



wwPDB EM Validation Summary Report ⓘ

Sep 21, 2026 – 05:05 PM EDT

PDB ID : 12UU / pdb_000012uu
EMDB ID : EMD-76772
Title : The AAV2 capsid in complex with IgG-Fab#3-4
Authors : Zachery, J.; Mietzsch, M.; McKenna, R.
Deposited on : 2026-04-20
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

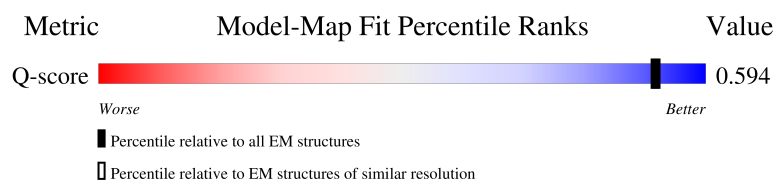
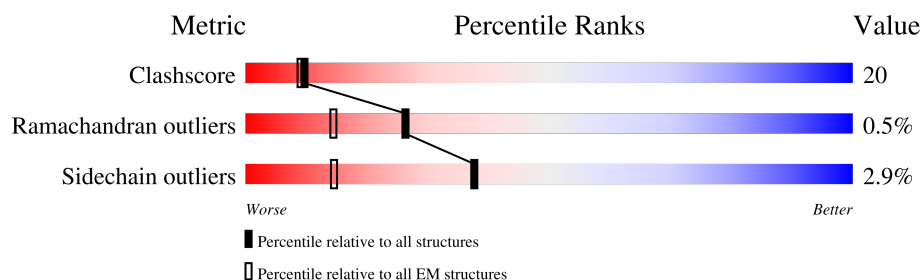
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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	12972 (2.41 - 3.41)

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

Mol	Chain	Length	Quality of chain
1	1	533	78% 17% . .
1	2	533	78% 17% . .
1	3	533	77% 17% . .
1	4	533	78% 17% . .

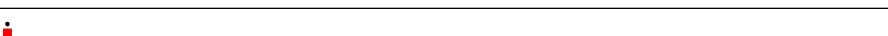
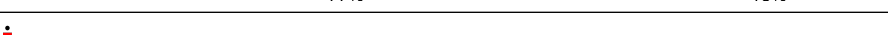
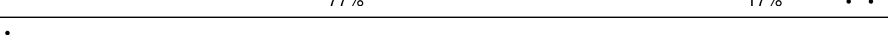
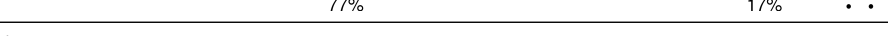
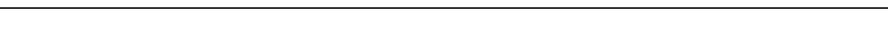
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Mol	Chain	Length	Quality of chain
1	5	533	 78%17% . .
1	6	533	 77%18% . .
1	7	533	 78%17% . .
1	8	533	 78%17% . .
1	A	533	 77%18% . .
1	B	533	 77%17% . .
1	C	533	 78%17% . .
1	D	533	 77%17% . .
1	E	533	 77%17% . .
1	F	533	 78%17% . .
1	G	533	 77%17% . .
1	H	533	 77%17% . .
1	I	533	 77%17% . .
1	J	533	 78%17% . .
1	K	533	 78%17% . .
1	L	533	 77%17% . .
1	M	533	 77%18% . .
1	N	533	 77%18% . .
1	O	533	 77%17% . .
1	P	533	 77%17% . .
1	Q	533	 78%17% . .
1	R	533	 77%18% . .
1	S	533	 78%17% . .
1	T	533	 77%17% . .
1	U	533	 77%17% . .

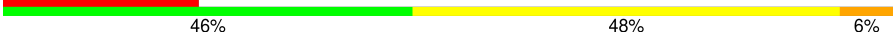
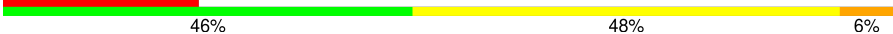
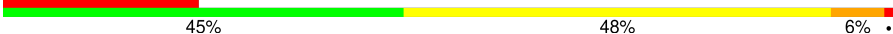
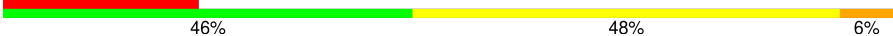
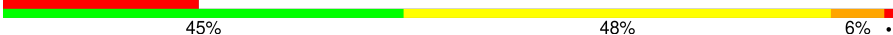
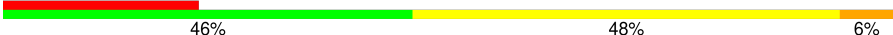
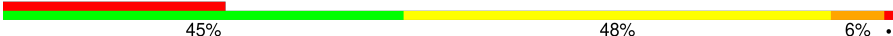
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Mol	Chain	Length	Quality of chain
1	V	533	
1	W	533	
1	X	533	
1	Y	533	
1	Z	533	
1	a	533	
1	b	533	
1	c	533	
1	d	533	
1	e	533	
1	f	533	
1	g	533	
1	h	533	
1	i	533	
1	j	533	
1	k	533	
1	l	533	
1	m	533	
1	n	533	
1	o	533	
1	p	533	
1	q	533	
1	r	533	
1	s	533	
1	t	533	

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Mol	Chain	Length	Quality of chain
1	u	533	 77% 17% . .
1	v	533	 78% 17% . .
1	w	533	 78% 17% . .
1	x	533	 78% 17% . .
1	y	533	 78% 17% . .
1	z	533	 78% 17% . .
2	1h	125	 22% 46% 48% 6% .
2	2h	125	 22% 46% 48% 6% .
2	3h	125	 22% 45% 48% 6% .
2	4h	125	 22% 46% 48% 6% .
2	5h	125	 22% 45% 48% 6% .
2	6h	125	 22% 46% 48% 6% .
2	7h	125	 25% 45% 48% 6% .
2	8h	125	 25% 45% 48% 6% .
2	Ah	125	 21% 45% 48% 6% .
2	Bh	125	 21% 46% 48% 6% .
2	Ch	125	 23% 45% 48% 6% .
2	Dh	125	 25% 45% 48% 6% .
2	Eh	125	 26% 46% 48% 6% .
2	Fh	125	 22% 46% 48% 6% .
2	Gh	125	 26% 45% 48% 6% .
2	Hh	125	 25% 46% 48% 6% .
2	Ih	125	 23% 45% 48% 6% .
2	Jh	125	 21% 45% 48% 6% .
2	Kh	125	 23% 45% 48% 6% .

