:Af:165:GLY:C	3:Af:167:LEU:H	2.28	0.42
14:Ai:8:PHE:O	14:Ai:9:GLY:C	2.62	0.42
2:I:617:ILE:O	2:I:648:PHE:HA	2.19	0.42
2:K:362:SER:O	2:K:386:SER:HA	2.20	0.42
2:l:310:GLU:CB	2:l:664:ALA:HB2	2.49	0.42
10:o:260:ASP:O	10:o:262:GLN:N	2.53	0.42
2:1:206:ALA:O	2:1:209:THR:O	2.37	0.42
4:5:299:VAL:HA	4:5:309:PHE:O	2.20	0.42
4:8:295:LEU:HA	4:8:571:ARG:O	2.20	0.42
7:A2:154:ARG:O	7:A2:158:GLN:HA	2.19	0.42
13:AK:246:LEU:O	13:AK:247:ASN:C	2.62	0.42
4:Al:254:LEU:O	4:Al:255:SER:C	2.63	0.42
14:Aq:4:PHE:O	14:Aq:5:ILE:C	2.62	0.42
5:R:75:LEU:O	5:R:91:ILE:HA	2.19	0.42
9:Z:89:ALA:O	9:Z:90:GLY:C	2.63	0.42
6:e:2:UNK:C	6:e:4:UNK:N	2.83	0.42
6:e:346:UNK:HA	6:e:360:UNK:C	2.50	0.42
6:g:193:UNK:O	6:g:194:UNK:O	2.38	0.42
10:o:258:LEU:C	10:o:260:ASP:H	2.28	0.42
3:7:207:LYS:O	3:7:208:ILE:C	2.62	0.41
4:8:442:ILE:O	4:8:453:CYS:HA	2.19	0.41
11:Al:85:CYS:O	11:Al:86:LEU:C	2.63	0.41
6:AL:394:UNK:HA	6:AL:408:UNK:HA	2.01	0.41
6:AX:213:UNK:CA	6:AX:232:UNK:O	2.68	0.41
3:Af:900:GLU:HA	3:Af:928:SER:O	2.20	0.41
3:Ak:813:THR:HA	3:Ak:840:ALA:O	2.20	0.41
6:At:213:UNK:CA	6:At:232:UNK:O	2.67	0.41
7:Au:136:ARG:O	7:Au:140:ASN:HA	2.20	0.41
6:Av:154:UNK:HA	6:Av:164:UNK:O	2.20	0.41
2:D:52:ILE:HA	2:D:75:ALA:HA	2.01	0.41
3:P:817:LEU:O	3:P:846:LEU:HA	2.20	0.41
7:h:162:GLU:O	7:h:163:LYS:C	2.63	0.41
9:n:772:GLN:O	9:n:773:CYS:C	2.63	0.41
6:s:454:UNK:O	6:s:455:UNK:C	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:324:SER:O	2:t:328:LYS:N	2.53	0.41
2:x:214:SER:O	2:x:215:GLN:C	2.62	0.41
2:y:133:ASP:O	2:y:136:ALA:HB3	2.20	0.41
6:A1:305:UNK:O	6:A1:306:UNK:C	2.68	0.41
2:AD:364:ILE:O	2:AD:388:TYR:HA	2.20	0.41
3:Af:761:ALA:HA	3:Af:790:ASP:O	2.19	0.41
2:B:513:VAL:O	2:B:533:THR:HA	2.20	0.41
2:G:565:LEU:O	2:G:566:GLY:C	2.63	0.41
2:I:40:PHE:HA	2:I:94:SER:O	2.19	0.41
10:a:38:VAL:O	10:a:39:GLU:C	2.62	0.41
6:g:157:UNK:O	6:g:158:UNK:C	2.68	0.41
2:u:170:GLU:O	2:u:171:GLY:C	2.63	0.41
2:w:499:PHE:O	2:w:500:GLU:C	2.62	0.41
2:x:454:GLN:O	2:x:455:ALA:C	2.62	0.41
2:y:45:SER:O	2:y:60:LYS:HA	2.20	0.41
2:1:206:ALA:HB1	2:1:226:GLY:O	2.21	0.41
2:AD:268:VAL:HA	2:AD:280:PRO:HA	2.02	0.41
6:AN:78:UNK:O	6:AN:79:UNK:C	2.68	0.41
12:AV:10:GLY:O	12:AV:11:GLN:C	2.63	0.41
4:Ah:432:ALA:O	4:Ah:433:ARG:C	2.63	0.41
2:G:579:PHE:HA	2:G:599:ARG:O	2.21	0.41
2:K:263:LEU:O	2:K:285:THR:HA	2.18	0.41
2:K:430:SER:C	2:K:432:TYR:H	2.28	0.41
12:AJ:265:ILE:O	12:AJ:267:PHE:N	2.53	0.41
2:Aa:71:HIS:O	2:Aa:72:PRO:C	2.62	0.41
2:Aa:306:TYR:O	2:Aa:666:ALA:HB1	2.21	0.41
4:Ah:285:GLN:O	4:Ah:577:TYR:HA	2.20	0.41
6:At:253:UNK:O	6:At:254:UNK:C	2.69	0.41
6:Ax:453:UNK:O	6:Ax:455:UNK:N	2.53	0.41
2:H:119:GLU:N	2:H:182:ASN:O	2.52	0.41
4:N:432:ALA:O	4:N:433:ARG:C	2.63	0.41
3:P:131:PRO:O	3:P:132:TYR:C	2.64	0.41
3:P:859:LEU:O	3:P:860:ALA:C	2.61	0.41
6:e:341:UNK:O	6:e:342:UNK:C	2.68	0.41
10:o:546:GLY:CA	10:o:552:ALA:HB3	2.51	0.41
3:4:279:MET:O	3:4:280:VAL:C	2.62	0.41
3:AR:614:VAL:O	3:AR:615:THR:C	2.63	0.41
3:Af:906:CYS:O	3:Af:934:ASN:HA	2.20	0.41
6:Av:430:UNK:O	6:Av:431:UNK:C	2.66	0.41
2:G:473:MET:HA	2:G:491:LEU:O	2.21	0.41
10:o:293:PRO:O	10:o:294:PRO:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:p:88:ILE:O	11:p:93:TRP:HA	2.20	0.41
4:5:300:ALA:O	4:5:308:VAL:HA	2.20	0.41
2:AD:514:THR:HA	2:AD:533:THR:HA	2.02	0.41
9:AG:163:SER:HA	9:AG:209:ALA:O	2.20	0.41
6:AL:108:UNK:O	6:AL:116:UNK:O	2.38	0.41
6:Av:385:UNK:HA	6:Av:399:UNK:HA	2.02	0.41
2:Az:513:VAL:O	2:Az:533:THR:HA	2.21	0.41
2:D:429:GLY:O	2:D:460:PHE:HA	2.20	0.41
2:G:170:GLU:O	2:G:171:GLY:C	2.62	0.41
5:O:94:GLN:O	5:O:95:PRO:C	2.64	0.41
3:P:909:THR:O	3:P:910:GLN:C	2.63	0.41
1:S:16:LYS:O	1:S:17:GLN:C	2.64	0.41
4:X:493:CYS:HA	4:X:504:LEU:O	2.21	0.41
6:g:440:UNK:O	6:g:441:UNK:C	2.68	0.41
2:1:430:SER:C	2:1:432:TYR:H	2.28	0.41
6:AN:58:UNK:O	6:AN:59:UNK:C	2.69	0.41
2:Ab:206:ALA:HB1	2:Ab:226:GLY:O	2.21	0.41
1:An:75:VAL:HA	1:An:85:GLU:O	2.21	0.41
6:Ax:305:UNK:O	6:Ax:306:UNK:C	2.68	0.41
2:Az:324:SER:O	2:Az:328:LYS:N	2.53	0.41
9:Z:177:ALA:O	9:Z:178:LEU:C	2.63	0.41
2:w:306:TYR:O	2:w:666:ALA:HB1	2.20	0.41
2:y:98:PRO:C	2:y:100:GLN:H	2.29	0.41
13:AW:137:HIS:O	13:AW:168:SER:HA	2.20	0.41
2:Aa:473:MET:HA	2:Aa:491:LEU:O	2.21	0.41
2:Ad:454:GLN:O	2:Ad:455:ALA:C	2.63	0.41
4:Ah:147:PRO:O	4:Ah:148:GLN:C	2.64	0.41
3:Ak:934:ASN:O	3:Ak:963:CYS:HA	2.21	0.41
4:Al:430:ASN:O	4:Al:446:GLY:HA3	2.21	0.41
3:M:727:VAL:O	3:M:755:LEU:HA	2.21	0.41
5:O:50:GLU:O	5:O:51:ALA:C	2.63	0.41
10:a:448:ARG:O	10:a:449:PRO:C	2.62	0.41
2:u:454:GLN:O	2:u:455:ALA:C	2.64	0.41
2:z:353:TYR:HA	2:z:362:SER:HA	2.02	0.41
3:4:435:ASN:O	3:4:436:SER:C	2.64	0.41
3:4:900:GLU:HA	3:4:928:SER:O	2.20	0.41
4:5:255:SER:O	4:5:257:GLY:N	2.54	0.41
6:A1:151:UNK:HA	6:A1:167:UNK:HA	2.02	0.41
2:AC:206:ALA:HB1	2:AC:226:GLY:O	2.20	0.41
2:AC:302:PRO:HA	2:AC:670:ARG:HA	2.03	0.41
