



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:58 AM UTC

PDB ID : 7VS5 / pdb\_00007vs5  
EMDB ID : EMD-32109  
Title : The expanded head structure of phage T4  
Authors : Fang, Q.; Tang, W.; Fokine, A.; Mahalingam, M.; Shao, Q.; Rossmann, M.G.;  
Rao, V.B.  
Deposited on : 2021-10-25  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

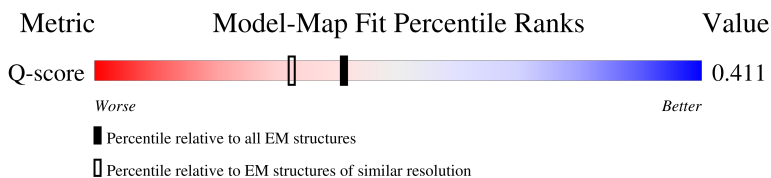
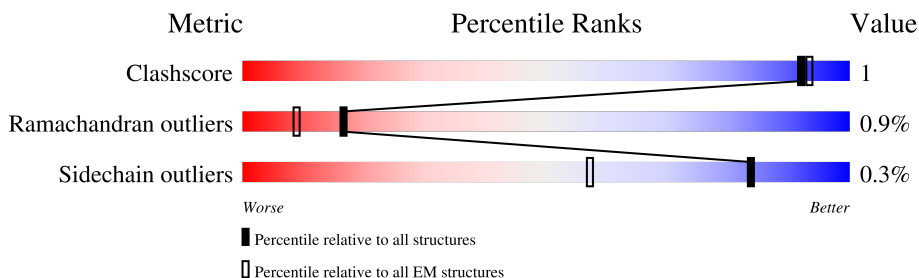
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



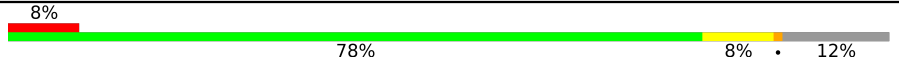

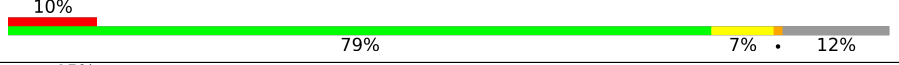

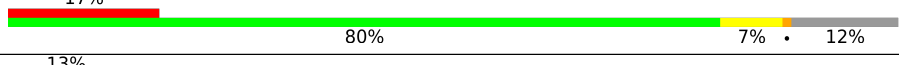
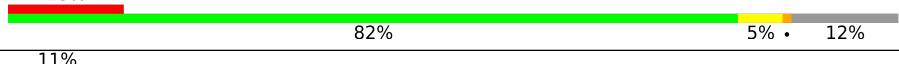
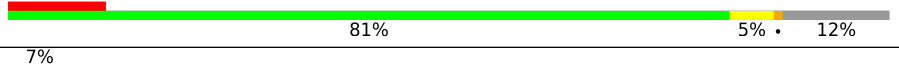

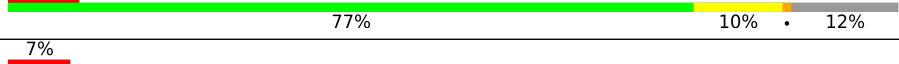


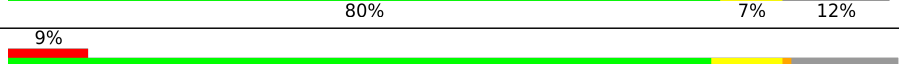
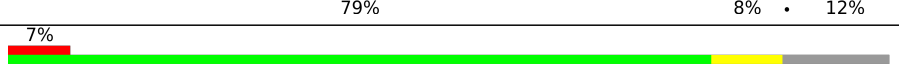
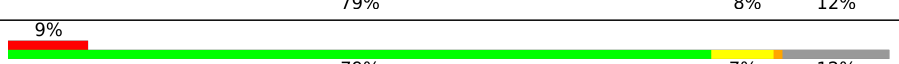

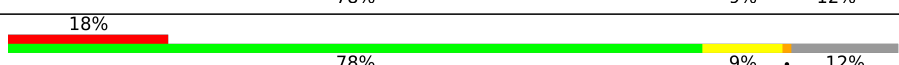
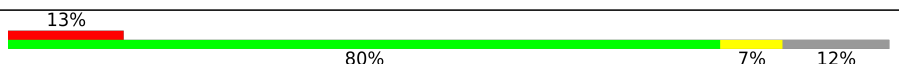
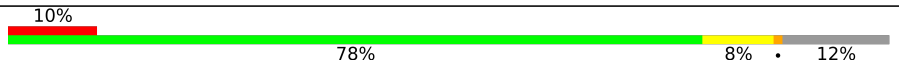
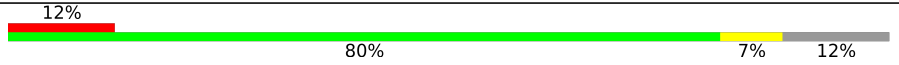


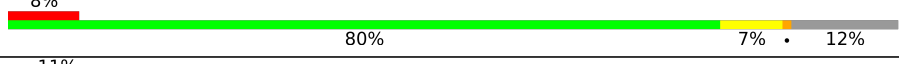
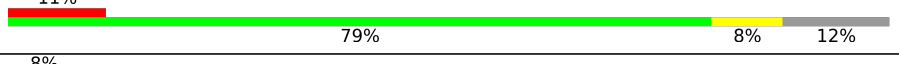


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 ( 2.90 - 3.90 )

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

Mol	Chain	Length	Quality of chain
1	aa	521	<p>5% (red), 80% (green), 7% (yellow), 12% (grey)</p>
1	ab	521	<p>81% (green), 7% (yellow), 12% (grey)</p>
1	ac	521	<p>5% (red), 80% (green), 7% (yellow), 12% (grey)</p>
1	ad	521	<p>5% (red), 81% (green), 6% (yellow), 12% (grey)</p>

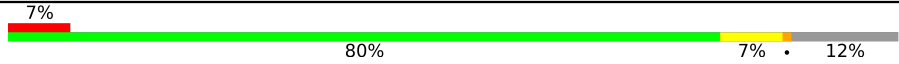

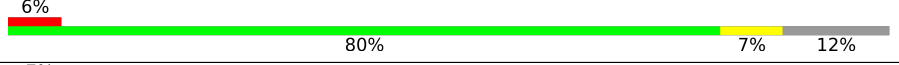

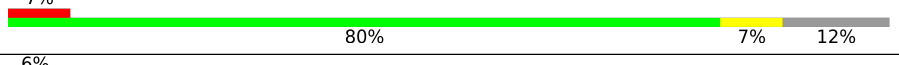
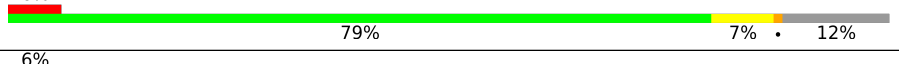
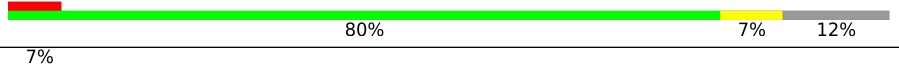

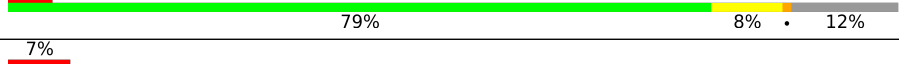


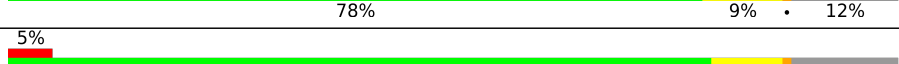
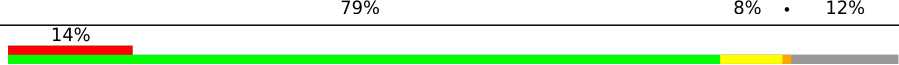
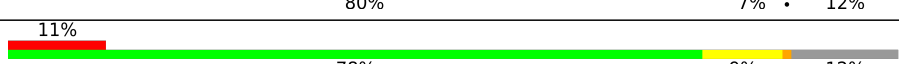

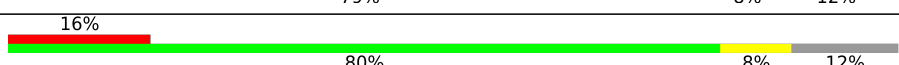
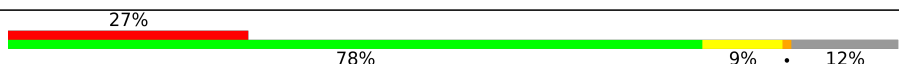
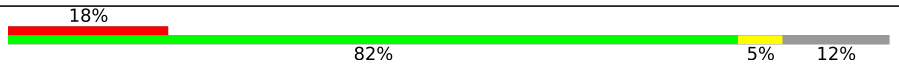
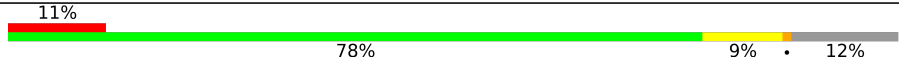


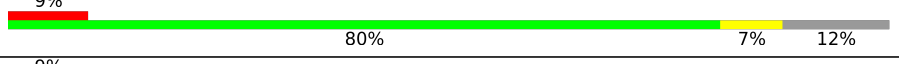
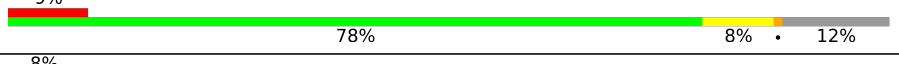


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Mol	Chain	Length	Quality of chain
1	ae	521	 8% 78% 8% • 12%
1	af	521	 7% 79% 9% • 12%
1	ag	521	 10% 79% 7% • 12%
1	ah	521	 15% 79% 8% • 12%
1	ai	521	 17% 80% 7% • 12%
1	aj	521	 13% 82% 5% • 12%
1	ak	521	 11% 81% 5% • 12%
1	al	521	 7% 79% 8% • 12%
1	am	521	 8% 77% 10% • 12%
1	an	521	 7% 79% 8% • 12%
1	ao	521	 6% 80% 7% • 12%
1	ap	521	 9% 80% 7% • 12%
1	aq	521	 9% 79% 8% • 12%
1	ar	521	 7% 79% 8% • 12%
1	as	521	 9% 79% 7% • 12%
1	at	521	 11% 78% 9% • 12%
1	au	521	 18% 78% 9% • 12%
1	av	521	 13% 80% 7% • 12%
1	aw	521	 10% 78% 8% • 12%
1	ax	521	 12% 80% 7% • 12%
1	ay	521	 7% 79% 6% • 12%
1	az	521	 5% 79% 8% • 12%
1	ba	521	 8% 80% 7% • 12%
1	bb	521	 11% 79% 8% • 12%
1	bc	521	 8% 81% 6% • 12%

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Mol	Chain	Length	Quality of chain
1	bd	521	
1	be	521	
1	bf	521	
1	bg	521	
1	bh	521	
1	bi	521	
1	bj	521	
1	bk	521	
1	bl	521	
1	bm	521	
1	bn	521	
1	bo	521	
1	bp	521	
1	bq	521	
1	br	521	
1	bs	521	
1	bt	521	
1	bu	521	
1	bv	521	
1	bw	521	
1	bx	521	
1	by	521	
1	bz	521	
1	ca	521	
1	cb	521	

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Mol	Chain	Length	Quality of chain
1	cc	521	11% 80% 7% 12%
1	cd	521	7% 80% 7% 12%
1	ce	521	7% 79% 8% 12%
1	cf	521	7% 81% 7% 12%
1	cg	521	12% 79% 8% 12%
1	ch	521	10% 79% 8% 12%
1	ci	521	18% 79% 8% 12%
1	cj	521	24% 78% 9% 12%
1	ck	521	16% 79% 7% 12%
1	cl	521	8% 79% 8% 12%
1	cm	521	9% 80% 7% 12%
1	cn	521	11% 80% 6% 12%
1	co	521	13% 79% 8% 12%
1	cp	521	16% 80% 7% 12%
1	cq	521	19% 78% 9% 12%
1	cr	521	24% 80% 7% 12%
1	cs	521	30% 80% 7% 12%
1	ct	521	15% 79% 8% 12%
1	cu	521	14% 80% 7% 12%
1	cv	521	18% 80% 7% 12%
1	cw	521	17% 77% 9% 12%
1	cx	521	18% 79% 8% 12%
1	cy	521	22% 78% 9% 12%
1	cz	521	15% 80% 7% 12%
1	da	521	18% 80% 7% 12%





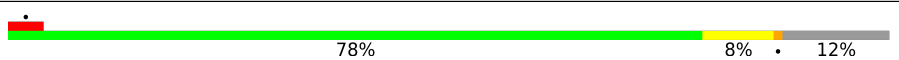
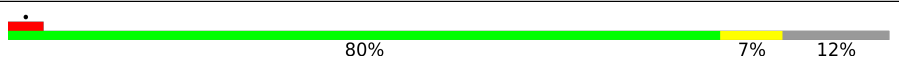
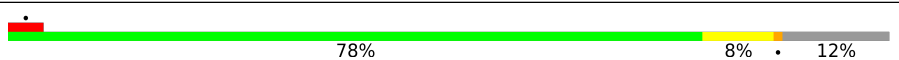
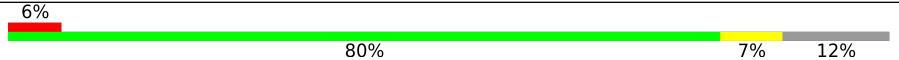
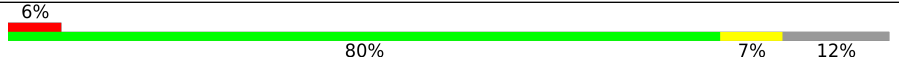
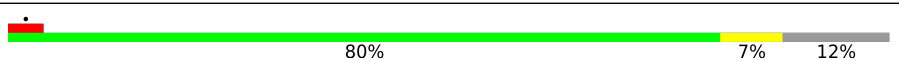
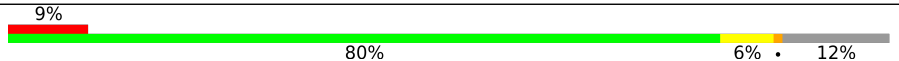
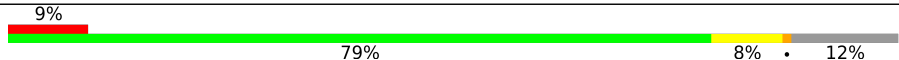


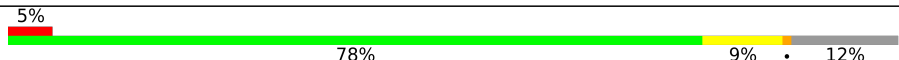
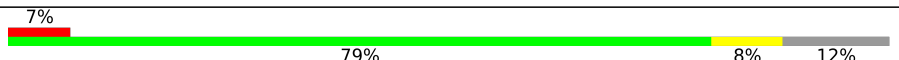
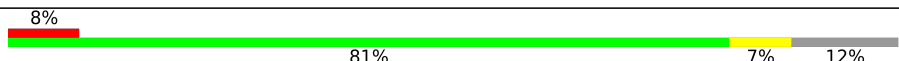
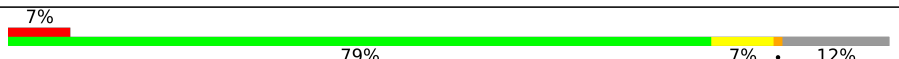
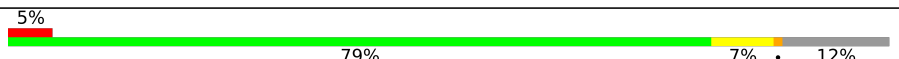

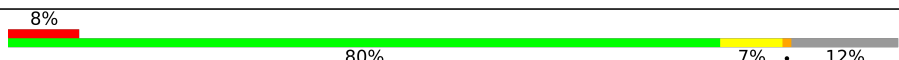
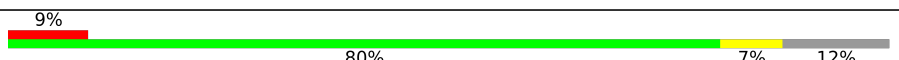
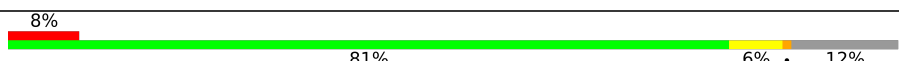
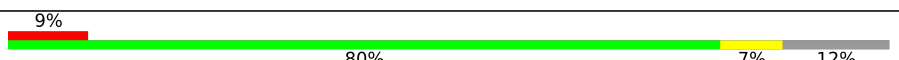
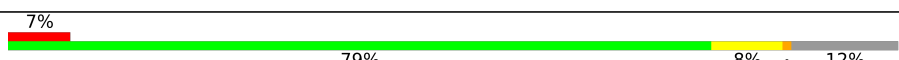
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Mol	Chain	Length	Quality of chain
1	db	521	11% 78% 9% 12%
1	dc	521	9% 79% 7% 12%
1	dd	521	16% 80% 7% 12%
1	de	521	17% 79% 7% 12%
1	df	521	16% 80% 7% 12%
1	dg	521	24% 79% 9% 12%
1	dh	521	22% 78% 9% 12%
1	di	521	17% 81% 6% 12%
1	dj	521	11% 79% 8% 12%
1	dk	521	16% 81% 7% 12%
1	dl	521	19% 78% 9% 12%
1	dm	521	8% 80% 7% 12%
1	dn	521	8% 81% 6% 12%
1	do	521	8% 79% 8% 12%
1	dp	521	10% 80% 7% 12%
1	dq	521	12% 79% 8% 12%
1	dr	521	8% 80% 7% 12%
1	ds	521	12% 81% 6% 12%
1	dt	521	14% 80% 7% 12%
1	du	521	13% 79% 7% 12%
1	dv	521	12% 81% 6% 12%
1	dw	521	12% 75% 6% 17%
1	dx	521	11% 80% 7% 12%
1	dy	521	9% 80% 7% 12%
1	dz	521	6% 80% 7% 12%

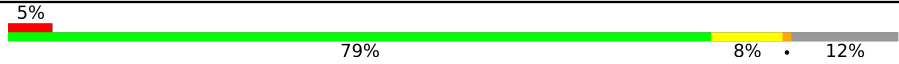
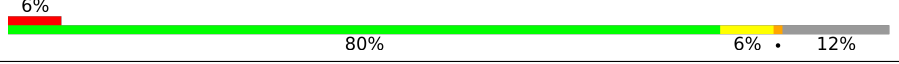
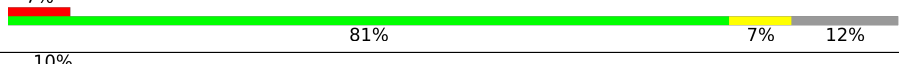


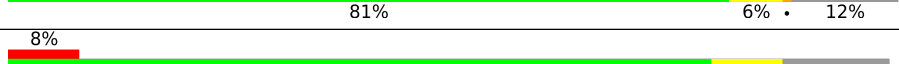
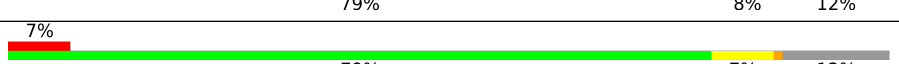
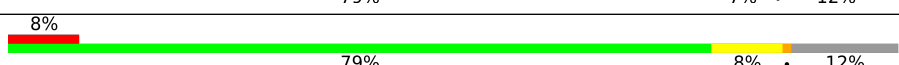
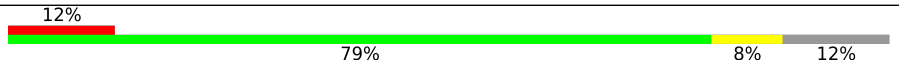


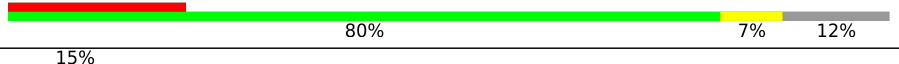
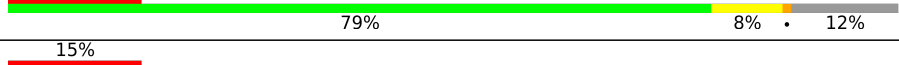

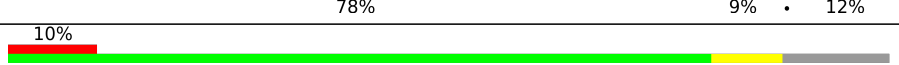










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Mol	Chain	Length	Quality of chain
1	ea	521	 6% 80% 7% • 12%
1	eb	521	 5% 78% 8% • 12%
1	ec	521	 6% 82% 5% • 12%
1	ed	521	 7% 78% 9% 12%
1	ee	521	 • 78% 8% • 12%
1	ef	521	 • 80% 7% 12%
1	eg	521	 • 78% 8% • 12%
1	eh	521	 6% 80% 7% 12%
1	ei	521	 6% 80% 7% 12%
1	ej	521	 • 80% 7% 12%
1	ek	521	 9% 80% 6% • 12%
1	el	521	 9% 79% 8% • 12%
1	em	521	 11% 80% 7% • 12%
1	en	521	 8% 79% 8% • 12%
1	eo	521	 5% 78% 9% • 12%
1	ep	521	 7% 79% 8% 12%
1	eq	521	 8% 81% 7% 12%
1	er	521	 7% 79% 7% • 12%
1	es	521	 5% 79% 7% • 12%
1	et	521	 7% 79% 8% 12%
1	eu	521	 8% 80% 7% • 12%
1	ev	521	 9% 80% 7% 12%
1	ew	521	 8% 81% 6% • 12%
1	ex	521	 9% 80% 7% 12%
1	ey	521	 7% 79% 8% • 12%

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Mol	Chain	Length	Quality of chain
1	ez	521	 5% 79% 8% • 12%
1	fa	521	 6% 80% 6% • 12%
1	fb	521	 7% 81% 7% 12%
1	fc	521	 10% 80% 6% • 12%
1	fd	521	 12% 80% 7% 12%
1	fe	521	 9% 81% 6% • 12%
1	ff	521	 8% 79% 8% 12%
1	fg	521	 7% 79% 7% • 12%
1	fh	521	 8% 79% 8% • 12%
1	fi	521	 12% 79% 8% 12%
1	fj	521	 14% 79% 7% • 12%
1	fk	521	 21% 78% 8% • 12%
1	fl	521	 20% 80% 7% 12%
1	fm	521	 15% 79% 8% • 12%
1	fn	521	 15% 79% 8% 12%
1	fo	521	 8% 78% 9% • 12%
1	fp	521	 10% 79% 8% 12%
1	fq	521	 5% 80% 7% • 12%
1	fr	521	 6% 79% 8% 12%
1	fs	521	 8% 79% 8% • 12%
1	ft	521	 6% 79% 8% 12%
1	fu	521	 7% 80% 7% • 12%
1	fv	521	 8% 80% 7% • 12%
1	fw	521	 12% 80% 7% • 12%
1	fx	521	 11% 80% 7% • 12%

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Mol	Chain	Length	Quality of chain
1	fy	521	9% 80% 7% • 12%
1	fz	521	8% 80% 7% • 12%
1	ga	521	18% 77% 10% 12%
1	gb	521	25% 79% 8% • 12%
1	gc	521	23% 77% 10% • 12%
1	gd	521	15% 80% 7% 12%
1	ge	521	10% 79% 8% • 12%
1	gf	521	11% 82% 6% 12%
1	gg	521	26% 79% 7% • 12%
1	gh	521	20% 80% 6% • 12%
1	gi	521	17% 80% 6% • 12%
1	gj	521	21% 78% 8% • 12%
1	gk	521	29% 80% 6% • 12%
1	gl	521	28% 76% 10% • 12%
1	gm	521	10% 80% 7% • 12%
1	gn	521	6% 79% 8% • 12%
1	go	521	8% 79% 8% • 12%
1	gp	521	15% 79% 8% 12%
1	gq	521	12% 79% 7% • 12%
1	gr	521	10% 79% 8% 12%
1	gs	521	26% 78% 9% • 12%
1	gt	521	22% 80% 7% • 12%
1	gu	521	16% 78% 9% • 12%
1	gv	521	13% 80% 7% 12%
1	gw	521	16% 80% 7% • 12%

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Mol	Chain	Length	Quality of chain
1	gx	521	19% 80% 7% 12%
1	gy	521	9% 79% 8% 12%
1	gz	521	10% 79% 8% 12%
1	ha	521	6% 80% 7% 12%
1	hb	521	5% 80% 7% 12%
1	hc	521	6% 80% 6% 12%
1	hd	521	10% 78% 9% 12%
2	he	427	22% 86% 11% .
2	hf	427	22% 87% 10% .
2	hg	427	22% 88% 8% ..
2	hh	427	24% 87% 10% .
2	hi	427	21% 87% 9% ..
2	hj	427	21% 88% 9% .
2	hk	427	22% 86% 10% ..
2	hl	427	18% 88% 8% ..
2	hm	427	21% 85% 11% ..
2	hn	427	17% 87% 10% .
2	ho	427	37% 87% 9% ..
3	hp	80	92% 86% 12% .
3	hq	80	61% 84% 15% .
3	hr	80	94% 89% 10% .
3	hs	80	96% 85% 12% ..
3	ht	80	99% 89% 10% .
3	hu	80	98% 81% 18% .
3	hv	80	75% 84% 15% .

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Mol	Chain	Length	Quality of chain
3	hw	80	95% 86% 12% .
3	hx	80	89% 90% 9% .
3	hy	80	99% 89% 10% .
3	hz	80	75% 81% 16% ..
3	ia	80	91% 86% 12% .
3	ib	80	89% 88% 11% .
3	ic	80	74% 88% 10% ..
3	id	80	99% 89% 10% .
3	ie	80	96% 86% 12% .
3	if	80	95% 90% 9% .
3	ig	80	91% 86% 12% .
3	ih	80	68% 84% 15% .
3	ii	80	88% 86% 12% .
3	ij	80	61% 81% 18% .
3	ik	80	81% 79% 19% ..
3	il	80	99% 86% 11% ..
3	im	80	95% 84% 15% .
3	in	80	98% 85% 14% .
3	io	80	99% 85% 14% .
3	ip	80	91% 86% 12% .
3	iq	80	99% 81% 18% .
3	ir	80	98% 85% 12% ..
3	is	80	98% 88% 11% .
3	it	80	95% 88% 11% .
3	iu	80	92% 79% 19% ..

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Mol	Chain	Length	Quality of chain
3	iv	80	98% 85% 14%
3	iw	80	98% 80% 19%
3	ix	80	99% 86% 12%
3	iy	80	99% 84% 15%
3	iz	80	82% 82% 16%
3	ja	80	59% 85% 14%
3	jb	80	99% 84% 15%
3	jc	80	99% 79% 20%
3	jd	80	95% 89% 10%
3	je	80	91% 82% 16%
3	jf	80	94% 81% 18%
3	yg	80	82% 78% 20%
3	jh	80	98% 82% 16%
3	ji	80	96% 81% 16%
3	jj	80	98% 92% 6%
3	jk	80	95% 91% 8%
3	jl	80	86% 84% 14%
3	jm	80	96% 89% 10%
3	jn	80	94% 84% 15%
3	jo	80	99% 85% 14%
3	jp	80	99% 91% 6%
3	jq	80	99% 88% 11%
3	jr	80	92% 84% 14%
3	js	80	84% 89% 10%
3	jt	80	98% 85% 14%

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Mol	Chain	Length	Quality of chain
3	ju	80	95% 84% 15% .
3	jv	80	99% 92% 6% .
3	jw	80	99% 82% 16% .
3	jx	80	91% 88% 11% .
3	jy	80	95% 86% 12% .
3	jz	80	99% 81% 16% ..
3	ka	80	99% 81% 16% ..
3	kb	80	98% 82% 16% .
3	kc	80	99% 88% 10% ..
3	kd	80	99% 89% 9% ..
3	ke	80	98% 82% 16% .
3	kf	80	99% 90% 9% .
3	kg	80	92% 81% 18% .
3	kh	80	88% 90% 9% .
3	ki	80	96% 90% 9% .
3	kj	80	99% 91% 8% .
3	kk	80	98% 82% 16% .
3	kl	80	99% 84% 15% .
3	km	80	99% 88% 11% .
3	kn	80	98% 84% 15% .
3	ko	80	99% 82% 16% .
3	kp	80	99% 78% 21% .
3	kq	80	99% 81% 16% ..
3	kr	80	98% 85% 14% .
3	ks	80	95% 86% 12% .

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Mol	Chain	Length	Quality of chain
3	kt	80	96% 84% 15% .
3	ku	80	95% 85% 12% ..
3	80	99% 81% 18% .	
3	kw	80	99% 89% 10% .
3	kx	80	99% 86% 11% ..
3	ky	80	99% 80% 19% .
3	kz	80	99% 89% 10% .
3	la	80	74% 81% 16% ..
3	lb	80	98% 84% 15% .
3	lc	80	95% 86% 12% .
3	ld	80	95% 89% 10% .
3	le	80	92% 85% 12% ..
3	lf	80	71% 85% 14% .
3	lg	80	99% 79% 20% .
3	lh	80	85% 89% 10% .
3	li	80	90% 84% 15% .
3	lj	80	86% 80% 19% .
3	lk	80	88% 85% 14% .
3	ll	80	89% 91% 6% ..
3	lm	80	85% 82% 16% .
3	ln	80	88% 89% 10% .
3	lo	80	96% 86% 12% .
3	lp	80	81% 79% 20% .
3	lq	80	69% 85% 14% .
3	lr	80	85% 94% 5% .

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Mol	Chain	Length	Quality of chain
3	ls	80	91% 89% 9%
3	lt	80	48% 78% 21%
3	lu	80	64% 81% 18%
3	lv	80	98% 82% 16%
3	lw	80	90% 85% 14%
3	lx	80	99% 88% 11%
3	ly	80	95% 86% 12%
3	lz	80	90% 82% 15%
3	ma	80	94% 88% 11%
3	mb	80	99% 88% 11%
3	mc	80	96% 92% 6%
3	md	80	91% 91% 8%
3	me	80	79% 84% 15%
3	mf	80	79% 82% 16%
3	mg	80	80% 89% 10%
3	mh	80	95% 85% 12%
3	mi	80	86% 85% 14%
3	mj	80	76% 80% 19%
3	mk	80	60% 85% 14%
3	ml	80	98% 90% 9%
3	mm	80	99% 84% 15%
3	mn	80	80% 84% 15%
3	mo	80	75% 81% 18%
3	mp	80	80% 86% 12%
3	mq	80	54% 84% 15%

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Mol	Chain	Length	Quality of chain
3	ms	80	99% 80% 19%
3	mt	80	99% 81% 18%
3	mu	80	96% 88% 11%
3	mv	80	99% 86% 12%
3	mw	80	95% 94% 5%
3	mx	80	96% 84% 14%
3	my	80	99% 81% 16%
3	mz	80	99% 80% 19%
3	na	80	99% 88% 11%
3	nb	80	99% 85% 14%
3	nc	80	92% 89% 10%
3	nd	80	95% 86% 11%
3	ne	80	99% 89% 10%
3	nf	80	95% 85% 14%
3	ng	80	88% 88% 11%
3	nh	80	98% 82% 15%
3	ni	80	99% 88% 11%
3	nj	80	99% 85% 12%
3	nk	80	96% 80% 19%
3	nl	80	99% 88% 11%
3	nm	80	98% 90% 9%
3	nn	80	96% 79% 20%
3	no	80	96% 86% 12%
3	np	80	96% 85% 14%
3	nq	80	92% 82% 15%

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Mol	Chain	Length	Quality of chain
3	ns	80	92% 86% 12% .
3	nt	80	99% 85% 12% ..
3	nu	80	99% 78% 20% ..
3	nv	80	92% 85% 12% ..
3	nw	80	88% 82% 15% ..
3	nx	80	98% 90% 9% .
3	ny	80	98% 82% 15% ..
3	nz	80	99% 91% 8% .
3	oa	80	99% 89% 10% .
3	ob	80	99% 82% 16% .
3	oc	80	98% 90% 9% .
3	od	80	96% 89% 10% .
3	oe	80	99% 80% 19% .
3	of	80	99% 86% 12% .
3	og	80	98% 90% 9% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 781038 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	aa	456	3425	2167	584	659	15	0	0
1	ab	456	3425	2167	584	659	15	0	0
1	ac	456	3425	2167	584	659	15	0	0
1	ad	456	3425	2167	584	659	15	0	0
1	ae	456	3425	2167	584	659	15	0	0
1	af	456	3425	2167	584	659	15	0	0
1	ag	456	3425	2167	584	659	15	0	0
1	ah	456	3425	2167	584	659	15	0	0
1	ai	456	3425	2167	584	659	15	0	0
1	aj	456	3425	2167	584	659	15	0	0
1	ak	456	3425	2167	584	659	15	0	0
1	al	456	3425	2167	584	659	15	0	0
1	am	456	3425	2167	584	659	15	0	0
1	an	456	3425	2167	584	659	15	0	0
1	ao	456	3425	2167	584	659	15	0	0
1	ap	456	3425	2167	584	659	15	0	0
1	aq	456	3425	2167	584	659	15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ar	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	as	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	at	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	au	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	av	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	aw	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ax	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ay	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	az	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ba	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bb	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bc	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bd	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	be	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bf	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bg	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bh	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bi	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bj	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bk	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	bl	456	Total 3425	C 2167	N 584	O 659	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	bm	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bn	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bo	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bp	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bq	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	br	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bs	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bt	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bu	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bv	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bw	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bx	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	by	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	bz	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ca	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	cb	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	cc	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	cd	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ce	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	cf	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	cg	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ch	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ci	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cj	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ck	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cl	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cm	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cn	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	co	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cp	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cq	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cr	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cs	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ct	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cu	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cv	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cw	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cx	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cy	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	cz	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	da	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	db	456	Total 3425	C 2167	N 584	O 659	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	dc	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dd	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	de	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	df	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dg	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dh	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	di	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dj	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dk	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dl	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dm	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dn	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	do	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dp	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dq	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dr	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ds	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dt	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	du	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dv	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dw	430	Total	C	N	O	S	0	0
			3249	2062	552	620	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	dx	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dy	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	dz	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ea	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	eb	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ec	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ed	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ee	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ef	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	eg	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	eh	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ei	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ej	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ek	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	el	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	em	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	en	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	eo	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ep	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	eq	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	er	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	es	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	et	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	eu	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ev	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ew	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ex	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ey	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ez	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fa	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fb	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fc	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fd	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fe	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ff	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fg	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fh	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fi	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fj	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fk	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fl	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fm	456	Total 3425	C 2167	N 584	O 659	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	fn	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fo	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fp	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fq	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fr	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fs	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ft	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fu	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fv	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fw	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fx	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fy	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	fz	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ga	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	gb	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	gc	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	gd	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	ge	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	gf	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	gg	456	Total 3425	C 2167	N 584	O 659	S 15	0	0
1	gh	456	Total 3425	C 2167	N 584	O 659	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	gi	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gj	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gk	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gl	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gm	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gn	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	go	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gp	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gq	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gr	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gs	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gt	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gu	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gv	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gw	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gx	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gy	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	gz	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	ha	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	hb	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
1	hc	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	hd	456	3425	2167	584	659	15	0	0

- Molecule 2 is a protein called Capsid vertex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	he	415	3208	2039	521	640	8	0	0
2	hf	415	3208	2039	521	640	8	0	0
2	hg	415	3208	2039	521	640	8	0	0
2	hh	415	3208	2039	521	640	8	0	0
2	hi	415	3208	2039	521	640	8	0	0
2	hj	415	3208	2039	521	640	8	0	0
2	hk	415	3208	2039	521	640	8	0	0
2	hl	415	3208	2039	521	640	8	0	0
2	hm	415	3208	2039	521	640	8	0	0
2	hn	415	3208	2039	521	640	8	0	0
2	ho	415	3208	2039	521	640	8	0	0

- Molecule 3 is a protein called Small outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	hp	79	633	403	106	124	0	0
3	hq	79	633	403	106	124	0	0
3	hr	79	633	403	106	124	0	0
3	hs	79	633	403	106	124	0	0
3	ht	79	633	403	106	124	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	hu	79	Total 633	C 403	N 106	O 124	0	0
3	hv	79	Total 633	C 403	N 106	O 124	0	0
3	hw	79	Total 633	C 403	N 106	O 124	0	0
3	hx	79	Total 633	C 403	N 106	O 124	0	0
3	hy	79	Total 633	C 403	N 106	O 124	0	0
3	hz	79	Total 633	C 403	N 106	O 124	0	0
3	ia	79	Total 633	C 403	N 106	O 124	0	0
3	ib	79	Total 633	C 403	N 106	O 124	0	0
3	ic	79	Total 633	C 403	N 106	O 124	0	0
3	id	79	Total 633	C 403	N 106	O 124	0	0
3	ie	79	Total 633	C 403	N 106	O 124	0	0
3	if	79	Total 633	C 403	N 106	O 124	0	0
3	ig	79	Total 633	C 403	N 106	O 124	0	0
3	ih	79	Total 633	C 403	N 106	O 124	0	0
3	ii	79	Total 633	C 403	N 106	O 124	0	0
3	ij	79	Total 633	C 403	N 106	O 124	0	0
3	ik	79	Total 633	C 403	N 106	O 124	0	0
3	il	79	Total 633	C 403	N 106	O 124	0	0
3	im	79	Total 633	C 403	N 106	O 124	0	0
3	in	79	Total 633	C 403	N 106	O 124	0	0
3	io	79	Total 633	C 403	N 106	O 124	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	ip	79	Total 633	C 403	N 106	O 124	0	0
3	iq	79	Total 633	C 403	N 106	O 124	0	0
3	ir	79	Total 633	C 403	N 106	O 124	0	0
3	is	79	Total 633	C 403	N 106	O 124	0	0
3	it	79	Total 633	C 403	N 106	O 124	0	0
3	iu	79	Total 633	C 403	N 106	O 124	0	0
3	iv	79	Total 633	C 403	N 106	O 124	0	0
3	iw	79	Total 633	C 403	N 106	O 124	0	0
3	ix	79	Total 633	C 403	N 106	O 124	0	0
3	iy	79	Total 633	C 403	N 106	O 124	0	0
3	iz	79	Total 633	C 403	N 106	O 124	0	0
3	ja	79	Total 633	C 403	N 106	O 124	0	0
3	jb	79	Total 633	C 403	N 106	O 124	0	0
3	jc	79	Total 633	C 403	N 106	O 124	0	0
3	jd	79	Total 633	C 403	N 106	O 124	0	0
3	je	79	Total 633	C 403	N 106	O 124	0	0
3	jf	79	Total 633	C 403	N 106	O 124	0	0
3	yg	79	Total 633	C 403	N 106	O 124	0	0
3	yh	79	Total 633	C 403	N 106	O 124	0	0
3	ji	79	Total 633	C 403	N 106	O 124	0	0
3	jj	79	Total 633	C 403	N 106	O 124	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	jk	79	Total 633	C 403	N 106	O 124	0	0
3	jl	79	Total 633	C 403	N 106	O 124	0	0
3	jm	79	Total 633	C 403	N 106	O 124	0	0
3	jn	79	Total 633	C 403	N 106	O 124	0	0
3	jo	79	Total 633	C 403	N 106	O 124	0	0
3	jp	79	Total 633	C 403	N 106	O 124	0	0
3	jq	79	Total 633	C 403	N 106	O 124	0	0
3	jr	79	Total 633	C 403	N 106	O 124	0	0
3	js	79	Total 633	C 403	N 106	O 124	0	0
3	jt	79	Total 633	C 403	N 106	O 124	0	0
3	ju	79	Total 633	C 403	N 106	O 124	0	0
3	jv	79	Total 633	C 403	N 106	O 124	0	0
3	jw	79	Total 633	C 403	N 106	O 124	0	0
3	jx	79	Total 633	C 403	N 106	O 124	0	0
3	jy	79	Total 633	C 403	N 106	O 124	0	0
3	jz	79	Total 633	C 403	N 106	O 124	0	0
3	ka	79	Total 633	C 403	N 106	O 124	0	0
3	kb	79	Total 633	C 403	N 106	O 124	0	0
3	kc	79	Total 633	C 403	N 106	O 124	0	0
3	kd	79	Total 633	C 403	N 106	O 124	0	0
3	ke	79	Total 633	C 403	N 106	O 124	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	kf	79	Total 633	C 403	N 106	O 124	0	0
3	kg	79	Total 633	C 403	N 106	O 124	0	0
3	kh	79	Total 633	C 403	N 106	O 124	0	0
3	ki	79	Total 633	C 403	N 106	O 124	0	0
3	kj	79	Total 633	C 403	N 106	O 124	0	0
3	kk	79	Total 633	C 403	N 106	O 124	0	0
3	kl	79	Total 633	C 403	N 106	O 124	0	0
3	km	79	Total 633	C 403	N 106	O 124	0	0
3	kn	79	Total 633	C 403	N 106	O 124	0	0
3	ko	79	Total 633	C 403	N 106	O 124	0	0
3	kp	79	Total 633	C 403	N 106	O 124	0	0
3	kq	79	Total 633	C 403	N 106	O 124	0	0
3	kr	79	Total 633	C 403	N 106	O 124	0	0
3	ks	79	Total 633	C 403	N 106	O 124	0	0
3	kt	79	Total 633	C 403	N 106	O 124	0	0
3	ku	79	Total 633	C 403	N 106	O 124	0	0
3	79	Total 633	C 403	N 106	O 124	0	0	
3	kw	79	Total 633	C 403	N 106	O 124	0	0
3	kx	79	Total 633	C 403	N 106	O 124	0	0
3	ky	79	Total 633	C 403	N 106	O 124	0	0
3	kz	79	Total 633	C 403	N 106	O 124	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	la	79	Total 633	C 403	N 106	O 124	0	0
3	lb	79	Total 633	C 403	N 106	O 124	0	0
3	lc	79	Total 633	C 403	N 106	O 124	0	0
3	ld	79	Total 633	C 403	N 106	O 124	0	0
3	le	79	Total 633	C 403	N 106	O 124	0	0
3	lf	79	Total 633	C 403	N 106	O 124	0	0
3	lg	79	Total 633	C 403	N 106	O 124	0	0
3	lh	79	Total 633	C 403	N 106	O 124	0	0
3	li	79	Total 633	C 403	N 106	O 124	0	0
3	lj	79	Total 633	C 403	N 106	O 124	0	0
3	lk	79	Total 633	C 403	N 106	O 124	0	0
3	ll	79	Total 633	C 403	N 106	O 124	0	0
3	lm	79	Total 633	C 403	N 106	O 124	0	0
3	ln	79	Total 633	C 403	N 106	O 124	0	0
3	lo	79	Total 633	C 403	N 106	O 124	0	0
3	lp	79	Total 633	C 403	N 106	O 124	0	0
3	lq	79	Total 633	C 403	N 106	O 124	0	0
3	lr	79	Total 633	C 403	N 106	O 124	0	0
3	ls	79	Total 633	C 403	N 106	O 124	0	0
3	lt	79	Total 633	C 403	N 106	O 124	0	0
3	lu	79	Total 633	C 403	N 106	O 124	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	lv	79	Total 633	C 403	N 106	O 124	0	0
3	lw	79	Total 633	C 403	N 106	O 124	0	0
3	lx	79	Total 633	C 403	N 106	O 124	0	0
3	ly	79	Total 633	C 403	N 106	O 124	0	0
3	lz	79	Total 633	C 403	N 106	O 124	0	0
3	ma	79	Total 633	C 403	N 106	O 124	0	0
3	mb	79	Total 633	C 403	N 106	O 124	0	0
3	mc	79	Total 633	C 403	N 106	O 124	0	0
3	md	79	Total 633	C 403	N 106	O 124	0	0
3	me	79	Total 633	C 403	N 106	O 124	0	0
3	mf	79	Total 633	C 403	N 106	O 124	0	0
3	mg	79	Total 633	C 403	N 106	O 124	0	0
3	mh	79	Total 633	C 403	N 106	O 124	0	0
3	mi	79	Total 633	C 403	N 106	O 124	0	0
3	mj	79	Total 633	C 403	N 106	O 124	0	0
3	mk	79	Total 633	C 403	N 106	O 124	0	0
3	ml	79	Total 633	C 403	N 106	O 124	0	0
3	mm	79	Total 633	C 403	N 106	O 124	0	0
3	mn	79	Total 633	C 403	N 106	O 124	0	0
3	mo	79	Total 633	C 403	N 106	O 124	0	0
3	mp	79	Total 633	C 403	N 106	O 124	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	mq	79	Total 633	C 403	N 106	O 124	0	0
3	ms	79	Total 633	C 403	N 106	O 124	0	0
3	mt	79	Total 633	C 403	N 106	O 124	0	0
3	mu	79	Total 633	C 403	N 106	O 124	0	0
3	mv	79	Total 633	C 403	N 106	O 124	0	0
3	mw	79	Total 633	C 403	N 106	O 124	0	0
3	mx	79	Total 633	C 403	N 106	O 124	0	0
3	my	79	Total 633	C 403	N 106	O 124	0	0
3	mz	79	Total 633	C 403	N 106	O 124	0	0
3	na	79	Total 633	C 403	N 106	O 124	0	0
3	nb	79	Total 633	C 403	N 106	O 124	0	0
3	nc	79	Total 633	C 403	N 106	O 124	0	0
3	nd	79	Total 633	C 403	N 106	O 124	0	0
3	ne	79	Total 633	C 403	N 106	O 124	0	0
3	nf	79	Total 633	C 403	N 106	O 124	0	0
3	ng	79	Total 633	C 403	N 106	O 124	0	0
3	nh	79	Total 633	C 403	N 106	O 124	0	0
3	ni	79	Total 633	C 403	N 106	O 124	0	0
3	nj	79	Total 633	C 403	N 106	O 124	0	0
3	nk	79	Total 633	C 403	N 106	O 124	0	0
3	nl	79	Total 633	C 403	N 106	O 124	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	nm	79	Total 633	C 403	N 106	O 124	0	0
3	nn	79	Total 633	C 403	N 106	O 124	0	0
3	no	79	Total 633	C 403	N 106	O 124	0	0
3	np	79	Total 633	C 403	N 106	O 124	0	0
3	nq	79	Total 633	C 403	N 106	O 124	0	0
3	ns	79	Total 633	C 403	N 106	O 124	0	0
3	nt	79	Total 633	C 403	N 106	O 124	0	0
3	nu	79	Total 633	C 403	N 106	O 124	0	0
3	nv	79	Total 633	C 403	N 106	O 124	0	0
3	nw	79	Total 633	C 403	N 106	O 124	0	0
3	nx	79	Total 633	C 403	N 106	O 124	0	0
3	ny	79	Total 633	C 403	N 106	O 124	0	0
3	nz	79	Total 633	C 403	N 106	O 124	0	0
3	oa	79	Total 633	C 403	N 106	O 124	0	0
3	ob	79	Total 633	C 403	N 106	O 124	0	0
3	oc	79	Total 633	C 403	N 106	O 124	0	0
3	od	79	Total 633	C 403	N 106	O 124	0	0
3	oe	79	Total 633	C 403	N 106	O 124	0	0
3	of	79	Total 633	C 403	N 106	O 124	0	0
3	og	79	Total 633	C 403	N 106	O 124	0	0

There are 344 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
hp	4	ALA	THR	conflict	UNP P03715
hp	28	VAL	ILE	conflict	UNP P03715
hq	4	ALA	THR	conflict	UNP P03715
hq	28	VAL	ILE	conflict	UNP P03715
hr	4	ALA	THR	conflict	UNP P03715
hr	28	VAL	ILE	conflict	UNP P03715
hs	4	ALA	THR	conflict	UNP P03715
hs	28	VAL	ILE	conflict	UNP P03715
ht	4	ALA	THR	conflict	UNP P03715
ht	28	VAL	ILE	conflict	UNP P03715
hu	4	ALA	THR	conflict	UNP P03715
hu	28	VAL	ILE	conflict	UNP P03715
hv	4	ALA	THR	conflict	UNP P03715
hv	28	VAL	ILE	conflict	UNP P03715
hw	4	ALA	THR	conflict	UNP P03715
hw	28	VAL	ILE	conflict	UNP P03715
hx	4	ALA	THR	conflict	UNP P03715
hx	28	VAL	ILE	conflict	UNP P03715
hy	4	ALA	THR	conflict	UNP P03715
hy	28	VAL	ILE	conflict	UNP P03715
hz	4	ALA	THR	conflict	UNP P03715
hz	28	VAL	ILE	conflict	UNP P03715
ia	4	ALA	THR	conflict	UNP P03715
ia	28	VAL	ILE	conflict	UNP P03715
ib	4	ALA	THR	conflict	UNP P03715
ib	28	VAL	ILE	conflict	UNP P03715
ic	4	ALA	THR	conflict	UNP P03715
ic	28	VAL	ILE	conflict	UNP P03715
id	4	ALA	THR	conflict	UNP P03715
id	28	VAL	ILE	conflict	UNP P03715
ie	4	ALA	THR	conflict	UNP P03715
ie	28	VAL	ILE	conflict	UNP P03715
if	4	ALA	THR	conflict	UNP P03715
if	28	VAL	ILE	conflict	UNP P03715
ig	4	ALA	THR	conflict	UNP P03715
ig	28	VAL	ILE	conflict	UNP P03715
ih	4	ALA	THR	conflict	UNP P03715
ih	28	VAL	ILE	conflict	UNP P03715
ii	4	ALA	THR	conflict	UNP P03715
ii	28	VAL	ILE	conflict	UNP P03715
ij	4	ALA	THR	conflict	UNP P03715
ij	28	VAL	ILE	conflict	UNP P03715
ik	4	ALA	THR	conflict	UNP P03715

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Chain	Residue	Modelled	Actual	Comment	Reference
ik	28	VAL	ILE	conflict	UNP P03715
il	4	ALA	THR	conflict	UNP P03715
il	28	VAL	ILE	conflict	UNP P03715
im	4	ALA	THR	conflict	UNP P03715
im	28	VAL	ILE	conflict	UNP P03715
in	4	ALA	THR	conflict	UNP P03715
in	28	VAL	ILE	conflict	UNP P03715
io	4	ALA	THR	conflict	UNP P03715
io	28	VAL	ILE	conflict	UNP P03715
ip	4	ALA	THR	conflict	UNP P03715
ip	28	VAL	ILE	conflict	UNP P03715
iq	4	ALA	THR	conflict	UNP P03715
iq	28	VAL	ILE	conflict	UNP P03715
ir	4	ALA	THR	conflict	UNP P03715
ir	28	VAL	ILE	conflict	UNP P03715
is	4	ALA	THR	conflict	UNP P03715
is	28	VAL	ILE	conflict	UNP P03715
it	4	ALA	THR	conflict	UNP P03715
it	28	VAL	ILE	conflict	UNP P03715
iu	4	ALA	THR	conflict	UNP P03715
iu	28	VAL	ILE	conflict	UNP P03715
iv	4	ALA	THR	conflict	UNP P03715
iv	28	VAL	ILE	conflict	UNP P03715
iw	4	ALA	THR	conflict	UNP P03715
iw	28	VAL	ILE	conflict	UNP P03715
ix	4	ALA	THR	conflict	UNP P03715
ix	28	VAL	ILE	conflict	UNP P03715
iy	4	ALA	THR	conflict	UNP P03715
iy	28	VAL	ILE	conflict	UNP P03715
iz	4	ALA	THR	conflict	UNP P03715
iz	28	VAL	ILE	conflict	UNP P03715
ja	4	ALA	THR	conflict	UNP P03715
ja	28	VAL	ILE	conflict	UNP P03715
jb	4	ALA	THR	conflict	UNP P03715
jb	28	VAL	ILE	conflict	UNP P03715
jc	4	ALA	THR	conflict	UNP P03715
jc	28	VAL	ILE	conflict	UNP P03715
jd	4	ALA	THR	conflict	UNP P03715
jd	28	VAL	ILE	conflict	UNP P03715
je	4	ALA	THR	conflict	UNP P03715
je	28	VAL	ILE	conflict	UNP P03715
jf	4	ALA	THR	conflict	UNP P03715

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Chain	Residue	Modelled	Actual	Comment	Reference
jf	28	VAL	ILE	conflict	UNP P03715
kg	4	ALA	THR	conflict	UNP P03715
kg	28	VAL	ILE	conflict	UNP P03715
kh	4	ALA	THR	conflict	UNP P03715
kh	28	VAL	ILE	conflict	UNP P03715
ki	4	ALA	THR	conflict	UNP P03715
ki	28	VAL	ILE	conflict	UNP P03715
kj	4	ALA	THR	conflict	UNP P03715
kj	28	VAL	ILE	conflict	UNP P03715
kk	4	ALA	THR	conflict	UNP P03715
kk	28	VAL	ILE	conflict	UNP P03715
kl	4	ALA	THR	conflict	UNP P03715
kl	28	VAL	ILE	conflict	UNP P03715
km	4	ALA	THR	conflict	UNP P03715
km	28	VAL	ILE	conflict	UNP P03715
kn	4	ALA	THR	conflict	UNP P03715
kn	28	VAL	ILE	conflict	UNP P03715
ko	4	ALA	THR	conflict	UNP P03715
ko	28	VAL	ILE	conflict	UNP P03715
kp	4	ALA	THR	conflict	UNP P03715
kp	28	VAL	ILE	conflict	UNP P03715
kq	4	ALA	THR	conflict	UNP P03715
kq	28	VAL	ILE	conflict	UNP P03715
kr	4	ALA	THR	conflict	UNP P03715
kr	28	VAL	ILE	conflict	UNP P03715
ks	4	ALA	THR	conflict	UNP P03715
ks	28	VAL	ILE	conflict	UNP P03715
kt	4	ALA	THR	conflict	UNP P03715
kt	28	VAL	ILE	conflict	UNP P03715
ku	4	ALA	THR	conflict	UNP P03715
ku	28	VAL	ILE	conflict	UNP P03715
kv	4	ALA	THR	conflict	UNP P03715
kv	28	VAL	ILE	conflict	UNP P03715
kx	4	ALA	THR	conflict	UNP P03715
kx	28	VAL	ILE	conflict	UNP P03715
ky	4	ALA	THR	conflict	UNP P03715
ky	28	VAL	ILE	conflict	UNP P03715
kz	4	ALA	THR	conflict	UNP P03715
kz	28	VAL	ILE	conflict	UNP P03715
ka	4	ALA	THR	conflict	UNP P03715

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Chain	Residue	Modelled	Actual	Comment	Reference
ka	28	VAL	ILE	conflict	UNP P03715
kb	4	ALA	THR	conflict	UNP P03715
kb	28	VAL	ILE	conflict	UNP P03715
kc	4	ALA	THR	conflict	UNP P03715
kc	28	VAL	ILE	conflict	UNP P03715
kd	4	ALA	THR	conflict	UNP P03715
kd	28	VAL	ILE	conflict	UNP P03715
ke	4	ALA	THR	conflict	UNP P03715
ke	28	VAL	ILE	conflict	UNP P03715
kf	4	ALA	THR	conflict	UNP P03715
kf	28	VAL	ILE	conflict	UNP P03715
kg	4	ALA	THR	conflict	UNP P03715
kg	28	VAL	ILE	conflict	UNP P03715
kh	4	ALA	THR	conflict	UNP P03715
kh	28	VAL	ILE	conflict	UNP P03715
ki	4	ALA	THR	conflict	UNP P03715
ki	28	VAL	ILE	conflict	UNP P03715
kj	4	ALA	THR	conflict	UNP P03715
kj	28	VAL	ILE	conflict	UNP P03715
kk	4	ALA	THR	conflict	UNP P03715
kk	28	VAL	ILE	conflict	UNP P03715
kl	4	ALA	THR	conflict	UNP P03715
kl	28	VAL	ILE	conflict	UNP P03715
km	4	ALA	THR	conflict	UNP P03715
km	28	VAL	ILE	conflict	UNP P03715
kn	4	ALA	THR	conflict	UNP P03715
kn	28	VAL	ILE	conflict	UNP P03715
ko	4	ALA	THR	conflict	UNP P03715
ko	28	VAL	ILE	conflict	UNP P03715
kp	4	ALA	THR	conflict	UNP P03715
kp	28	VAL	ILE	conflict	UNP P03715
kq	4	ALA	THR	conflict	UNP P03715
kq	28	VAL	ILE	conflict	UNP P03715
kr	4	ALA	THR	conflict	UNP P03715
kr	28	VAL	ILE	conflict	UNP P03715
ks	4	ALA	THR	conflict	UNP P03715
ks	28	VAL	ILE	conflict	UNP P03715
kt	4	ALA	THR	conflict	UNP P03715
kt	28	VAL	ILE	conflict	UNP P03715
ku	4	ALA	THR	conflict	UNP P03715
ku	28	VAL	ILE	conflict	UNP P03715
kv	4	ALA	THR	conflict	UNP P03715

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Chain	Residue	Modelled	Actual	Comment	Reference
kv	28	VAL	ILE	conflict	UNP P03715
kw	4	ALA	THR	conflict	UNP P03715
kw	28	VAL	ILE	conflict	UNP P03715
kx	4	ALA	THR	conflict	UNP P03715
kx	28	VAL	ILE	conflict	UNP P03715
ky	4	ALA	THR	conflict	UNP P03715
ky	28	VAL	ILE	conflict	UNP P03715
kz	4	ALA	THR	conflict	UNP P03715
kz	28	VAL	ILE	conflict	UNP P03715
la	4	ALA	THR	conflict	UNP P03715
la	28	VAL	ILE	conflict	UNP P03715
lb	4	ALA	THR	conflict	UNP P03715
lb	28	VAL	ILE	conflict	UNP P03715
lc	4	ALA	THR	conflict	UNP P03715
lc	28	VAL	ILE	conflict	UNP P03715
ld	4	ALA	THR	conflict	UNP P03715
ld	28	VAL	ILE	conflict	UNP P03715
le	4	ALA	THR	conflict	UNP P03715
le	28	VAL	ILE	conflict	UNP P03715
lf	4	ALA	THR	conflict	UNP P03715
lf	28	VAL	ILE	conflict	UNP P03715
lg	4	ALA	THR	conflict	UNP P03715
lg	28	VAL	ILE	conflict	UNP P03715
lh	4	ALA	THR	conflict	UNP P03715
lh	28	VAL	ILE	conflict	UNP P03715
li	4	ALA	THR	conflict	UNP P03715
li	28	VAL	ILE	conflict	UNP P03715
lj	4	ALA	THR	conflict	UNP P03715
lj	28	VAL	ILE	conflict	UNP P03715
lk	4	ALA	THR	conflict	UNP P03715
lk	28	VAL	ILE	conflict	UNP P03715
ll	4	ALA	THR	conflict	UNP P03715
ll	28	VAL	ILE	conflict	UNP P03715
lm	4	ALA	THR	conflict	UNP P03715
lm	28	VAL	ILE	conflict	UNP P03715
ln	4	ALA	THR	conflict	UNP P03715
ln	28	VAL	ILE	conflict	UNP P03715
lo	4	ALA	THR	conflict	UNP P03715
lo	28	VAL	ILE	conflict	UNP P03715
lp	4	ALA	THR	conflict	UNP P03715
lp	28	VAL	ILE	conflict	UNP P03715
lq	4	ALA	THR	conflict	UNP P03715

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Chain	Residue	Modelled	Actual	Comment	Reference
lq	28	VAL	ILE	conflict	UNP P03715
lr	4	ALA	THR	conflict	UNP P03715
lr	28	VAL	ILE	conflict	UNP P03715
ls	4	ALA	THR	conflict	UNP P03715
ls	28	VAL	ILE	conflict	UNP P03715
lt	4	ALA	THR	conflict	UNP P03715
lt	28	VAL	ILE	conflict	UNP P03715
lu	4	ALA	THR	conflict	UNP P03715
lu	28	VAL	ILE	conflict	UNP P03715
lv	4	ALA	THR	conflict	UNP P03715
lv	28	VAL	ILE	conflict	UNP P03715
lw	4	ALA	THR	conflict	UNP P03715
lw	28	VAL	ILE	conflict	UNP P03715
lx	4	ALA	THR	conflict	UNP P03715
lx	28	VAL	ILE	conflict	UNP P03715
ly	4	ALA	THR	conflict	UNP P03715
ly	28	VAL	ILE	conflict	UNP P03715
lz	4	ALA	THR	conflict	UNP P03715
lz	28	VAL	ILE	conflict	UNP P03715
ma	4	ALA	THR	conflict	UNP P03715
ma	28	VAL	ILE	conflict	UNP P03715
mb	4	ALA	THR	conflict	UNP P03715
mb	28	VAL	ILE	conflict	UNP P03715
mc	4	ALA	THR	conflict	UNP P03715
mc	28	VAL	ILE	conflict	UNP P03715
md	4	ALA	THR	conflict	UNP P03715
md	28	VAL	ILE	conflict	UNP P03715
me	4	ALA	THR	conflict	UNP P03715
me	28	VAL	ILE	conflict	UNP P03715
mf	4	ALA	THR	conflict	UNP P03715
mf	28	VAL	ILE	conflict	UNP P03715
mg	4	ALA	THR	conflict	UNP P03715
mg	28	VAL	ILE	conflict	UNP P03715
mh	4	ALA	THR	conflict	UNP P03715
mh	28	VAL	ILE	conflict	UNP P03715
mi	4	ALA	THR	conflict	UNP P03715
mi	28	VAL	ILE	conflict	UNP P03715
mj	4	ALA	THR	conflict	UNP P03715
mj	28	VAL	ILE	conflict	UNP P03715
mk	4	ALA	THR	conflict	UNP P03715
mk	28	VAL	ILE	conflict	UNP P03715
ml	4	ALA	THR	conflict	UNP P03715

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Chain	Residue	Modelled	Actual	Comment	Reference
ml	28	VAL	ILE	conflict	UNP P03715
mm	4	ALA	THR	conflict	UNP P03715
mm	28	VAL	ILE	conflict	UNP P03715
mn	4	ALA	THR	conflict	UNP P03715
mn	28	VAL	ILE	conflict	UNP P03715
mo	4	ALA	THR	conflict	UNP P03715
mo	28	VAL	ILE	conflict	UNP P03715
mp	4	ALA	THR	conflict	UNP P03715
mp	28	VAL	ILE	conflict	UNP P03715
mq	4	ALA	THR	conflict	UNP P03715
mq	28	VAL	ILE	conflict	UNP P03715
ms	4	ALA	THR	conflict	UNP P03715
ms	28	VAL	ILE	conflict	UNP P03715
mt	4	ALA	THR	conflict	UNP P03715
mt	28	VAL	ILE	conflict	UNP P03715
mu	4	ALA	THR	conflict	UNP P03715
mu	28	VAL	ILE	conflict	UNP P03715
mv	4	ALA	THR	conflict	UNP P03715
mv	28	VAL	ILE	conflict	UNP P03715
mw	4	ALA	THR	conflict	UNP P03715
mw	28	VAL	ILE	conflict	UNP P03715
mx	4	ALA	THR	conflict	UNP P03715
mx	28	VAL	ILE	conflict	UNP P03715
my	4	ALA	THR	conflict	UNP P03715
my	28	VAL	ILE	conflict	UNP P03715
mz	4	ALA	THR	conflict	UNP P03715
mz	28	VAL	ILE	conflict	UNP P03715
na	4	ALA	THR	conflict	UNP P03715
na	28	VAL	ILE	conflict	UNP P03715
nb	4	ALA	THR	conflict	UNP P03715
nb	28	VAL	ILE	conflict	UNP P03715
nc	4	ALA	THR	conflict	UNP P03715
nc	28	VAL	ILE	conflict	UNP P03715
nd	4	ALA	THR	conflict	UNP P03715
nd	28	VAL	ILE	conflict	UNP P03715
ne	4	ALA	THR	conflict	UNP P03715
ne	28	VAL	ILE	conflict	UNP P03715
nf	4	ALA	THR	conflict	UNP P03715
nf	28	VAL	ILE	conflict	UNP P03715
ng	4	ALA	THR	conflict	UNP P03715
ng	28	VAL	ILE	conflict	UNP P03715
nh	4	ALA	THR	conflict	UNP P03715

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Chain	Residue	Modelled	Actual	Comment	Reference
nh	28	VAL	ILE	conflict	UNP P03715
ni	4	ALA	THR	conflict	UNP P03715
ni	28	VAL	ILE	conflict	UNP P03715
nj	4	ALA	THR	conflict	UNP P03715
nj	28	VAL	ILE	conflict	UNP P03715
nk	4	ALA	THR	conflict	UNP P03715
nk	28	VAL	ILE	conflict	UNP P03715
nl	4	ALA	THR	conflict	UNP P03715
nl	28	VAL	ILE	conflict	UNP P03715
nm	4	ALA	THR	conflict	UNP P03715
nm	28	VAL	ILE	conflict	UNP P03715
nn	4	ALA	THR	conflict	UNP P03715
nn	28	VAL	ILE	conflict	UNP P03715
no	4	ALA	THR	conflict	UNP P03715
no	28	VAL	ILE	conflict	UNP P03715
np	4	ALA	THR	conflict	UNP P03715
np	28	VAL	ILE	conflict	UNP P03715
nq	4	ALA	THR	conflict	UNP P03715
nq	28	VAL	ILE	conflict	UNP P03715
ns	4	ALA	THR	conflict	UNP P03715
ns	28	VAL	ILE	conflict	UNP P03715
nt	4	ALA	THR	conflict	UNP P03715
nt	28	VAL	ILE	conflict	UNP P03715
nu	4	ALA	THR	conflict	UNP P03715
nu	28	VAL	ILE	conflict	UNP P03715
nv	4	ALA	THR	conflict	UNP P03715
nv	28	VAL	ILE	conflict	UNP P03715
nw	4	ALA	THR	conflict	UNP P03715
nw	28	VAL	ILE	conflict	UNP P03715
nx	4	ALA	THR	conflict	UNP P03715
nx	28	VAL	ILE	conflict	UNP P03715
ny	4	ALA	THR	conflict	UNP P03715
ny	28	VAL	ILE	conflict	UNP P03715
nz	4	ALA	THR	conflict	UNP P03715
nz	28	VAL	ILE	conflict	UNP P03715
oa	4	ALA	THR	conflict	UNP P03715
oa	28	VAL	ILE	conflict	UNP P03715
ob	4	ALA	THR	conflict	UNP P03715
ob	28	VAL	ILE	conflict	UNP P03715
oc	4	ALA	THR	conflict	UNP P03715
oc	28	VAL	ILE	conflict	UNP P03715
od	4	ALA	THR	conflict	UNP P03715

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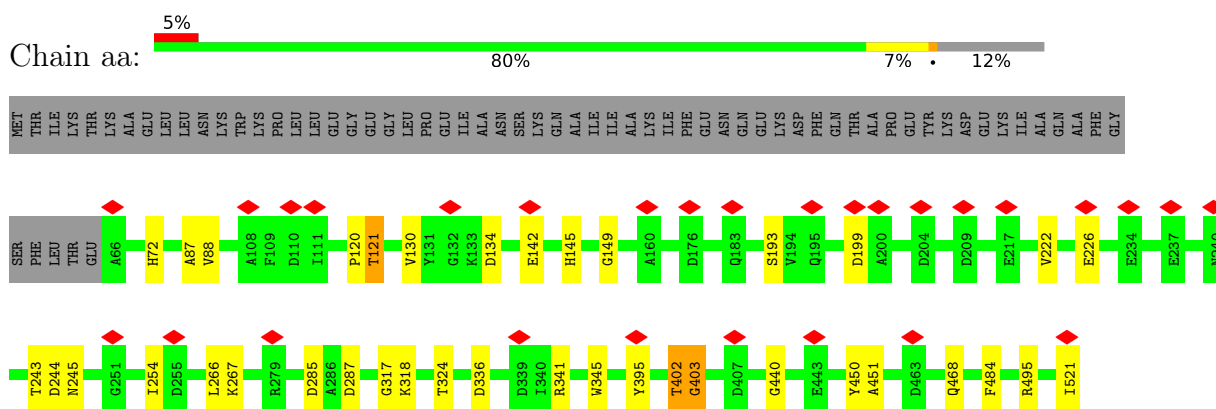
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Chain	Residue	Modelled	Actual	Comment	Reference
od	28	VAL	ILE	conflict	UNP P03715
oe	4	ALA	THR	conflict	UNP P03715
oe	28	VAL	ILE	conflict	UNP P03715
of	4	ALA	THR	conflict	UNP P03715
of	28	VAL	ILE	conflict	UNP P03715
og	4	ALA	THR	conflict	UNP P03715
og	28	VAL	ILE	conflict	UNP P03715

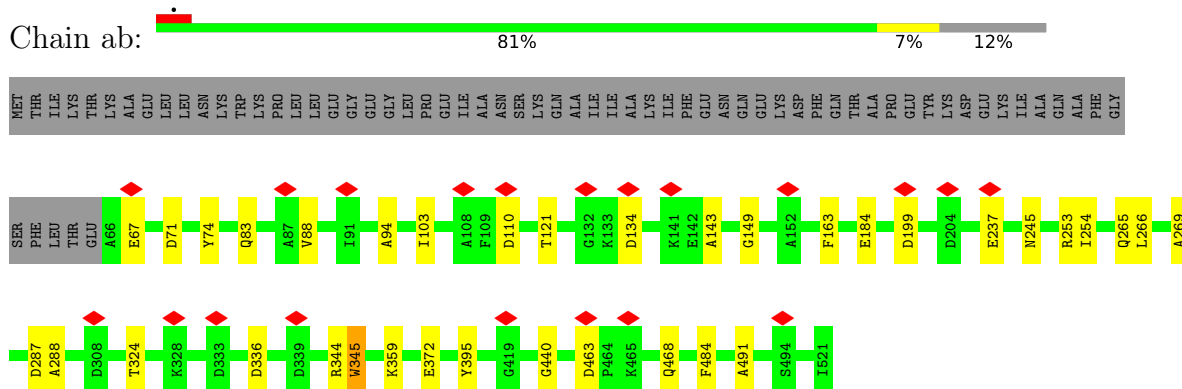
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

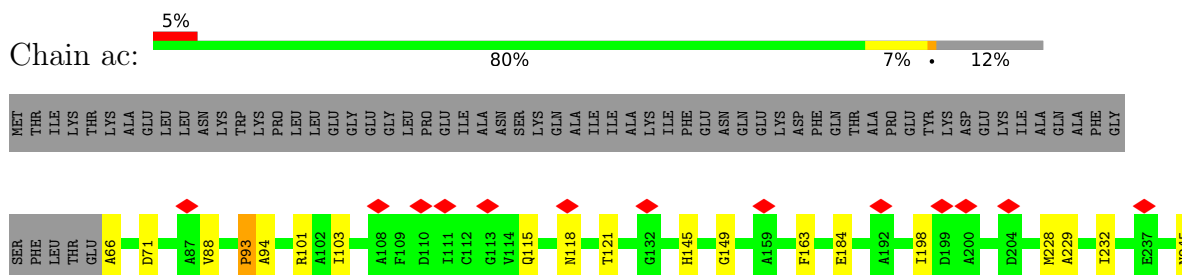
- Molecule 1: Major capsid protein

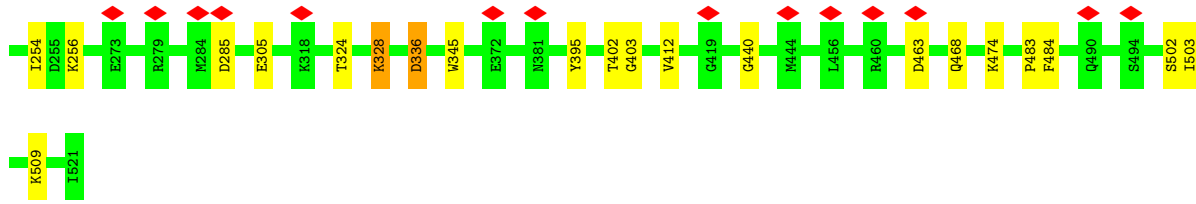


- Molecule 1: Major capsid protein

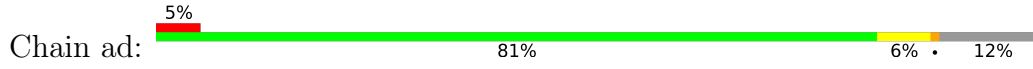


- Molecule 1: Major capsid protein

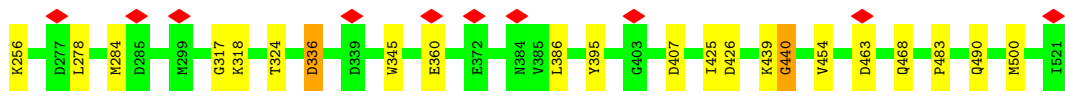
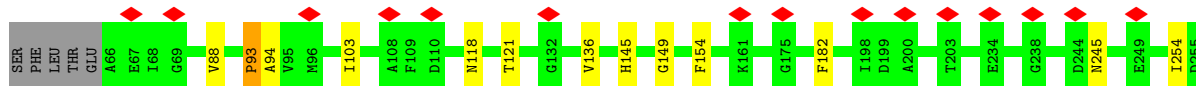




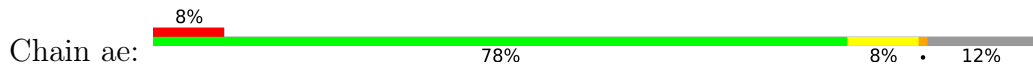
• Molecule 1: Major capsid protein



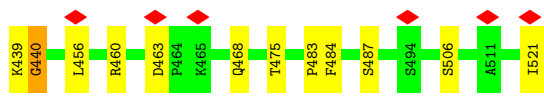
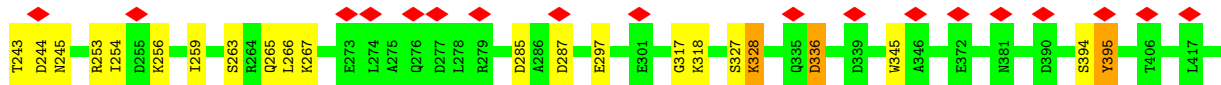
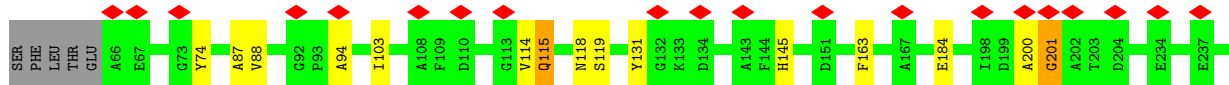
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	GLY	GLY	LEU	PRO	PRO	GLU	ILE	ALA	ASN	SER	SER	LYS	GLN	ALA	ILE	ALA	ALA	LYS	ILE	ILE	ALA	ALA	LYS	ILE	PHE	PHE	GLU	ASN	GLN	LYS	LYS	ASP	PHE	GLN	THR	ALA	ALA	PRO	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	ALA	GLN	ALA	PHE	PHE	GLY
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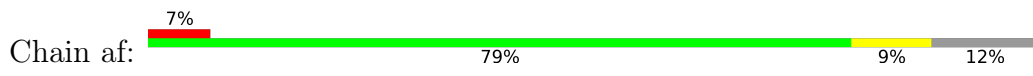
• Molecule 1: Major capsid protein



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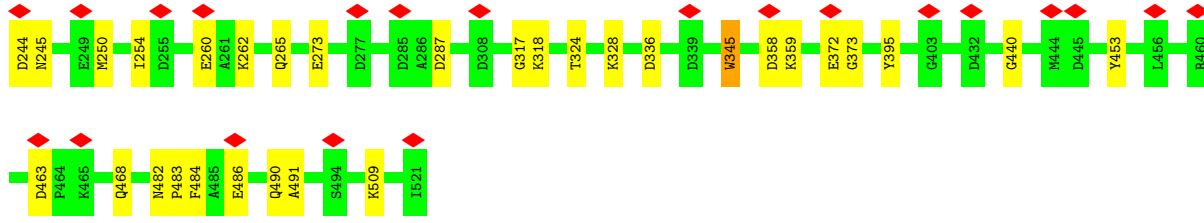


• Molecule 1: Major capsid protein

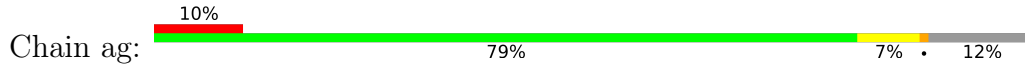


MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	GLY	GLY	LEU	PRO	PRO	GLU	ILE	ALA	ASN	SER	SER	LYS	GLN	ALA	ILE	ILE	ALA	ALA	LYS	LYS	ILE	PHE	PHE	GLU	ASN	GLN	LYS	LYS	ASP	PHE	GLN	THR	ALA	ALA	PRO	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	ALA	GLN	ALA	PHE	PHE	GLY
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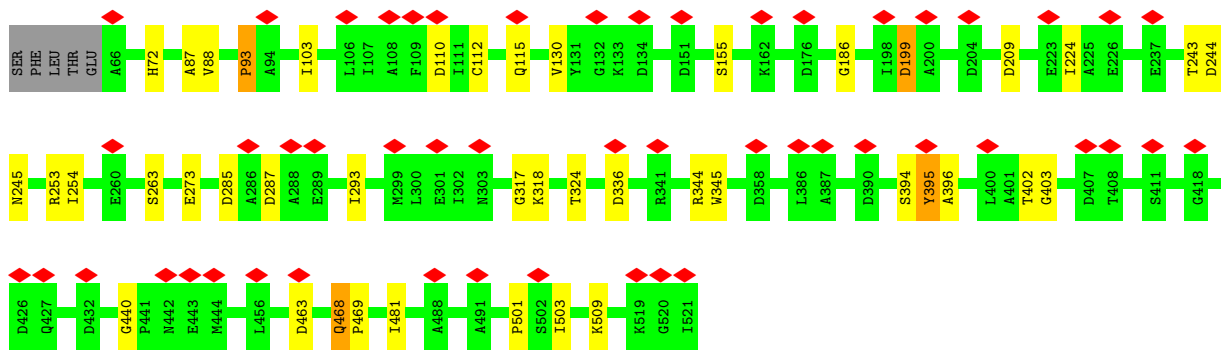




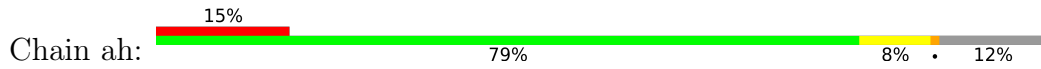
• Molecule 1: Major capsid protein



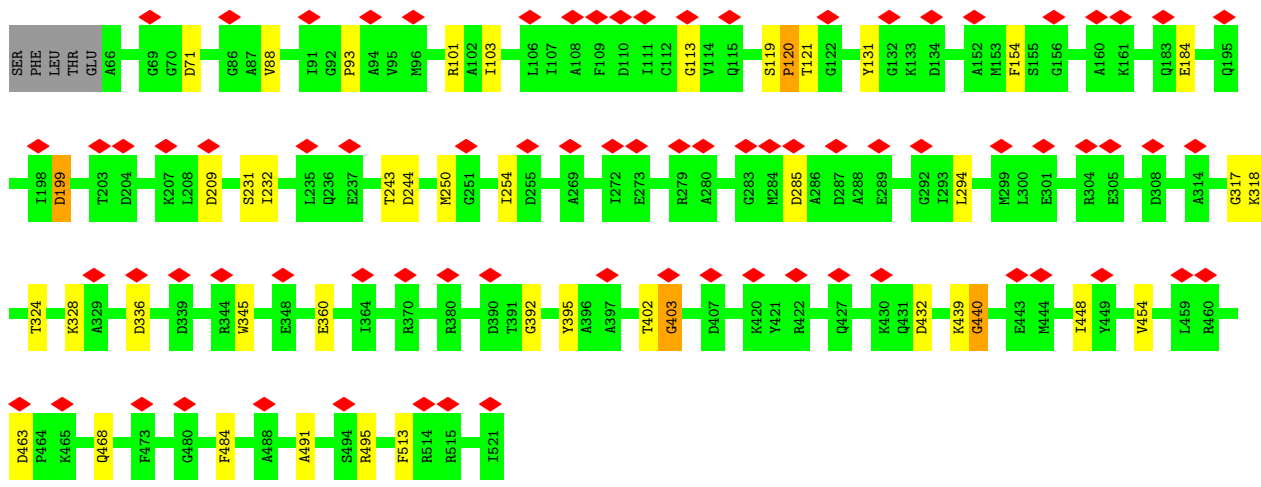
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLY	LYS	ASP	PHE	GLN	THR	ALA	PRO	PRO	GLY	TVR	LYS	ASP	LYS	ILE	ALA	GLN	ALA	PHE	PHE	GLY
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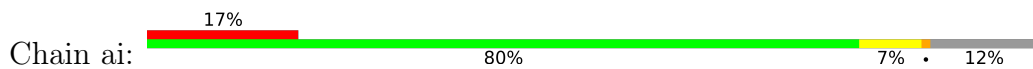
• Molecule 1: Major capsid protein

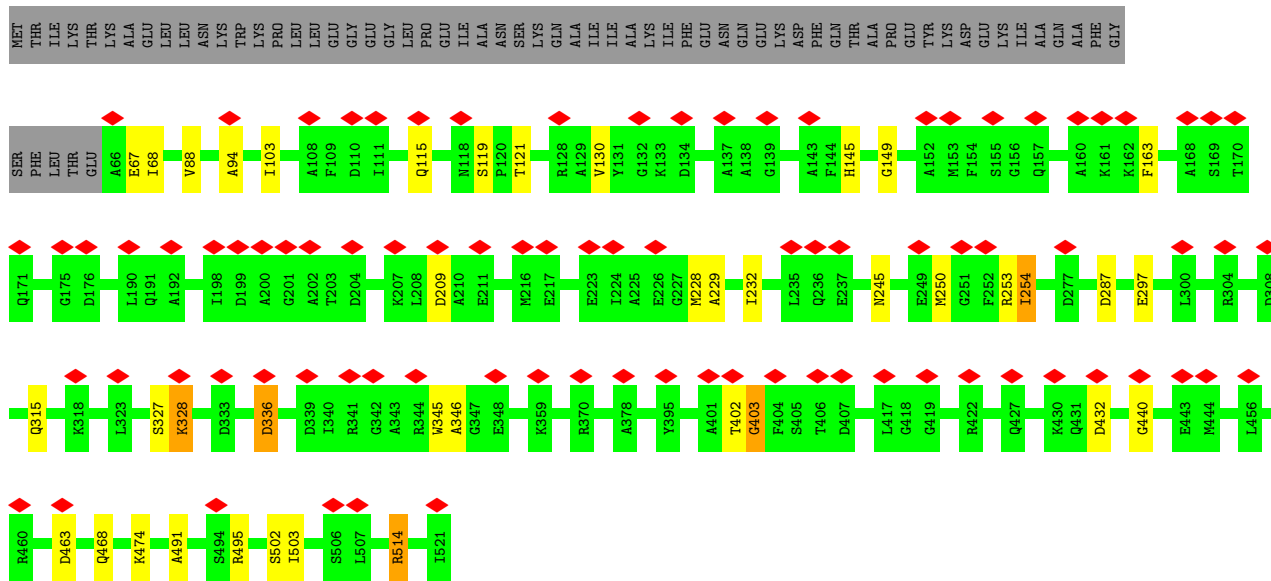


MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLY	LYS	ASP	PHE	GLN	THR	ALA	PRO	PRO	GLY	TVR	LYS	ASP	LYS	ILE	ALA	GLN	ALA	PHE	PHE	GLY
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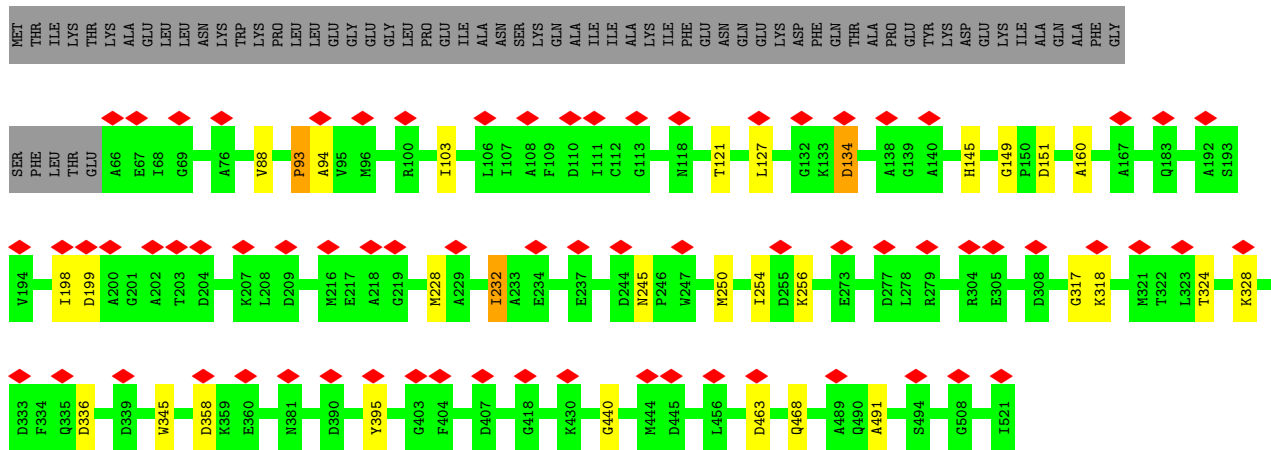
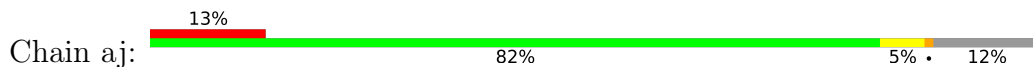


• Molecule 1: Major capsid protein

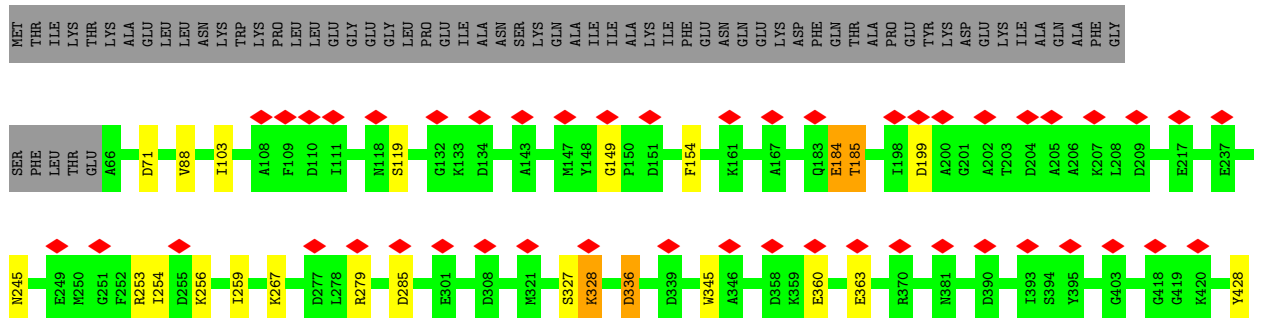
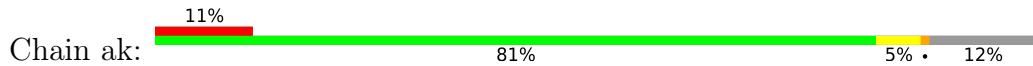




• Molecule 1: Major capsid protein

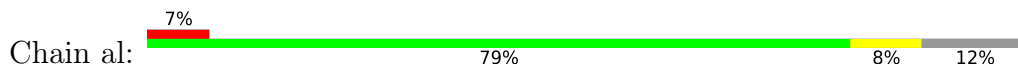


• Molecule 1: Major capsid protein

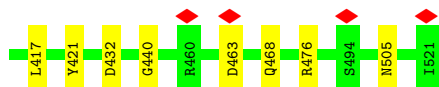
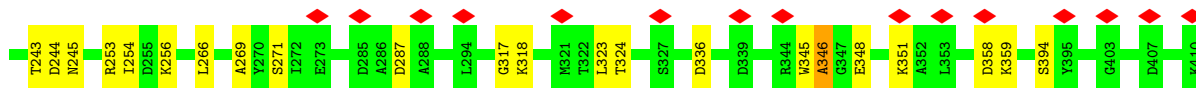




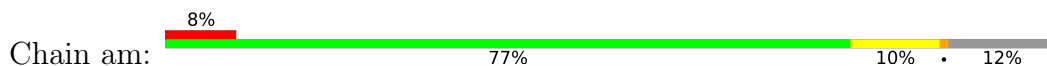
• Molecule 1: Major capsid protein



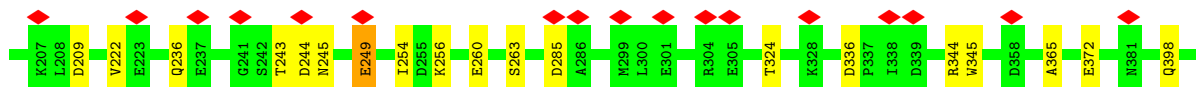
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	LEU	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	LYS	ASP	PHE	GLN	THR	ALA	PRO	PRO	GLY	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	PHE	ALA	GLY
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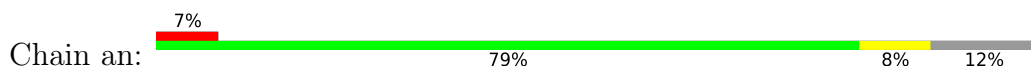
• Molecule 1: Major capsid protein