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Mol	Chain	Length	Quality of chain
2	Lh	125	
2	Mh	125	
2	Nh	125	
2	Oh	125	
2	Ph	125	
2	Qh	125	
2	Rh	125	
2	Sh	125	
2	Th	125	
2	Uh	125	
2	Vh	125	
2	Wh	125	
2	Xh	125	
2	Yh	125	
2	Zh	125	
2	ah	125	
2	bh	125	
2	ch	125	
2	dh	125	
2	eh	125	
2	fh	125	
2	gh	125	
2	hh	125	
2	ih	125	
2	jh	125	

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Mol	Chain	Length	Quality of chain
2	kh	125	21% 45% 48% 6%
2	lh	125	21% 45% 48% 6%
2	mh	125	21% 45% 48% 6%
2	nh	125	26% 45% 48% 6%
2	oh	125	23% 45% 48% 6%
2	ph	125	22% 45% 48% 6%
2	qh	125	26% 46% 48% 6%
2	rh	125	23% 45% 48% 6%
2	sh	125	22% 46% 48% 6%
2	th	125	21% 46% 48% 6%
2	uh	125	21% 46% 48% 6%
2	vh	125	21% 45% 48% 6%
2	wh	125	22% 46% 48% 6%
2	xh	125	23% 45% 48% 6%
2	yh	125	25% 46% 48% 6%
2	zh	125	25% 45% 48% 6%
3	1l	107	21% 60% 36% •
3	2l	107	21% 61% 36% •
3	3l	107	21% 62% 33% 6%
3	4l	107	21% 59% 36% 6%
3	5l	107	21% 62% 33% 6%
3	6l	107	21% 61% 36% •
3	7l	107	21% 60% 36% 5%
3	8l	107	23% 62% 34% 5%
3	Al	107	18% 61% 34% 6%

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Mol	Chain	Length	Quality of chain
3	B1	107	
3	C1	107	
3	D1	107	
3	E1	107	
3	F1	107	
3	G1	107	
3	H1	107	
3	I1	107	
3	J1	107	
3	K1	107	
3	L1	107	
3	M1	107	
3	N1	107	
3	O1	107	
3	P1	107	
3	Q1	107	
3	R1	107	
3	S1	107	
3	T1	107	
3	U1	107	
3	V1	107	
3	W1	107	
3	X1	107	
3	Y1	107	
3	Z1	107	

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Mol	Chain	Length	Quality of chain
3	al	107	
3	bl	107	
3	cl	107	
3	dl	107	
3	el	107	
3	fl	107	
3	gl	107	
3	hl	107	
3	il	107	
3	jl	107	
3	kl	107	
3	ll	107	
3	ml	107	
3	nl	107	
3	ol	107	
3	pl	107	
3	ql	107	
3	rl	107	
3	sl	107	
3	tl	107	
3	ul	107	
3	vl	107	
3	wl	107	
3	xl	107	
3	yl	107	

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Mol	Chain	Length	Quality of chain
3	zl	107	21% 60% 35% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 354540 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	B	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	C	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	D	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	E	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	F	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	G	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	H	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	I	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	J	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	K	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	L	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	M	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	N	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	O	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	P	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		
1	Q	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	S	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	T	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	U	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	V	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	W	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	X	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	Y	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	Z	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	1	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	2	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	3	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	4	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	5	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	6	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	a	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	b	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	c	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	d	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	e	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	f	516	Total 4135	C 2603	N 722	O 797	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	h	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	i	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	j	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	k	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	l	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	m	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	n	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	o	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	p	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	q	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	r	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	s	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	t	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	u	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	v	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	w	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	x	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	y	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	z	516	Total 4135	C 2603	N 722	O 797	S 13	0	0
1	7	516	Total 4135	C 2603	N 722	O 797	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	516	Total	C	N	O	S	0	0
			4135	2603	722	797	13		

- Molecule 2 is a protein called IgG Fab3-4 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ah	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Bh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Ch	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Dh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Eh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Fh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Gh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Hh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Ih	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Jh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Kh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Lh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Mh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Nh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Oh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Ph	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Qh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		
2	Rh	125	Total	C	N	O	S	0	0
			989	632	165	187	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Sh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	Th	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	Uh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	Vh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	Wh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	Xh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	Yh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	Zh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	1h	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	2h	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	3h	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	4h	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	5h	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	6h	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	ah	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	bh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	ch	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	dh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	eh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	fh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	gh	125	Total 989	C 632	N 165	O 187	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	hh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	ih	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	jh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	kh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	lh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	mh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	nh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	oh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	ph	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	qh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	rh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	sh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	th	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	uh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	vh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	wh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	xh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	yh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	zh	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	7h	125	Total 989	C 632	N 165	O 187	S 5	0	0
2	8h	125	Total 989	C 632	N 165	O 187	S 5	0	0

- Molecule 3 is a protein called IgG Fab3-4 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Al	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Bl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Cl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Dl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	El	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Fl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Gl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Hl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Il	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Jl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Kl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Ll	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Ml	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Nl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Ol	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Pl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Ql	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Rl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Sl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Tl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Ul	107	Total 785	C 482	N 135	O 166	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Vl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Wl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Xl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Yl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	Zl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	1l	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	2l	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	3l	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	4l	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	5l	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	6l	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	al	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	bl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	cl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	dl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	el	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	fl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	gl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	hl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	il	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	jl	107	Total 785	C 482	N 135	O 166	S 2	0	0

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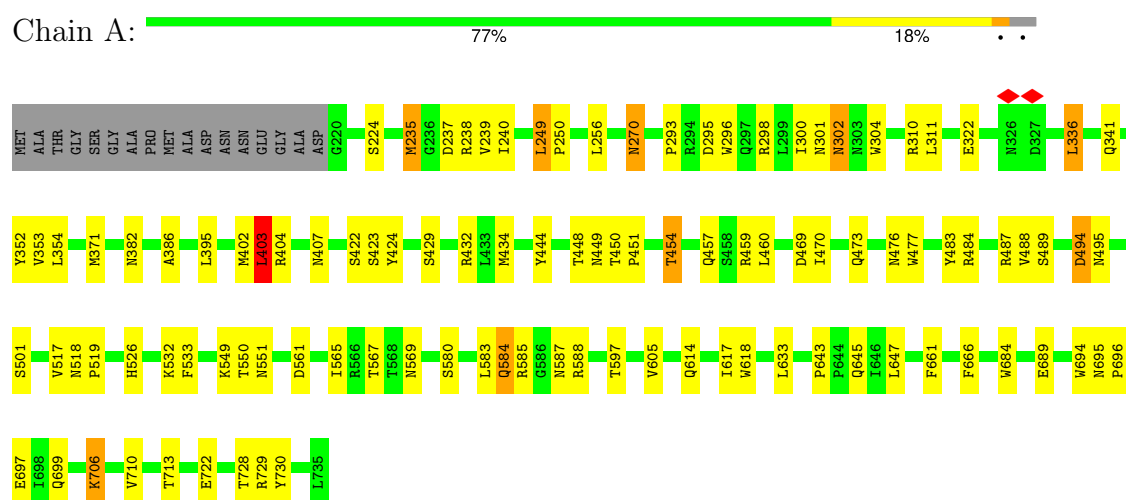
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	kl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	ll	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	ml	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	nl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	ol	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	pl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	ql	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	rl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	sl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	tl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	ul	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	vl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	wl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	xl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	yl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	zl	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	7l	107	Total 785	C 482	N 135	O 166	S 2	0	0
3	8l	107	Total 785	C 482	N 135	O 166	S 2	0	0