12:AJ:146:GLY:O	12:AJ:147:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AU:531:CYS:O	14:AU:532:LEU:C	2.63	0.41
14:AU:850:ALA:HB1	14:AU:880:ALA:HB2	2.02	0.41
2:B:442:LYS:O	2:B:443:GLY:C	2.63	0.41
2:C:20:MET:O	2:C:21:VAL:C	2.64	0.41
2:G:43:ARG:HA	2:G:63:THR:O	2.21	0.41
3:M:903:LEU:O	3:M:905:ASP:N	2.54	0.41
9:Z:719:GLU:HA	9:Z:746:LEU:HA	2.03	0.41
7:f:136:ARG:O	7:f:140:ASN:N	2.54	0.41
6:g:380:UNK:O	6:g:381:UNK:C	2.69	0.41
10:o:24:LYS:HA	10:o:56:HIS:O	2.20	0.41
11:p:31:PHE:O	11:p:55:HIS:HA	2.21	0.41
12:q:313:MET:O	12:q:314:ALA:HB2	2.21	0.41
2:y:52:ILE:O	2:y:54:SER:N	2.54	0.41
2:A:212:TYR:HA	2:A:222:GLU:O	2.21	0.41
9:AG:315:PRO:O	9:AG:316:VAL:C	2.64	0.41
10:AH:176:ASP:HA	10:AH:197:ALA:HB3	2.02	0.41
6:AL:109:UNK:HA	6:AL:116:UNK:O	2.21	0.41
3:AR:874:LEU:O	3:AR:903:LEU:HA	2.21	0.41
3:AR:932:GLY:O	3:AR:961:GLY:O	2.39	0.41
4:AS:431:SER:O	4:AS:445:GLY:C	2.64	0.41
3:Af:132:TYR:O	3:Af:133:GLN:C	2.63	0.41
14:Aq:812:LEU:O	14:Aq:813:LYS:C	2.64	0.41
6:At:346:UNK:HA	6:At:360:UNK:C	2.51	0.41
6:Ax:108:UNK:O	6:Ax:109:UNK:C	2.69	0.41
2:L:206:ALA:O	2:L:226:GLY:HA2	2.21	0.41
1:S:50:LEU:O	1:S:54:MET:N	2.54	0.41
12:c:182:VAL:O	12:c:183:GLU:C	2.64	0.41
2:v:268:VAL:HA	2:v:280:PRO:HA	2.03	0.41
2:A:623:PRO:O	2:A:629:CYS:HA	2.21	0.40
9:AG:50:GLU:O	9:AG:52:ALA:N	2.54	0.40
9:AG:322:PRO:C	10:AH:554:ALA:HB2	2.46	0.40
3:AR:899:GLN:O	3:AR:927:LYS:N	2.54	0.40
14:AU:775:GLU:HA	14:AU:802:LEU:HA	2.03	0.40
13:AW:66:VAL:HA	13:AW:91:VAL:O	2.20	0.40
2:Aa:430:SER:C	2:Aa:432:TYR:H	2.29	0.40
2:Ab:436:GLU:O	2:Ab:437:GLY:C	2.64	0.40
4:Ah:534:ILE:O	4:Ah:547:GLN:HA	2.22	0.40
14:Aq:267:MET:O	14:Aq:268:LEU:C	2.64	0.40
2:B:473:MET:HA	2:B:491:LEU:O	2.21	0.40
4:X:366:PRO:HA	4:X:387:GLU:C	2.46	0.40
9:Z:712:GLU:O	9:Z:713:ASN:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:121:ARG:O	13:d:124:ALA:HB3	2.21	0.40
2:z:38:LYS:O	2:z:68:SER:HA	2.22	0.40
3:7:839:CYS:O	3:7:840:ALA:HB3	2.20	0.40
12:AJ:139:HIS:O	12:AJ:170:SER:HA	2.20	0.40
6:AN:253:UNK:O	6:AN:254:UNK:C	2.70	0.40
3:AR:885:LYS:O	3:AR:886:LEU:C	2.64	0.40
6:At:56:UNK:O	6:At:57:UNK:C	2.69	0.40
2:D:602:PHE:O	2:D:603:PRO:C	2.64	0.40
2:I:494:SER:O	2:I:576:PRO:HA	2.20	0.40
14:Y:659:TYR:O	14:Y:660:PRO:C	2.63	0.40
2:z:268:VAL:HA	2:z:280:PRO:HA	2.04	0.40
3:4:904:VAL:HA	3:4:932:GLY:H	1.86	0.40
4:5:568:THR:O	4:5:574:ALA:HB1	2.22	0.40
4:8:349:CYS:HA	4:8:360:ALA:HA	2.04	0.40
2:AB:206:ALA:HB1	2:AB:226:GLY:C	2.46	0.40
3:AF:118:ASP:O	3:AF:119:SER:C	2.64	0.40
3:AF:132:TYR:O	3:AF:133:GLN:C	2.62	0.40
10:AH:507:THR:O	10:AH:508:ASN:C	2.65	0.40
2:Ac:170:GLU:O	2:Ac:171:GLY:C	2.63	0.40
6:Ax:110:UNK:N	6:Ax:117:UNK:HA	2.37	0.40
2:C:313:LEU:O	2:C:314:GLN:C	2.63	0.40
2:G:617:ILE:O	2:G:648:PHE:HA	2.21	0.40
2:I:324:SER:O	2:I:328:LYS:N	2.54	0.40
6:g:433:UNK:O	6:g:434:UNK:CB	2.69	0.40
5:6:50:GLU:O	5:6:51:ALA:C	2.64	0.40
4:8:306:ARG:O	4:8:320:ASN:HA	2.21	0.40
3:AF:133:GLN:O	3:AF:135:THR:N	2.54	0.40
10:AH:615:TYR:O	10:AH:618:ALA:HB3	2.21	0.40
6:AL:253:UNK:O	6:AL:254:UNK:C	2.69	0.40
3:Ak:945:CYS:CB	3:Ak:972:ALA:HB1	2.51	0.40
2:G:585:THR:O	2:G:587:VAL:N	2.54	0.40
2:J:514:THR:HA	2:J:533:THR:HA	2.04	0.40
7:f:139:PHE:O	7:f:140:ASN:C	2.64	0.40
2:m:44:GLY:O	2:m:62:ASP:HA	2.20	0.40
2:m:581:LEU:HA	2:m:597:PHE:O	2.22	0.40
2:u:116:ILE:HA	2:u:184:THR:O	2.21	0.40
2:1:206:ALA:O	2:1:226:GLY:HA2	2.22	0.40
2:AB:651:ASP:O	2:AB:652:PHE:C	2.65	0.40
7:AY:157:ASN:O	7:AY:158:GLN:C	2.64	0.40
2:Ab:45:SER:O	2:Ab:59:GLY:HA3	2.21	0.40
2:Ac:324:SER:O	2:Ac:328:LYS:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:473:MET:HA	2:J:491:LEU:O	2.21	0.40
2:L:45:SER:O	2:L:60:LYS:HA	2.22	0.40
3:M:877:ASN:O	3:M:878:PRO:C	2.65	0.40
4:N:160:GLY:O	4:N:161:PHE:C	2.63	0.40
9:Z:532:LYS:HA	9:Z:577:LEU:HA	2.03	0.40
12:c:102:ASN:O	12:c:103:TYR:C	2.64	0.40
2:m:101:GLU:O	2:m:102:VAL:C	2.63	0.40
6:s:286:UNK:HA	6:s:303:UNK:HA	2.04	0.40
2:v:514:THR:HA	2:v:533:THR:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	134/440 (30%)	127 (95%)	7 (5%)	0	100	100
1	An	134/440 (30%)	130 (97%)	4 (3%)	0	100	100
1	S	134/440 (30%)	128 (96%)	6 (4%)	0	100	100
1	j	134/440 (30%)	128 (96%)	6 (4%)	0	100	100
2	1	680/682 (100%)	616 (91%)	63 (9%)	1 (0%)	48	83
2	2	680/682 (100%)	626 (92%)	54 (8%)	0	100	100
2	3	680/682 (100%)	624 (92%)	56 (8%)	0	100	100
2	A	680/682 (100%)	613 (90%)	67 (10%)	0	100	100
2	AB	680/682 (100%)	641 (94%)	38 (6%)	1 (0%)	48	83
2	AC	680/682 (100%)	650 (96%)	29 (4%)	1 (0%)	48	83
2	AD	680/682 (100%)	639 (94%)	41 (6%)	0	100	100
2	Aa	680/682 (100%)	633 (93%)	47 (7%)	0	100	100
2	Ab	680/682 (100%)	645 (95%)	35 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ac	680/682 (100%)	650 (96%)	28 (4%)	2 (0%)	36	72
2	Ad	680/682 (100%)	638 (94%)	42 (6%)	0	100	100