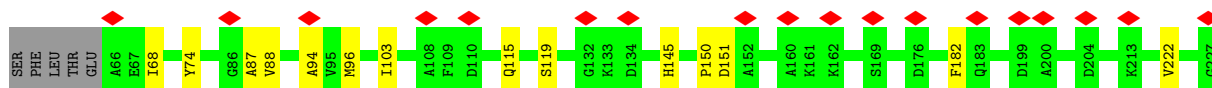
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	PRO	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLY	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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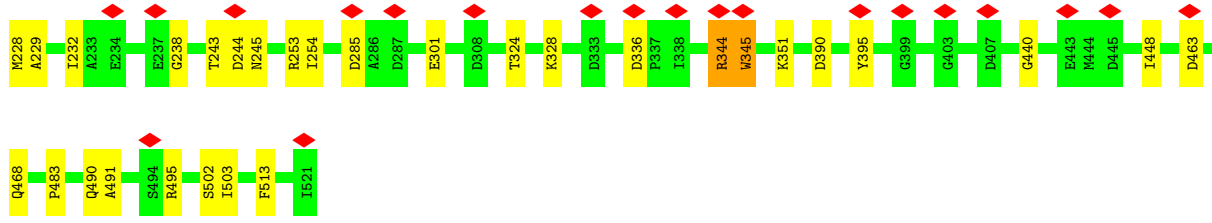


• Molecule 1: Major capsid protein

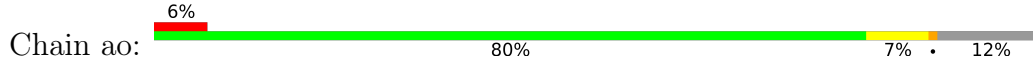


MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	PRO	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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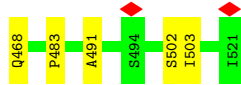




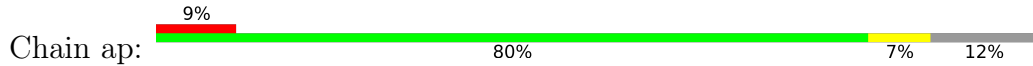
• Molecule 1: Major capsid protein



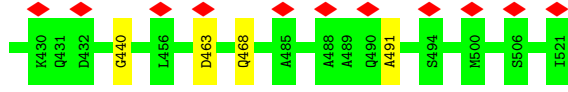
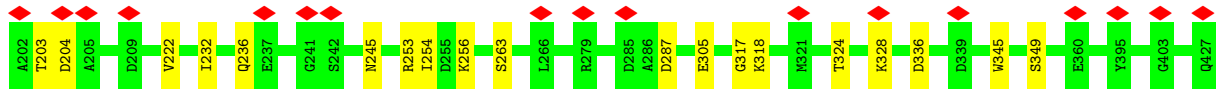
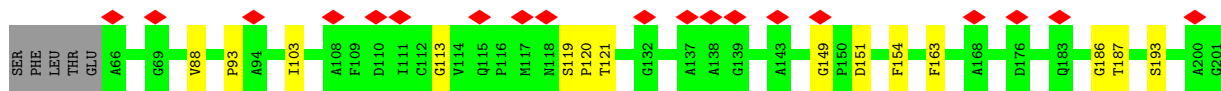
MET	THR	ILE	THR	LYS	LYS	ALA	GLU	LEU	LEU	ASN	LYS	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLY	PRO	PRO	GLU	ILE	ALA	ALA	ILE	ILE	ALA	LYS	LYS	ILE	PHE	GLU	ASN	GLN	GLN	ALA	ILE	ILE	ALA	ALA	LYS	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	PHE	GLY
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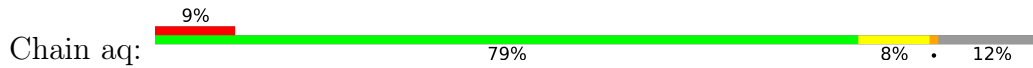
• Molecule 1: Major capsid protein



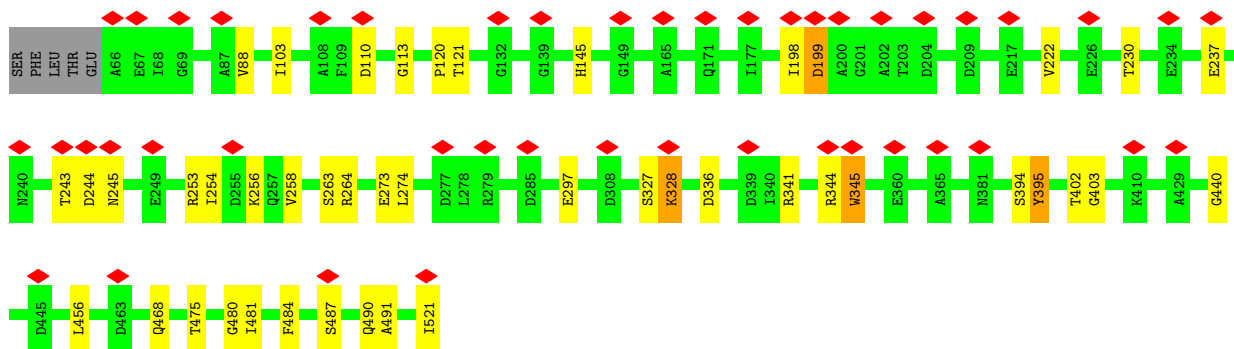
MET	THR	ILE	THR	LYS	LYS	ALA	GLU	LEU	LEU	ASN	LYS	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLY	PRO	PRO	GLU	ILE	ALA	ALA	ILE	ILE	ALA	LYS	LYS	ILE	PHE	GLU	ASN	GLN	GLN	ALA	ILE	ILE	ALA	ALA	LYS	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	PHE	GLY
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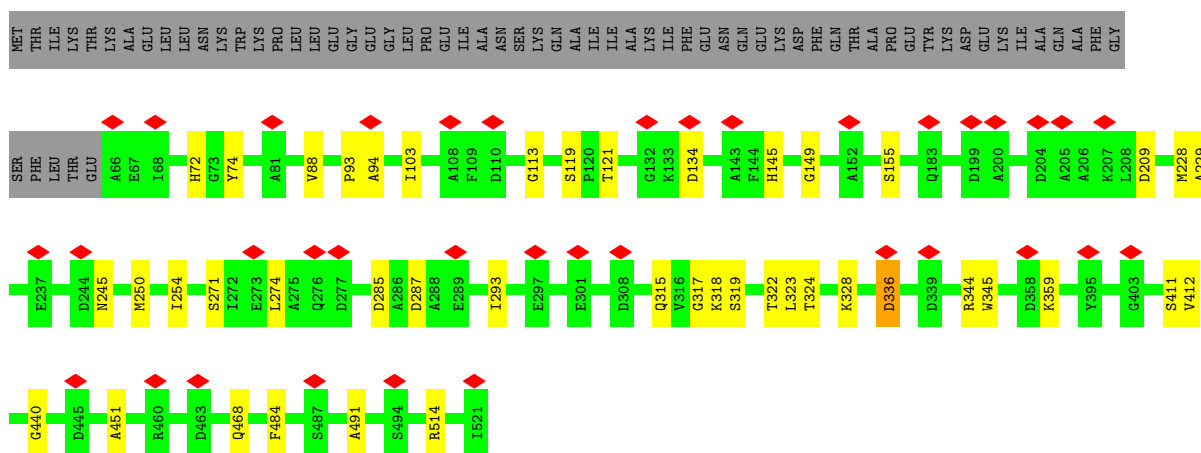
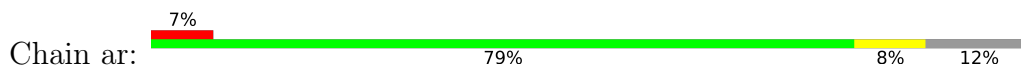
• Molecule 1: Major capsid protein



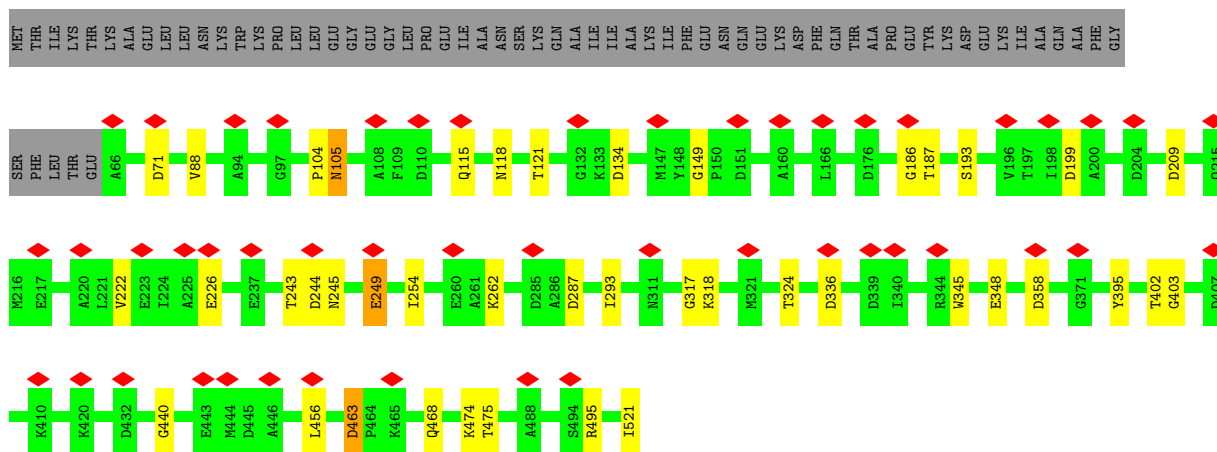
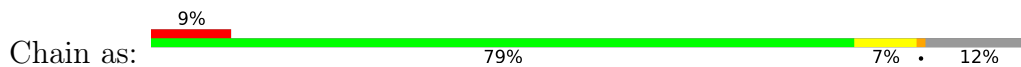
MET	THR	ILE	THR	LYS	LYS	ALA	GLU	LEU	LEU	ASN	LYS	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLY	PRO	PRO	GLU	ILE	ALA	ALA	ASN	SER	LYS	GLN	GLN	ALA	ILE	ILE	ALA	ALA	LYS	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	PHE	GLY
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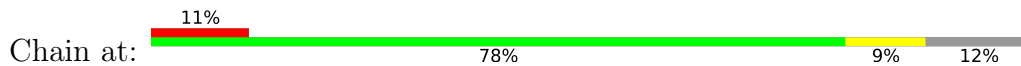
• Molecule 1: Major capsid protein

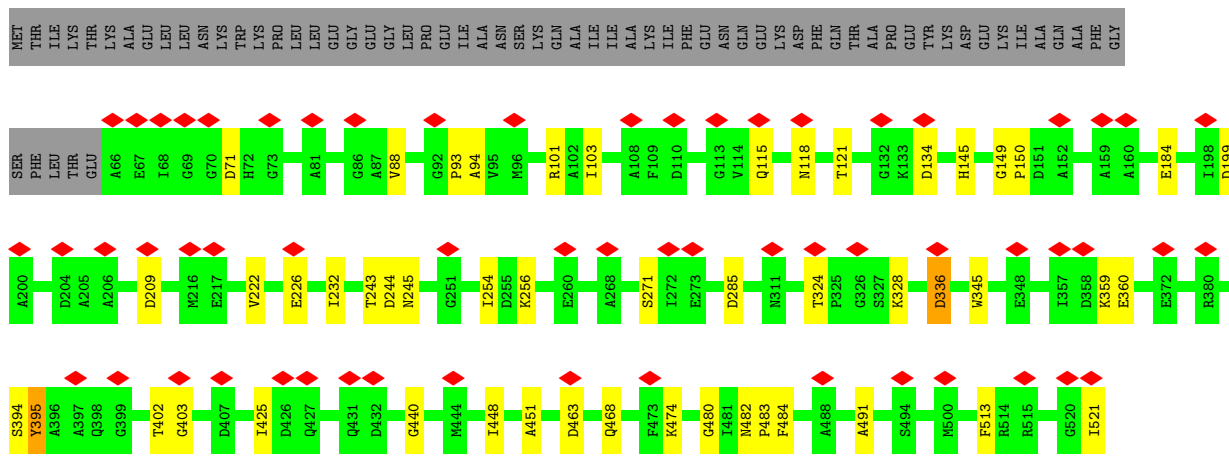


• Molecule 1: Major capsid protein

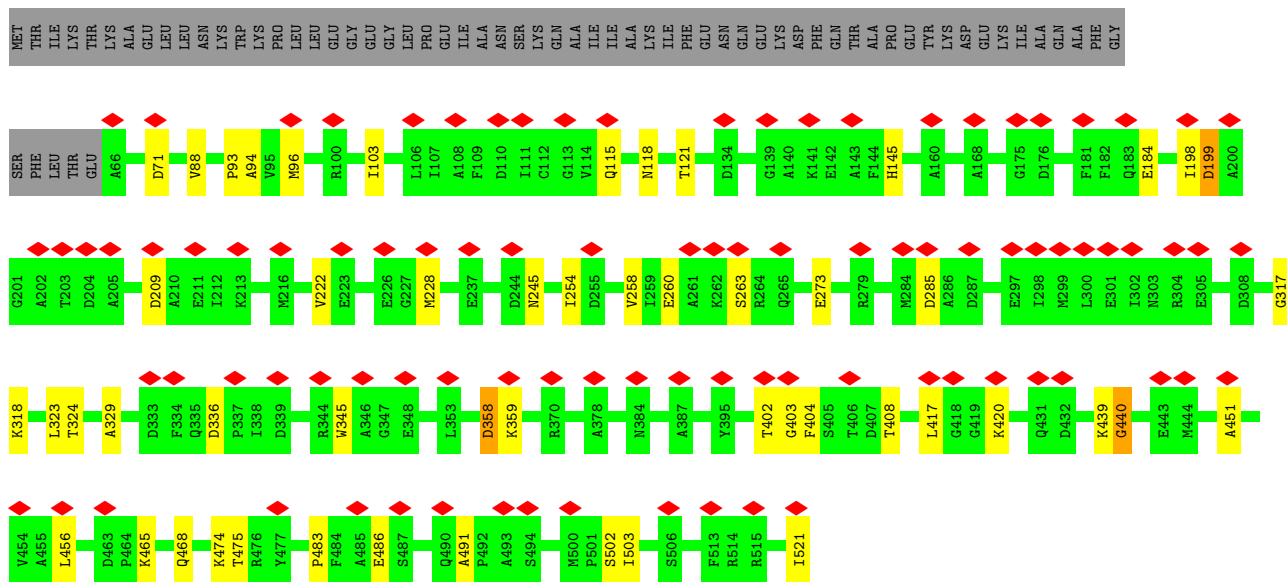
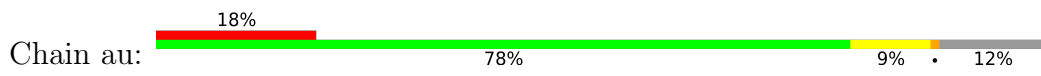


• Molecule 1: Major capsid protein

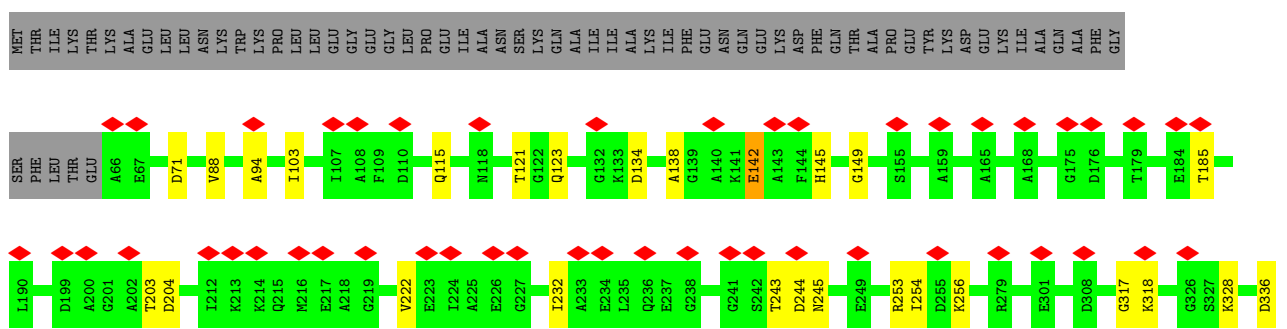
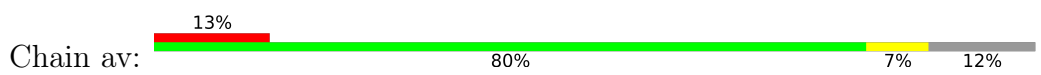


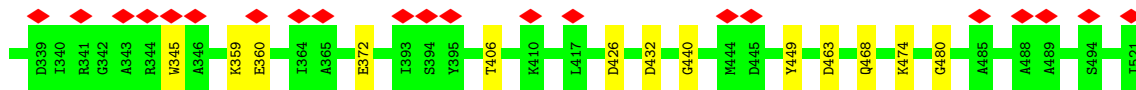


• Molecule 1: Major capsid protein

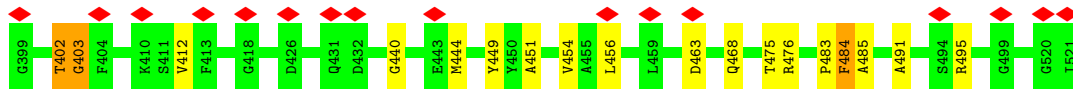
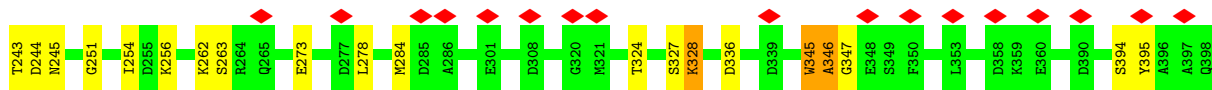
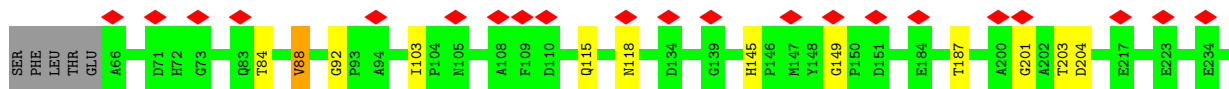
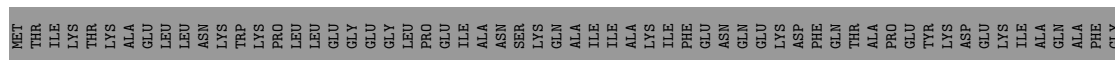
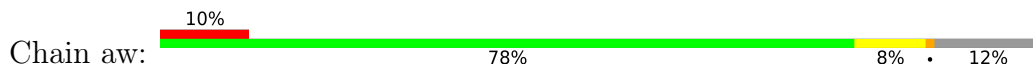


• Molecule 1: Major capsid protein

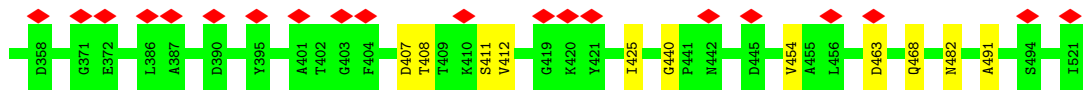
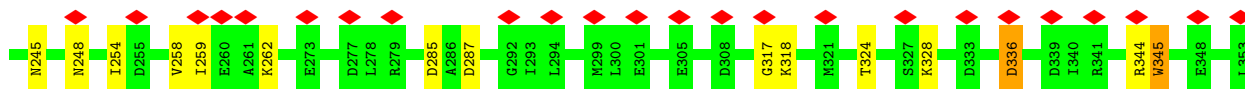
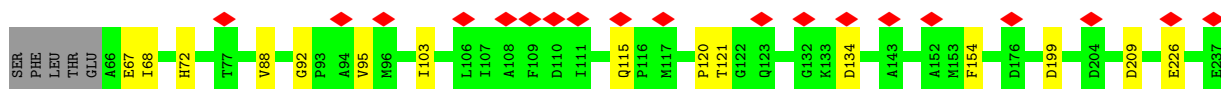
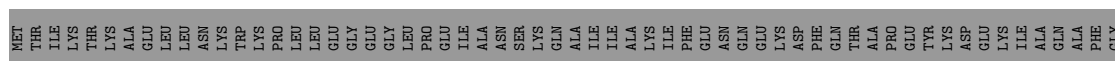
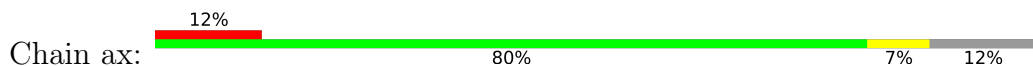




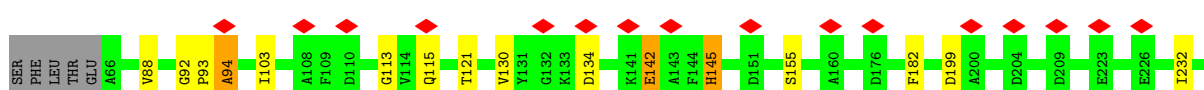
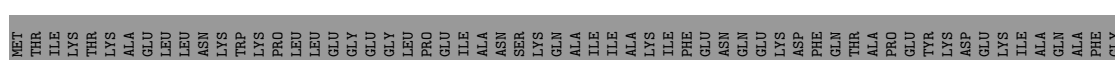
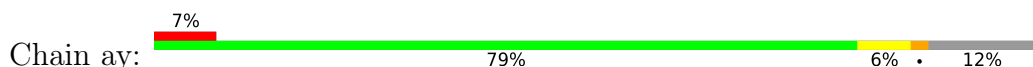
• Molecule 1: Major capsid protein

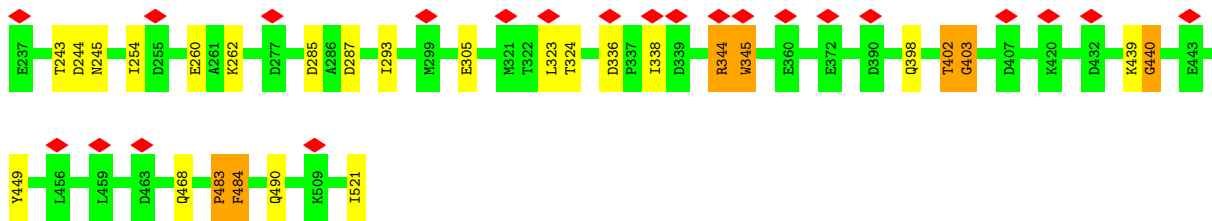


• Molecule 1: Major capsid protein

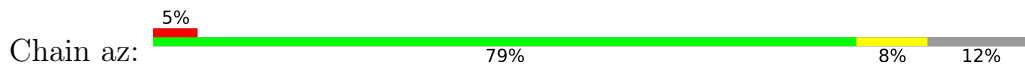


• Molecule 1: Major capsid protein

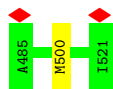
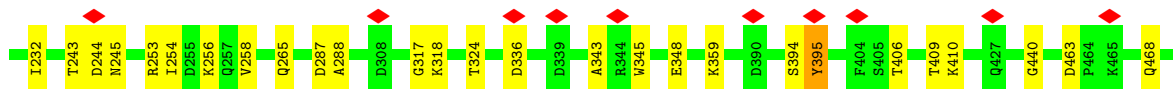
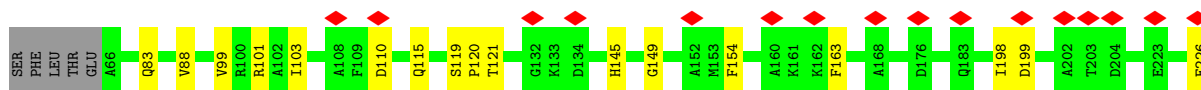




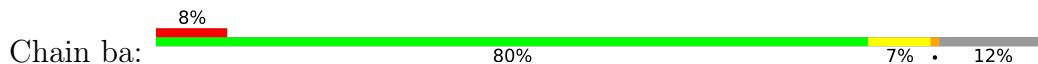
• Molecule 1: Major capsid protein



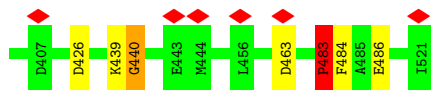
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	ASP	LYS	TRP	LYS	PRO	LEU	LEU	LEU	GLY	GLY	GLY	PRO	GLU	ILE	ALA	ASN	SER	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	PRO	GLU	TYR	LYS	ASP	GLU	ILE	ALA	GLN	ALA	PHE	GLY
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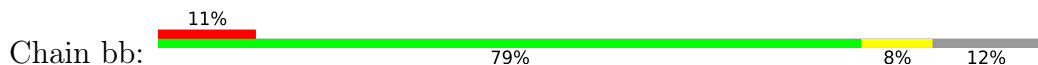
• Molecule 1: Major capsid protein



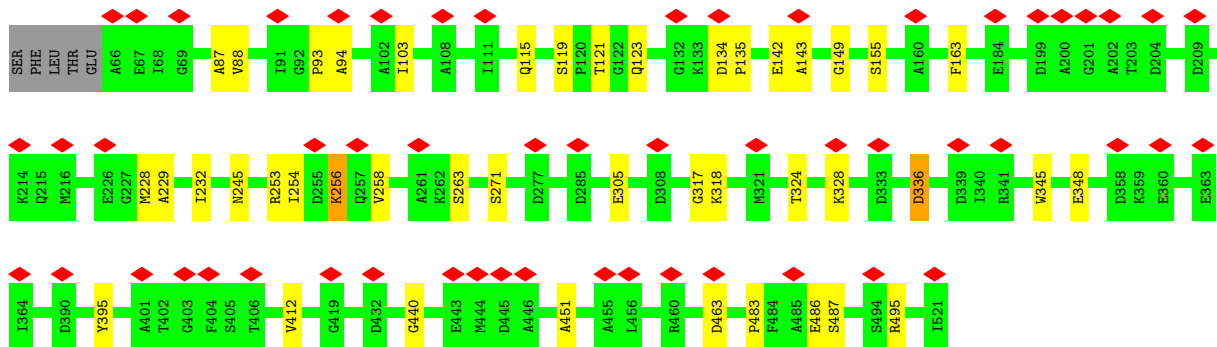
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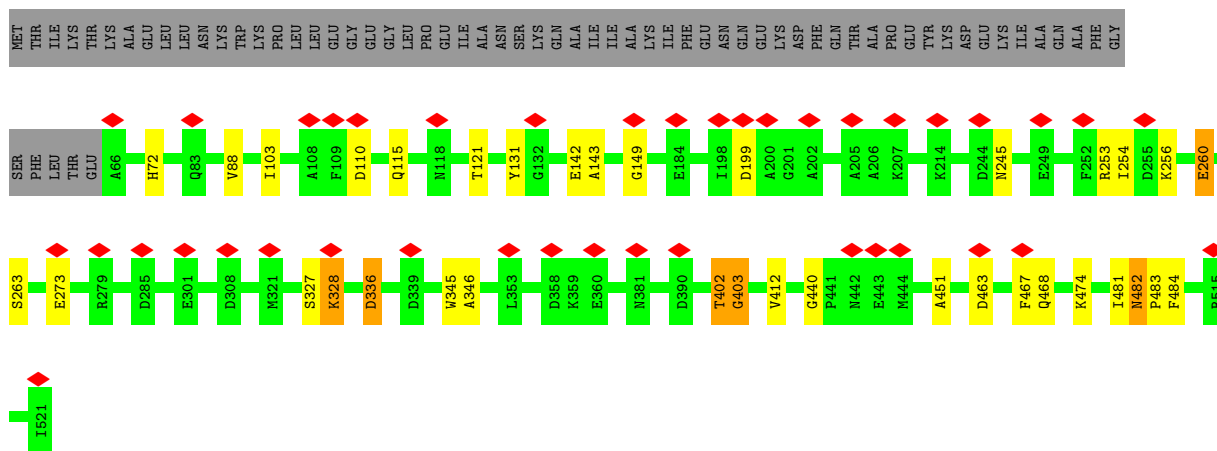
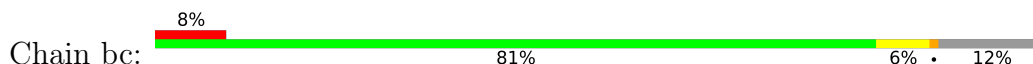
• Molecule 1: Major capsid protein



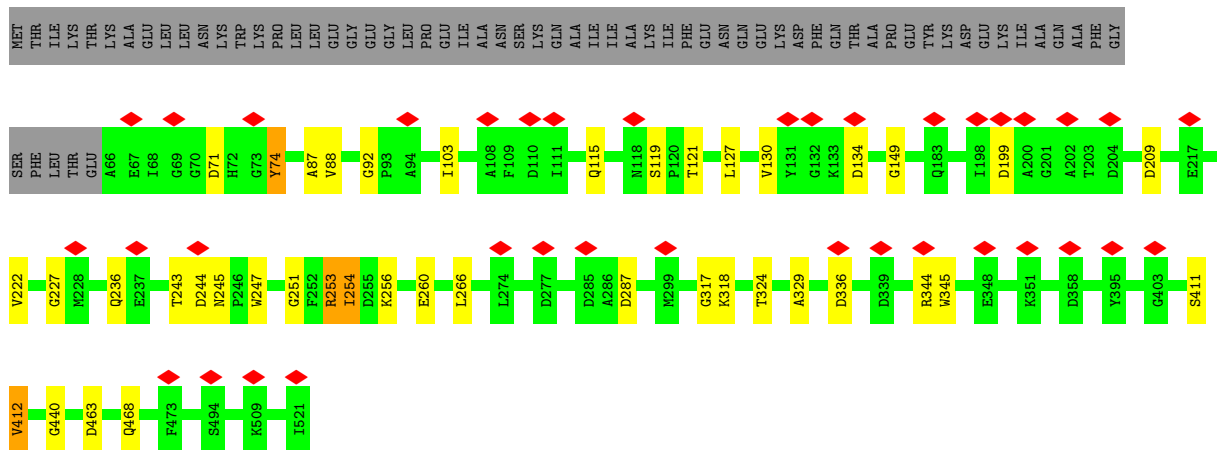
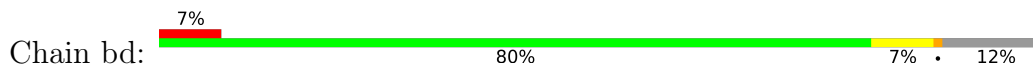
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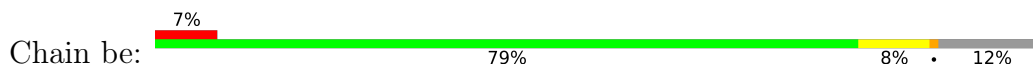
• Molecule 1: Major capsid protein

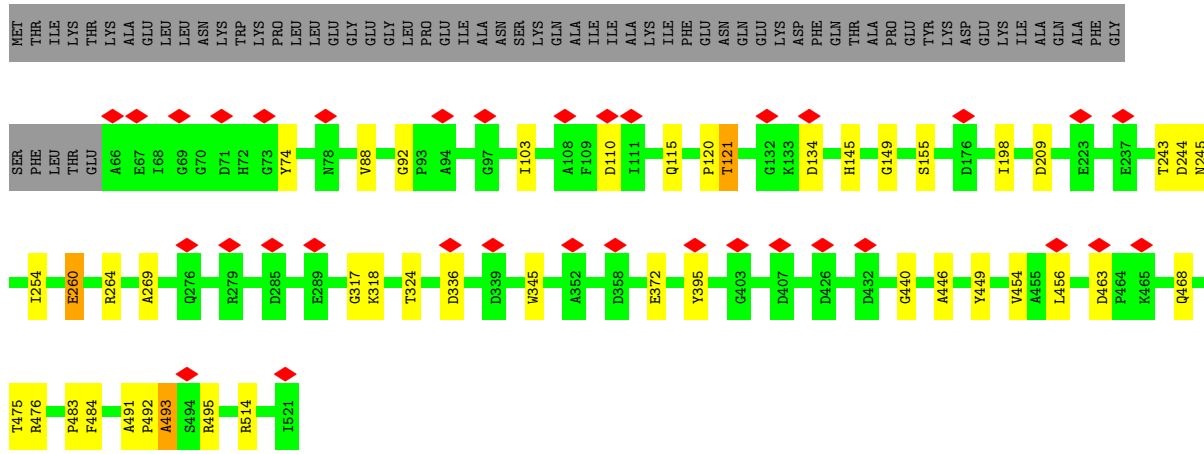


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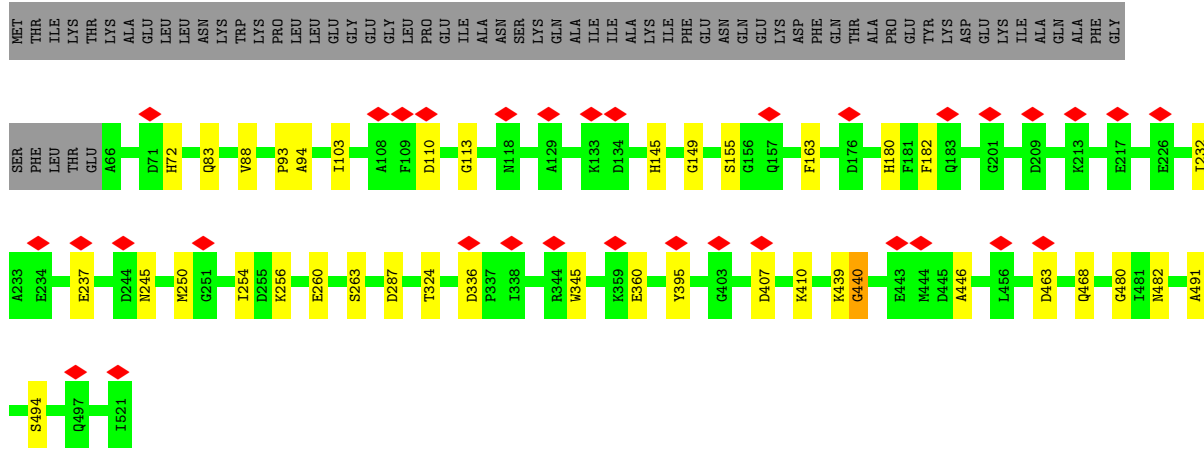
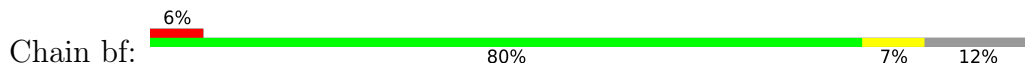


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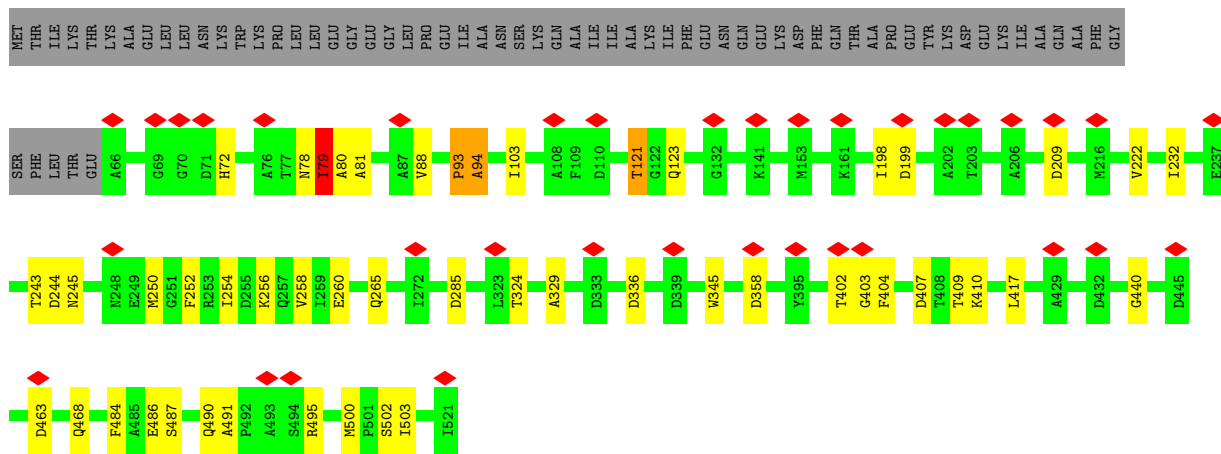
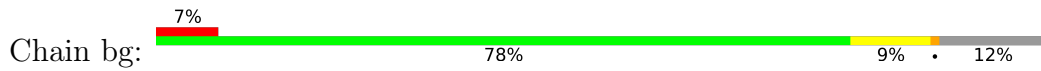




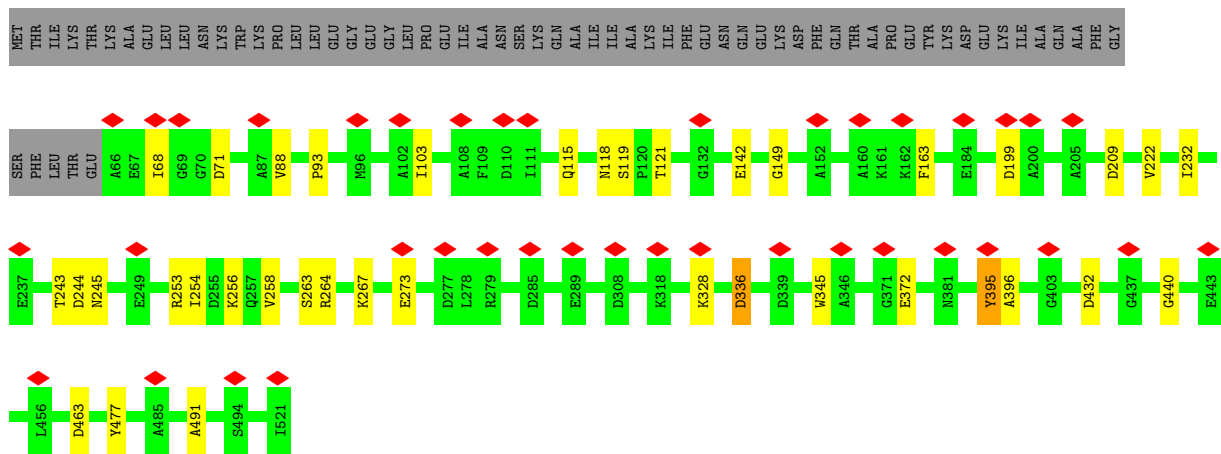
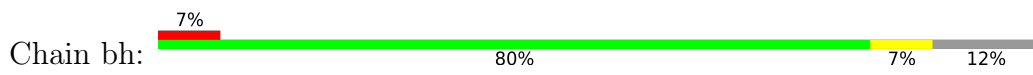
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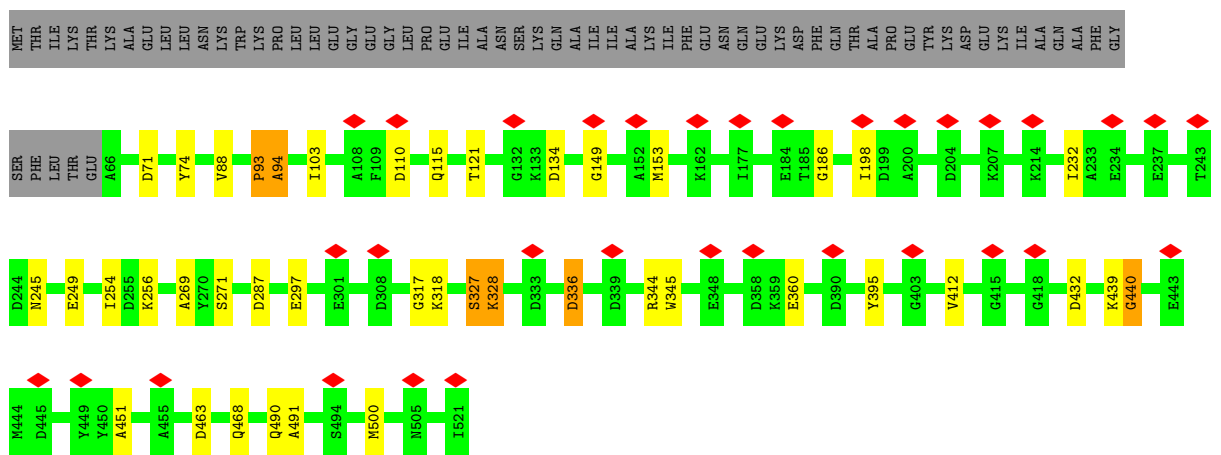
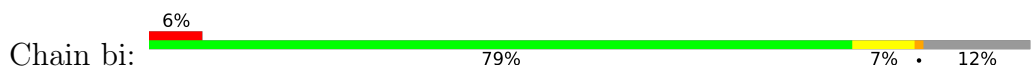
• Molecule 1: Major capsid protein



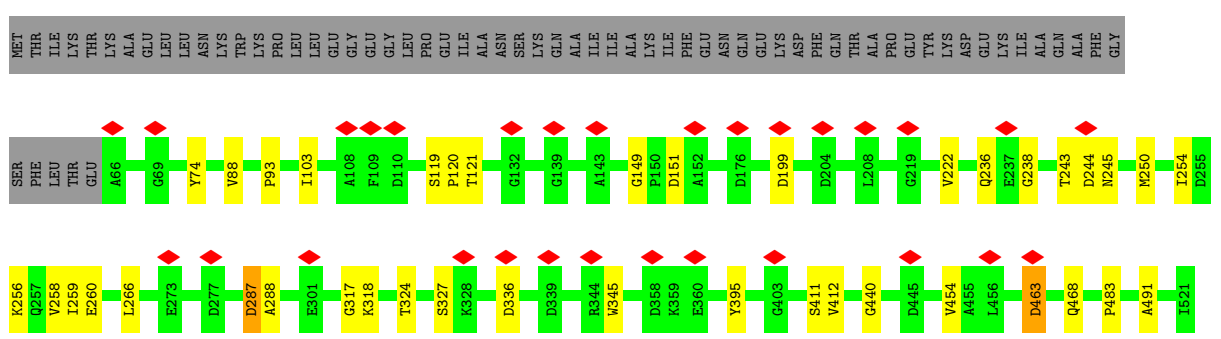
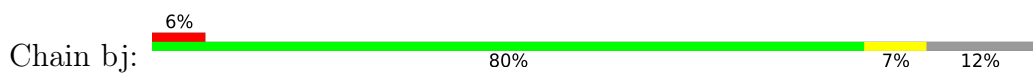
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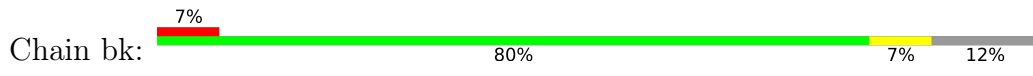
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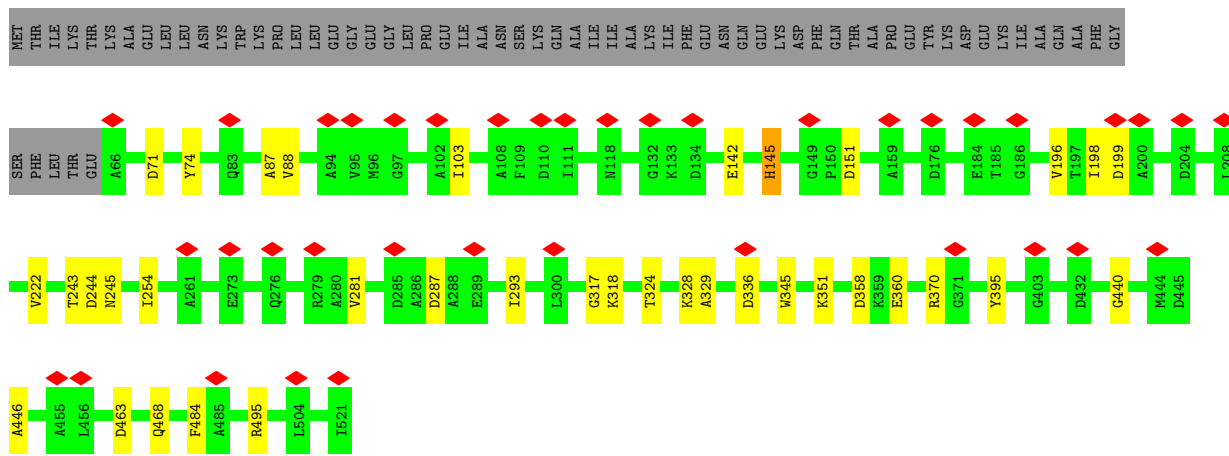


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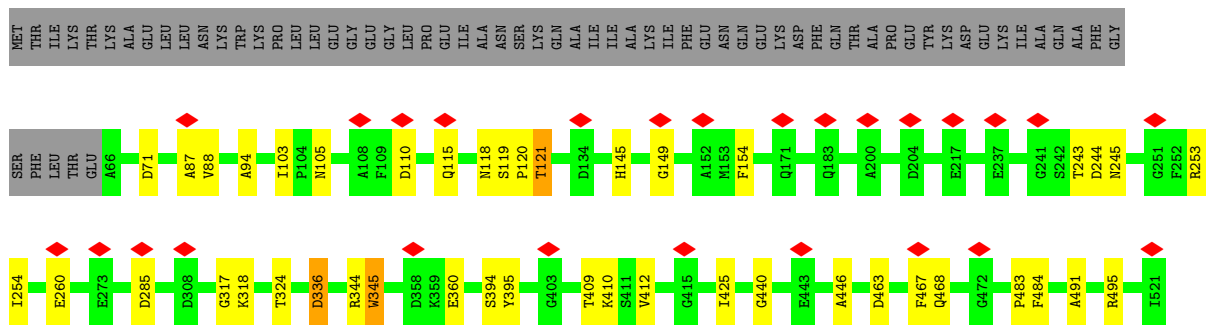
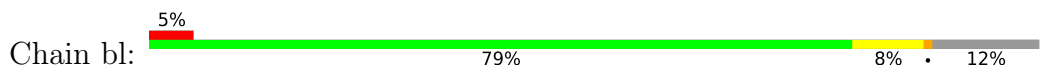


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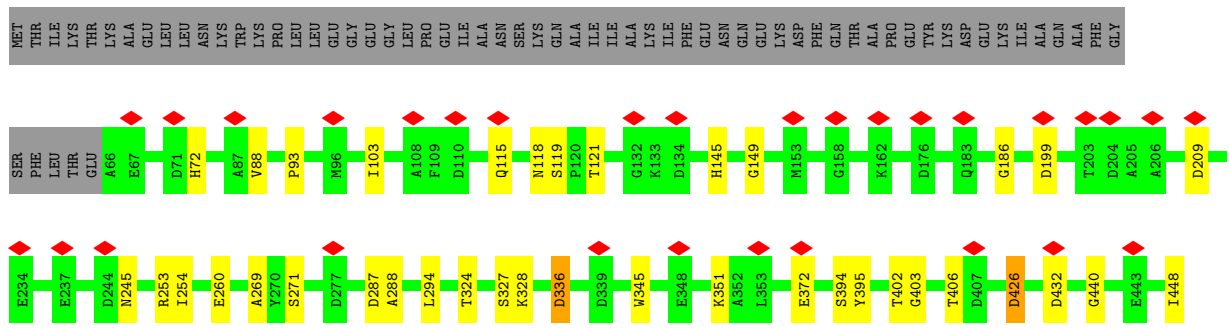
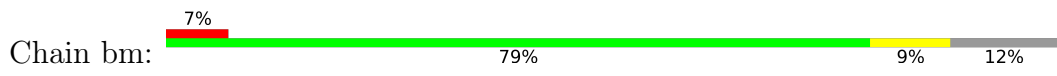




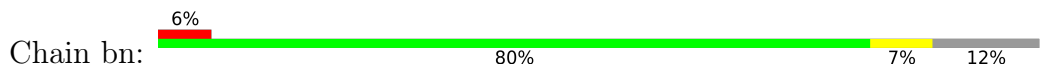
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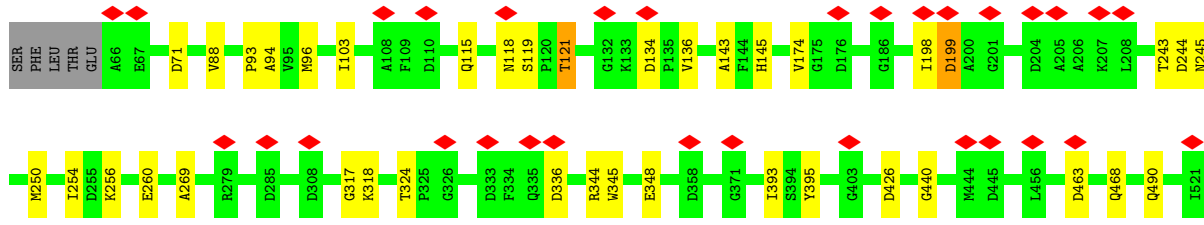


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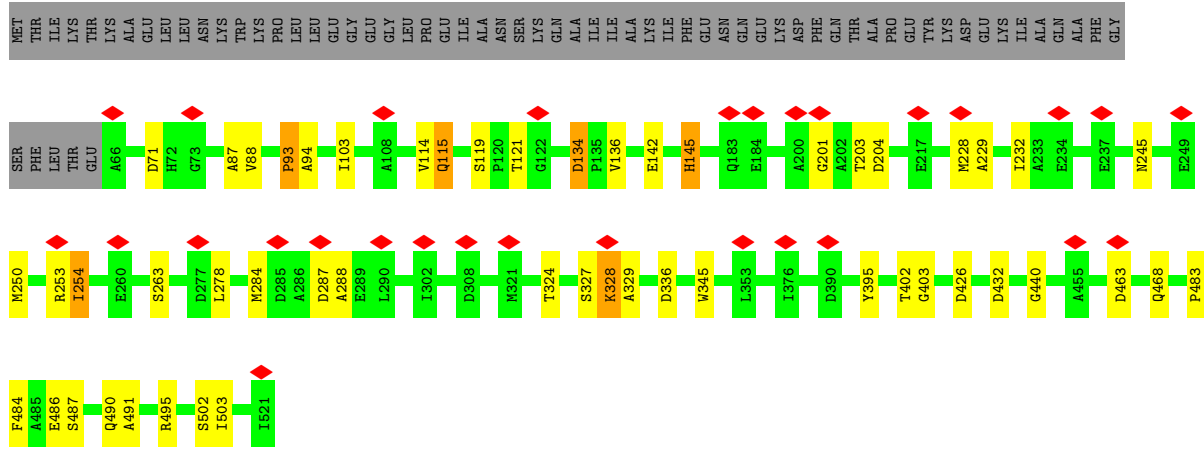
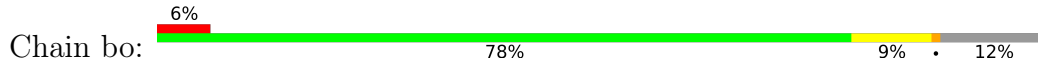


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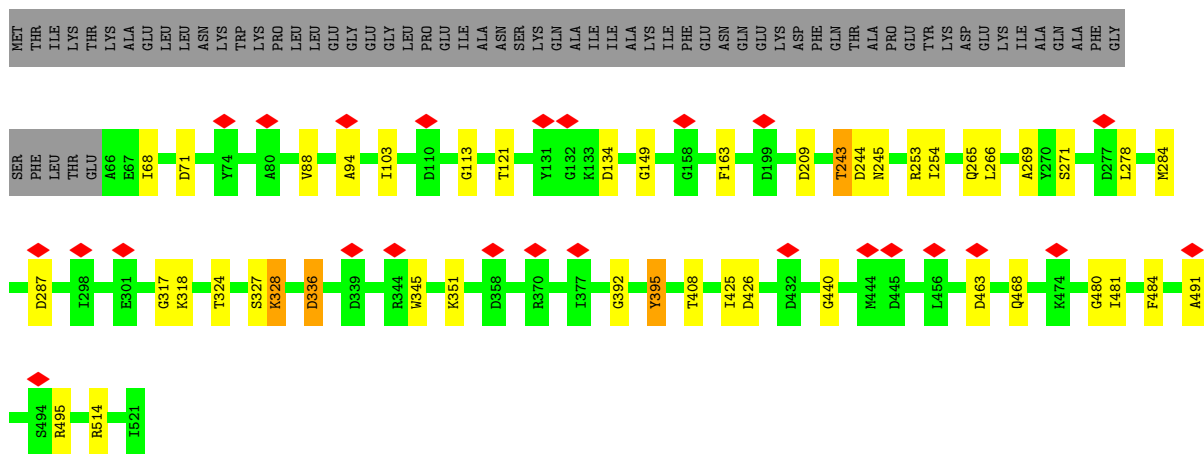
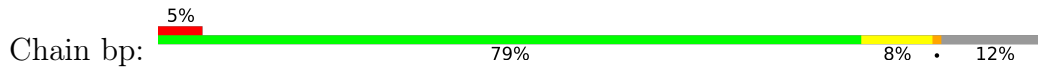




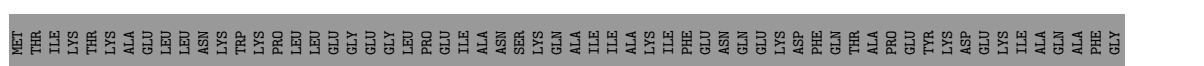
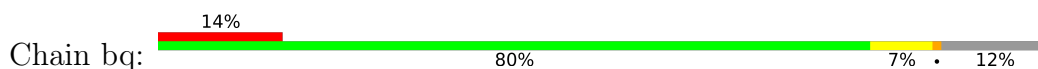
• Molecule 1: Major capsid protein

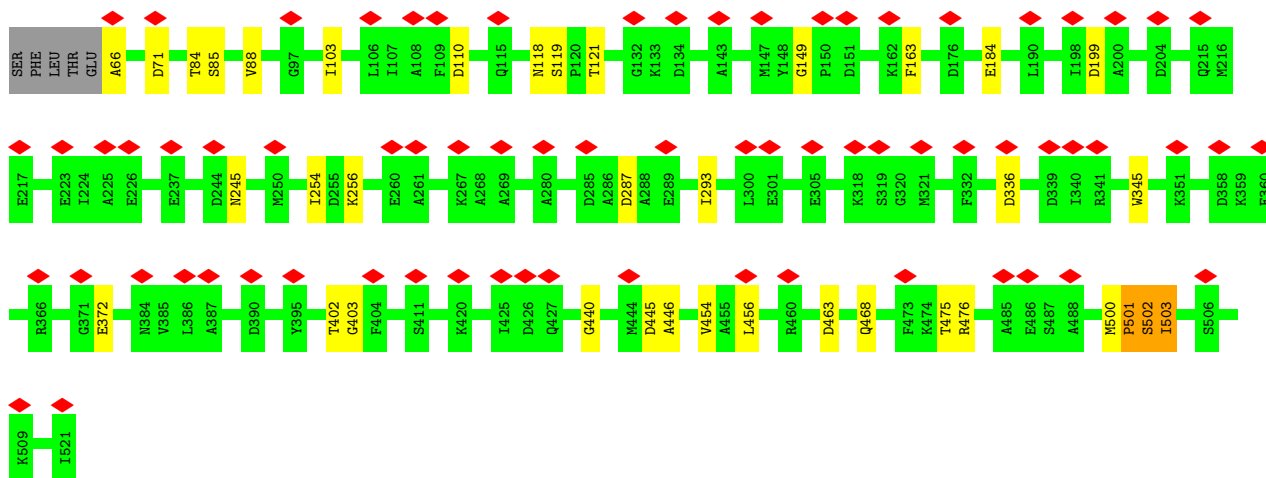


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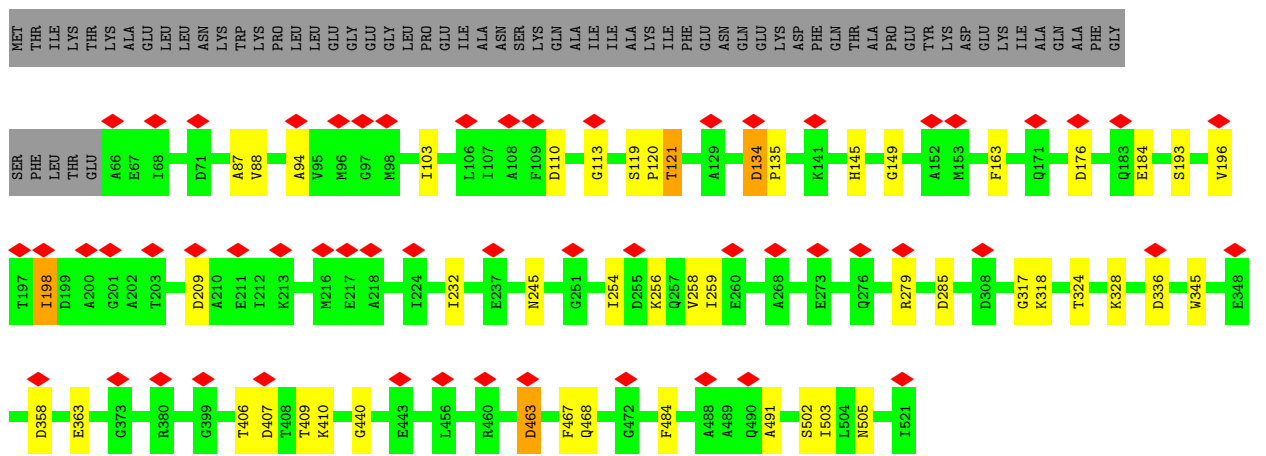
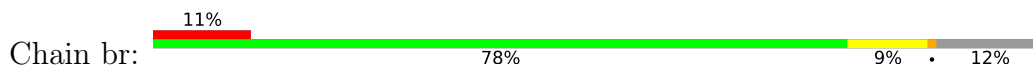


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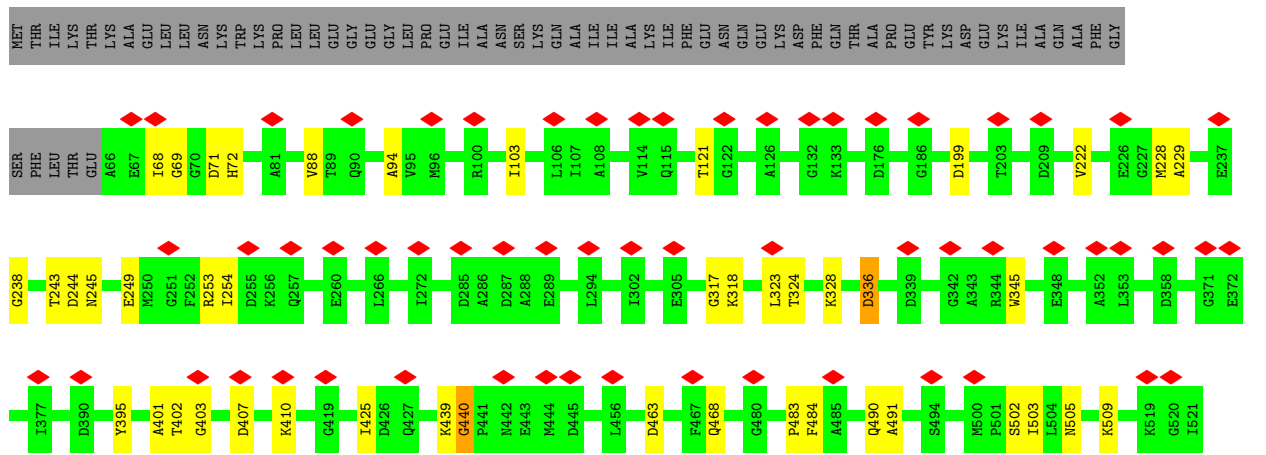
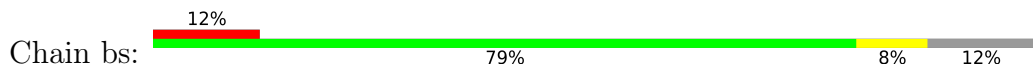




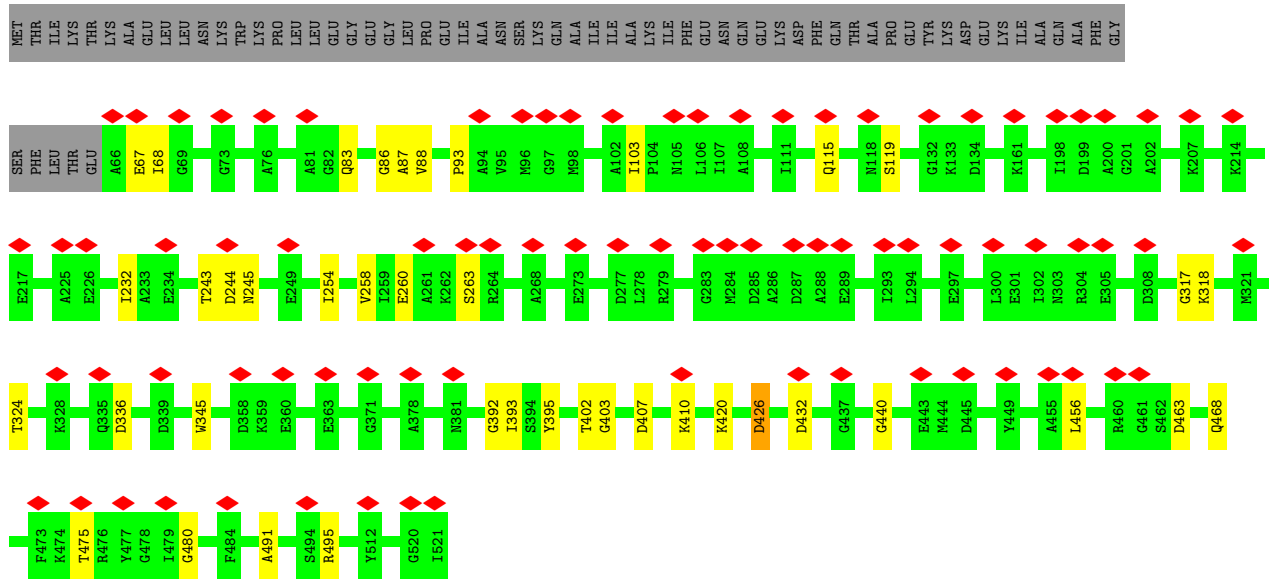
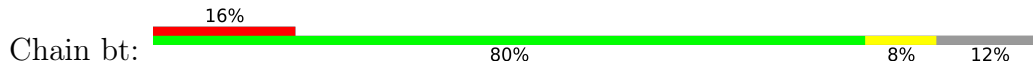
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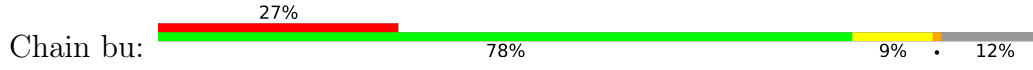
• Molecule 1: Major capsid protein



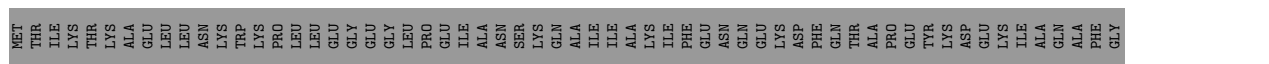
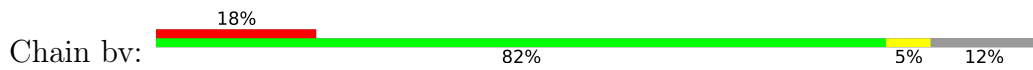
• Molecule 1: Major capsid protein

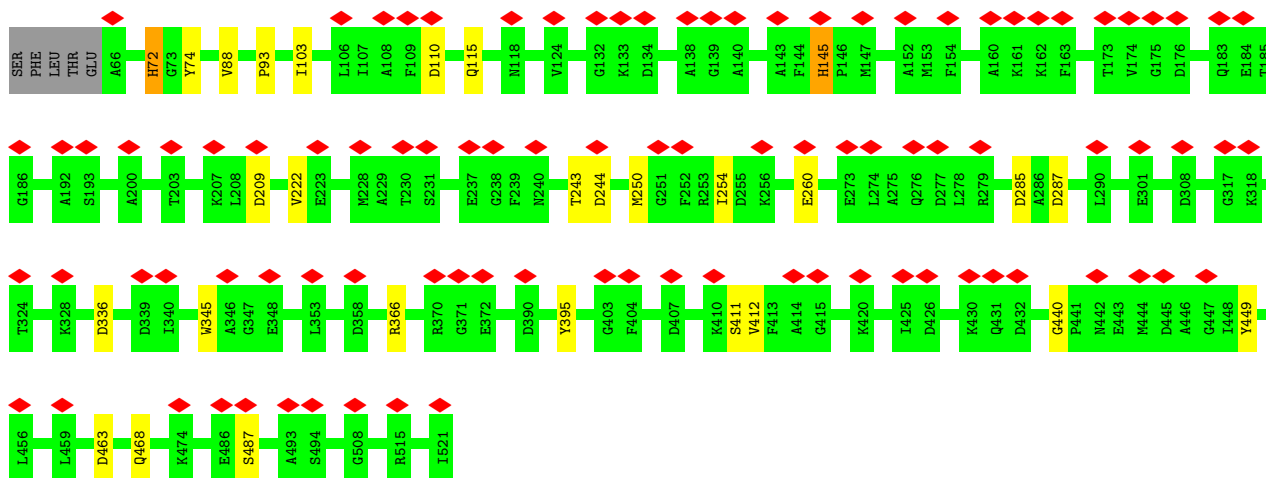


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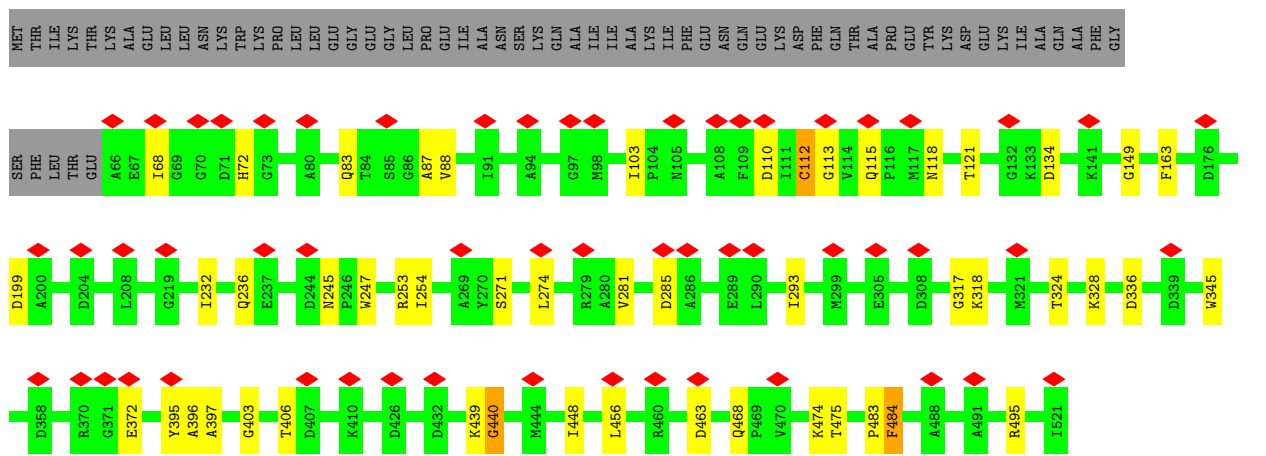
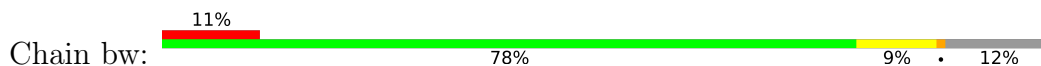


• Molecule 1: Major capsid protein

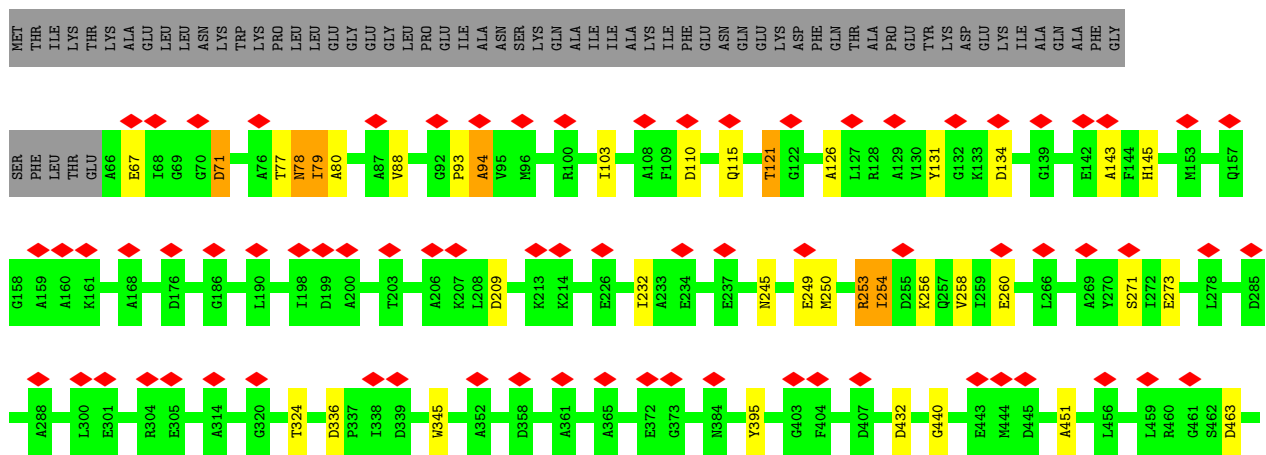
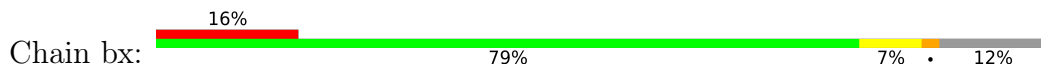


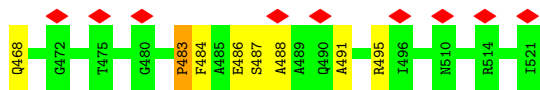


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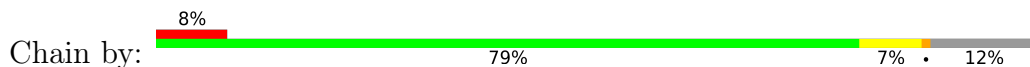


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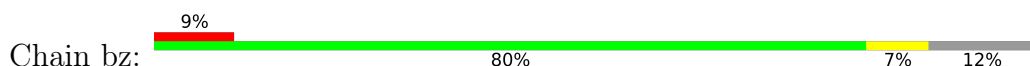
• Molecule 1: Major capsid protein



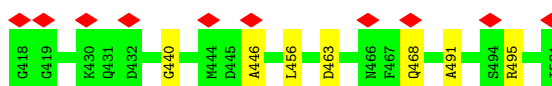
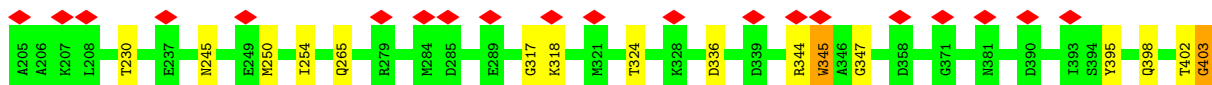
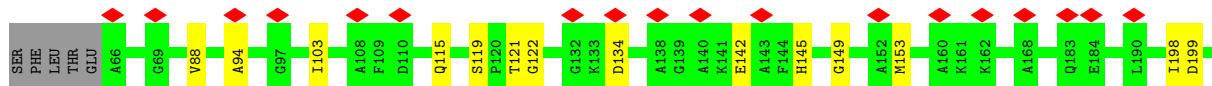
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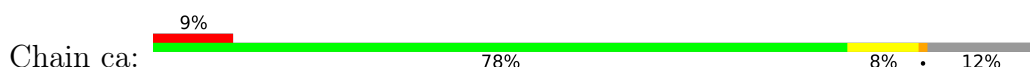
• Molecule 1: Major capsid protein



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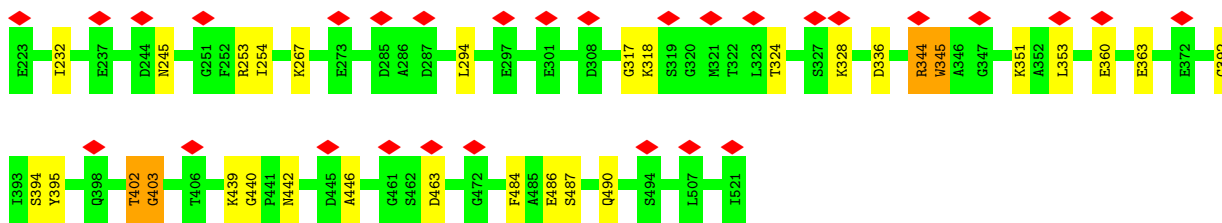


• Molecule 1: Major capsid protein

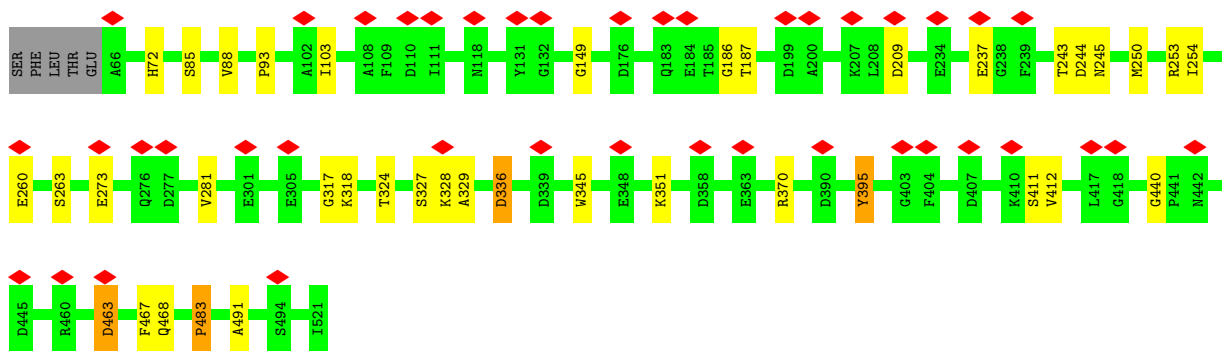
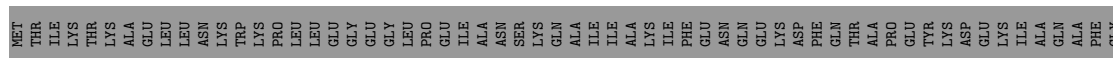
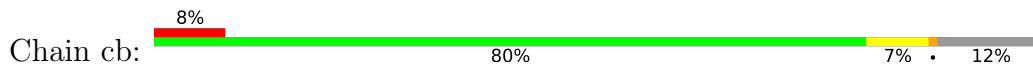


MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	LYS	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	PRO	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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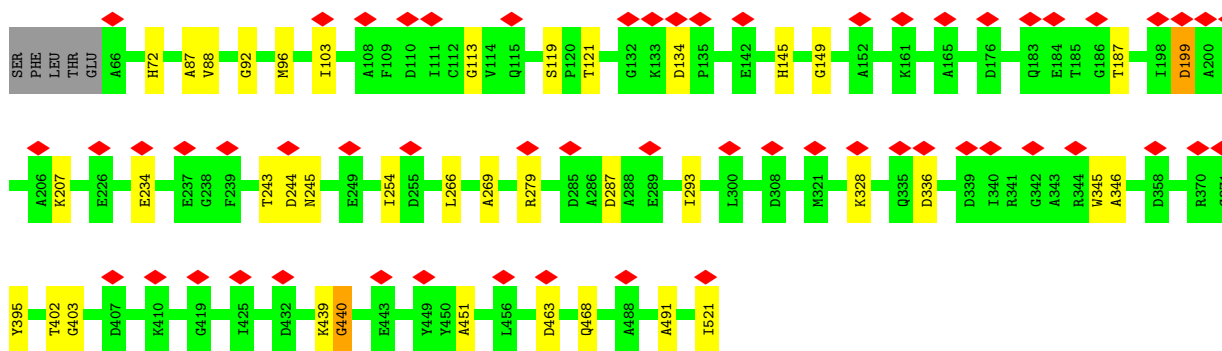
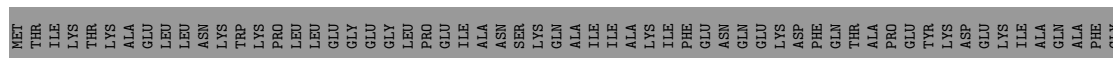
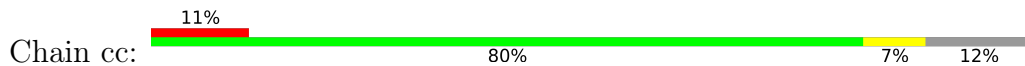




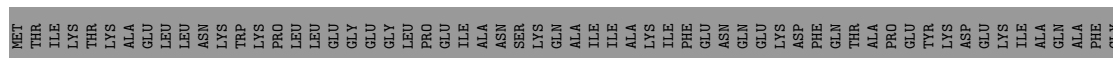
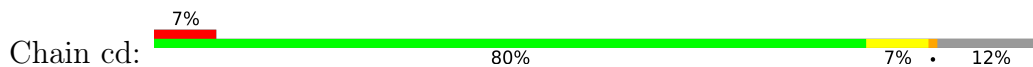
• Molecule 1: Major capsid protein

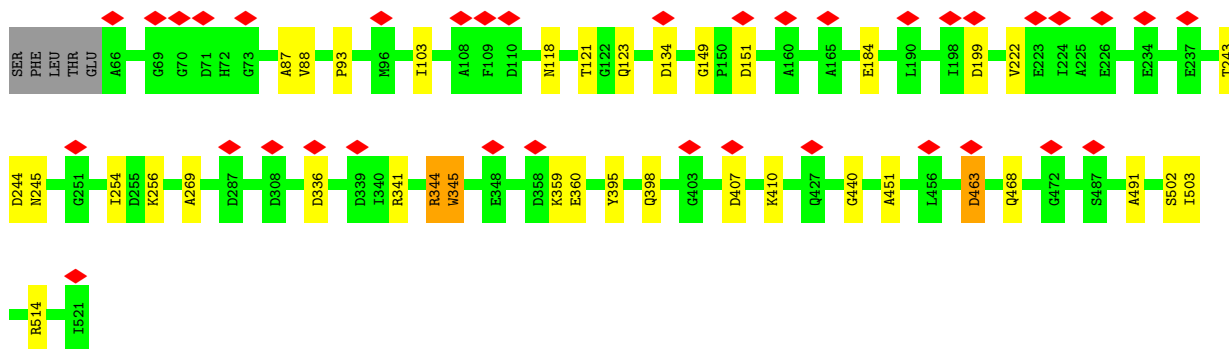


• Molecule 1: Major capsid protein

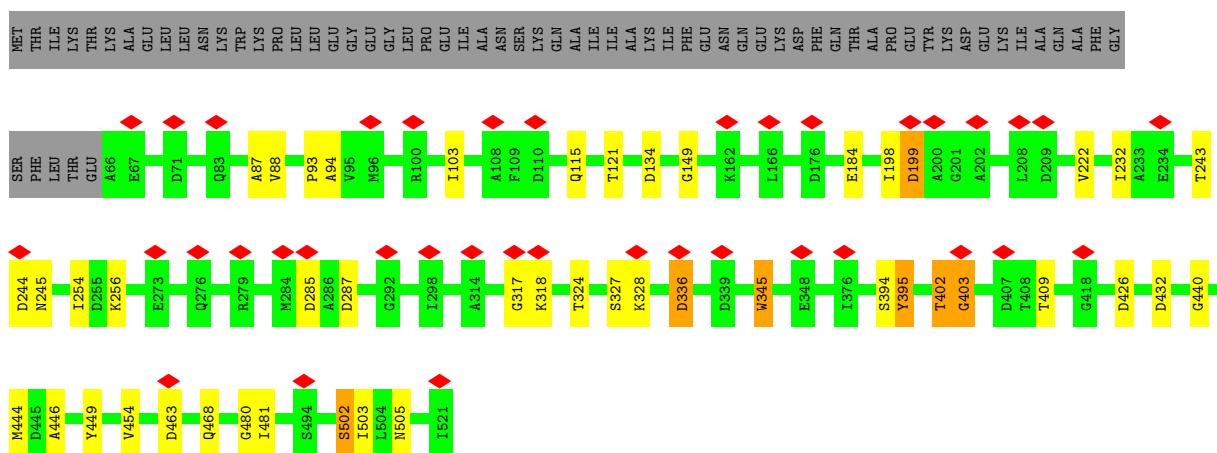
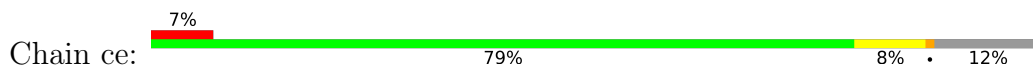


• Molecule 1: Major capsid protein

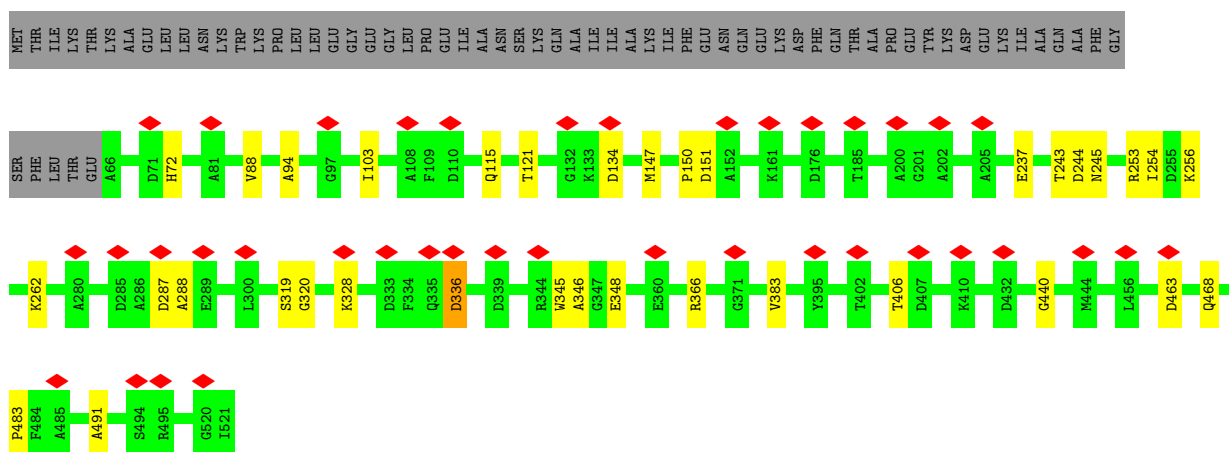
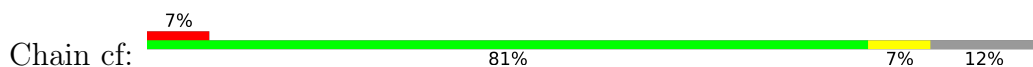




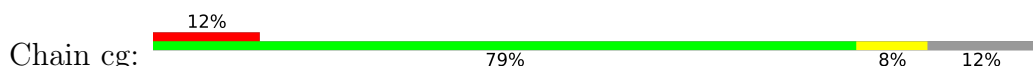
• Molecule 1: Major capsid protein

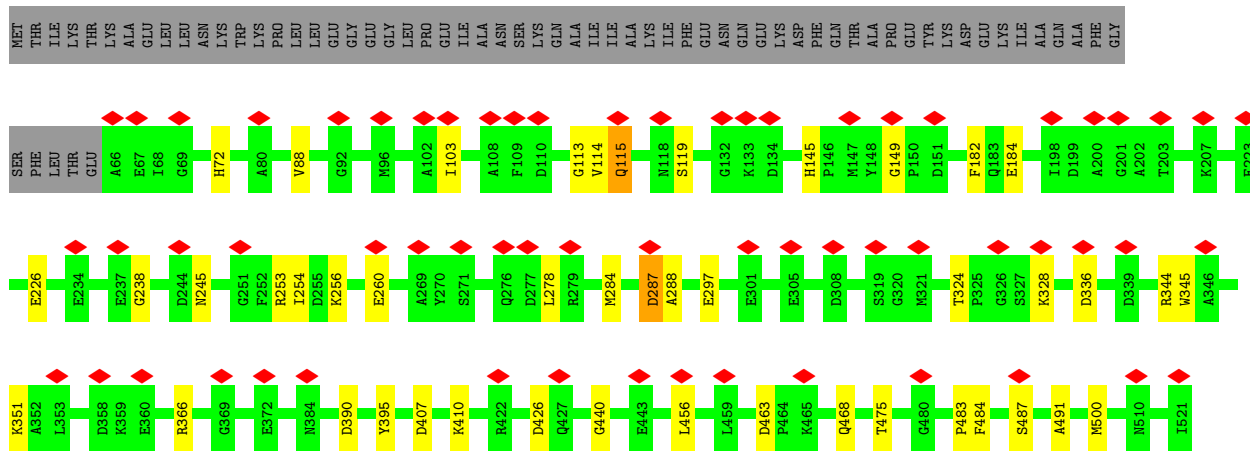


• Molecule 1: Major capsid protein

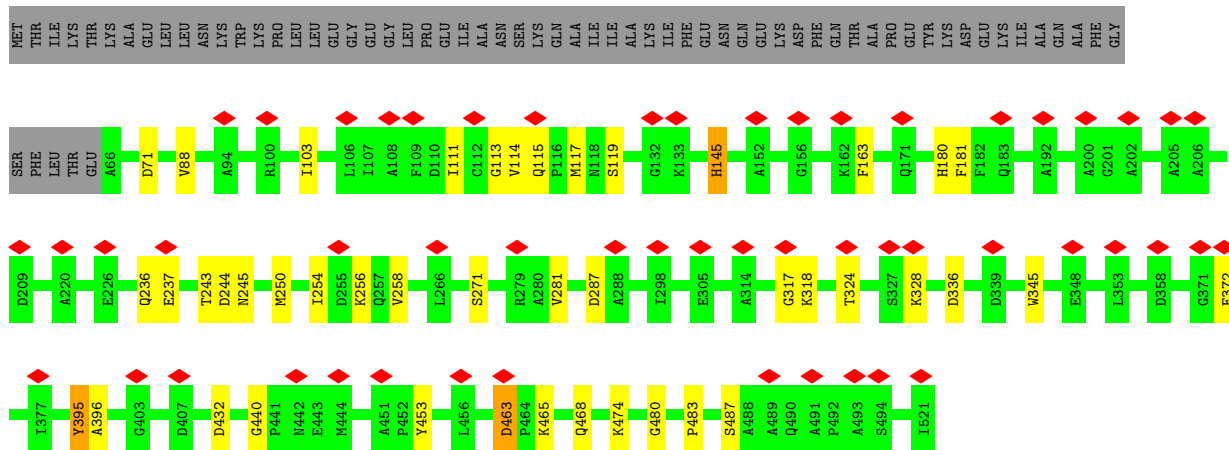
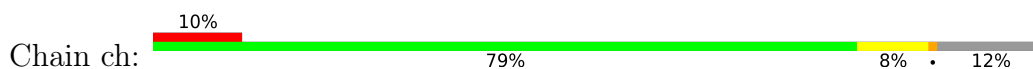


• Molecule 1: Major capsid protein

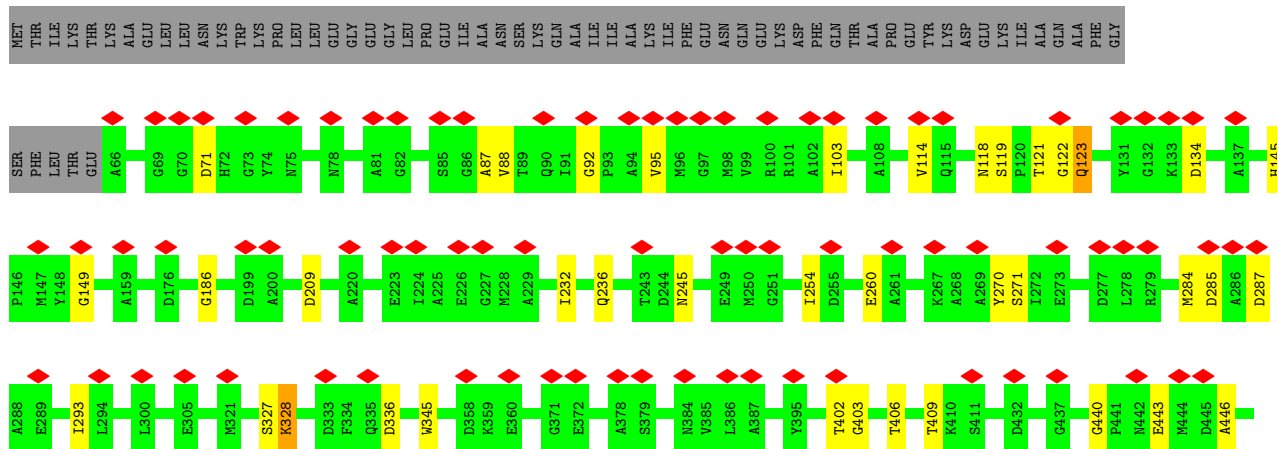
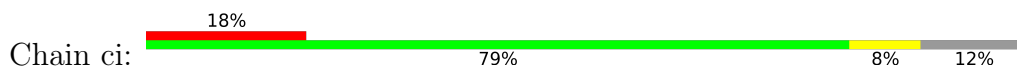