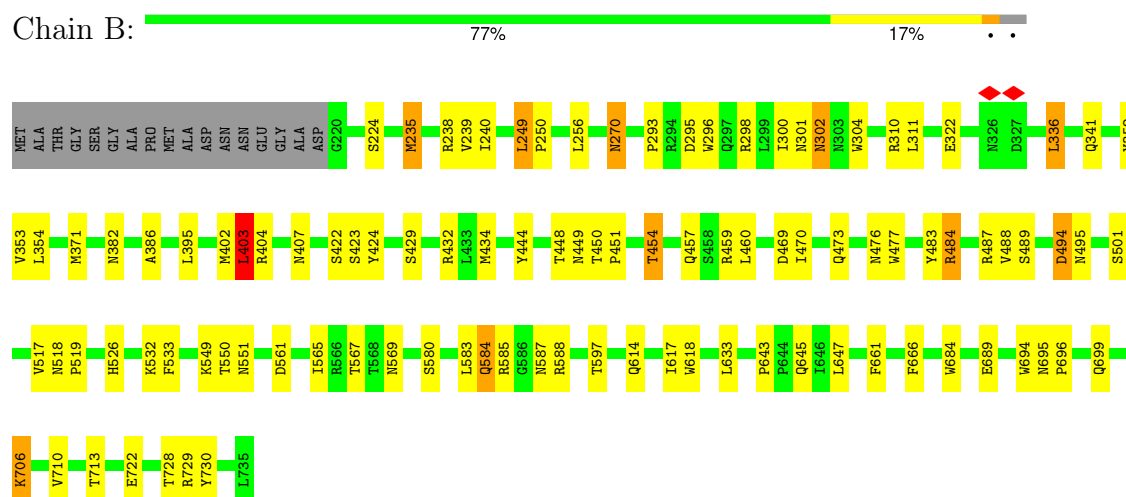
3 Residue-property plots

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

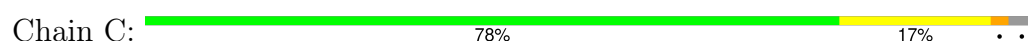
• Molecule 1: Capsid protein VP1

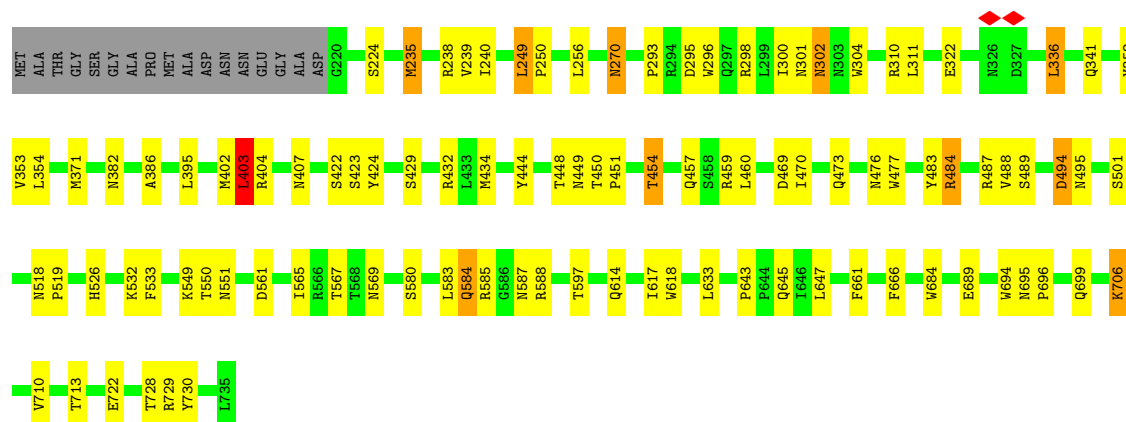


• Molecule 1: Capsid protein VP1



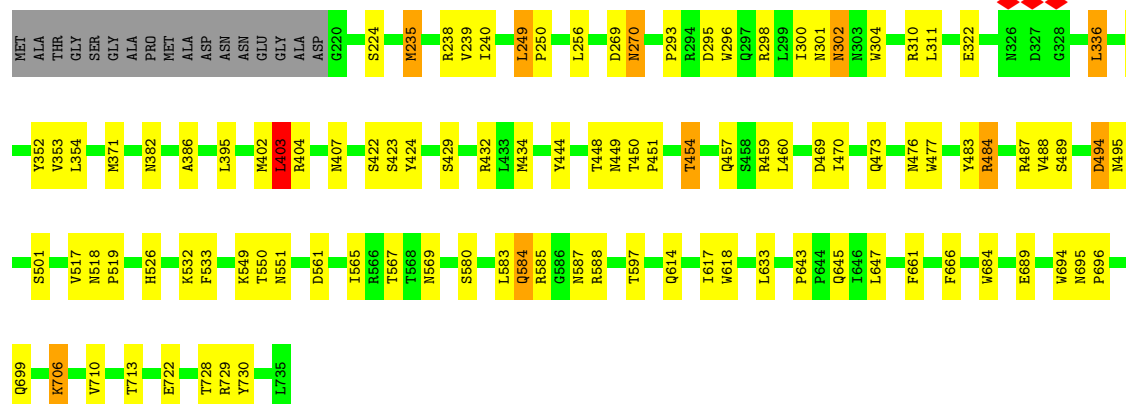
• Molecule 1: Capsid protein VP1





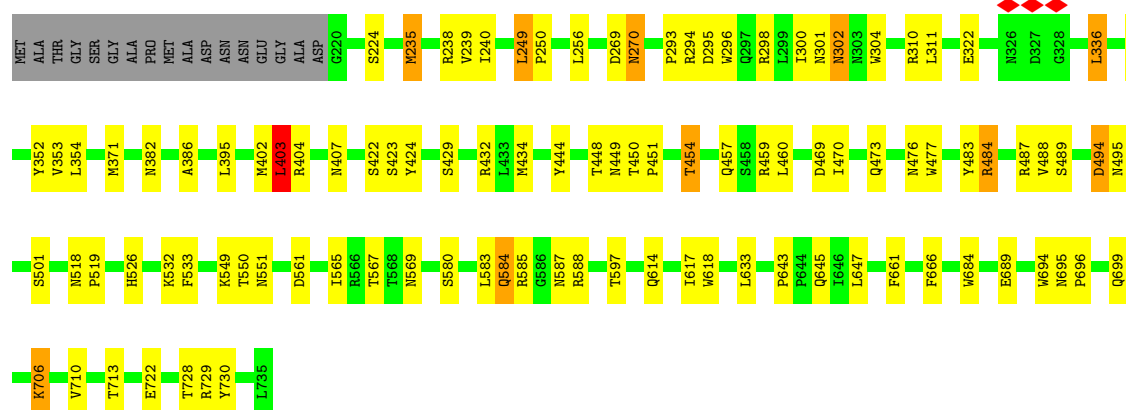