2	Az	680/682 (100%)	631 (93%)	48 (7%)	1 (0%)	48	83
2	B	680/682 (100%)	634 (93%)	46 (7%)	0	100	100
2	C	680/682 (100%)	647 (95%)	33 (5%)	0	100	100
2	D	680/682 (100%)	631 (93%)	49 (7%)	0	100	100
2	E	680/682 (100%)	642 (94%)	37 (5%)	1 (0%)	48	83
2	F	680/682 (100%)	646 (95%)	34 (5%)	0	100	100
2	G	680/682 (100%)	615 (90%)	64 (9%)	1 (0%)	48	83
2	H	680/682 (100%)	631 (93%)	49 (7%)	0	100	100
2	I	680/682 (100%)	637 (94%)	43 (6%)	0	100	100
2	J	680/682 (100%)	625 (92%)	54 (8%)	1 (0%)	48	83
2	K	680/682 (100%)	631 (93%)	47 (7%)	2 (0%)	36	72
2	L	680/682 (100%)	638 (94%)	42 (6%)	0	100	100
2	l	680/682 (100%)	640 (94%)	40 (6%)	0	100	100
2	m	680/682 (100%)	633 (93%)	47 (7%)	0	100	100
2	t	680/682 (100%)	635 (93%)	45 (7%)	0	100	100
2	u	680/682 (100%)	631 (93%)	49 (7%)	0	100	100
2	v	680/682 (100%)	630 (93%)	49 (7%)	1 (0%)	48	83
2	w	680/682 (100%)	640 (94%)	40 (6%)	0	100	100
2	x	680/682 (100%)	622 (92%)	58 (8%)	0	100	100
2	y	680/682 (100%)	633 (93%)	45 (7%)	2 (0%)	36	72
2	z	680/682 (100%)	628 (92%)	52 (8%)	0	100	100
3	4	945/1163 (81%)	880 (93%)	63 (7%)	2 (0%)	43	78
3	7	945/1163 (81%)	859 (91%)	86 (9%)	0	100	100
3	AF	945/1163 (81%)	873 (92%)	72 (8%)	0	100	100
3	AR	945/1163 (81%)	878 (93%)	66 (7%)	1 (0%)	48	83
3	Af	945/1163 (81%)	874 (92%)	70 (7%)	1 (0%)	48	83
3	Ak	945/1163 (81%)	867 (92%)	77 (8%)	1 (0%)	48	83
3	M	945/1163 (81%)	881 (93%)	61 (6%)	3 (0%)	36	72
3	P	945/1163 (81%)	873 (92%)	69 (7%)	3 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	5	363/581 (62%)	307 (85%)	56 (15%)	0	100	100
4	8	363/581 (62%)	320 (88%)	42 (12%)	1 (0%)	36	72
4	AS	363/581 (62%)	327 (90%)	34 (9%)	2 (1%)	21	59
4	Ah	363/581 (62%)	316 (87%)	46 (13%)	1 (0%)	36	72
4	Al	363/581 (62%)	317 (87%)	44 (12%)	2 (1%)	21	59
4	N	363/581 (62%)	313 (86%)	48 (13%)	2 (1%)	21	59
4	Q	363/581 (62%)	321 (88%)	41 (11%)	1 (0%)	36	72
4	X	363/581 (62%)	325 (90%)	38 (10%)	0	100	100
5	6	117/164 (71%)	110 (94%)	7 (6%)	0	100	100
5	9	87/164 (53%)	77 (88%)	10 (12%)	0	100	100
5	AQ	117/164 (71%)	113 (97%)	4 (3%)	0	100	100
5	Aj	117/164 (71%)	111 (95%)	6 (5%)	0	100	100
5	Am	87/164 (53%)	78 (90%)	8 (9%)	1 (1%)	11	46
5	O	117/164 (71%)	109 (93%)	8 (7%)	0	100	100
5	R	87/164 (53%)	77 (88%)	10 (12%)	0	100	100
5	i	87/164 (53%)	76 (87%)	10 (12%)	1 (1%)	11	46
7	A2	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
7	AM	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
7	AO	161/163 (99%)	150 (93%)	10 (6%)	1 (1%)	21	59
7	AY	161/163 (99%)	155 (96%)	6 (4%)	0	100	100
7	AZ	161/163 (99%)	156 (97%)	5 (3%)	0	100	100
7	Au	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
7	Aw	161/163 (99%)	155 (96%)	6 (4%)	0	100	100
7	Ay	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
7	f	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
7	h	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
8	AA	61/228 (27%)	57 (93%)	4 (7%)	0	100	100
8	AE	137/228 (60%)	133 (97%)	4 (3%)	0	100	100
8	AP	139/228 (61%)	132 (95%)	7 (5%)	0	100	100
8	AT	78/228 (34%)	78 (100%)	0	0	100	100
8	Ae	137/228 (60%)	133 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Ag	139/228 (61%)	132 (95%)	7 (5%)	0	100	100
8	Ao	137/228 (60%)	137 (100%)	0	0	100	100
8	Ap	78/228 (34%)	76 (97%)	2 (3%)	0	100	100
8	T	61/228 (27%)	56 (92%)	5 (8%)	0	100	100
8	k	137/228 (60%)	136 (99%)	1 (1%)	0	100	100
9	AG	964/993 (97%)	892 (92%)	71 (7%)	1 (0%)	48	83
9	Z	964/993 (97%)	884 (92%)	80 (8%)	0	100	100
9	n	964/993 (97%)	911 (94%)	53 (6%)	0	100	100
10	AH	623/782 (80%)	576 (92%)	47 (8%)	0	100	100
10	a	623/782 (80%)	580 (93%)	43 (7%)	0	100	100
10	o	623/782 (80%)	575 (92%)	47 (8%)	1 (0%)	43	78
11	AI	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
11	b	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
11	p	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
12	AJ	438/449 (98%)	410 (94%)	28 (6%)	0	100	100
12	AV	438/449 (98%)	415 (95%)	23 (5%)	0	100	100
12	Ar	438/449 (98%)	412 (94%)	26 (6%)	0	100	100
12	c	438/449 (98%)	408 (93%)	30 (7%)	0	100	100
12	q	438/449 (98%)	418 (95%)	20 (5%)	0	100	100
13	AK	429/445 (96%)	403 (94%)	26 (6%)	0	100	100
13	AW	429/445 (96%)	409 (95%)	20 (5%)	0	100	100
13	As	429/445 (96%)	408 (95%)	21 (5%)	0	100	100
13	d	429/445 (96%)	407 (95%)	22 (5%)	0	100	100
13	r	429/445 (96%)	411 (96%)	18 (4%)	0	100	100
14	AU	931/937 (99%)	884 (95%)	46 (5%)	1 (0%)	48	83
14	Ai	931/937 (99%)	880 (94%)	49 (5%)	2 (0%)	43	78
14	Aq	931/937 (99%)	875 (94%)	56 (6%)	0	100	100
14	Y	931/937 (99%)	881 (95%)	48 (5%)	2 (0%)	43	78
15	U	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
15	V	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
15	W	72/76 (95%)	68 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	49761/56970 (87%)	46345 (93%)	3372 (7%)	44 (0%)	49 83