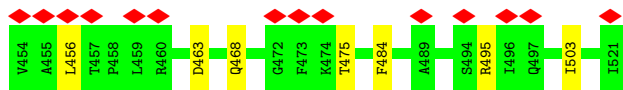


• Molecule 1: Major capsid protein

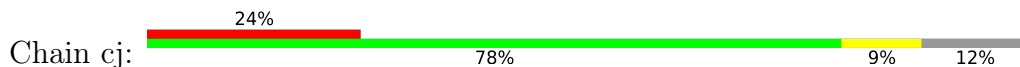


• Molecule 1: Major capsid protein

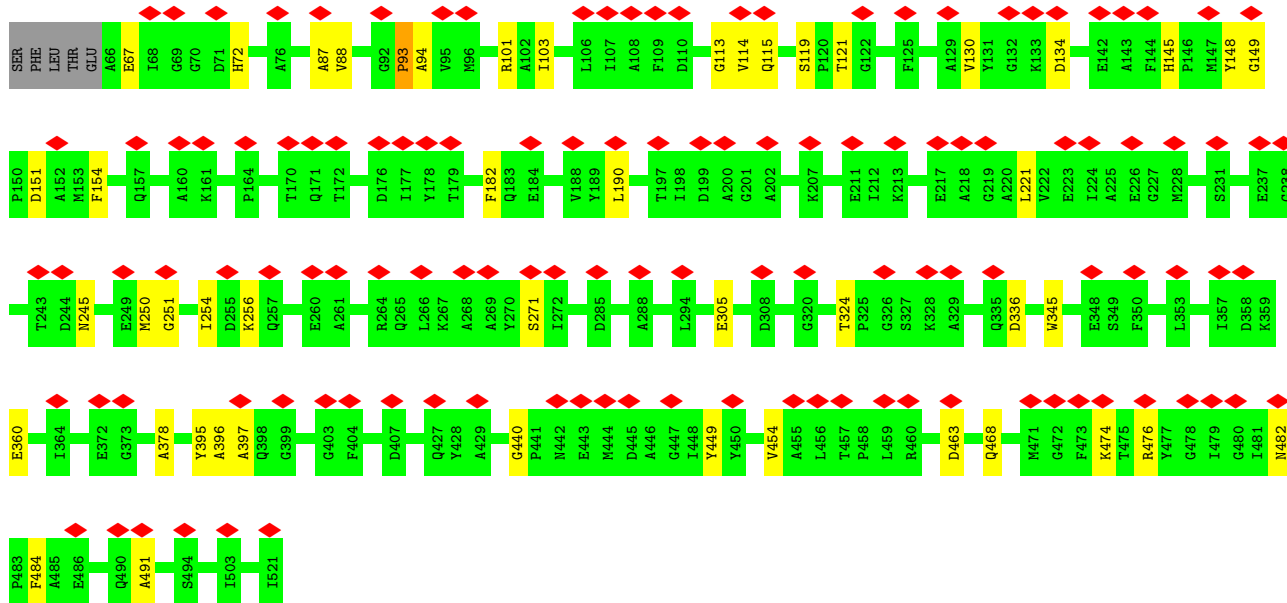




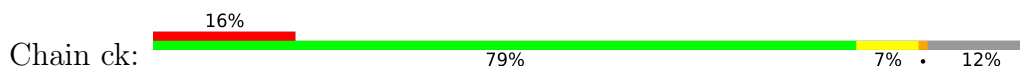
• Molecule 1: Major capsid protein



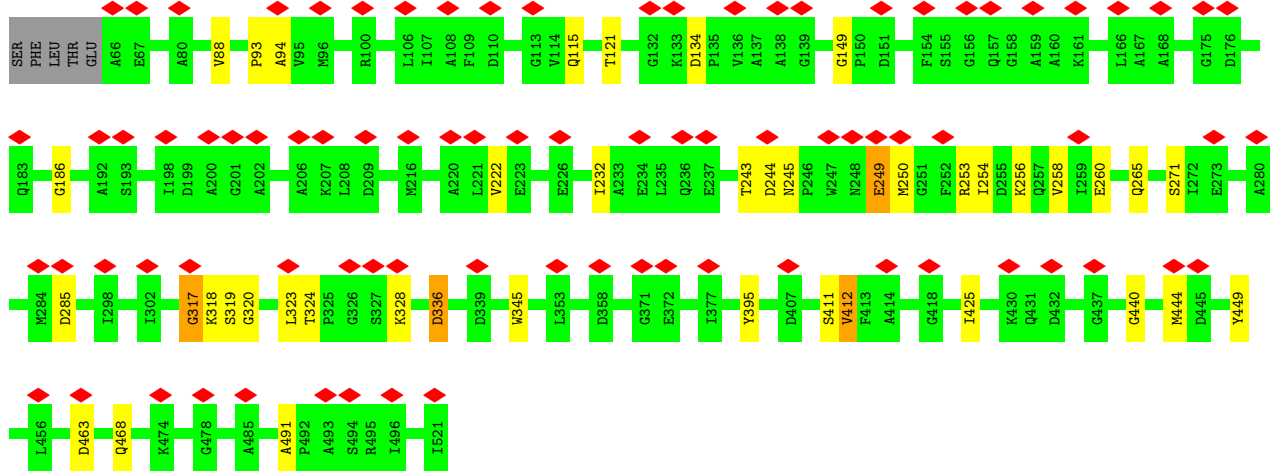
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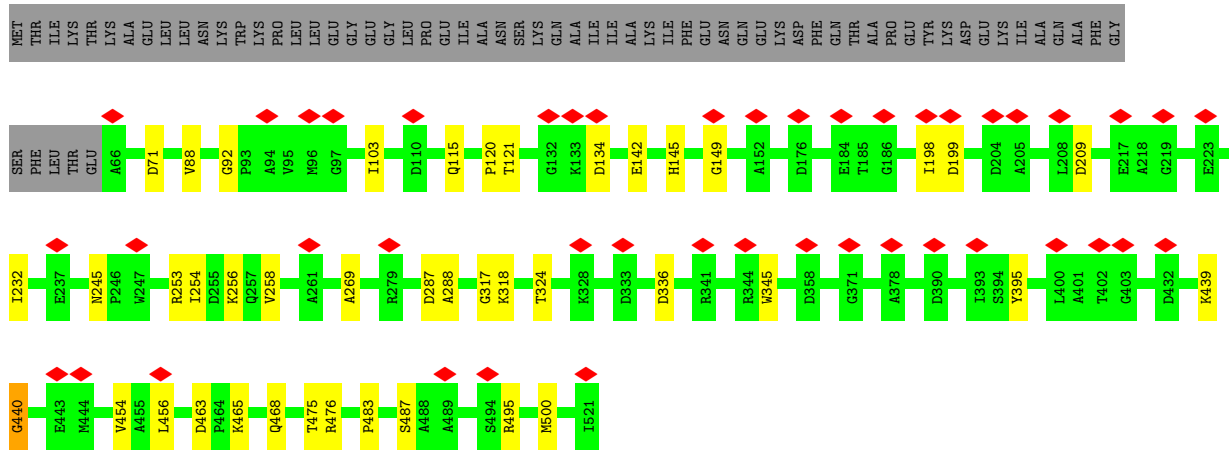
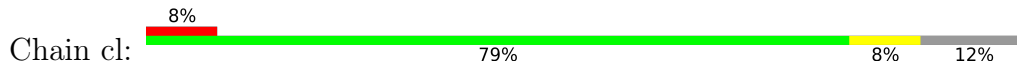
• Molecule 1: Major capsid protein



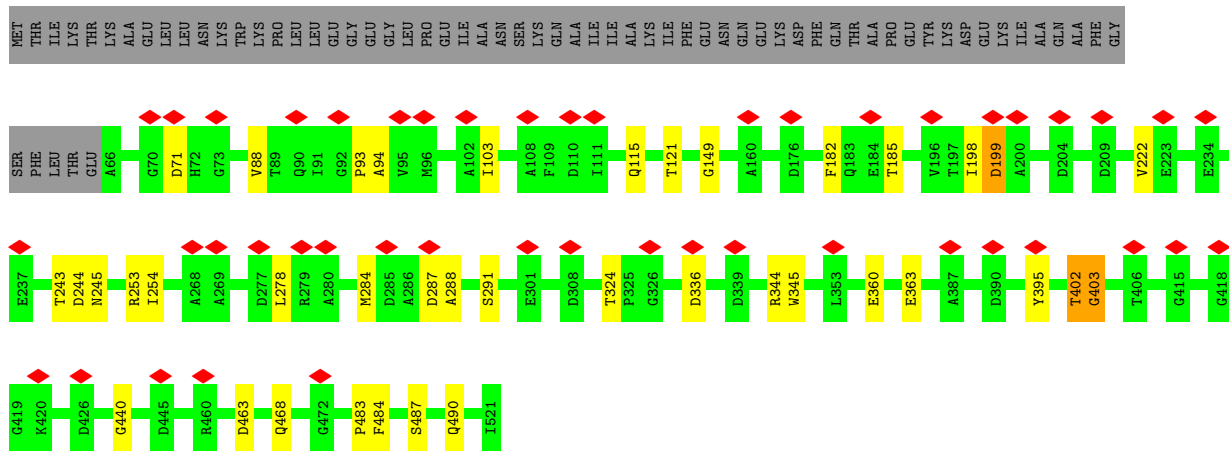
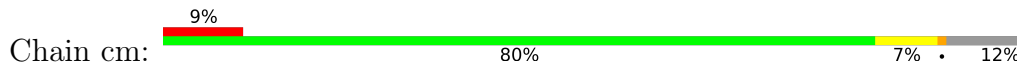
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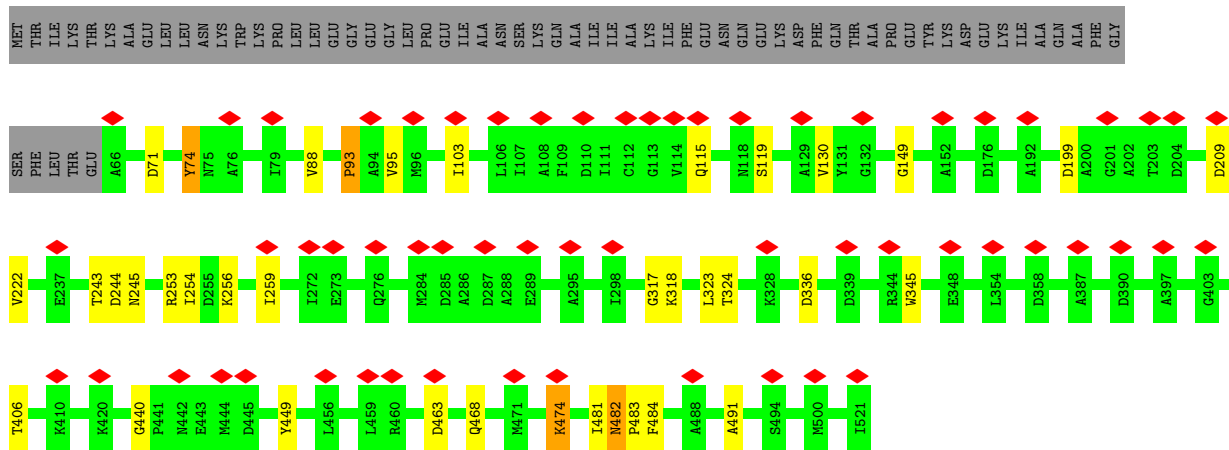
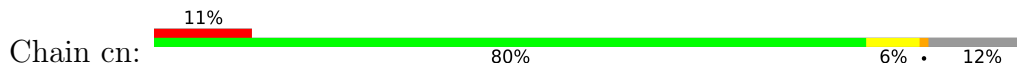
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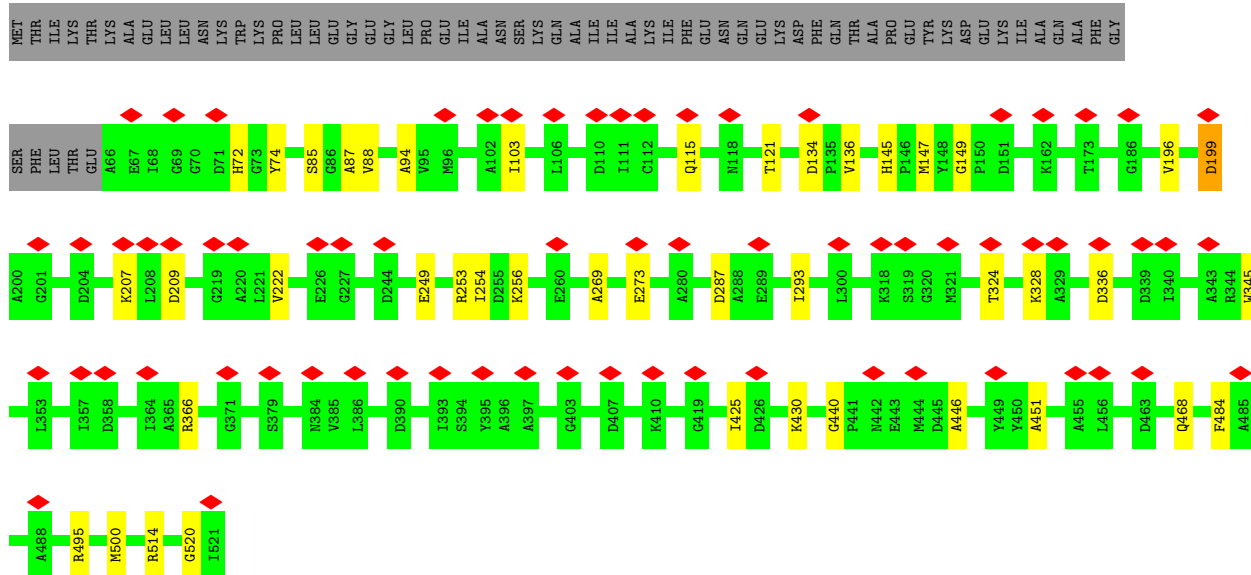
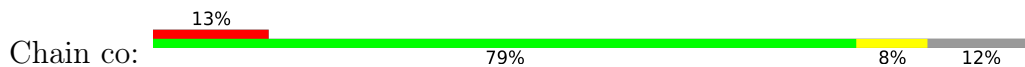
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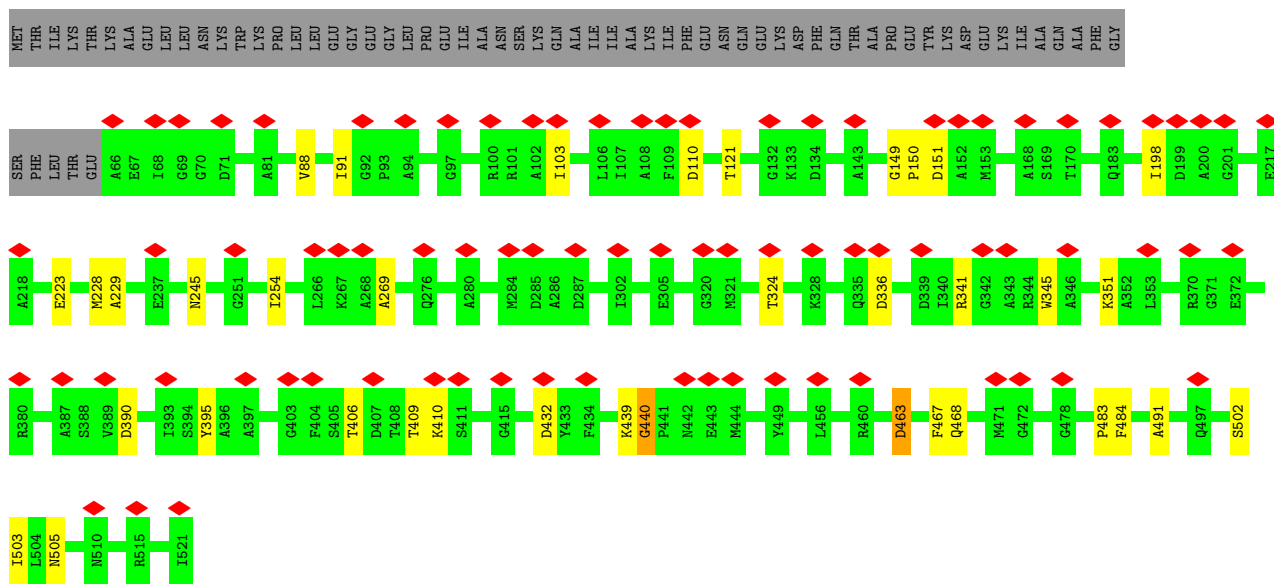
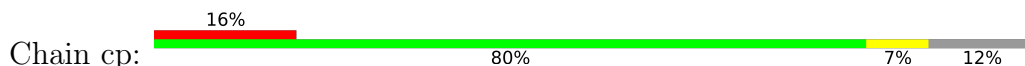
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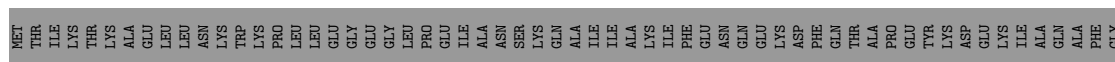
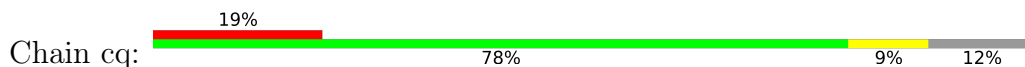
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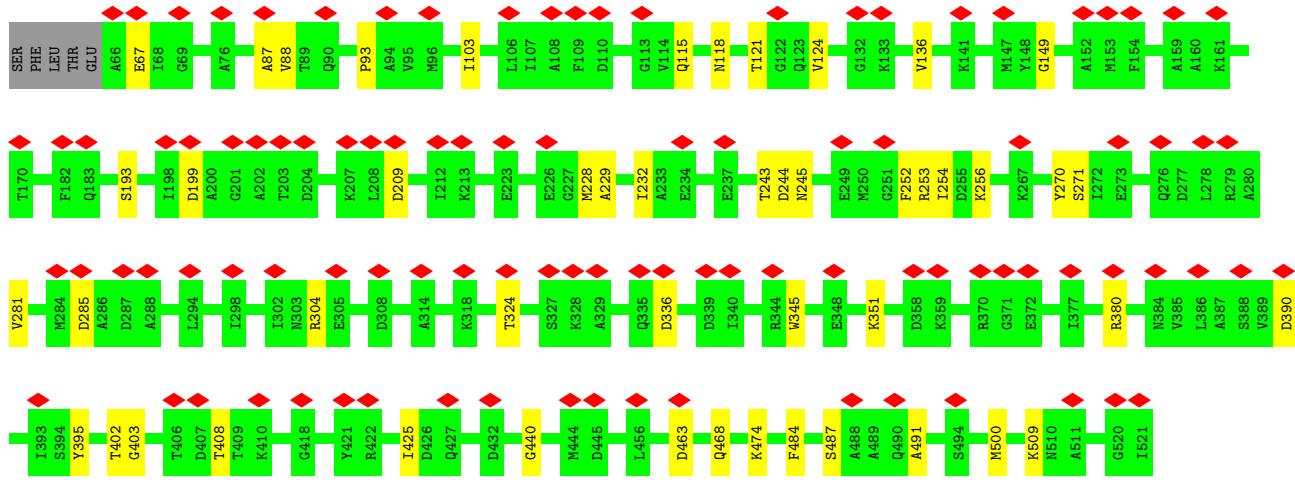


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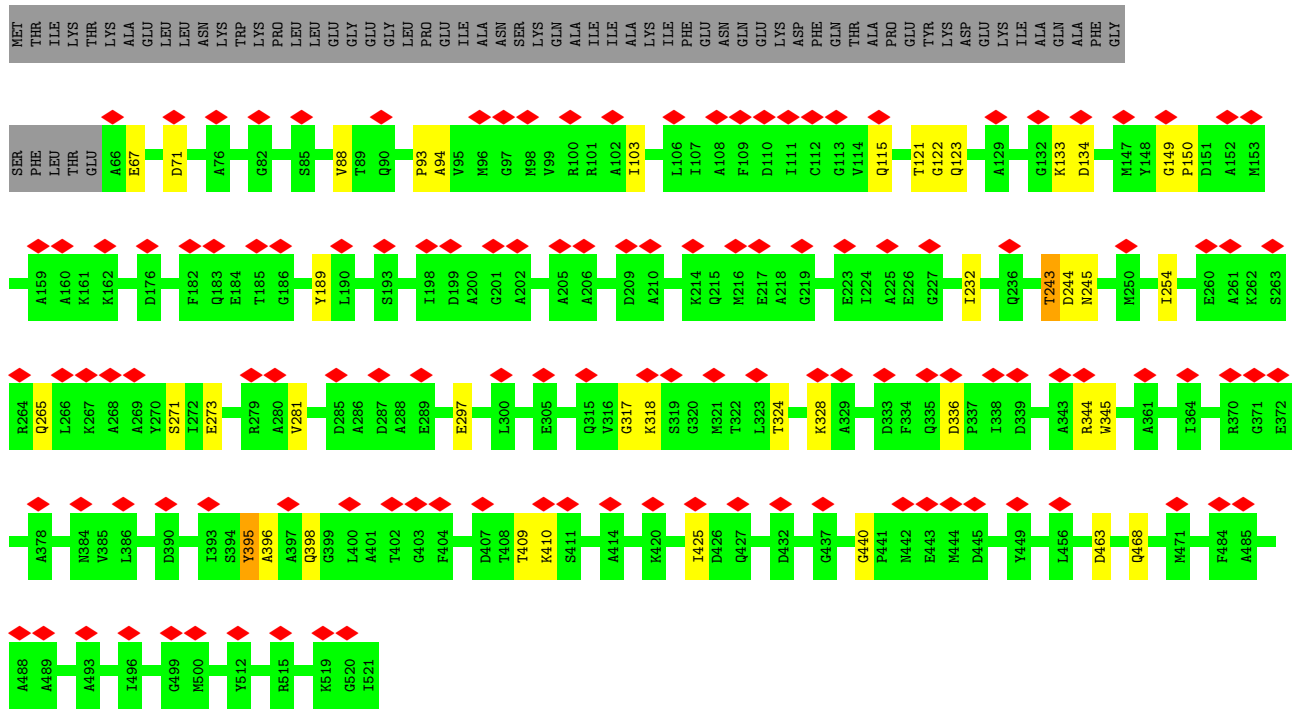
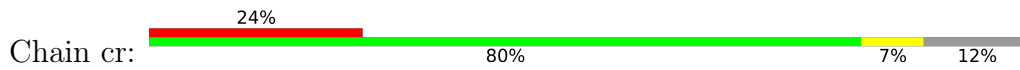


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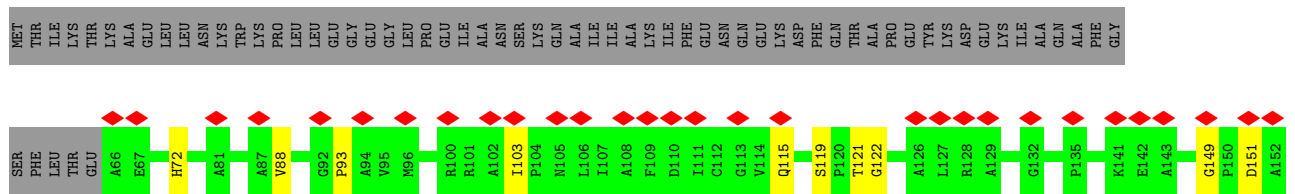
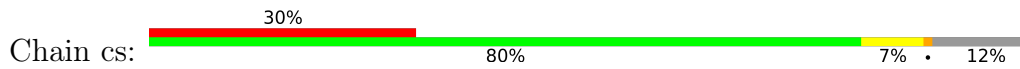


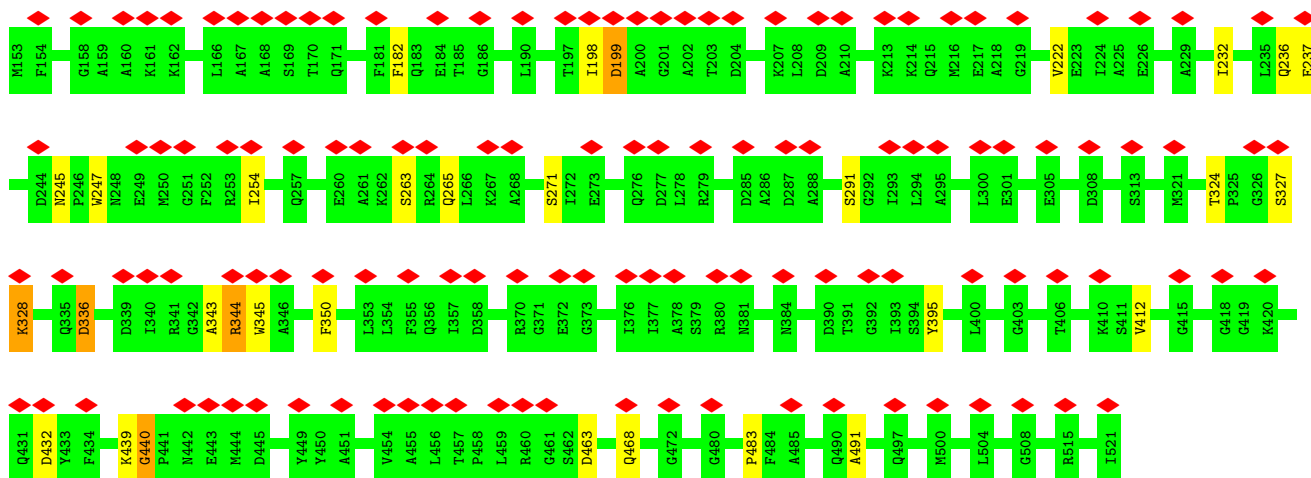


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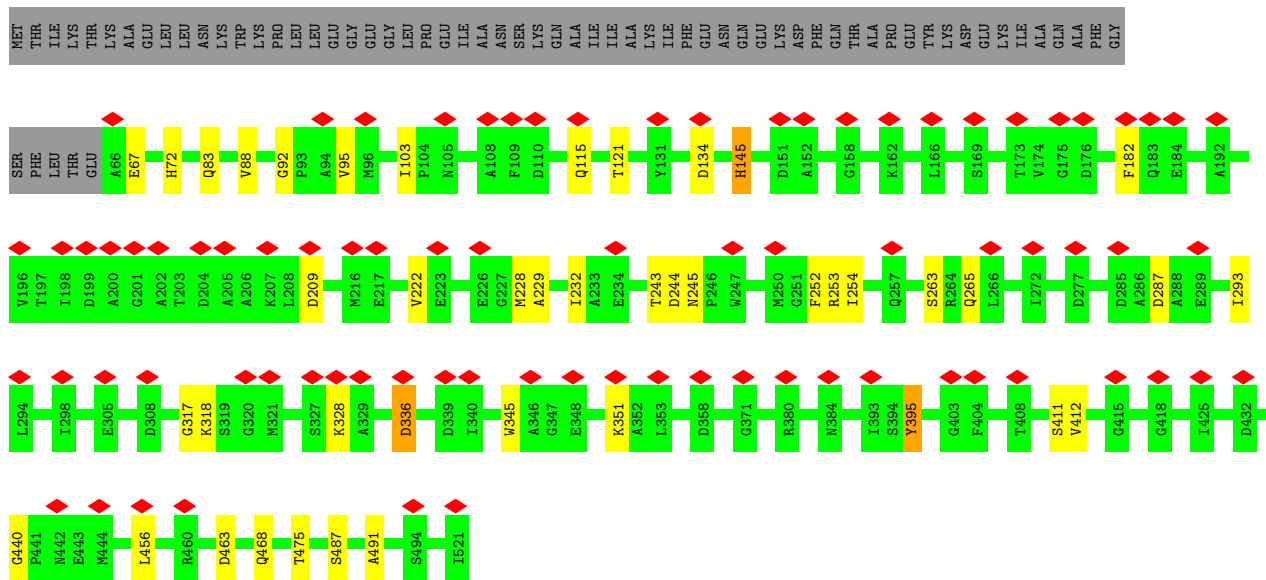
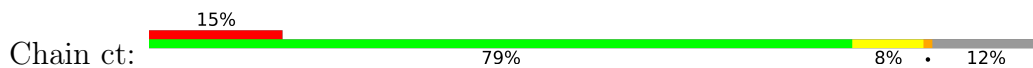


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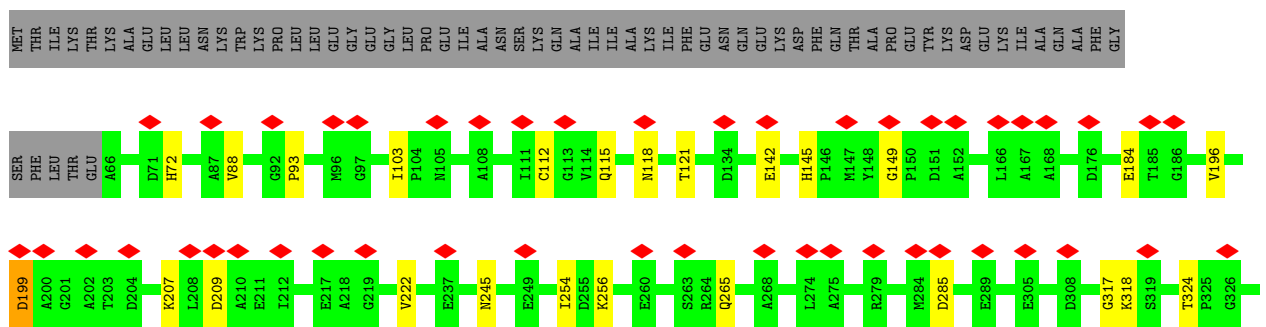
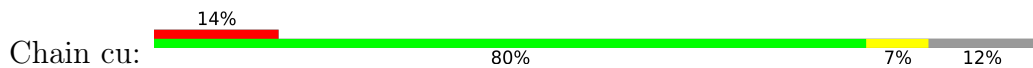


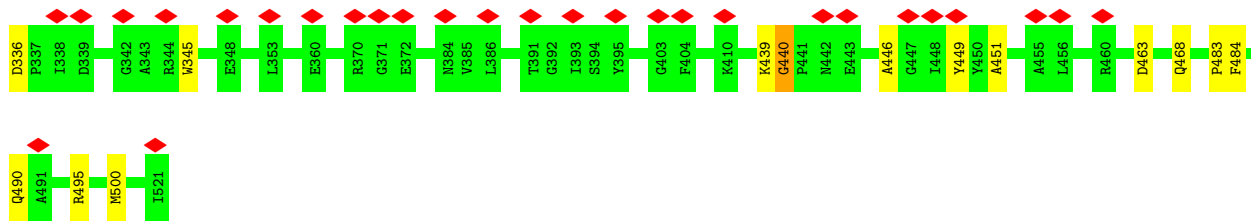


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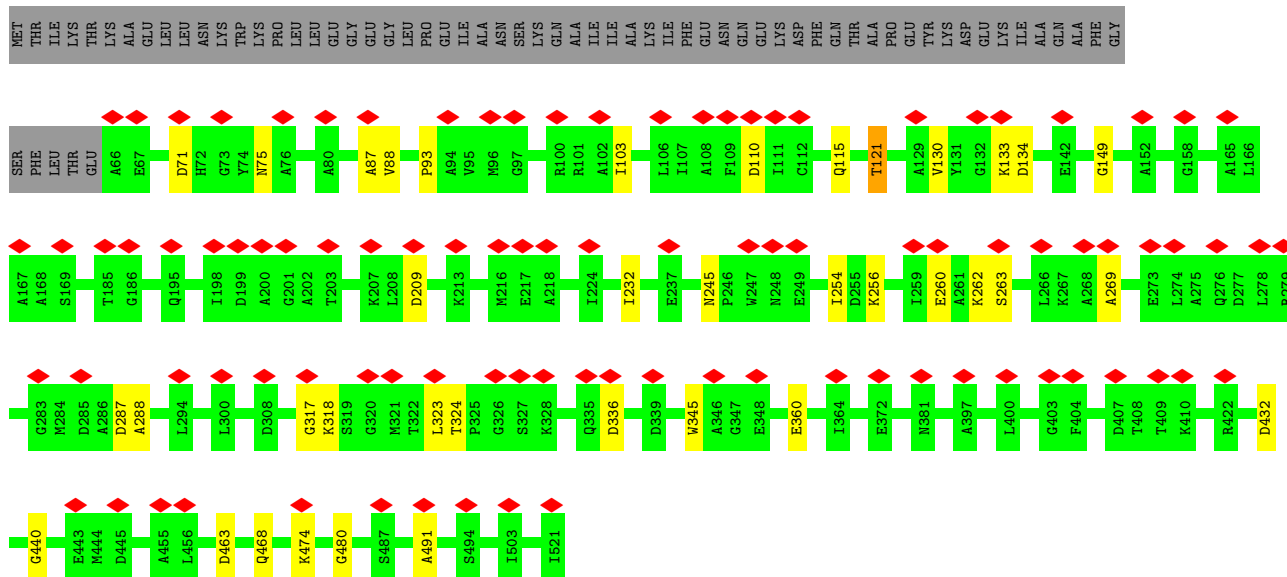
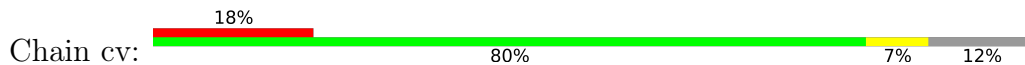


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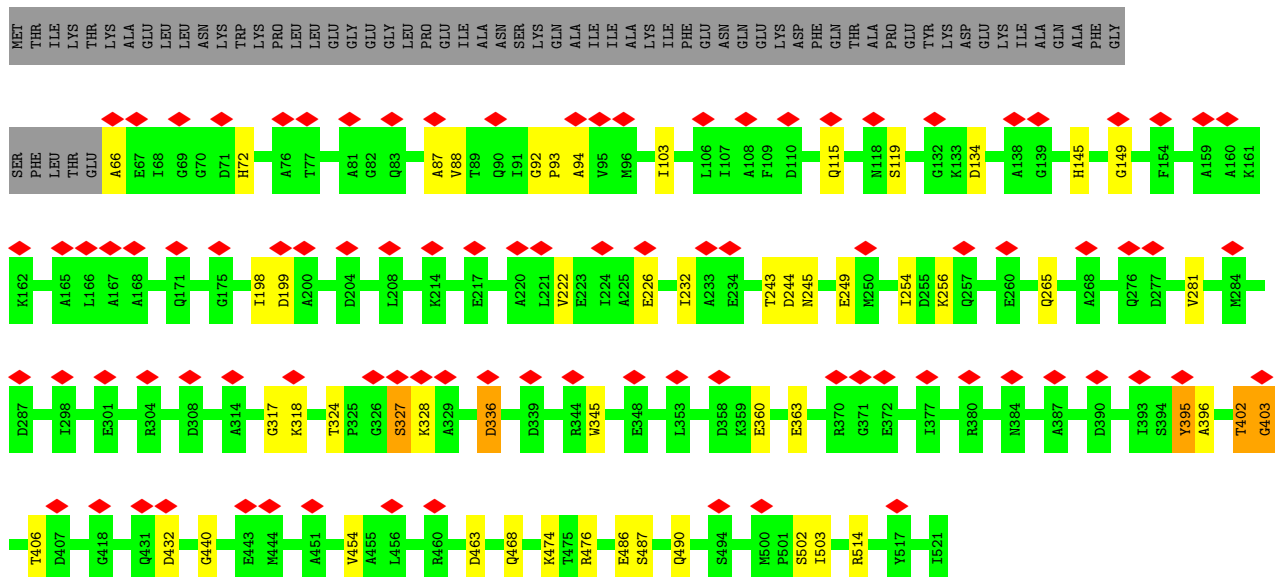
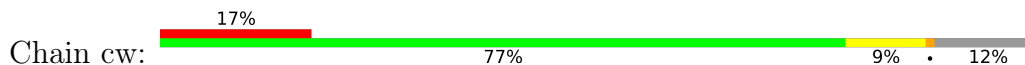




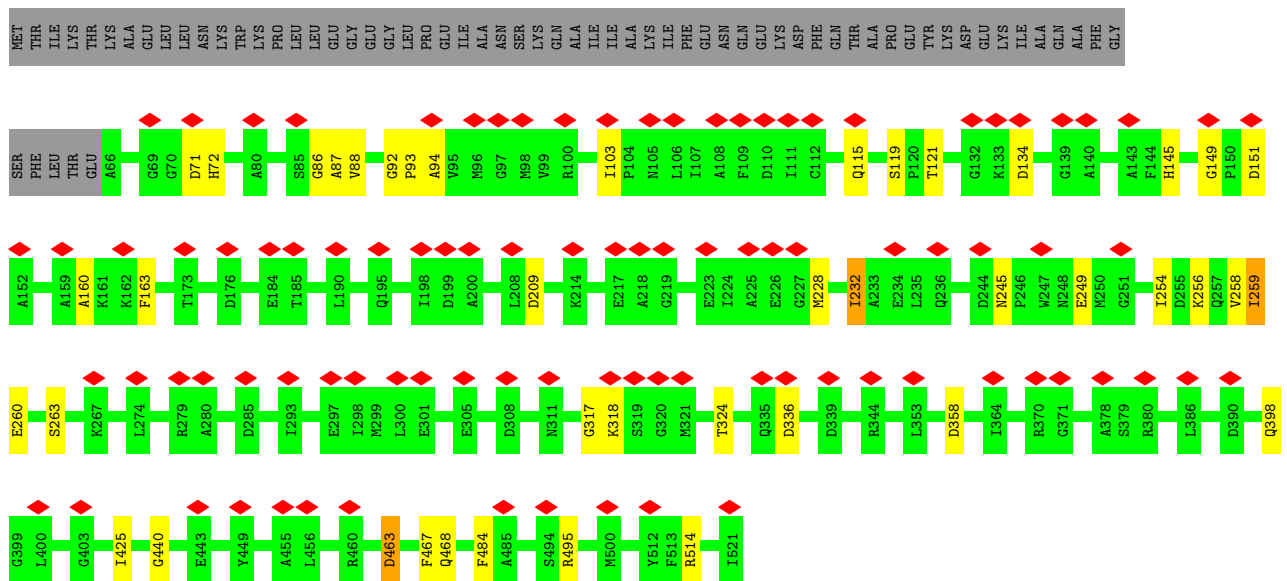
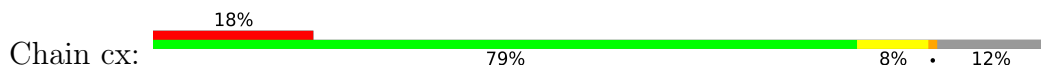
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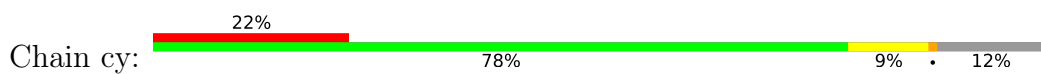
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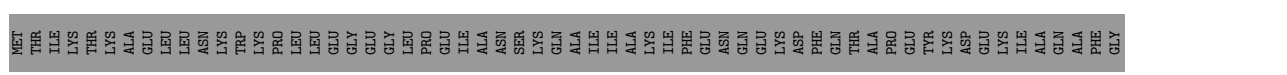
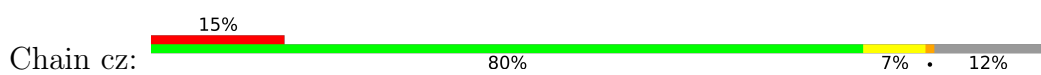
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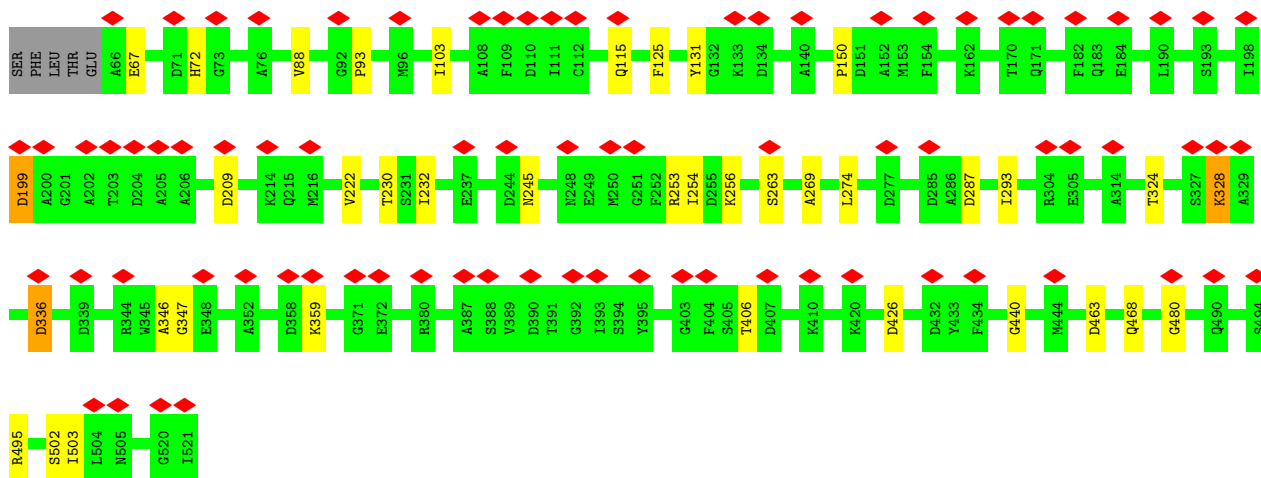


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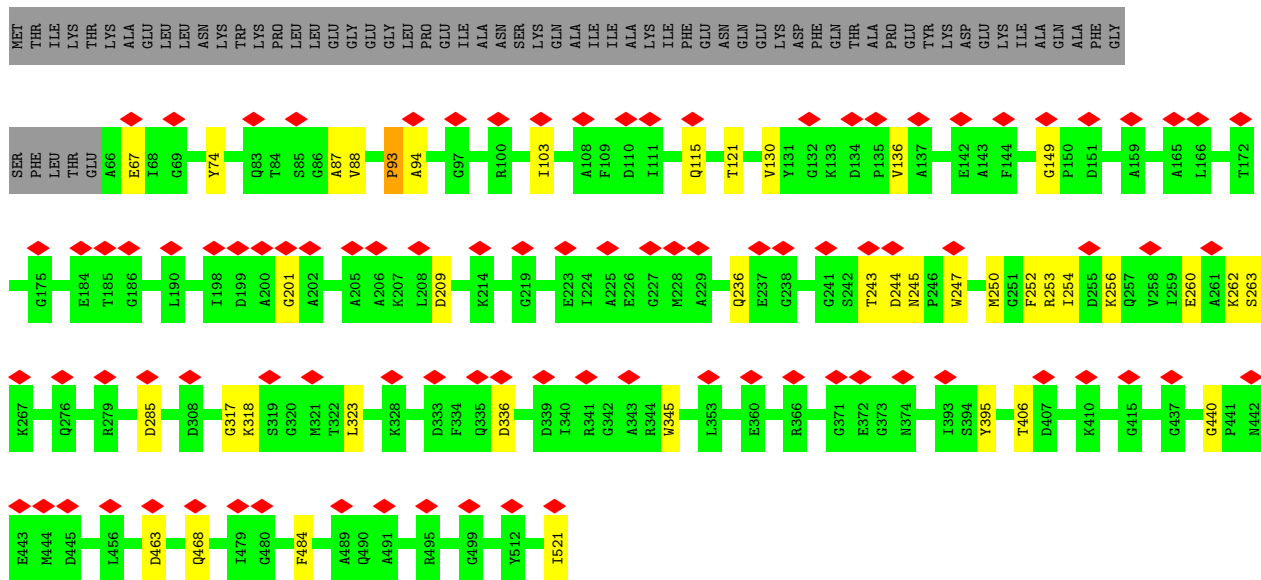
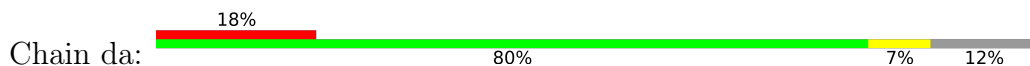


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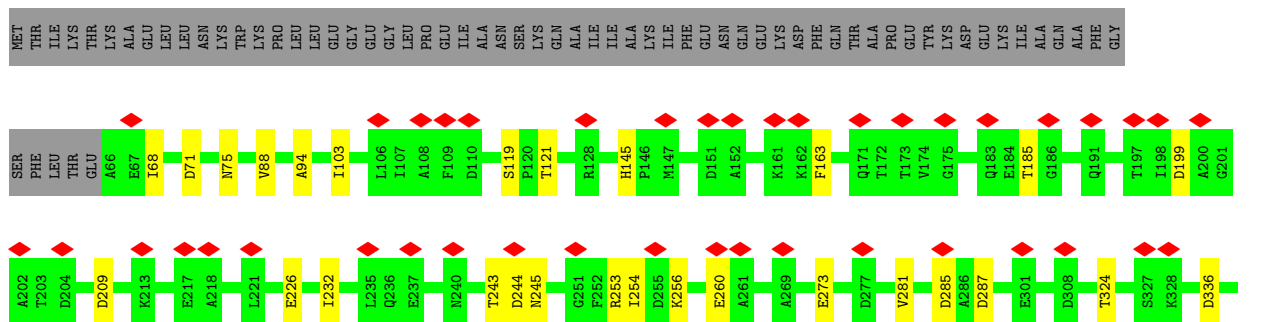
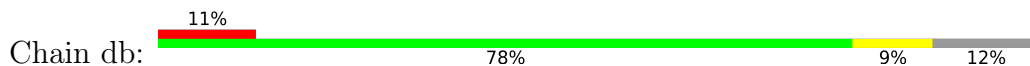




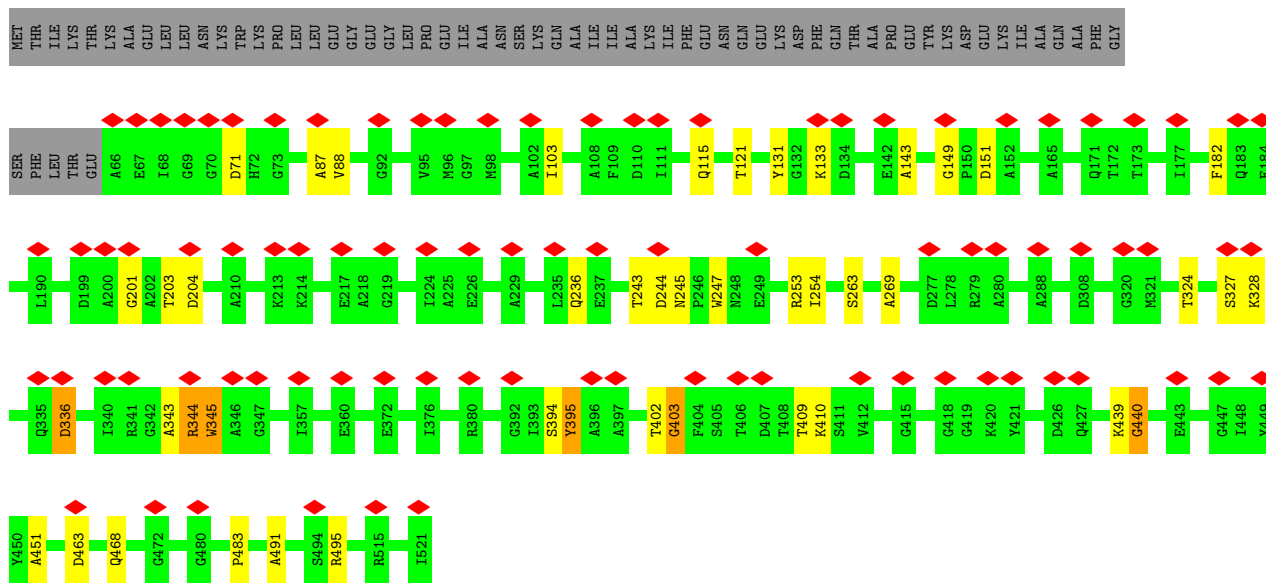
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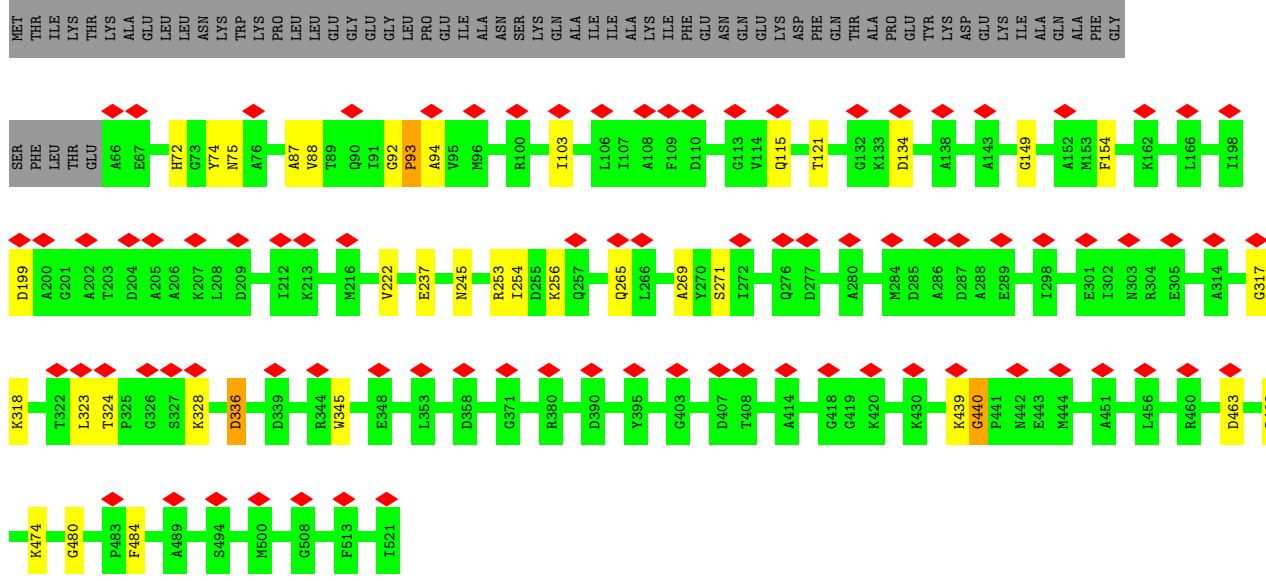
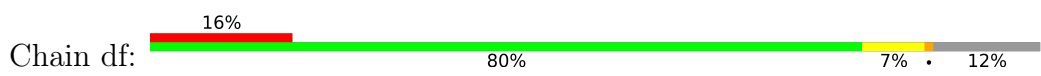
• Molecule 1: Major capsid protein



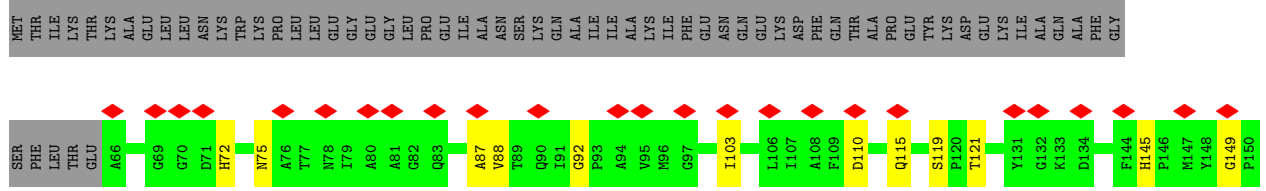
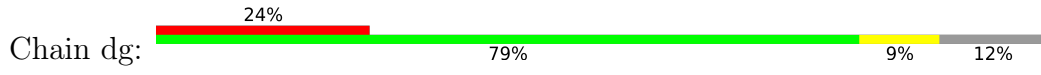


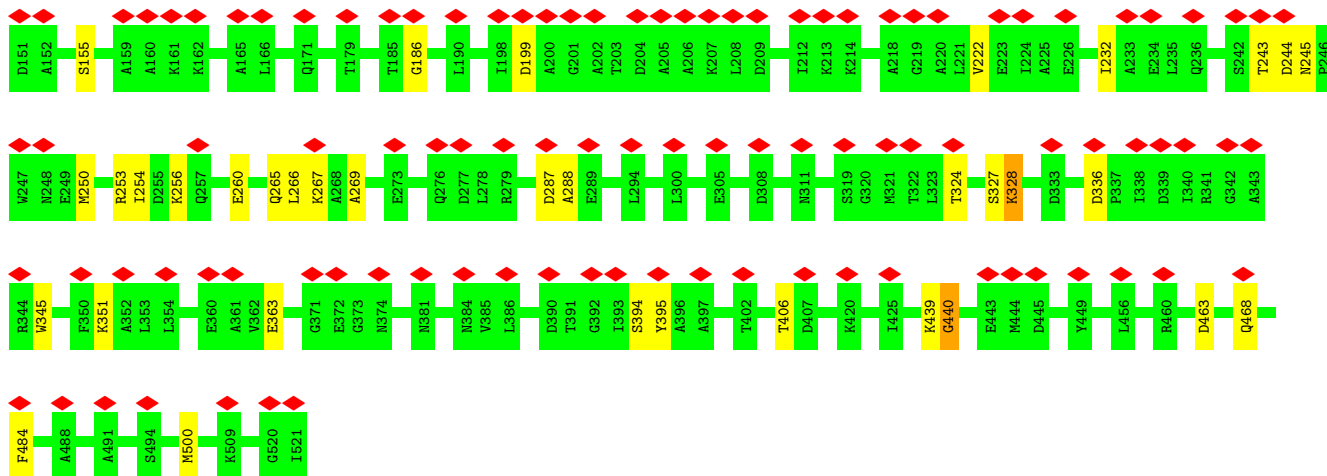


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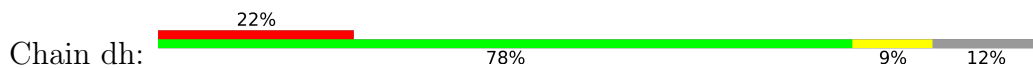


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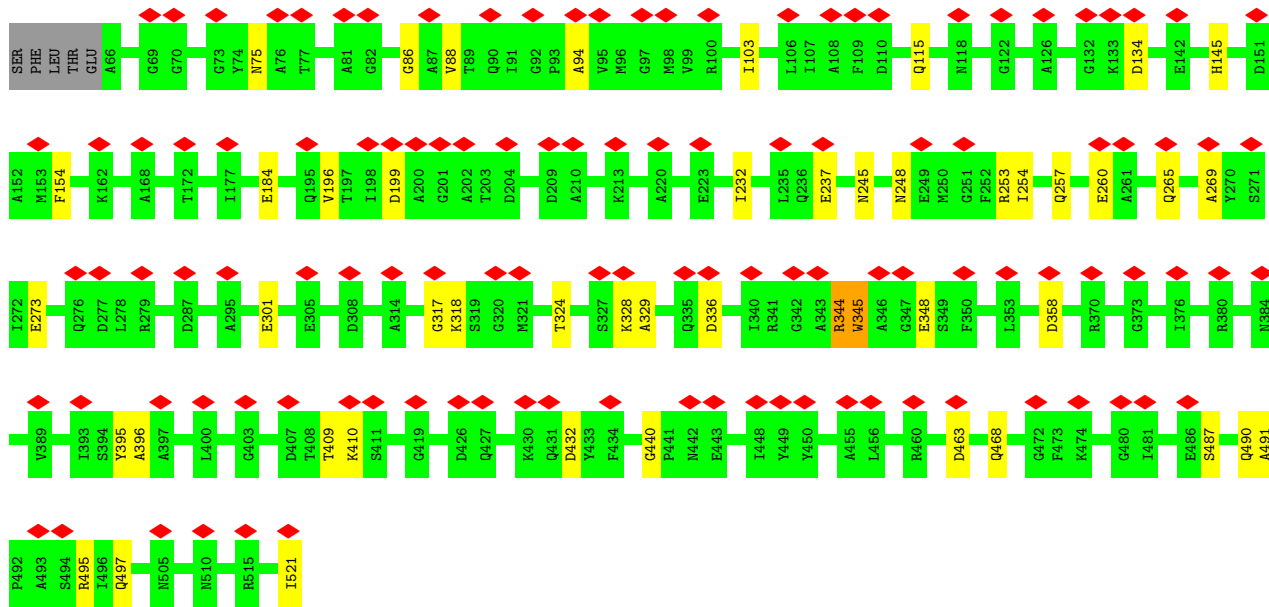




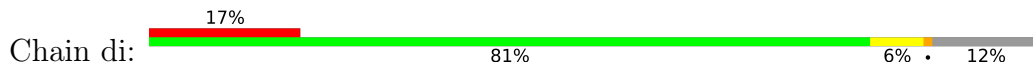
● Molecule 1: Major capsid protein



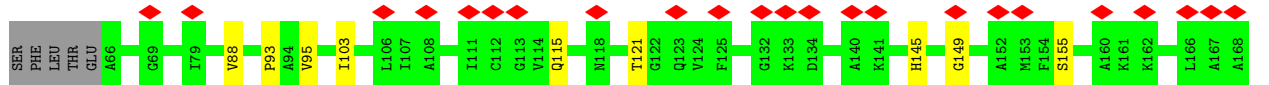
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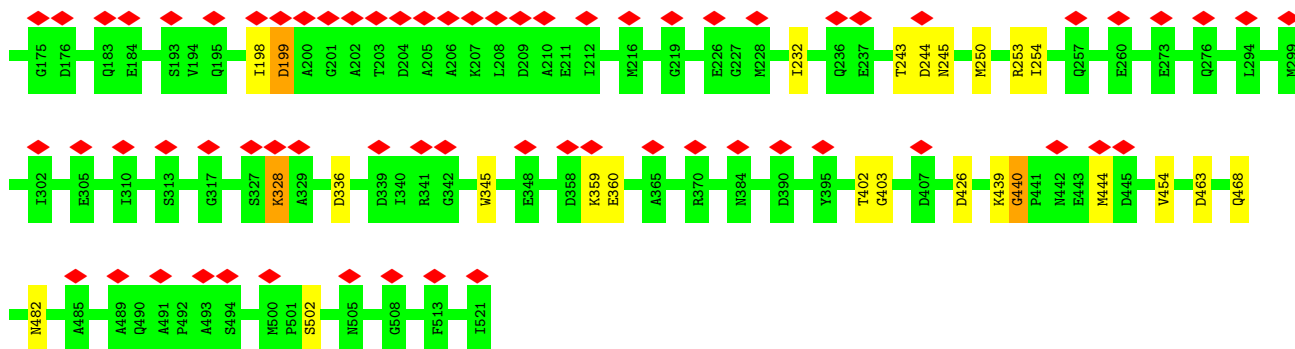


● Molecule 1: Major capsid protein

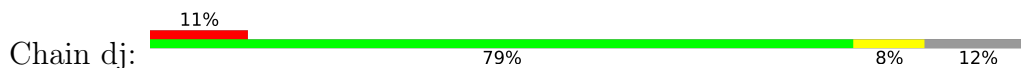


MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	LYS	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLU	GLY	LEU	PRO	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLN	GLU	LYS	ASP	PHE	THR	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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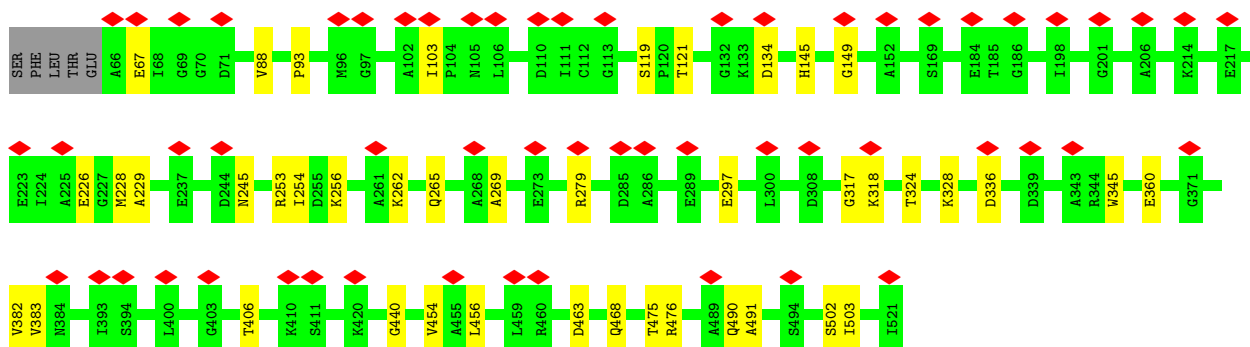




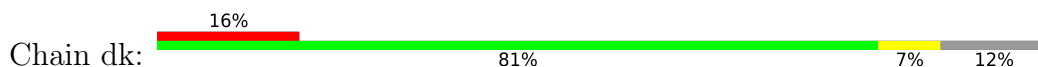
• Molecule 1: Major capsid protein



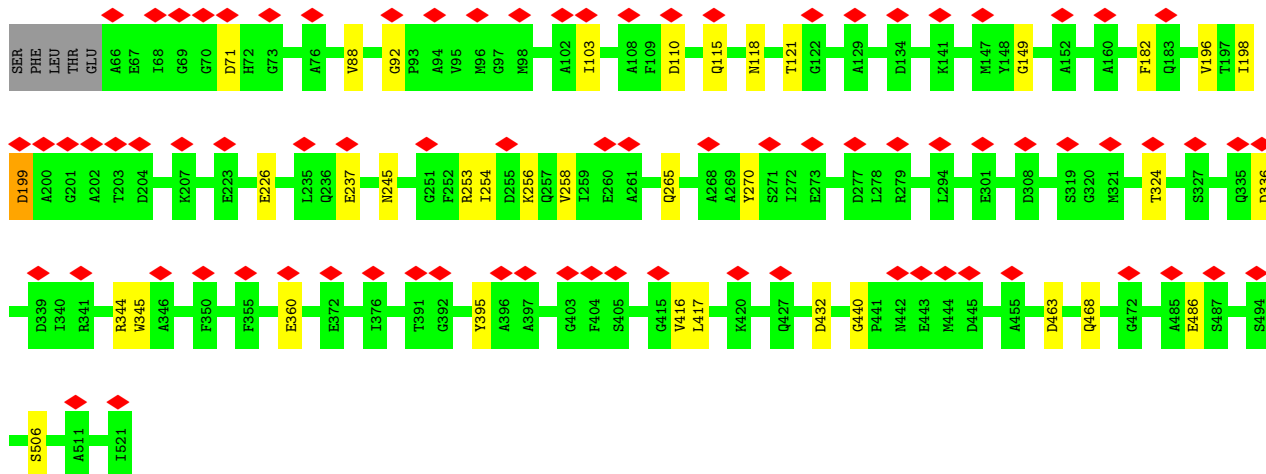
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	ASN	TRP	LYS	PRO	LEU	GLY	GLY	PRO	GLN	ALA	ILE	ILE	ALA	LYS	PHE	GLU	ASN	GLN	GLY	LYS	ASP	PHE	GLN	THR	PRO	GLU	TYR	LYS	ASP	GLY	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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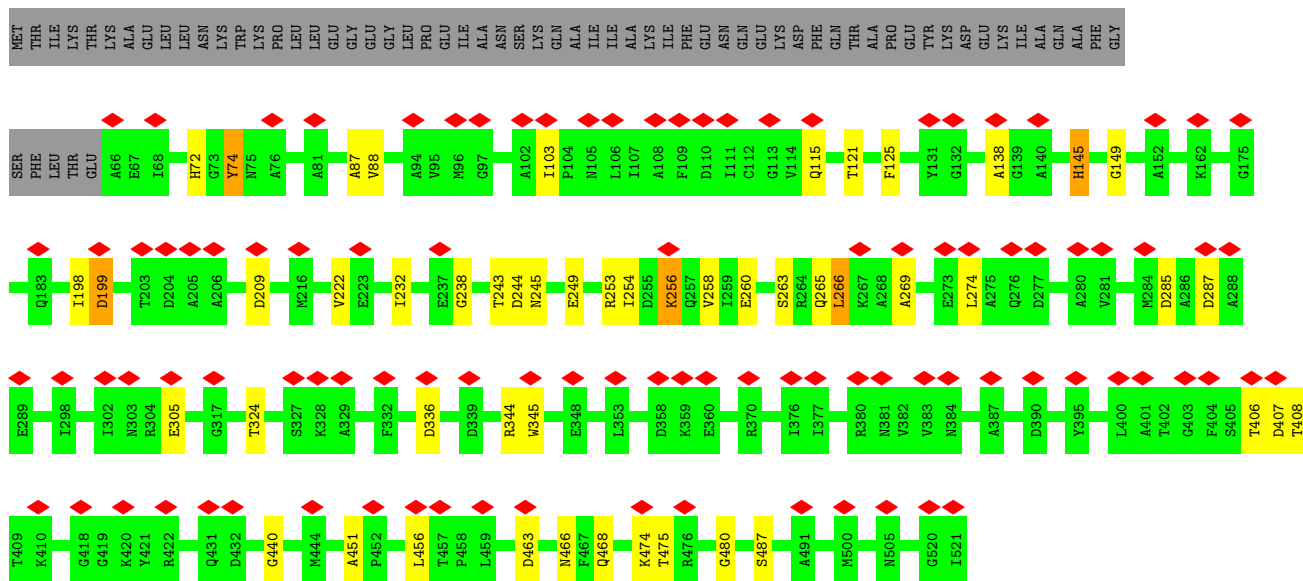
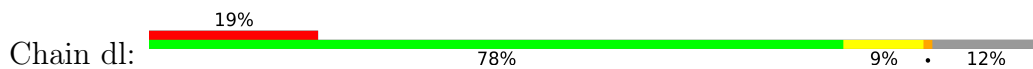
• Molecule 1: Major capsid protein



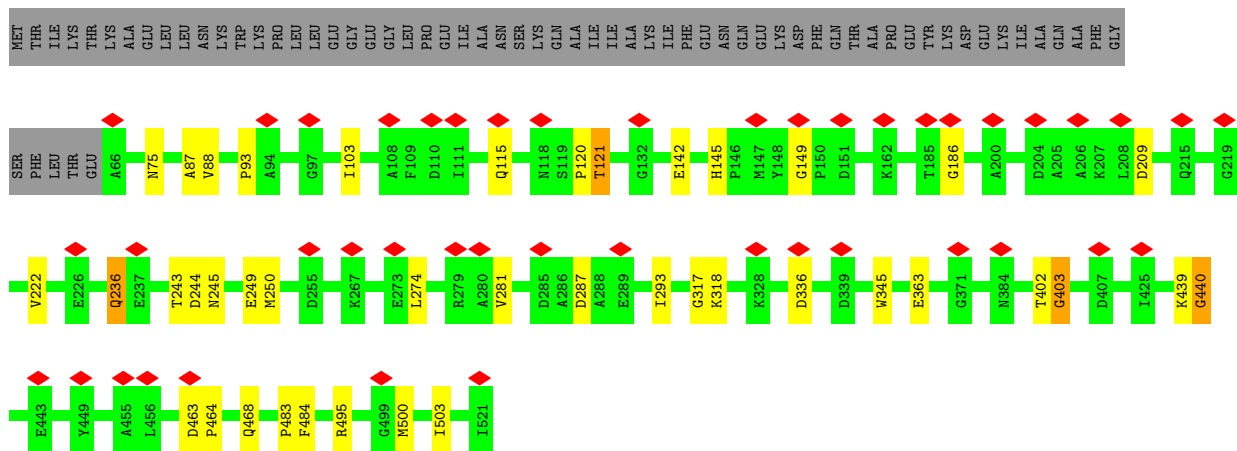
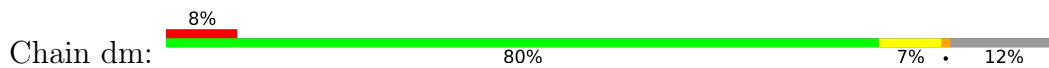
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	ASN	TRP	LYS	PRO	LEU	GLY	GLY	PRO	GLN	ALA	ILE	ILE	ALA	LYS	PHE	GLU	ASN	GLN	GLY	LYS	ASP	PHE	GLN	THR	PRO	GLU	TYR	LYS	ASP	GLY	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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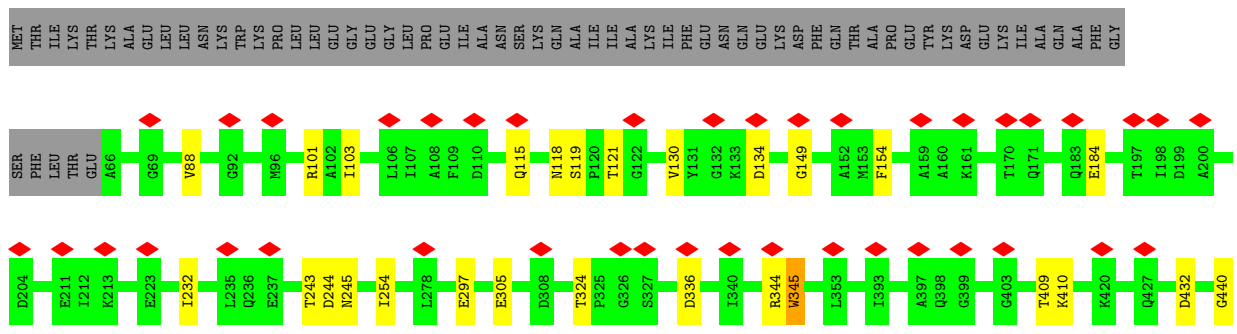
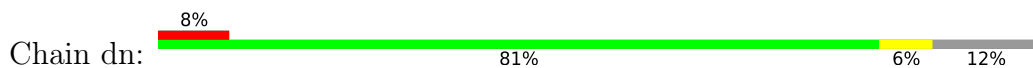
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

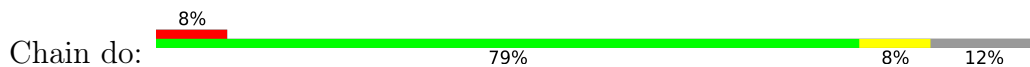


• Molecule 1: Major capsid protein

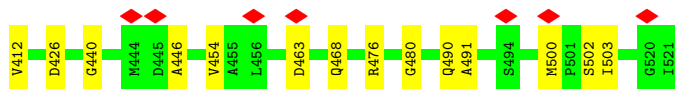
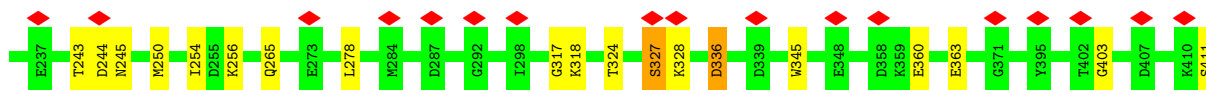
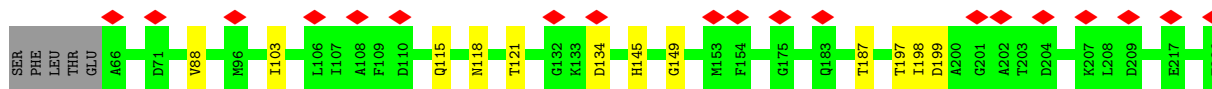




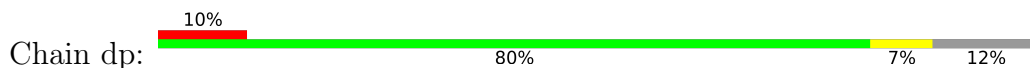
• Molecule 1: Major capsid protein



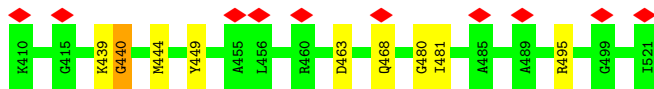
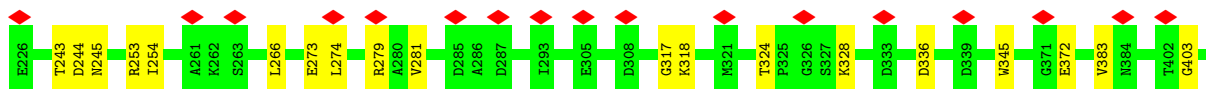
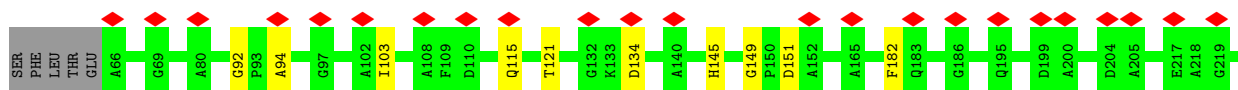
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	LYS	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLY	GLU	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	ALA	ILE	PHE	GLU	GLU	ASN	GLN	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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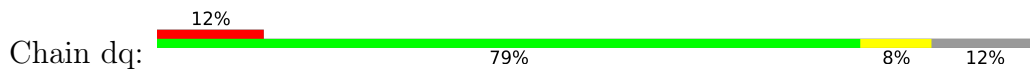
• Molecule 1: Major capsid protein



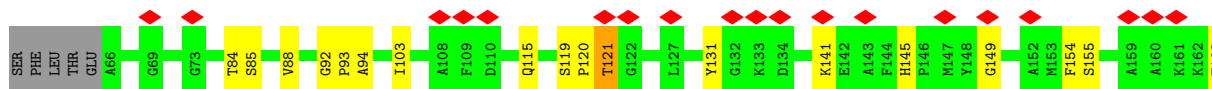
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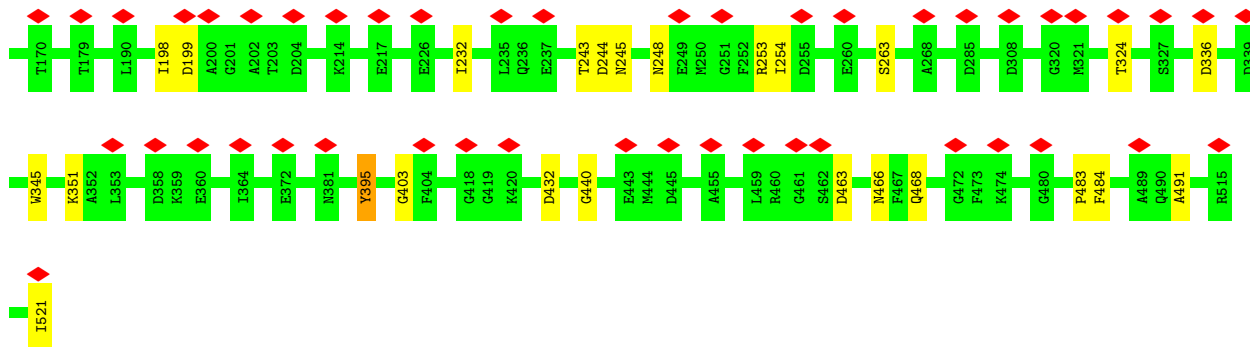


• Molecule 1: Major capsid protein

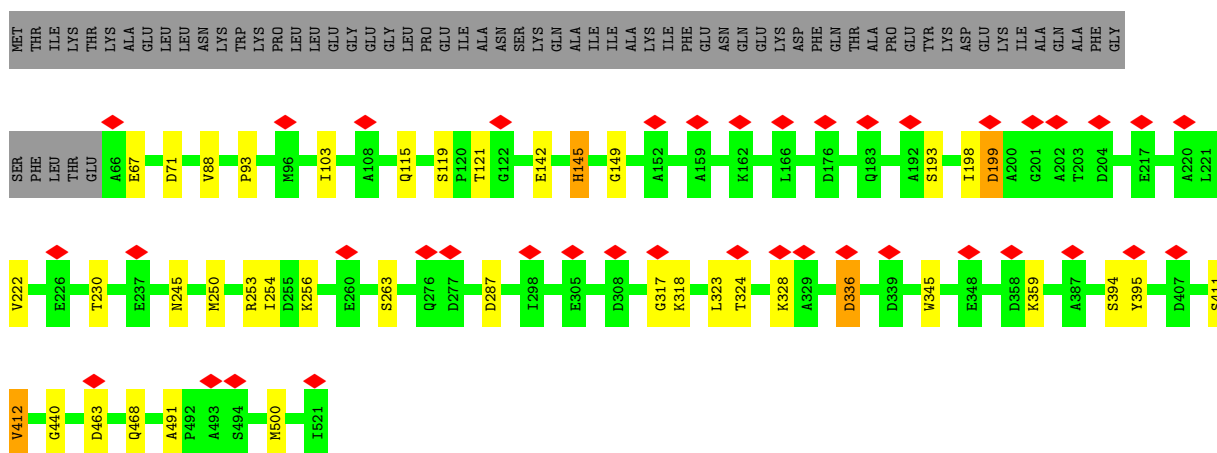
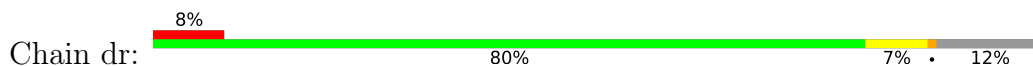


MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	LYS	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLY	GLU	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLU	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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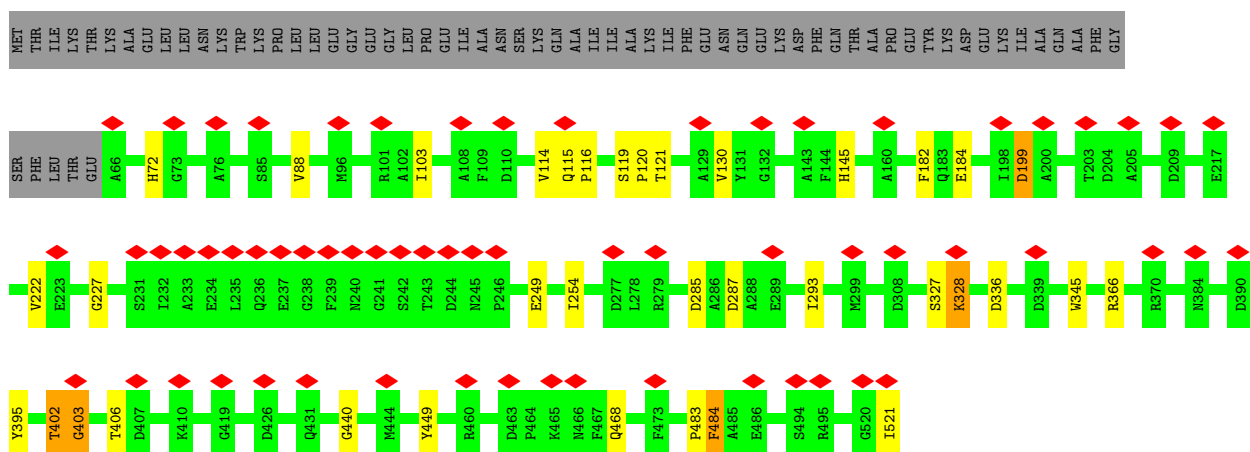
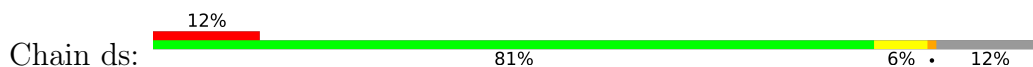




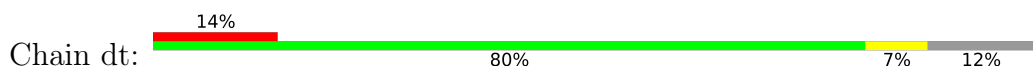
• Molecule 1: Major capsid protein

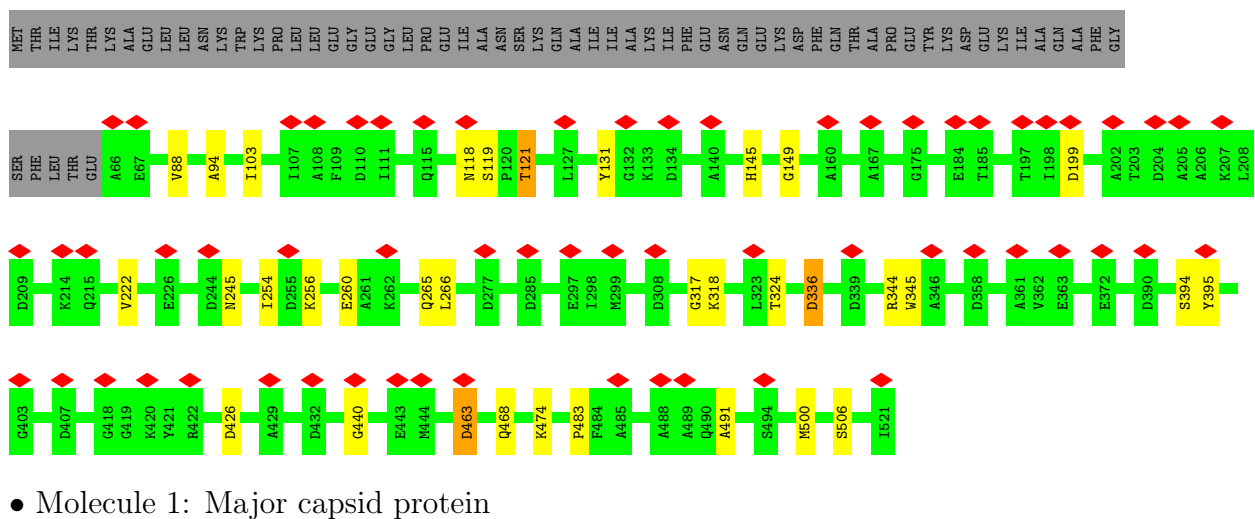
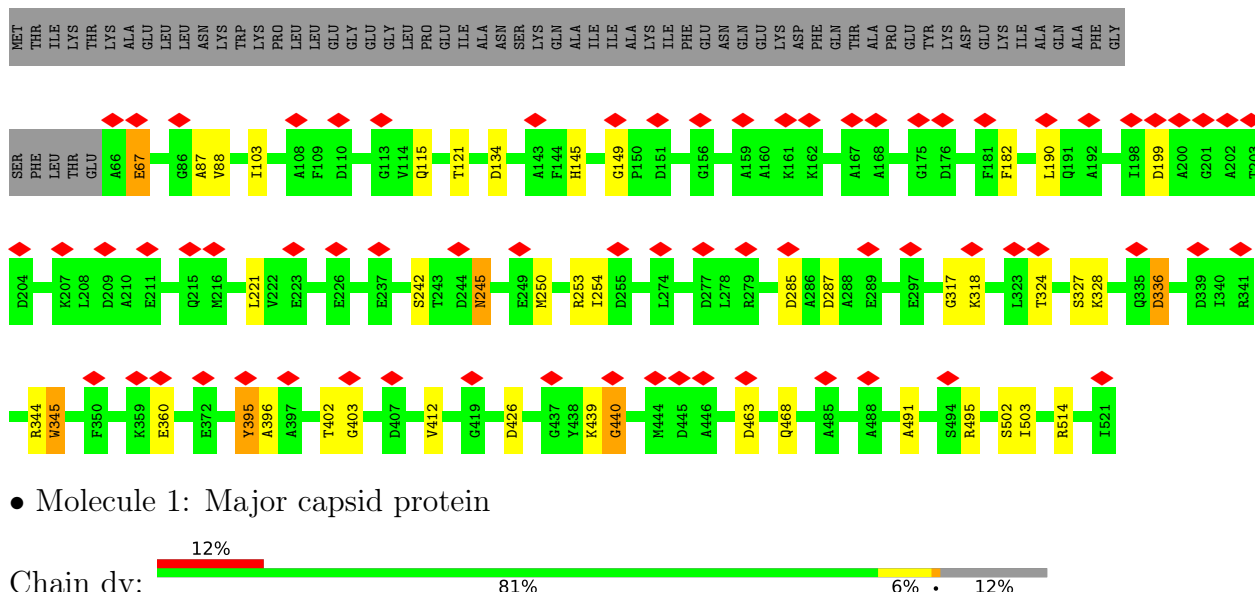
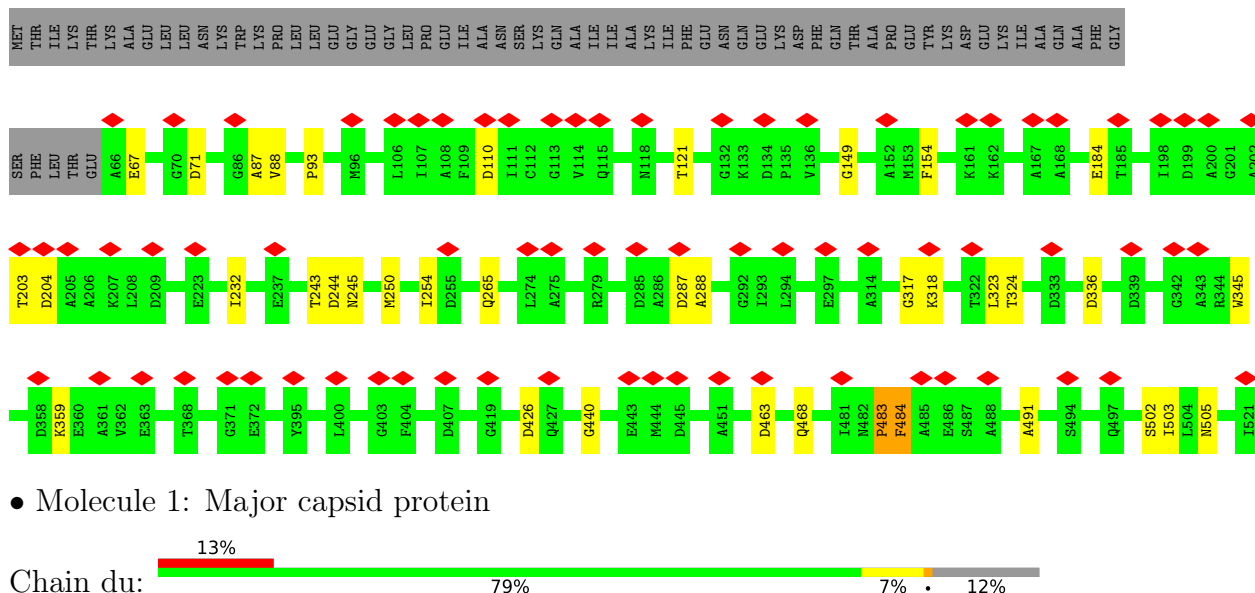


• Molecule 1: Major capsid protein

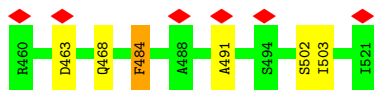


• Molecule 1: Major capsid protein

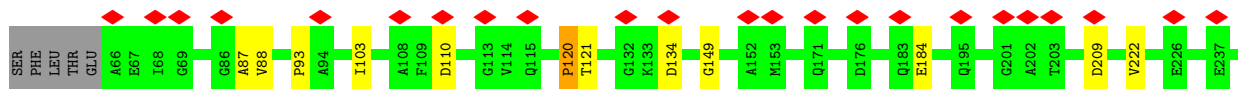
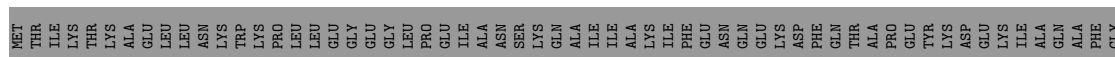
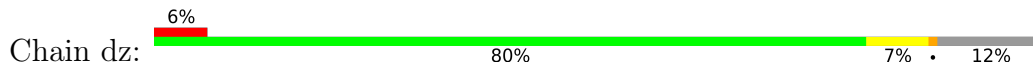




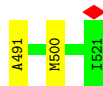
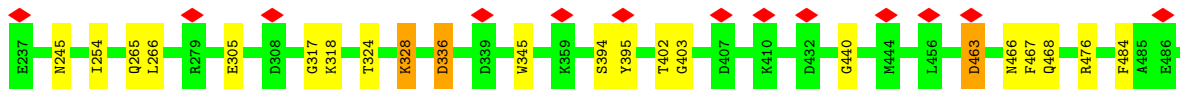
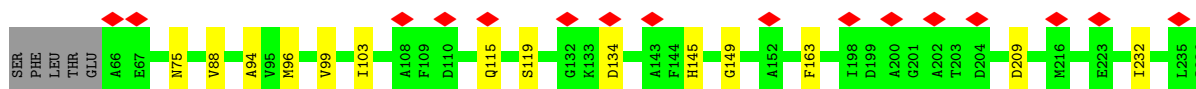
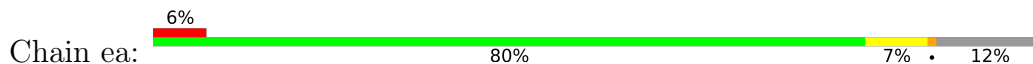




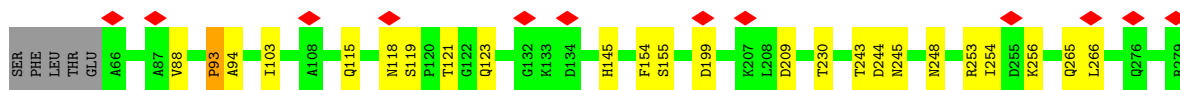
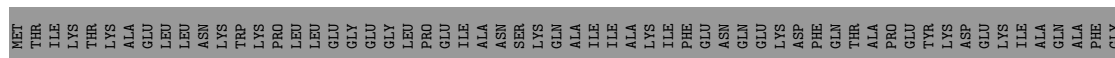
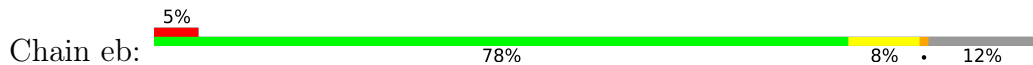
• Molecule 1: Major capsid protein