• Molecule 1: Capsid protein VP1

Chain D: 77% 17%



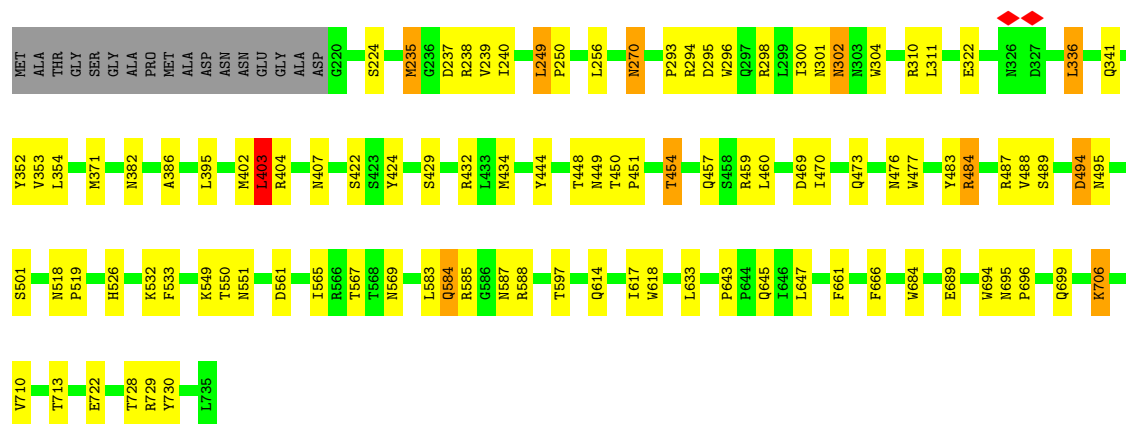
• Molecule 1: Capsid protein VP1

Chain E: 77% 17%

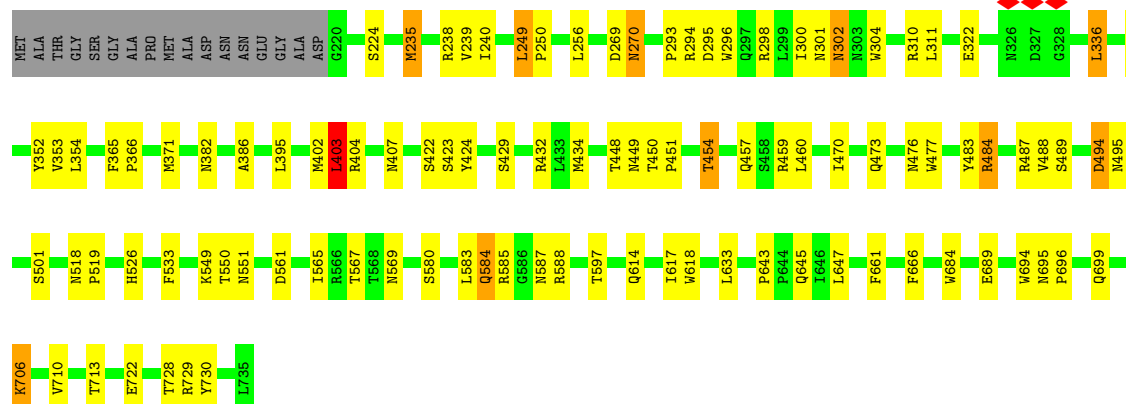
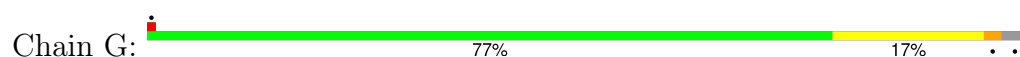


• Molecule 1: Capsid protein VP1

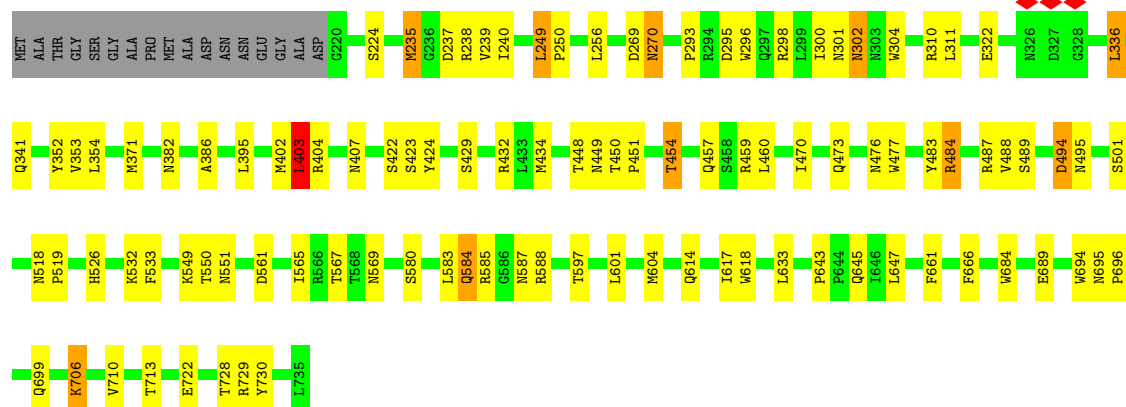
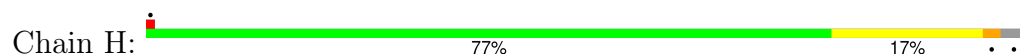
Chain F: 78% 17%