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	453	VAL
3	4	904	VAL
3	4	1056	TRP
4	AS	439	ASP
4	AS	572	ASP
14	Ai	926	PHE
14	Ai	928	VAL
4	Al	439	ASP
2	K	175	ILE
3	M	904	VAL
3	P	751	SER
14	Y	926	PHE
14	Y	928	VAL
3	AR	848	HIS
14	AU	928	VAL
2	Ac	239	ASN
2	J	625	ILE
3	M	405	PHE
5	i	105	LEU
10	o	261	SER
2	y	53	SER
4	8	439	ASP
2	AC	431	PHE
3	Af	308	SER
3	Ak	848	HIS
2	E	53	SER
3	P	308	SER
3	P	682	VAL
4	Q	439	ASP
9	AG	317	GLY
7	AO	80	LYS
2	G	586	ASN
3	M	566	GLN
2	v	99	ASP
2	AB	239	ASN
5	Am	71	MET
2	Az	53	SER

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Mol	Chain	Res	Type
4	N	276	GLU
2	Ac	431	PHE
4	Ah	276	GLU
4	Al	155	PRO
2	K	239	ASN
2	y	282	TYR
4	N	155	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

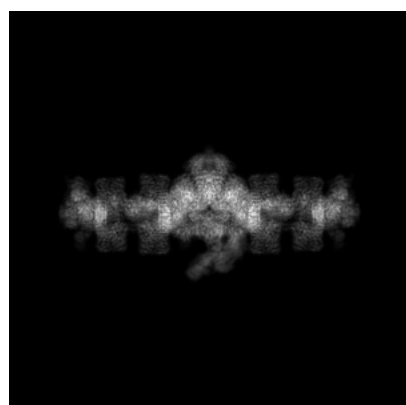
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55609. These allow visual inspection of the internal detail of the map and identification of artifacts.

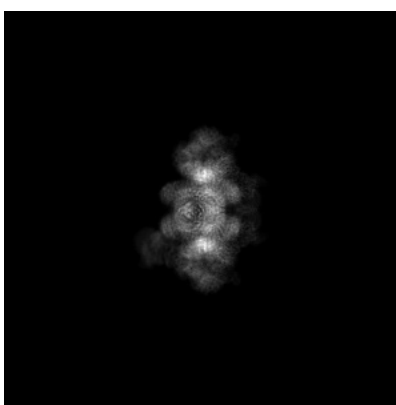
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

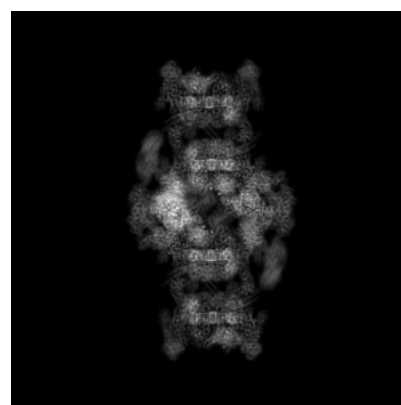
6.1.1 Primary map



X



Y



Z

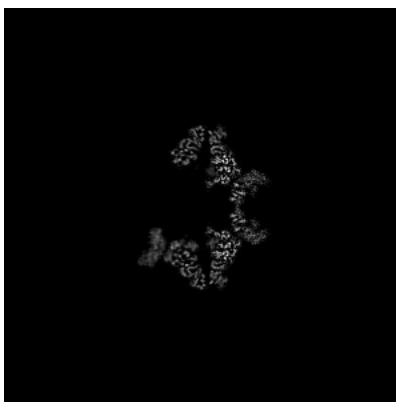
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240

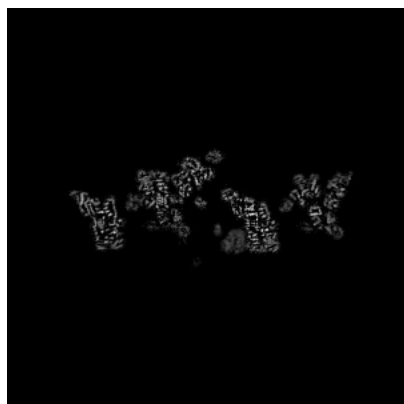


Z Index: 240

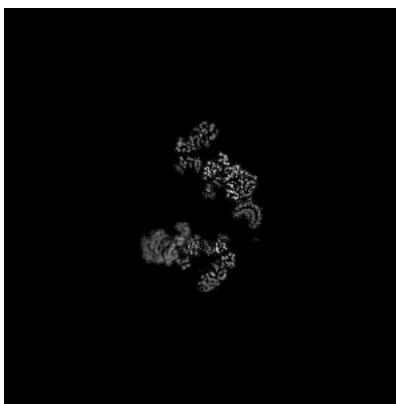
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