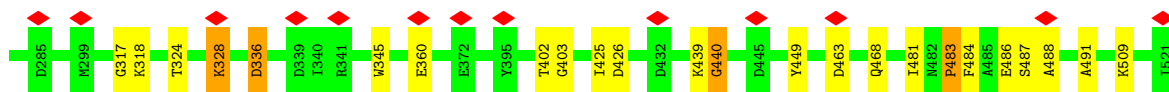


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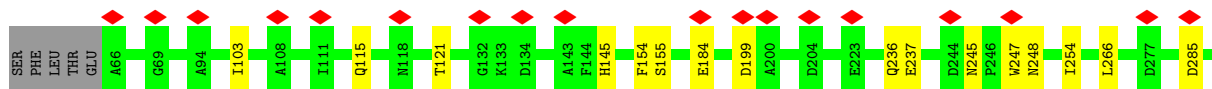
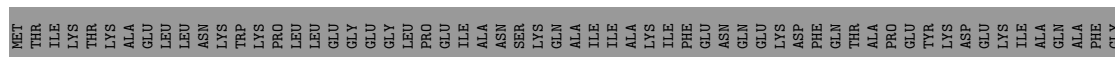
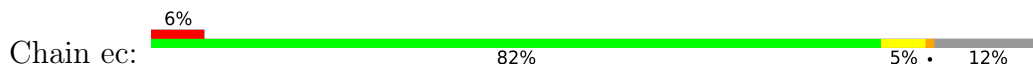


• Molecule 1: Major capsid protein

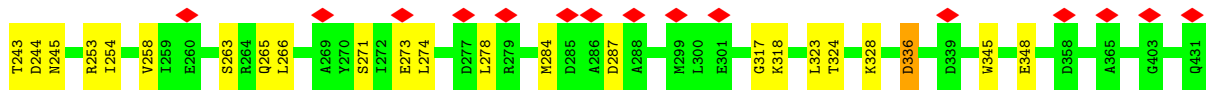
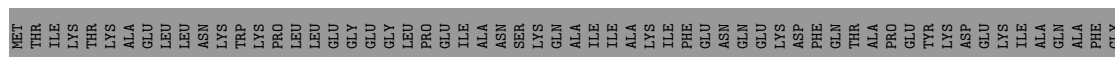
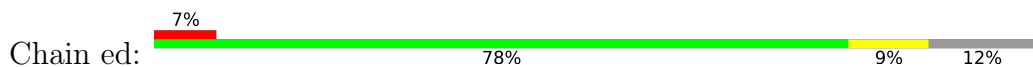




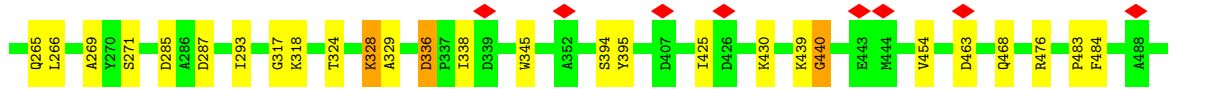
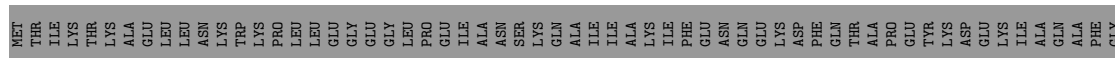
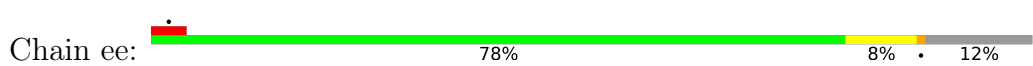
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

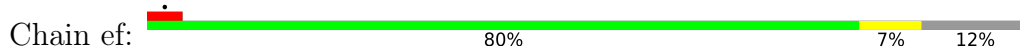


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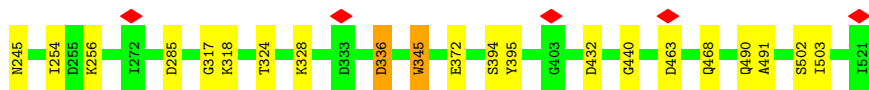




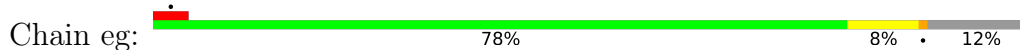
• Molecule 1: Major capsid protein



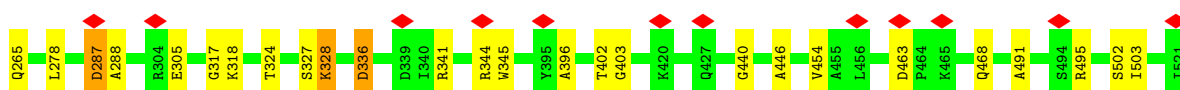
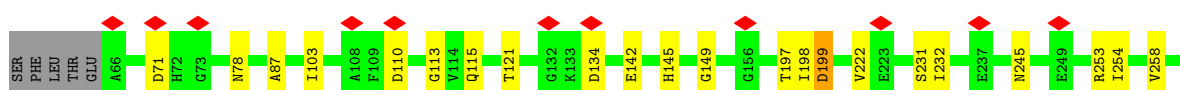
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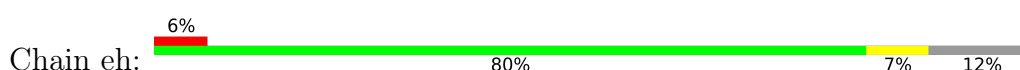
• Molecule 1: Major capsid protein



MET	THR	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	PRO	ILE	ALA	ASN	SER	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	LYS	ASP	PHE	GLN	THR	ALA	PRO	PRO	GLU	TYR	LYS	ASP	GLU	ILE	ALA	GLN	ALA	PHE	ALA	GLY
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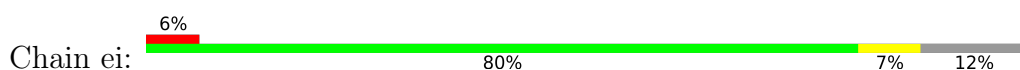
• Molecule 1: Major capsid protein



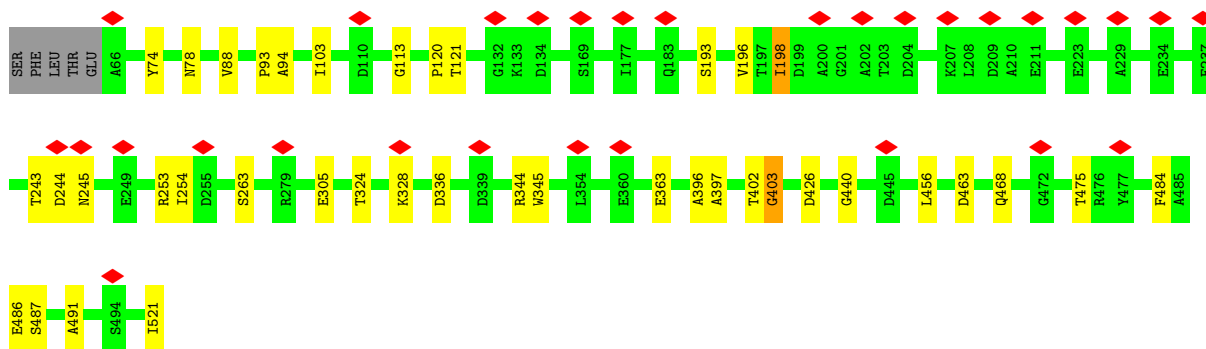
MET	THR	ILE	LYS	THR	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	LYS	ASP	PHE	GLN	THR	ALA	PRO	PRO	GLU	TYR	LYS	ASP	GLU	ILE	ALA	GLN	ALA	PHE	ALA	GLY
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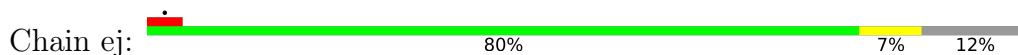
• Molecule 1: Major capsid protein



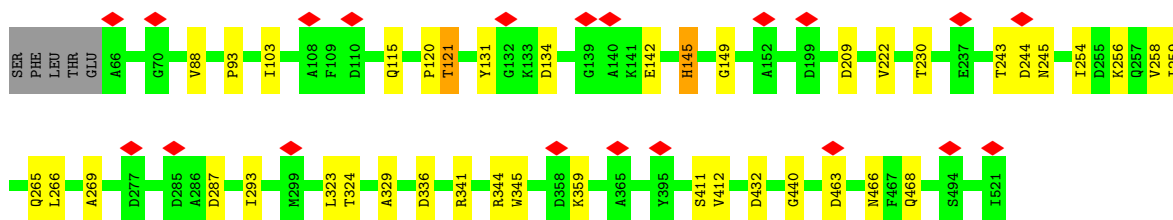
MET	THR	ILE	LYS	THR	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	PRO	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	LYS	ASP	PHE	GLN	THR	ALA	PRO	PRO	GLU	TYR	LYS	ASP	GLU	ILE	ALA	GLN	ALA	PHE	ALA	GLY
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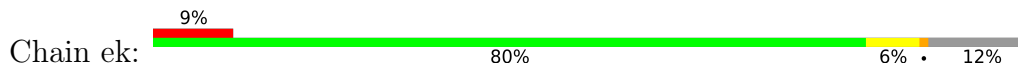
• Molecule 1: Major capsid protein



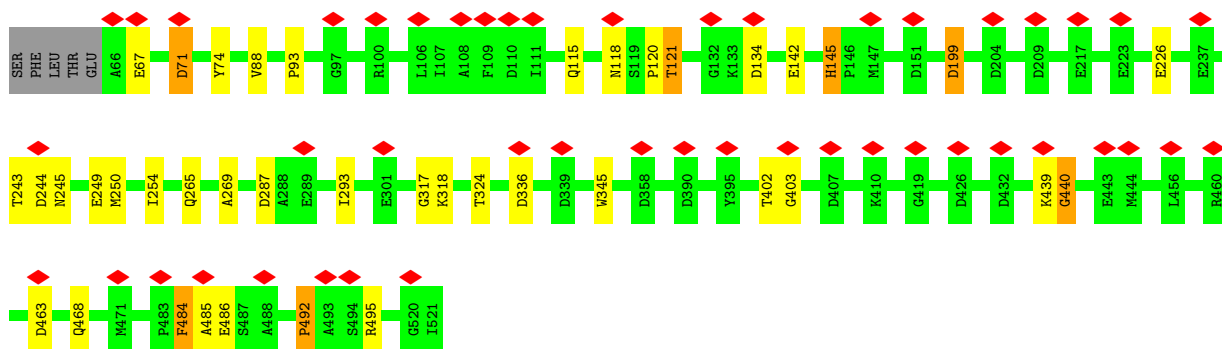
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	GLY	GLY	PRO	ILE	ALA	SER	LYS	GLN	ALA	ILE	ILE	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	ASP	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	ILE	LYS	ALA	GLN	ALA	PHE	GLY
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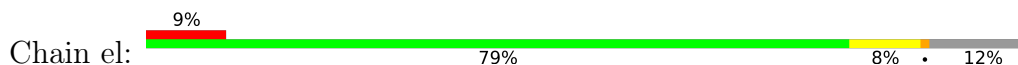
• Molecule 1: Major capsid protein



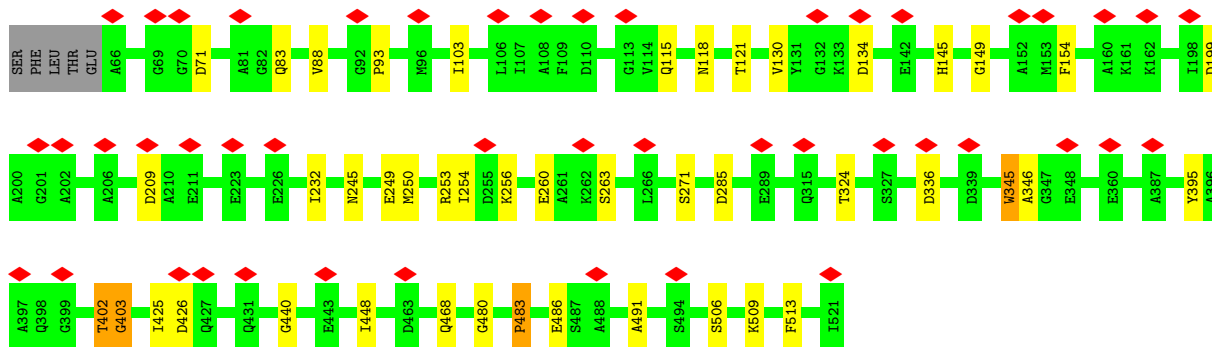
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	GLY	GLY	PRO	ILE	ALA	SER	LYS	GLN	ALA	ILE	ILE	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	ASP	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	ILE	LYS	ALA	GLN	ALA	PHE	GLY
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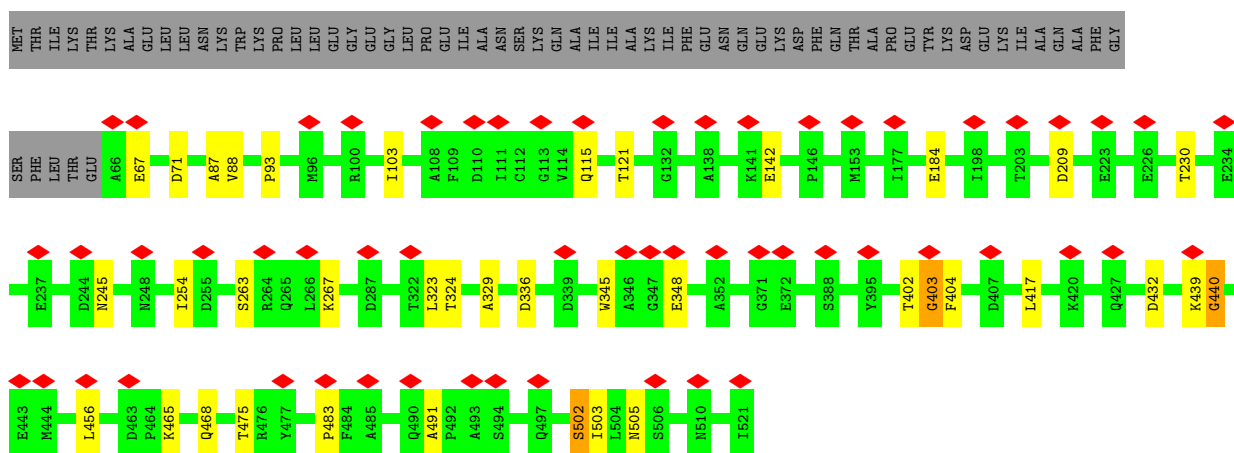
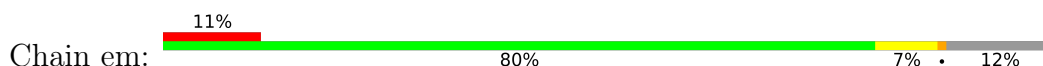
• Molecule 1: Major capsid protein



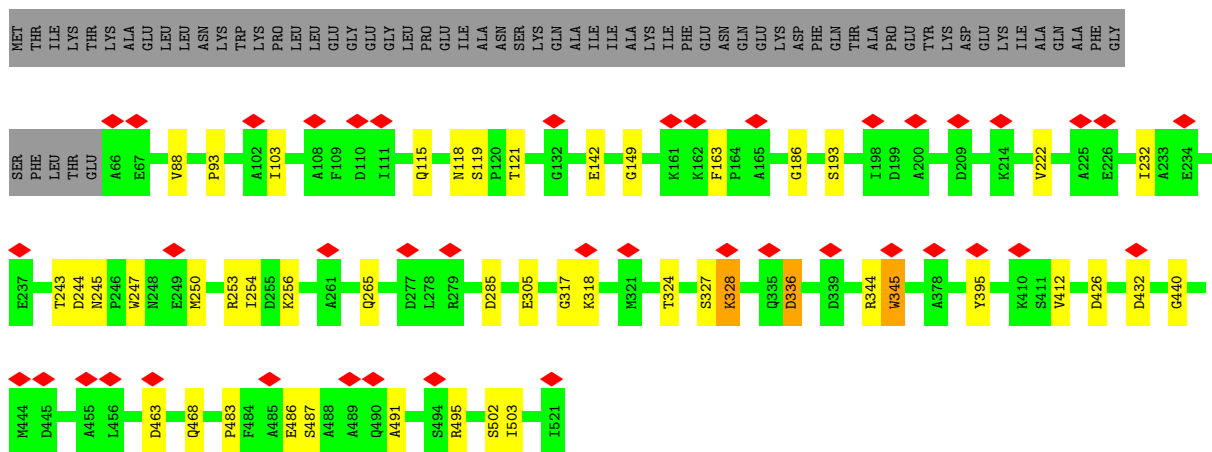
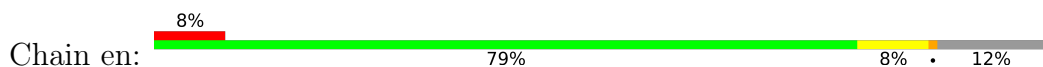
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	GLY	GLY	PRO	ILE	ALA	SER	LYS	GLN	ALA	ILE	ILE	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	ASP	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	ILE	LYS	ALA	GLN	ALA	PHE	GLY
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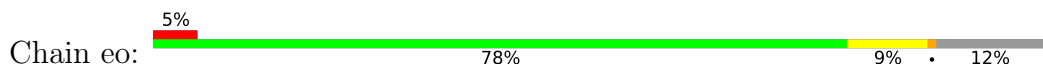
• Molecule 1: Major capsid protein

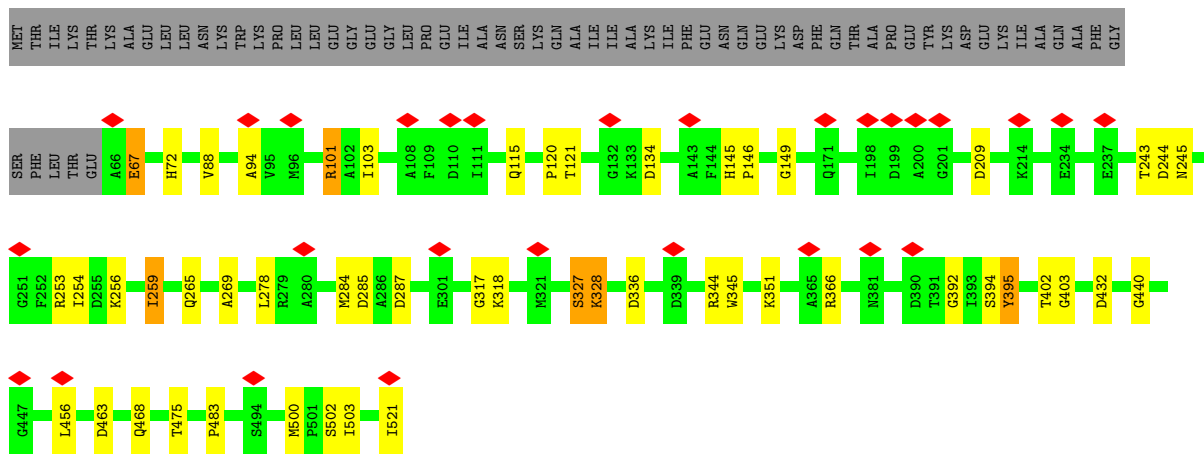


• Molecule 1: Major capsid protein

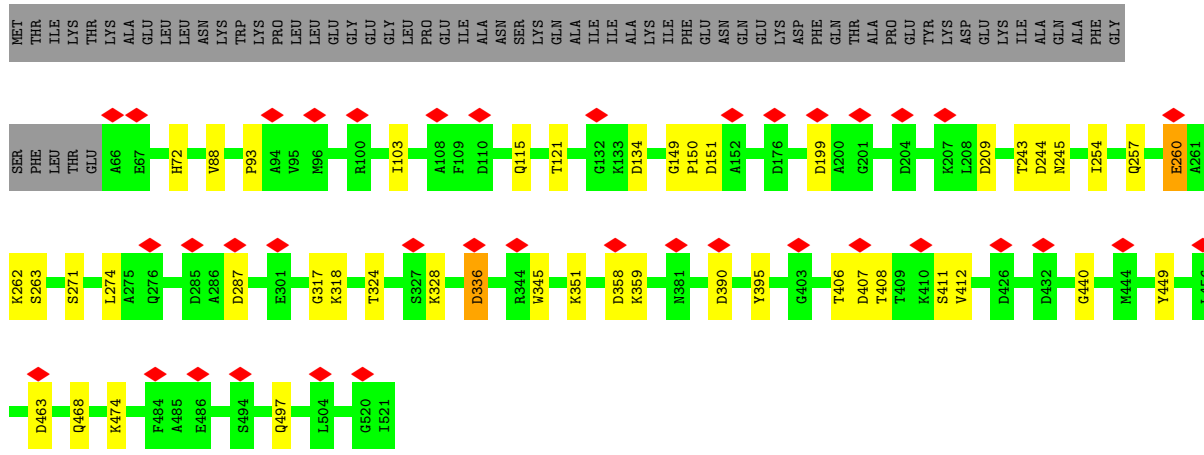
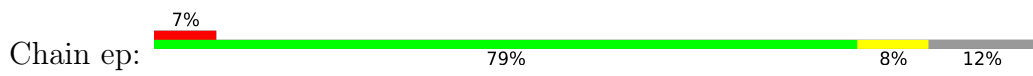


• Molecule 1: Major capsid protein

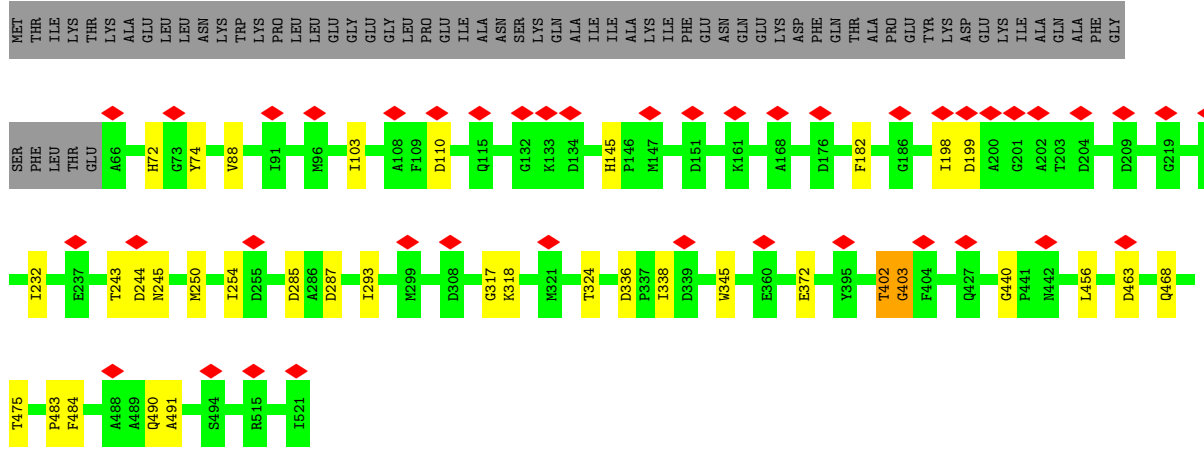
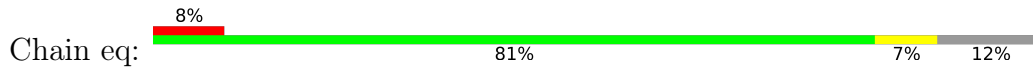




• Molecule 1: Major capsid protein



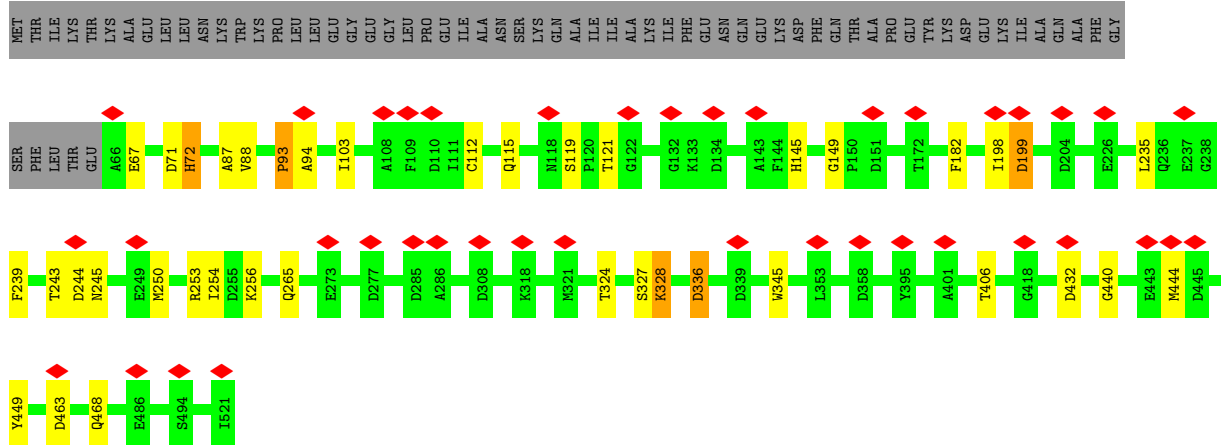
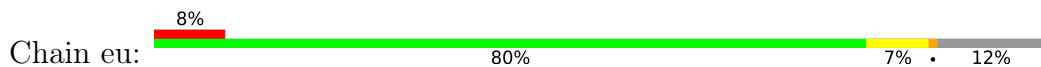
• Molecule 1: Major capsid protein



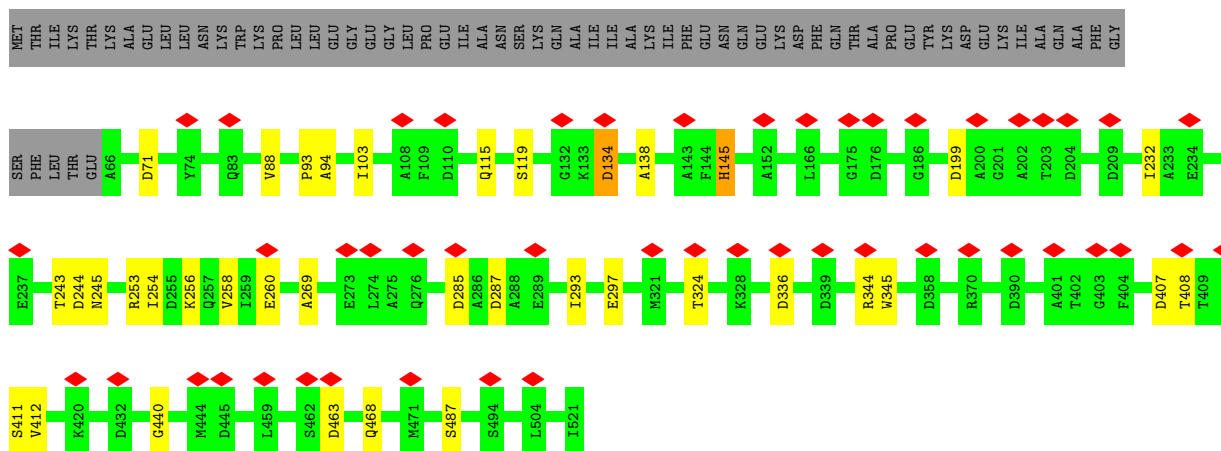
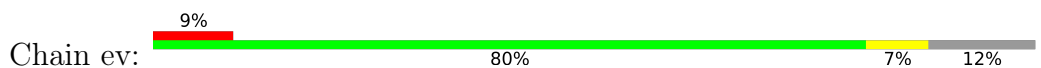
• Molecule 1: Major capsid protein



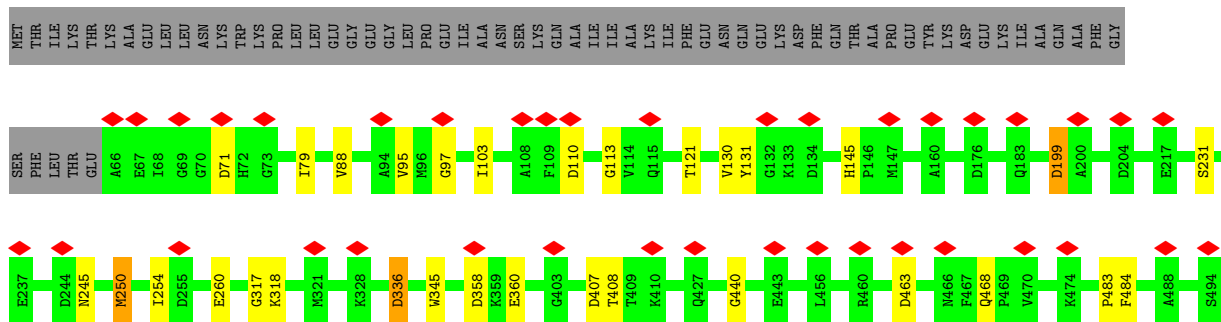
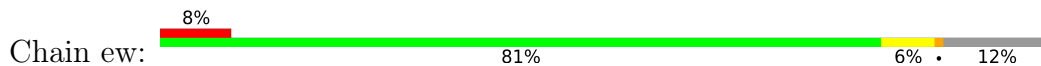
- Molecule 1: Major capsid protein

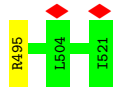


- Molecule 1: Major capsid protein

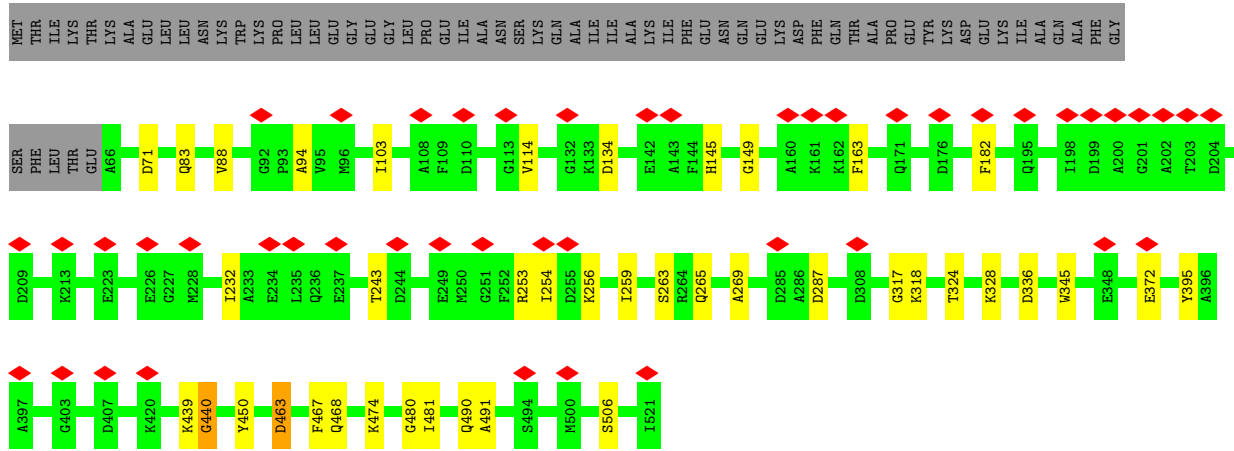
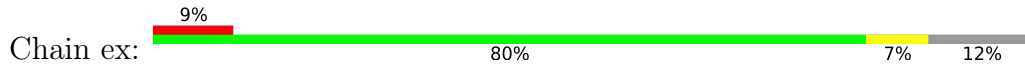


- Molecule 1: Major capsid protein

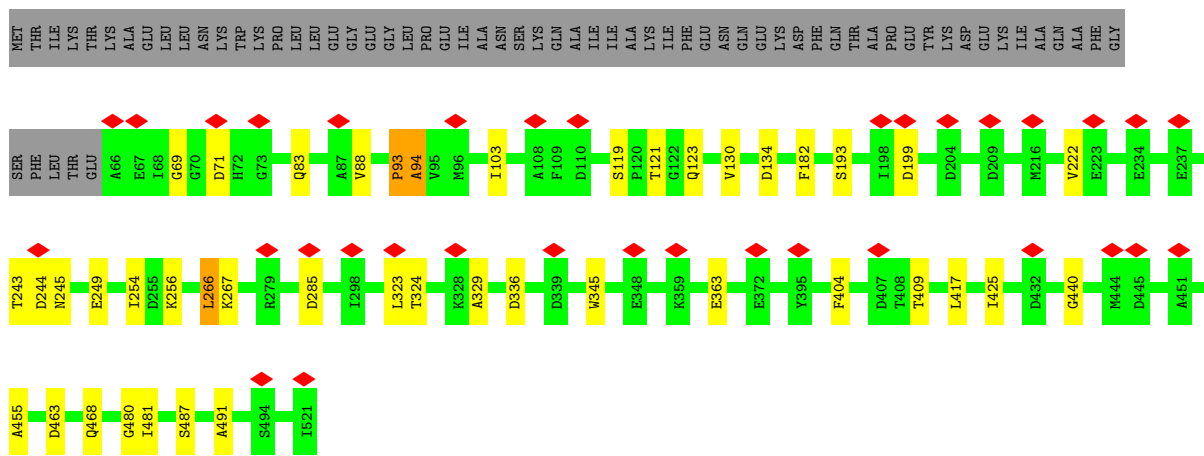
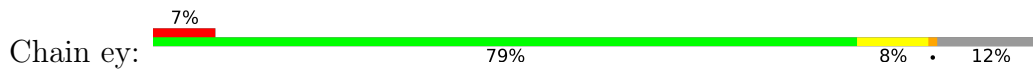




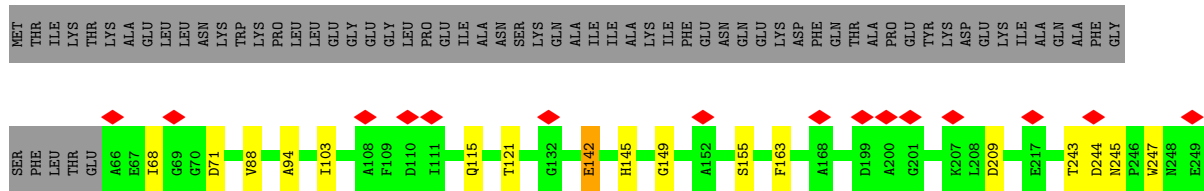
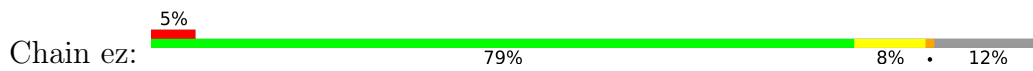
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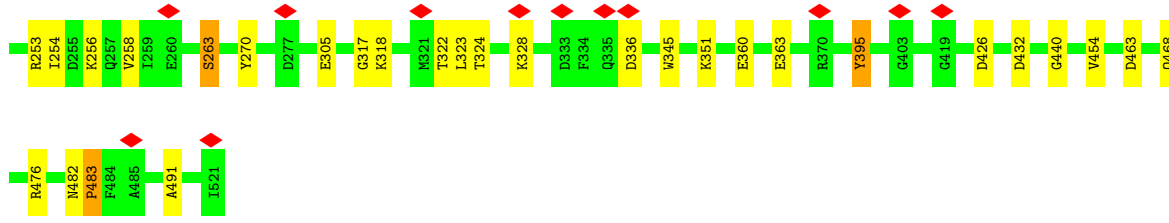


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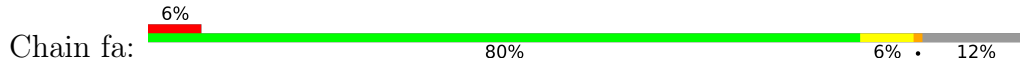


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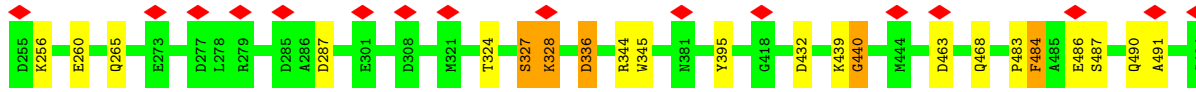
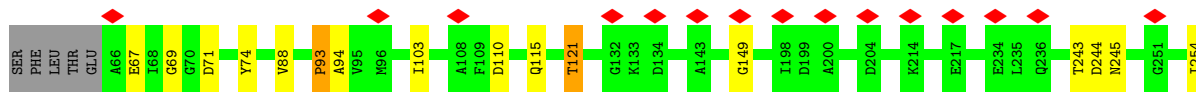




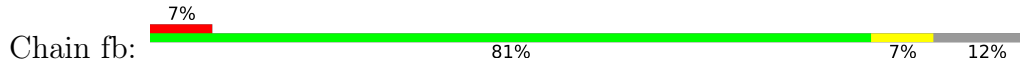
• Molecule 1: Major capsid protein



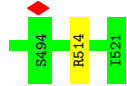
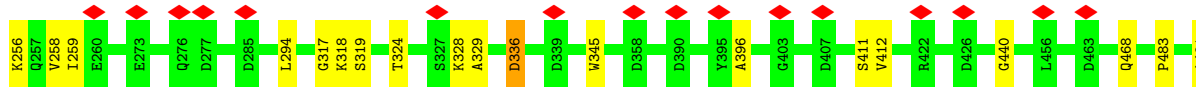
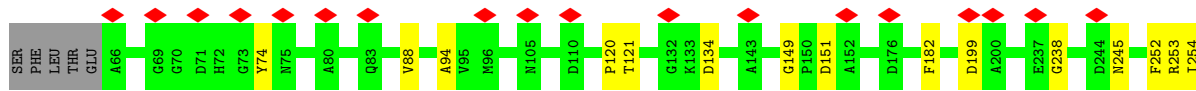
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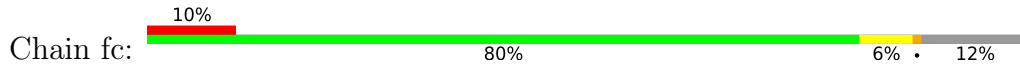
• Molecule 1: Major capsid protein



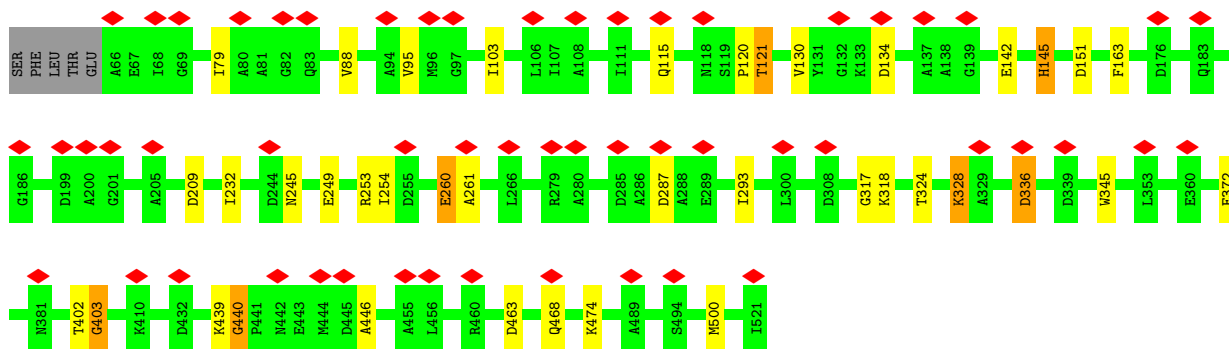
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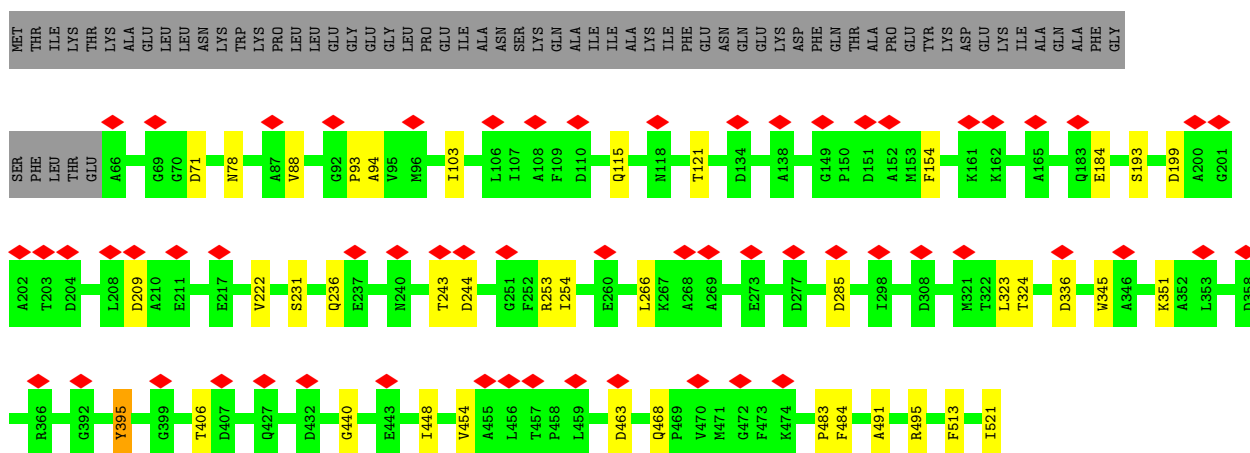
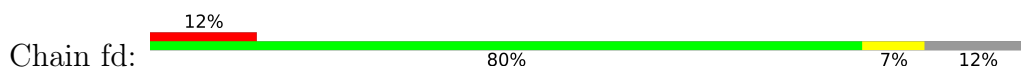
• Molecule 1: Major capsid protein



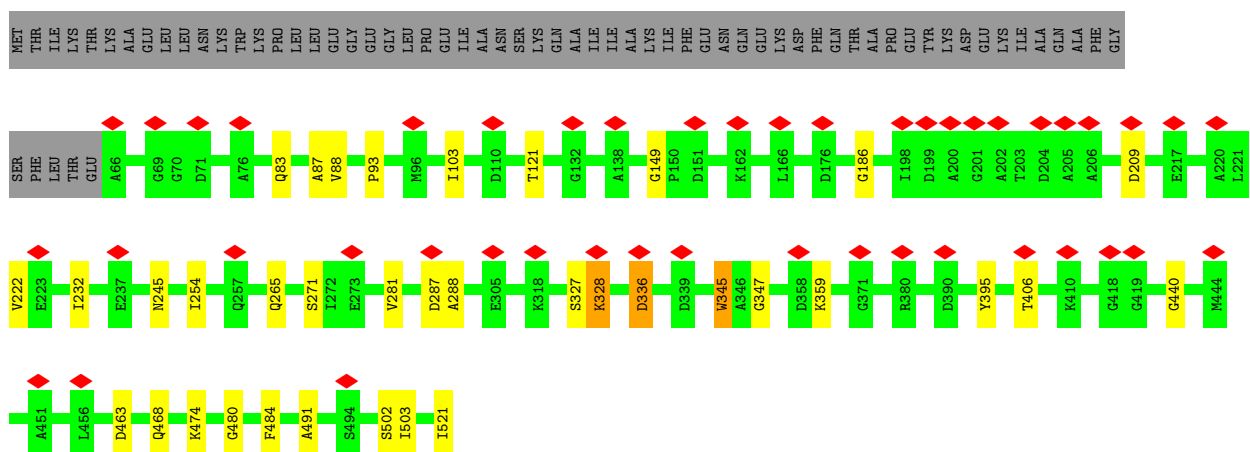
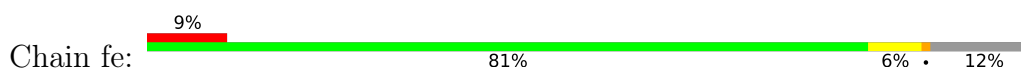
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• Molecule 1: Major capsid protein

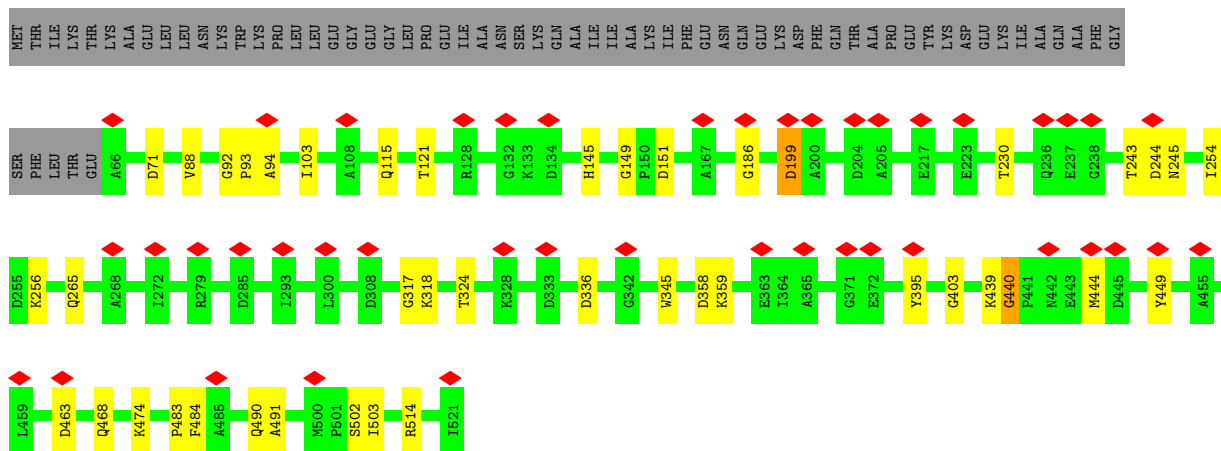


• Molecule 1: Major capsid protein

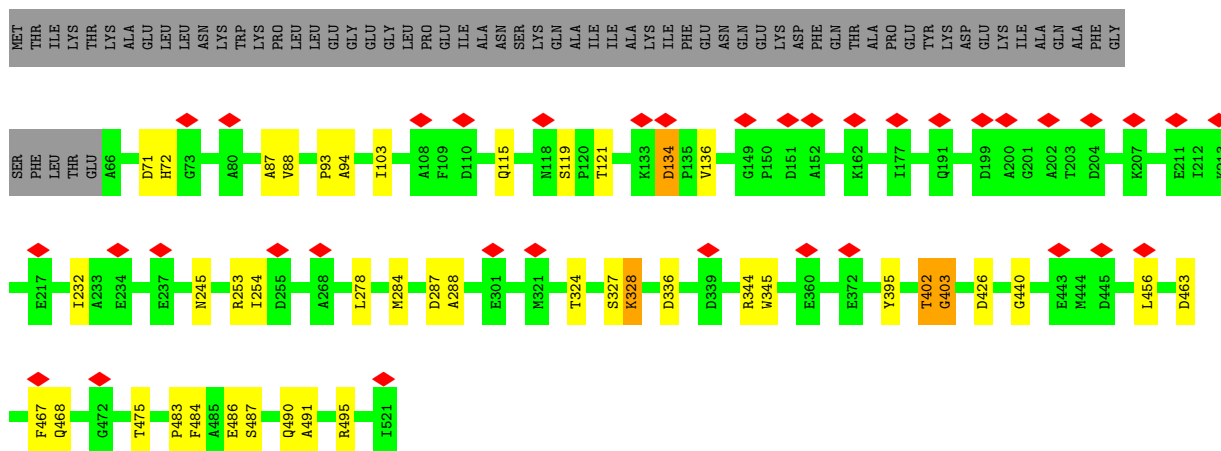
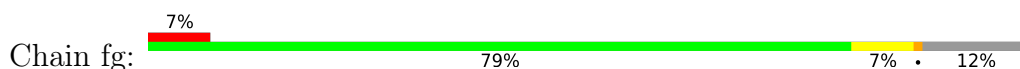


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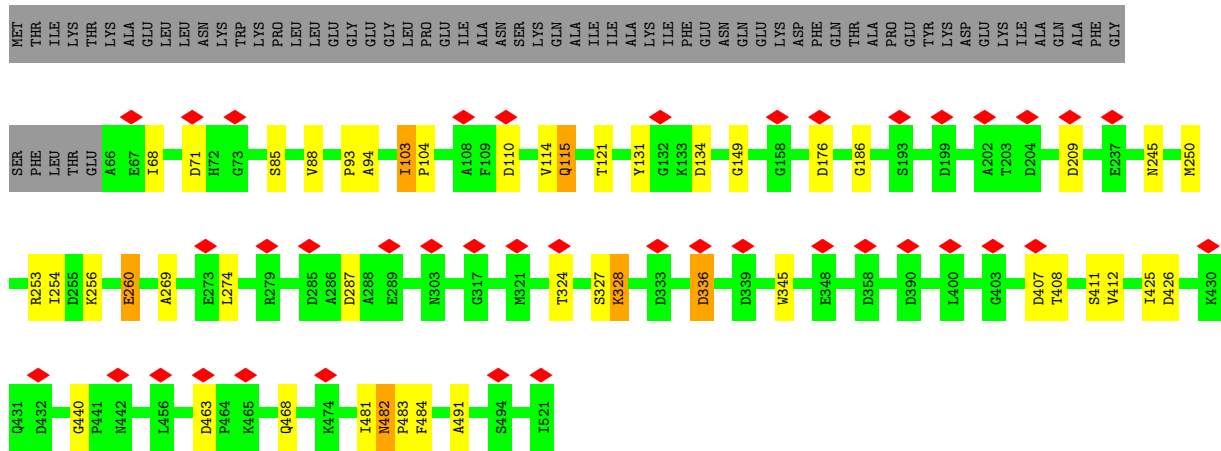
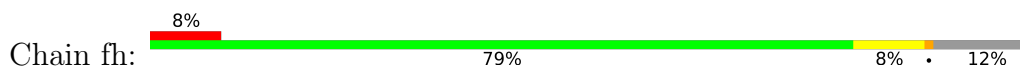




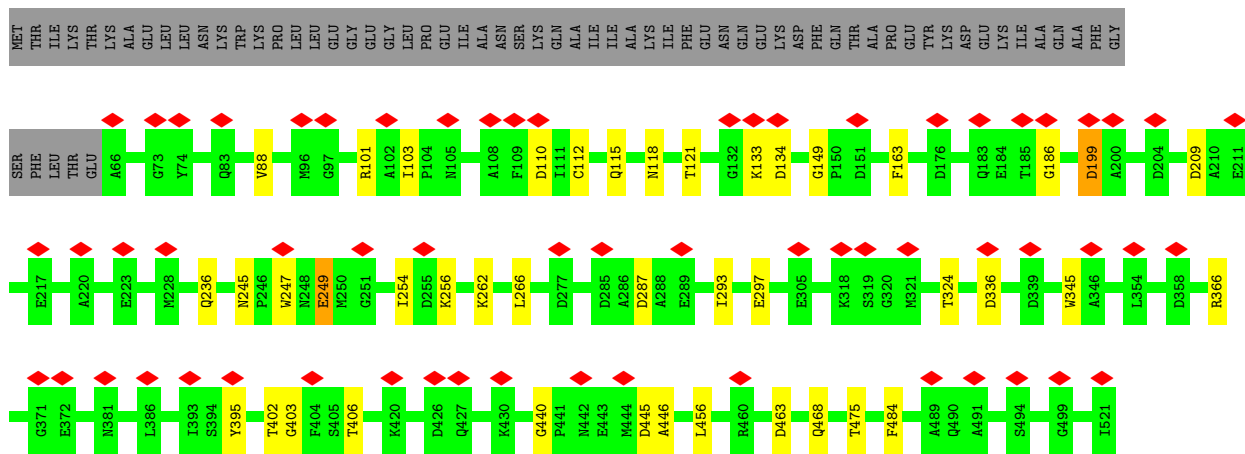
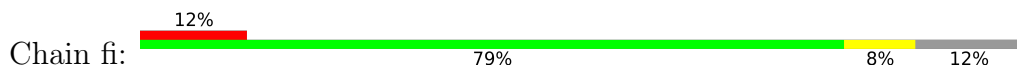
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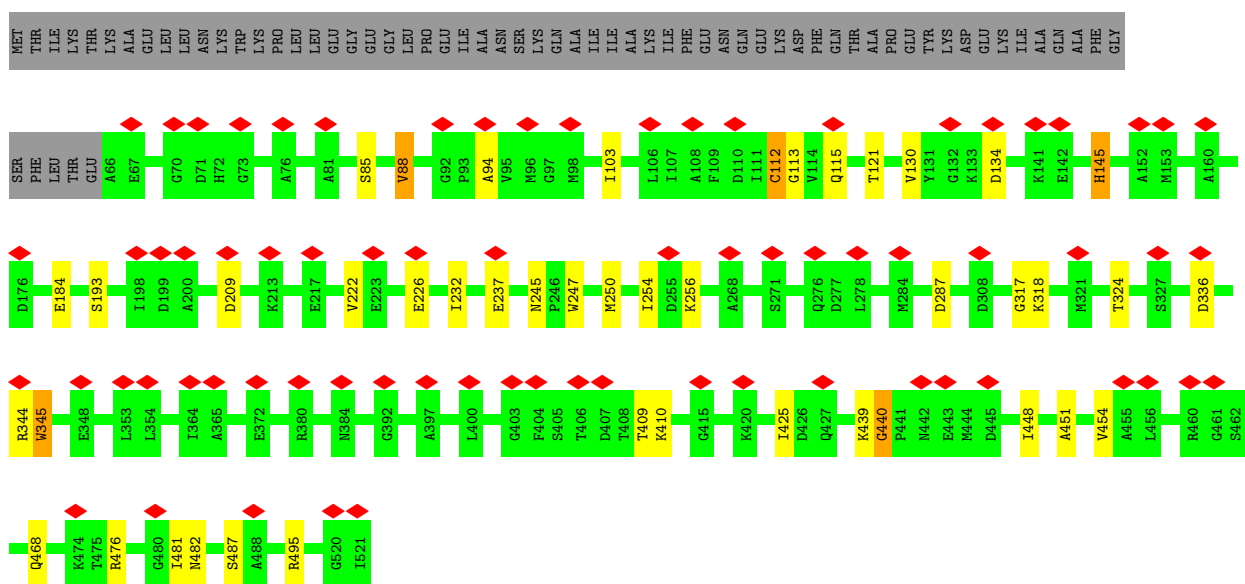
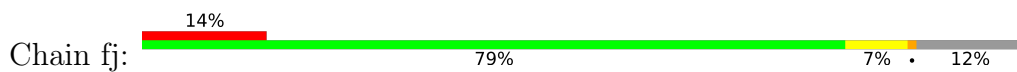
• Molecule 1: Major capsid protein



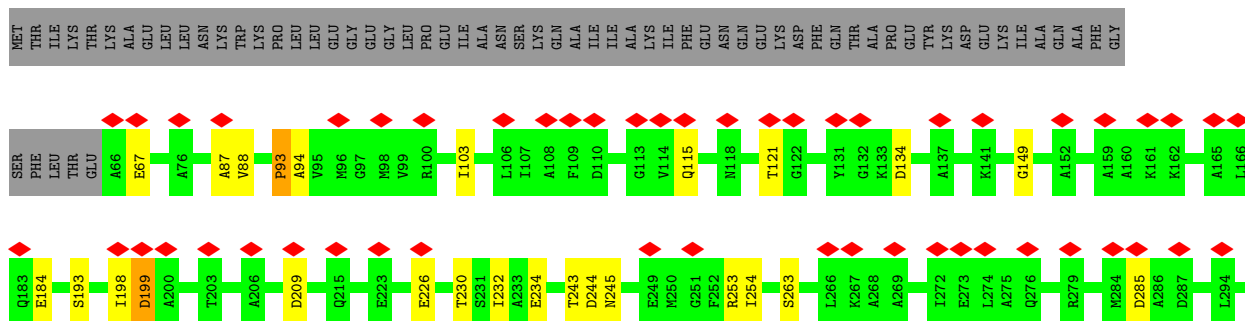
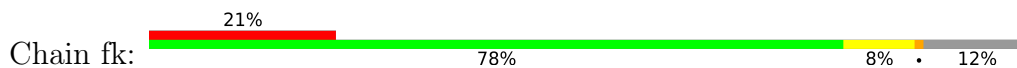
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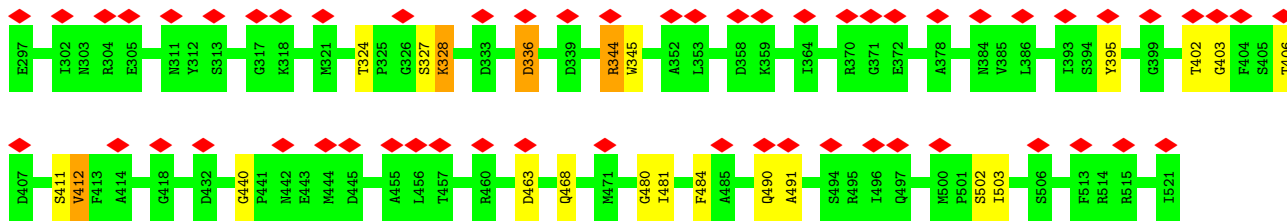


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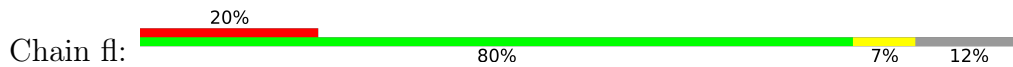


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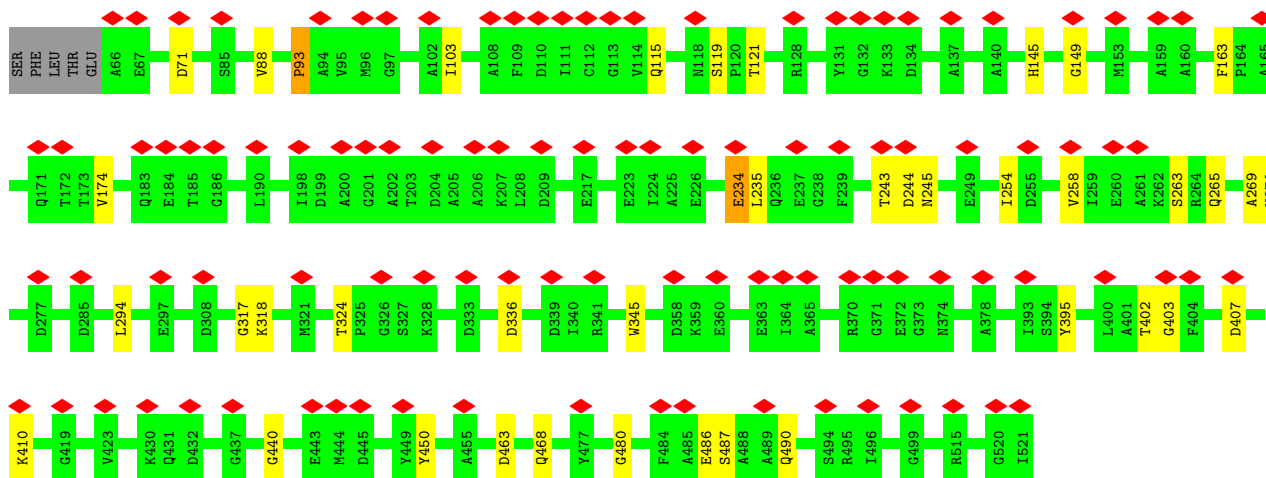




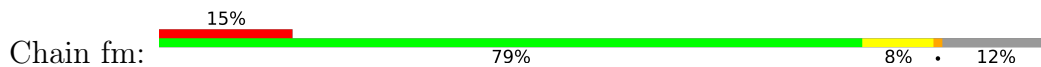
• Molecule 1: Major capsid protein



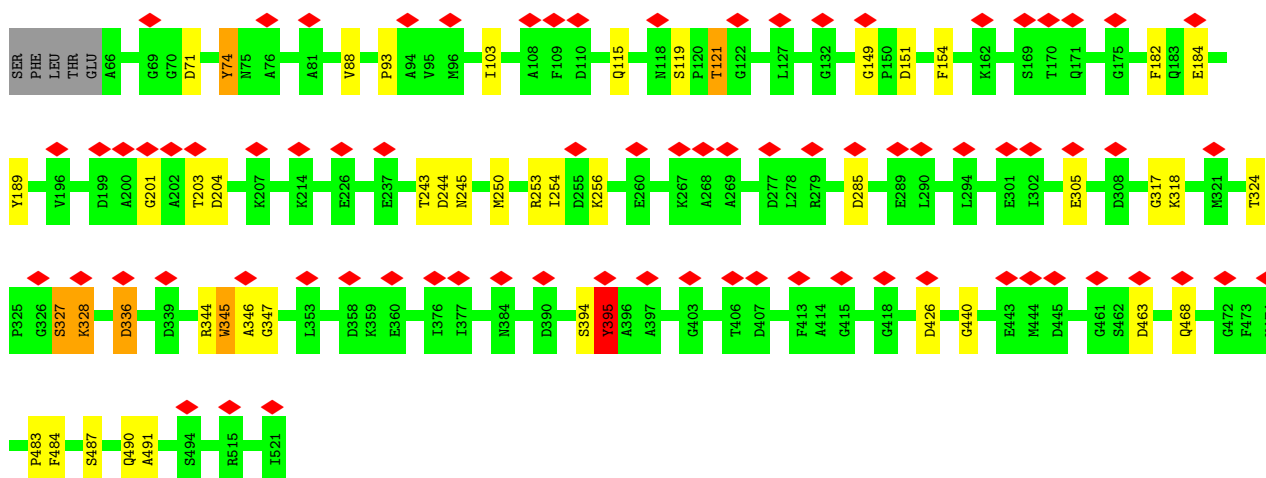
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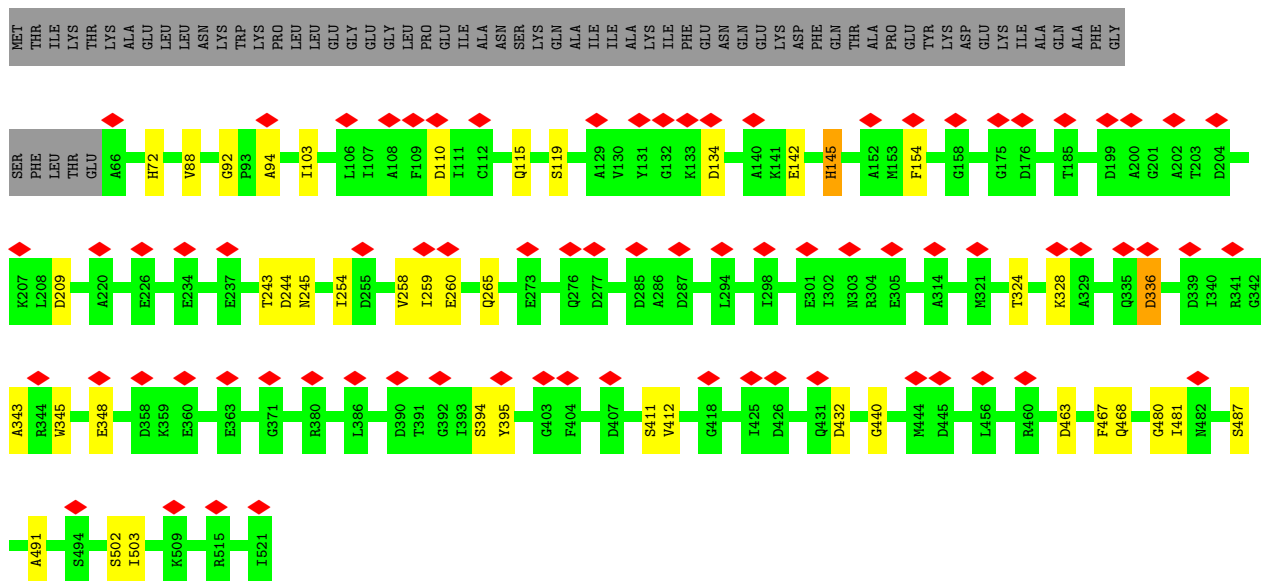
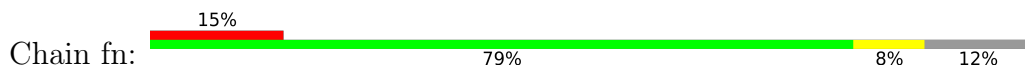
• Molecule 1: Major capsid protein



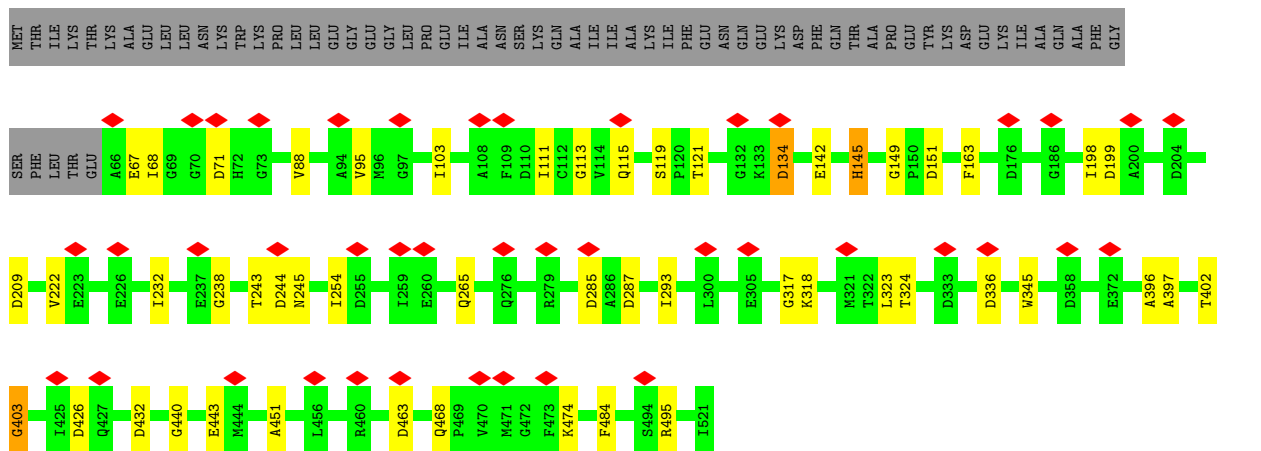
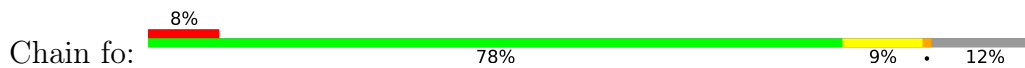
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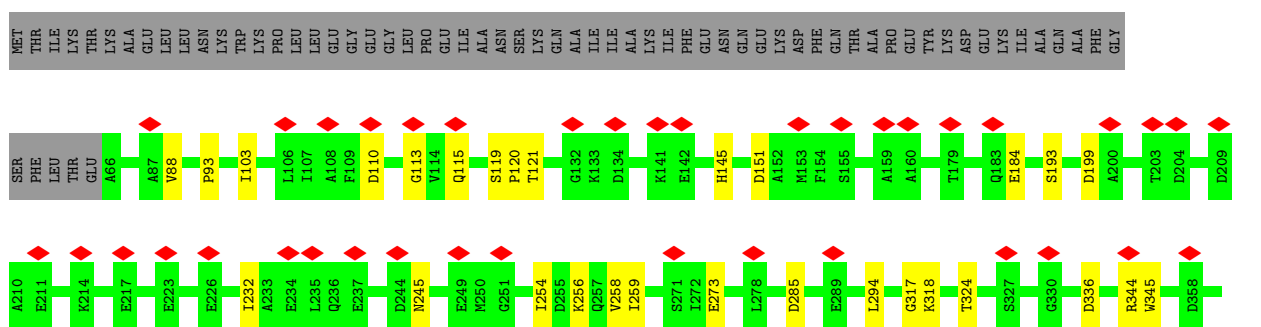
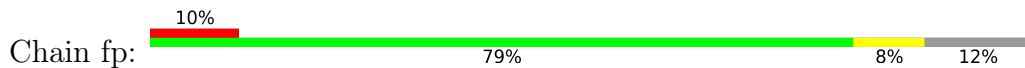
• Molecule 1: Major capsid protein

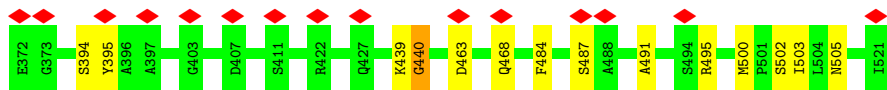


• Molecule 1: Major capsid protein

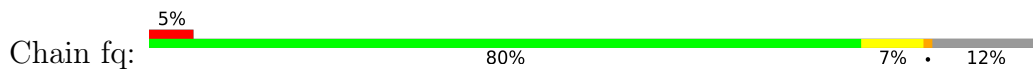


• Molecule 1: Major capsid protein

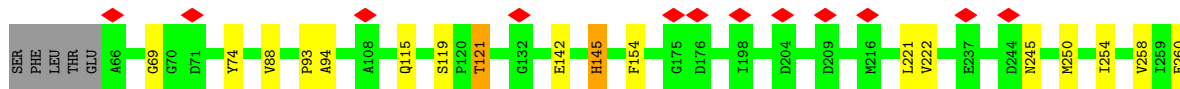




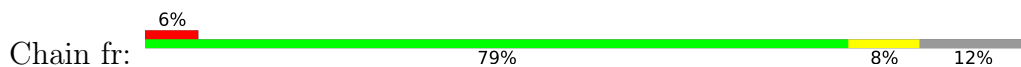
• Molecule 1: Major capsid protein



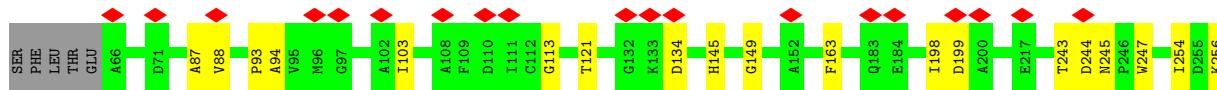
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	LYS	TRP	PRO	LEU	LEU	GLU	GLY	GLY	PRO	GLU	ILE	ALA	ASN	LYS	GLN	ALA	ILE	ILE	LYS	ILE	PHE	GLU	ASN	GLN	GLU	GLN	LYS	LYS	ASP	PHE	GLN	THR	ALA	ALA	PRO	GLU	TYR	LYS	ASP	LYS	ILE	ILE	GLN	ALA	PHE	GLY
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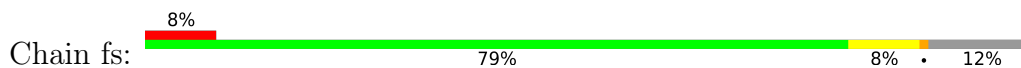
• Molecule 1: Major capsid protein



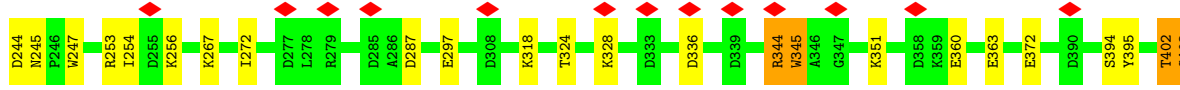
MET	THR	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLY	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	LYS	ILE	PHE	GLU	ASN	GLN	LYS	GLU	ASP	PHE	GLN	THR	ALA	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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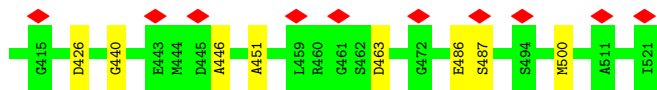


• Molecule 1: Major capsid protein

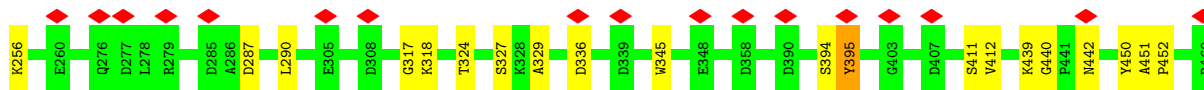
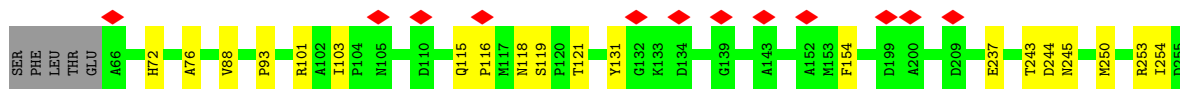
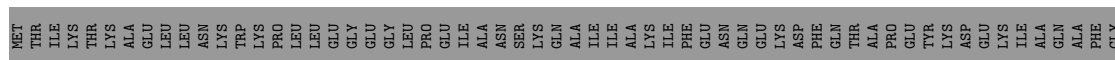
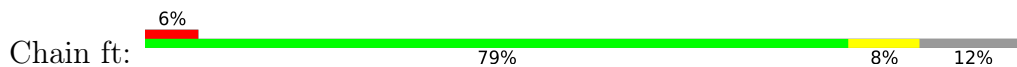


MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLY	PRO	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	LYS	ILE	PHE	GLU	ASN	GLN	LYS	ASP	PHE	GLN	THR	ALA	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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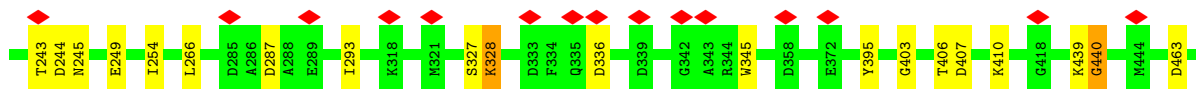
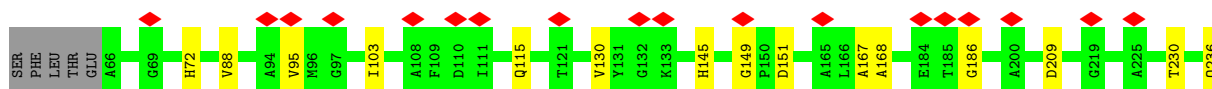
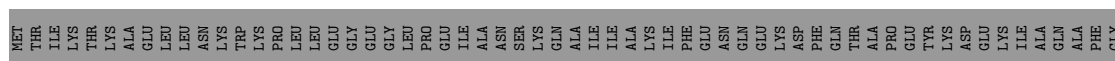
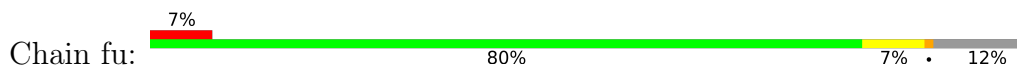




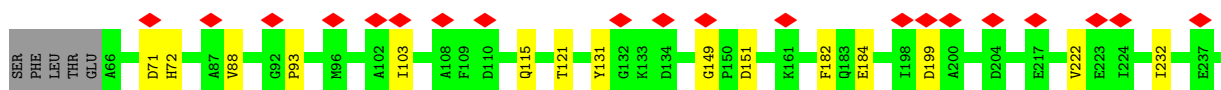
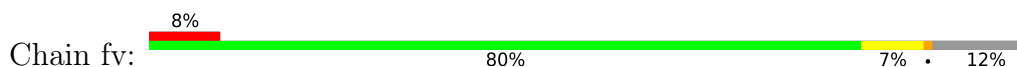
• Molecule 1: Major capsid protein

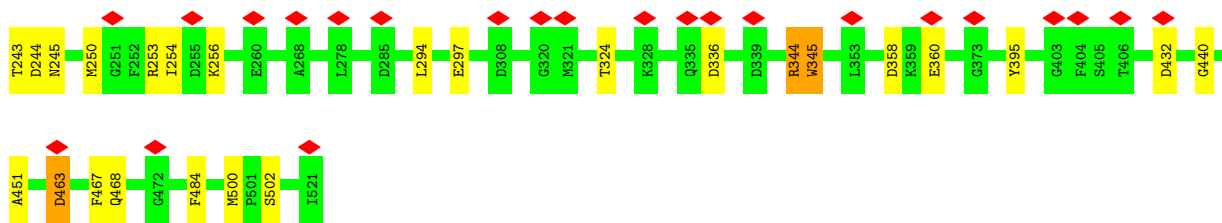


• Molecule 1: Major capsid protein

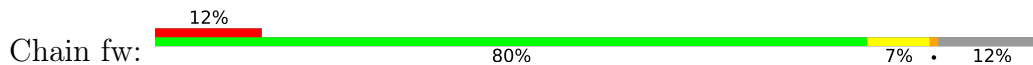


• Molecule 1: Major capsid protein

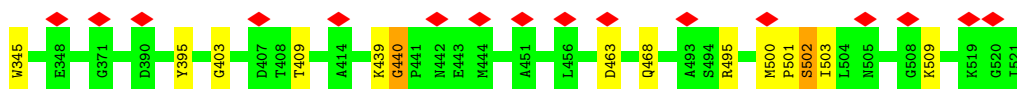
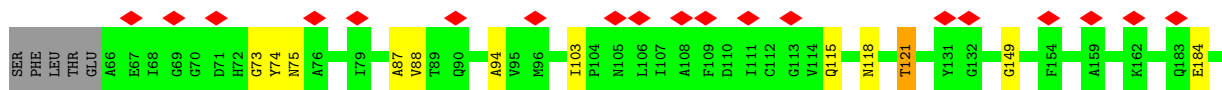




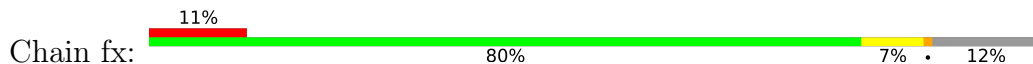
• Molecule 1: Major capsid protein



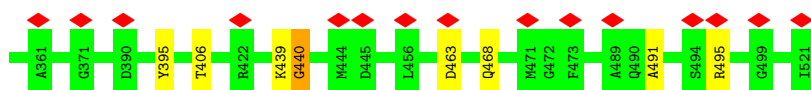
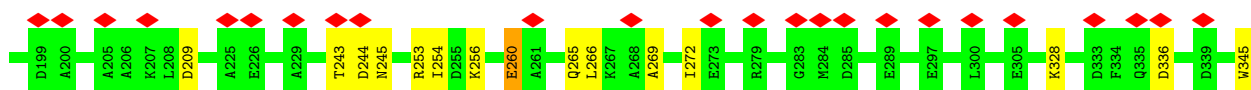
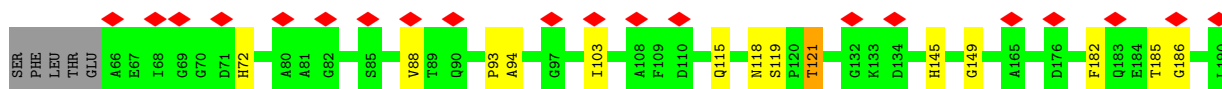
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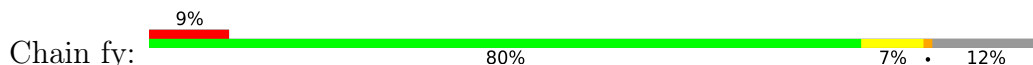
• Molecule 1: Major capsid protein



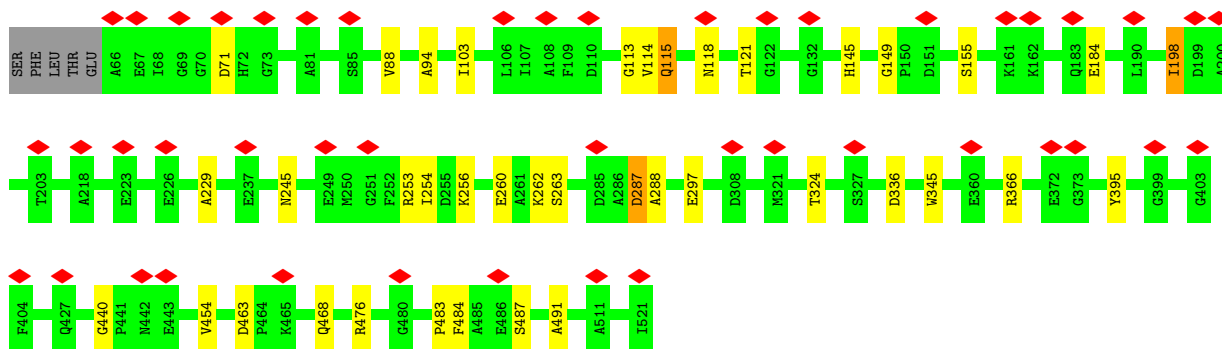
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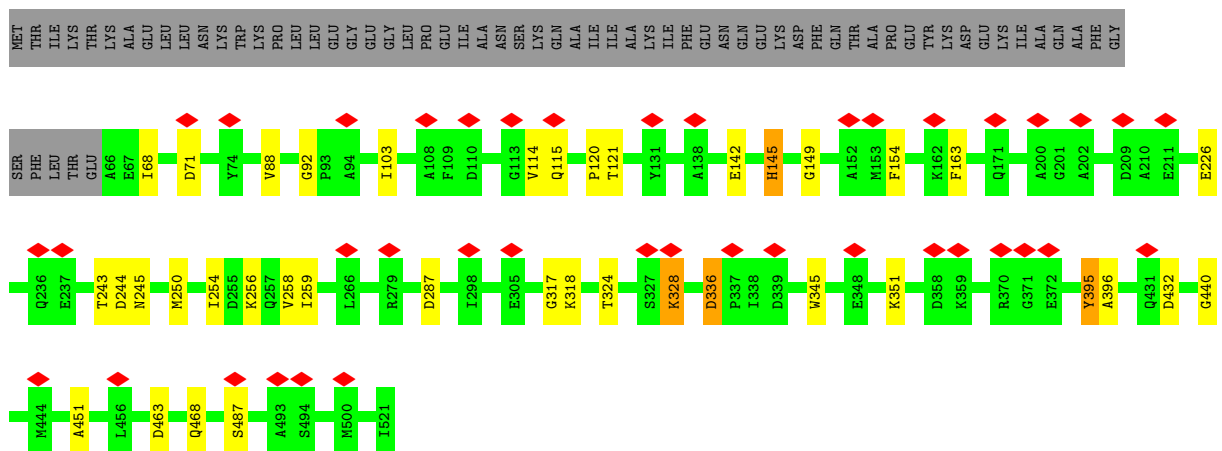
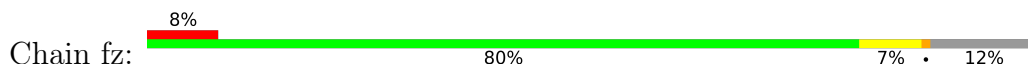
• Molecule 1: Major capsid protein



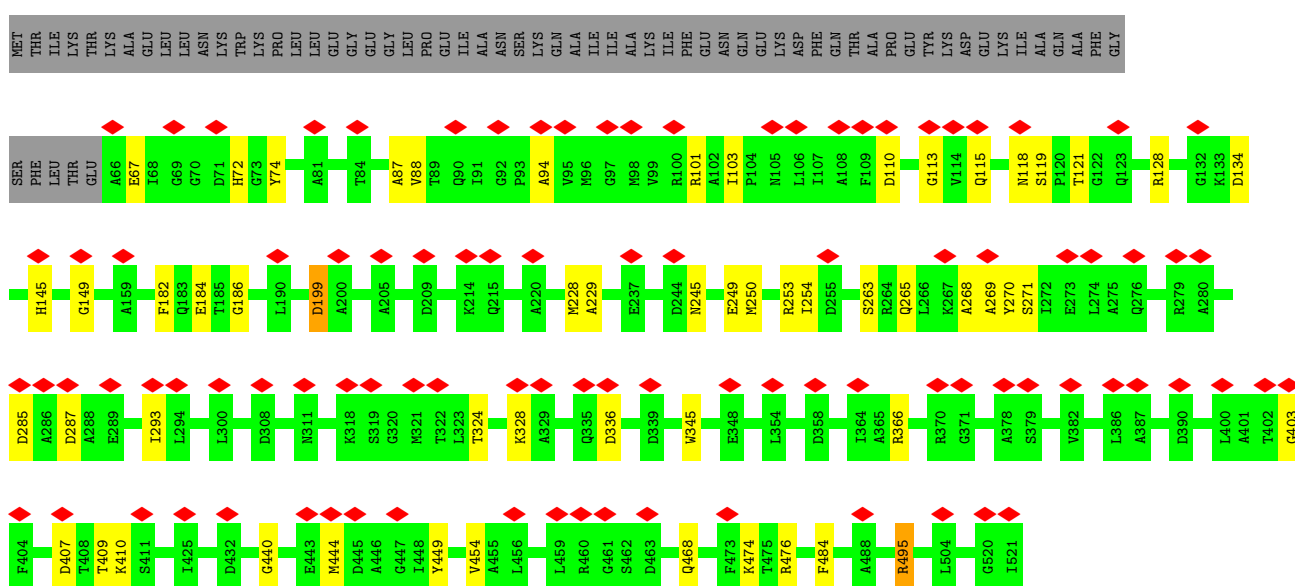
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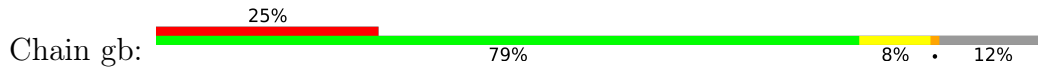
• Molecule 1: Major capsid protein



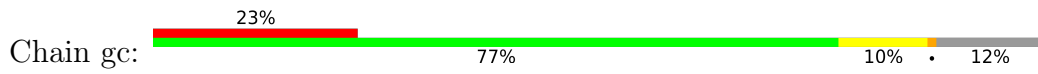
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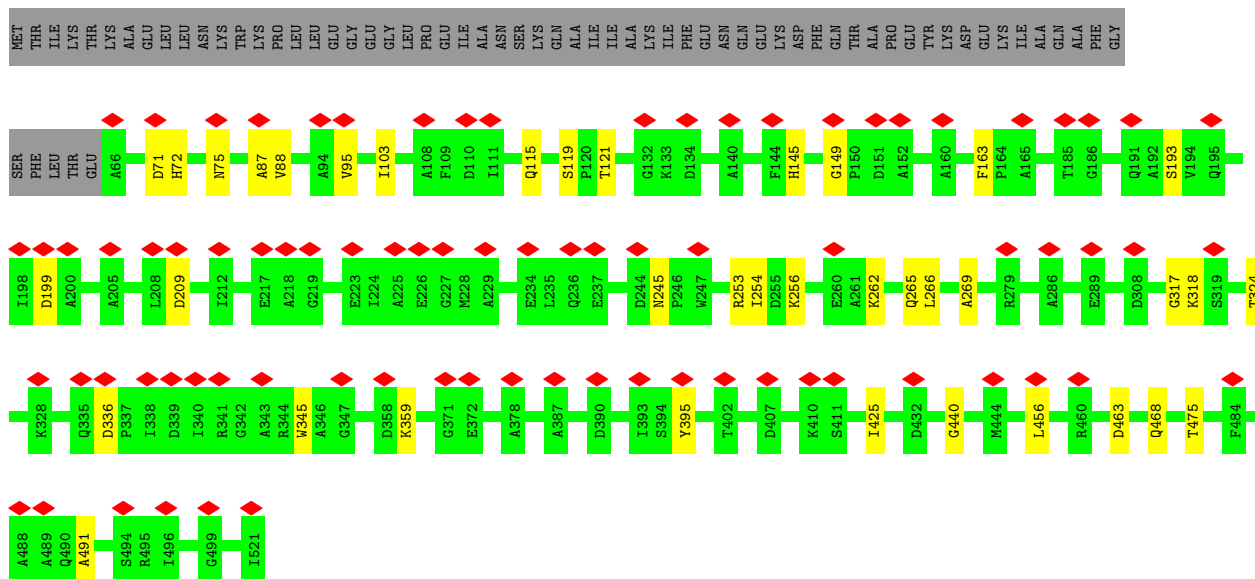
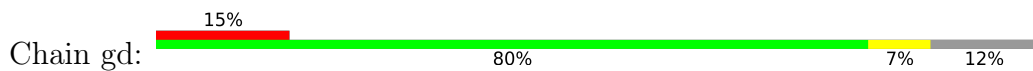
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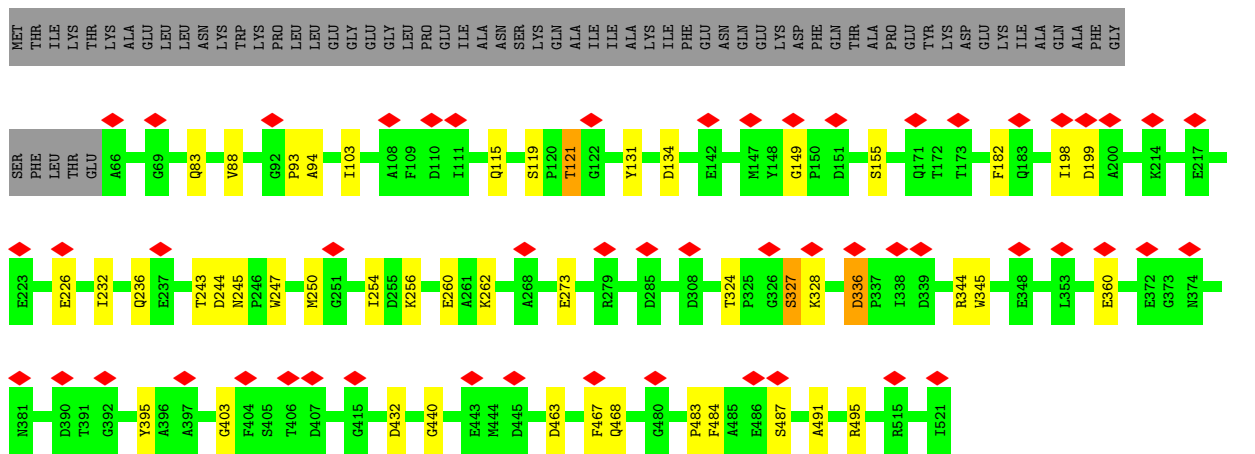
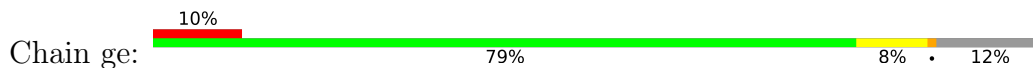
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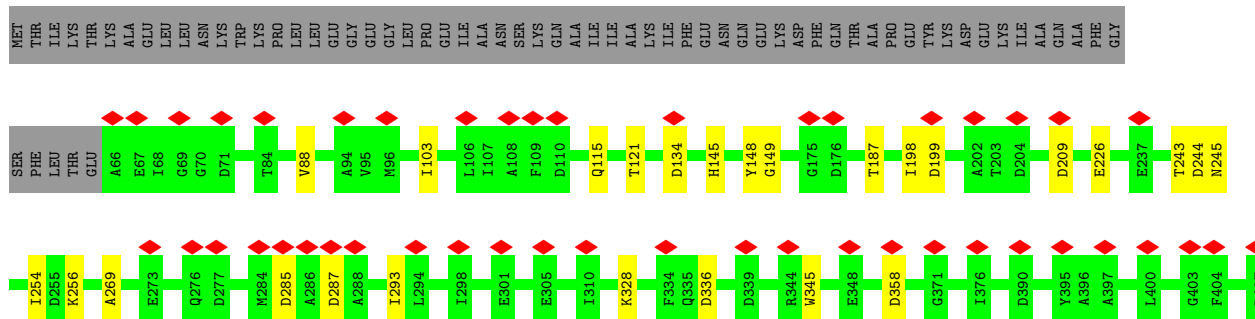
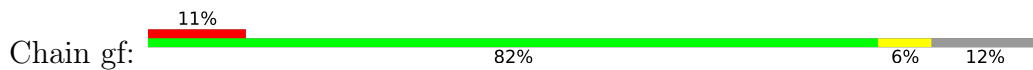
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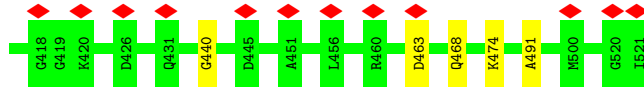