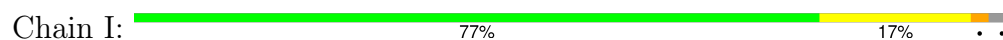
• Molecule 1: Capsid protein VP1

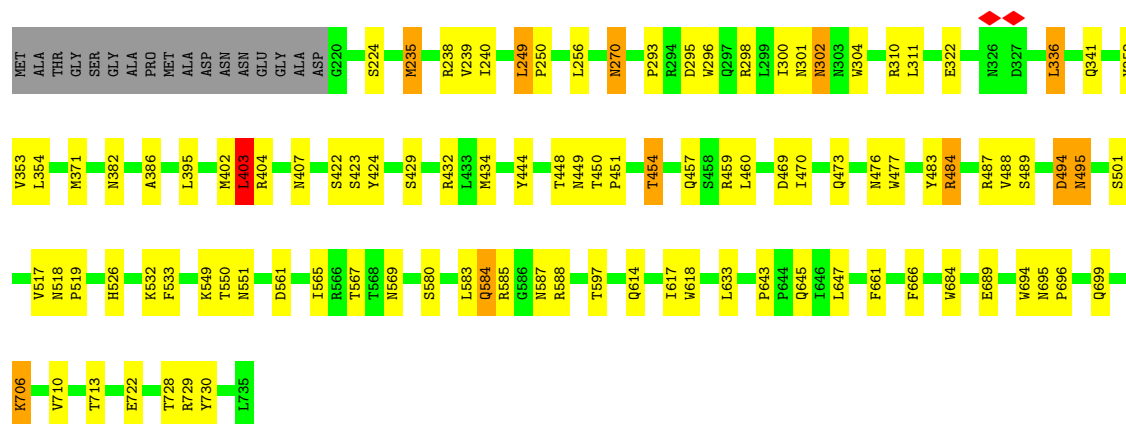


• Molecule 1: Capsid protein VP1



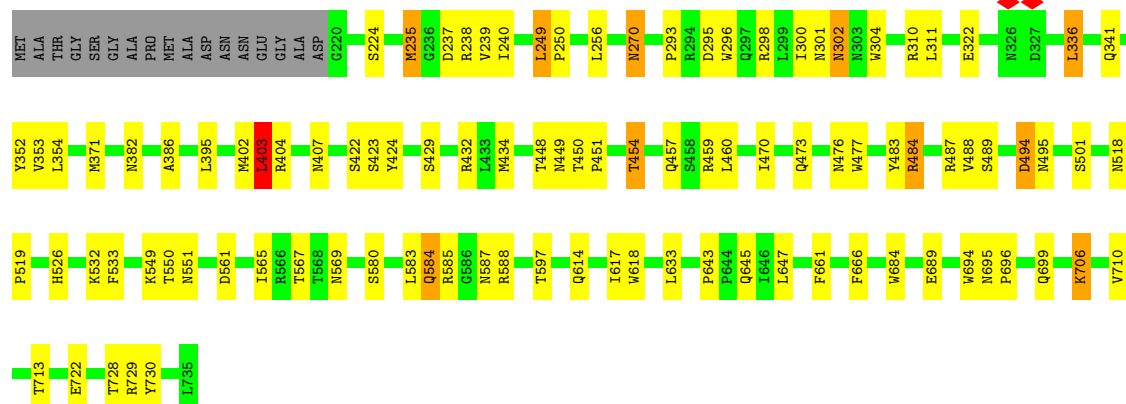
• Molecule 1: Capsid protein VP1





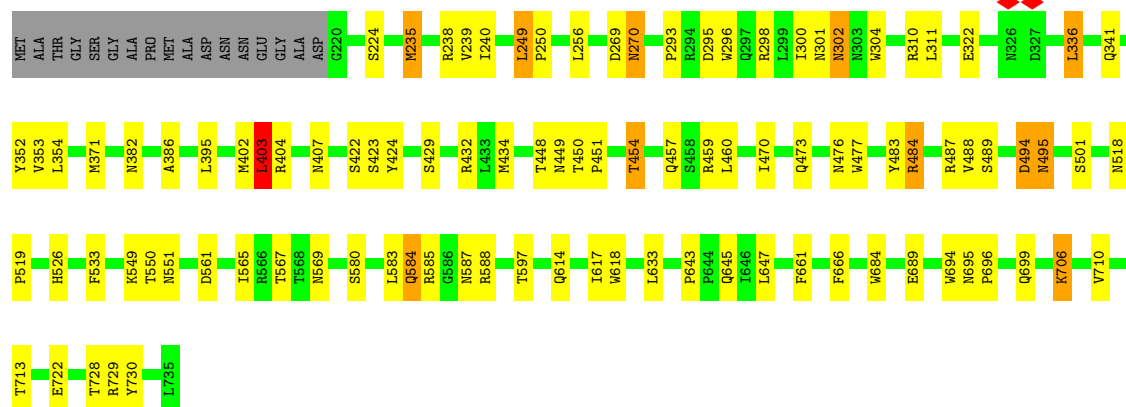
• Molecule 1: Capsid protein VP1

Chain J: 78% 17%



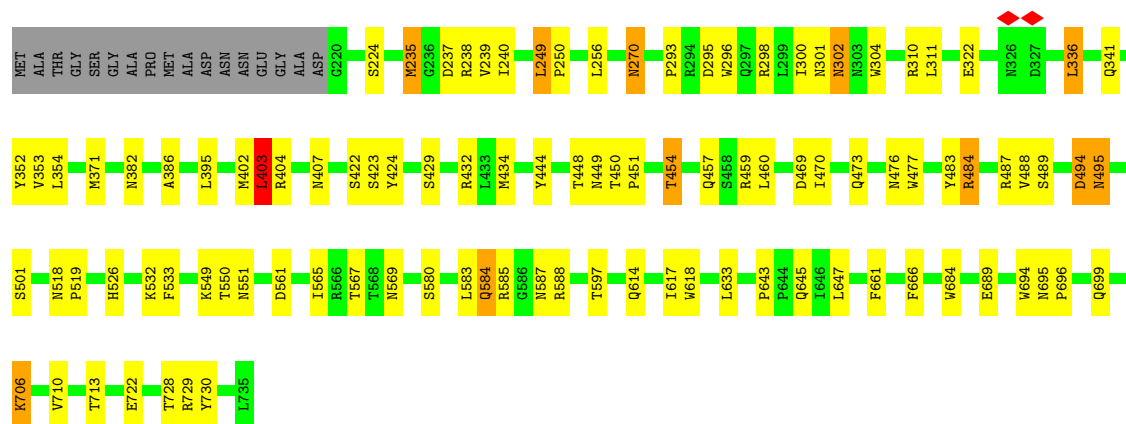
• Molecule 1: Capsid protein VP1

Chain K: 78% 17%



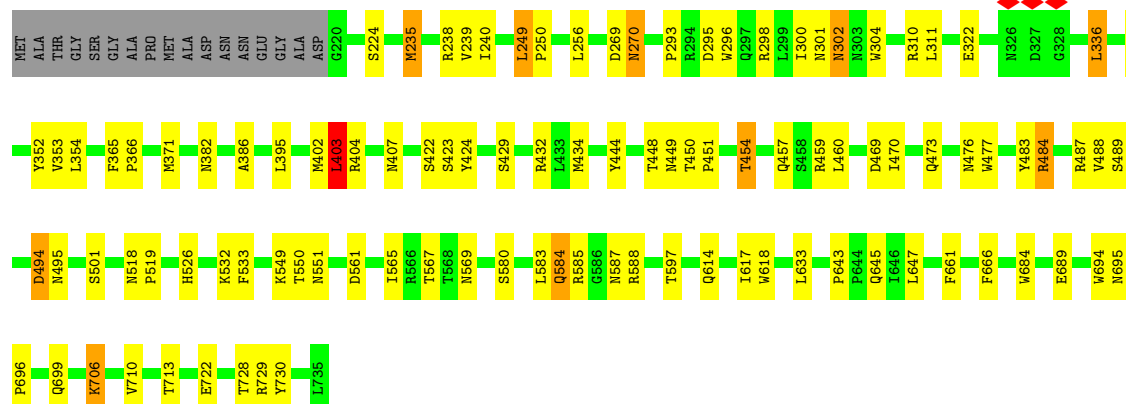
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Chain L: 77% 17%