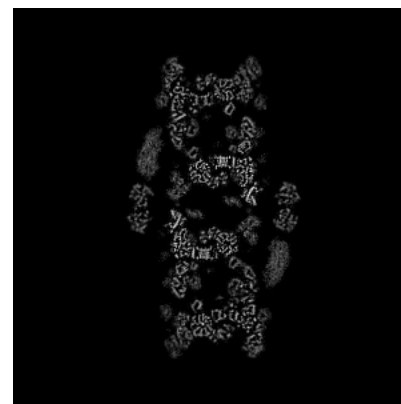
6.3.1 Primary map



X Index: 221



Y Index: 253

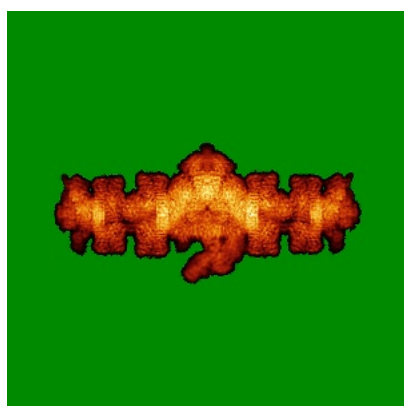


Z Index: 241

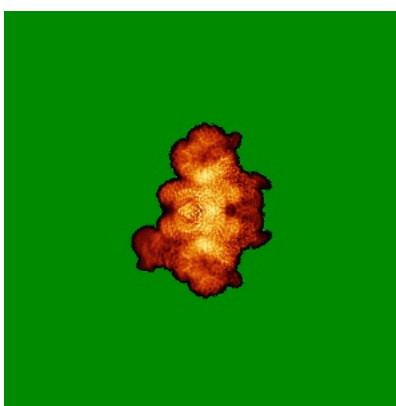
The images above show the largest variance slices of the map in three orthogonal directions.

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

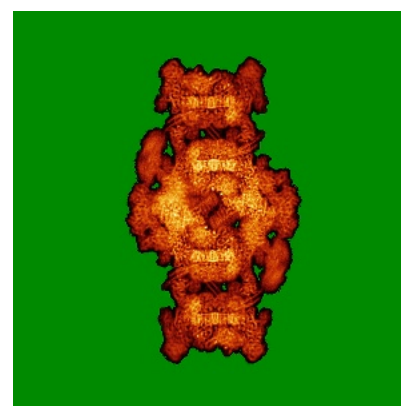
6.4.1 Primary map



X



Y

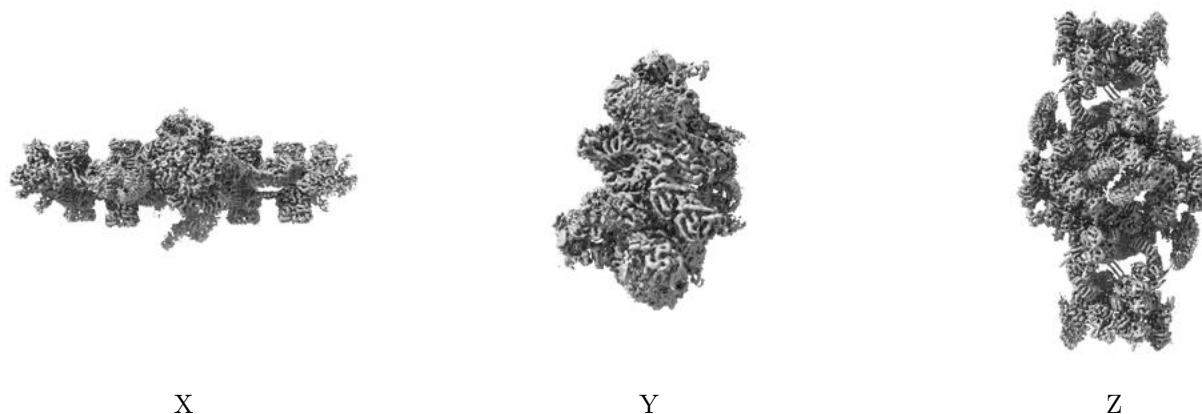


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

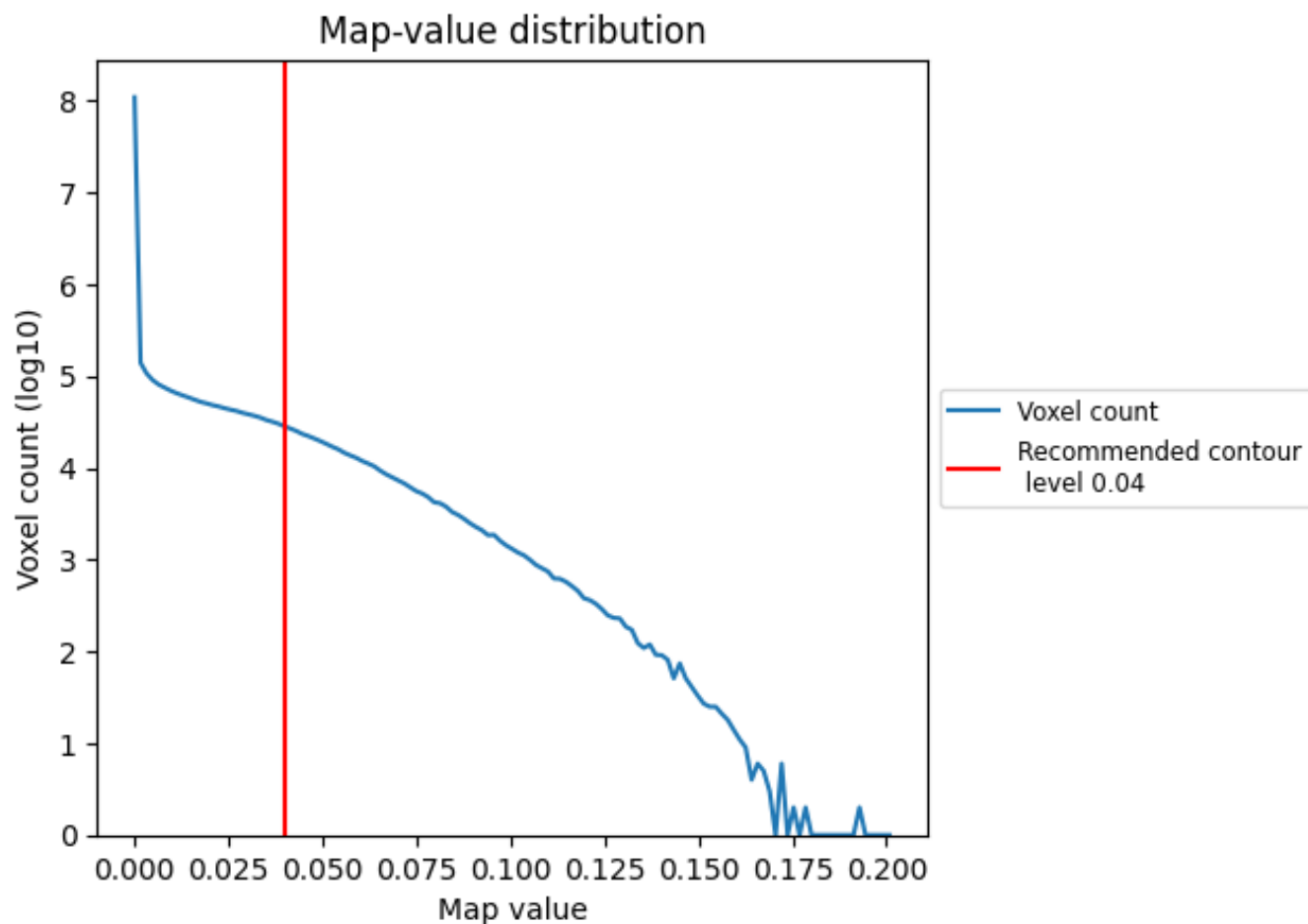
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