• Molecule 1: Major capsid protein

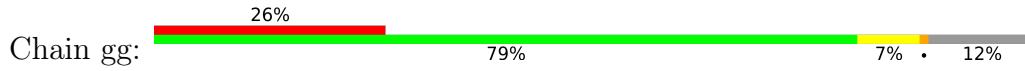


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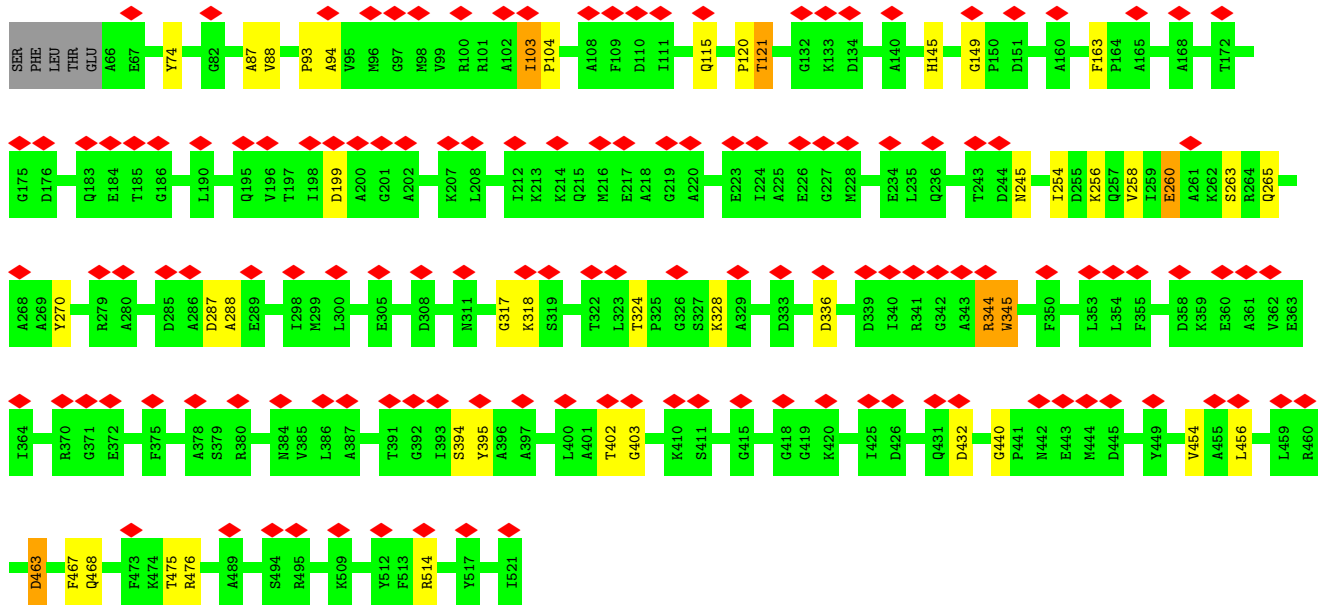




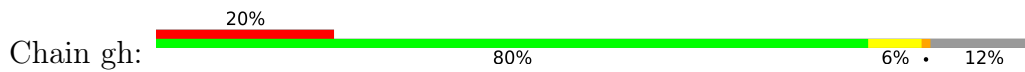
• Molecule 1: Major capsid protein



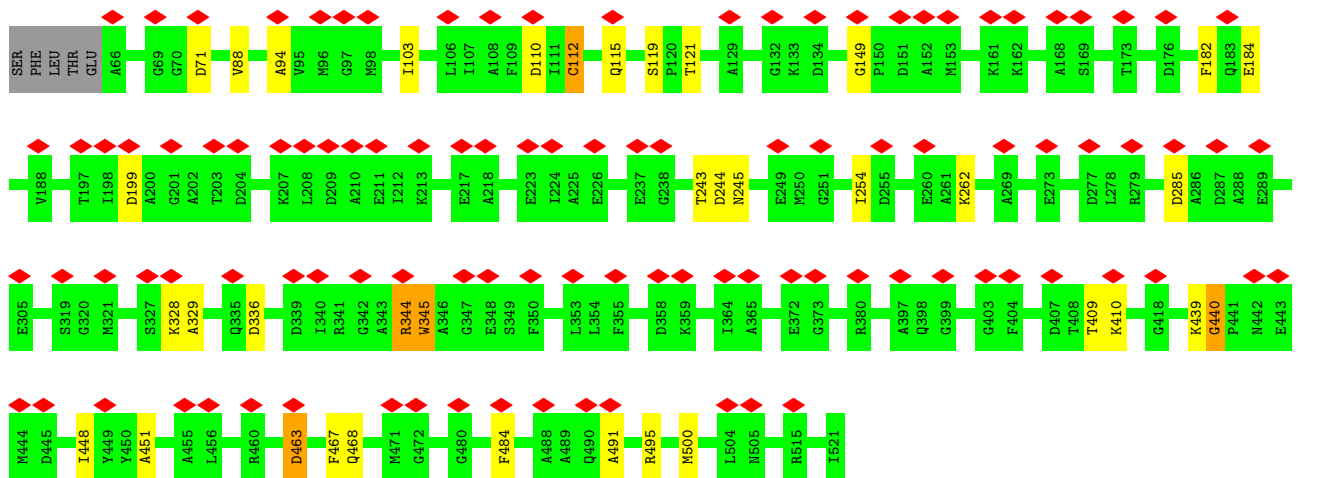
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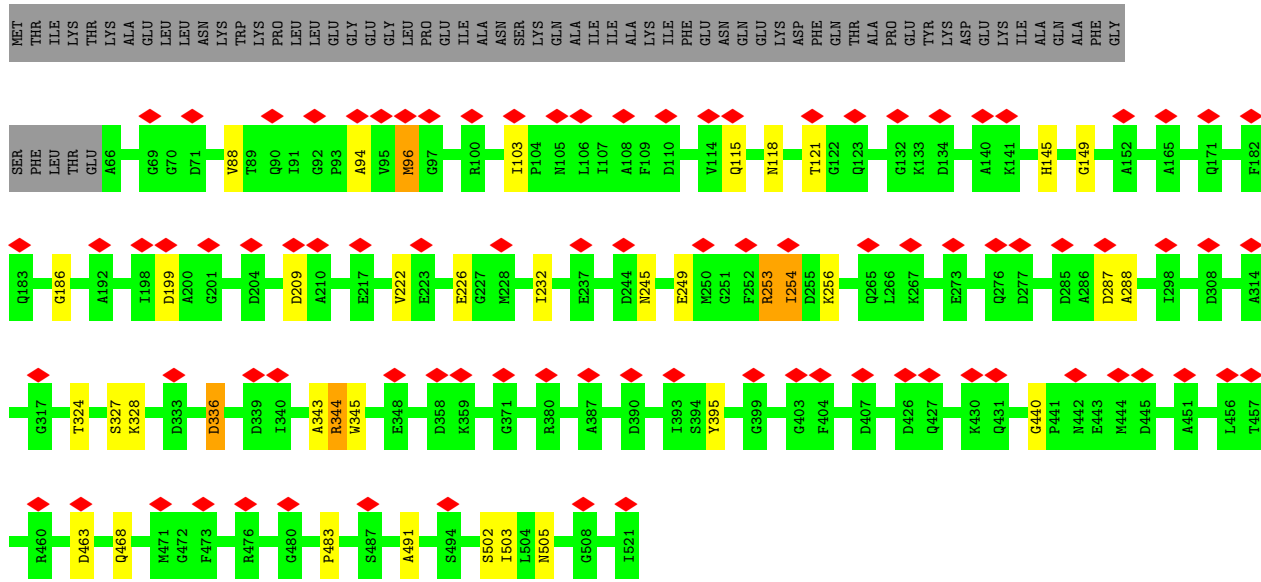
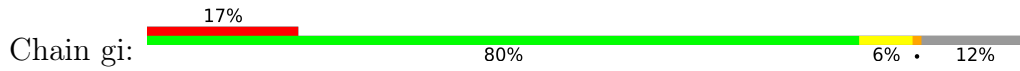
• Molecule 1: Major capsid protein



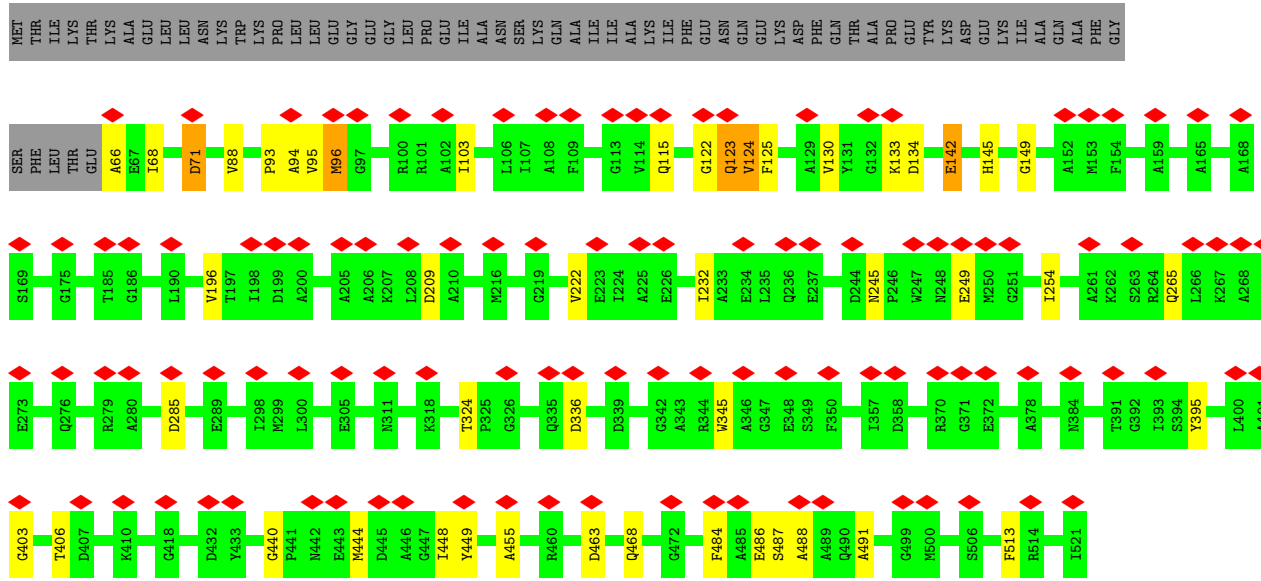
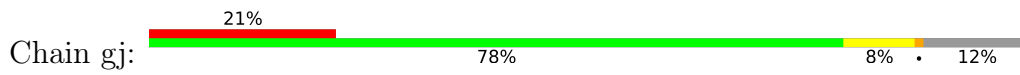
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLU	PRO	GLU	LEU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLU	GLY	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TVR	LYS	ASP	GLU	LYS	ILE	ILE	GLN	ALA	ALA	PHE	GLY
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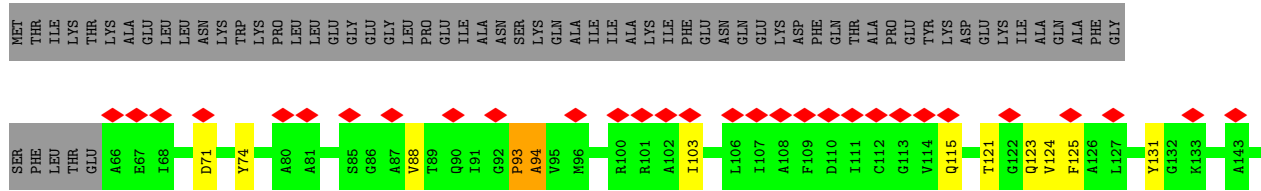
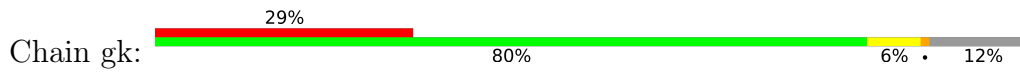
• Molecule 1: Major capsid protein

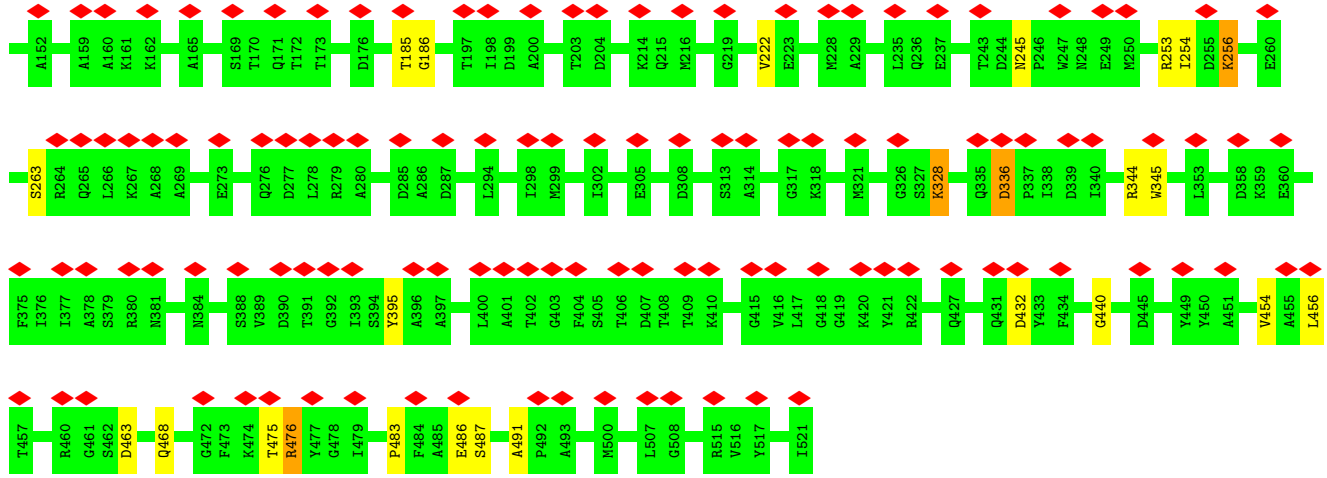


• Molecule 1: Major capsid protein

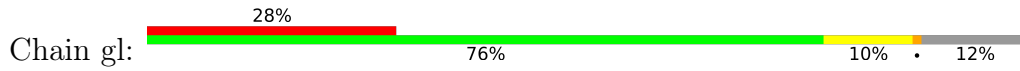


• Molecule 1: Major capsid protein

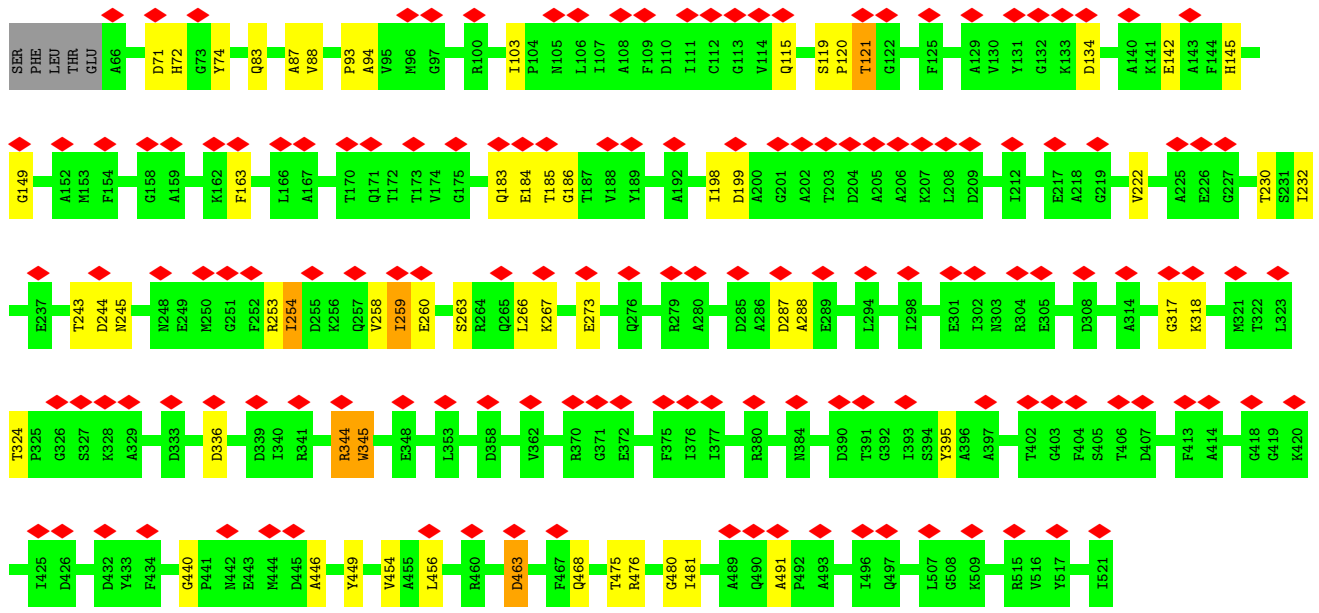




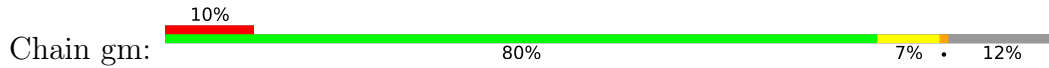
• Molecule 1: Major capsid protein



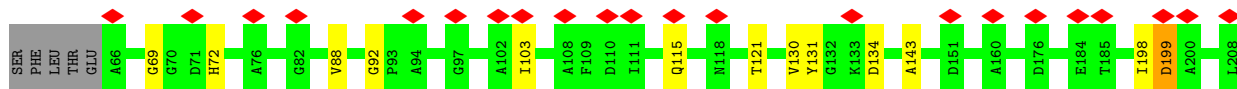
MET	THR	ILE	LYS	THR	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLU	GLY	ASN	PRO	LEU	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLU	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	GLN	ALA	PHE	GLY
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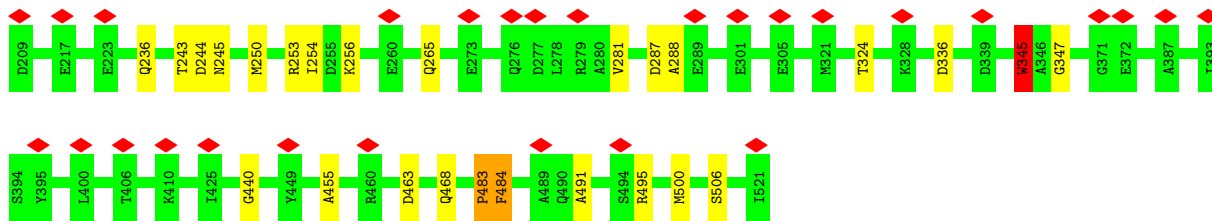


• Molecule 1: Major capsid protein

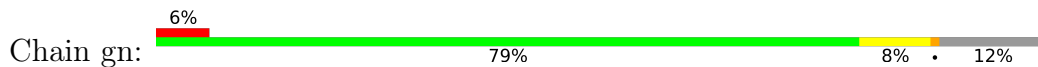


MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLU	GLY	GLU	GLY	GLU	ASN	PRO	LEU	GLU	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLU	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TYR	LYS	ASP	GLU	LYS	ILE	ALA	GLN	ALA	PHE	GLY
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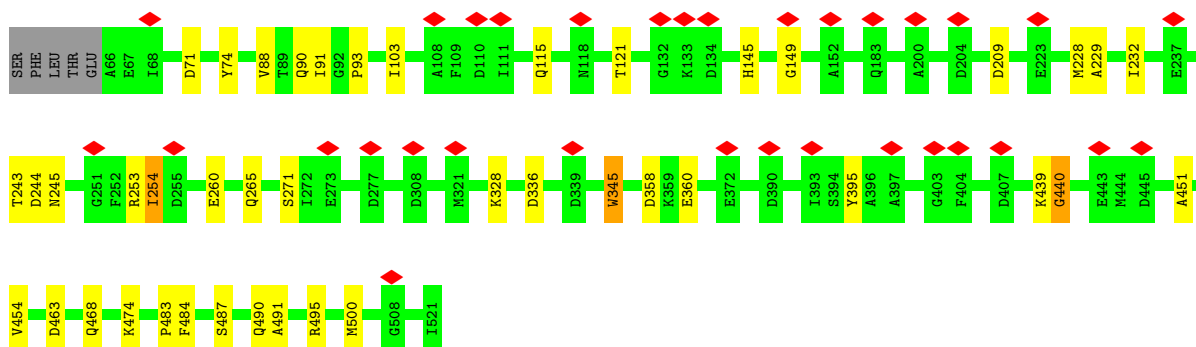




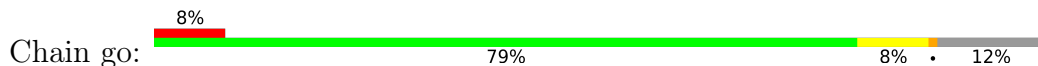
• Molecule 1: Major capsid protein



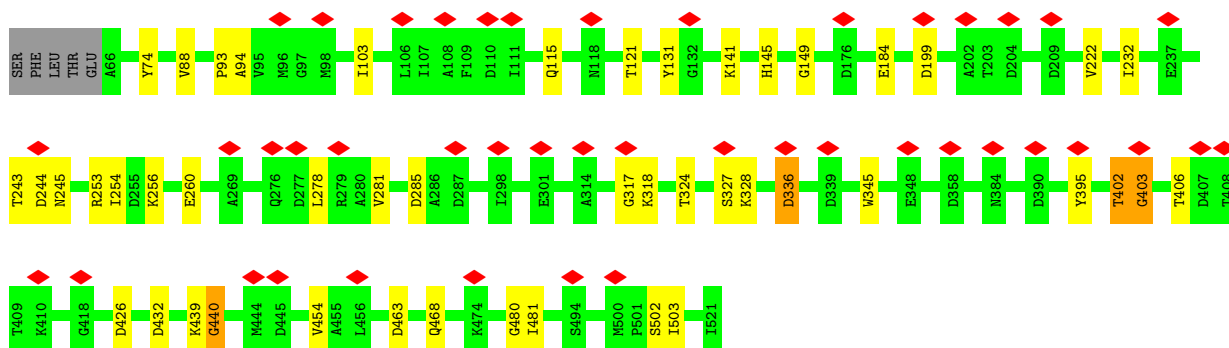
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	LEU	PRO	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TVR	LYS	ASP	ILE	ALA	GLN	ALA	PHE	GLY
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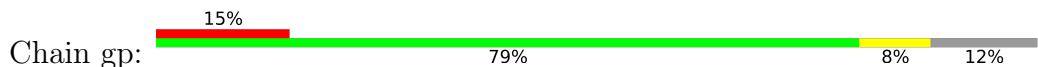
• Molecule 1: Major capsid protein



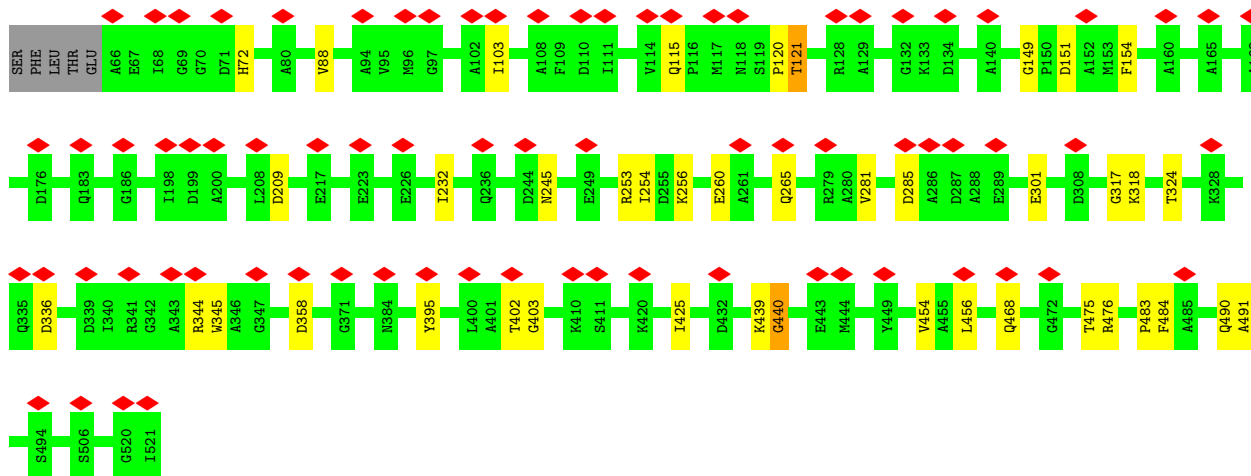
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	LEU	PRO	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TVR	LYS	ASP	ILE	ALA	GLN	ALA	PHE	GLY
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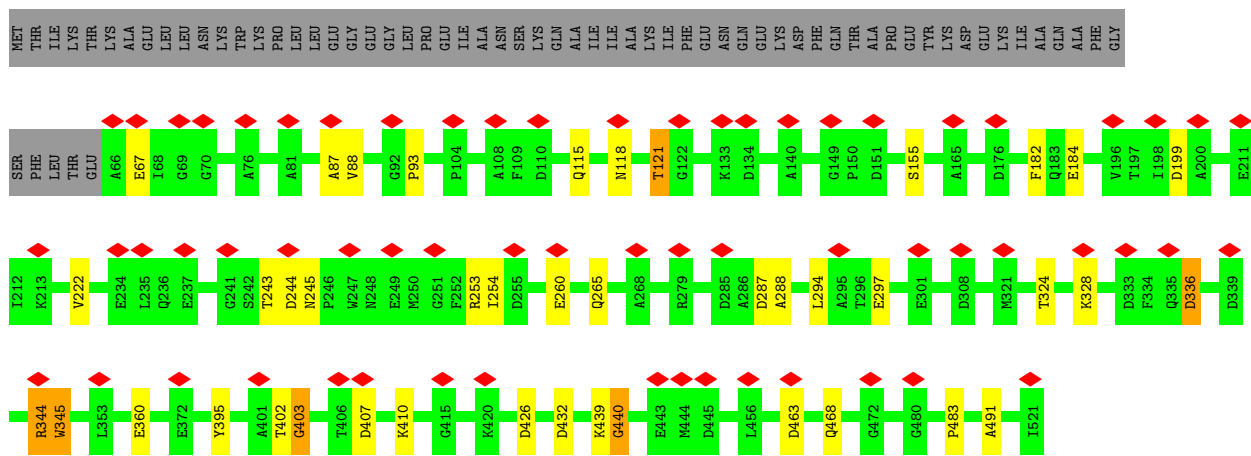
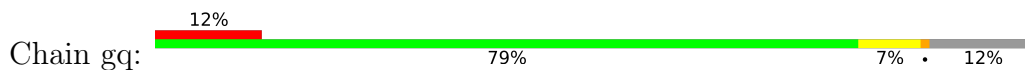
• Molecule 1: Major capsid protein



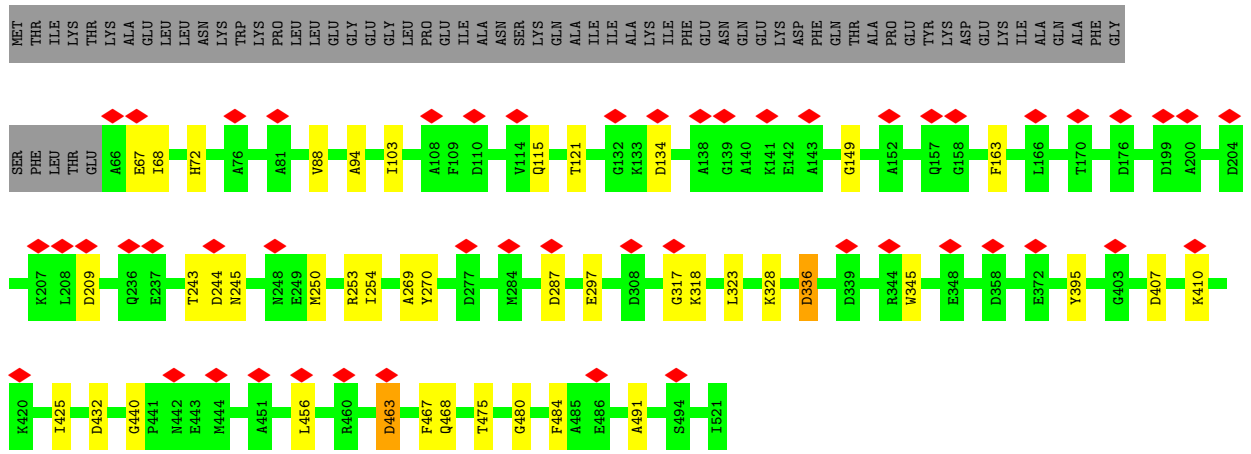
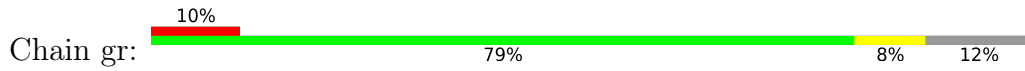
MET	THR	ILE	LYS	THR	LYS	ALA	GLU	LEU	LEU	ASN	TRP	LYS	PRO	LEU	LEU	GLY	GLY	GLY	LEU	PRO	ILE	ALA	ASN	SER	LYS	GLN	ALA	ILE	ILE	ALA	LYS	ILE	PHE	GLU	ASN	GLN	GLU	LYS	ASP	PHE	GLN	THR	ALA	PRO	GLU	TVR	LYS	ASP	ILE	ALA	GLN	ALA	PHE	GLY
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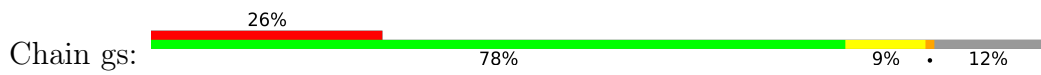
• Molecule 1: Major capsid protein



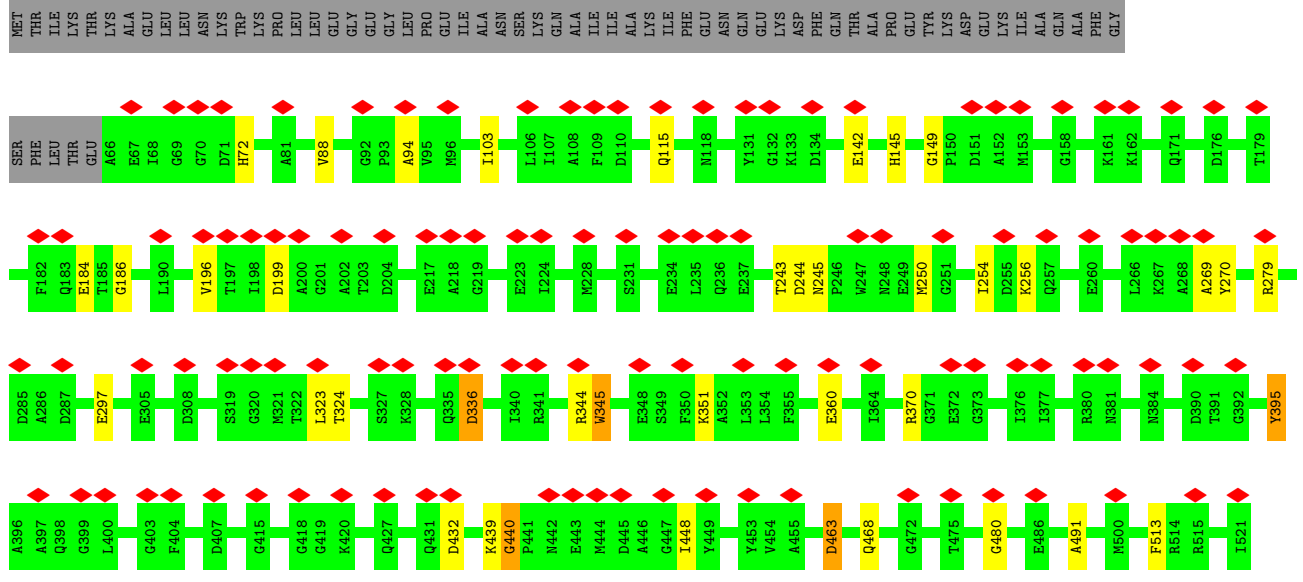
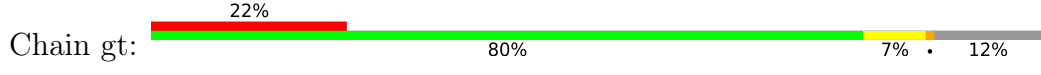
• Molecule 1: Major capsid protein



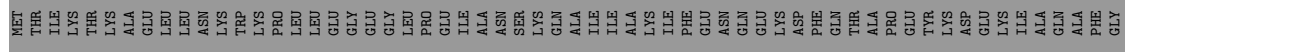
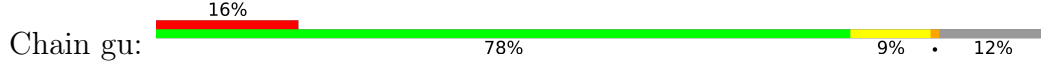
• Molecule 1: Major capsid protein

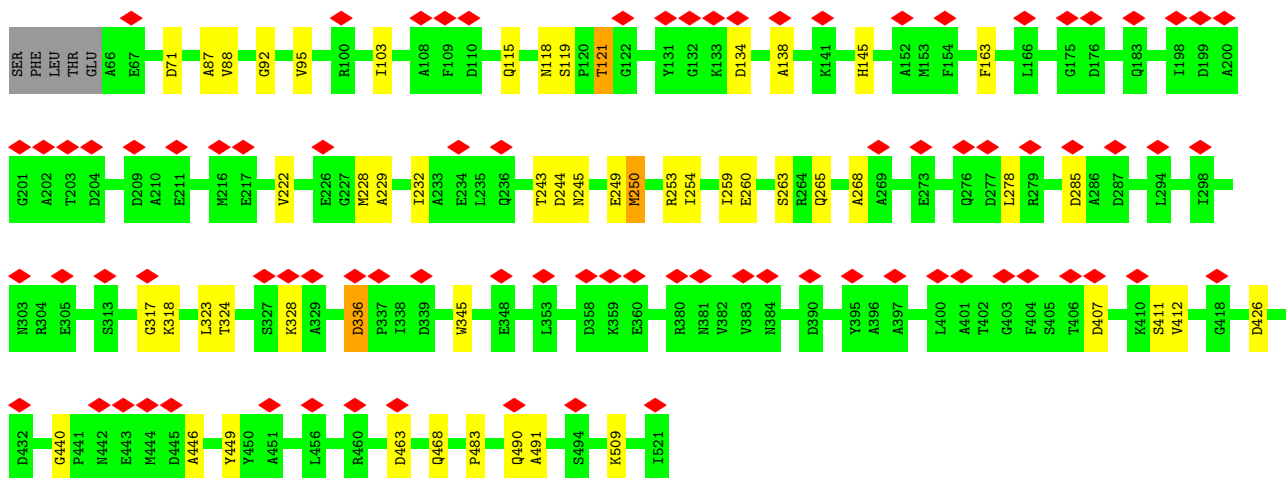


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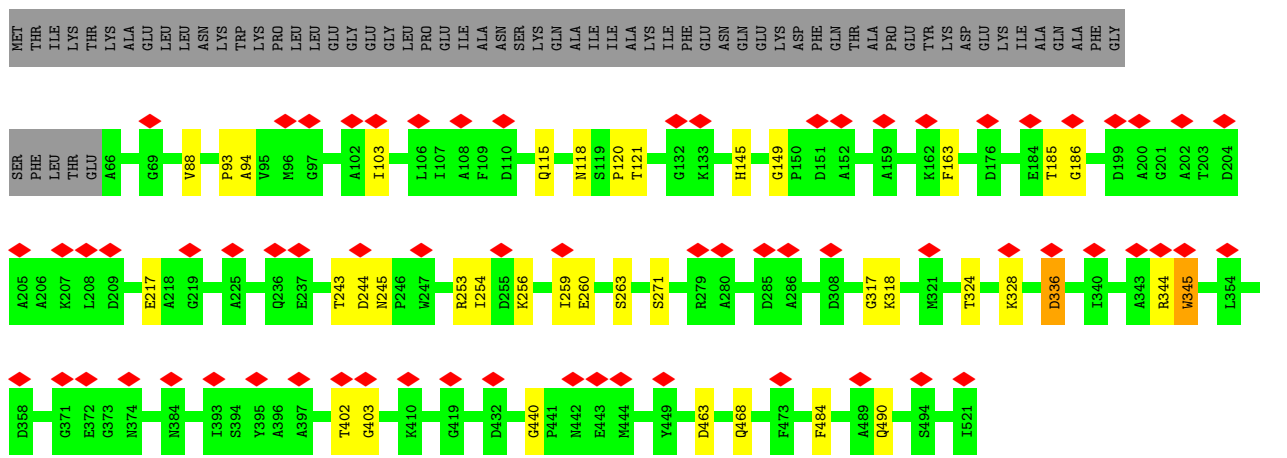
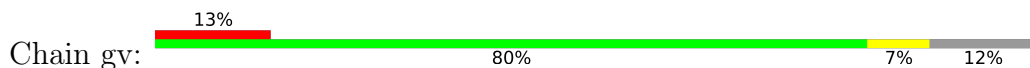


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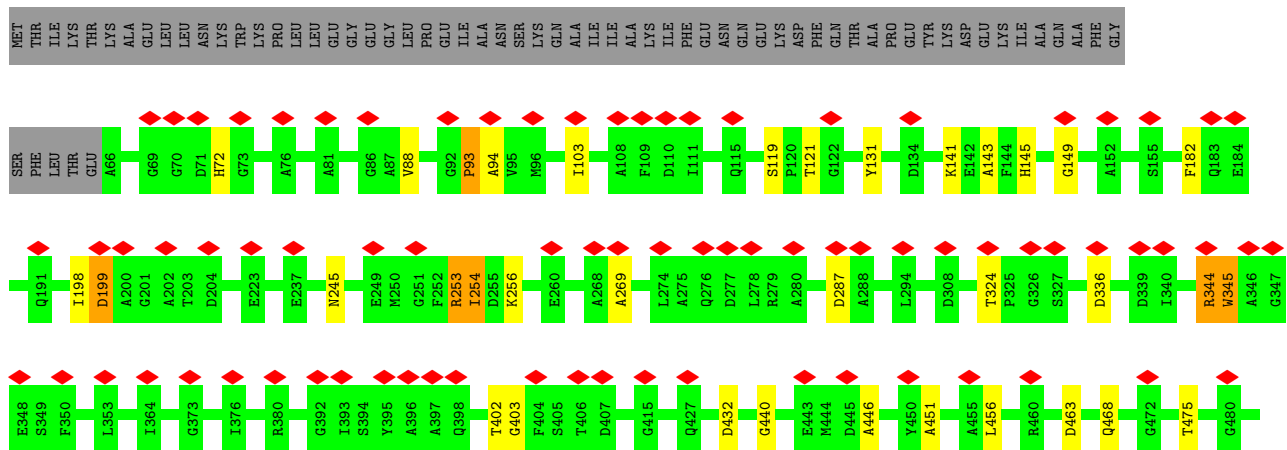
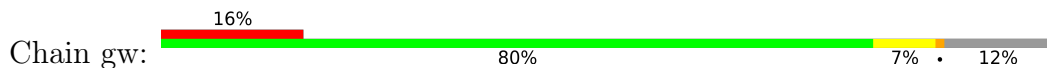


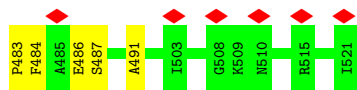


• Molecule 1: Major capsid protein

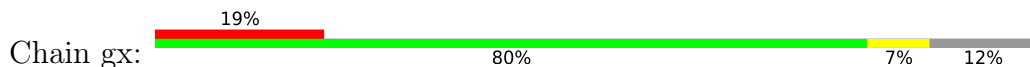


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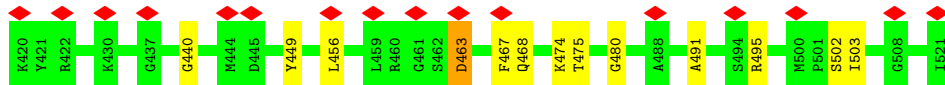
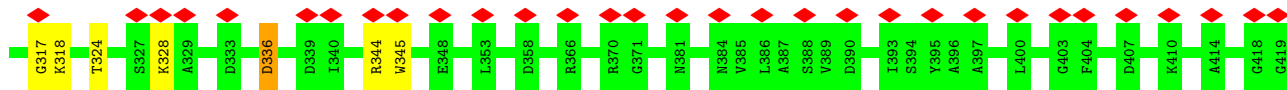
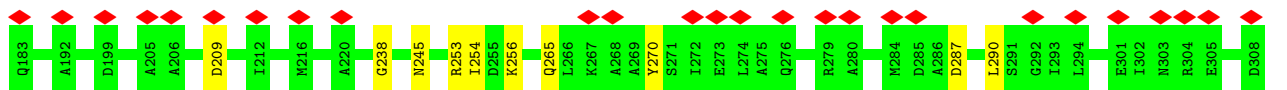
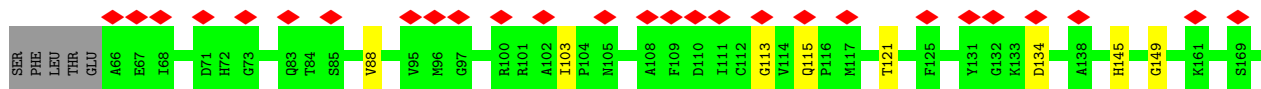




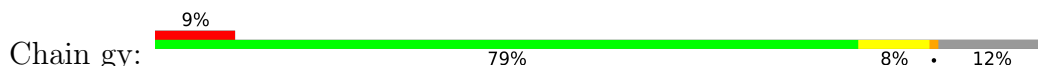
• Molecule 1: Major capsid protein



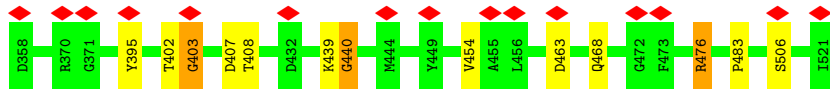
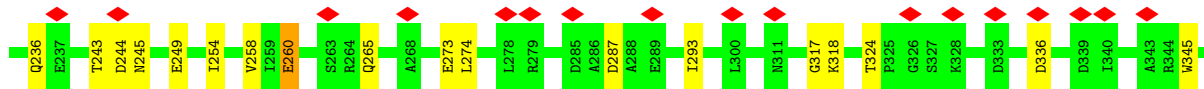
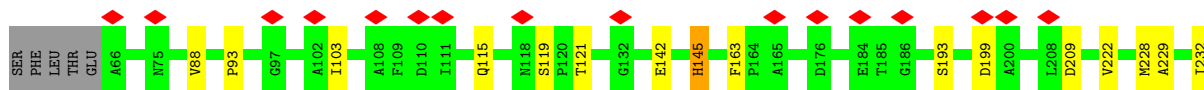
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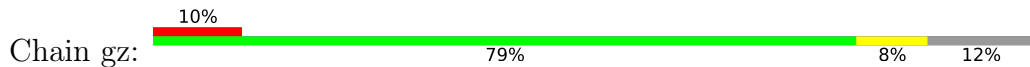
• Molecule 1: Major capsid protein



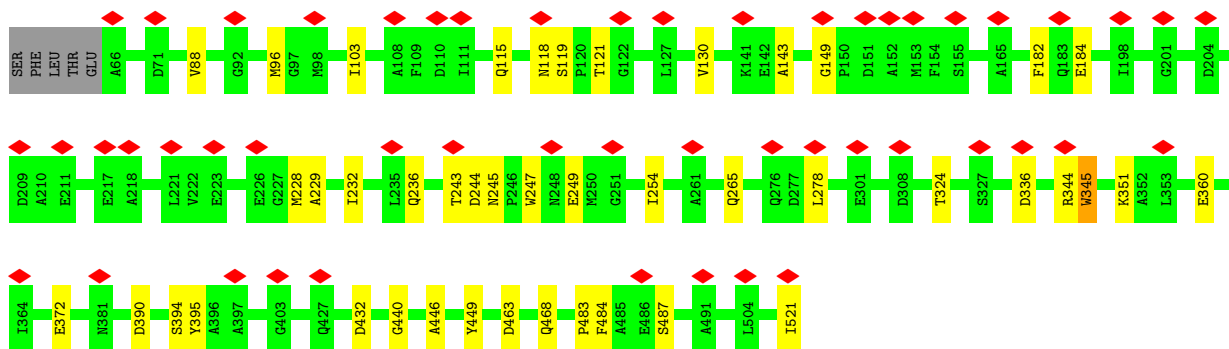
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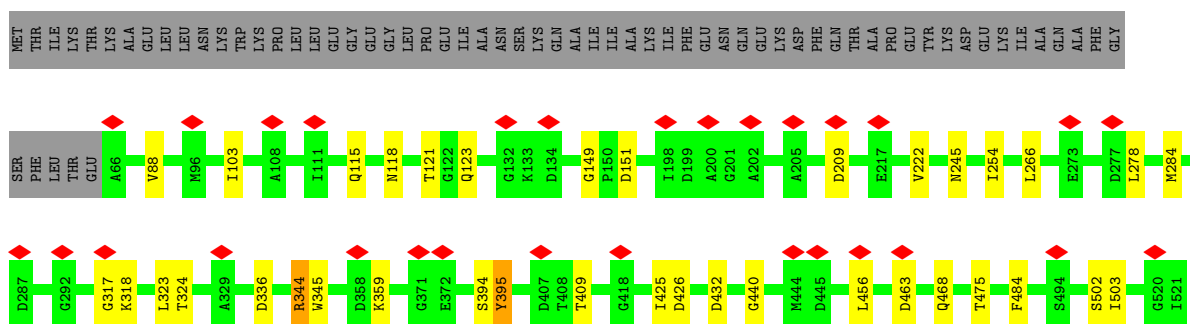
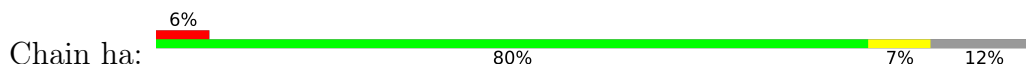
• Molecule 1: Major capsid protein



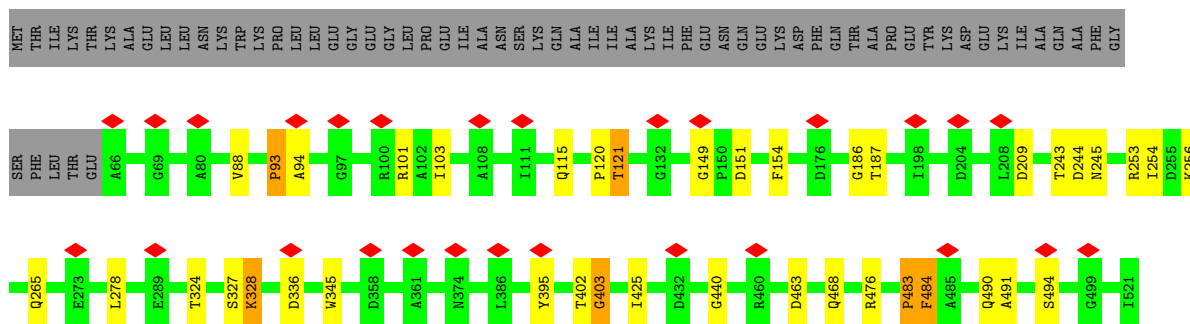
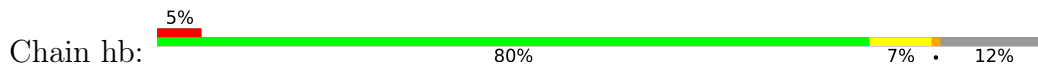
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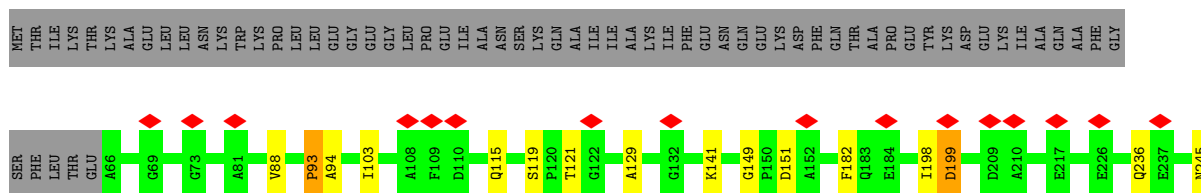
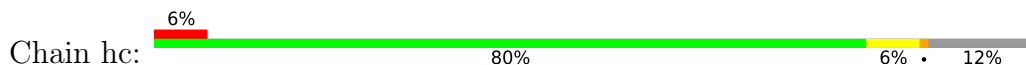
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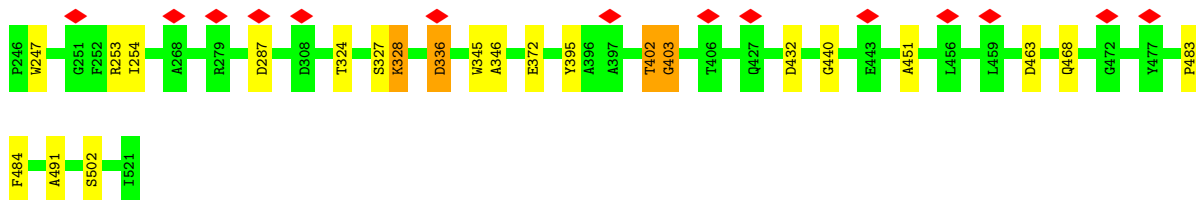


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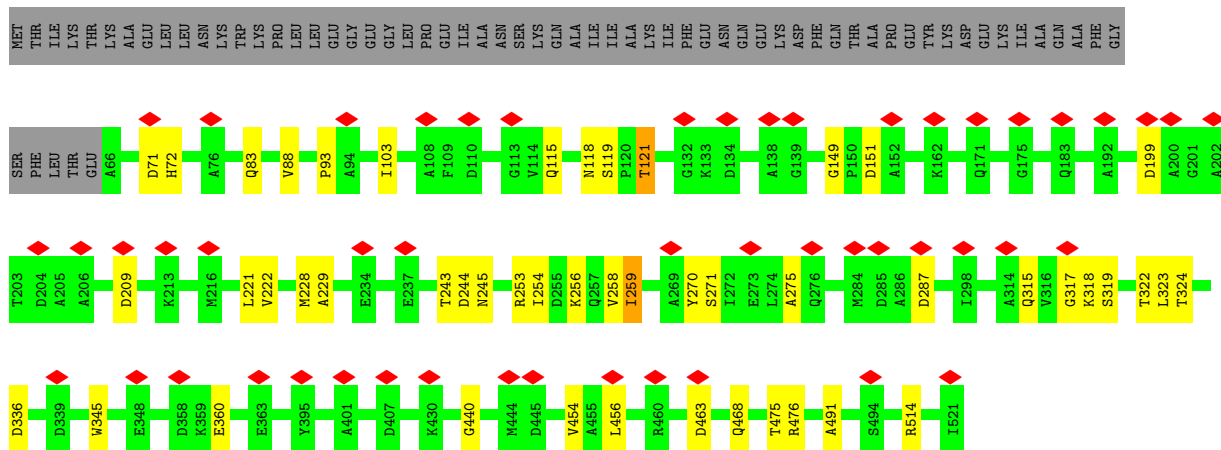
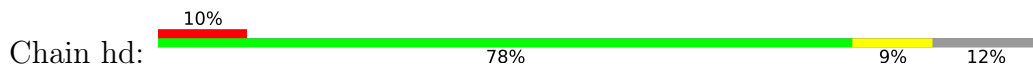


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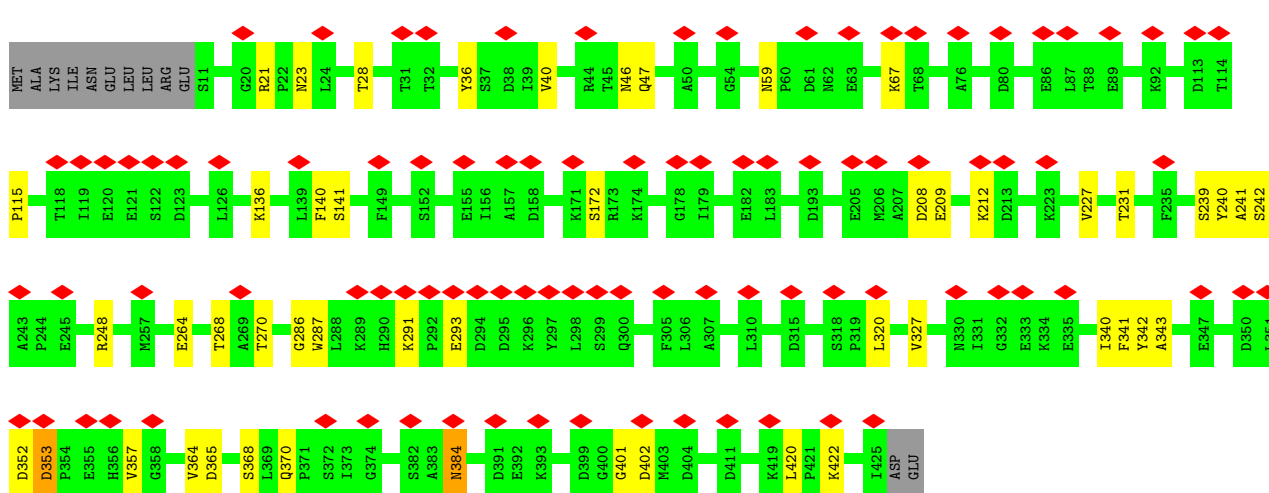
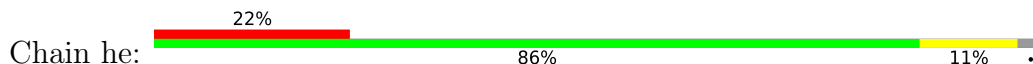




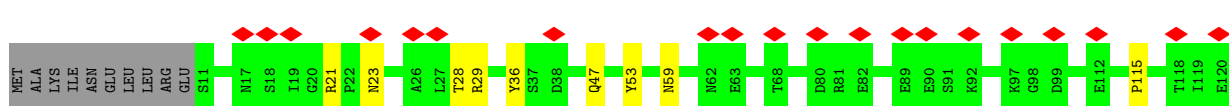
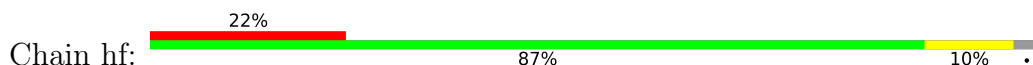
• Molecule 1: Major capsid protein

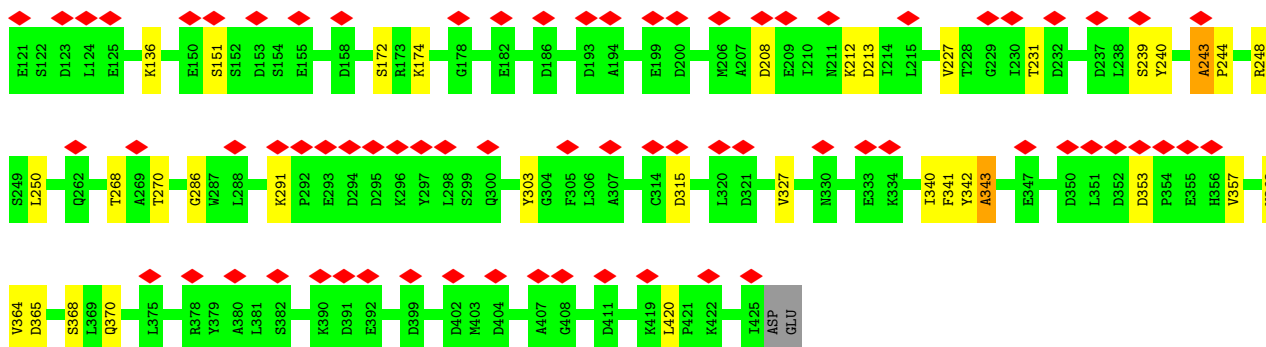


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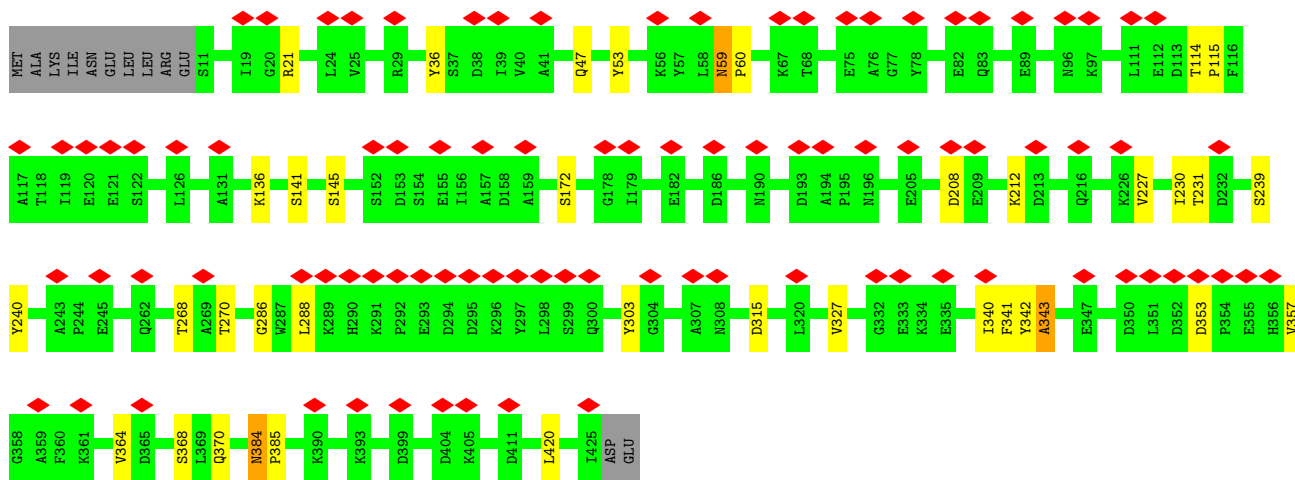
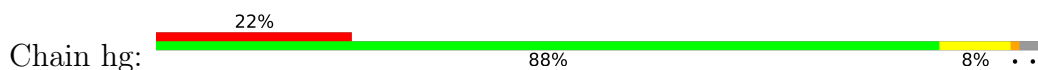


• Molecule 2: Capsid vertex protein

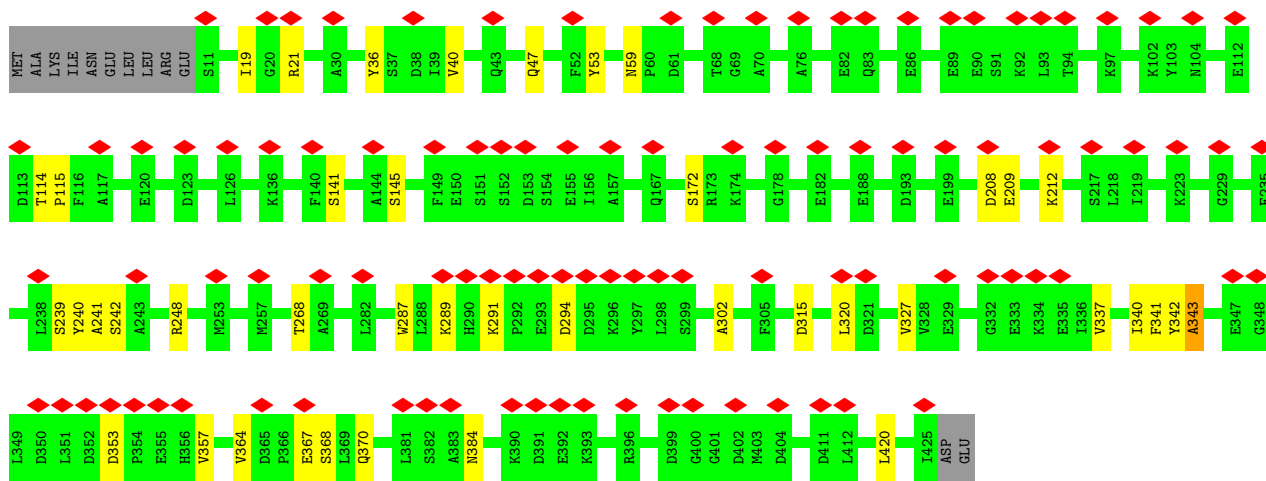
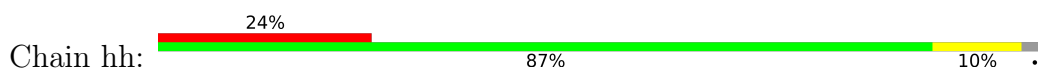




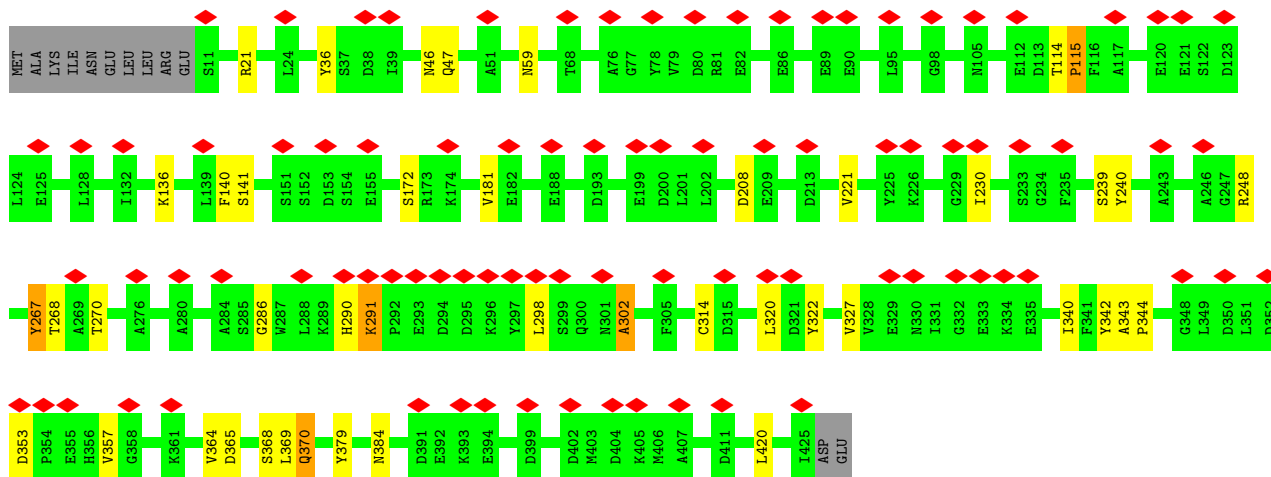
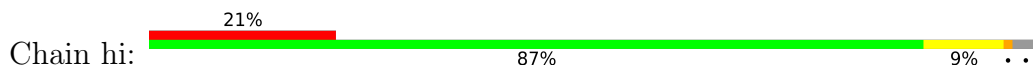
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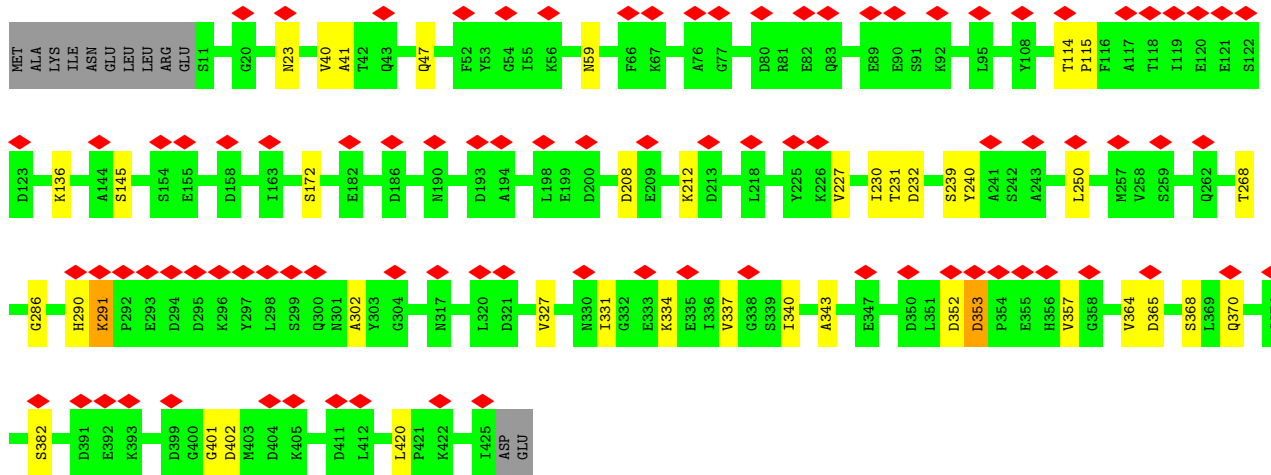
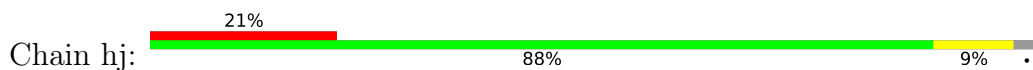
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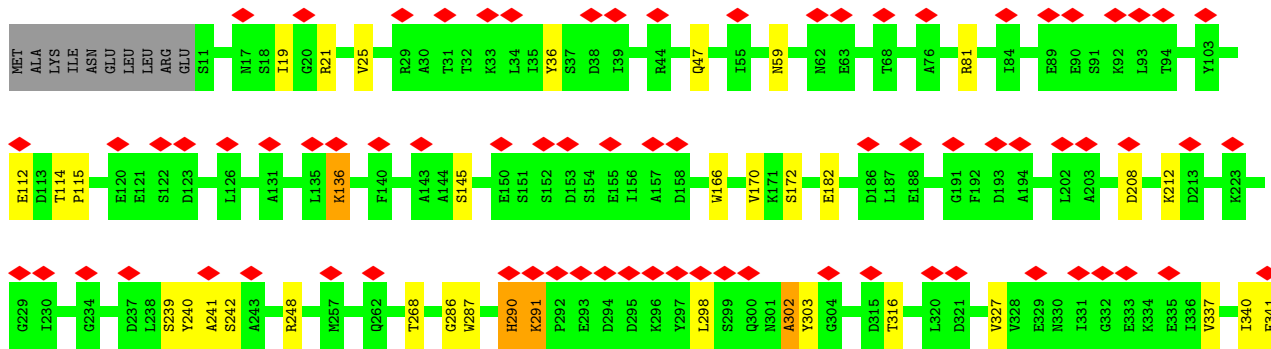
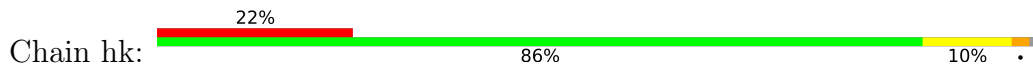
• Molecule 2: Capsid vertex protein



• Molecule 2: Capsid vertex protein

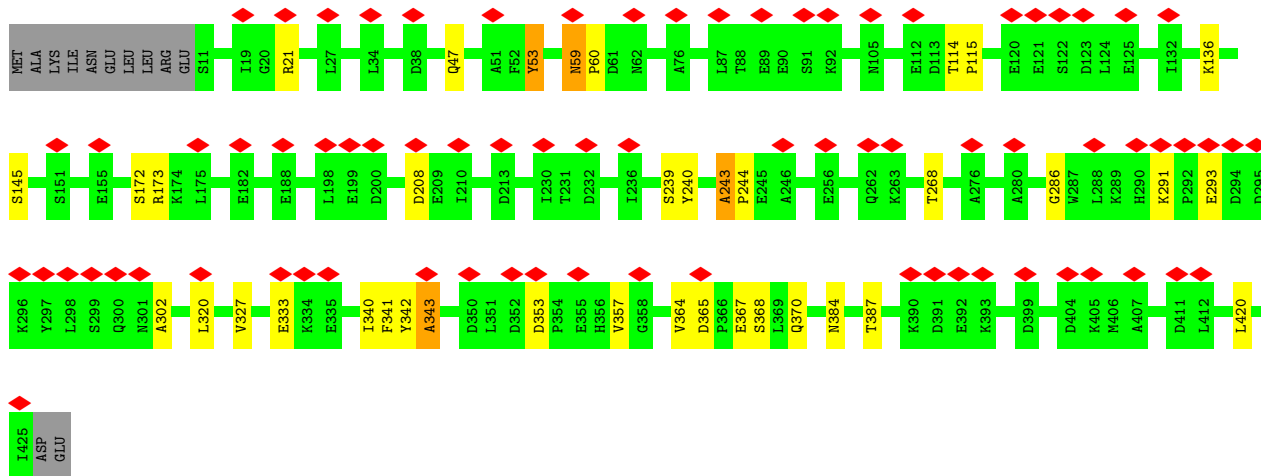
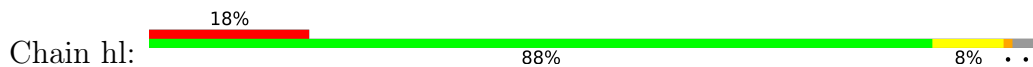


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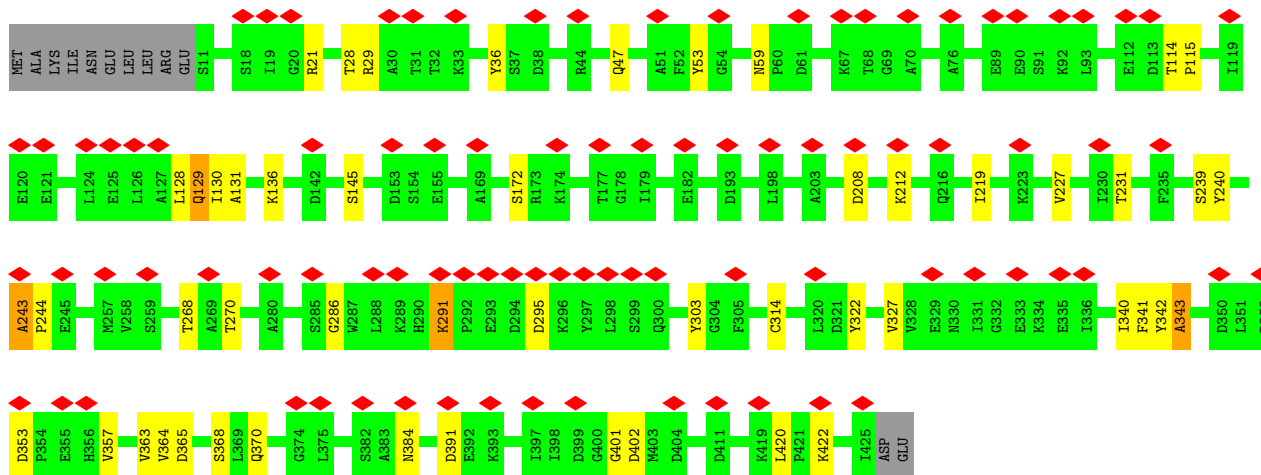
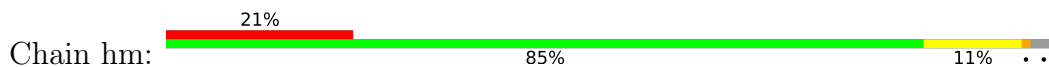




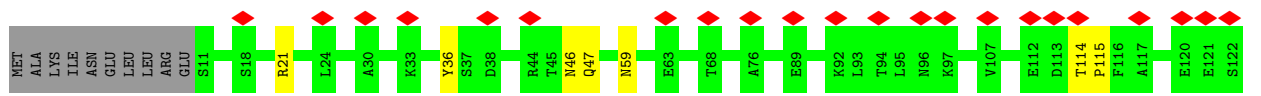
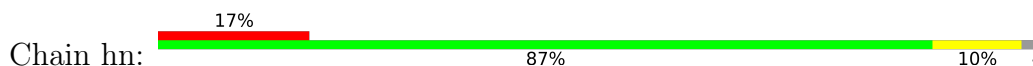
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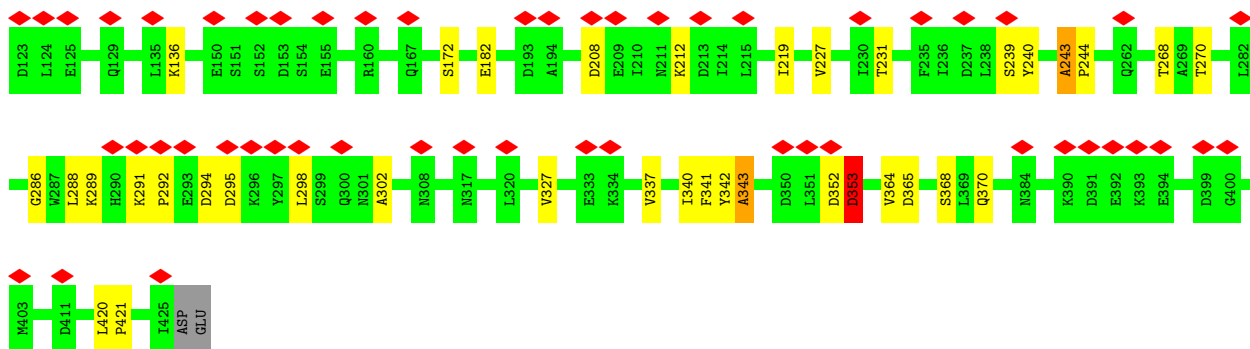


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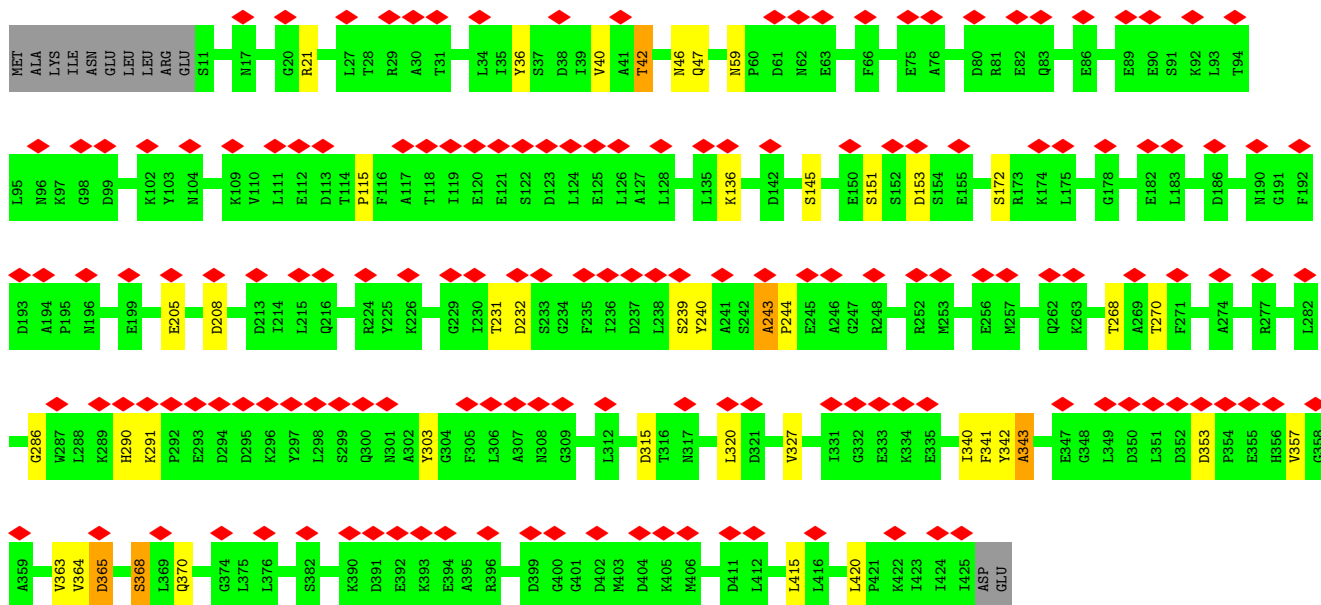
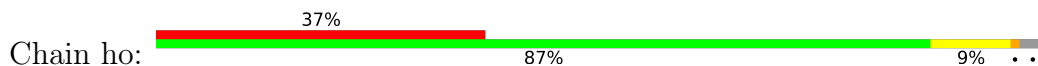


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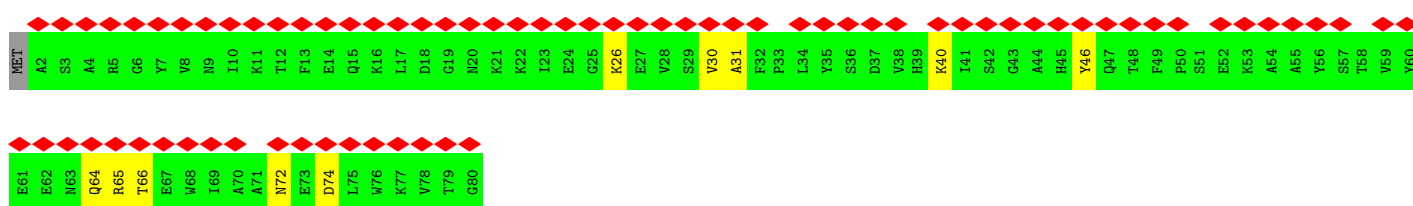
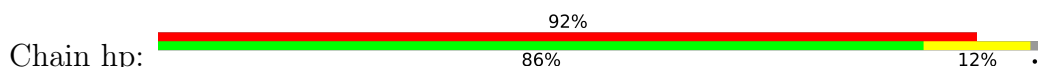




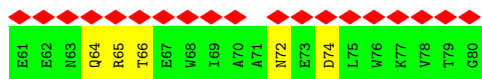
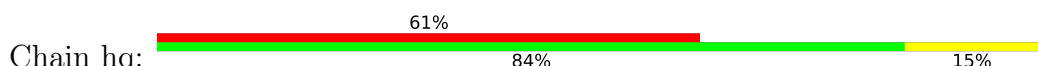
• Molecule 2: Capsid vertex protein

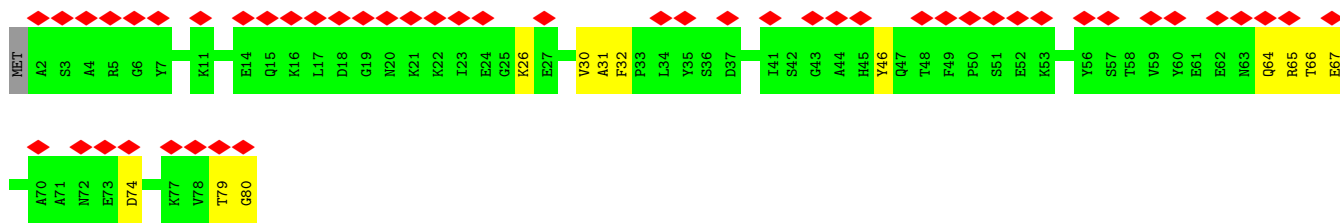


• Molecule 3: Small outer capsid protein

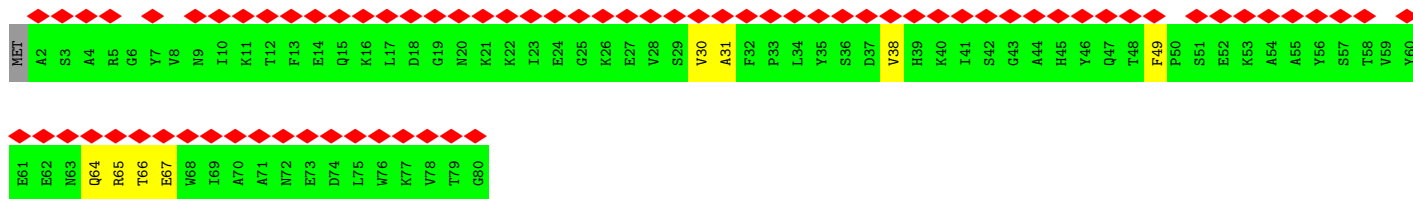
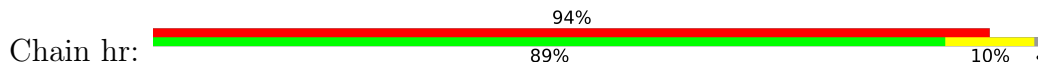


• Molecule 3: Small outer capsid protein

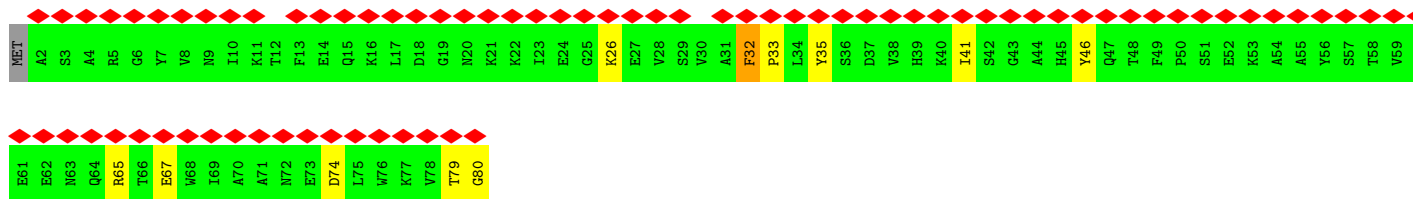
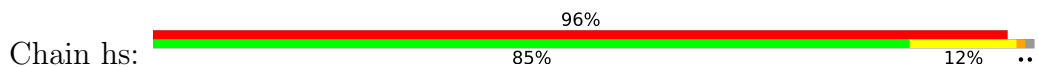




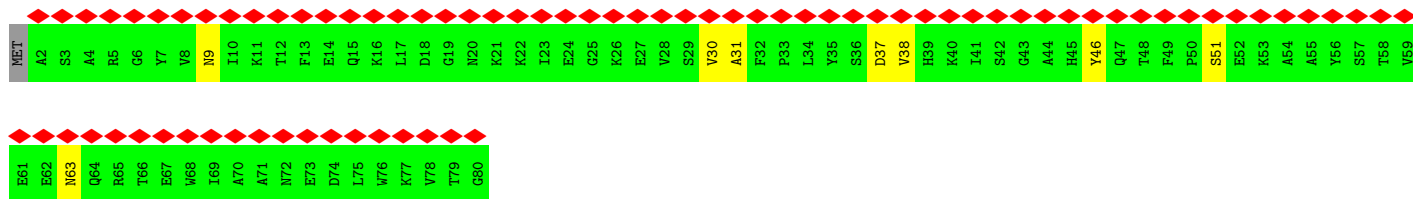
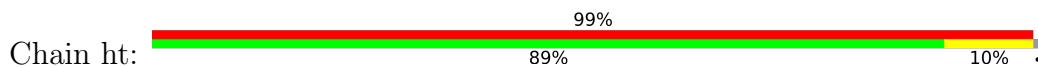
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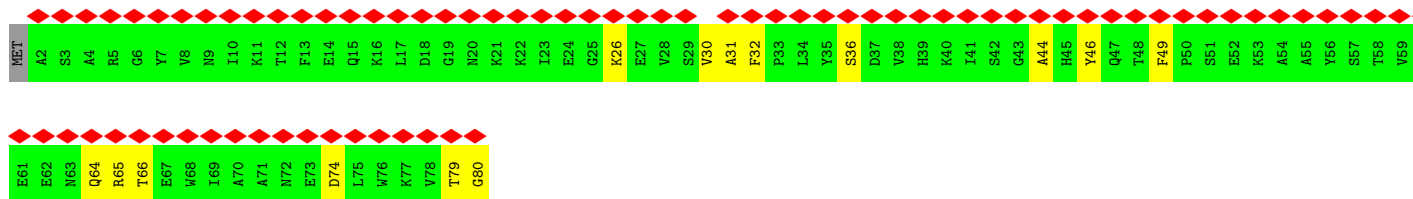
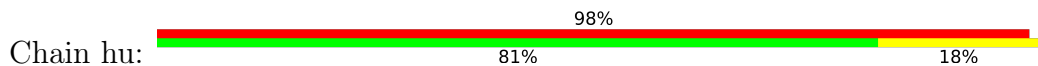
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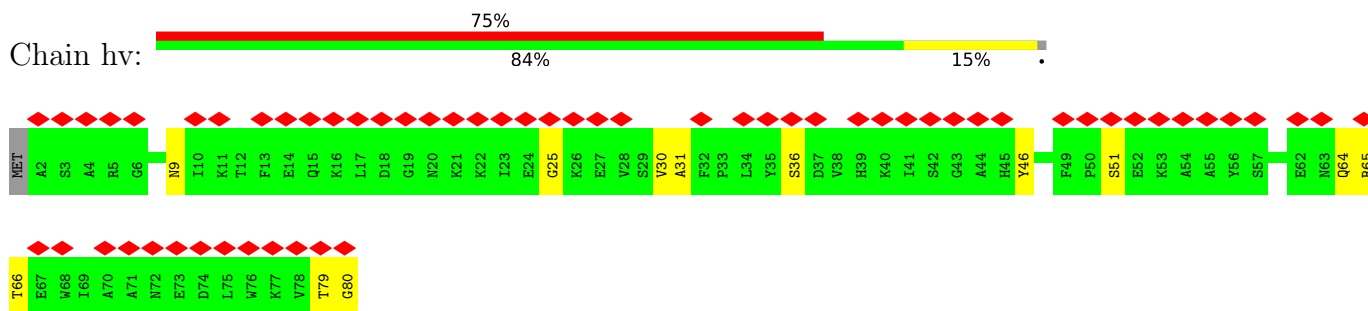
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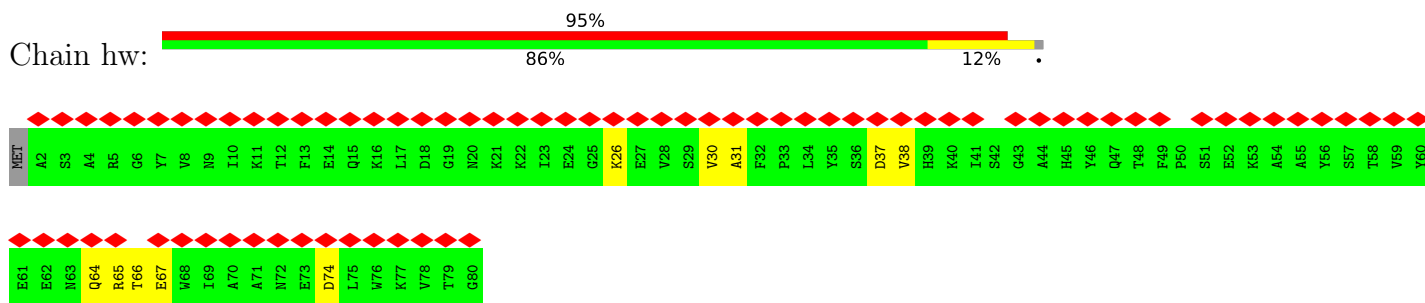
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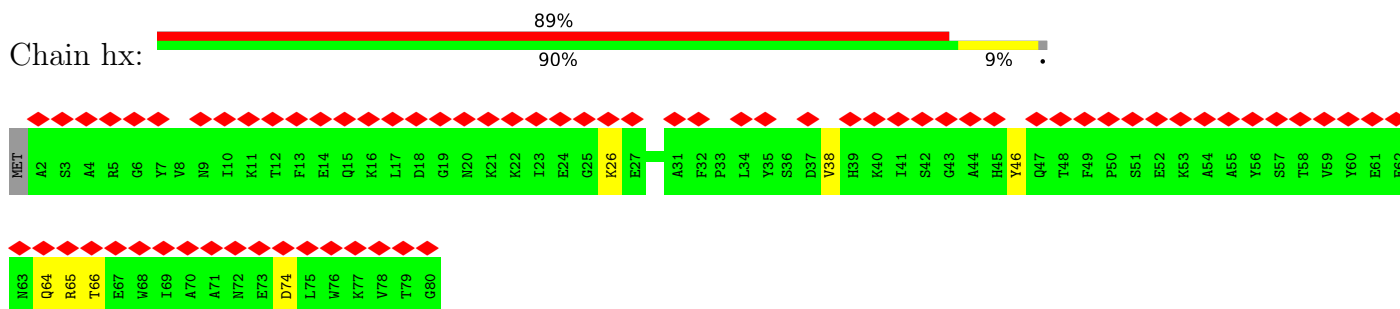
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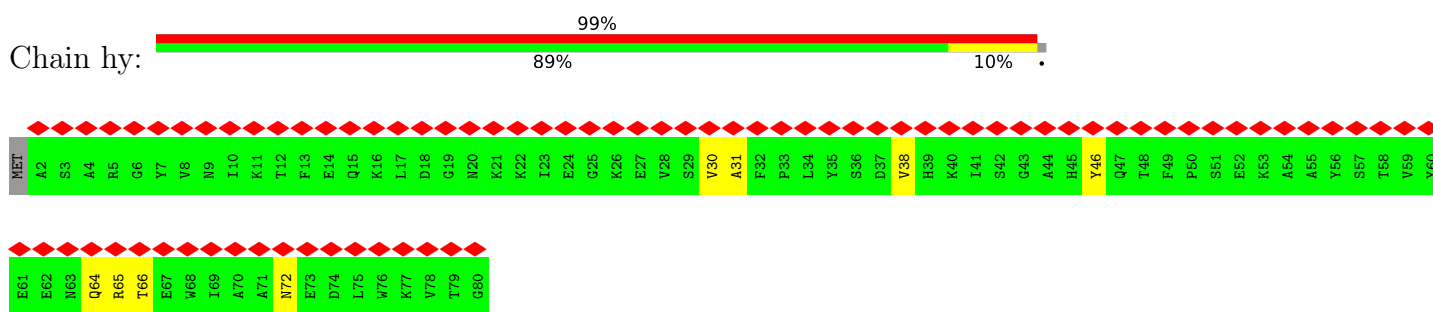
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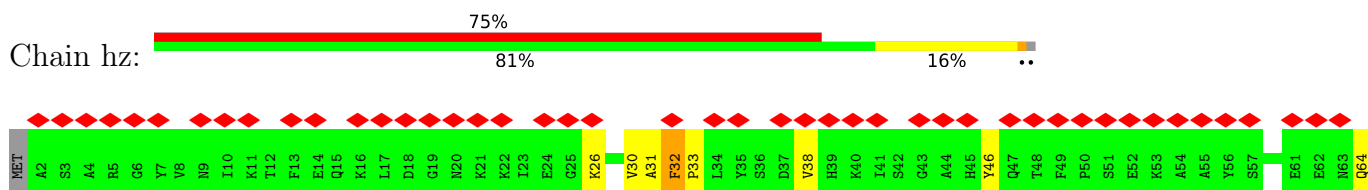
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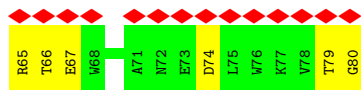