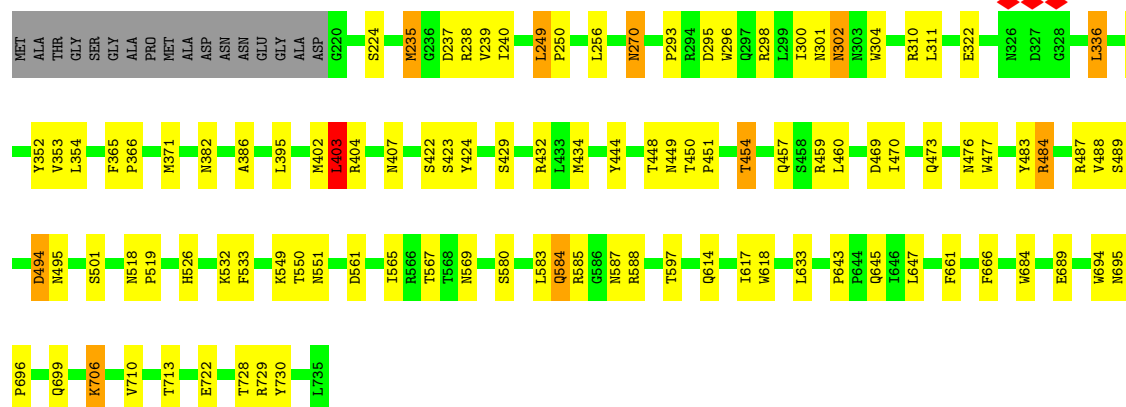
• Molecule 1: Capsid protein VP1

Chain M: 77% 18%



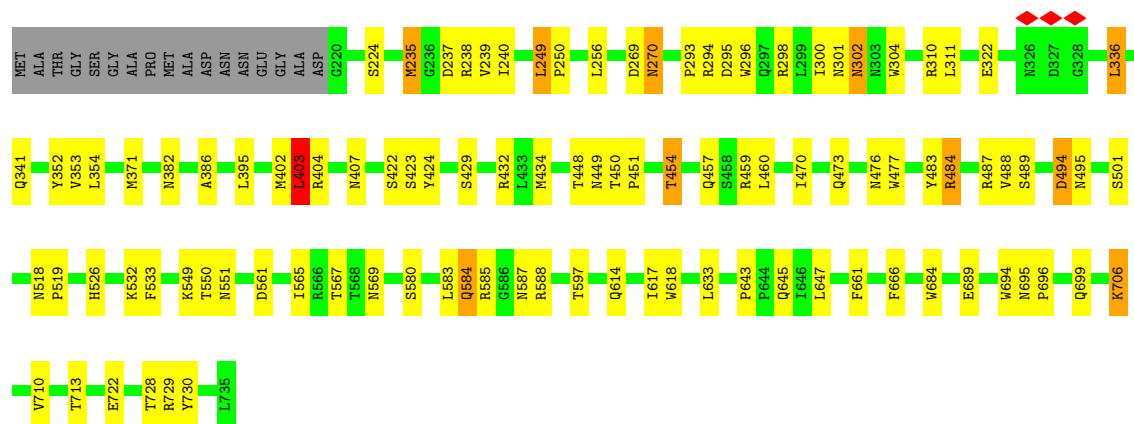
• Molecule 1: Capsid protein VP1

Chain N: 77% 18%



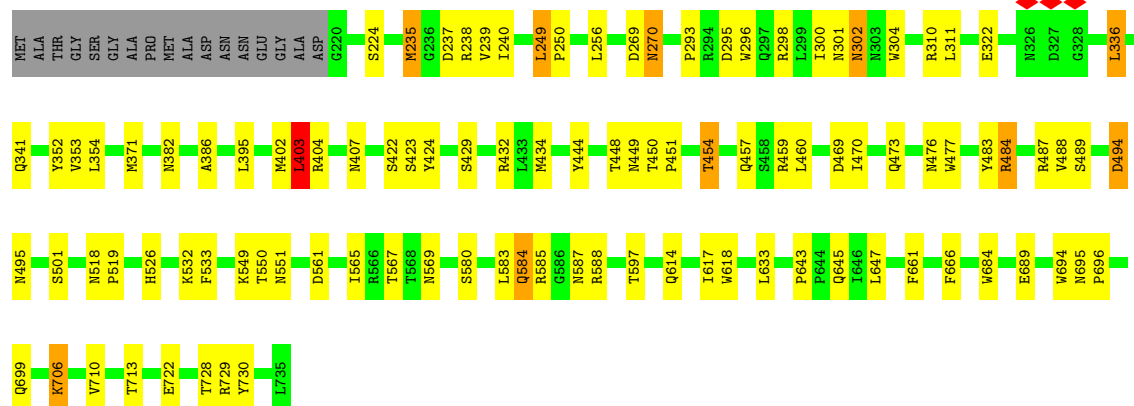
• Molecule 1: Capsid protein VP1

Chain O: 77% 17%



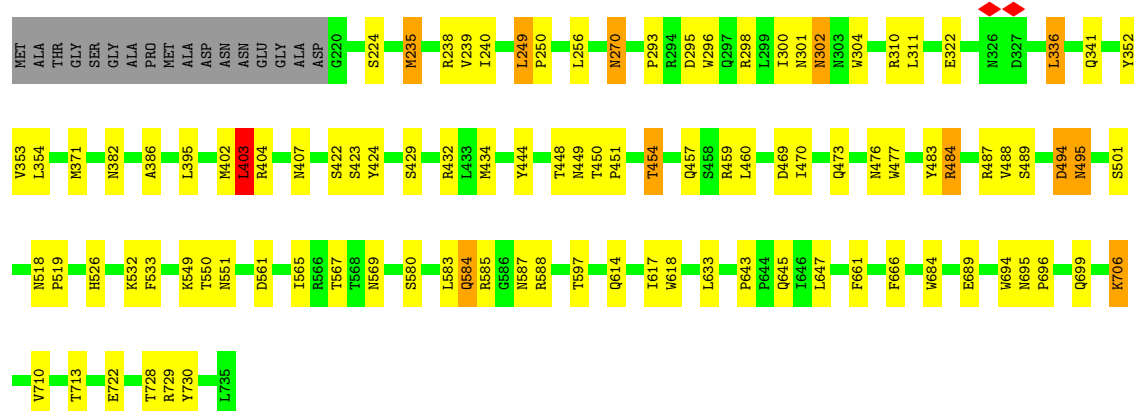
• Molecule 1: Capsid protein VP1

Chain P: 77% 17%



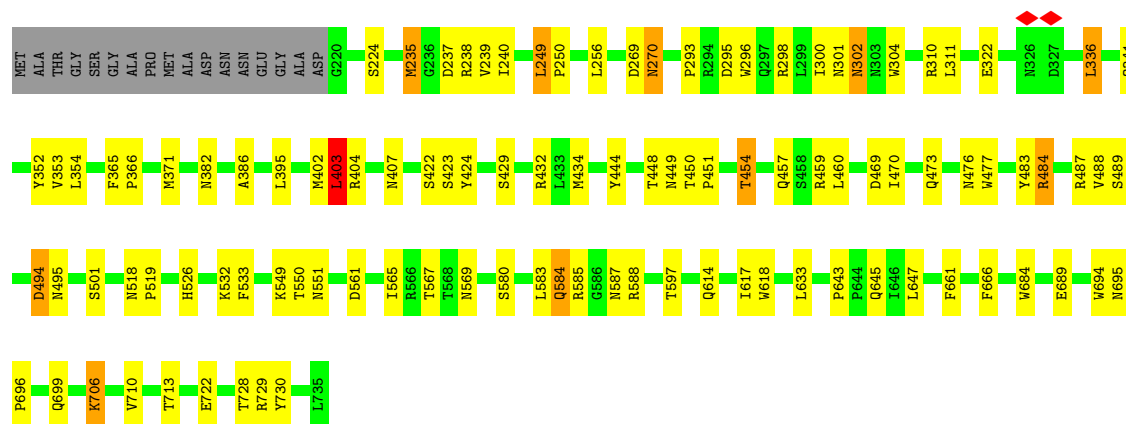
• Molecule 1: Capsid protein VP1

Chain Q: 78% 17%