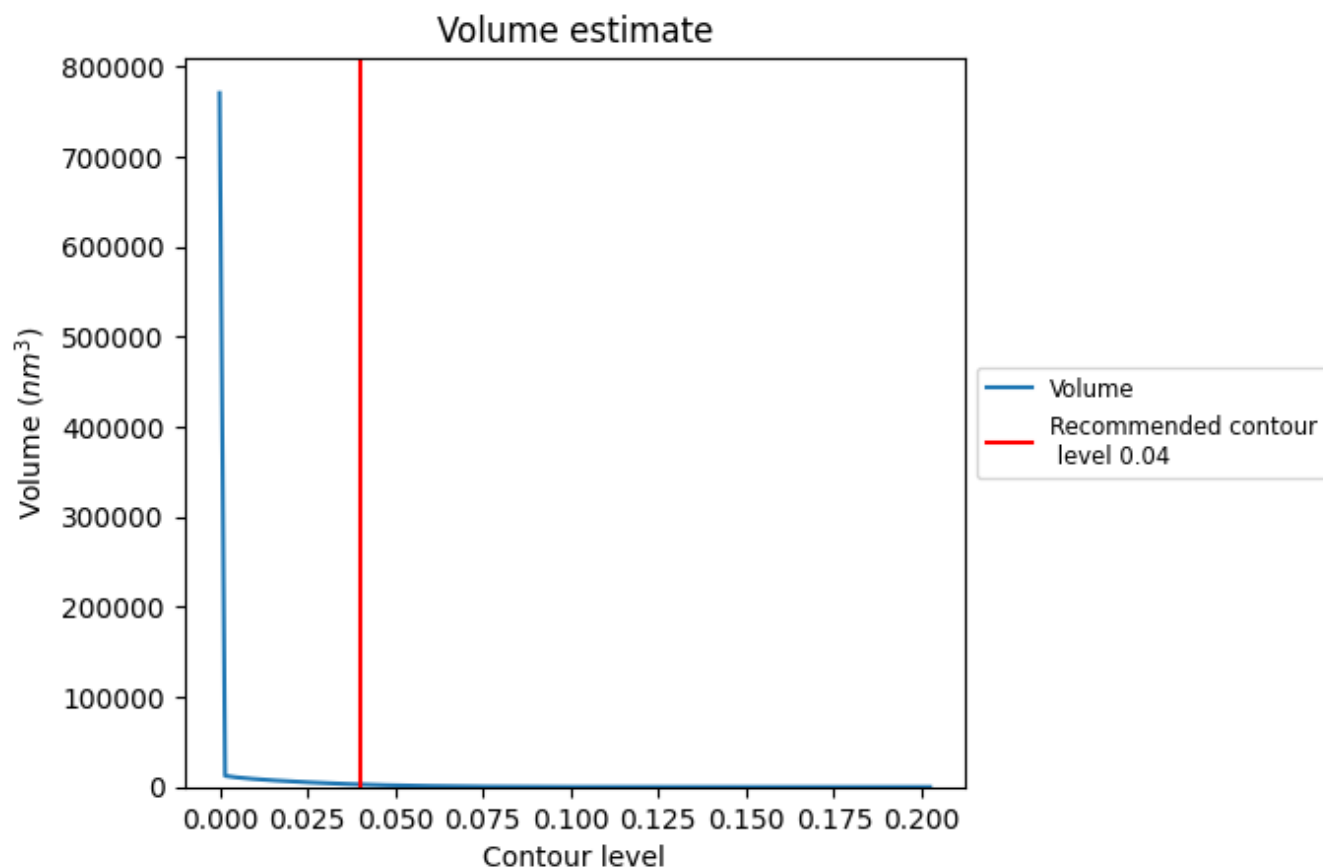
This section contains the results of statistical analysis of the map.

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.

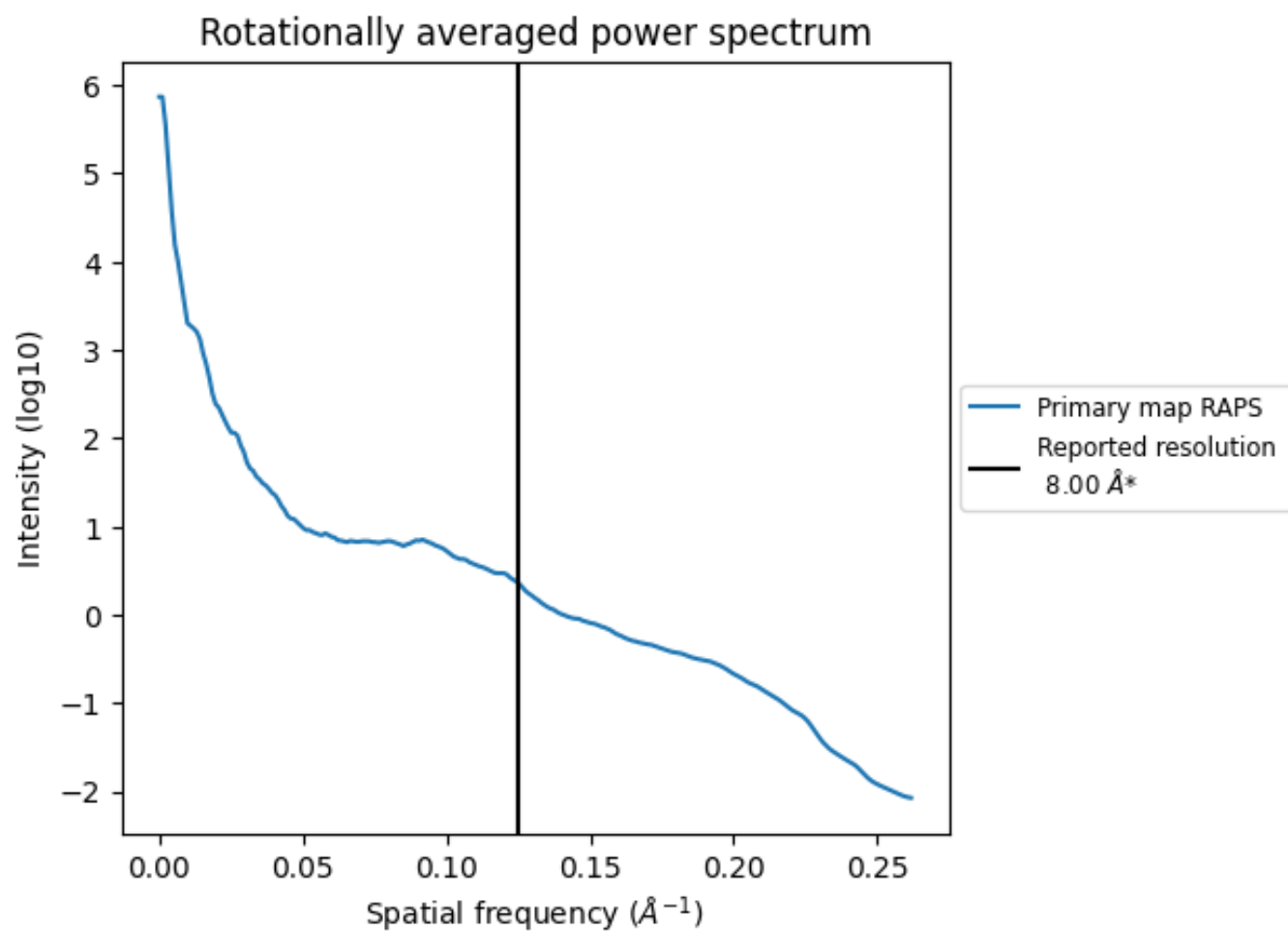
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2781 nm^3 ; this corresponds to an approximate mass of 2512 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 0.125 Å⁻¹