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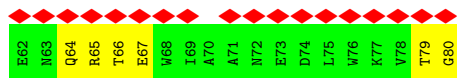
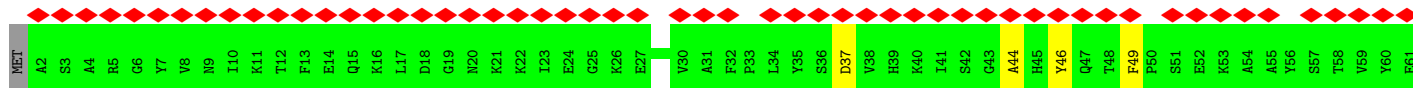
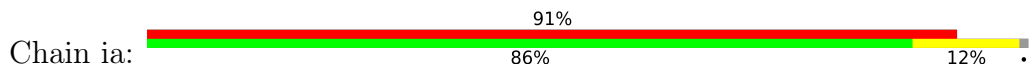


• Molecule 3: Small outer capsid protein

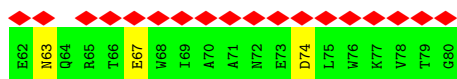
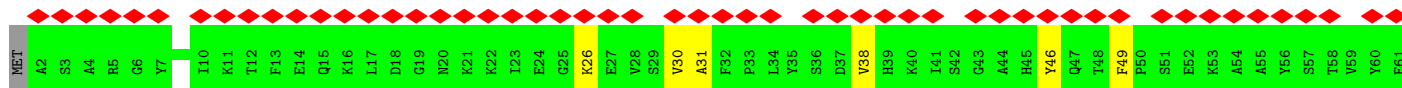
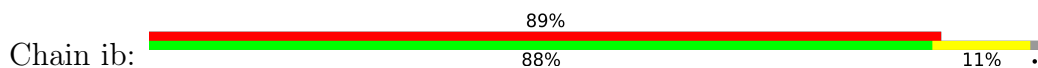




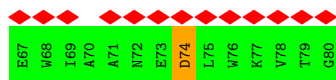
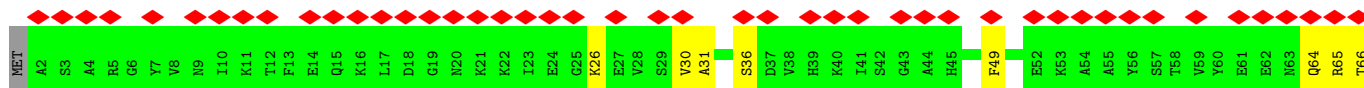
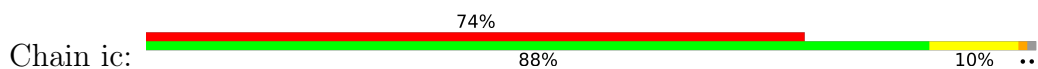
• Molecule 3: Small outer capsid protein



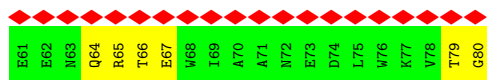
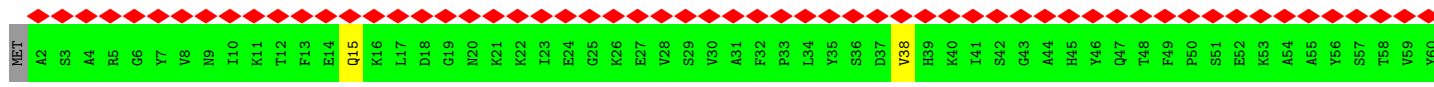
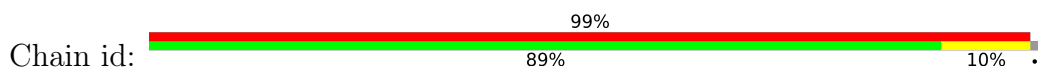
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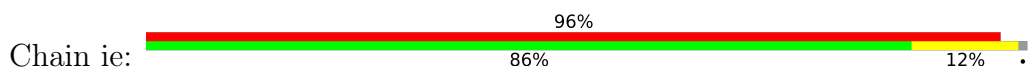
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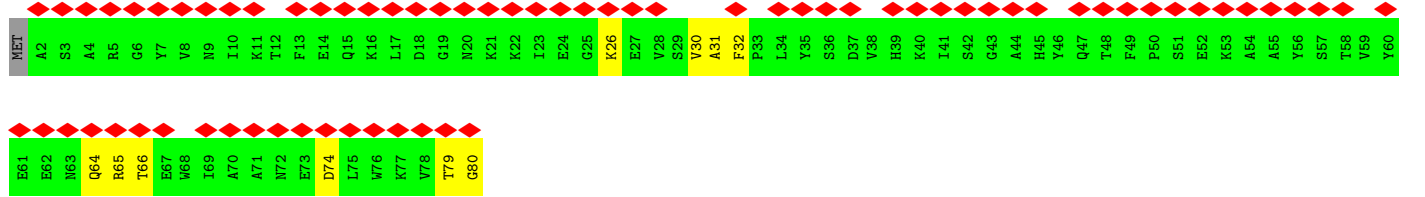
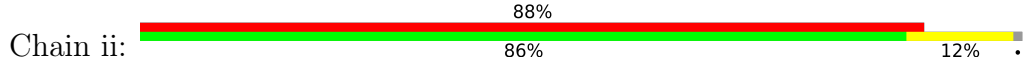
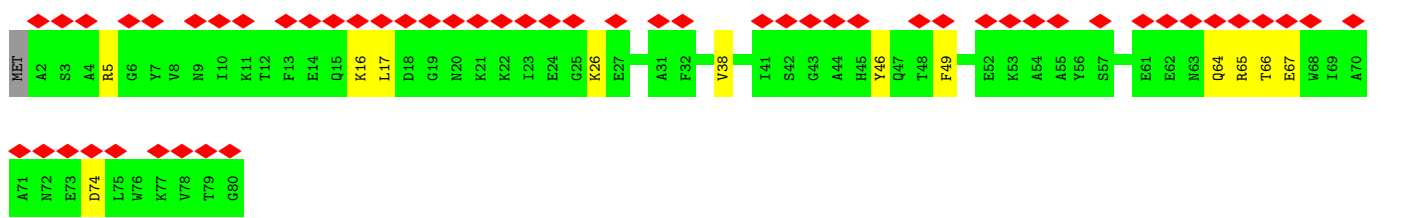
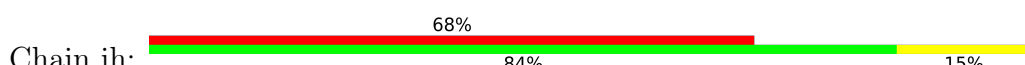
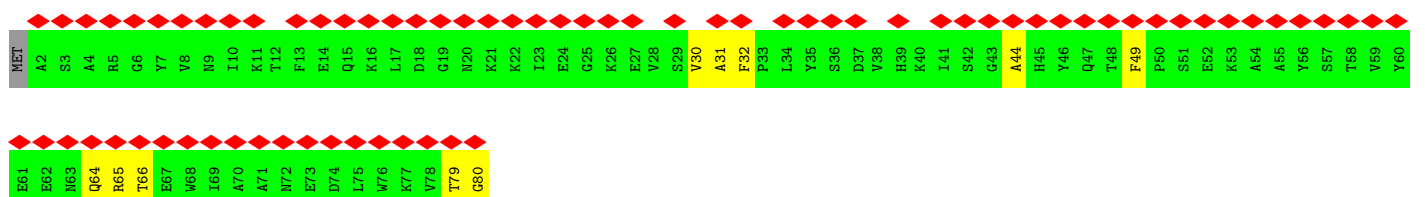
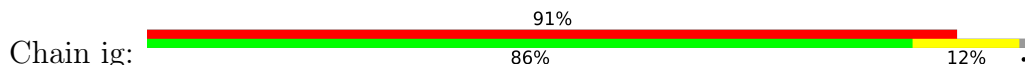
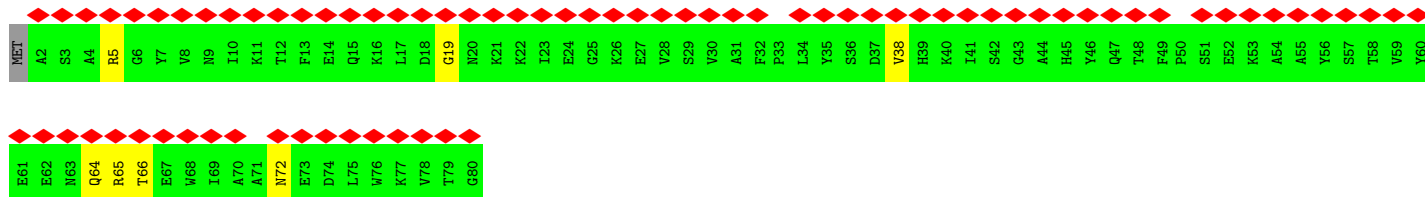
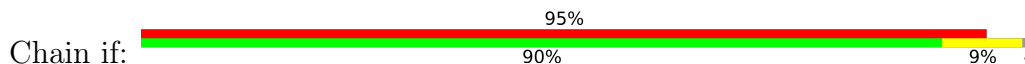
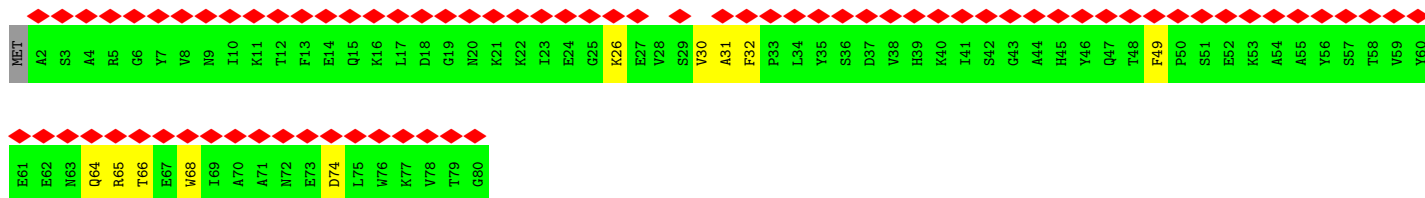


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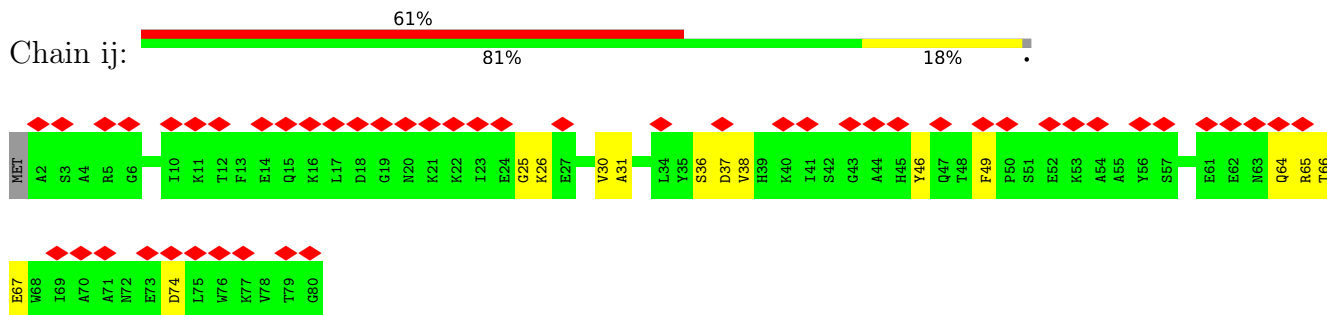


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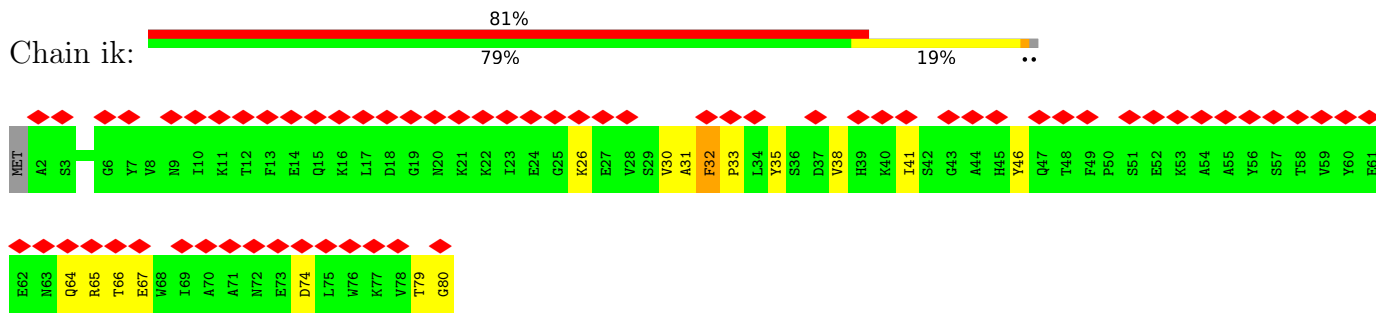




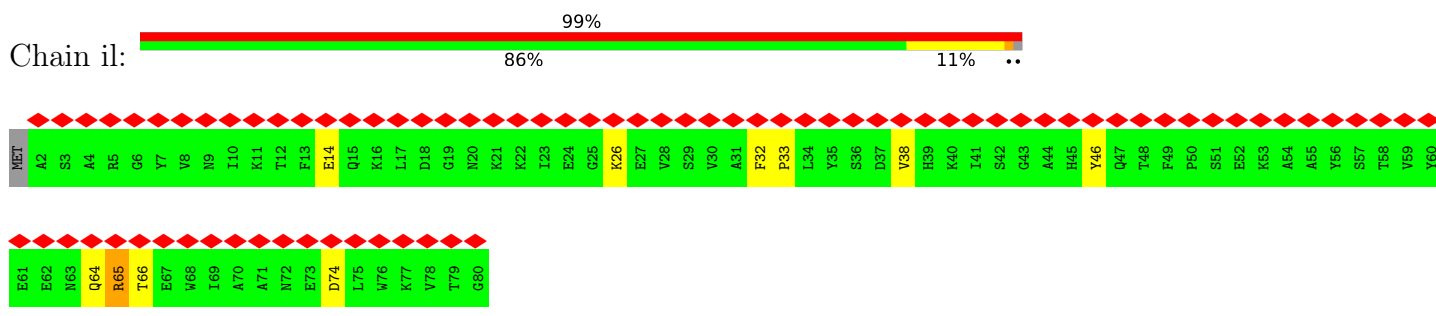
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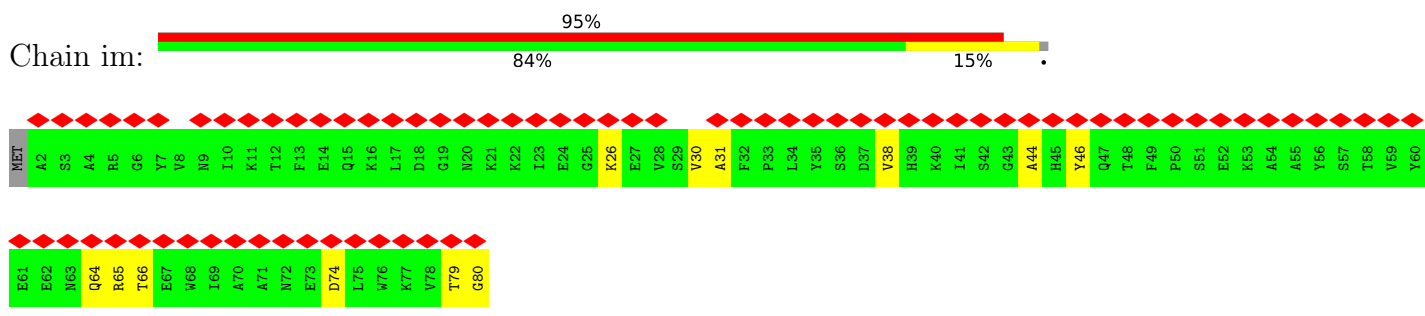
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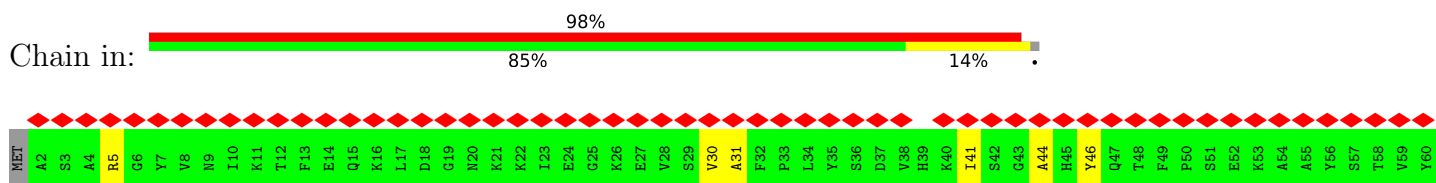
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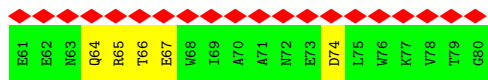


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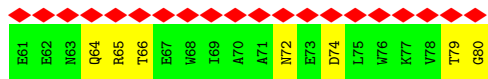
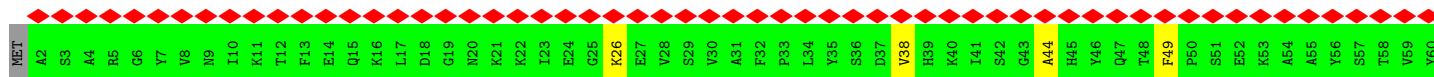
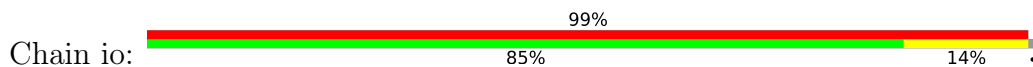


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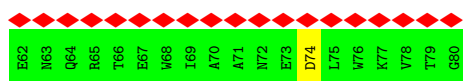
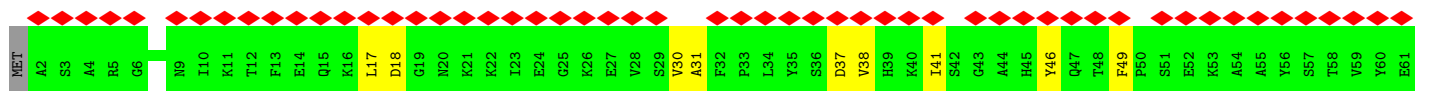
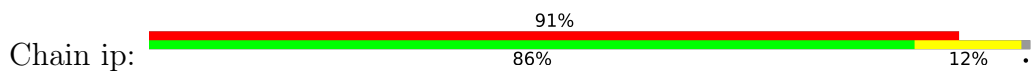




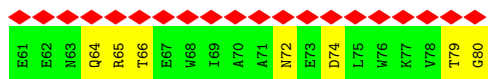
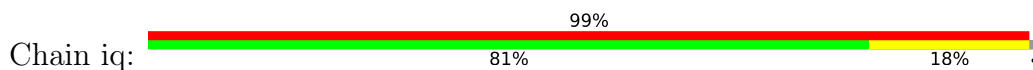
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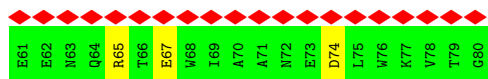
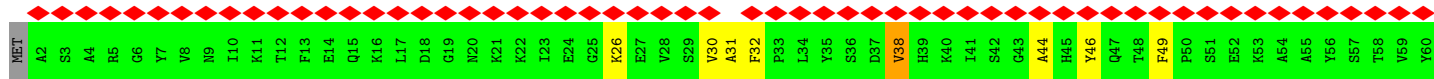
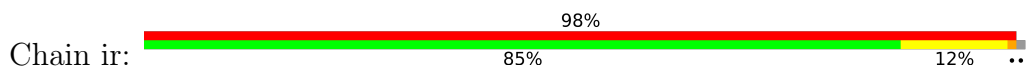
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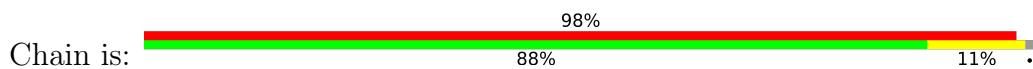
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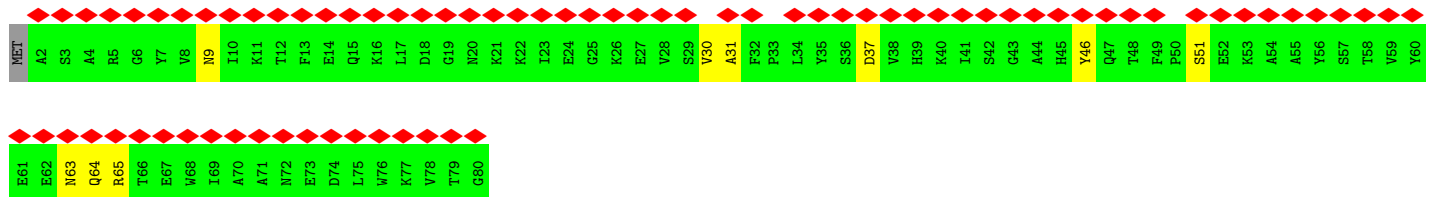
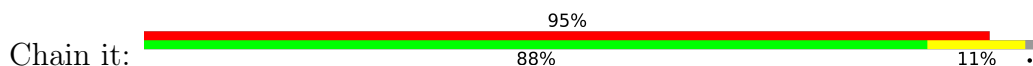


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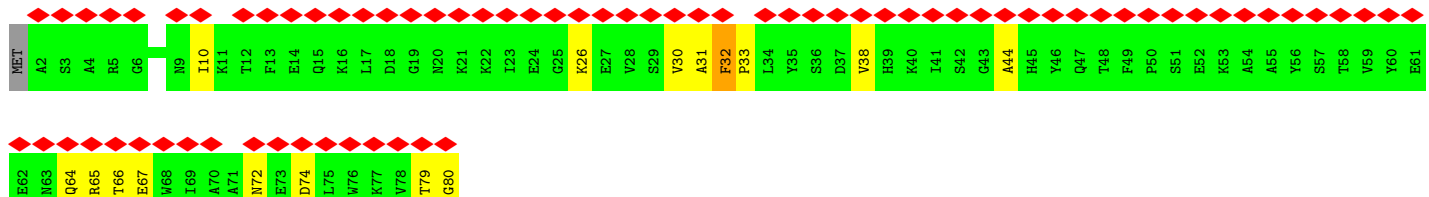
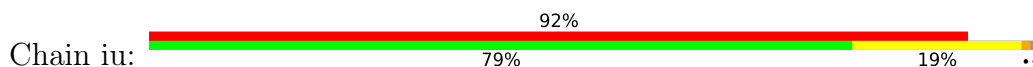




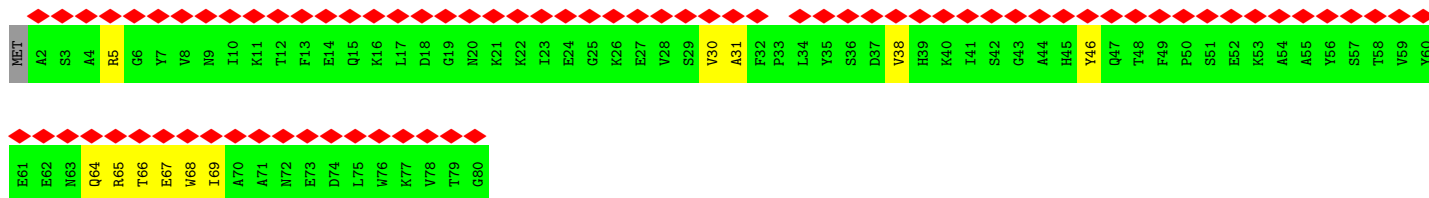
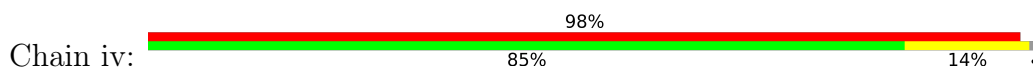
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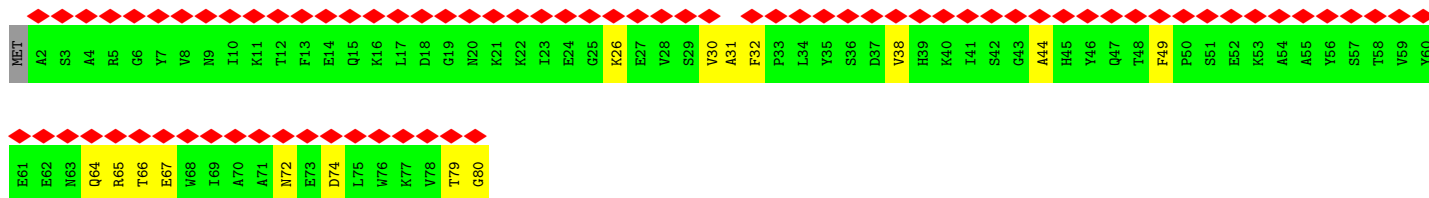
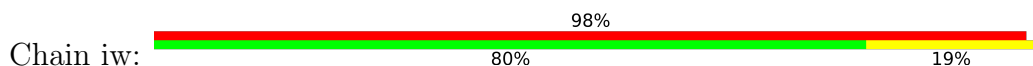
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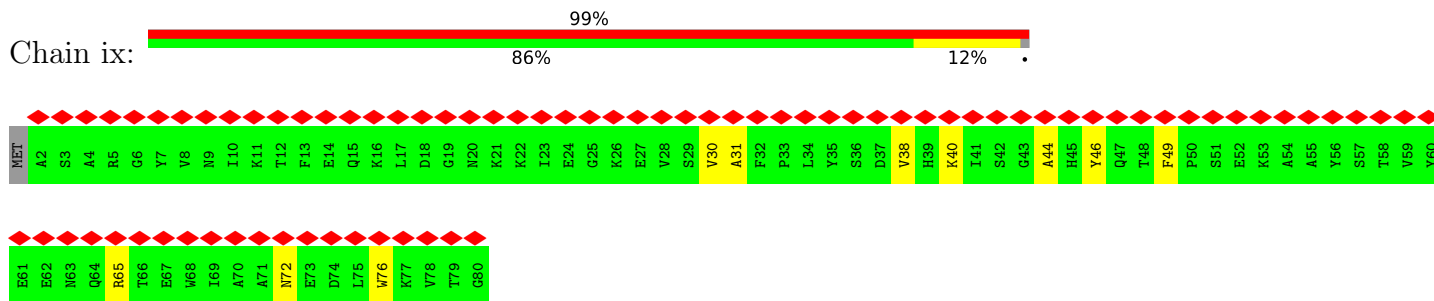
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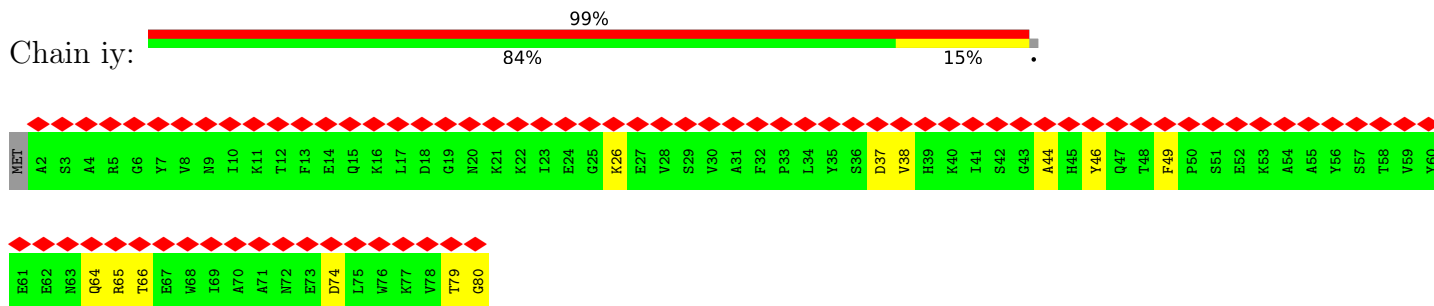
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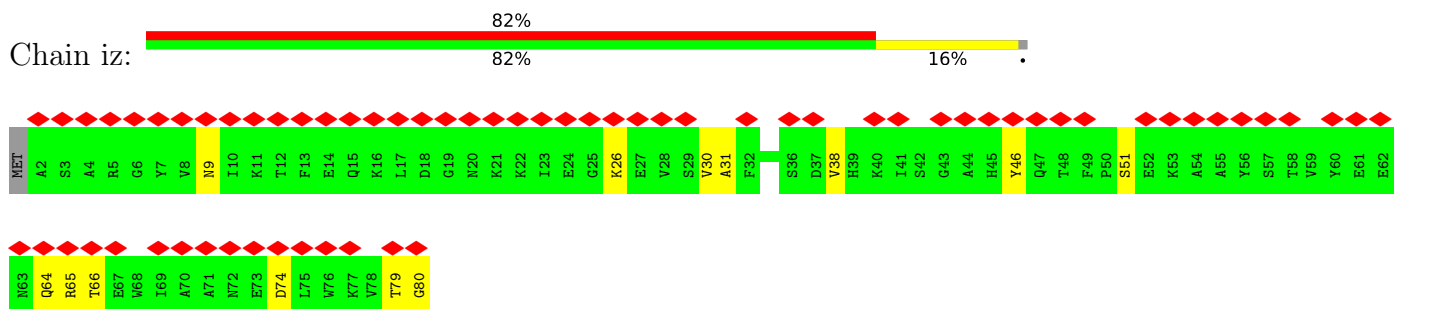
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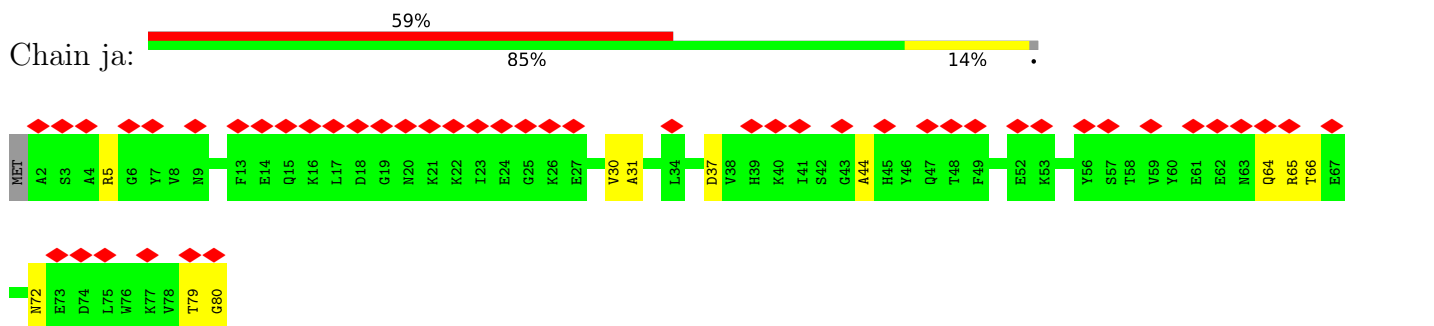
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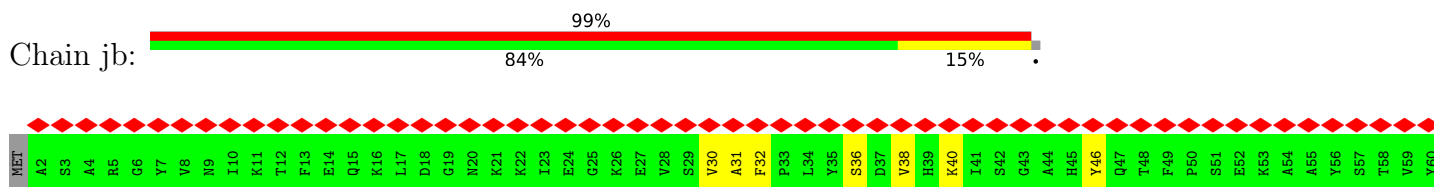
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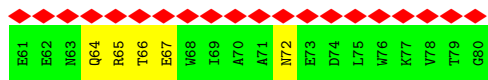


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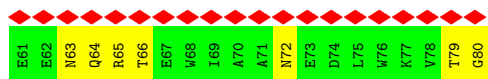
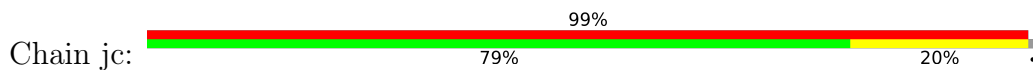


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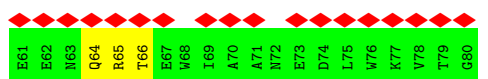
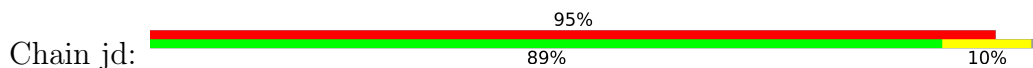




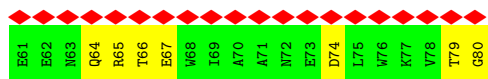
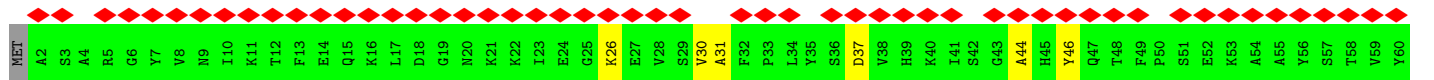
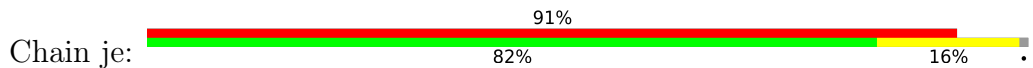
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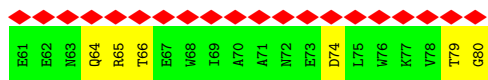
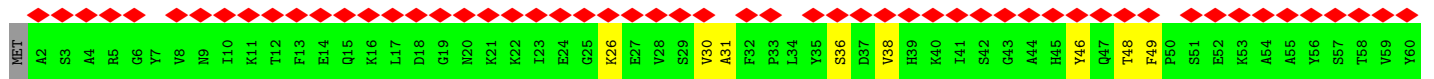
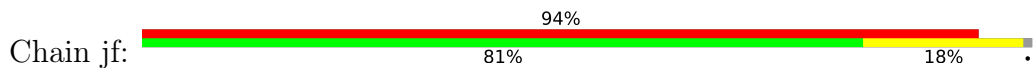
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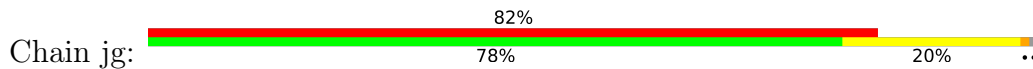
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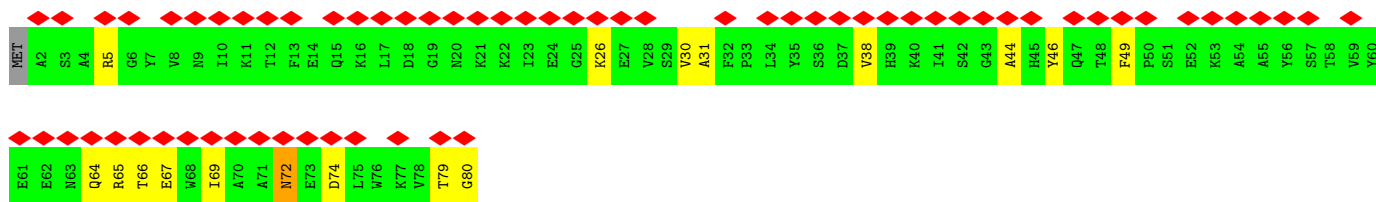


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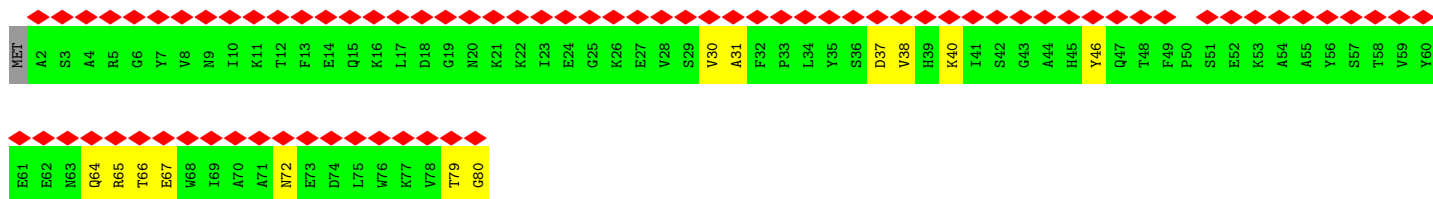
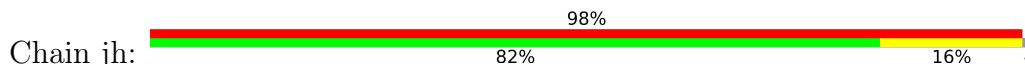


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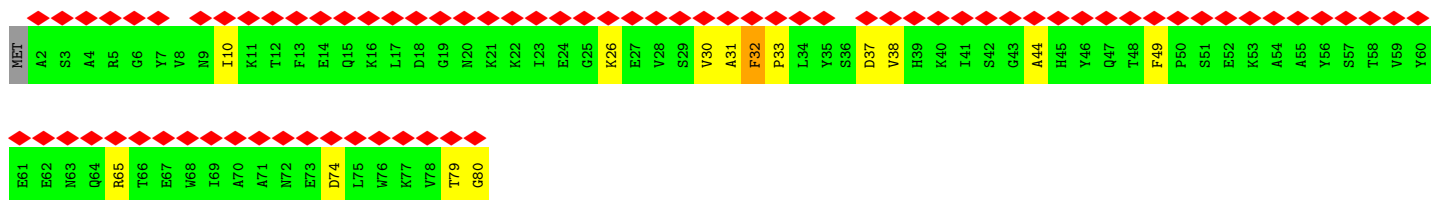
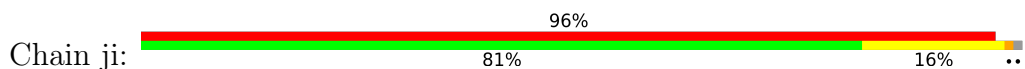




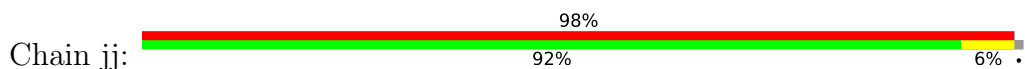
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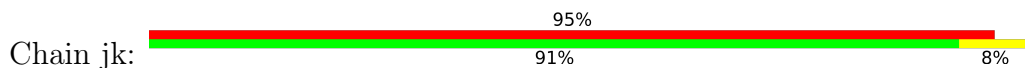
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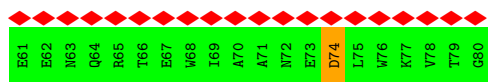
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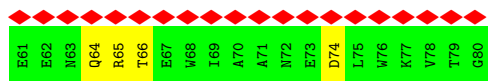
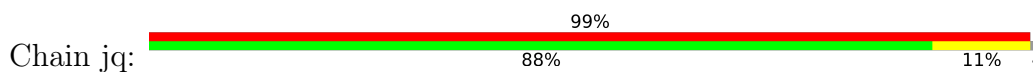
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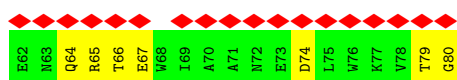
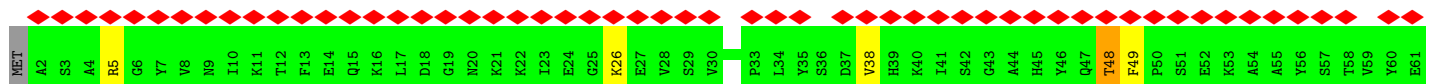
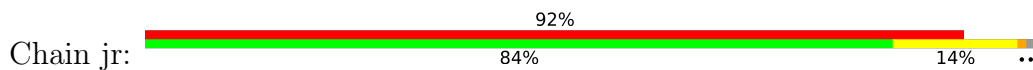




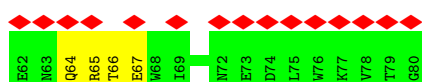
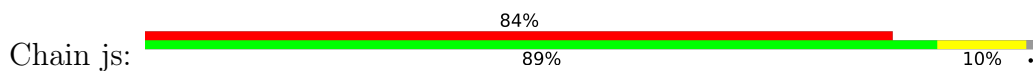
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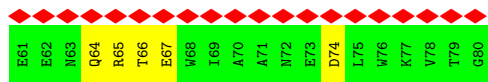
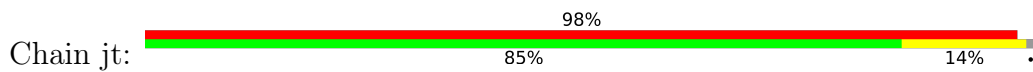
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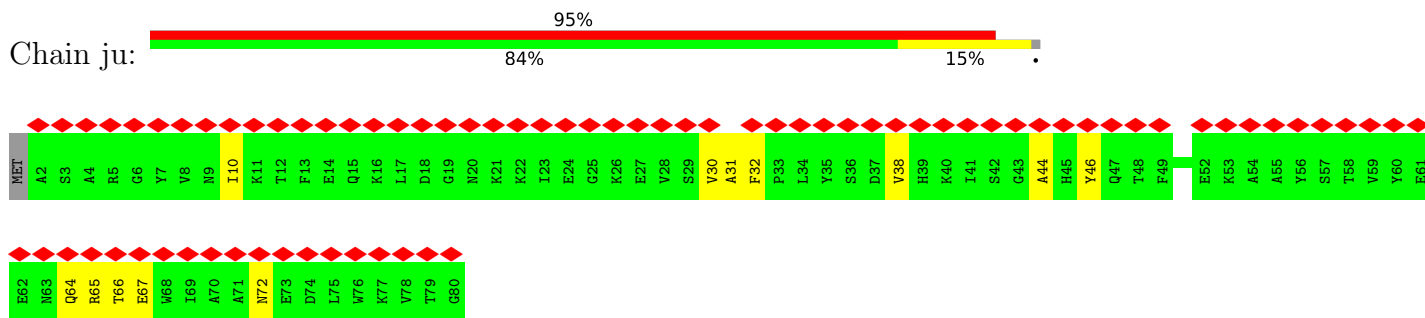
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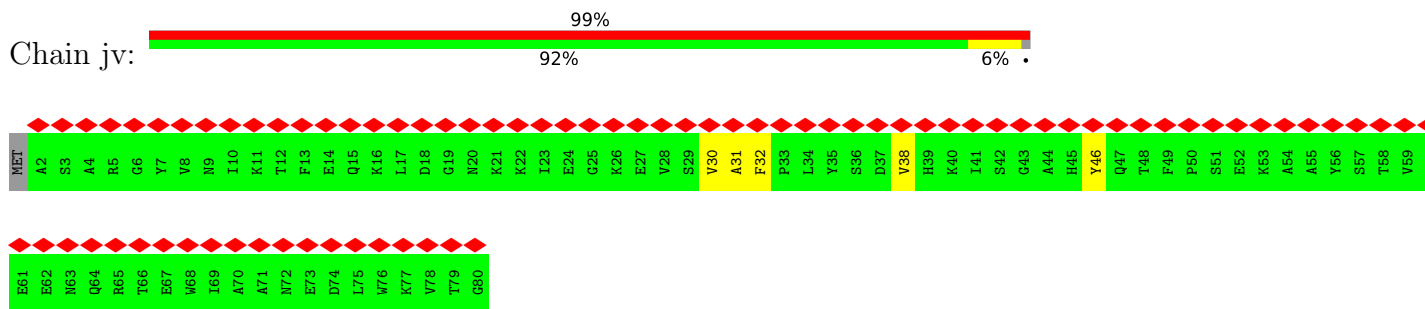
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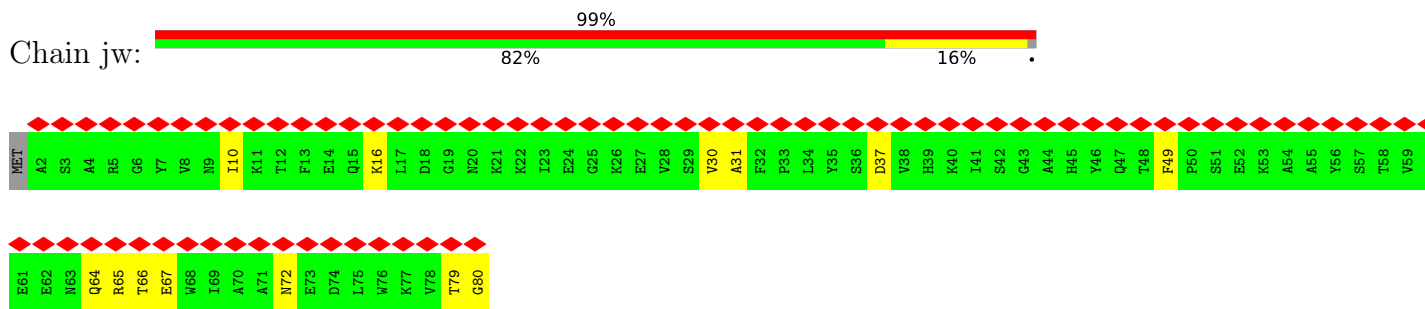
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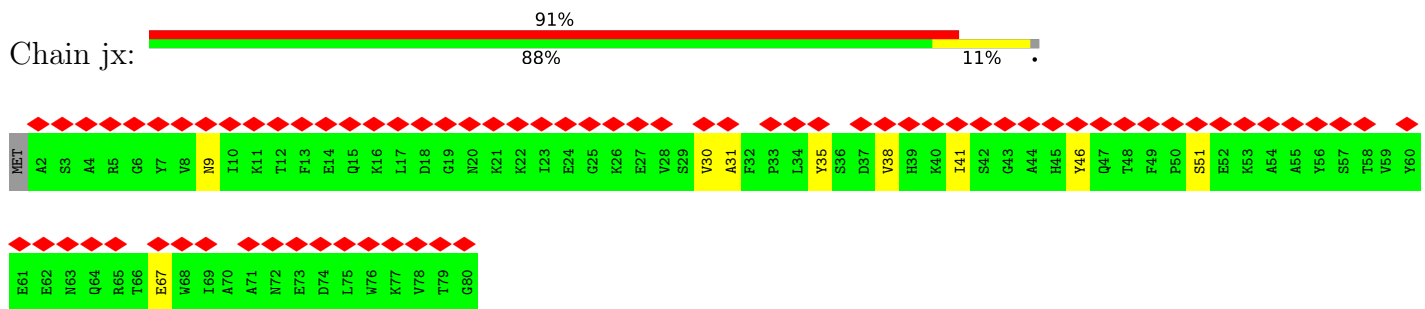
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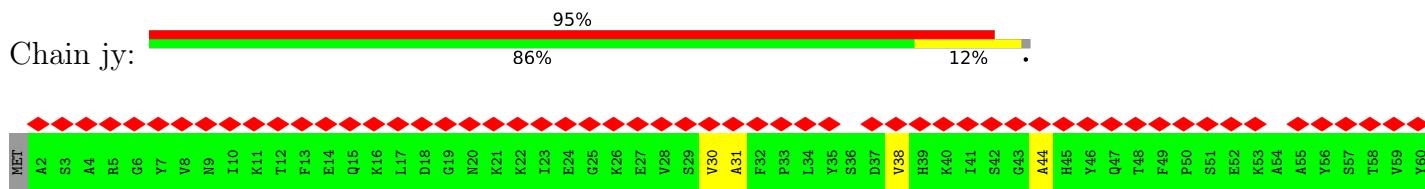
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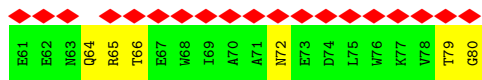


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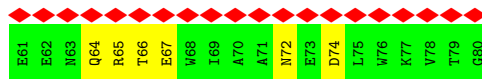
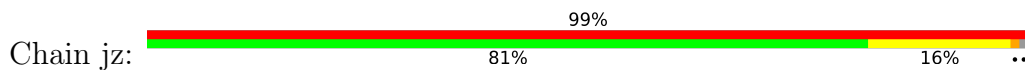


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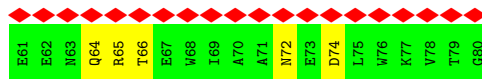
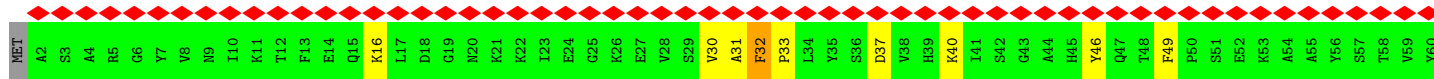
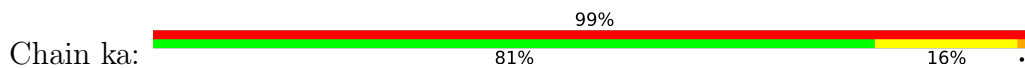




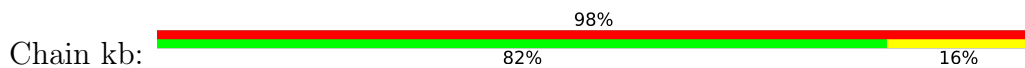
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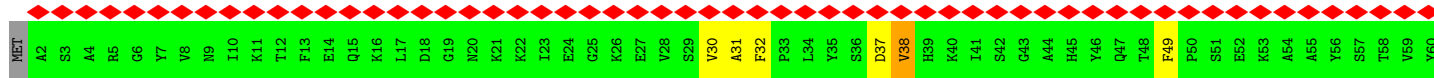
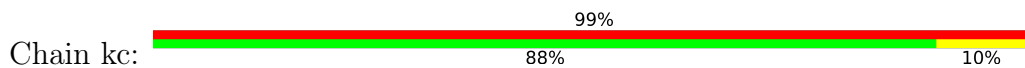
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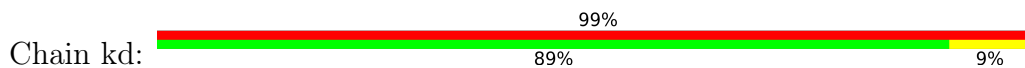
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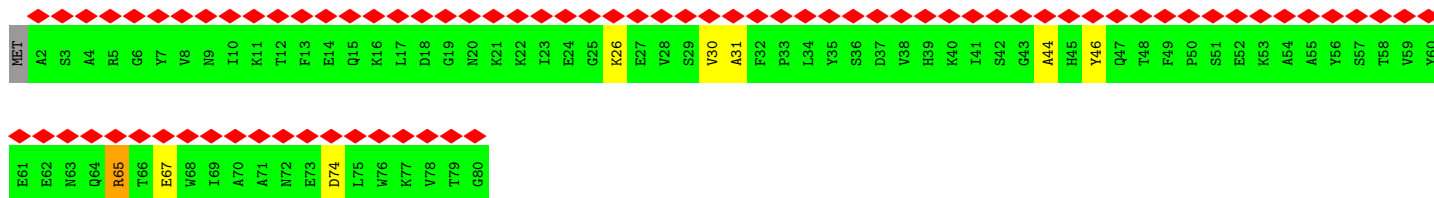


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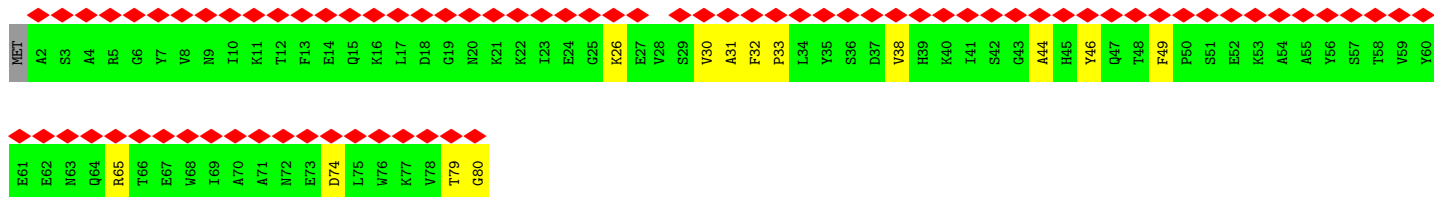
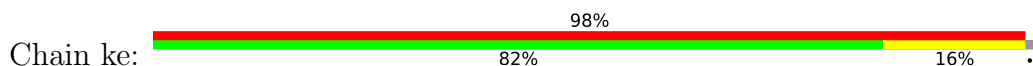


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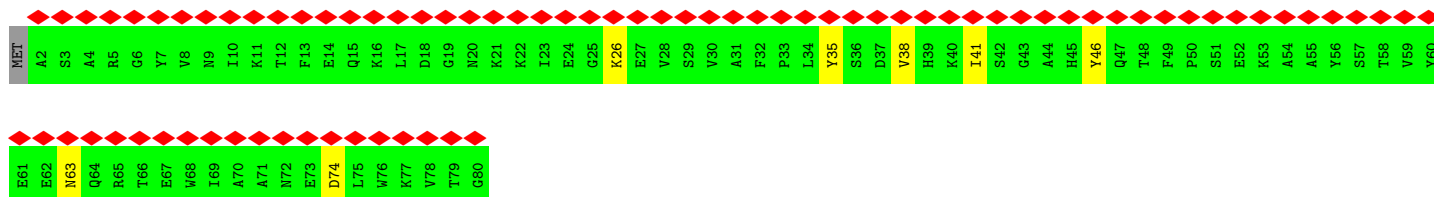
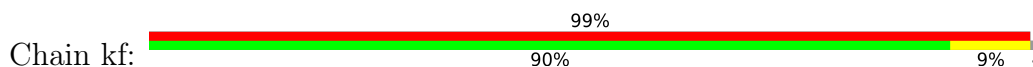




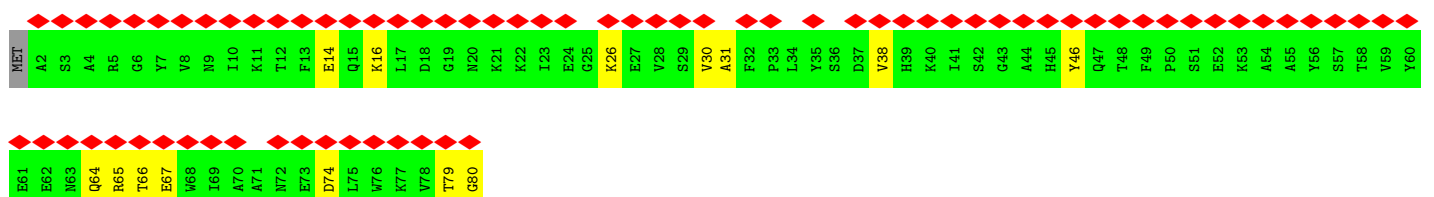
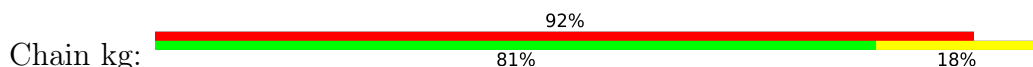
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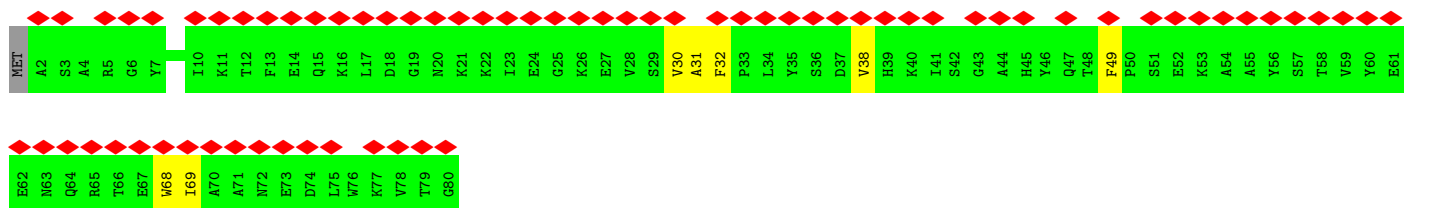
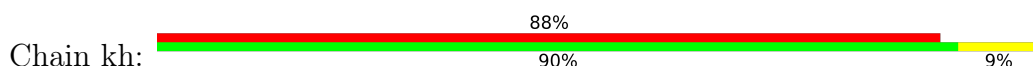
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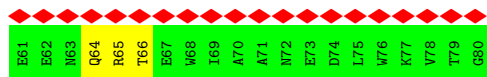
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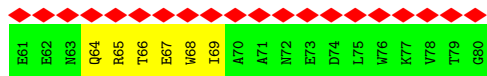
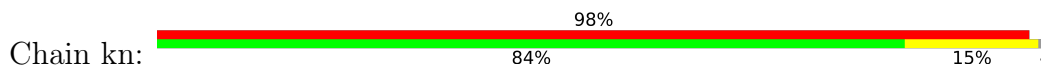
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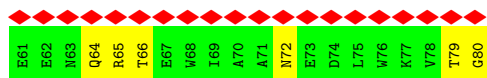
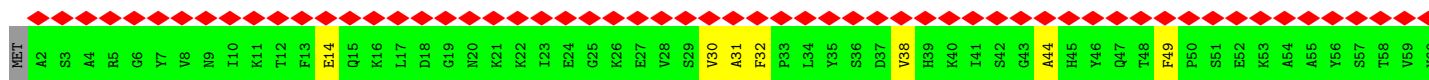
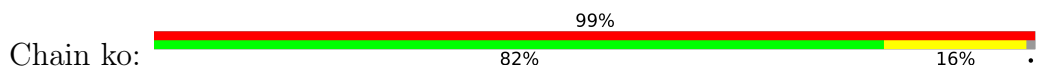




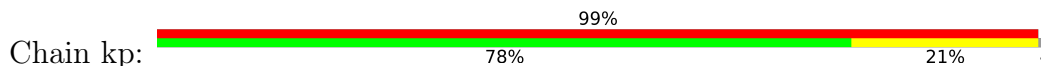
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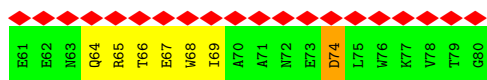
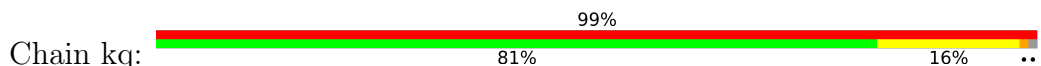
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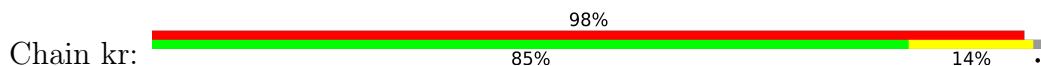
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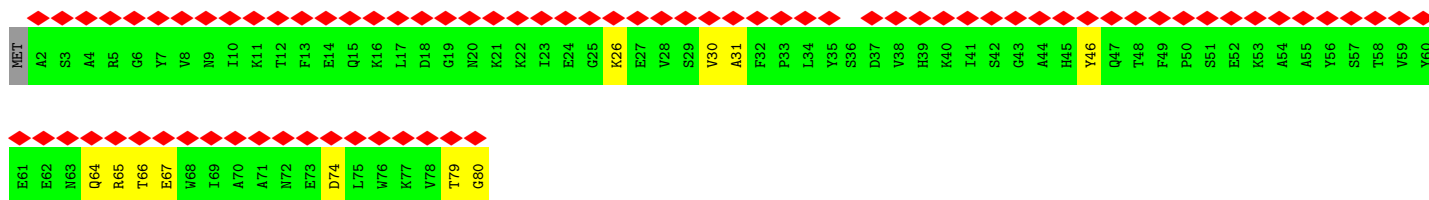


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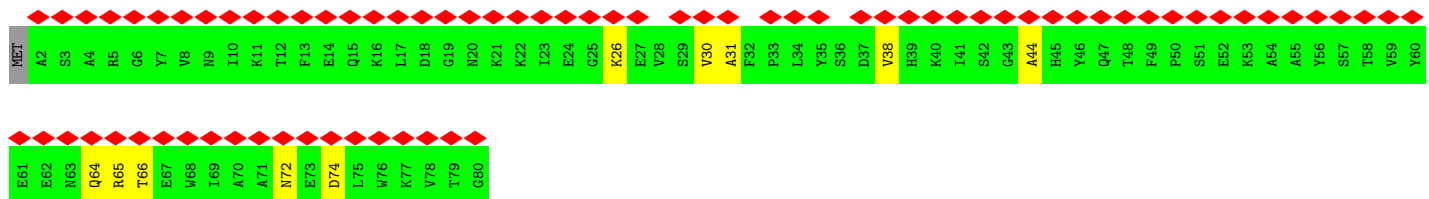
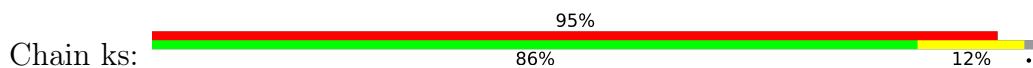


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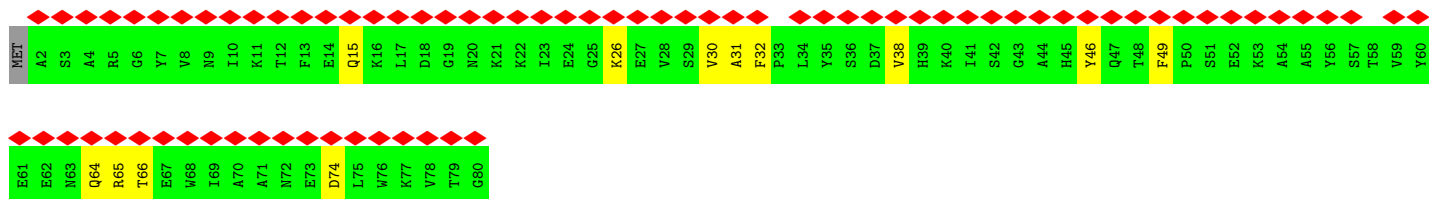
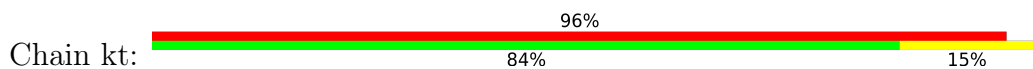




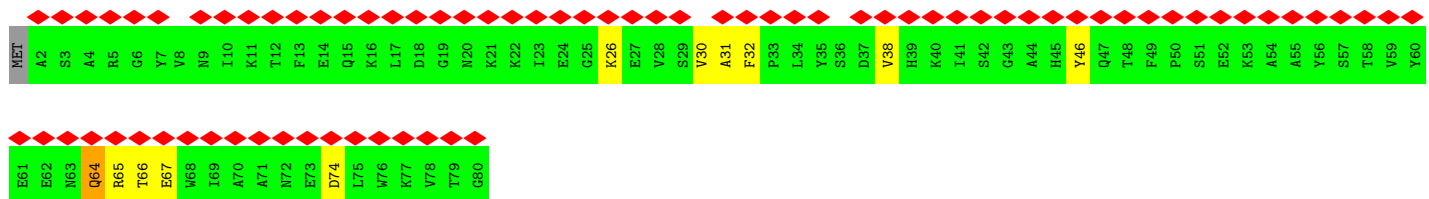
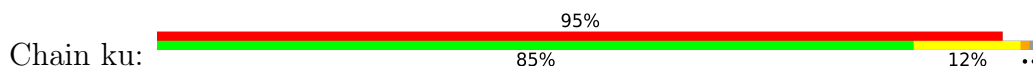
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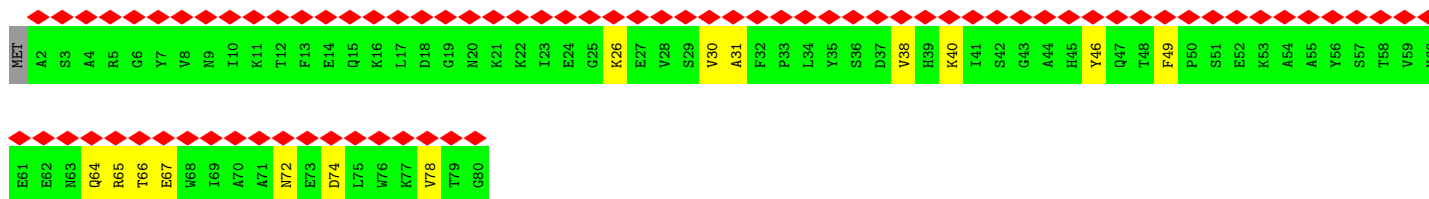
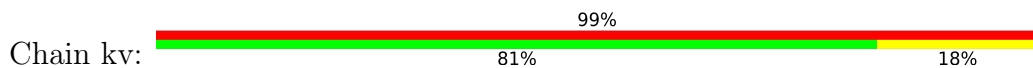
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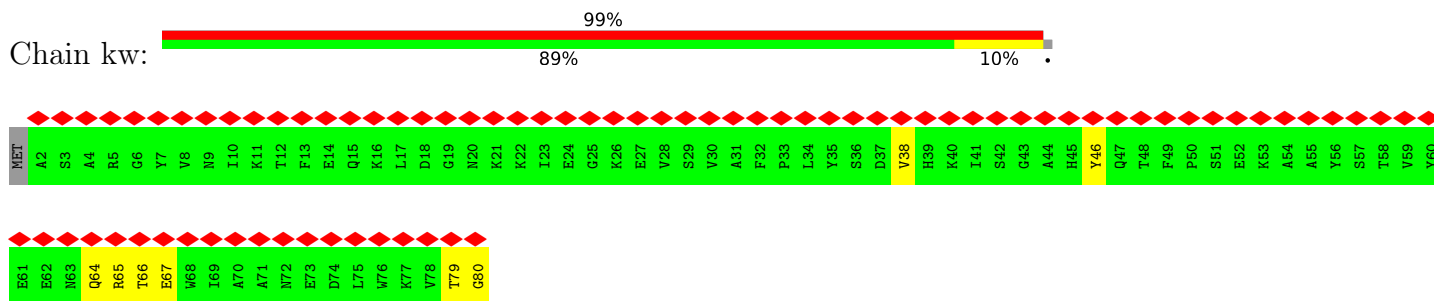
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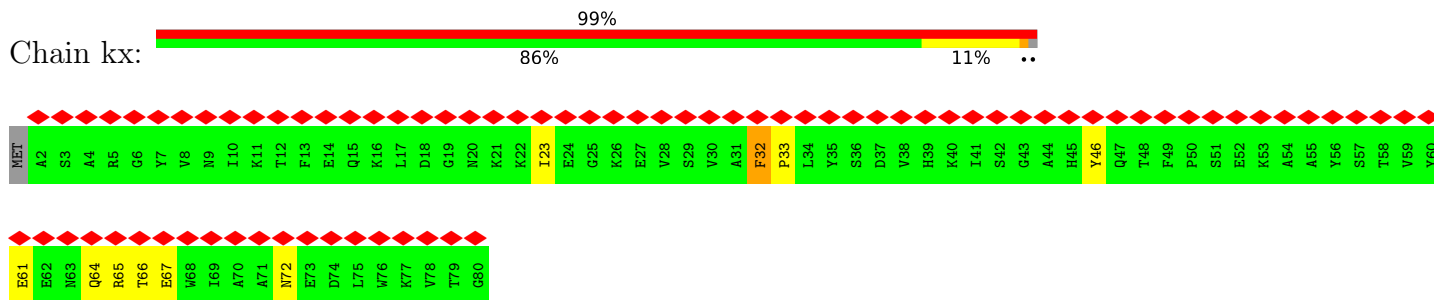
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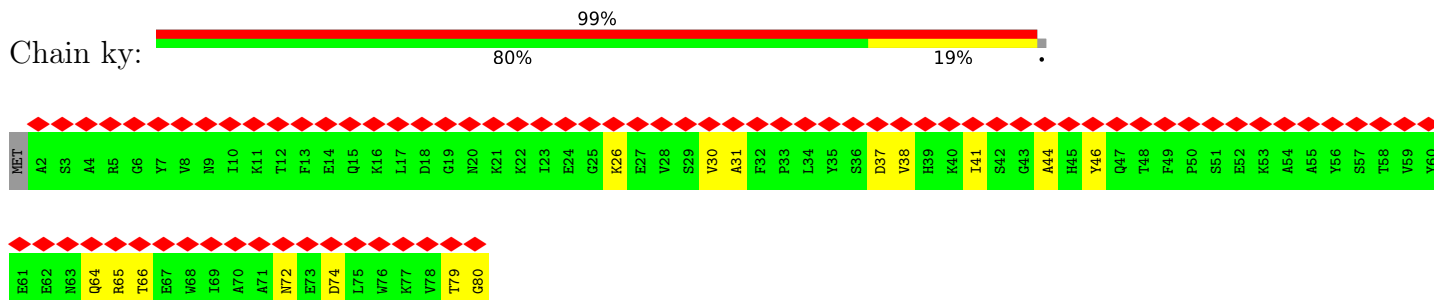
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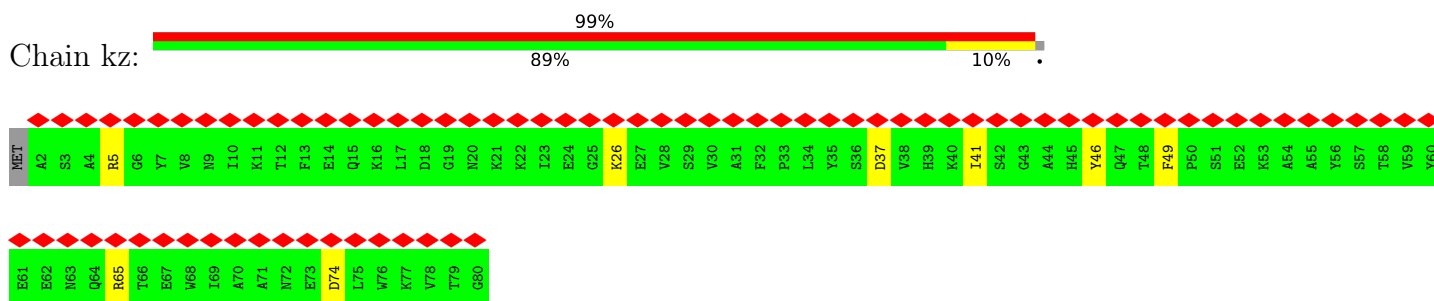
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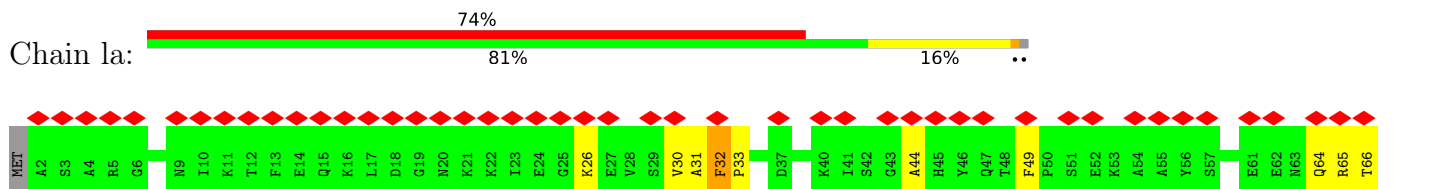
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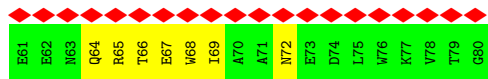
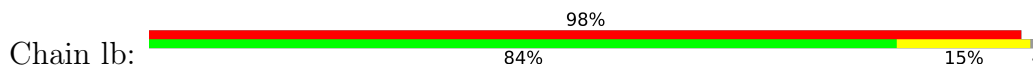


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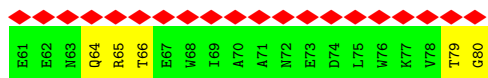
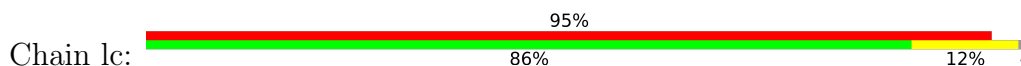




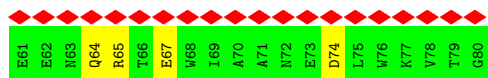
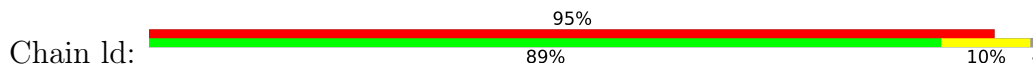
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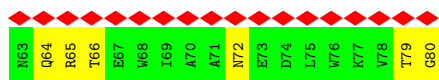
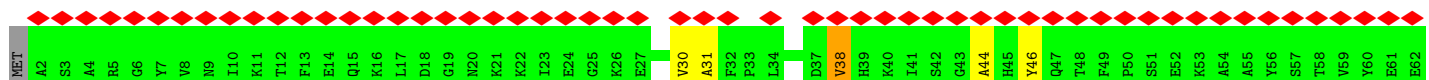
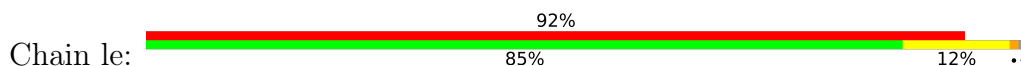
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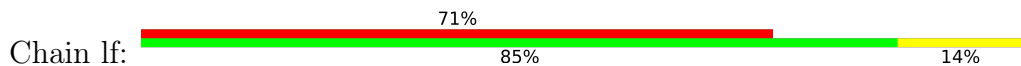
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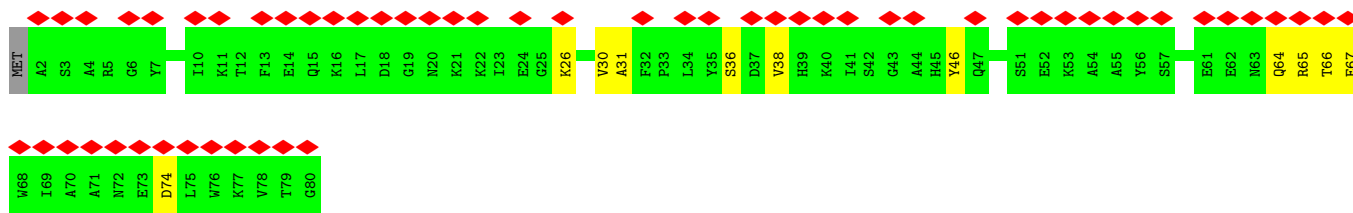


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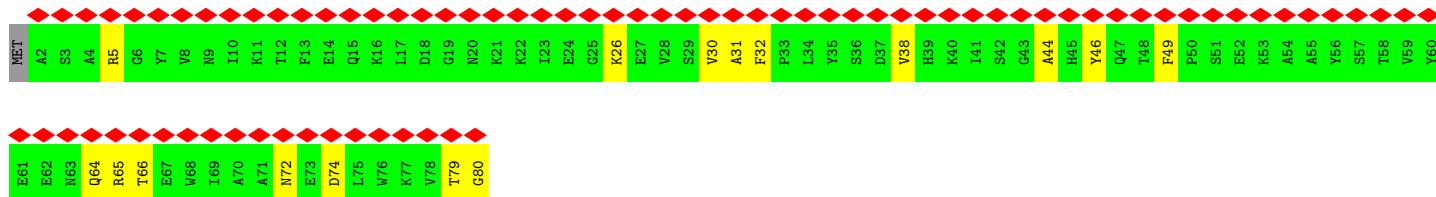
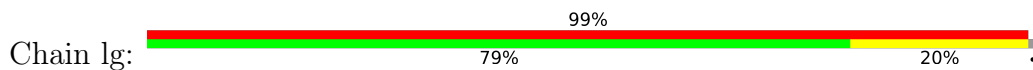


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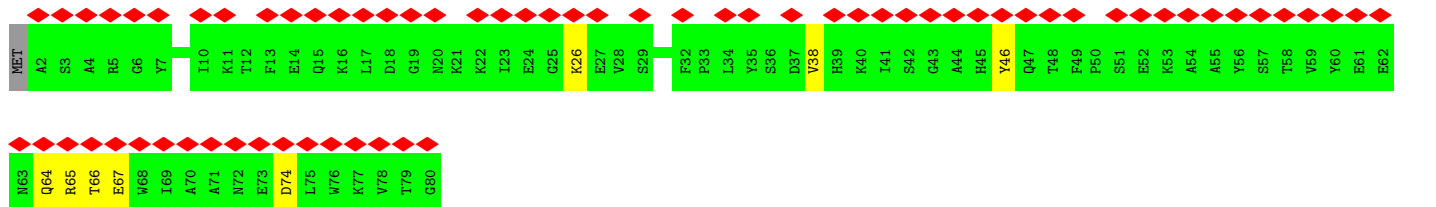
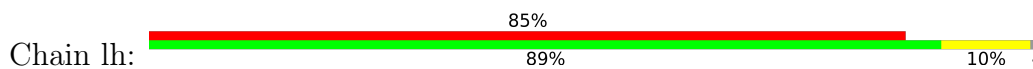




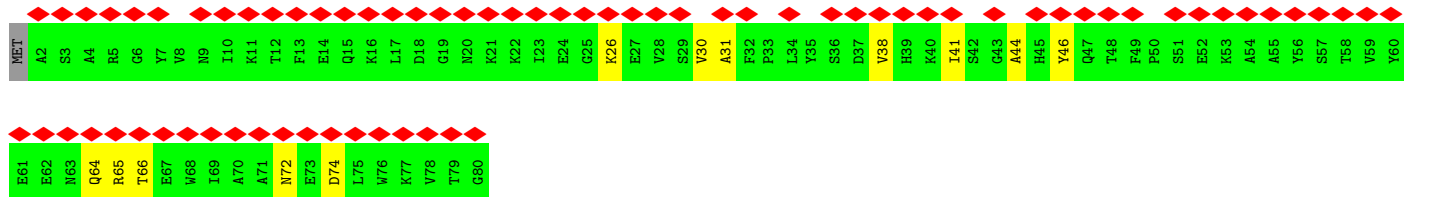
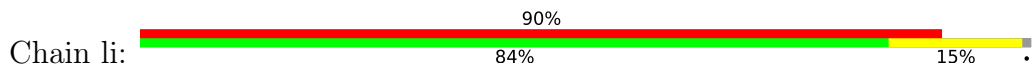
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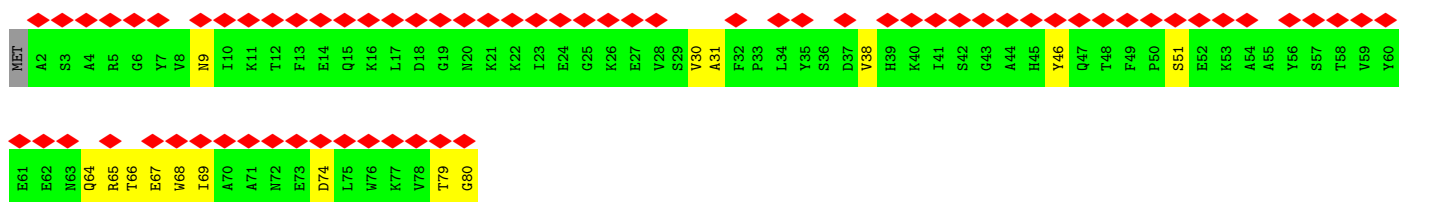
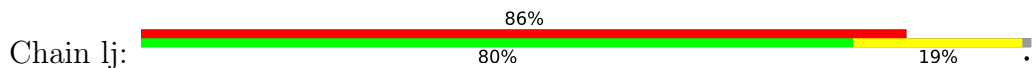
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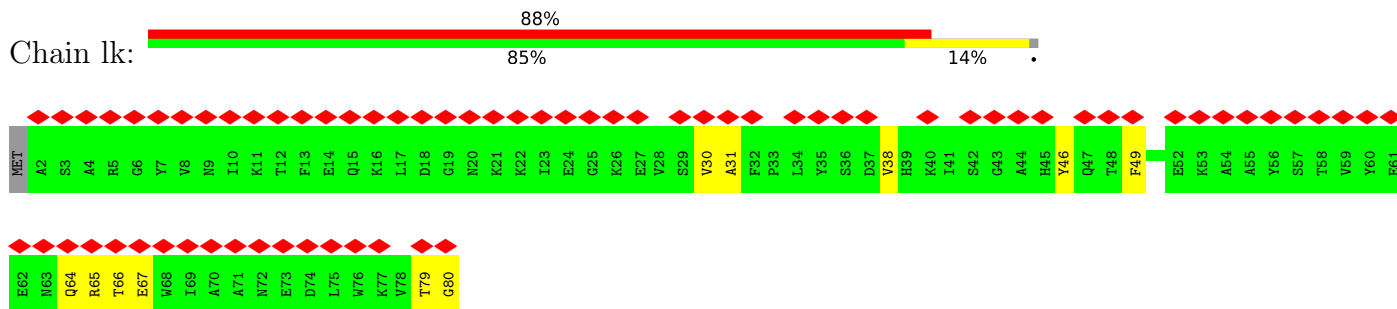
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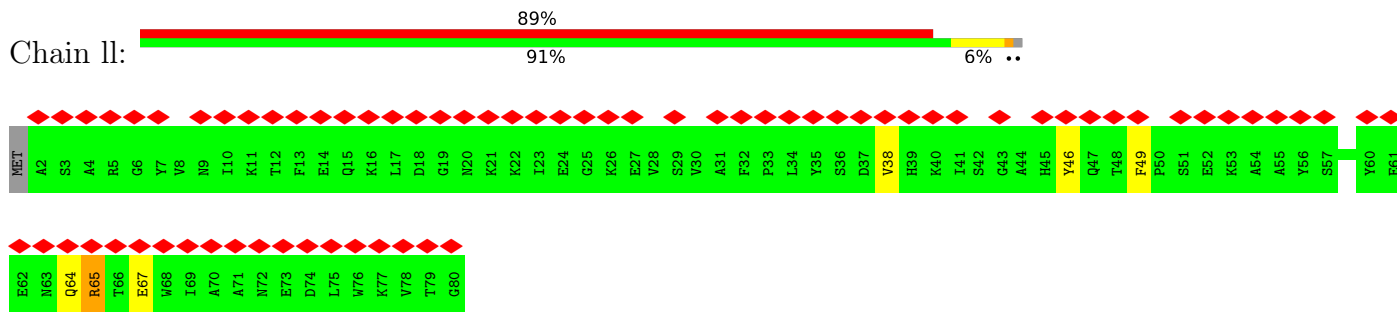
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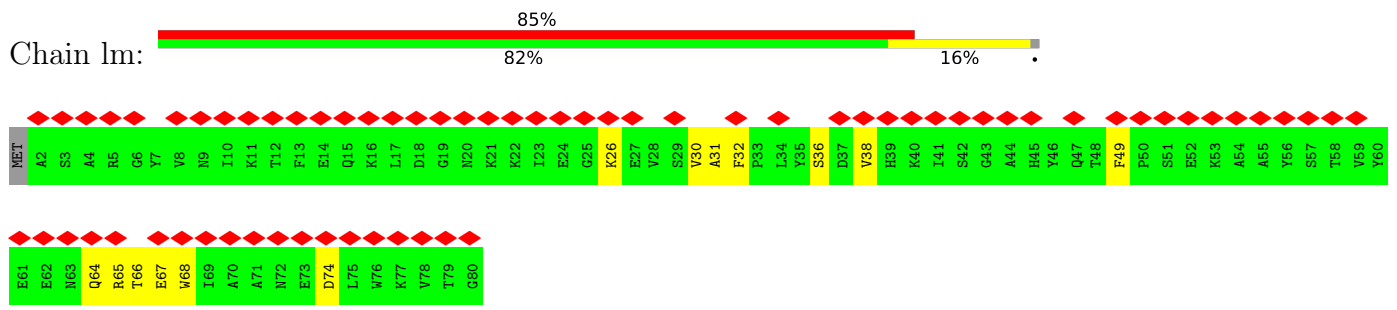
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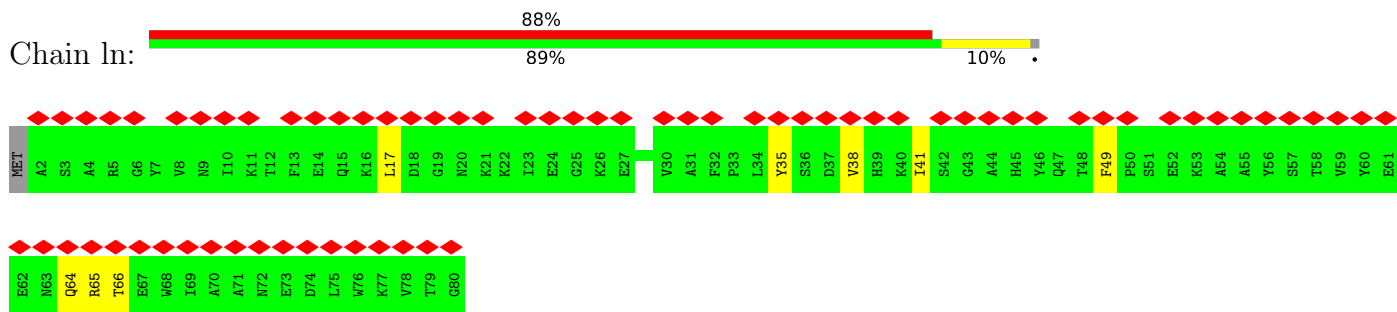
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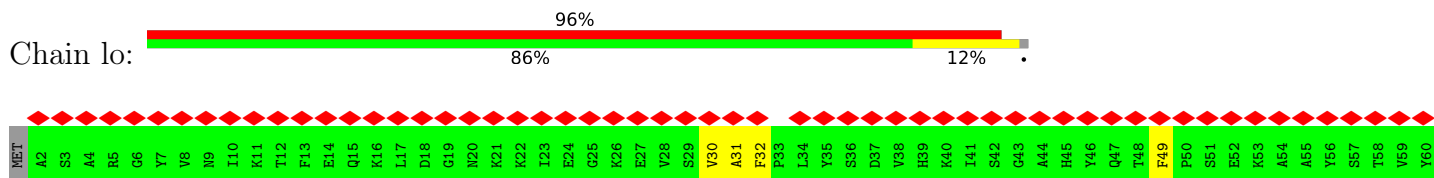
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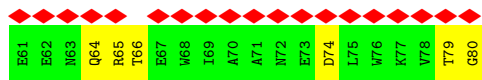