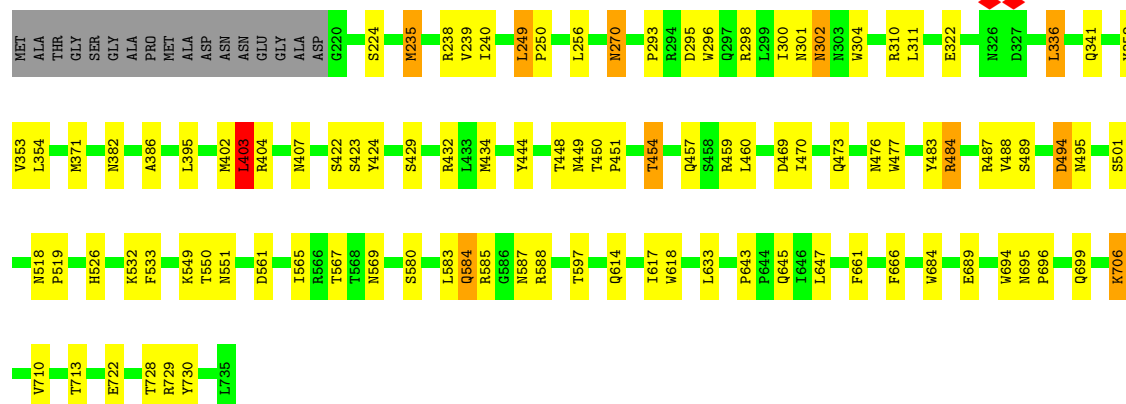
• Molecule 1: Capsid protein VP1

Chain R: 77% 18%



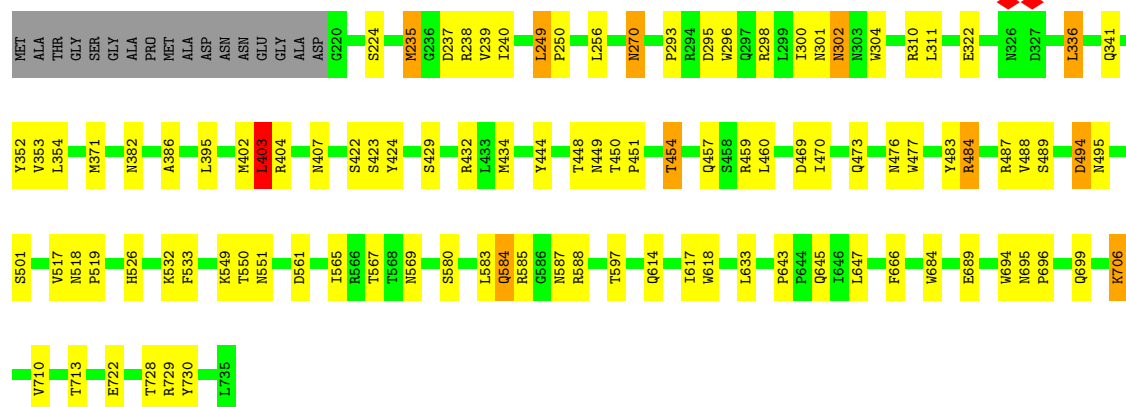
• Molecule 1: Capsid protein VP1

Chain S: 78% 17%



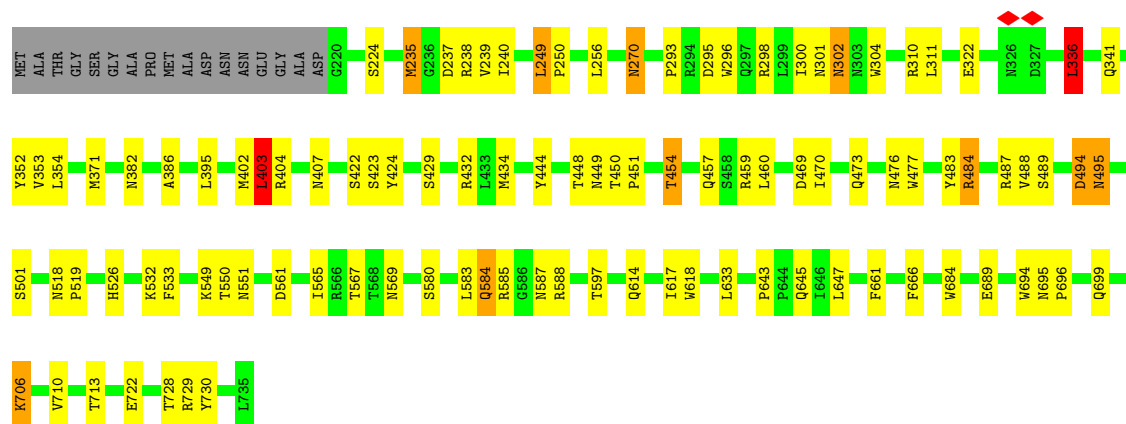
• Molecule 1: Capsid protein VP1

Chain T: 77% 17%



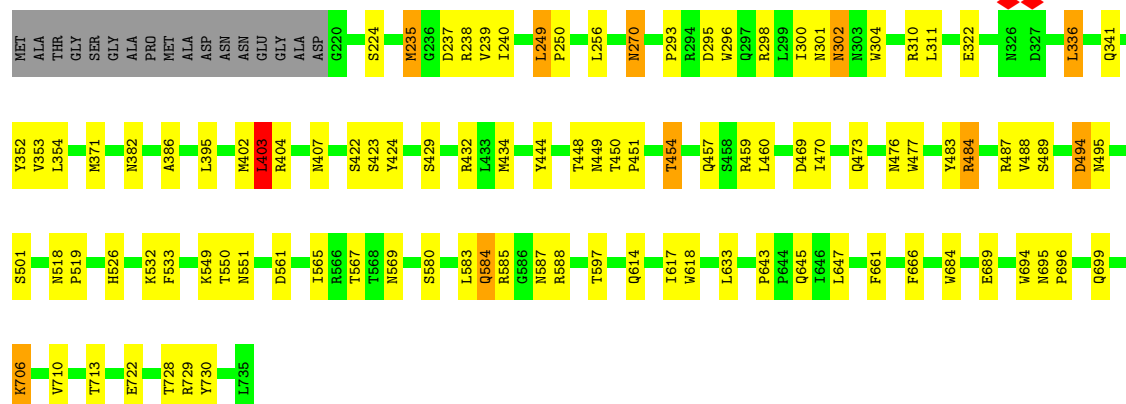
• Molecule 1: Capsid protein VP1

Chain U: 77% 17%



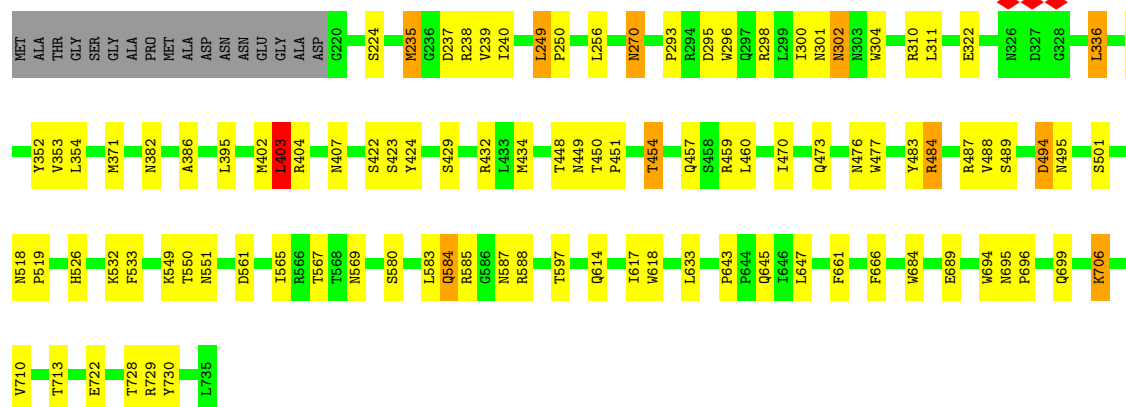
• Molecule 1: Capsid protein VP1

Chain V: 77% 17% ..