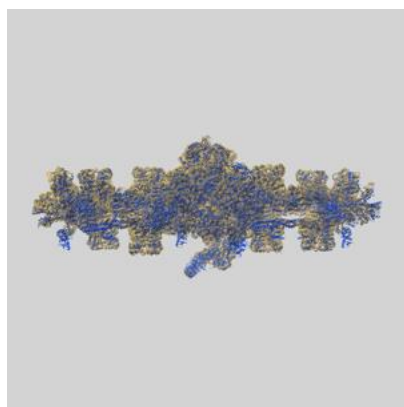
8 Fourier-Shell correlation

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

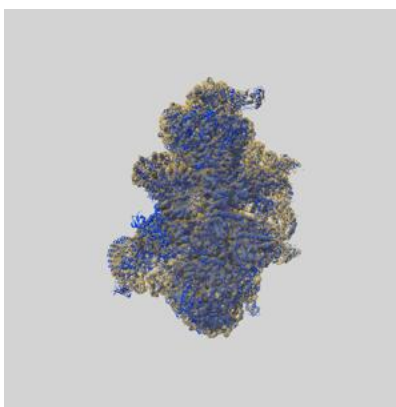
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55609 and PDB model 9T68. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

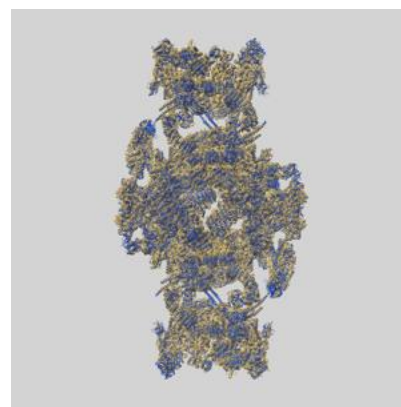
9.1 Map-model overlay [i](#)



X



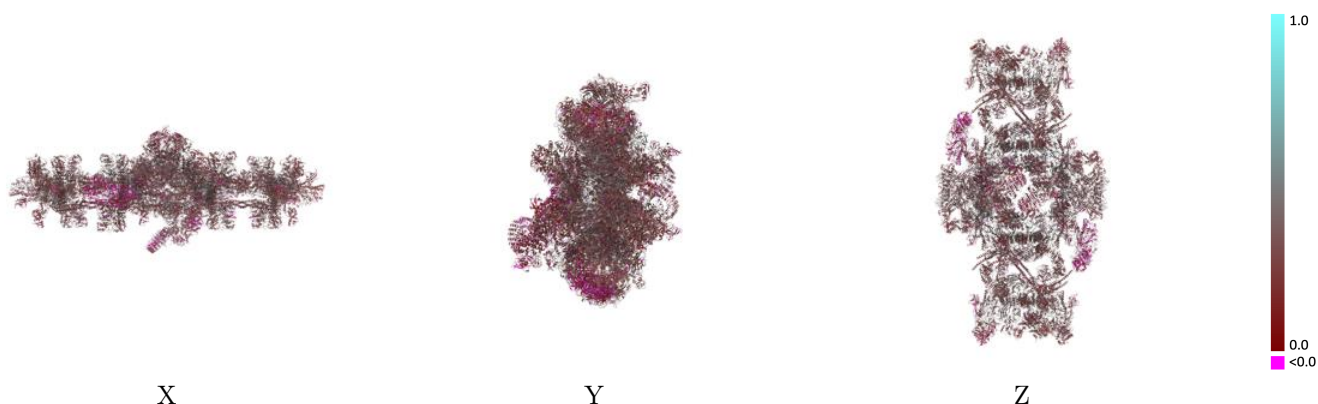
Y



Z

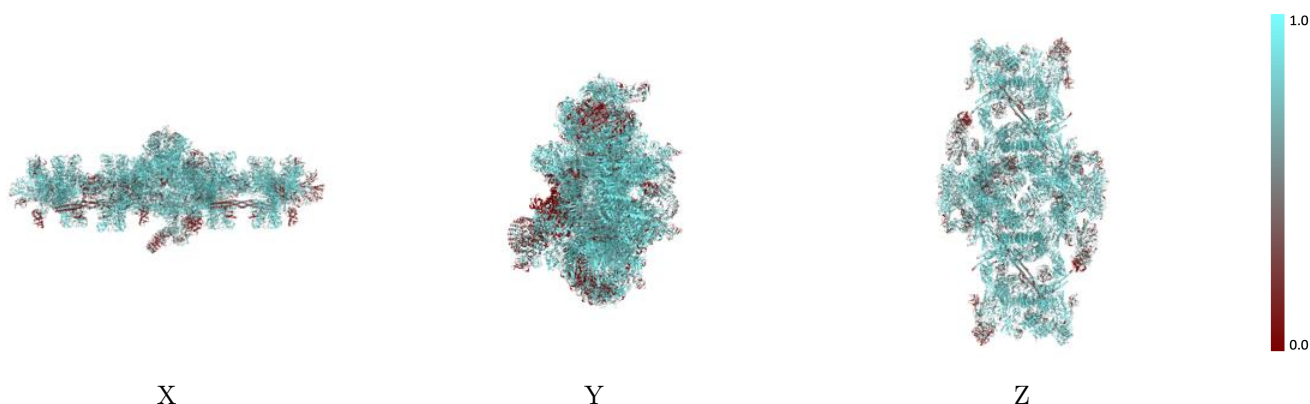
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