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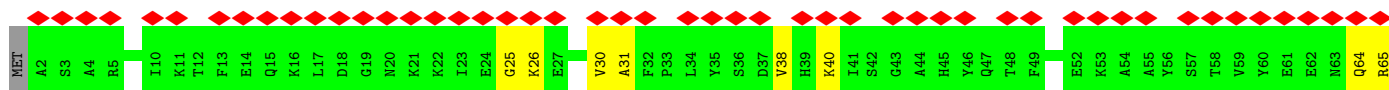
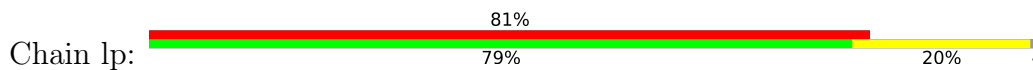


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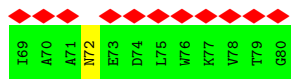
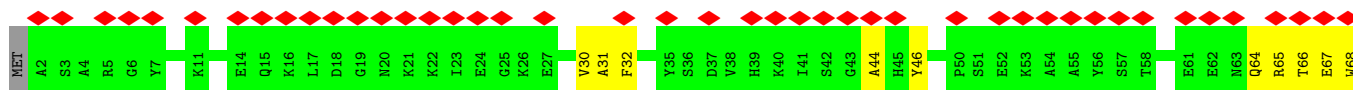
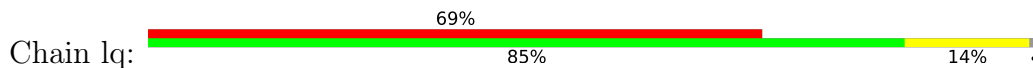




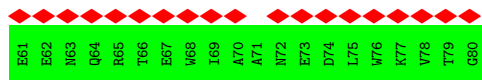
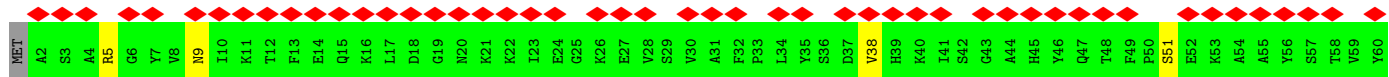
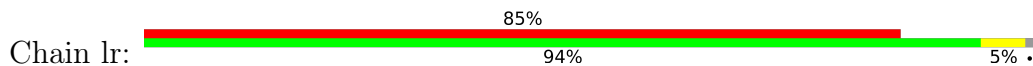
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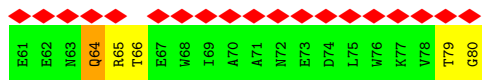
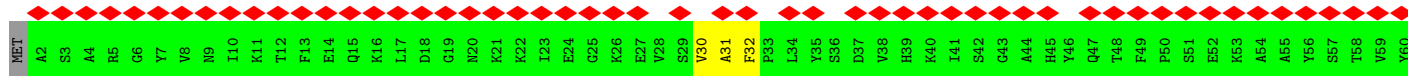
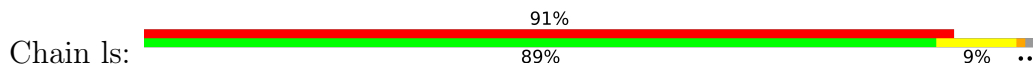
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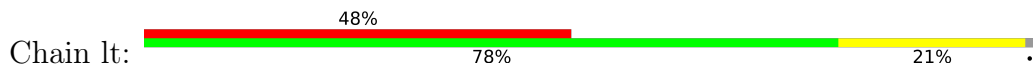
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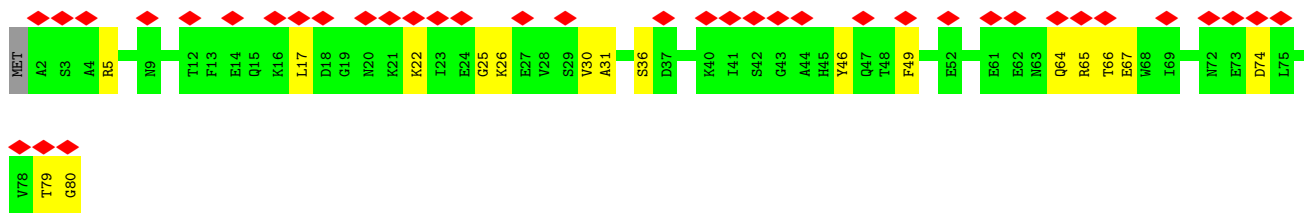


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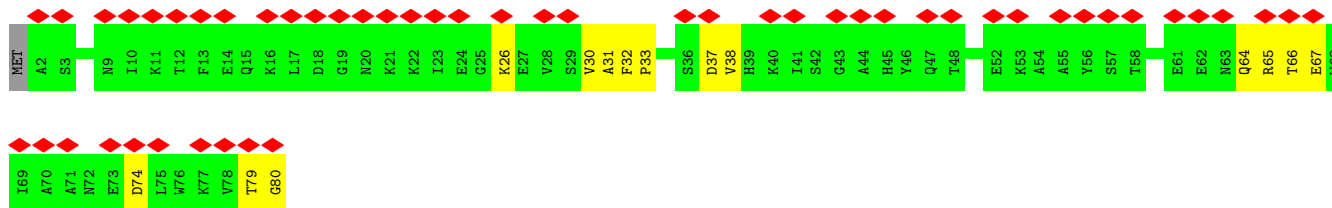
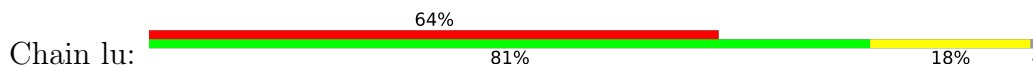


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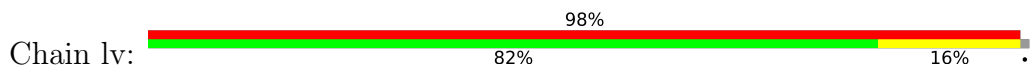




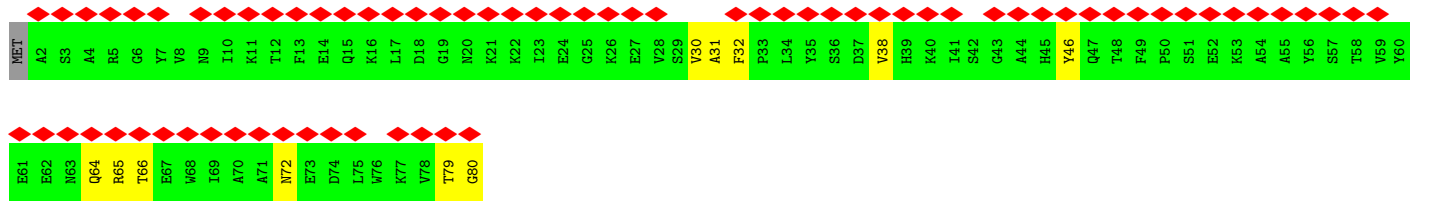
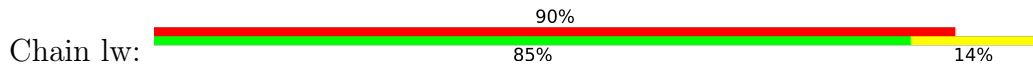
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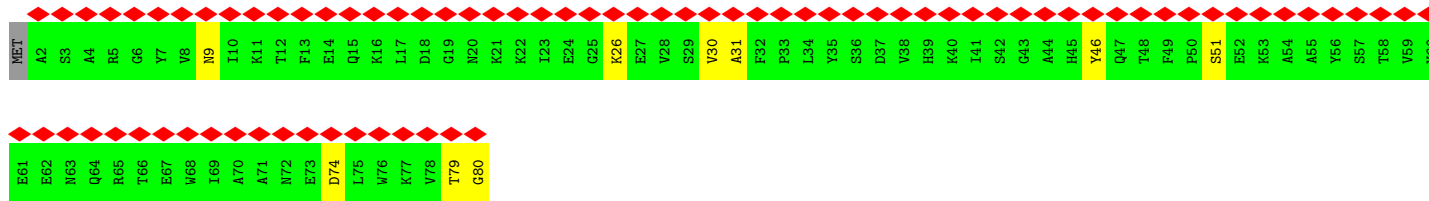
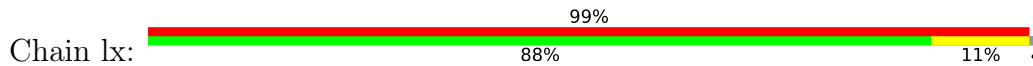
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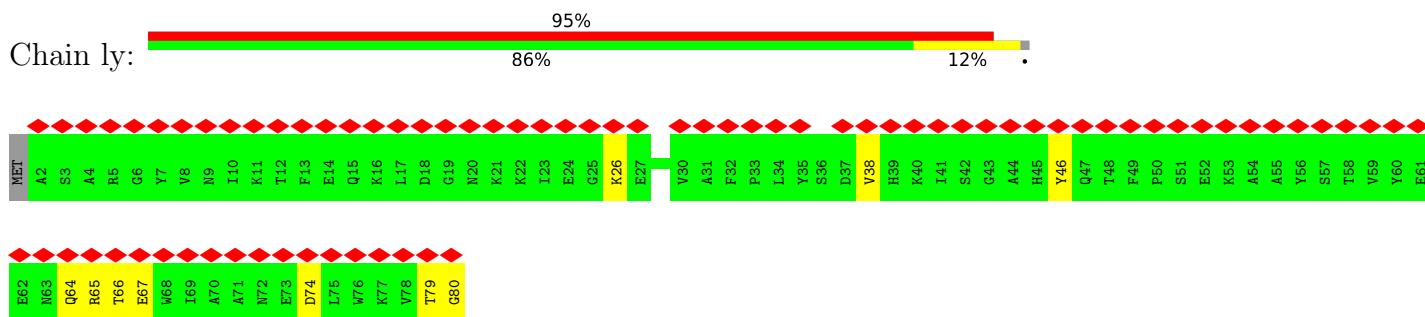
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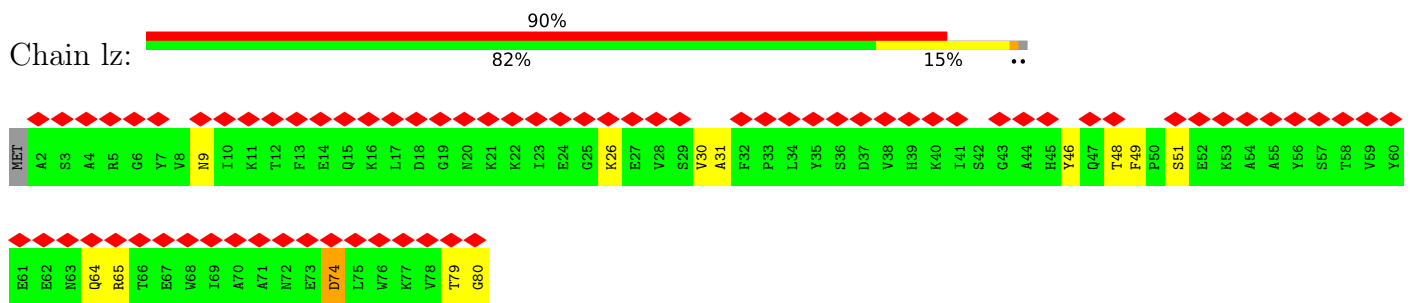
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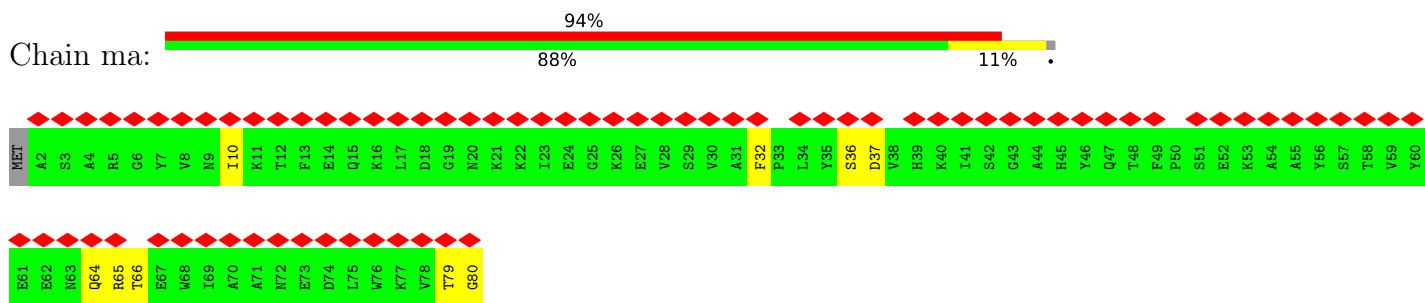
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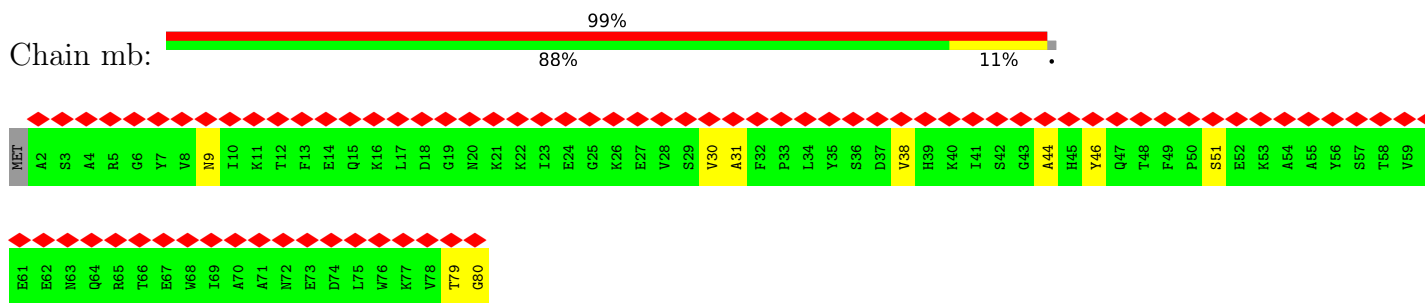
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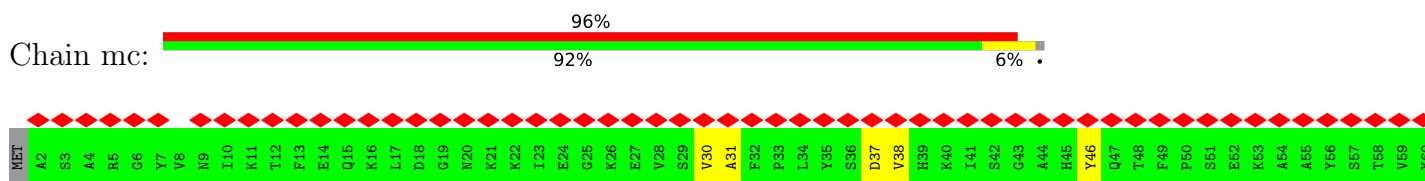
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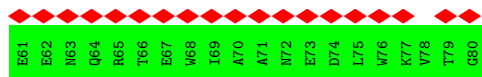


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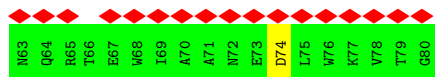


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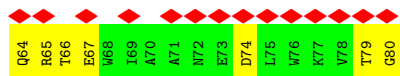
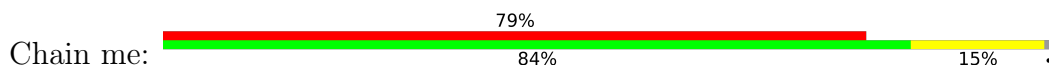




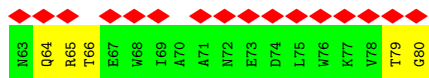
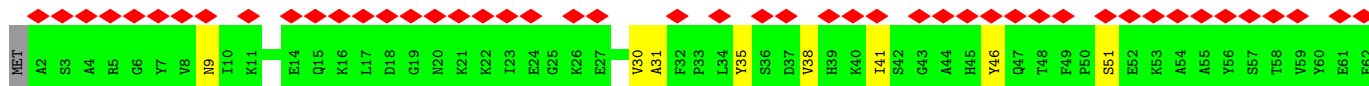
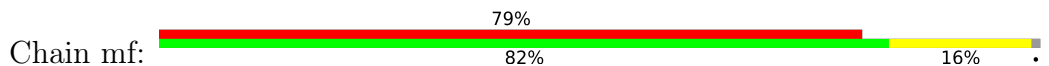
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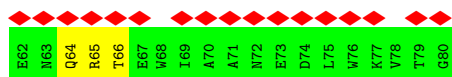
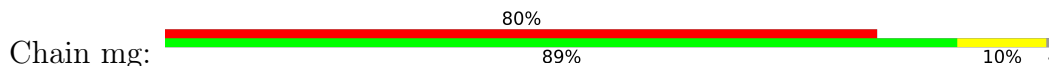
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• Molecule 3: Small outer capsid protein

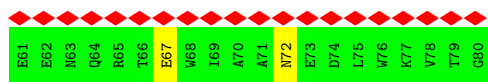


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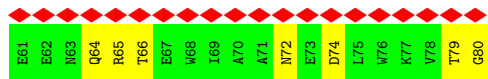
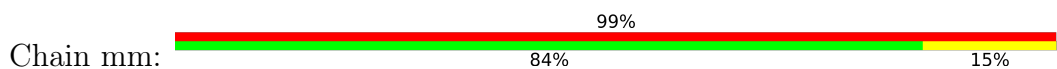


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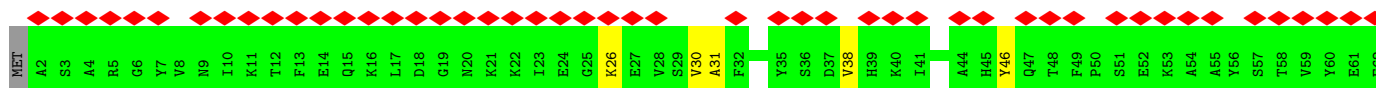
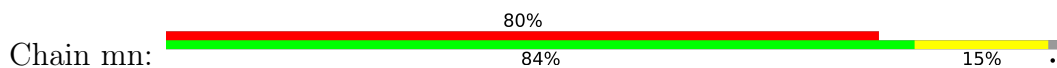




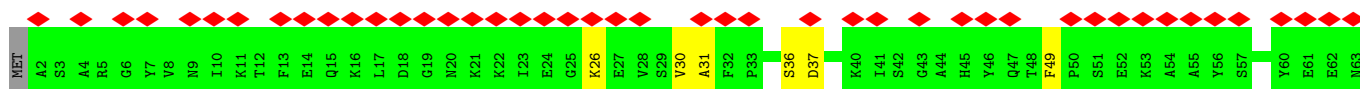
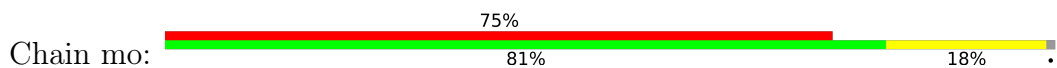
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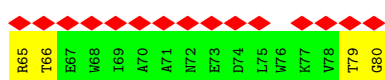
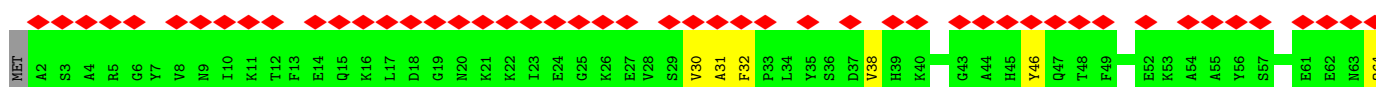
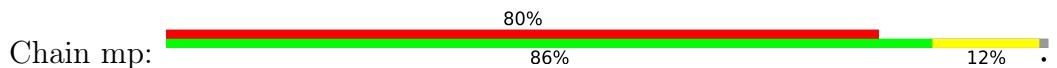
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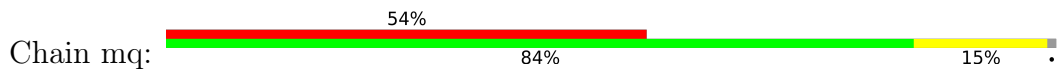
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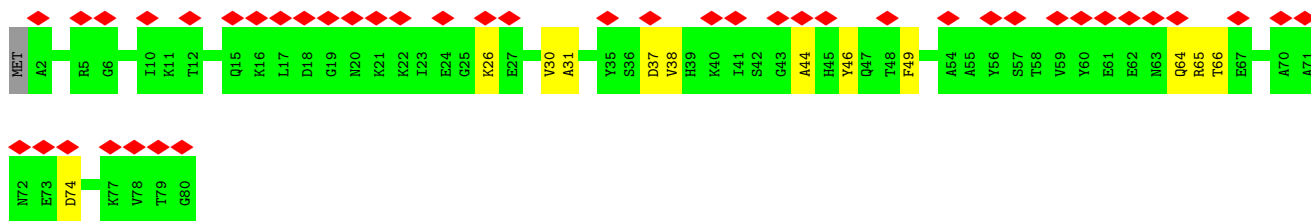


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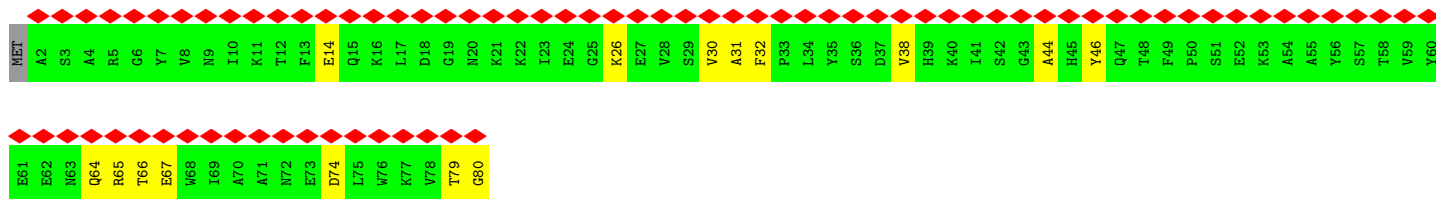
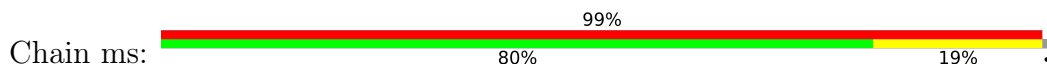


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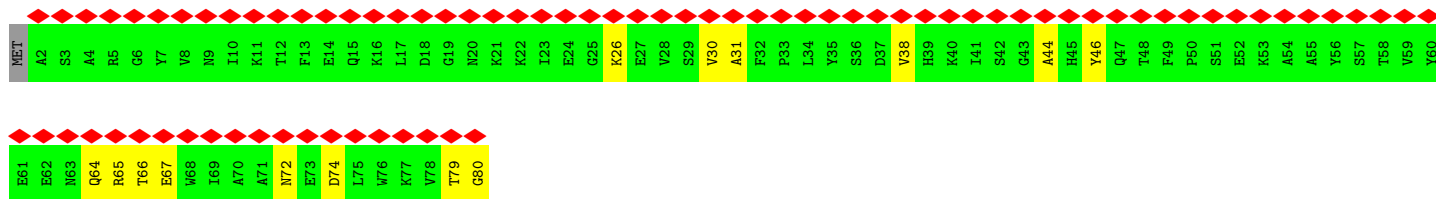
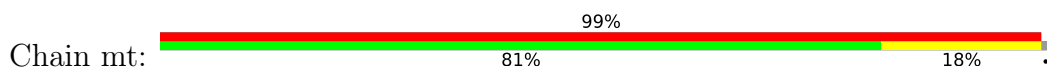




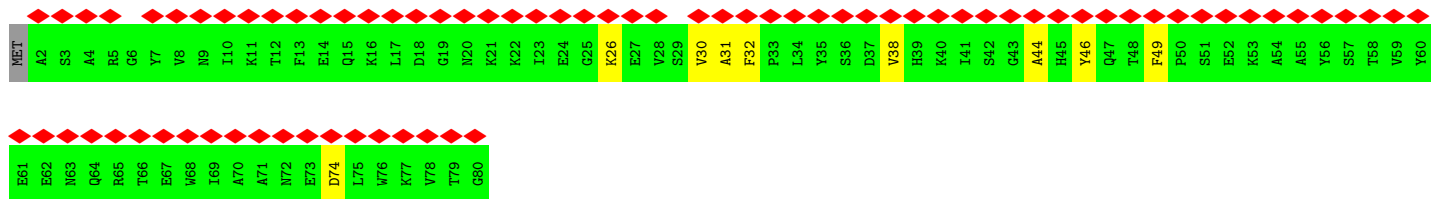
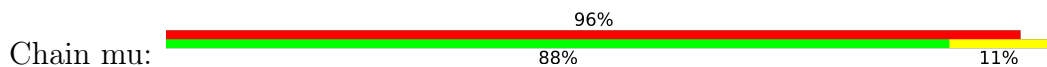
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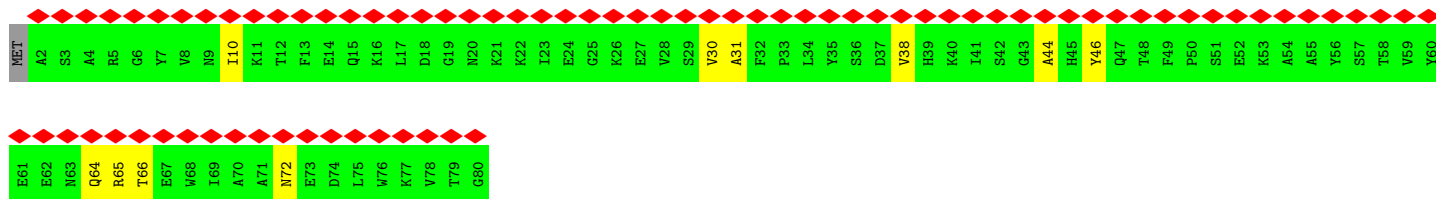
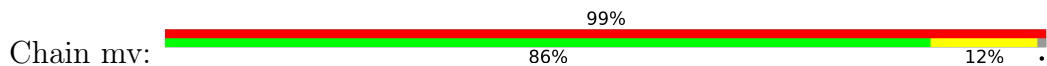
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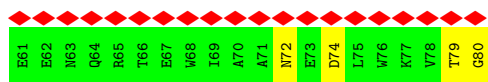
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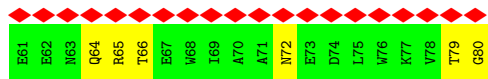
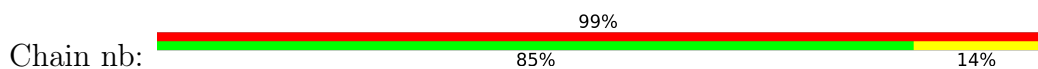
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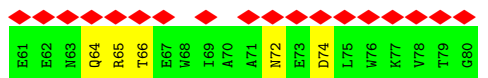
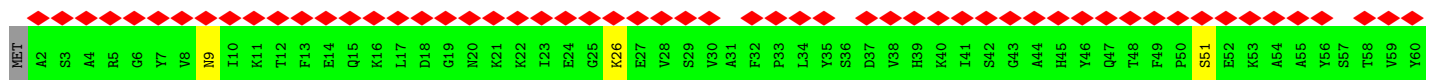
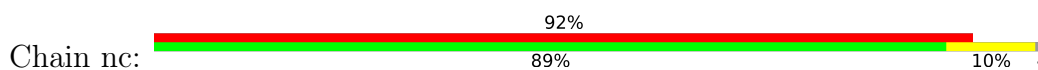




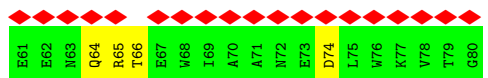
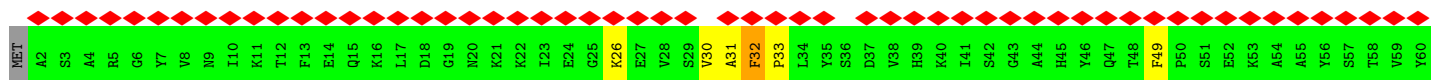
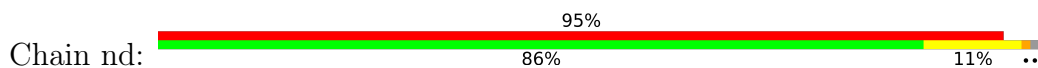
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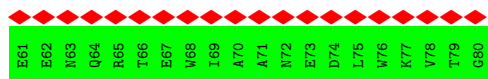
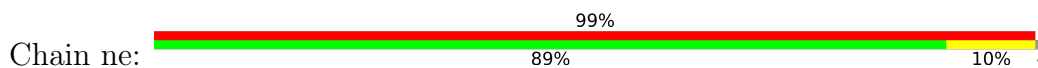
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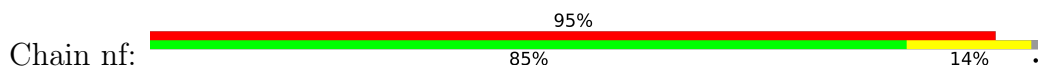
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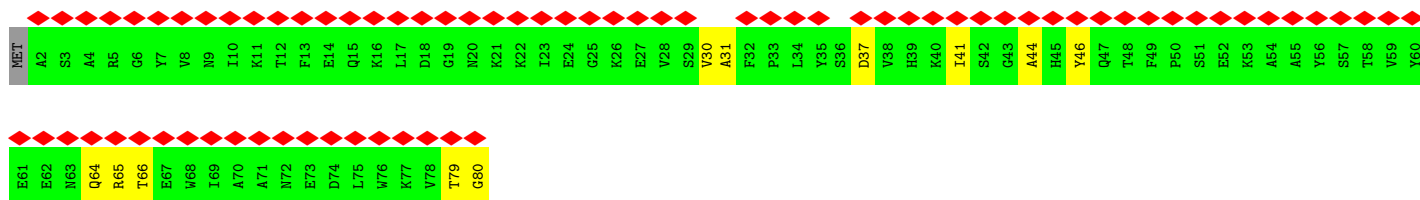


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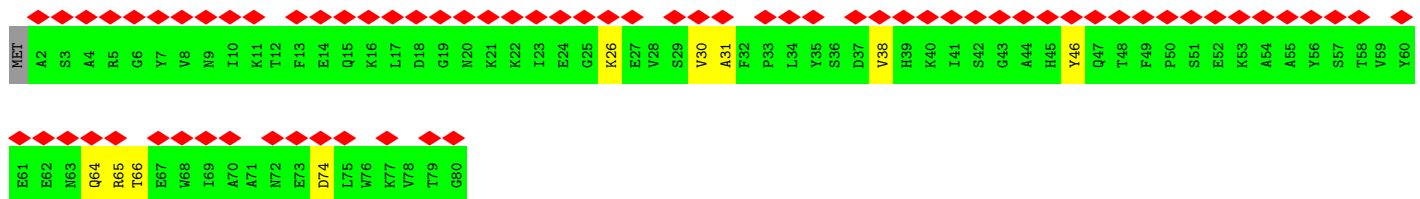
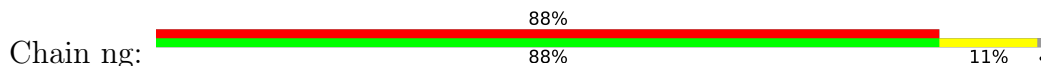


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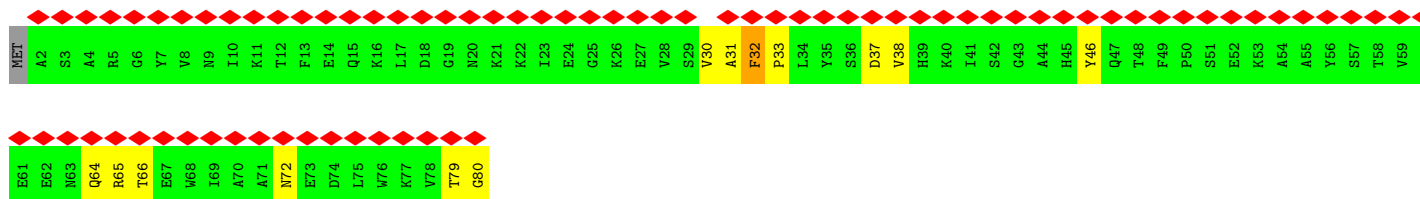
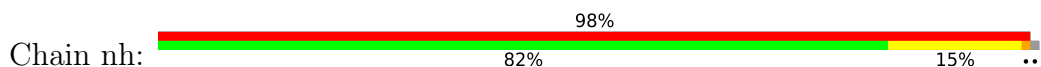




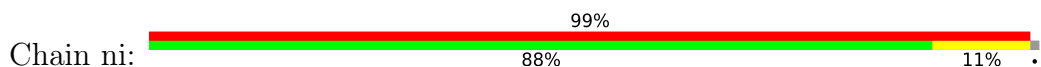
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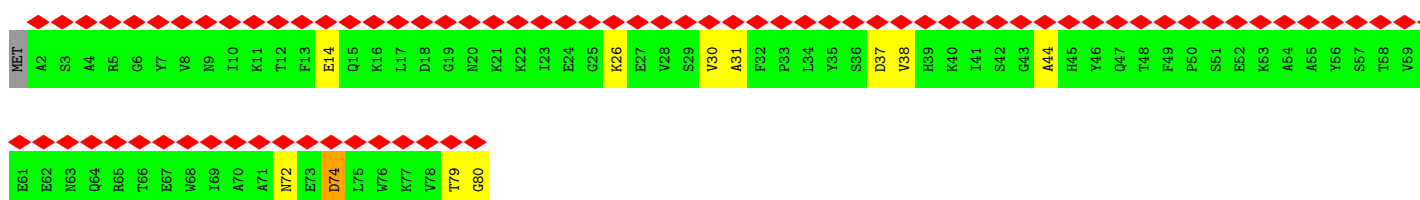
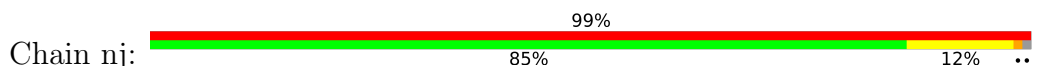
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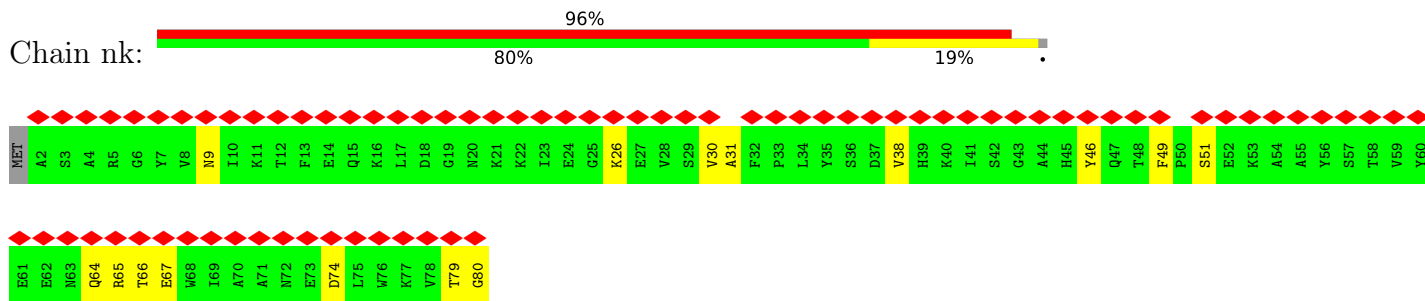
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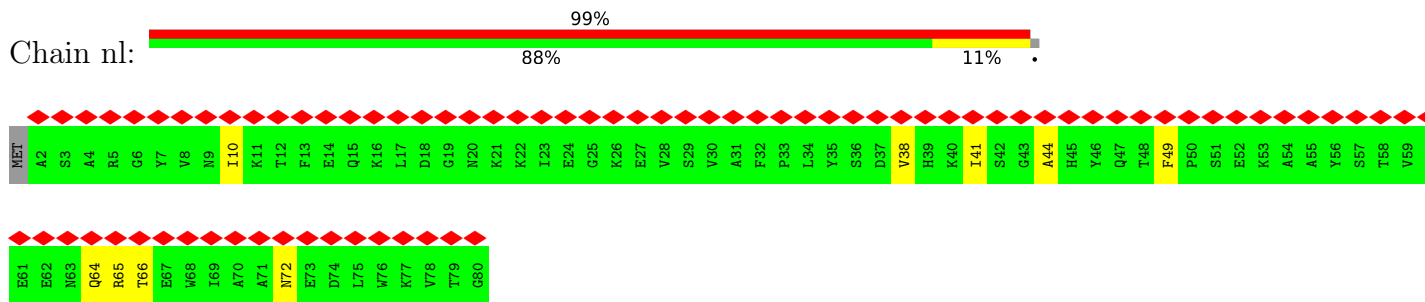
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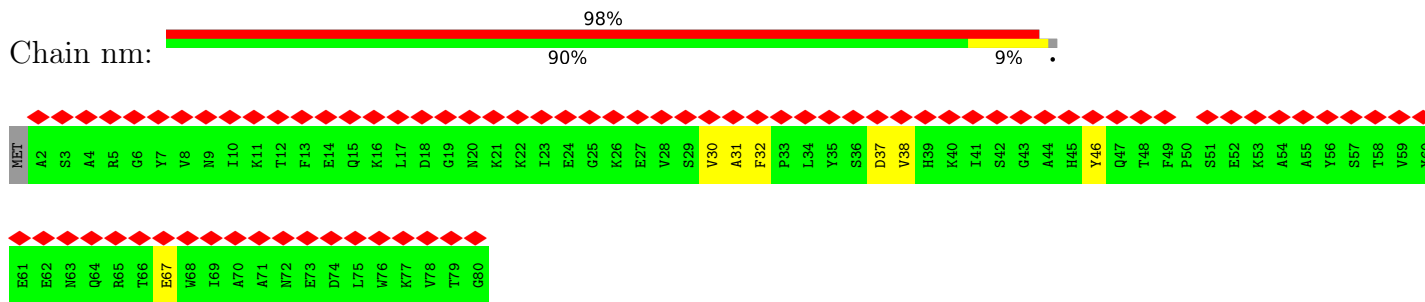
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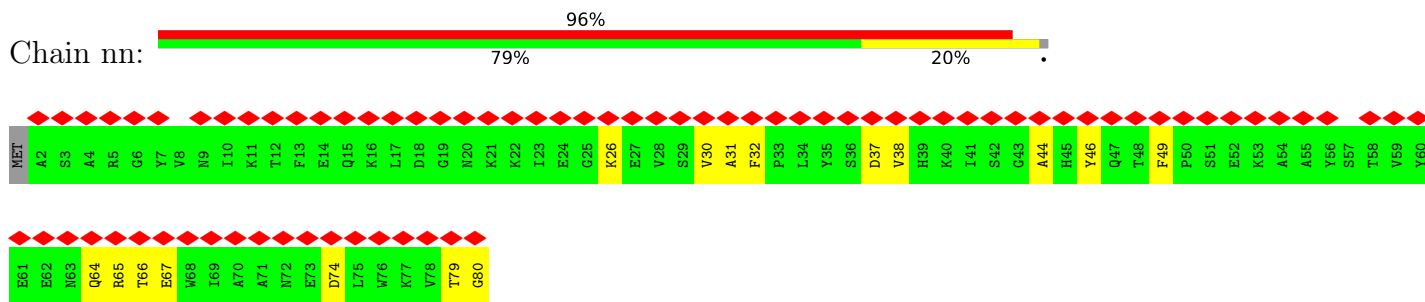
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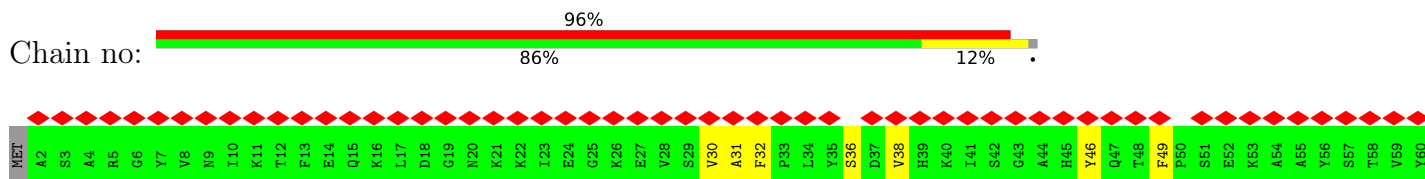
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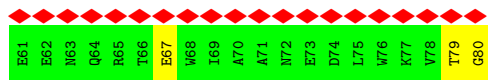


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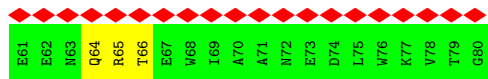
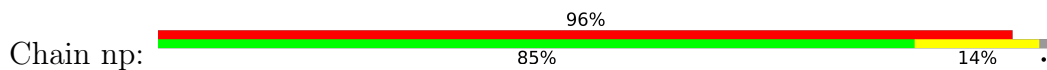


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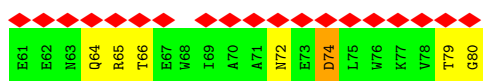
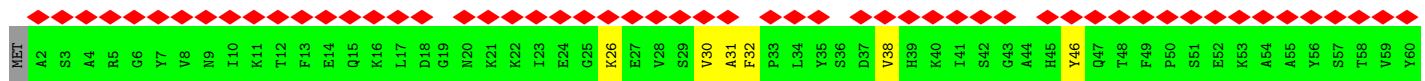
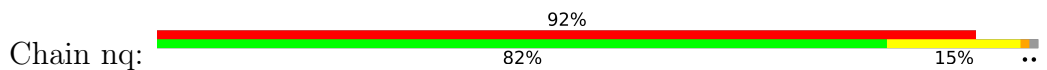




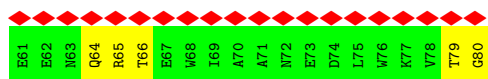
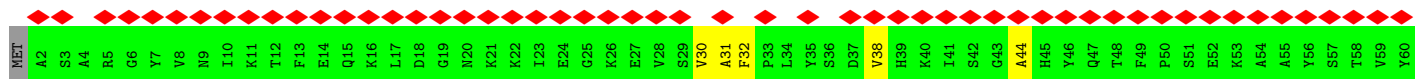
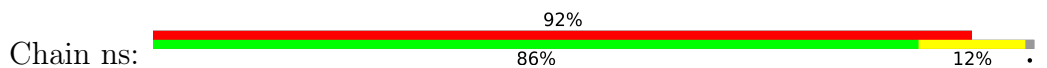
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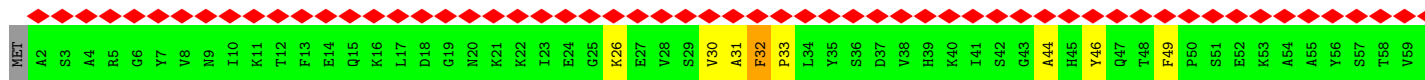
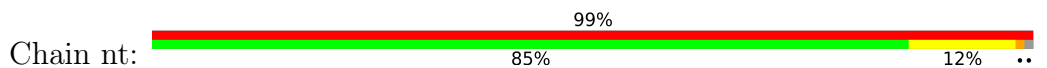
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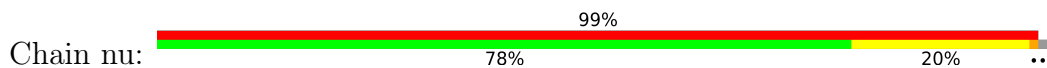
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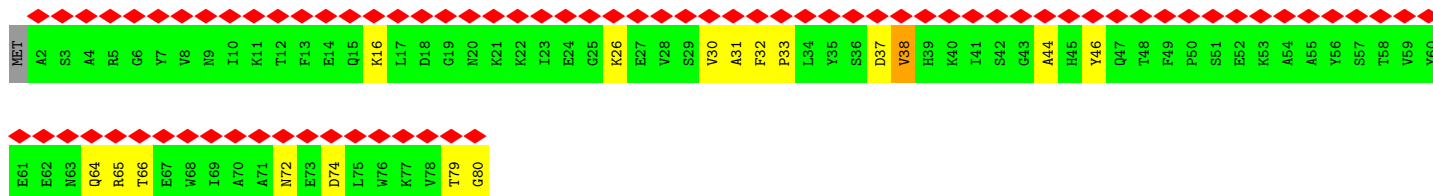


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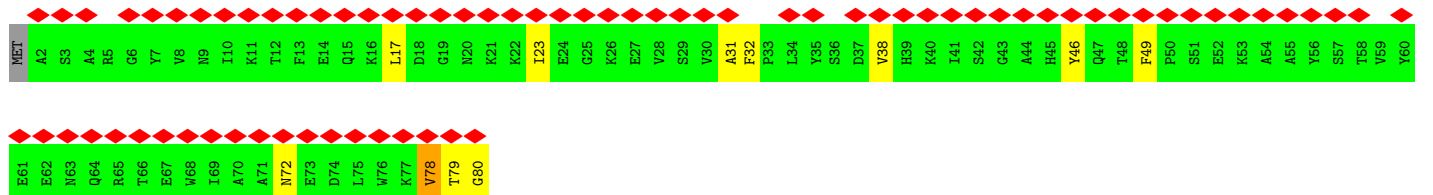
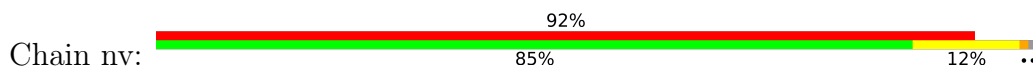


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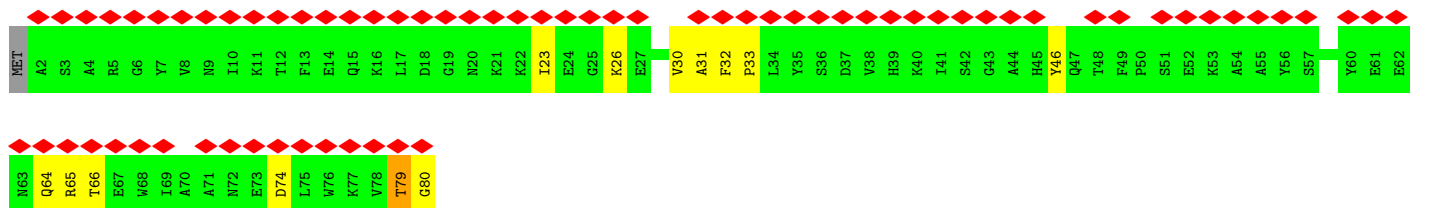
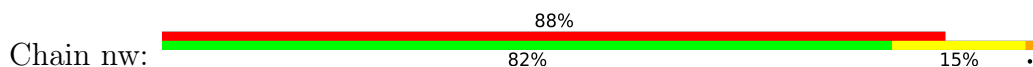




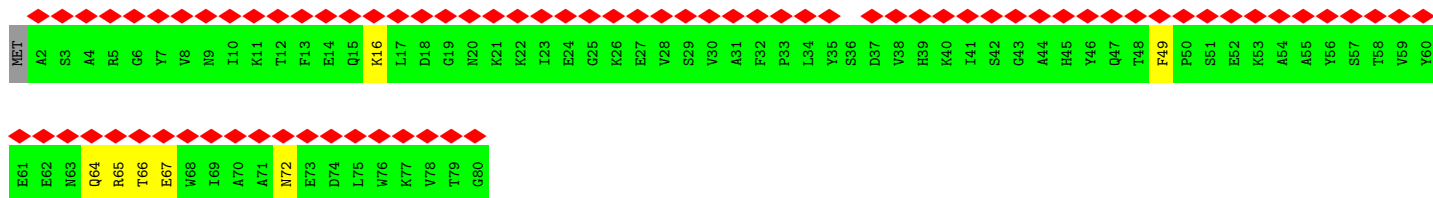
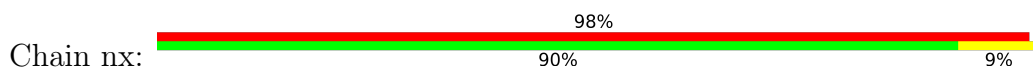
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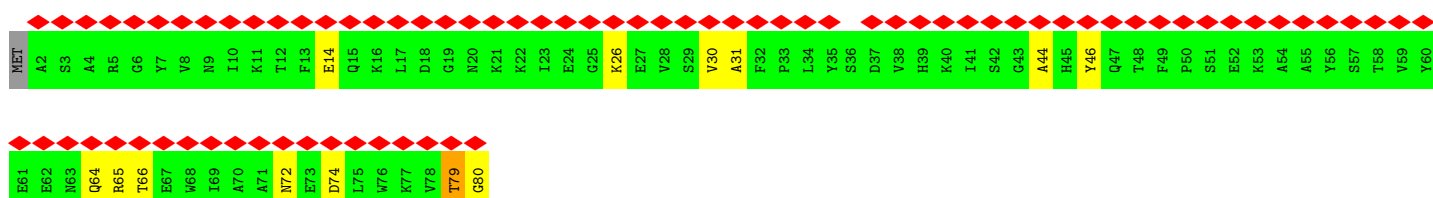
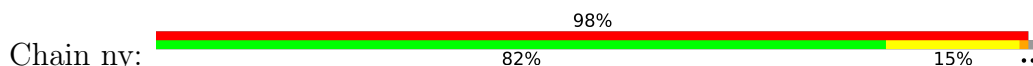
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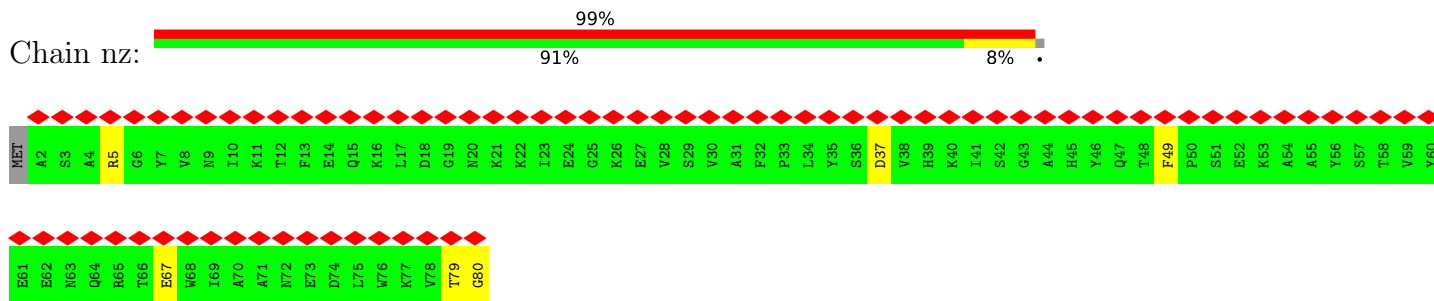
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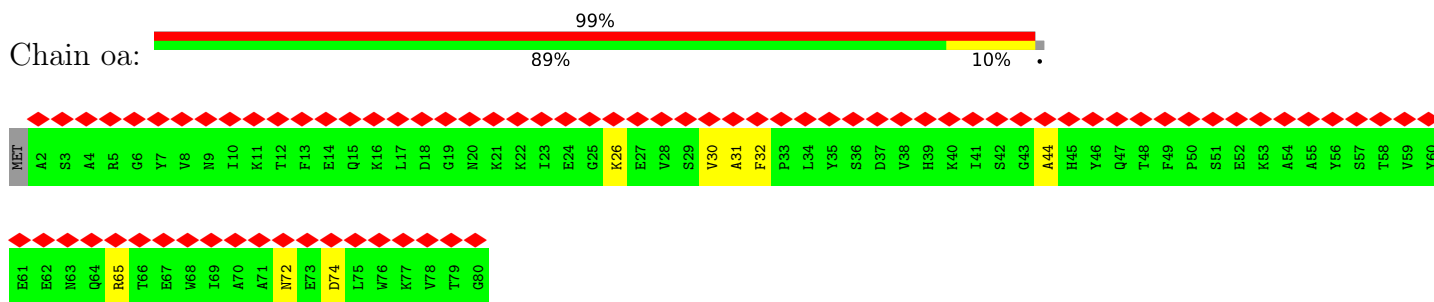
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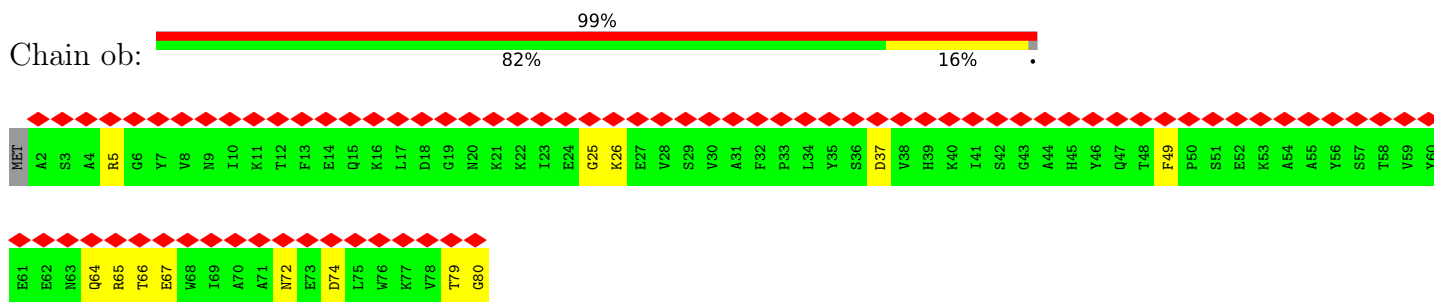
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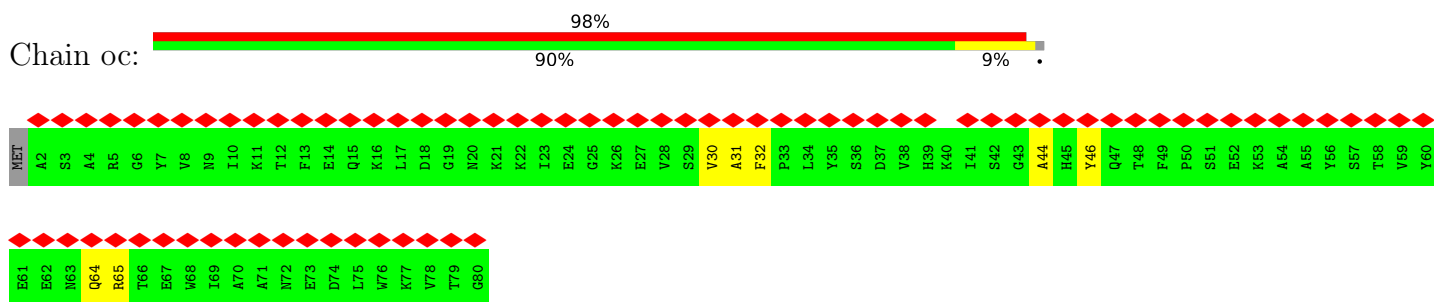
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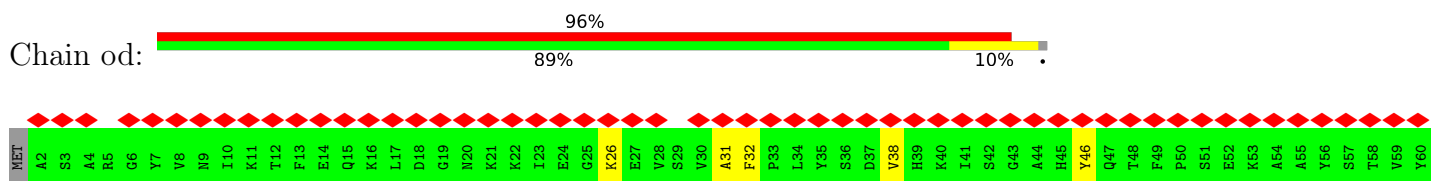
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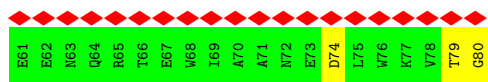


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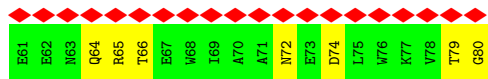
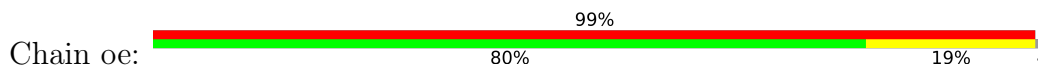


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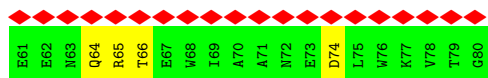
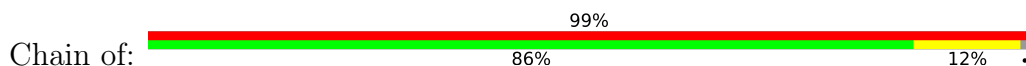




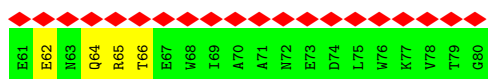
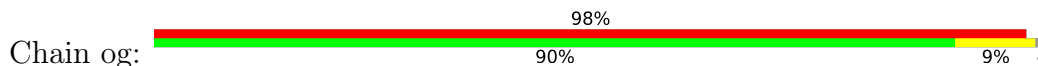
• Molecule 3: Small outer capsid protein



• Molecule 3: Small outer capsid protein



• Molecule 3: Small outer capsid protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	53608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	23.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.990	Depositor
Minimum map value	-0.745	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	1382.4, 1382.4, 1382.4	wwPDB
Map dimensions	960, 960, 960	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.44, 1.44, 1.44	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	aa	0.98	0/3493	1.33	31/4731 (0.7%)
1	ab	0.96	0/3493	1.34	30/4731 (0.6%)
1	ac	0.95	0/3493	1.32	38/4731 (0.8%)
1	ad	0.96	0/3493	1.36	32/4731 (0.7%)
1	ae	0.98	0/3493	1.37	40/4731 (0.8%)
1	af	0.96	0/3493	1.33	35/4731 (0.7%)
1	ag	0.96	1/3493 (0.0%)	1.35	35/4731 (0.7%)
1	ah	0.95	0/3493	1.33	34/4731 (0.7%)
1	ai	0.96	1/3493 (0.0%)	1.32	32/4731 (0.7%)
1	aj	0.94	1/3493 (0.0%)	1.33	32/4731 (0.7%)
1	ak	0.95	0/3493	1.32	29/4731 (0.6%)
1	al	0.98	1/3493 (0.0%)	1.36	35/4731 (0.7%)
1	am	0.95	0/3493	1.37	44/4731 (0.9%)
1	an	0.98	1/3493 (0.0%)	1.35	38/4731 (0.8%)
1	ao	0.97	1/3493 (0.0%)	1.33	29/4731 (0.6%)
1	ap	0.95	0/3493	1.34	38/4731 (0.8%)
1	aq	0.96	0/3493	1.33	25/4731 (0.5%)
1	ar	0.95	0/3493	1.33	36/4731 (0.8%)
1	as	1.00	0/3493	1.37	36/4731 (0.8%)
1	at	0.98	2/3493 (0.1%)	1.38	50/4731 (1.1%)
1	au	0.98	3/3493 (0.1%)	1.33	35/4731 (0.7%)
1	av	0.94	0/3493	1.35	31/4731 (0.7%)
1	aw	0.97	2/3493 (0.1%)	1.39	39/4731 (0.8%)
1	ax	0.97	0/3493	1.35	37/4731 (0.8%)
1	ay	0.96	1/3493 (0.0%)	1.34	33/4731 (0.7%)
1	az	0.96	1/3493 (0.0%)	1.33	35/4731 (0.7%)
1	ba	0.97	1/3493 (0.0%)	1.35	35/4731 (0.7%)
1	bb	0.97	0/3493	1.36	38/4731 (0.8%)
1	bc	0.94	0/3493	1.33	31/4731 (0.7%)
1	bd	0.96	0/3493	1.33	40/4731 (0.8%)
1	be	0.97	0/3493	1.37	33/4731 (0.7%)
1	bf	1.00	2/3493 (0.1%)	1.35	31/4731 (0.7%)
1	bg	0.97	0/3493	1.35	41/4731 (0.9%)
1	bh	0.94	0/3493	1.36	34/4731 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	bi	0.97	0/3493	1.36	38/4731 (0.8%)
1	bj	0.97	0/3493	1.33	34/4731 (0.7%)
1	bk	0.97	0/3493	1.32	33/4731 (0.7%)
1	bl	0.96	1/3493 (0.0%)	1.35	35/4731 (0.7%)
1	bm	0.96	1/3493 (0.0%)	1.33	39/4731 (0.8%)
1	bn	0.99	0/3493	1.32	28/4731 (0.6%)
1	bo	0.97	1/3493 (0.0%)	1.35	44/4731 (0.9%)
1	bp	0.95	0/3493	1.35	46/4731 (1.0%)
1	bq	0.94	0/3493	1.35	38/4731 (0.8%)
1	br	0.96	1/3493 (0.0%)	1.36	43/4731 (0.9%)
1	bs	0.97	1/3493 (0.0%)	1.35	32/4731 (0.7%)
1	bt	0.95	0/3493	1.35	37/4731 (0.8%)
1	bu	0.98	0/3493	1.39	37/4731 (0.8%)
1	bv	0.97	0/3493	1.33	24/4731 (0.5%)
1	bw	0.94	0/3493	1.38	40/4731 (0.8%)
1	bx	0.97	1/3493 (0.0%)	1.33	38/4731 (0.8%)
1	by	0.98	0/3493	1.37	36/4731 (0.8%)
1	bz	0.98	2/3493 (0.1%)	1.36	27/4731 (0.6%)
1	ca	0.96	0/3493	1.36	40/4731 (0.8%)
1	cb	0.97	0/3493	1.35	31/4731 (0.7%)
1	cc	0.97	0/3493	1.35	42/4731 (0.9%)
1	cd	0.95	0/3493	1.32	33/4731 (0.7%)
1	ce	0.99	0/3493	1.34	43/4731 (0.9%)
1	cf	0.95	0/3493	1.32	28/4731 (0.6%)
1	cg	0.95	1/3493 (0.0%)	1.32	33/4731 (0.7%)
1	ch	0.97	1/3493 (0.0%)	1.34	33/4731 (0.7%)
1	ci	0.97	1/3493 (0.0%)	1.40	51/4731 (1.1%)
1	cj	0.96	0/3493	1.36	45/4731 (1.0%)
1	ck	0.97	1/3493 (0.0%)	1.37	41/4731 (0.9%)
1	cl	0.97	0/3493	1.33	32/4731 (0.7%)
1	cm	0.97	0/3493	1.36	32/4731 (0.7%)
1	cn	0.96	2/3493 (0.1%)	1.36	41/4731 (0.9%)
1	co	0.97	0/3493	1.36	41/4731 (0.9%)
1	cp	0.96	0/3493	1.32	27/4731 (0.6%)
1	cq	0.96	0/3493	1.38	42/4731 (0.9%)
1	cr	0.96	1/3493 (0.0%)	1.34	33/4731 (0.7%)
1	cs	0.93	1/3493 (0.0%)	1.37	43/4731 (0.9%)
1	ct	0.95	1/3493 (0.0%)	1.34	38/4731 (0.8%)
1	cu	0.95	0/3493	1.33	34/4731 (0.7%)
1	cv	0.95	1/3493 (0.0%)	1.33	35/4731 (0.7%)
1	cw	0.95	0/3493	1.35	42/4731 (0.9%)
1	cx	0.94	1/3493 (0.0%)	1.35	40/4731 (0.8%)
1	cy	0.96	0/3493	1.34	37/4731 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	cz	0.94	0/3493	1.36	36/4731 (0.8%)
1	da	0.95	1/3493 (0.0%)	1.35	32/4731 (0.7%)
1	db	0.97	1/3493 (0.0%)	1.35	37/4731 (0.8%)
1	dc	0.94	0/3493	1.35	41/4731 (0.9%)
1	dd	0.95	0/3493	1.35	40/4731 (0.8%)
1	de	0.95	0/3493	1.37	38/4731 (0.8%)
1	df	0.97	1/3493 (0.0%)	1.35	38/4731 (0.8%)
1	dg	0.96	0/3493	1.37	42/4731 (0.9%)
1	dh	0.98	1/3493 (0.0%)	1.36	34/4731 (0.7%)
1	di	0.97	1/3493 (0.0%)	1.37	31/4731 (0.7%)
1	dj	0.98	0/3493	1.32	33/4731 (0.7%)
1	dk	0.98	0/3493	1.38	36/4731 (0.8%)
1	dl	0.96	2/3493 (0.1%)	1.37	44/4731 (0.9%)
1	dm	0.95	0/3493	1.38	40/4731 (0.8%)
1	dn	0.96	0/3493	1.33	31/4731 (0.7%)
1	do	0.98	1/3493 (0.0%)	1.34	39/4731 (0.8%)
1	dp	0.94	1/3493 (0.0%)	1.35	31/4731 (0.7%)
1	dq	0.96	1/3493 (0.0%)	1.34	37/4731 (0.8%)
1	dr	0.98	2/3493 (0.1%)	1.33	39/4731 (0.8%)
1	ds	0.94	0/3493	1.36	30/4731 (0.6%)
1	dt	0.97	1/3493 (0.0%)	1.34	30/4731 (0.6%)
1	du	0.98	1/3493 (0.0%)	1.34	35/4731 (0.7%)
1	dv	0.95	0/3493	1.33	33/4731 (0.7%)
1	dw	0.95	1/3315 (0.0%)	1.33	31/4488 (0.7%)
1	dx	0.97	0/3493	1.34	34/4731 (0.7%)
1	dy	0.98	0/3493	1.37	36/4731 (0.8%)
1	dz	0.96	0/3493	1.36	35/4731 (0.7%)
1	ea	0.98	1/3493 (0.0%)	1.31	38/4731 (0.8%)
1	eb	0.97	1/3493 (0.0%)	1.36	36/4731 (0.8%)
1	ec	0.95	1/3493 (0.0%)	1.31	20/4731 (0.4%)
1	ed	0.95	1/3493 (0.0%)	1.34	35/4731 (0.7%)
1	ee	1.01	0/3493	1.38	39/4731 (0.8%)
1	ef	1.02	0/3493	1.33	31/4731 (0.7%)
1	eg	0.99	2/3493 (0.1%)	1.35	44/4731 (0.9%)
1	eh	0.97	0/3493	1.35	36/4731 (0.8%)
1	ei	0.98	0/3493	1.35	31/4731 (0.7%)
1	ej	0.98	0/3493	1.33	41/4731 (0.9%)
1	ek	0.97	0/3493	1.38	35/4731 (0.7%)
1	el	0.94	0/3493	1.37	48/4731 (1.0%)
1	em	0.98	1/3493 (0.0%)	1.32	28/4731 (0.6%)
1	en	0.93	1/3493 (0.0%)	1.36	39/4731 (0.8%)
1	eo	0.98	0/3493	1.36	41/4731 (0.9%)
1	ep	0.95	0/3493	1.33	31/4731 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	eq	0.97	0/3493	1.33	34/4731 (0.7%)
1	er	0.98	1/3493 (0.0%)	1.34	39/4731 (0.8%)
1	es	0.96	0/3493	1.33	39/4731 (0.8%)
1	et	0.94	0/3493	1.33	38/4731 (0.8%)
1	eu	0.96	2/3493 (0.1%)	1.36	34/4731 (0.7%)
1	ev	0.95	1/3493 (0.0%)	1.33	30/4731 (0.6%)
1	ew	0.98	0/3493	1.35	26/4731 (0.5%)
1	ex	0.98	1/3493 (0.0%)	1.35	38/4731 (0.8%)
1	ey	0.97	1/3493 (0.0%)	1.36	43/4731 (0.9%)
1	ez	0.96	1/3493 (0.0%)	1.34	36/4731 (0.8%)
1	fa	0.95	0/3493	1.34	36/4731 (0.8%)
1	fb	0.99	0/3493	1.32	26/4731 (0.5%)
1	fc	0.97	0/3493	1.35	37/4731 (0.8%)
1	fd	0.95	1/3493 (0.0%)	1.35	35/4731 (0.7%)
1	fe	0.94	0/3493	1.35	35/4731 (0.7%)
1	ff	0.96	0/3493	1.33	38/4731 (0.8%)
1	fg	0.97	0/3493	1.35	39/4731 (0.8%)
1	fh	0.96	0/3493	1.36	41/4731 (0.9%)
1	fi	0.95	0/3493	1.36	40/4731 (0.8%)
1	fj	0.98	1/3493 (0.0%)	1.35	29/4731 (0.6%)
1	fk	0.95	0/3493	1.37	50/4731 (1.1%)
1	fl	0.95	0/3493	1.35	39/4731 (0.8%)
1	fm	0.94	0/3493	1.35	45/4731 (1.0%)
1	fn	0.98	1/3493 (0.0%)	1.35	39/4731 (0.8%)
1	fo	0.98	1/3493 (0.0%)	1.40	52/4731 (1.1%)
1	fp	0.98	1/3493 (0.0%)	1.32	37/4731 (0.8%)
1	fq	0.99	1/3493 (0.0%)	1.33	32/4731 (0.7%)
1	fr	0.98	3/3493 (0.1%)	1.34	34/4731 (0.7%)
1	fs	0.98	1/3493 (0.0%)	1.36	44/4731 (0.9%)
1	ft	0.98	0/3493	1.37	33/4731 (0.7%)
1	fu	0.95	0/3493	1.35	36/4731 (0.8%)
1	fv	0.96	0/3493	1.34	38/4731 (0.8%)
1	fw	0.96	0/3493	1.32	28/4731 (0.6%)
1	fx	0.94	0/3493	1.34	37/4731 (0.8%)
1	fy	0.95	1/3493 (0.0%)	1.30	30/4731 (0.6%)
1	fz	0.98	1/3493 (0.0%)	1.34	32/4731 (0.7%)
1	ga	0.94	0/3493	1.38	49/4731 (1.0%)
1	gb	0.92	0/3493	1.33	40/4731 (0.8%)
1	gc	0.94	0/3493	1.37	42/4731 (0.9%)
1	gd	0.96	0/3493	1.36	40/4731 (0.8%)
1	ge	0.95	0/3493	1.35	35/4731 (0.7%)
1	gf	0.96	0/3493	1.35	34/4731 (0.7%)
1	gg	0.95	0/3493	1.36	36/4731 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	gh	0.95	0/3493	1.36	36/4731 (0.8%)
1	gi	0.97	0/3493	1.33	37/4731 (0.8%)
1	gj	0.98	2/3493 (0.1%)	1.41	50/4731 (1.1%)
1	gk	0.95	0/3493	1.36	32/4731 (0.7%)
1	gl	0.95	0/3493	1.40	54/4731 (1.1%)
1	gm	0.96	0/3493	1.34	39/4731 (0.8%)
1	gn	0.97	1/3493 (0.0%)	1.35	41/4731 (0.9%)
1	go	0.95	1/3493 (0.0%)	1.34	37/4731 (0.8%)
1	gp	0.94	0/3493	1.34	36/4731 (0.8%)
1	gq	0.93	0/3493	1.34	29/4731 (0.6%)
1	gr	0.94	1/3493 (0.0%)	1.33	35/4731 (0.7%)
1	gs	0.93	1/3493 (0.0%)	1.36	46/4731 (1.0%)
1	gt	0.95	3/3493 (0.1%)	1.34	28/4731 (0.6%)
1	gu	0.95	1/3493 (0.0%)	1.36	48/4731 (1.0%)
1	gv	0.93	1/3493 (0.0%)	1.34	36/4731 (0.8%)
1	gw	0.97	1/3493 (0.0%)	1.36	42/4731 (0.9%)
1	gx	0.99	0/3493	1.34	36/4731 (0.8%)
1	gy	0.97	0/3493	1.34	40/4731 (0.8%)
1	gz	0.94	0/3493	1.34	28/4731 (0.6%)
1	ha	0.99	1/3493 (0.0%)	1.33	29/4731 (0.6%)
1	hb	0.97	0/3493	1.31	38/4731 (0.8%)
1	hc	0.96	0/3493	1.34	39/4731 (0.8%)
1	hd	0.99	1/3493 (0.0%)	1.35	35/4731 (0.7%)
2	he	0.92	0/3263	1.27	32/4430 (0.7%)
2	hf	0.94	0/3263	1.29	34/4430 (0.8%)
2	hg	0.94	0/3263	1.28	31/4430 (0.7%)
2	hh	0.94	0/3263	1.28	37/4430 (0.8%)
2	hi	0.94	0/3263	1.28	40/4430 (0.9%)
2	hj	0.95	0/3263	1.31	37/4430 (0.8%)
2	hk	0.96	1/3263 (0.0%)	1.30	40/4430 (0.9%)
2	hl	0.96	1/3263 (0.0%)	1.28	33/4430 (0.7%)
2	hm	0.96	0/3263	1.30	39/4430 (0.9%)
2	hn	0.94	1/3263 (0.0%)	1.27	32/4430 (0.7%)
2	ho	0.96	1/3263 (0.0%)	1.30	37/4430 (0.8%)
3	hp	0.83	0/648	1.18	1/876 (0.1%)
3	hq	0.85	0/648	1.19	4/876 (0.5%)
3	hr	0.87	0/648	1.19	4/876 (0.5%)
3	hs	0.84	0/648	1.18	4/876 (0.5%)
3	ht	0.88	0/648	1.18	3/876 (0.3%)
3	hu	0.89	0/648	1.16	6/876 (0.7%)
3	hv	0.88	0/648	1.21	2/876 (0.2%)
3	hw	0.86	0/648	1.21	3/876 (0.3%)
3	hx	0.85	0/648	1.20	2/876 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	hy	0.84	0/648	1.24	3/876 (0.3%)
3	hz	0.90	0/648	1.24	5/876 (0.6%)
3	ia	0.89	0/648	1.17	6/876 (0.7%)
3	ib	0.87	0/648	1.21	5/876 (0.6%)
3	ic	0.89	0/648	1.19	3/876 (0.3%)
3	id	0.85	0/648	1.20	3/876 (0.3%)
3	ie	0.82	0/648	1.13	4/876 (0.5%)
3	if	0.87	0/648	1.31	3/876 (0.3%)
3	ig	0.86	0/648	1.20	5/876 (0.6%)
3	ih	0.88	0/648	1.25	9/876 (1.0%)
3	ii	0.86	0/648	1.16	2/876 (0.2%)
3	ij	0.89	0/648	1.23	7/876 (0.8%)
3	ik	0.87	0/648	1.14	5/876 (0.6%)
3	il	0.88	0/648	1.18	3/876 (0.3%)
3	im	0.91	0/648	1.17	3/876 (0.3%)
3	in	0.85	0/648	1.23	5/876 (0.6%)
3	io	0.84	0/648	1.22	5/876 (0.6%)
3	ip	0.87	0/648	1.27	9/876 (1.0%)
3	iq	0.89	1/648 (0.2%)	1.18	4/876 (0.5%)
3	ir	0.89	0/648	1.18	6/876 (0.7%)
3	is	0.84	0/648	1.18	4/876 (0.5%)
3	it	0.86	0/648	1.18	2/876 (0.2%)
3	iu	0.89	1/648 (0.2%)	1.23	6/876 (0.7%)
3	iv	0.92	1/648 (0.2%)	1.22	3/876 (0.3%)
3	iw	0.85	0/648	1.21	8/876 (0.9%)
3	ix	0.86	0/648	1.17	4/876 (0.5%)
3	iy	0.86	0/648	1.21	6/876 (0.7%)
3	iz	0.89	0/648	1.19	2/876 (0.2%)
3	ja	0.94	2/648 (0.3%)	1.19	2/876 (0.2%)
3	jb	0.88	0/648	1.25	5/876 (0.6%)
3	jc	0.87	1/648 (0.2%)	1.19	5/876 (0.6%)
3	jd	0.87	0/648	1.17	3/876 (0.3%)
3	je	0.86	0/648	1.17	4/876 (0.5%)
3	jf	0.89	0/648	1.19	2/876 (0.2%)
3	jg	0.91	1/648 (0.2%)	1.21	7/876 (0.8%)
3	jh	0.89	0/648	1.20	4/876 (0.5%)
3	ji	0.87	0/648	1.22	8/876 (0.9%)
3	jj	0.87	0/648	1.17	4/876 (0.5%)
3	jk	0.87	0/648	1.17	6/876 (0.7%)
3	jl	0.91	0/648	1.24	3/876 (0.3%)
3	jm	0.87	0/648	1.21	3/876 (0.3%)
3	jn	0.86	0/648	1.23	8/876 (0.9%)
3	jo	0.91	1/648 (0.2%)	1.18	3/876 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	jp	0.86	0/648	1.17	3/876 (0.3%)
3	jq	0.88	0/648	1.19	2/876 (0.2%)
3	jr	0.82	0/648	1.23	4/876 (0.5%)
3	js	0.83	0/648	1.16	4/876 (0.5%)
3	jt	0.84	0/648	1.21	5/876 (0.6%)
3	ju	0.89	1/648 (0.2%)	1.19	5/876 (0.6%)
3	jv	0.90	0/648	1.19	4/876 (0.5%)
3	jw	0.89	1/648 (0.2%)	1.22	5/876 (0.6%)
3	jx	0.87	0/648	1.17	3/876 (0.3%)
3	jy	0.87	0/648	1.20	3/876 (0.3%)
3	jz	0.91	0/648	1.23	10/876 (1.1%)
3	ka	0.83	0/648	1.16	7/876 (0.8%)
3	kb	0.89	0/648	1.17	3/876 (0.3%)
3	kc	0.88	0/648	1.21	7/876 (0.8%)
3	kd	0.87	0/648	1.29	4/876 (0.5%)
3	ke	0.90	0/648	1.25	5/876 (0.6%)
3	kf	0.91	0/648	1.18	2/876 (0.2%)
3	kg	0.90	0/648	1.20	3/876 (0.3%)
3	kh	0.90	0/648	1.21	5/876 (0.6%)
3	ki	0.89	0/648	1.19	2/876 (0.2%)
3	kj	0.87	0/648	1.21	3/876 (0.3%)
3	kk	0.88	0/648	1.19	4/876 (0.5%)
3	kl	0.88	0/648	1.23	3/876 (0.3%)
3	km	0.83	0/648	1.22	5/876 (0.6%)
3	kn	0.89	0/648	1.22	5/876 (0.6%)
3	ko	0.89	0/648	1.22	7/876 (0.8%)
3	kp	0.88	0/648	1.22	6/876 (0.7%)
3	kq	0.89	0/648	1.23	7/876 (0.8%)
3	kr	0.85	0/648	1.19	2/876 (0.2%)
3	ks	0.85	0/648	1.21	3/876 (0.3%)
3	kt	0.87	0/648	1.19	7/876 (0.8%)
3	ku	0.89	0/648	1.22	6/876 (0.7%)
3	0.87	0/648	1.25	8/876 (0.9%)	
3	kx	0.86	0/648	1.21	3/876 (0.3%)
3	ky	0.88	0/648	1.28	6/876 (0.7%)
3	ky	0.86	0/648	1.22	6/876 (0.7%)
3	kz	0.83	0/648	1.23	6/876 (0.7%)
3	la	0.86	0/648	1.18	6/876 (0.7%)
3	lb	0.84	0/648	1.24	5/876 (0.6%)
3	lc	0.84	0/648	1.18	4/876 (0.5%)
3	ld	0.86	0/648	1.16	4/876 (0.5%)
3	le	0.88	0/648	1.27	4/876 (0.5%)
3	lf	0.93	0/648	1.24	3/876 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	lg	0.91	1/648 (0.2%)	1.20	6/876 (0.7%)
3	lh	0.88	0/648	1.26	3/876 (0.3%)
3	li	0.89	0/648	1.23	5/876 (0.6%)
3	lj	0.89	0/648	1.24	4/876 (0.5%)
3	lk	0.87	0/648	1.15	5/876 (0.6%)
3	ll	0.87	0/648	1.18	5/876 (0.6%)
3	lm	0.88	0/648	1.20	6/876 (0.7%)
3	ln	0.85	0/648	1.20	4/876 (0.5%)
3	lo	0.79	0/648	1.17	5/876 (0.6%)
3	lp	0.91	0/648	1.21	3/876 (0.3%)
3	lq	0.88	1/648 (0.2%)	1.17	5/876 (0.6%)
3	lr	0.90	0/648	1.18	2/876 (0.2%)
3	ls	0.84	0/648	1.17	3/876 (0.3%)
3	lt	0.94	1/648 (0.2%)	1.25	7/876 (0.8%)
3	lu	0.88	0/648	1.18	3/876 (0.3%)
3	lv	0.87	0/648	1.20	5/876 (0.6%)
3	lw	0.86	0/648	1.24	5/876 (0.6%)
3	lx	0.84	0/648	1.17	1/876 (0.1%)
3	ly	0.84	0/648	1.17	3/876 (0.3%)
3	lz	0.91	0/648	1.26	5/876 (0.6%)
3	ma	0.89	0/648	1.16	4/876 (0.5%)
3	mb	0.85	0/648	1.20	3/876 (0.3%)
3	mc	0.88	0/648	1.16	3/876 (0.3%)
3	md	0.88	0/648	1.16	3/876 (0.3%)
3	me	0.89	0/648	1.21	3/876 (0.3%)
3	mf	0.91	0/648	1.19	2/876 (0.2%)
3	mg	0.86	0/648	1.20	4/876 (0.5%)
3	mh	0.82	0/648	1.12	3/876 (0.3%)
3	mi	0.86	0/648	1.25	4/876 (0.5%)
3	mj	0.88	0/648	1.26	5/876 (0.6%)
3	mk	0.91	0/648	1.16	1/876 (0.1%)
3	ml	0.91	1/648 (0.2%)	1.24	4/876 (0.5%)
3	mm	0.86	1/648 (0.2%)	1.17	2/876 (0.2%)
3	mn	0.93	0/648	1.23	2/876 (0.2%)
3	mo	0.91	1/648 (0.2%)	1.19	4/876 (0.5%)
3	mp	0.88	0/648	1.13	2/876 (0.2%)
3	mq	0.90	0/648	1.23	6/876 (0.7%)
3	ms	0.84	0/648	1.28	6/876 (0.7%)
3	mt	0.84	0/648	1.21	5/876 (0.6%)
3	mu	0.89	0/648	1.19	5/876 (0.6%)
3	mv	0.86	0/648	1.23	5/876 (0.6%)
3	mw	0.89	0/648	1.23	3/876 (0.3%)
3	mx	0.89	1/648 (0.2%)	1.23	6/876 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	my	0.88	0/648	1.25	6/876 (0.7%)
3	mz	0.89	0/648	1.24	8/876 (0.9%)
3	na	0.84	0/648	1.22	5/876 (0.6%)
3	nb	0.87	0/648	1.20	5/876 (0.6%)
3	nc	0.84	0/648	1.20	0/876
3	nd	0.86	0/648	1.15	4/876 (0.5%)
3	ne	0.85	0/648	1.17	3/876 (0.3%)
3	nf	0.88	0/648	1.22	4/876 (0.5%)
3	ng	0.89	0/648	1.19	2/876 (0.2%)
3	nh	0.88	0/648	1.18	6/876 (0.7%)
3	ni	0.84	0/648	1.20	5/876 (0.6%)
3	nj	0.82	0/648	1.24	5/876 (0.6%)
3	nk	0.88	0/648	1.21	5/876 (0.6%)
3	nl	0.87	0/648	1.22	7/876 (0.8%)
3	nm	0.91	0/648	1.24	4/876 (0.5%)
3	nn	0.88	0/648	1.22	9/876 (1.0%)
3	no	0.92	0/648	1.23	7/876 (0.8%)
3	np	0.88	0/648	1.22	4/876 (0.5%)
3	nq	0.88	0/648	1.24	6/876 (0.7%)
3	ns	0.89	0/648	1.23	4/876 (0.5%)
3	nt	0.84	0/648	1.24	7/876 (0.8%)
3	nu	0.90	0/648	1.21	5/876 (0.6%)
3	nv	0.88	0/648	1.21	5/876 (0.6%)
3	nw	0.85	0/648	1.23	3/876 (0.3%)
3	nx	0.84	0/648	1.27	5/876 (0.6%)
3	ny	0.86	0/648	1.18	4/876 (0.5%)
3	nz	0.85	0/648	1.23	5/876 (0.6%)
3	oa	0.81	0/648	1.14	4/876 (0.5%)
3	ob	0.86	0/648	1.30	8/876 (0.9%)
3	oc	0.81	0/648	1.18	5/876 (0.6%)
3	od	0.85	0/648	1.19	2/876 (0.2%)
3	oe	0.86	0/648	1.24	7/876 (0.8%)
3	of	0.87	0/648	1.22	6/876 (0.7%)
3	og	0.82	0/648	1.17	1/876 (0.1%)
All	All	0.95	114/796869 (0.0%)	1.33	7933/1079125 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	aq	0	1

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	gj	96	MET	SD-CE	-9.24	1.56	1.79
1	at	483	PRO	C-N	-6.56	1.25	1.33
1	do	145	HIS	CB-CG	-6.48	1.41	1.50
1	ec	145	HIS	CB-CG	-6.41	1.41	1.50
1	fj	145	HIS	CB-CG	-6.38	1.41	1.50

The worst 5 of 7933 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	dm	236	GLN	CA-C-N	13.89	146.71	121.70
1	dm	236	GLN	C-N-CA	13.89	146.71	121.70
1	ek	486	GLU	N-CA-C	-13.32	95.45	112.23
1	ba	154	PHE	N-CA-C	-11.27	98.19	113.18
1	gj	96	MET	N-CA-C	10.95	123.22	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	aq	480	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aa	3425	0	3371	9	0
1	ab	3425	0	3371	8	0
1	ac	3425	0	3371	8	0
1	ad	3425	0	3371	7	0
1	ae	3425	0	3371	14	0
1	af	3425	0	3371	13	0
1	ag	3425	0	3371	11	0
1	ah	3425	0	3371	10	0
1	ai	3425	0	3371	13	0
1	aj	3425	0	3371	8	0
1	ak	3425	0	3371	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	al	3425	0	3371	13	0
1	am	3425	0	3371	15	0
1	an	3425	0	3371	9	0
1	ao	3425	0	3371	13	0
1	ap	3425	0	3371	4	0
1	aq	3425	0	3371	16	0
1	ar	3425	0	3371	13	0
1	as	3425	0	3371	8	0
1	at	3425	0	3371	9	0
1	au	3425	0	3371	15	0
1	av	3425	0	3371	8	0
1	aw	3425	0	3371	17	0
1	ax	3425	0	3371	12	0
1	ay	3425	0	3371	16	0
1	az	3425	0	3371	12	0
1	ba	3425	0	3371	13	0
1	bb	3425	0	3371	8	0
1	bc	3425	0	3371	13	0
1	bd	3425	0	3371	11	0
1	be	3425	0	3371	12	0
1	bf	3425	0	3371	8	0
1	bg	3425	0	3371	11	0
1	bh	3425	0	3371	9	0
1	bi	3425	0	3371	12	0
1	bj	3425	0	3371	10	0
1	bk	3425	0	3371	5	0
1	bl	3425	0	3371	12	0
1	bm	3425	0	3371	9	0
1	bn	3425	0	3371	12	0
1	bo	3425	0	3371	14	0
1	bp	3425	0	3371	6	0
1	bq	3425	0	3371	6	0
1	br	3425	0	3371	10	0
1	bs	3425	0	3371	11	0
1	bt	3425	0	3371	9	0
1	bu	3425	0	3371	12	0
1	bv	3425	0	3371	6	0
1	bw	3425	0	3371	12	0
1	bx	3425	0	3371	12	0
1	by	3425	0	3371	11	0
1	bz	3425	0	3371	9	0
1	ca	3425	0	3371	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	cb	3425	0	3371	14	0
1	cc	3425	0	3371	8	0
1	cd	3425	0	3371	10	0
1	ce	3425	0	3371	13	0
1	cf	3425	0	3371	10	0
1	cg	3425	0	3371	12	0
1	ch	3425	0	3371	11	0
1	ci	3425	0	3371	6	0
1	cj	3425	0	3371	8	0
1	ck	3425	0	3371	8	0
1	cl	3425	0	3371	8	0
1	cm	3425	0	3371	8	0
1	cn	3425	0	3371	5	0
1	co	3425	0	3371	6	0
1	cp	3425	0	3371	12	0
1	cq	3425	0	3371	9	0
1	cr	3425	0	3371	11	0
1	cs	3425	0	3371	8	0
1	ct	3425	0	3371	9	0
1	cu	3425	0	3371	8	0
1	cv	3425	0	3371	7	0
1	cw	3425	0	3371	13	0
1	cx	3425	0	3371	10	0
1	cy	3425	0	3371	12	0
1	cz	3425	0	3371	8	0
1	da	3425	0	3371	10	0
1	db	3425	0	3371	12	0
1	dc	3425	0	3371	10	0
1	dd	3425	0	3371	7	0
1	de	3425	0	3371	13	0
1	df	3425	0	3371	7	0
1	dg	3425	0	3371	9	0
1	dh	3425	0	3371	14	0
1	di	3425	0	3371	7	0
1	dj	3425	0	3371	9	0
1	dk	3425	0	3371	5	0
1	dl	3425	0	3371	12	0
1	dm	3425	0	3371	6	0
1	dn	3425	0	3371	7	0
1	do	3425	0	3371	10	0
1	dp	3425	0	3371	8	0
1	dq	3425	0	3371	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	dr	3425	0	3371	7	0
1	ds	3425	0	3371	7	0
1	dt	3425	0	3371	9	0
1	du	3425	0	3371	15	0
1	dv	3425	0	3371	11	0
1	dw	3249	0	3209	14	0
1	dx	3425	0	3371	10	0
1	dy	3425	0	3371	10	0
1	dz	3425	0	3371	8	0
1	ea	3425	0	3371	10	0
1	eb	3425	0	3371	17	0
1	ec	3425	0	3371	15	0
1	ed	3425	0	3371	20	0
1	ee	3425	0	3371	15	0
1	ef	3425	0	3371	11	0
1	eg	3425	0	3371	11	0
1	eh	3425	0	3371	4	0
1	ei	3425	0	3371	8	0
1	ej	3425	0	3371	8	0
1	ek	3425	0	3371	13	0
1	el	3425	0	3371	8	0
1	em	3425	0	3371	10	0
1	en	3425	0	3371	11	0
1	eo	3425	0	3371	15	0
1	ep	3425	0	3371	14	0
1	eq	3425	0	3371	6	0
1	er	3425	0	3371	12	0
1	es	3425	0	3371	11	0
1	et	3425	0	3371	9	0
1	eu	3425	0	3371	9	0
1	ev	3425	0	3371	10	0
1	ew	3425	0	3371	8	0
1	ex	3425	0	3371	8	0
1	ey	3425	0	3371	8	0
1	ez	3425	0	3371	11	0
1	fa	3425	0	3371	10	0
1	fb	3425	0	3371	7	0
1	fc	3425	0	3371	8	0
1	fd	3425	0	3371	6	0
1	fe	3425	0	3371	10	0
1	ff	3425	0	3371	8	0
1	fg	3425	0	3371	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	fh	3425	0	3371	11	0
1	fi	3425	0	3371	8	0
1	fj	3425	0	3371	19	0
1	fk	3425	0	3371	10	0
1	fl	3425	0	3371	7	0
1	fm	3425	0	3371	14	0
1	fn	3425	0	3371	9	0
1	fo	3425	0	3371	8	0
1	fp	3425	0	3371	10	0
1	fq	3425	0	3371	9	0
1	fr	3425	0	3371	8	0
1	fs	3425	0	3371	9	0
1	ft	3425	0	3371	12	0
1	fu	3425	0	3371	8	0
1	fv	3425	0	3371	9	0
1	fw	3425	0	3371	16	0
1	fx	3425	0	3371	7	0
1	fy	3425	0	3371	14	0
1	fz	3425	0	3371	11	0
1	ga	3425	0	3371	11	0
1	gb	3425	0	3371	11	0
1	gc	3425	0	3371	17	0
1	gd	3425	0	3371	6	0
1	ge	3425	0	3371	15	0
1	gf	3425	0	3371	4	0
1	gg	3425	0	3371	12	0
1	gh	3425	0	3371	9	0
1	gi	3425	0	3371	10	0
1	gj	3425	0	3371	12	0
1	gk	3425	0	3371	8	0
1	gl	3425	0	3371	16	0
1	gm	3425	0	3371	12	0
1	gn	3425	0	3371	8	0
1	go	3425	0	3371	12	0
1	gp	3425	0	3371	11	0
1	gq	3425	0	3371	14	0
1	gr	3425	0	3371	12	0
1	gs	3425	0	3371	11	0
1	gt	3425	0	3371	9	0
1	gu	3425	0	3371	11	0
1	gv	3425	0	3371	6	0
1	gw	3425	0	3371	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	gx	3425	0	3371	9	0
1	gy	3425	0	3371	10	0
1	gz	3425	0	3371	12	0
1	ha	3425	0	3371	9	0
1	hb	3425	0	3371	7	0
1	hc	3425	0	3371	8	0
1	hd	3425	0	3371	13	0
2	he	3208	0	3205	14	0
2	hf	3208	0	3205	7	0
2	hg	3208	0	3205	9	0
2	hh	3208	0	3205	6	0
2	hi	3208	0	3205	10	0
2	hj	3208	0	3205	7	0
2	hk	3208	0	3205	11	0
2	hl	3208	0	3205	6	0
2	hm	3208	0	3205	10	0
2	hn	3208	0	3205	10	0
2	ho	3208	0	3205	7	0
3	hp	633	0	608	4	0
3	hq	633	0	608	4	0
3	hr	633	0	608	2	0
3	hs	633	0	608	4	0
3	ht	633	0	608	3	0
3	hu	633	0	608	5	0
3	hv	633	0	608	5	0
3	hw	633	0	608	3	0
3	hx	633	0	608	2	0
3	hy	633	0	608	2	0
3	hz	633	0	608	5	0
3	ia	633	0	608	2	0
3	ib	633	0	608	3	0
3	ic	633	0	608	4	0
3	id	633	0	608	2	0
3	ie	633	0	608	4	0
3	if	633	0	608	1	0
3	ig	633	0	608	3	0
3	ih	633	0	608	2	0
3	ii	633	0	608	5	0
3	ij	633	0	608	4	0
3	ik	633	0	608	6	0
3	il	633	0	608	3	0
3	im	633	0	608	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	in	633	0	608	2	0
3	io	633	0	608	3	0
3	ip	633	0	608	1	0
3	iq	633	0	608	4	0
3	ir	633	0	608	4	0
3	is	633	0	608	2	0
3	it	633	0	608	4	0
3	iu	633	0	608	6	0
3	iv	633	0	608	3	0
3	iw	633	0	608	4	0
3	ix	633	0	608	3	0
3	iy	633	0	608	3	0
3	iz	633	0	608	5	0
3	ja	633	0	608	3	0
3	jb	633	0	608	4	0
3	jc	633	0	608	6	0
3	jd	633	0	608	3	0
3	je	633	0	608	4	0
3	jf	633	0	608	6	0
3	jg	633	0	608	5	0
3	jh	633	0	608	4	0
3	ji	633	0	608	4	0
3	jj	633	0	608	1	0
3	jk	633	0	608	1	0
3	jl	633	0	608	4	0
3	jm	633	0	608	2	0
3	jn	633	0	608	3	0
3	jo	633	0	608	4	0
3	jp	633	0	608	2	0
3	jq	633	0	608	3	0
3	jr	633	0	608	4	0
3	js	633	0	608	2	0
3	jt	633	0	608	3	0
3	ju	633	0	608	3	0
3	jv	633	0	608	1	0
3	jw	633	0	608	4	0
3	jx	633	0	608	3	0
3	jy	633	0	608	3	0
3	jz	633	0	608	3	0
3	ka	633	0	608	6	0
3	kb	633	0	608	5	0
3	kc	633	0	608	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	kd	633	0	608	2	0
3	ke	633	0	608	5	0
3	kf	633	0	608	3	0
3	kg	633	0	608	6	0
3	kh	633	0	608	2	0
3	ki	633	0	608	2	0
3	kj	633	0	608	2	0
3	kk	633	0	608	5	0
3	kl	633	0	608	5	0
3	km	633	0	608	2	0
3	kn	633	0	608	4	0
3	ko	633	0	608	4	0
3	kp	633	0	608	5	0
3	kq	633	0	608	4	0
3	kr	633	0	608	4	0
3	ks	633	0	608	3	0
3	kt	633	0	608	3	0
3	ku	633	0	608	3	0
3	633	0	608	3	0	
3	kw	633	0	608	2	0
3	kx	633	0	608	2	0
3	ky	633	0	608	4	0
3	kz	633	0	608	1	0
3	la	633	0	608	5	0
3	lb	633	0	608	4	0
3	lc	633	0	608	3	0
3	ld	633	0	608	2	0
3	le	633	0	608	5	0
3	lf	633	0	608	4	0
3	lg	633	0	608	5	0
3	lh	633	0	608	2	0
3	li	633	0	608	3	0
3	lj	633	0	608	5	0
3	lk	633	0	608	3	0
3	ll	633	0	608	1	0
3	lm	633	0	608	5	0
3	ln	633	0	608	2	0
3	lo	633	0	608	4	0
3	lp	633	0	608	6	0
3	lq	633	0	608	3	0
3	lr	633	0	608	1	0
3	ls	633	0	608	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	lt	633	0	608	5	0
3	lu	633	0	608	5	0
3	lv	633	0	608	4	0
3	lw	633	0	608	3	0
3	lx	633	0	608	4	0
3	ly	633	0	608	3	0
3	lz	633	0	608	5	0
3	ma	633	0	608	3	0
3	mb	633	0	608	3	0
3	mc	633	0	608	1	0
3	md	633	0	608	2	0
3	me	633	0	608	4	0
3	mf	633	0	608	5	0
3	mg	633	0	608	2	0
3	mh	633	0	608	4	0
3	mi	633	0	608	3	0
3	mj	633	0	608	5	0
3	mk	633	0	608	5	0
3	ml	633	0	608	1	0
3	mm	633	0	608	4	0
3	mn	633	0	608	5	0
3	mo	633	0	608	5	0
3	mp	633	0	608	4	0
3	mq	633	0	608	3	0
3	ms	633	0	608	4	0
3	mt	633	0	608	4	0
3	mu	633	0	608	3	0
3	mv	633	0	608	2	0
3	mw	633	0	608	1	0
3	mx	633	0	608	3	0
3	my	633	0	608	6	0
3	mz	633	0	608	4	0
3	na	633	0	608	2	0
3	nb	633	0	608	3	0
3	nc	633	0	608	4	0
3	nd	633	0	608	4	0
3	ne	633	0	608	3	0
3	nf	633	0	608	3	0
3	ng	633	0	608	3	0
3	nh	633	0	608	4	0
3	ni	633	0	608	2	0
3	nj	633	0	608	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	nk	633	0	608	5	0
3	nl	633	0	608	1	0
3	nm	633	0	608	2	0
3	nn	633	0	608	4	0
3	no	633	0	608	3	0
3	np	633	0	608	3	0
3	nq	633	0	608	4	0
3	ns	633	0	608	3	0
3	nt	633	0	608	3	0
3	nu	633	0	608	7	0
3	nv	633	0	608	4	0
3	nw	633	0	608	6	0
3	nx	633	0	608	2	0
3	ny	633	0	608	6	0
3	nz	633	0	608	1	0
3	oa	633	0	608	2	0
3	ob	633	0	608	3	0
3	oc	633	0	608	1	0
3	od	633	0	608	3	0
3	oe	633	0	608	4	0
3	of	633	0	608	2	0
3	og	633	0	608	2	0
All	All	781038	0	766675	2284	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 1.