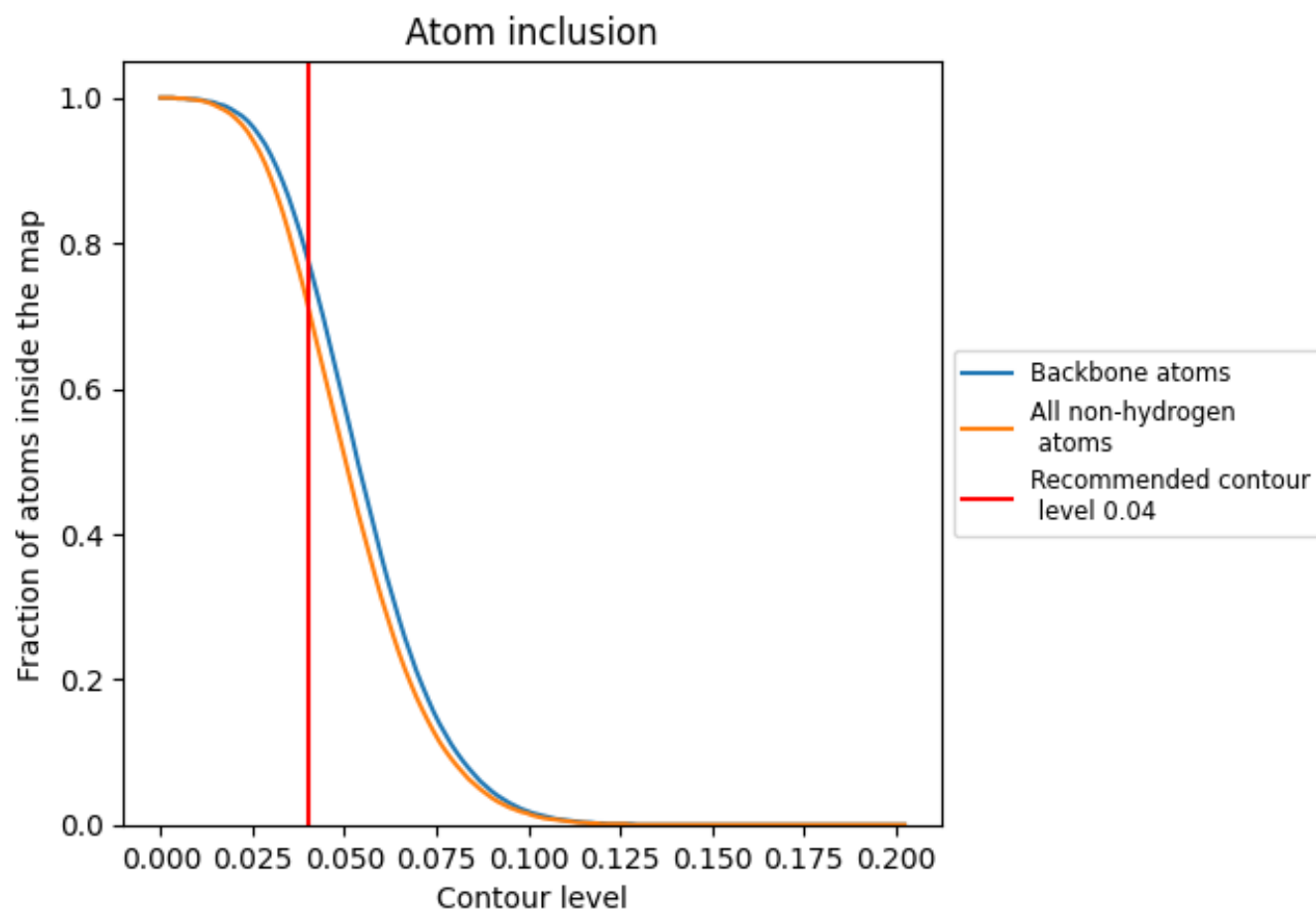
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7160	 0.3040
0	 0.8440	 0.3560
1	 0.7990	 0.3310
2	 0.4420	 0.1520
3	 0.4870	 0.1390
4	 0.8770	 0.3360
5	 0.8630	 0.3580
6	 0.8870	 0.3420
7	 0.8730	 0.3300
8	 0.8440	 0.3430
9	 0.8800	 0.3380
A	 0.8990	 0.3740
A1	 0.5820	 0.2990
A2	 0.3620	 0.2650
AA	 0.7620	 0.2740
AB	 0.6940	 0.3130
AC	 0.3400	 0.2490
AD	 0.6260	 0.3140
AE	 0.1020	 0.2090
AF	 0.8070	 0.3220
AG	 0.7590	 0.2810
AH	 0.7410	 0.3050
AI	 0.9310	 0.3560
AJ	 0.8700	 0.3370
AK	 0.8630	 0.3300
AL	 0.6600	 0.3340
AM	 0.1070	 0.2070
AN	 0.9360	 0.3910
AO	 0.6020	 0.2560
AP	 0.4590	 0.2720
AQ	 0.8260	 0.3210
AR	 0.8250	 0.3190
AS	 0.7840	 0.3320
AT	 0.1710	 0.2580
AU	 0.7360	 0.3070



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Chain	Atom inclusion	Q-score
AV	 0.7140	 0.2970
AW	 0.8160	 0.3170
AX	 0.6620	 0.3270
AY	 0.0800	 0.2150
AZ	 0.5240	 0.2600
Aa	 0.7560	 0.3390
Ab	 0.6920	 0.3140
Ac	 0.3480	 0.2500
Ad	 0.6300	 0.3140
Ae	 0.1020	 0.2130
Af	 0.8050	 0.3230
Ag	 0.4660	 0.2790
Ah	 0.7330	 0.3230
Ai	 0.7480	 0.3030
Aj	 0.8310	 0.3340
Ak	 0.8280	 0.3220
Al	 0.7840	 0.3320
Am	 0.8370	 0.3290
An	 0.7840	 0.3300
Ao	 0.0890	 0.2000
Ap	 0.1710	 0.2540
Aq	 0.7300	 0.3070
Ar	 0.7340	 0.3040
As	 0.8220	 0.3170
At	 0.6550	 0.3300
Au	 0.0860	 0.2170
Av	 0.8770	 0.3690
Aw	 0.5150	 0.2710
Ax	 0.5780	 0.3020
Ay	 0.3650	 0.2640
Az	 0.8520	 0.3580
B	 0.8640	 0.3670
C	 0.7630	 0.3220
D	 0.7420	 0.3210
E	 0.7360	 0.3260
F	 0.7420	 0.3180
G	 0.8700	 0.3530
H	 0.8610	 0.3490
I	 0.6370	 0.2700
J	 0.8100	 0.3370
K	 0.4530	 0.1500
L	 0.4850	 0.1300

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Chain	Atom inclusion	Q-score
M	 0.8790	 0.3390
N	 0.8800	 0.3690
O	 0.8880	 0.3450
P	 0.8830	 0.3320
Q	 0.8600	 0.3470
R	 0.8980	 0.3490
S	 0.8630	 0.3590
T	 0.7880	 0.2960
U	 0.5080	 0.2740
V	 0.1170	 0.2780
W	 0.0160	 0.2350
X	 0.7340	 0.3230
Y	 0.7500	 0.3070
Z	 0.7640	 0.2820
a	 0.7580	 0.3080
b	 0.9350	 0.3620
c	 0.8740	 0.3410
d	 0.8750	 0.3320
e	 0.6970	 0.3350
f	 0.1460	 0.1860
g	 0.9220	 0.3760
h	 0.6140	 0.2600
i	 0.8300	 0.3210
j	 0.8010	 0.3310
k	 0.0990	 0.2140
l	 0.7580	 0.3380
m	 0.8900	 0.3720
n	 0.4180	 0.1730
o	 0.6070	 0.1960
p	 0.8510	 0.2550
q	 0.3810	 0.2010
r	 0.0790	 0.1230
s	 0.8810	 0.3670
t	 0.7670	 0.3250
u	 0.7410	 0.3250
v	 0.7350	 0.3280
w	 0.7380	 0.3140
x	 0.8650	 0.3520
y	 0.8510	 0.3440
z	 0.6260	 0.2760