The worst 5 of 2284 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ea:99:VAL:HG21	1:eb:483:PRO:HG3	1.35	1.09
1:ca:99:VAL:HG21	1:cb:483:PRO:HB2	1.67	0.76
1:fq:121:THR:HG22	1:fq:260:GLU:HG2	1.74	0.69
3:hv:9:ASN:ND2	3:hv:51:SER:OG	2.26	0.69
1:an:74:TYR:CE2	1:ao:260:GLU:HG2	2.28	0.69

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	aa	454/521 (87%)	429 (94%)	20 (4%)	5 (1%)	11	38
1	ab	454/521 (87%)	433 (95%)	16 (4%)	5 (1%)	11	38
1	ac	454/521 (87%)	427 (94%)	24 (5%)	3 (1%)	18	47
1	ad	454/521 (87%)	422 (93%)	29 (6%)	3 (1%)	18	47
1	ae	454/521 (87%)	432 (95%)	18 (4%)	4 (1%)	14	42
1	af	454/521 (87%)	429 (94%)	21 (5%)	4 (1%)	14	42
1	ag	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	ah	454/521 (87%)	429 (94%)	19 (4%)	6 (1%)	9	33
1	ai	454/521 (87%)	425 (94%)	26 (6%)	3 (1%)	18	47
1	aj	454/521 (87%)	431 (95%)	20 (4%)	3 (1%)	18	47
1	ak	454/521 (87%)	429 (94%)	21 (5%)	4 (1%)	14	42
1	al	454/521 (87%)	433 (95%)	17 (4%)	4 (1%)	14	42
1	am	454/521 (87%)	428 (94%)	24 (5%)	2 (0%)	30	59
1	an	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	ao	454/521 (87%)	425 (94%)	26 (6%)	3 (1%)	18	47
1	ap	454/521 (87%)	426 (94%)	26 (6%)	2 (0%)	30	59
1	aq	454/521 (87%)	424 (93%)	24 (5%)	6 (1%)	9	33
1	ar	454/521 (87%)	430 (95%)	22 (5%)	2 (0%)	30	59
1	as	454/521 (87%)	429 (94%)	20 (4%)	5 (1%)	11	38
1	at	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	au	454/521 (87%)	426 (94%)	24 (5%)	4 (1%)	14	42
1	av	454/521 (87%)	428 (94%)	22 (5%)	4 (1%)	14	42
1	aw	454/521 (87%)	423 (93%)	29 (6%)	2 (0%)	30	59
1	ax	454/521 (87%)	427 (94%)	25 (6%)	2 (0%)	30	59
1	ay	454/521 (87%)	428 (94%)	22 (5%)	4 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	az	454/521 (87%)	428 (94%)	23 (5%)	3 (1%)	18	47
1	ba	454/521 (87%)	422 (93%)	29 (6%)	3 (1%)	18	47
1	bb	454/521 (87%)	433 (95%)	16 (4%)	5 (1%)	11	38
1	bc	454/521 (87%)	425 (94%)	26 (6%)	3 (1%)	18	47
1	bd	454/521 (87%)	430 (95%)	23 (5%)	1 (0%)	43	71
1	be	454/521 (87%)	427 (94%)	22 (5%)	5 (1%)	11	38
1	bf	454/521 (87%)	429 (94%)	20 (4%)	5 (1%)	11	38
1	bg	454/521 (87%)	426 (94%)	21 (5%)	7 (2%)	8	30
1	bh	454/521 (87%)	429 (94%)	20 (4%)	5 (1%)	11	38
1	bi	454/521 (87%)	423 (93%)	27 (6%)	4 (1%)	14	42
1	bj	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	bk	454/521 (87%)	431 (95%)	19 (4%)	4 (1%)	14	42
1	bl	454/521 (87%)	429 (94%)	21 (5%)	4 (1%)	14	42
1	bm	454/521 (87%)	429 (94%)	19 (4%)	6 (1%)	9	33
1	bn	454/521 (87%)	429 (94%)	21 (5%)	4 (1%)	14	42
1	bo	454/521 (87%)	427 (94%)	21 (5%)	6 (1%)	9	33
1	bp	454/521 (87%)	429 (94%)	19 (4%)	6 (1%)	9	33
1	bq	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	br	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	bs	454/521 (87%)	426 (94%)	23 (5%)	5 (1%)	11	38
1	bt	454/521 (87%)	424 (93%)	25 (6%)	5 (1%)	11	38
1	bu	454/521 (87%)	432 (95%)	19 (4%)	3 (1%)	18	47
1	bv	454/521 (87%)	431 (95%)	20 (4%)	3 (1%)	18	47
1	bw	454/521 (87%)	431 (95%)	20 (4%)	3 (1%)	18	47
1	bx	454/521 (87%)	427 (94%)	19 (4%)	8 (2%)	6	26
1	by	454/521 (87%)	424 (93%)	23 (5%)	7 (2%)	8	30
1	bz	454/521 (87%)	432 (95%)	17 (4%)	5 (1%)	11	38
1	ca	454/521 (87%)	431 (95%)	20 (4%)	3 (1%)	18	47
1	cb	454/521 (87%)	427 (94%)	24 (5%)	3 (1%)	18	47
1	cc	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	cd	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ce	454/521 (87%)	423 (93%)	25 (6%)	6 (1%)	9	33
1	cf	454/521 (87%)	432 (95%)	20 (4%)	2 (0%)	30	59
1	cg	454/521 (87%)	428 (94%)	23 (5%)	3 (1%)	18	47
1	ch	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	ci	454/521 (87%)	430 (95%)	21 (5%)	3 (1%)	18	47
1	cj	454/521 (87%)	432 (95%)	19 (4%)	3 (1%)	18	47
1	ck	454/521 (87%)	429 (94%)	21 (5%)	4 (1%)	14	42
1	cl	454/521 (87%)	427 (94%)	21 (5%)	6 (1%)	9	33
1	cm	454/521 (87%)	427 (94%)	22 (5%)	5 (1%)	11	38
1	cn	454/521 (87%)	426 (94%)	24 (5%)	4 (1%)	14	42
1	co	454/521 (87%)	431 (95%)	19 (4%)	4 (1%)	14	42
1	cp	454/521 (87%)	424 (93%)	26 (6%)	4 (1%)	14	42
1	cq	454/521 (87%)	424 (93%)	24 (5%)	6 (1%)	9	33
1	cr	454/521 (87%)	427 (94%)	24 (5%)	3 (1%)	18	47
1	cs	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	ct	454/521 (87%)	427 (94%)	24 (5%)	3 (1%)	18	47
1	cu	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	cv	454/521 (87%)	428 (94%)	23 (5%)	3 (1%)	18	47
1	cw	454/521 (87%)	425 (94%)	22 (5%)	7 (2%)	8	30
1	cx	454/521 (87%)	423 (93%)	28 (6%)	3 (1%)	18	47
1	cy	454/521 (87%)	426 (94%)	23 (5%)	5 (1%)	11	38
1	cz	454/521 (87%)	432 (95%)	19 (4%)	3 (1%)	18	47
1	da	454/521 (87%)	430 (95%)	21 (5%)	3 (1%)	18	47
1	db	454/521 (87%)	426 (94%)	22 (5%)	6 (1%)	9	33
1	dc	454/521 (87%)	425 (94%)	26 (6%)	3 (1%)	18	47
1	dd	454/521 (87%)	427 (94%)	25 (6%)	2 (0%)	30	59
1	de	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	df	454/521 (87%)	430 (95%)	21 (5%)	3 (1%)	18	47
1	dg	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	dh	454/521 (87%)	429 (94%)	18 (4%)	7 (2%)	8	30
1	di	454/521 (87%)	431 (95%)	20 (4%)	3 (1%)	18	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	dj	454/521 (87%)	426 (94%)	26 (6%)	2 (0%)	30	59
1	dk	454/521 (87%)	426 (94%)	23 (5%)	5 (1%)	11	38
1	dl	454/521 (87%)	426 (94%)	25 (6%)	3 (1%)	18	47
1	dm	454/521 (87%)	432 (95%)	20 (4%)	2 (0%)	30	59
1	dn	454/521 (87%)	432 (95%)	18 (4%)	4 (1%)	14	42
1	do	454/521 (87%)	429 (94%)	22 (5%)	3 (1%)	18	47
1	dp	454/521 (87%)	422 (93%)	28 (6%)	4 (1%)	14	42
1	dq	454/521 (87%)	427 (94%)	22 (5%)	5 (1%)	11	38
1	dr	454/521 (87%)	429 (94%)	22 (5%)	3 (1%)	18	47
1	ds	454/521 (87%)	425 (94%)	24 (5%)	5 (1%)	11	38
1	dt	454/521 (87%)	430 (95%)	22 (5%)	2 (0%)	30	59
1	du	454/521 (87%)	431 (95%)	18 (4%)	5 (1%)	11	38
1	dv	454/521 (87%)	426 (94%)	25 (6%)	3 (1%)	18	47
1	dw	428/521 (82%)	400 (94%)	24 (6%)	4 (1%)	14	42
1	dx	454/521 (87%)	431 (95%)	19 (4%)	4 (1%)	14	42
1	dy	454/521 (87%)	428 (94%)	23 (5%)	3 (1%)	18	47
1	dz	454/521 (87%)	432 (95%)	19 (4%)	3 (1%)	18	47
1	ea	454/521 (87%)	427 (94%)	24 (5%)	3 (1%)	18	47
1	eb	454/521 (87%)	431 (95%)	19 (4%)	4 (1%)	14	42
1	ec	454/521 (87%)	426 (94%)	23 (5%)	5 (1%)	11	38
1	ed	454/521 (87%)	431 (95%)	20 (4%)	3 (1%)	18	47
1	ee	454/521 (87%)	431 (95%)	20 (4%)	3 (1%)	18	47
1	ef	454/521 (87%)	432 (95%)	19 (4%)	3 (1%)	18	47
1	eg	454/521 (87%)	428 (94%)	23 (5%)	3 (1%)	18	47
1	eh	454/521 (87%)	426 (94%)	25 (6%)	3 (1%)	18	47
1	ei	454/521 (87%)	431 (95%)	19 (4%)	4 (1%)	14	42
1	ej	454/521 (87%)	434 (96%)	17 (4%)	3 (1%)	18	47
1	ek	454/521 (87%)	431 (95%)	19 (4%)	4 (1%)	14	42
1	el	454/521 (87%)	429 (94%)	22 (5%)	3 (1%)	18	47
1	em	454/521 (87%)	423 (93%)	28 (6%)	3 (1%)	18	47
1	en	454/521 (87%)	424 (93%)	26 (6%)	4 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	eo	454/521 (87%)	425 (94%)	24 (5%)	5 (1%)	11	38
1	ep	454/521 (87%)	426 (94%)	24 (5%)	4 (1%)	14	42
1	eq	454/521 (87%)	430 (95%)	21 (5%)	3 (1%)	18	47
1	er	454/521 (87%)	434 (96%)	17 (4%)	3 (1%)	18	47
1	es	454/521 (87%)	424 (93%)	26 (6%)	4 (1%)	14	42
1	et	454/521 (87%)	426 (94%)	24 (5%)	4 (1%)	14	42
1	eu	454/521 (87%)	425 (94%)	25 (6%)	4 (1%)	14	42
1	ev	454/521 (87%)	432 (95%)	20 (4%)	2 (0%)	30	59
1	ew	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	ex	454/521 (87%)	430 (95%)	19 (4%)	5 (1%)	11	38
1	ey	454/521 (87%)	429 (94%)	20 (4%)	5 (1%)	11	38
1	ez	454/521 (87%)	430 (95%)	19 (4%)	5 (1%)	11	38
1	fa	454/521 (87%)	423 (93%)	27 (6%)	4 (1%)	14	42
1	fb	454/521 (87%)	428 (94%)	21 (5%)	5 (1%)	11	38
1	fc	454/521 (87%)	429 (94%)	23 (5%)	2 (0%)	30	59
1	fd	454/521 (87%)	429 (94%)	19 (4%)	6 (1%)	9	33
1	fe	454/521 (87%)	424 (93%)	27 (6%)	3 (1%)	18	47
1	ff	454/521 (87%)	432 (95%)	18 (4%)	4 (1%)	14	42
1	fg	454/521 (87%)	427 (94%)	22 (5%)	5 (1%)	11	38
1	fh	454/521 (87%)	429 (94%)	20 (4%)	5 (1%)	11	38
1	fi	454/521 (87%)	427 (94%)	24 (5%)	3 (1%)	18	47
1	fj	454/521 (87%)	429 (94%)	21 (5%)	4 (1%)	14	42
1	fk	454/521 (87%)	429 (94%)	22 (5%)	3 (1%)	18	47
1	fl	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	fm	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	fn	454/521 (87%)	427 (94%)	24 (5%)	3 (1%)	18	47
1	fo	454/521 (87%)	428 (94%)	23 (5%)	3 (1%)	18	47
1	fp	454/521 (87%)	431 (95%)	19 (4%)	4 (1%)	14	42
1	fq	454/521 (87%)	423 (93%)	26 (6%)	5 (1%)	11	38
1	fr	454/521 (87%)	429 (94%)	20 (4%)	5 (1%)	11	38
1	fs	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ft	454/521 (87%)	429 (94%)	22 (5%)	3 (1%)	18	47
1	fu	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	fv	454/521 (87%)	428 (94%)	21 (5%)	5 (1%)	11	38
1	fw	454/521 (87%)	424 (93%)	23 (5%)	7 (2%)	8	30
1	fx	454/521 (87%)	431 (95%)	18 (4%)	5 (1%)	11	38
1	fy	454/521 (87%)	426 (94%)	22 (5%)	6 (1%)	9	33
1	fz	454/521 (87%)	428 (94%)	22 (5%)	4 (1%)	14	42
1	ga	454/521 (87%)	427 (94%)	23 (5%)	4 (1%)	14	42
1	gb	454/521 (87%)	431 (95%)	17 (4%)	6 (1%)	9	33
1	gc	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	gd	454/521 (87%)	430 (95%)	22 (5%)	2 (0%)	30	59
1	ge	454/521 (87%)	425 (94%)	23 (5%)	6 (1%)	9	33
1	gf	454/521 (87%)	432 (95%)	19 (4%)	3 (1%)	18	47
1	gg	454/521 (87%)	433 (95%)	17 (4%)	4 (1%)	14	42
1	gh	454/521 (87%)	426 (94%)	23 (5%)	5 (1%)	11	38
1	gi	454/521 (87%)	426 (94%)	24 (5%)	4 (1%)	14	42
1	gj	454/521 (87%)	423 (93%)	27 (6%)	4 (1%)	14	42
1	gk	454/521 (87%)	428 (94%)	20 (4%)	6 (1%)	9	33
1	gl	454/521 (87%)	431 (95%)	18 (4%)	5 (1%)	11	38
1	gm	454/521 (87%)	433 (95%)	17 (4%)	4 (1%)	14	42
1	gn	454/521 (87%)	427 (94%)	22 (5%)	5 (1%)	11	38
1	go	454/521 (87%)	426 (94%)	23 (5%)	5 (1%)	11	38
1	gp	454/521 (87%)	427 (94%)	26 (6%)	1 (0%)	43	71
1	gq	454/521 (87%)	429 (94%)	20 (4%)	5 (1%)	11	38
1	gr	454/521 (87%)	428 (94%)	21 (5%)	5 (1%)	11	38
1	gs	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	gt	454/521 (87%)	427 (94%)	21 (5%)	6 (1%)	9	33
1	gu	454/521 (87%)	431 (95%)	21 (5%)	2 (0%)	30	59
1	gv	454/521 (87%)	427 (94%)	24 (5%)	3 (1%)	18	47
1	gw	454/521 (87%)	430 (95%)	19 (4%)	5 (1%)	11	38
1	gx	454/521 (87%)	433 (95%)	20 (4%)	1 (0%)	43	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	gy	454/521 (87%)	429 (94%)	23 (5%)	2 (0%)	30	59
1	gz	454/521 (87%)	430 (95%)	20 (4%)	4 (1%)	14	42
1	ha	454/521 (87%)	429 (94%)	21 (5%)	4 (1%)	14	42
1	hb	454/521 (87%)	432 (95%)	19 (4%)	3 (1%)	18	47
1	hc	454/521 (87%)	425 (94%)	25 (6%)	4 (1%)	14	42
1	hd	454/521 (87%)	431 (95%)	20 (4%)	3 (1%)	18	47
2	he	413/427 (97%)	393 (95%)	16 (4%)	4 (1%)	12	40
2	hf	413/427 (97%)	389 (94%)	19 (5%)	5 (1%)	10	35
2	hg	413/427 (97%)	385 (93%)	24 (6%)	4 (1%)	12	40
2	hh	413/427 (97%)	386 (94%)	23 (6%)	4 (1%)	12	40
2	hi	413/427 (97%)	389 (94%)	20 (5%)	4 (1%)	12	40
2	hj	413/427 (97%)	389 (94%)	21 (5%)	3 (1%)	18	47
2	hk	413/427 (97%)	388 (94%)	20 (5%)	5 (1%)	10	35
2	hl	413/427 (97%)	384 (93%)	23 (6%)	6 (2%)	8	30
2	hm	413/427 (97%)	387 (94%)	19 (5%)	7 (2%)	7	28
2	hn	413/427 (97%)	390 (94%)	17 (4%)	6 (2%)	8	30
2	ho	413/427 (97%)	388 (94%)	20 (5%)	5 (1%)	10	35
3	hp	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	hq	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	hr	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	hs	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ht	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	hu	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	hv	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	hw	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	hx	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	hy	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	hz	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	ia	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	ib	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	ic	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	id	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	ie	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	if	77/80 (96%)	72 (94%)	3 (4%)	2 (3%)	4	21
3	ig	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	ih	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	33
3	ii	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ij	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	ik	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	il	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	im	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	in	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	io	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	ip	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	iq	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	ir	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	is	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	it	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	iu	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	iv	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	iw	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ix	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	iy	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	iz	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	33
3	ja	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	jb	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	jc	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	jd	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	33
3	je	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	jf	77/80 (96%)	71 (92%)	5 (6%)	1 (1%)	9	33
3	jg	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	jh	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	ji	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	jj	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	jk	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
3	jl	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	jm	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	jn	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	jo	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	jp	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	jq	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	jr	77/80 (96%)	70 (91%)	6 (8%)	1 (1%)	9	33
3	js	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	jt	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ju	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	33
3	jv	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	jw	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	jx	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	jy	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	jz	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ka	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	33
3	kb	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	kc	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	kd	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ke	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	kf	77/80 (96%)	73 (95%)	4 (5%)	0	100	100
3	kg	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	kh	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	ki	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	kj	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
3	kk	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	kl	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	km	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	kn	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	ko	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	kp	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	33
3	kq	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	kr	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ks	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	kt	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	33
3	ku	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33	
3	kw	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	kx	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ky	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	kz	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	la	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lb	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lc	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ld	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
3	le	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	lf	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lg	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	lh	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	li	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lj	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	lk	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ll	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	lm	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	ln	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	lo	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	lp	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lq	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	lr	77/80 (96%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	ls	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lt	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	lu	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lv	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	lw	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lx	77/80 (96%)	73 (95%)	4 (5%)	0	100	100
3	ly	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	lz	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	ma	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	mb	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	mc	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	md	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	me	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	mf	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	mg	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	mh	77/80 (96%)	71 (92%)	5 (6%)	1 (1%)	9	33
3	mi	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	mj	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	mk	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	ml	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	mm	77/80 (96%)	76 (99%)	0	1 (1%)	9	33
3	mn	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	mo	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	mp	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	33
3	mq	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	ms	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	mt	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	mu	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	mv	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	mw	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
3	mx	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	my	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	mz	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	na	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	nb	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	nc	77/80 (96%)	71 (92%)	5 (6%)	1 (1%)	9	33
3	nd	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	ne	77/80 (96%)	73 (95%)	4 (5%)	0	100	100
3	nf	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	ng	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	nh	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	ni	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	nj	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
3	nk	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	nl	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	nm	77/80 (96%)	73 (95%)	4 (5%)	0	100	100
3	nn	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	no	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
3	np	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	nq	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	ns	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	nt	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	nu	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	nv	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
3	nw	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	nx	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	ny	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	nz	77/80 (96%)	73 (95%)	4 (5%)	0	100	100
3	oa	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	ob	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	oc	77/80 (96%)	74 (96%)	2 (3%)	1 (1%)	9	33
3	od	77/80 (96%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	oe	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
3	of	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	33
3	og	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	33
All	All	102205/115363 (89%)	96599 (94%)	4674 (5%)	932 (1%)	16	42

5 of 932 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	aa	395	TYR
1	ad	395	TYR
1	ag	254	ILE
1	ag	395	TYR
1	ai	254	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aa	345/400 (86%)	345 (100%)	0	100	100
1	ab	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ac	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	ad	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ae	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	af	345/400 (86%)	345 (100%)	0	100	100
1	ag	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ah	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	ai	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	aj	345/400 (86%)	345 (100%)	0	100	100
1	ak	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	al	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	am	345/400 (86%)	343 (99%)	2 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	an	345/400 (86%)	345 (100%)	0	100	100
1	ao	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ap	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	aq	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ar	345/400 (86%)	345 (100%)	0	100	100
1	as	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	at	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	au	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	av	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	aw	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	ax	345/400 (86%)	345 (100%)	0	100	100
1	ay	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	az	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ba	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bb	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	bc	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	bd	345/400 (86%)	345 (100%)	0	100	100
1	be	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	bf	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bg	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bh	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	bi	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bj	345/400 (86%)	345 (100%)	0	100	100
1	bk	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bl	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bm	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bn	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bo	345/400 (86%)	345 (100%)	0	100	100
1	bp	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bq	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	br	345/400 (86%)	343 (99%)	2 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	bs	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bt	345/400 (86%)	345 (100%)	0	100	100
1	bu	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	bv	345/400 (86%)	345 (100%)	0	100	100
1	bw	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	bx	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	by	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	bz	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	ca	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	cb	345/400 (86%)	345 (100%)	0	100	100
1	cc	345/400 (86%)	345 (100%)	0	100	100
1	cd	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	ce	345/400 (86%)	345 (100%)	0	100	100
1	cf	345/400 (86%)	345 (100%)	0	100	100
1	cg	345/400 (86%)	345 (100%)	0	100	100
1	ch	345/400 (86%)	345 (100%)	0	100	100
1	ci	345/400 (86%)	345 (100%)	0	100	100
1	cj	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	ck	345/400 (86%)	345 (100%)	0	100	100
1	cl	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	cm	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	cn	345/400 (86%)	345 (100%)	0	100	100
1	co	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	cp	345/400 (86%)	345 (100%)	0	100	100
1	cq	345/400 (86%)	345 (100%)	0	100	100
1	cr	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	cs	345/400 (86%)	345 (100%)	0	100	100
1	ct	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	cu	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	cv	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	cw	345/400 (86%)	344 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	cx	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	cy	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	cz	345/400 (86%)	345 (100%)	0	100	100
1	da	345/400 (86%)	345 (100%)	0	100	100
1	db	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	dc	345/400 (86%)	345 (100%)	0	100	100
1	dd	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	de	345/400 (86%)	345 (100%)	0	100	100
1	df	345/400 (86%)	345 (100%)	0	100	100
1	dg	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	dh	345/400 (86%)	345 (100%)	0	100	100
1	di	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	dj	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	dk	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	dl	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	dm	345/400 (86%)	341 (99%)	4 (1%)	63	72
1	dn	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	do	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	dp	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	dq	345/400 (86%)	345 (100%)	0	100	100
1	dr	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ds	345/400 (86%)	345 (100%)	0	100	100
1	dt	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	du	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	dv	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	dw	329/400 (82%)	328 (100%)	1 (0%)	86	84
1	dx	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	dy	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	dz	345/400 (86%)	345 (100%)	0	100	100
1	ea	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	eb	345/400 (86%)	343 (99%)	2 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ec	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ed	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	ee	345/400 (86%)	345 (100%)	0	100	100
1	ef	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	eg	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	eh	345/400 (86%)	341 (99%)	4 (1%)	63	72
1	ei	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	ej	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ek	345/400 (86%)	345 (100%)	0	100	100
1	el	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	em	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	en	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	eo	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	ep	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	eq	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	er	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	es	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	et	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	eu	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ev	345/400 (86%)	345 (100%)	0	100	100
1	ew	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	ex	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ey	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	ez	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	fa	345/400 (86%)	345 (100%)	0	100	100
1	fb	345/400 (86%)	345 (100%)	0	100	100
1	fc	345/400 (86%)	341 (99%)	4 (1%)	63	72
1	fd	345/400 (86%)	345 (100%)	0	100	100
1	fe	345/400 (86%)	345 (100%)	0	100	100
1	ff	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fg	345/400 (86%)	345 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	fh	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fi	345/400 (86%)	341 (99%)	4 (1%)	63	72
1	fj	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	fk	345/400 (86%)	345 (100%)	0	100	100
1	fl	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	fm	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fn	345/400 (86%)	345 (100%)	0	100	100
1	fo	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fp	345/400 (86%)	345 (100%)	0	100	100
1	fq	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fr	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	fs	345/400 (86%)	340 (99%)	5 (1%)	59	70
1	ft	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fu	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fv	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fw	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fx	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	fy	345/400 (86%)	345 (100%)	0	100	100
1	fz	345/400 (86%)	345 (100%)	0	100	100
1	ga	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	gb	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gc	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gd	345/400 (86%)	345 (100%)	0	100	100
1	ge	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gf	345/400 (86%)	345 (100%)	0	100	100
1	gg	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	gh	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gi	345/400 (86%)	345 (100%)	0	100	100
1	gj	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gk	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gl	345/400 (86%)	344 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	gm	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gn	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	go	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gp	345/400 (86%)	345 (100%)	0	100	100
1	gq	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	gr	345/400 (86%)	345 (100%)	0	100	100
1	gs	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	gt	345/400 (86%)	339 (98%)	6 (2%)	53	67
1	gu	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	gv	345/400 (86%)	343 (99%)	2 (1%)	78	80
1	gw	345/400 (86%)	345 (100%)	0	100	100
1	gx	345/400 (86%)	345 (100%)	0	100	100
1	gy	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	gz	345/400 (86%)	341 (99%)	4 (1%)	63	72
1	ha	345/400 (86%)	345 (100%)	0	100	100
1	hb	345/400 (86%)	342 (99%)	3 (1%)	70	76
1	hc	345/400 (86%)	344 (100%)	1 (0%)	86	84
1	hd	345/400 (86%)	344 (100%)	1 (0%)	86	84
2	he	350/361 (97%)	348 (99%)	2 (1%)	78	80
2	hf	350/361 (97%)	347 (99%)	3 (1%)	70	76
2	hg	350/361 (97%)	349 (100%)	1 (0%)	86	84
2	hh	350/361 (97%)	349 (100%)	1 (0%)	86	84
2	hi	350/361 (97%)	349 (100%)	1 (0%)	86	84
2	hj	350/361 (97%)	350 (100%)	0	100	100
2	hk	350/361 (97%)	349 (100%)	1 (0%)	86	84
2	hl	350/361 (97%)	348 (99%)	2 (1%)	78	80
2	hm	350/361 (97%)	348 (99%)	2 (1%)	78	80
2	hn	350/361 (97%)	349 (100%)	1 (0%)	86	84
2	ho	350/361 (97%)	349 (100%)	1 (0%)	86	84
3	hp	66/67 (98%)	66 (100%)	0	100	100
3	hq	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	hr	66/67 (98%)	66 (100%)	0	100	100
3	hs	66/67 (98%)	66 (100%)	0	100	100
3	ht	66/67 (98%)	66 (100%)	0	100	100
3	hu	66/67 (98%)	66 (100%)	0	100	100
3	hv	66/67 (98%)	66 (100%)	0	100	100
3	hw	66/67 (98%)	66 (100%)	0	100	100
3	hx	66/67 (98%)	66 (100%)	0	100	100
3	hy	66/67 (98%)	66 (100%)	0	100	100
3	hz	66/67 (98%)	66 (100%)	0	100	100
3	ia	66/67 (98%)	66 (100%)	0	100	100
3	ib	66/67 (98%)	66 (100%)	0	100	100
3	ic	66/67 (98%)	66 (100%)	0	100	100
3	id	66/67 (98%)	66 (100%)	0	100	100
3	ie	66/67 (98%)	66 (100%)	0	100	100
3	if	66/67 (98%)	66 (100%)	0	100	100
3	ig	66/67 (98%)	66 (100%)	0	100	100
3	ih	66/67 (98%)	66 (100%)	0	100	100
3	ii	66/67 (98%)	66 (100%)	0	100	100
3	ij	66/67 (98%)	66 (100%)	0	100	100
3	ik	66/67 (98%)	66 (100%)	0	100	100
3	il	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	im	66/67 (98%)	66 (100%)	0	100	100
3	in	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	io	66/67 (98%)	66 (100%)	0	100	100
3	ip	66/67 (98%)	66 (100%)	0	100	100
3	iq	66/67 (98%)	66 (100%)	0	100	100
3	ir	66/67 (98%)	66 (100%)	0	100	100
3	is	66/67 (98%)	66 (100%)	0	100	100
3	it	66/67 (98%)	66 (100%)	0	100	100
3	iu	66/67 (98%)	66 (100%)	0	100	100
3	iv	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	iw	66/67 (98%)	66 (100%)	0	100	100
3	ix	66/67 (98%)	66 (100%)	0	100	100
3	iy	66/67 (98%)	66 (100%)	0	100	100
3	iz	66/67 (98%)	66 (100%)	0	100	100
3	ja	66/67 (98%)	66 (100%)	0	100	100
3	jb	66/67 (98%)	66 (100%)	0	100	100
3	jc	66/67 (98%)	66 (100%)	0	100	100
3	jd	66/67 (98%)	66 (100%)	0	100	100
3	je	66/67 (98%)	66 (100%)	0	100	100
3	jf	66/67 (98%)	66 (100%)	0	100	100
3	jg	66/67 (98%)	66 (100%)	0	100	100
3	jh	66/67 (98%)	66 (100%)	0	100	100
3	ji	66/67 (98%)	66 (100%)	0	100	100
3	jj	66/67 (98%)	66 (100%)	0	100	100
3	jk	66/67 (98%)	66 (100%)	0	100	100
3	jl	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	jm	66/67 (98%)	66 (100%)	0	100	100
3	jn	66/67 (98%)	66 (100%)	0	100	100
3	jo	66/67 (98%)	66 (100%)	0	100	100
3	jp	66/67 (98%)	66 (100%)	0	100	100
3	jq	66/67 (98%)	66 (100%)	0	100	100
3	jr	66/67 (98%)	66 (100%)	0	100	100
3	js	66/67 (98%)	66 (100%)	0	100	100
3	jt	66/67 (98%)	66 (100%)	0	100	100
3	ju	66/67 (98%)	66 (100%)	0	100	100
3	jv	66/67 (98%)	66 (100%)	0	100	100
3	jw	66/67 (98%)	66 (100%)	0	100	100
3	jx	66/67 (98%)	66 (100%)	0	100	100
3	jy	66/67 (98%)	66 (100%)	0	100	100
3	jz	66/67 (98%)	66 (100%)	0	100	100
3	ka	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	kb	66/67 (98%)	66 (100%)	0	100	100
3	kc	66/67 (98%)	66 (100%)	0	100	100
3	kd	66/67 (98%)	66 (100%)	0	100	100
3	ke	66/67 (98%)	66 (100%)	0	100	100
3	kf	66/67 (98%)	66 (100%)	0	100	100
3	kg	66/67 (98%)	66 (100%)	0	100	100
3	kh	66/67 (98%)	66 (100%)	0	100	100
3	ki	66/67 (98%)	66 (100%)	0	100	100
3	kj	66/67 (98%)	66 (100%)	0	100	100
3	kk	66/67 (98%)	66 (100%)	0	100	100
3	kl	66/67 (98%)	66 (100%)	0	100	100
3	km	66/67 (98%)	66 (100%)	0	100	100
3	kn	66/67 (98%)	66 (100%)	0	100	100
3	ko	66/67 (98%)	66 (100%)	0	100	100
3	kp	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	kq	66/67 (98%)	66 (100%)	0	100	100
3	kr	66/67 (98%)	66 (100%)	0	100	100
3	ks	66/67 (98%)	66 (100%)	0	100	100
3	kt	66/67 (98%)	66 (100%)	0	100	100
3	ku	66/67 (98%)	66 (100%)	0	100	100
3	66/67 (98%)	65 (98%)	1 (2%)	57	69	
3	kw	66/67 (98%)	66 (100%)	0	100	100
3	kx	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	ky	66/67 (98%)	66 (100%)	0	100	100
3	kz	66/67 (98%)	66 (100%)	0	100	100
3	la	66/67 (98%)	66 (100%)	0	100	100
3	lb	66/67 (98%)	66 (100%)	0	100	100
3	lc	66/67 (98%)	66 (100%)	0	100	100
3	ld	66/67 (98%)	66 (100%)	0	100	100
3	le	66/67 (98%)	66 (100%)	0	100	100
3	lf	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	lg	66/67 (98%)	66 (100%)	0	100	100
3	lh	66/67 (98%)	66 (100%)	0	100	100
3	li	66/67 (98%)	66 (100%)	0	100	100
3	lj	66/67 (98%)	66 (100%)	0	100	100
3	lk	66/67 (98%)	66 (100%)	0	100	100
3	ll	66/67 (98%)	66 (100%)	0	100	100
3	lm	66/67 (98%)	66 (100%)	0	100	100
3	ln	66/67 (98%)	66 (100%)	0	100	100
3	lo	66/67 (98%)	66 (100%)	0	100	100
3	lp	66/67 (98%)	66 (100%)	0	100	100
3	lq	66/67 (98%)	66 (100%)	0	100	100
3	lr	66/67 (98%)	66 (100%)	0	100	100
3	ls	66/67 (98%)	66 (100%)	0	100	100
3	lt	66/67 (98%)	66 (100%)	0	100	100
3	lu	66/67 (98%)	66 (100%)	0	100	100
3	lv	66/67 (98%)	64 (97%)	2 (3%)	36	59
3	lw	66/67 (98%)	66 (100%)	0	100	100
3	lx	66/67 (98%)	66 (100%)	0	100	100
3	ly	66/67 (98%)	66 (100%)	0	100	100
3	lz	66/67 (98%)	66 (100%)	0	100	100
3	ma	66/67 (98%)	66 (100%)	0	100	100
3	mb	66/67 (98%)	66 (100%)	0	100	100
3	mc	66/67 (98%)	66 (100%)	0	100	100
3	md	66/67 (98%)	66 (100%)	0	100	100
3	me	66/67 (98%)	66 (100%)	0	100	100
3	mf	66/67 (98%)	66 (100%)	0	100	100
3	mg	66/67 (98%)	66 (100%)	0	100	100
3	mh	66/67 (98%)	66 (100%)	0	100	100
3	mi	66/67 (98%)	66 (100%)	0	100	100
3	mj	66/67 (98%)	66 (100%)	0	100	100
3	mk	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	ml	66/67 (98%)	66 (100%)	0	100	100
3	mm	66/67 (98%)	66 (100%)	0	100	100
3	mn	66/67 (98%)	66 (100%)	0	100	100
3	mo	66/67 (98%)	66 (100%)	0	100	100
3	mp	66/67 (98%)	66 (100%)	0	100	100
3	mq	66/67 (98%)	66 (100%)	0	100	100
3	ms	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	mt	66/67 (98%)	66 (100%)	0	100	100
3	mu	66/67 (98%)	66 (100%)	0	100	100
3	mv	66/67 (98%)	66 (100%)	0	100	100
3	mw	66/67 (98%)	66 (100%)	0	100	100
3	mx	66/67 (98%)	66 (100%)	0	100	100
3	my	66/67 (98%)	66 (100%)	0	100	100
3	mz	66/67 (98%)	66 (100%)	0	100	100
3	na	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	nb	66/67 (98%)	66 (100%)	0	100	100
3	nc	66/67 (98%)	66 (100%)	0	100	100
3	nd	66/67 (98%)	66 (100%)	0	100	100
3	ne	66/67 (98%)	66 (100%)	0	100	100
3	nf	66/67 (98%)	66 (100%)	0	100	100
3	ng	66/67 (98%)	66 (100%)	0	100	100
3	nh	66/67 (98%)	66 (100%)	0	100	100
3	ni	66/67 (98%)	66 (100%)	0	100	100
3	nj	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	nk	66/67 (98%)	66 (100%)	0	100	100
3	nl	66/67 (98%)	66 (100%)	0	100	100
3	nm	66/67 (98%)	66 (100%)	0	100	100
3	nn	66/67 (98%)	66 (100%)	0	100	100
3	no	66/67 (98%)	66 (100%)	0	100	100
3	np	66/67 (98%)	66 (100%)	0	100	100
3	nq	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	ns	66/67 (98%)	66 (100%)	0	100	100
3	nt	66/67 (98%)	66 (100%)	0	100	100
3	nu	66/67 (98%)	66 (100%)	0	100	100
3	nv	66/67 (98%)	65 (98%)	1 (2%)	57	69
3	nw	66/67 (98%)	66 (100%)	0	100	100
3	nx	66/67 (98%)	66 (100%)	0	100	100
3	ny	66/67 (98%)	66 (100%)	0	100	100
3	nz	66/67 (98%)	66 (100%)	0	100	100
3	oa	66/67 (98%)	66 (100%)	0	100	100
3	ob	66/67 (98%)	66 (100%)	0	100	100
3	oc	66/67 (98%)	66 (100%)	0	100	100
3	od	66/67 (98%)	66 (100%)	0	100	100
3	oe	66/67 (98%)	66 (100%)	0	100	100
3	of	66/67 (98%)	66 (100%)	0	100	100
3	og	66/67 (98%)	65 (98%)	1 (2%)	57	69
All	All	79356/89895 (88%)	79096 (100%)	260 (0%)	84	84

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	hd	360	GLU
2	hh	209	GLU
1	dj	279	ARG
1	dd	514	ARG
2	hm	53	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 553 such sidechains are listed below:

Mol	Chain	Res	Type
3	ia	64	GLN
3	jc	64	GLN
3	hy	64	GLN
3	lq	64	GLN
1	dh	115	GLN

### 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.

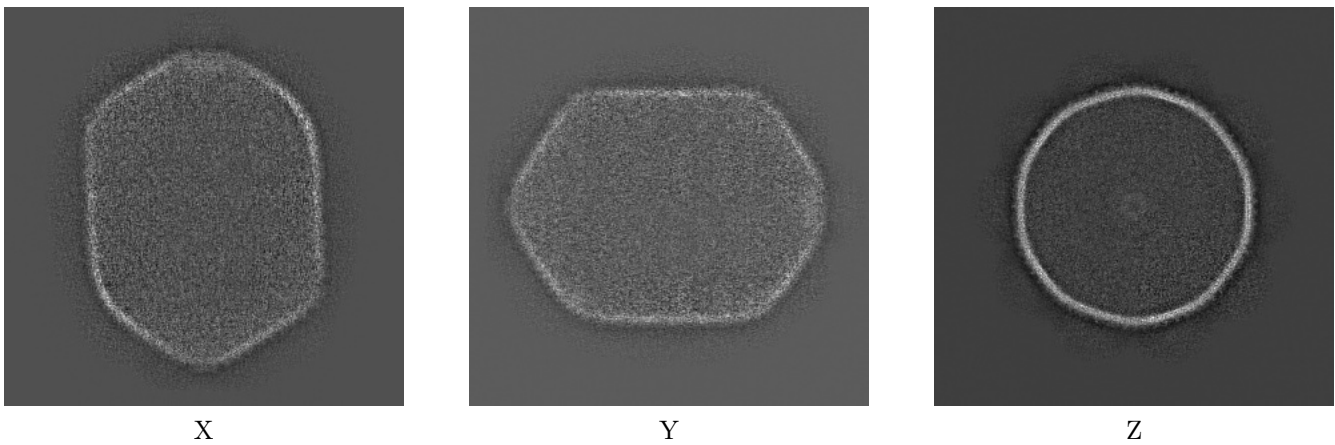
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32109. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

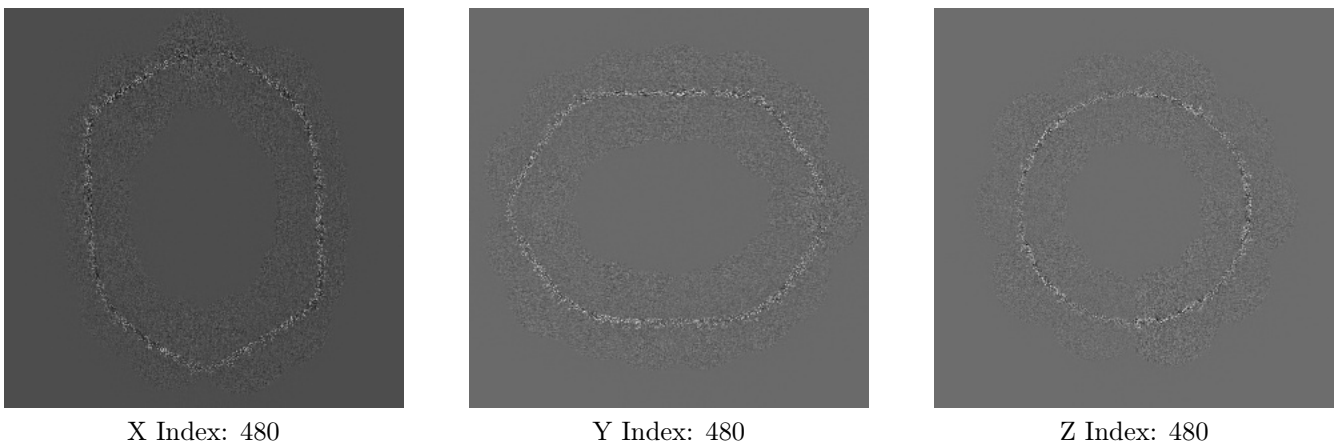
#### 6.1.1 Primary map



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

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

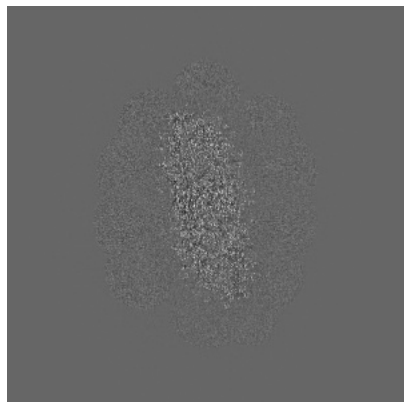
#### 6.2.1 Primary map



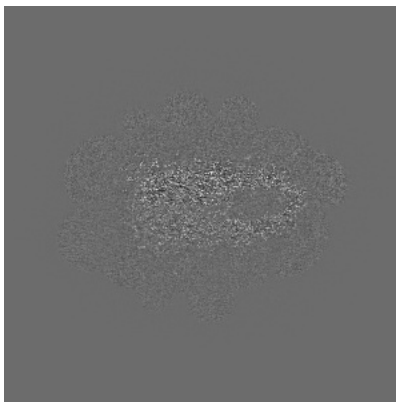
The images above show central slices of the map in three orthogonal directions.

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

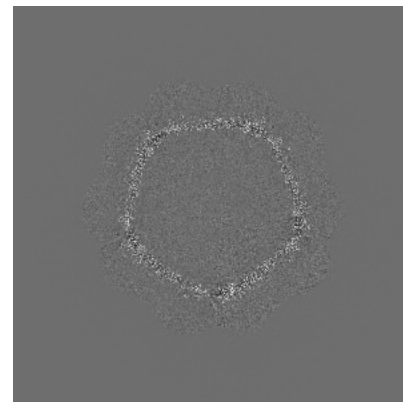
### 6.3.1 Primary map



X Index: 750



Y Index: 212

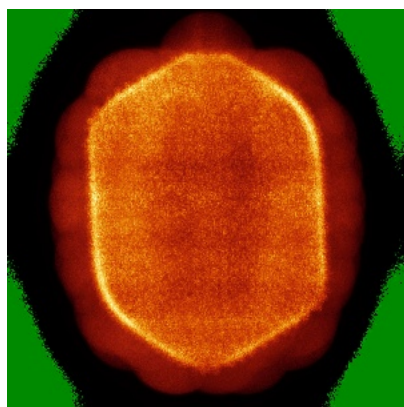


Z Index: 750

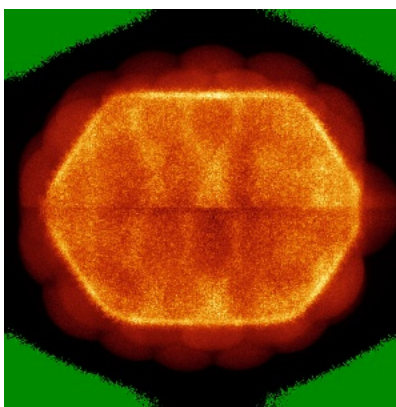
The images above show the largest variance slices of the map in three orthogonal directions.

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

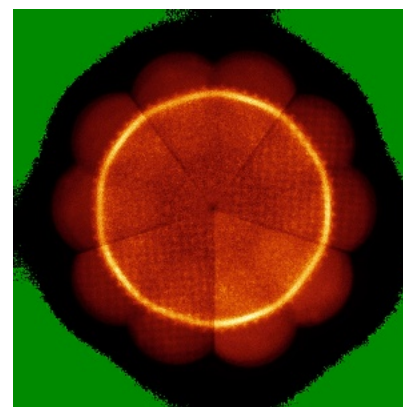
### 6.4.1 Primary map



X



Y

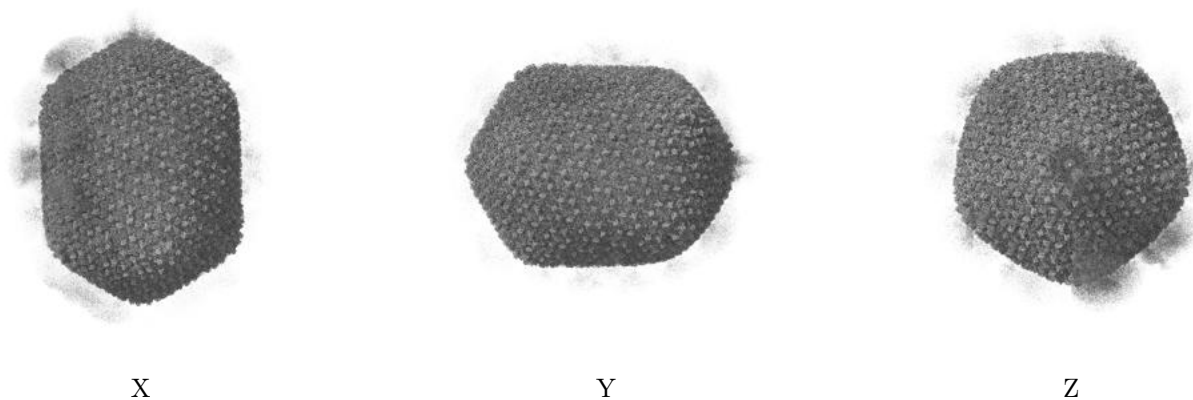


Z

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

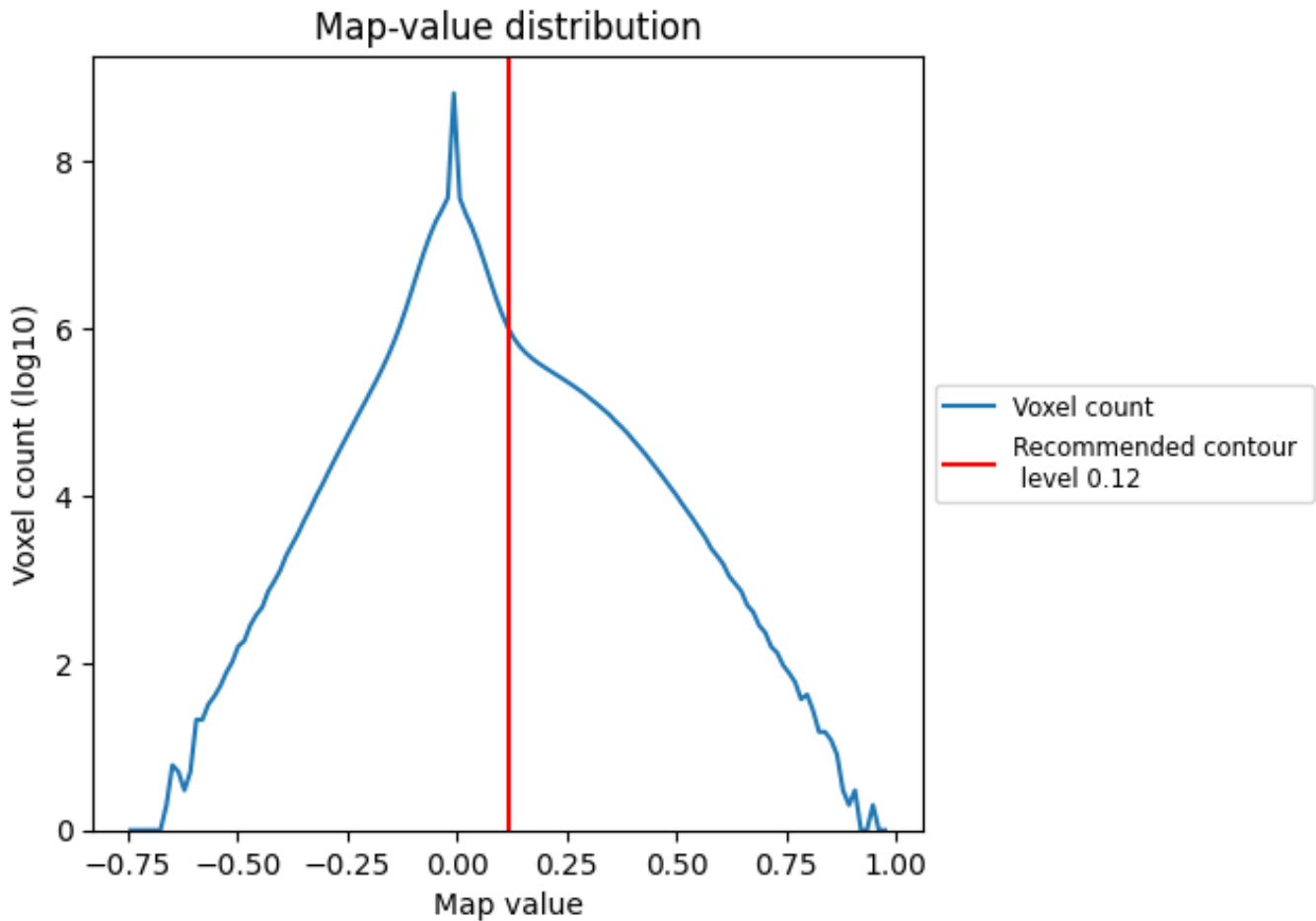
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

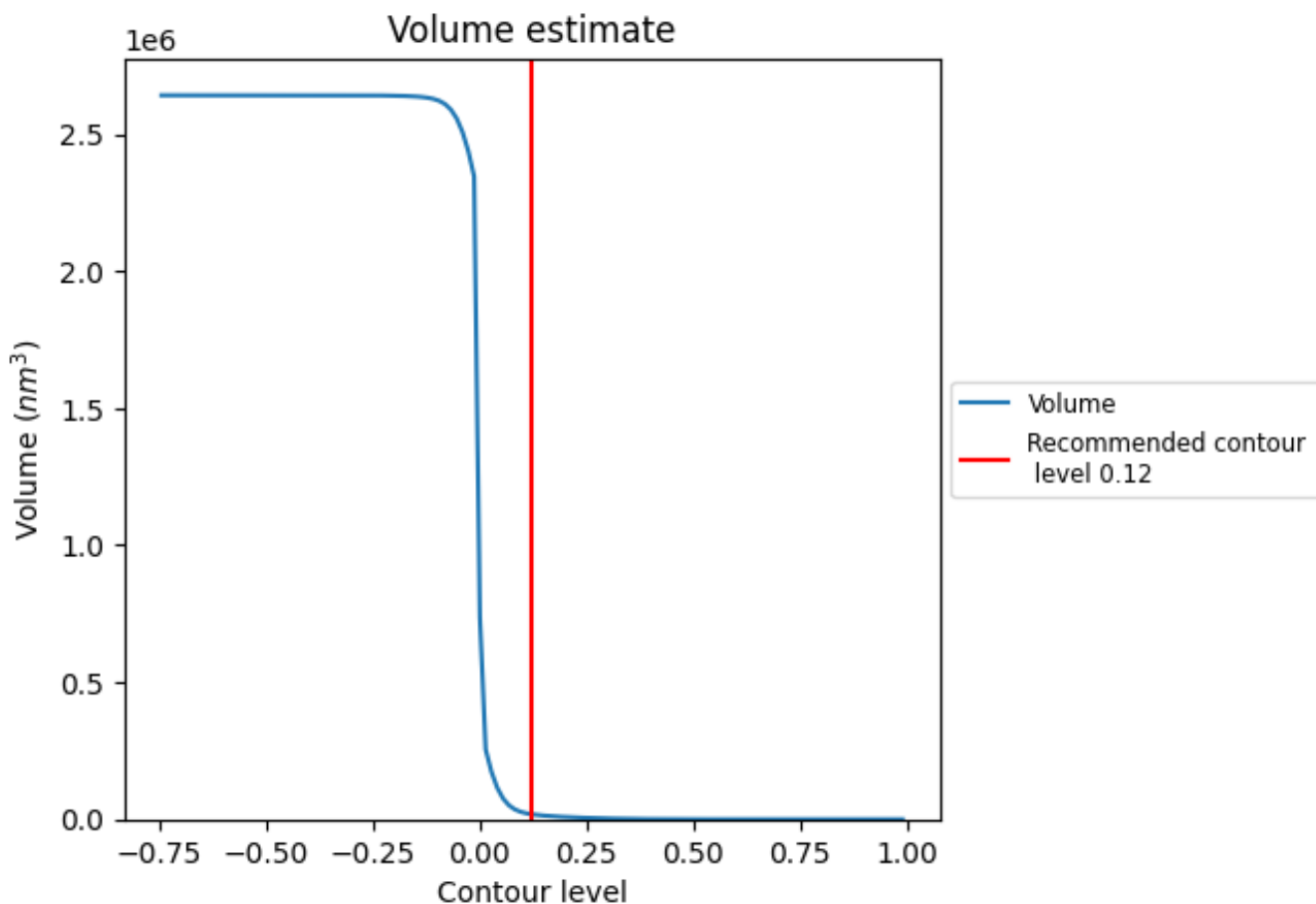
This section contains the results of statistical analysis of the map.

### 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.

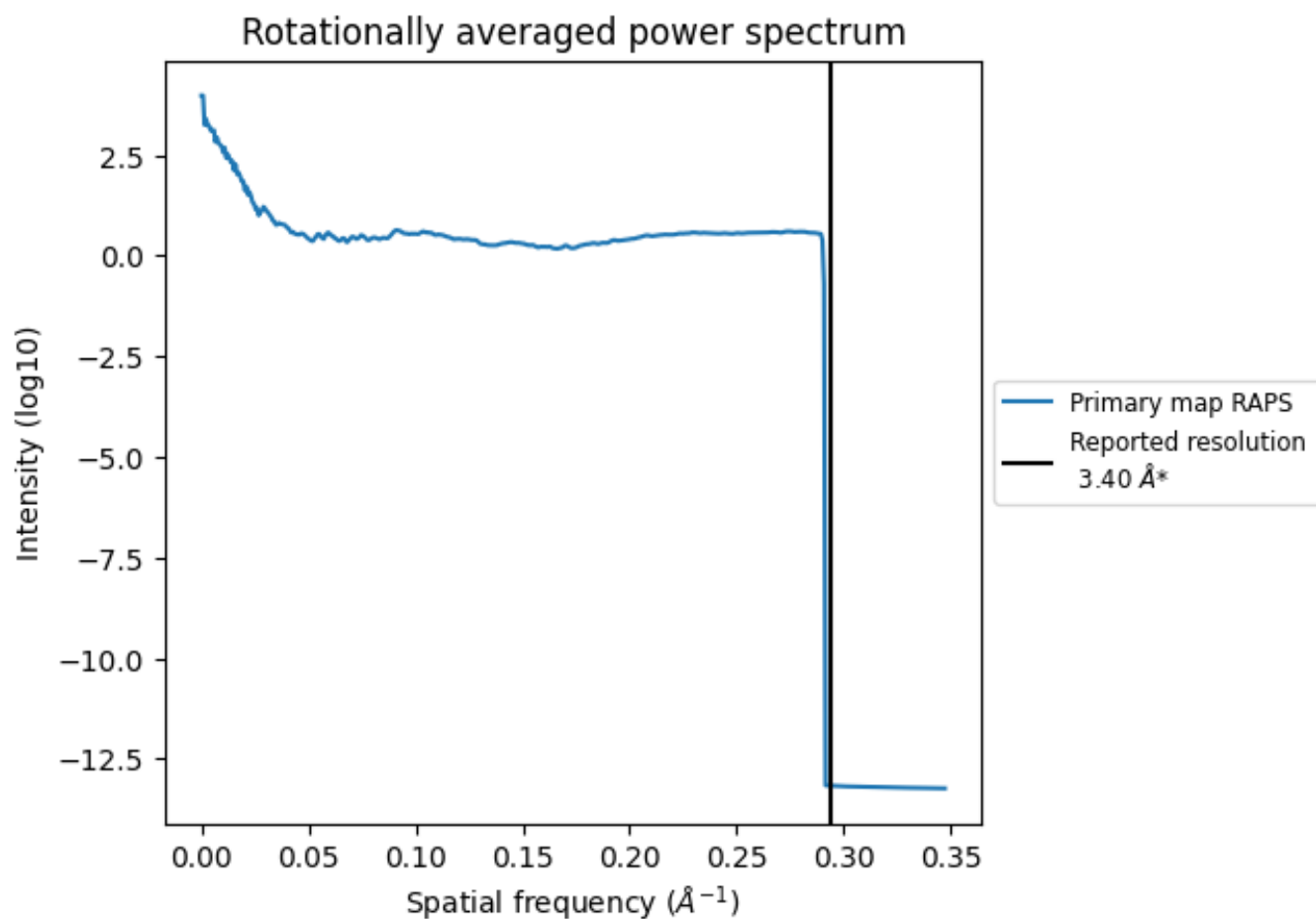
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $19040 \text{ nm}^3$ ; this corresponds to an approximate mass of 17199 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

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

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

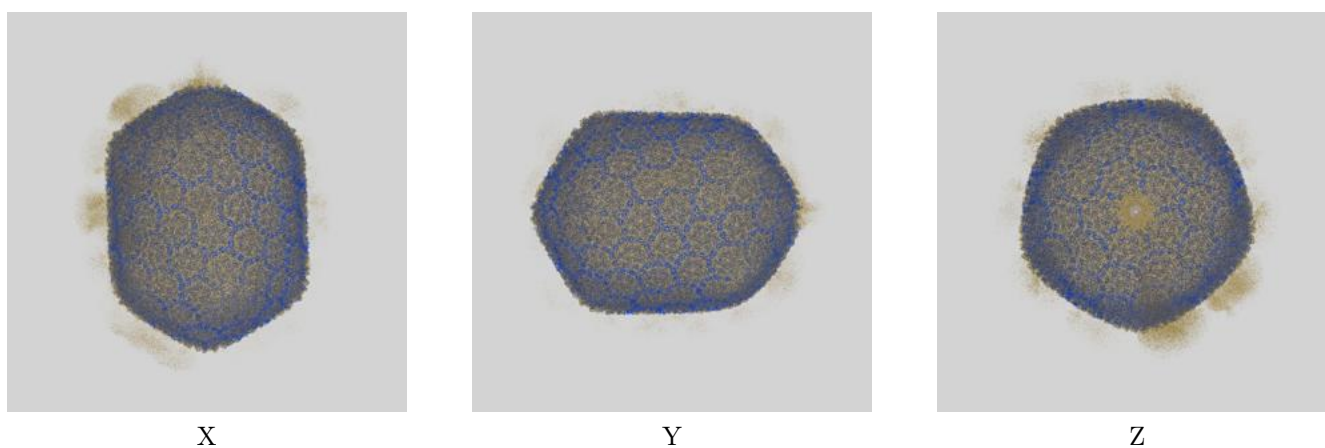
This section contains information regarding the fit between EMDB map EMD-32109 and PDB model 7VS5. Per-residue inclusion information can be found in section 3 on page 45.

### 9.1 Map-model overlays

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



#### 9.1.2 Map-model assembly overlay [i](#)



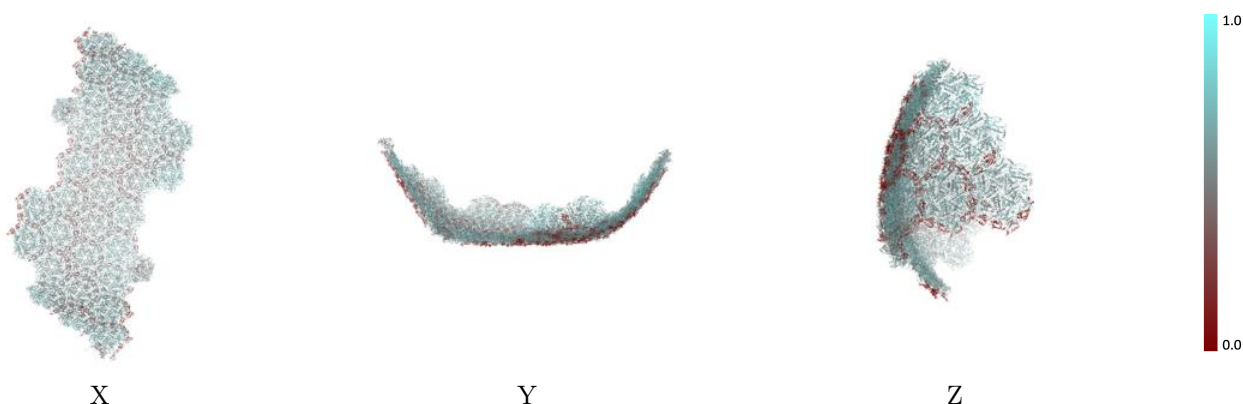
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



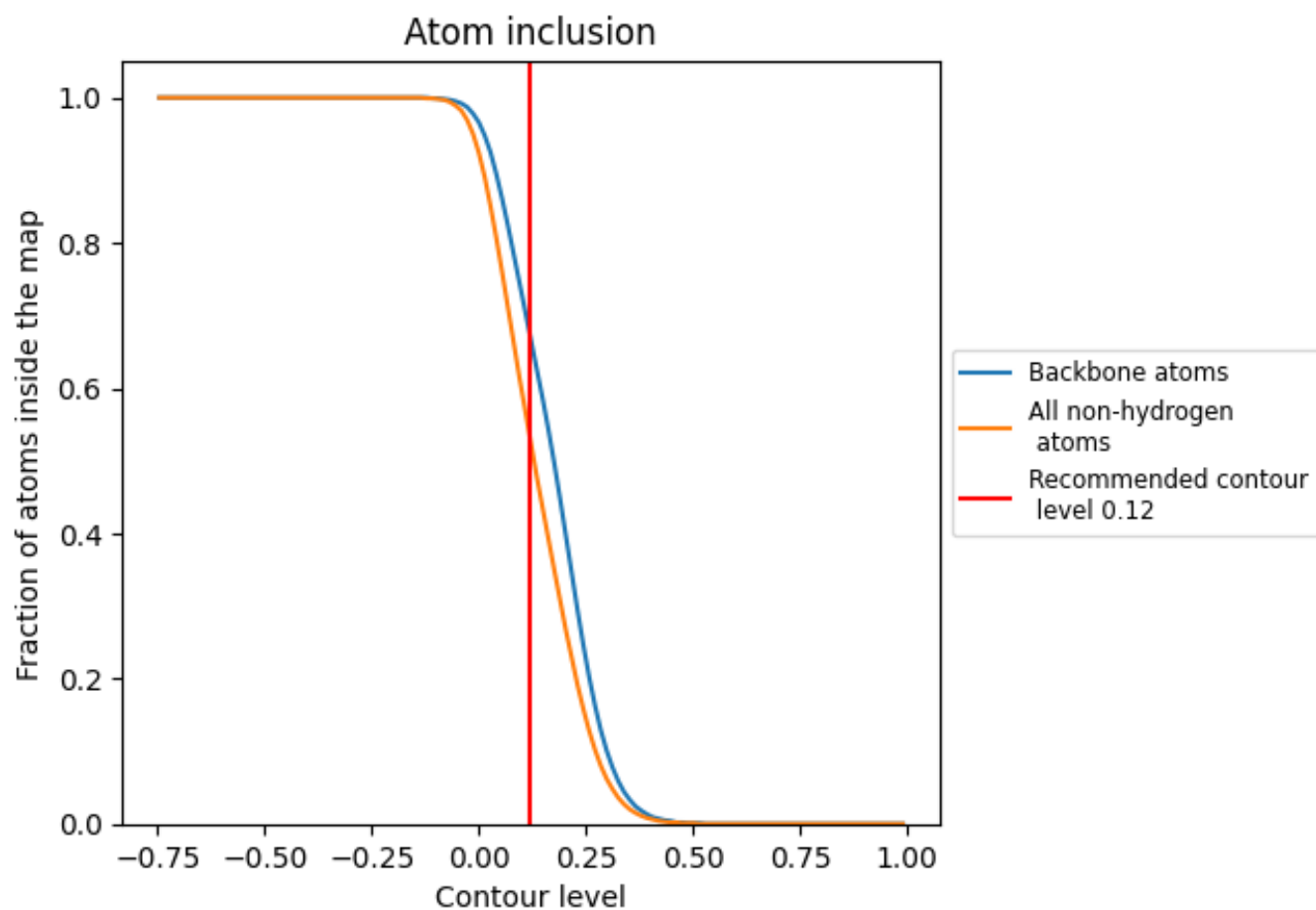
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 53% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5310	 0.4110
aa	 0.6410	 0.4500
ab	 0.6440	 0.4540
ac	 0.6290	 0.4510
ad	 0.6480	 0.4510
ae	 0.6210	 0.4420
af	 0.6080	 0.4390
ag	 0.6150	 0.4320
ah	 0.5430	 0.4180
ai	 0.5370	 0.4310
aj	 0.5580	 0.4400
ak	 0.5830	 0.4450
al	 0.6200	 0.4390
am	 0.5860	 0.4360
an	 0.6040	 0.4480
ao	 0.6080	 0.4490
ap	 0.6040	 0.4390
aq	 0.6210	 0.4400
ar	 0.6070	 0.4430
as	 0.6120	 0.4240
at	 0.5910	 0.4240
au	 0.5420	 0.4120
av	 0.5740	 0.4300
aw	 0.5890	 0.4340
ax	 0.5760	 0.4230
ay	 0.6070	 0.4480
az	 0.6070	 0.4480
ba	 0.6170	 0.4360
bb	 0.6140	 0.4370
bc	 0.6070	 0.4360
bd	 0.6090	 0.4360
be	 0.6310	 0.4540
bf	 0.6190	 0.4460
bg	 0.6470	 0.4420
bh	 0.6300	 0.4470



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Chain	Atom inclusion	Q-score
bi	 0.6160	 0.4420
bj	 0.6380	 0.4410
bk	 0.6460	 0.4370
bl	 0.6390	 0.4460
bm	 0.6380	 0.4480
bn	 0.6490	 0.4450
bo	 0.6550	 0.4410
bp	 0.6580	 0.4500
bq	 0.5880	 0.4150
br	 0.6200	 0.4230
bs	 0.6060	 0.4170
bt	 0.5740	 0.4120
bu	 0.5110	 0.4020
bv	 0.5470	 0.4130
bw	 0.5960	 0.4400
bx	 0.5630	 0.4250
by	 0.5990	 0.4360
bz	 0.6070	 0.4380
ca	 0.6060	 0.4390
cb	 0.6050	 0.4390
cc	 0.6130	 0.4300
cd	 0.6410	 0.4360
ce	 0.6470	 0.4270
cf	 0.6270	 0.4350
cg	 0.6050	 0.4260
ch	 0.5950	 0.4260
ci	 0.5780	 0.4030
cj	 0.5210	 0.3920
ck	 0.5790	 0.4010
cl	 0.6340	 0.4180
cm	 0.6350	 0.4240
cn	 0.6160	 0.4200
co	 0.5920	 0.4150
cp	 0.5720	 0.4050
cq	 0.5470	 0.3920
cr	 0.5140	 0.3840
cs	 0.5050	 0.3970
ct	 0.5700	 0.4100
cu	 0.5700	 0.4070
cv	 0.5510	 0.4060
cw	 0.5500	 0.4110
cx	 0.5440	 0.4080





















































































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Chain	Atom inclusion	Q-score
cy	0.5310	0.4020
cz	0.5650	0.4100
da	0.5540	0.4170
db	0.5990	0.4300
dc	0.6040	0.4270
dd	0.5810	0.4070
de	0.5750	0.3930
df	0.5640	0.4020
dg	0.5190	0.3820
dh	0.5330	0.4050
di	0.5690	0.3920
dj	0.6480	0.4030
dk	0.5910	0.4020
dl	0.5420	0.3920
dm	0.6290	0.4340
dn	0.6280	0.4260
do	0.6240	0.4230
dp	0.6180	0.4200
dq	0.6010	0.4270
dr	0.6180	0.4320
ds	0.5710	0.4130
dt	0.5600	0.4290
du	0.5550	0.4370
dv	0.5750	0.4340
dw	0.5820	0.4280
dx	0.5900	0.4110
dy	0.6120	0.4470
dz	0.6330	0.4500
ea	0.6420	0.4450
eb	0.6450	0.4450
ec	0.6420	0.4470
ed	0.6130	0.4440
ee	0.6780	0.4480
ef	0.6660	0.4550
eg	0.6410	0.4490
eh	0.6330	0.4470
ei	0.6680	0.4450
ej	0.6940	0.4550
ek	0.6150	0.4410
el	0.6050	0.4310
em	0.6010	0.4380
en	0.6110	0.4440





















































































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Chain	Atom inclusion	Q-score
eo	 0.6450	 0.4450
ep	 0.6360	 0.4390
eq	 0.6130	 0.4340
er	 0.6220	 0.4380
es	 0.6060	 0.4400
et	 0.6180	 0.4470
eu	 0.6200	 0.4400
ev	 0.6150	 0.4350
ew	 0.6160	 0.4460
ex	 0.6110	 0.4380
ey	 0.6420	 0.4460
ez	 0.6380	 0.4480
fa	 0.6280	 0.4470
fb	 0.6340	 0.4470
fc	 0.6200	 0.4330
fd	 0.5810	 0.4290
fe	 0.6060	 0.4370
ff	 0.6200	 0.4290
fg	 0.6230	 0.4400
fh	 0.6340	 0.4460
fi	 0.6060	 0.4160
fj	 0.5930	 0.4170
fk	 0.5370	 0.4110
fl	 0.5380	 0.4180
fm	 0.5710	 0.4300
fn	 0.5710	 0.4200
fo	 0.6120	 0.4350
fp	 0.5940	 0.4270
fq	 0.6530	 0.4420
fr	 0.6560	 0.4420
fs	 0.6440	 0.4390
ft	 0.6400	 0.4500
fu	 0.6520	 0.4310
fv	 0.6260	 0.4360
fw	 0.6010	 0.4230
fx	 0.6010	 0.4220
fy	 0.6350	 0.4190
fz	 0.6340	 0.4140
ga	 0.5430	 0.4100
gb	 0.4950	 0.4060
gc	 0.5240	 0.4090
gd	 0.5750	 0.4170





















































































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Chain	Atom inclusion	Q-score
ge	 0.6070	 0.4280
gf	 0.6100	 0.4230
gg	 0.5300	 0.3810
gh	 0.5530	 0.4000
gi	 0.5530	 0.3930
gj	 0.5330	 0.3740
gk	 0.5040	 0.3700
gl	 0.5050	 0.3660
gm	 0.6280	 0.4270
gn	 0.6180	 0.4310
go	 0.6120	 0.4290
gp	 0.5820	 0.4240
gq	 0.5790	 0.4280
gr	 0.6150	 0.4250
gs	 0.5130	 0.3970
gt	 0.5270	 0.4040
gu	 0.5670	 0.4110
gv	 0.6070	 0.4140
gw	 0.5930	 0.3880
gx	 0.5490	 0.3940
gy	 0.6200	 0.4230
gz	 0.6410	 0.4100
ha	 0.6750	 0.4090
hb	 0.6830	 0.4200
hc	 0.6570	 0.4270
hd	 0.6120	 0.4220
he	 0.5230	 0.4120
hf	 0.5150	 0.4120
hg	 0.5190	 0.4100
hh	 0.5280	 0.4200
hi	 0.5280	 0.4170
hj	 0.5300	 0.4020
hk	 0.5440	 0.3970
hl	 0.5650	 0.3930
hm	 0.5500	 0.4050
hn	 0.5600	 0.4180
ho	 0.4430	 0.3960
hp	 0.1610	 0.3340
hq	 0.3490	 0.4020
hr	 0.1250	 0.3660
hs	 0.0820	 0.3390
ht	 0.0390	 0.3410

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Chain	Atom inclusion	Q-score
hu	 0.0970	 0.3150
hv	 0.2320	 0.3690
hw	 0.1660	 0.3680
hx	 0.1780	 0.3590
hy	 0.1090	 0.3500
hz	 0.2590	 0.3470
ia	 0.1930	 0.3410
ib	 0.1880	 0.3910
ic	 0.2750	 0.3610
id	 0.0260	 0.3640
ie	 0.1090	 0.3560
if	 0.0920	 0.3440
ig	 0.1170	 0.3630
ih	 0.3040	 0.3810
ii	 0.1950	 0.3690
ij	 0.3330	 0.3750
ik	 0.2270	 0.3670
il	 0.0480	 0.3220
im	 0.1410	 0.3510
in	 0.0970	 0.3490
io	 0.0390	 0.3040
ip	 0.1250	 0.3680
iq	 0.0450	 0.3060
ir	 0.0690	 0.3280
is	 0.0850	 0.3240
it	 0.1290	 0.3610
iu	 0.1510	 0.3460
iv	 0.0870	 0.3450
iw	 0.0680	 0.3320
ix	 0.0150	 0.3290
iy	 0.0300	 0.3230
iz	 0.2330	 0.3540
ja	 0.3310	 0.4040
jb	 0.0160	 0.3460
jc	 0.0030	 0.2720
jd	 0.1090	 0.3620
je	 0.1370	 0.3570
jf	 0.1800	 0.3750
jg	 0.2690	 0.3730
jh	 0.0970	 0.3070
ji	 0.1090	 0.3170
jj	 0.1090	 0.3120

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Chain	Atom inclusion	Q-score
jk	■ 0.1040	■ 0.3250
jl	■ 0.2330	■ 0.3570
jm	■ 0.1240	■ 0.3580
jn	■ 0.0920	■ 0.3160
jo	■ 0.0900	■ 0.3160
jp	■ 0.0190	■ 0.3040
jq	■ 0.0480	■ 0.2950
jr	■ 0.1780	■ 0.3620
js	■ 0.2240	■ 0.3500
jt	■ 0.1110	■ 0.3020
ju	■ 0.1290	■ 0.3220
jv	■ 0.0390	■ 0.3160
jw	■ 0.0550	■ 0.3060
jx	■ 0.1900	■ 0.3280
jy	■ 0.1410	■ 0.3110
jz	■ 0.0180	■ 0.2470
ka	■ 0.0110	■ 0.2560
kb	■ 0.0950	■ 0.2890
kc	■ 0.0530	■ 0.2920
kd	■ 0.0400	■ 0.2610
ke	■ 0.0560	■ 0.2540
kf	■ 0.0800	■ 0.2910
kg	■ 0.1190	■ 0.2830
kh	■ 0.1590	■ 0.3360
ki	■ 0.1300	■ 0.3270
kj	■ 0.0480	■ 0.2260
kk	■ 0.0630	■ 0.2270
kl	■ 0.0160	■ 0.2720
km	■ 0.0020	■ 0.2700
kn	■ 0.0580	■ 0.3000
ko	■ 0.0340	■ 0.2700
kp	■ 0.0150	■ 0.2780
kq	■ 0.0640	■ 0.2830
kr	■ 0.0630	■ 0.2810
ks	■ 0.1190	■ 0.3150
kt	■ 0.1030	■ 0.3100
ku	■ 0.1290	■ 0.3280
■ 0.0100	■ 0.2520	
kw	■ 0.0160	■ 0.2560
kx	■ 0.0190	■ 0.2000
ky	■ 0.0000	■ 0.1780
kz	■ 0.0180	■ 0.1810



















































































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Chain	Atom inclusion	Q-score
la	0.2480	0.3480
lb	0.0900	0.3270
lc	0.1380	0.3200
ld	0.1210	0.3600
le	0.1720	0.3540
lf	0.2540	0.3690
lg	0.0560	0.3450
lh	0.2280	0.3620
li	0.1690	0.3410
lj	0.1980	0.3550
lk	0.2060	0.3610
ll	0.1770	0.3520
lm	0.2140	0.3760
ln	0.1930	0.3320
lo	0.1240	0.3420
lp	0.2150	0.3440
lq	0.3070	0.3450
lr	0.2190	0.3690
ls	0.1720	0.3600
lt	0.4210	0.3940
lu	0.3220	0.3610
lv	0.0690	0.3270
lw	0.1900	0.3580
lx	0.1190	0.3500
ly	0.0950	0.3190
lz	0.1720	0.3600
ma	0.1210	0.3390
mb	0.0550	0.3330
mc	0.1170	0.3720
md	0.1820	0.3570
me	0.2880	0.3720
mf	0.2650	0.3480
mg	0.2410	0.3710
mh	0.1240	0.3120
mi	0.2170	0.3620
mj	0.2850	0.3720
mk	0.3440	0.3750
ml	0.0770	0.3400
mm	0.0220	0.3130
mn	0.2440	0.3380
mo	0.2730	0.3580
mp	0.2690	0.3500

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Chain	Atom inclusion	Q-score
mq	 0.3910	 0.3850
ms	 0.0800	 0.3220
mt	 0.0640	 0.3440
mu	 0.0720	 0.2690
mv	 0.0790	 0.2990
mw	 0.1480	 0.3570
mx	 0.1130	 0.3260
my	 0.0580	 0.3050
mz	 0.0760	 0.3010
na	 0.0130	 0.2930
nb	 0.0220	 0.2690
nc	 0.1510	 0.3370
nd	 0.1610	 0.3630
ne	 0.0660	 0.3110
nf	 0.1090	 0.2800
ng	 0.2040	 0.3520
nh	 0.0550	 0.2950
ni	 0.0110	 0.2740
nj	 0.0110	 0.2560
nk	 0.0560	 0.3190
nl	 0.0710	 0.2830
nm	 0.0420	 0.2720
nn	 0.0900	 0.2880
no	 0.1510	 0.3400
np	 0.1010	 0.3550
nq	 0.1240	 0.3010
ns	 0.1610	 0.2900
nt	 0.0060	 0.2260
nu	 0.0050	 0.1990
nv	 0.1370	 0.2860
nw	 0.1990	 0.3080
nx	 0.0660	 0.3170
ny	 0.0510	 0.3210
nz	 0.0300	 0.2830
oa	 0.0290	 0.2920
ob	 0.0350	 0.2100
oc	 0.0190	 0.2520
od	 0.1030	 0.2500
oe	 0.0580	 0.2160
of	 0.0270	 0.2860
og	 0.0500	 0.2520