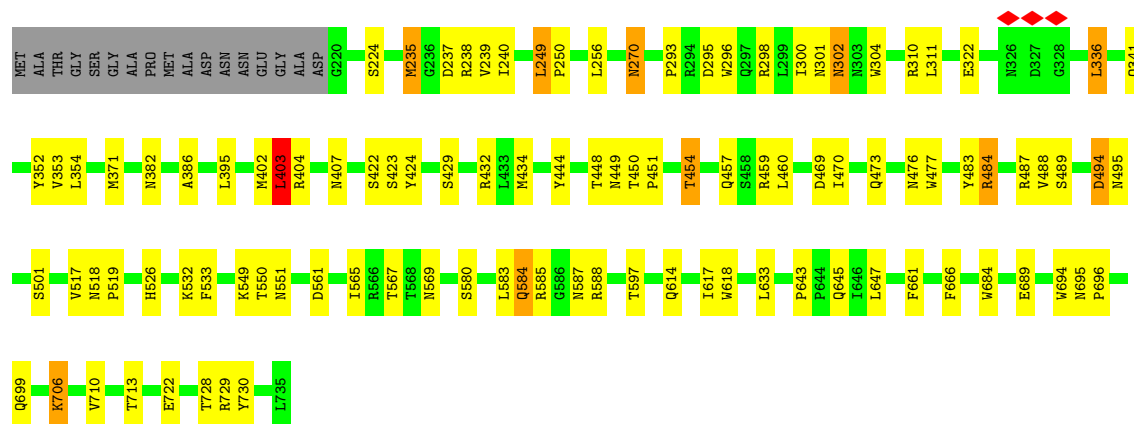
• Molecule 1: Capsid protein VP1

Chain W: 78% 17% ..

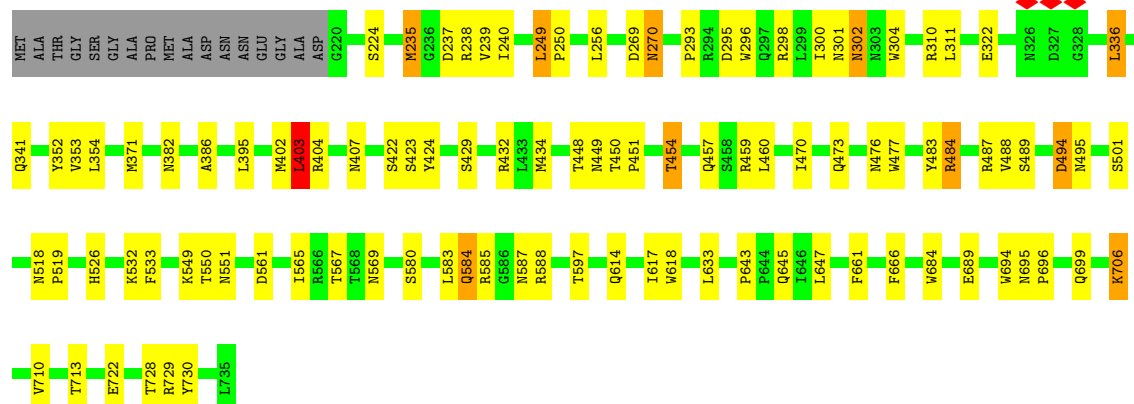
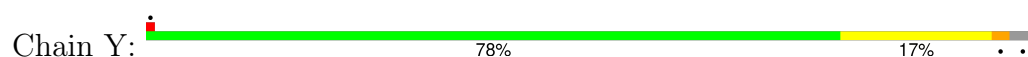


• Molecule 1: Capsid protein VP1

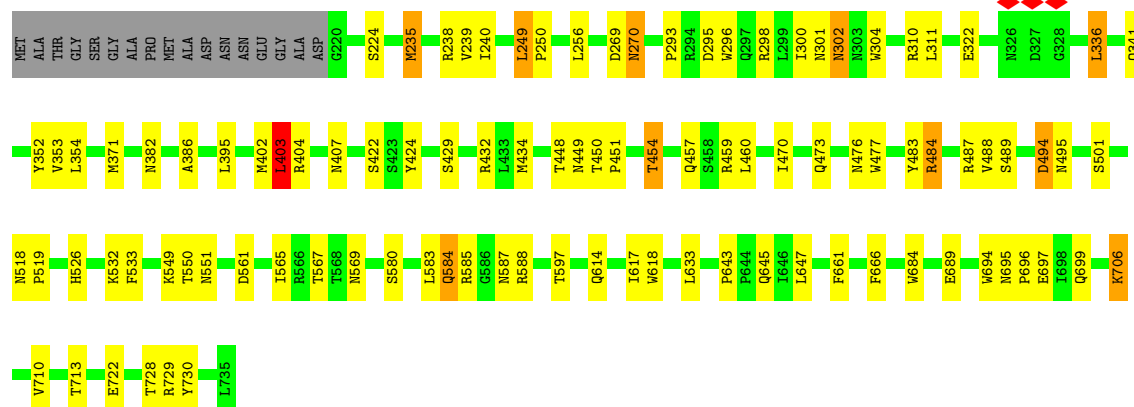
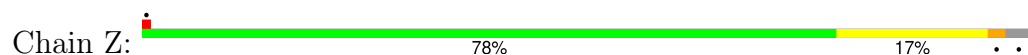
Chain X: 77% 17% ..



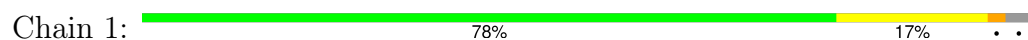
• Molecule 1: Capsid protein VP1

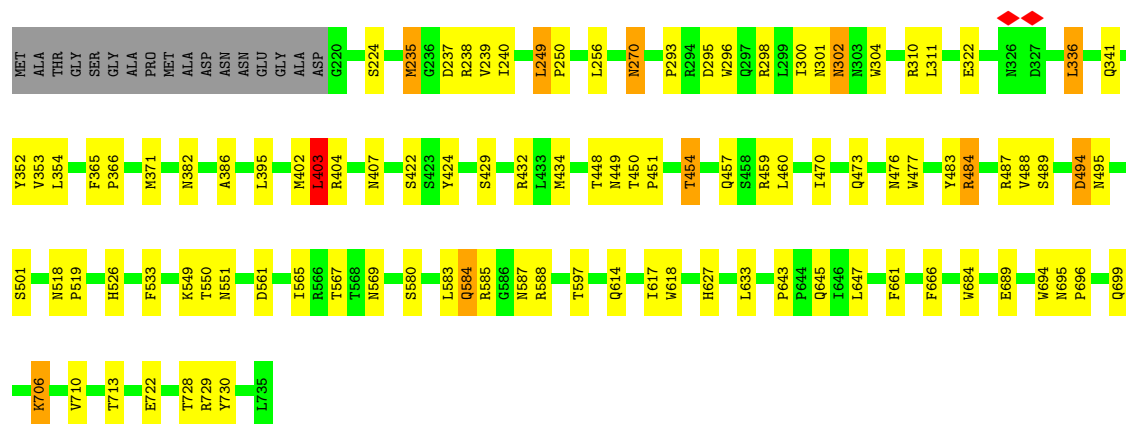


• Molecule 1: Capsid protein VP1



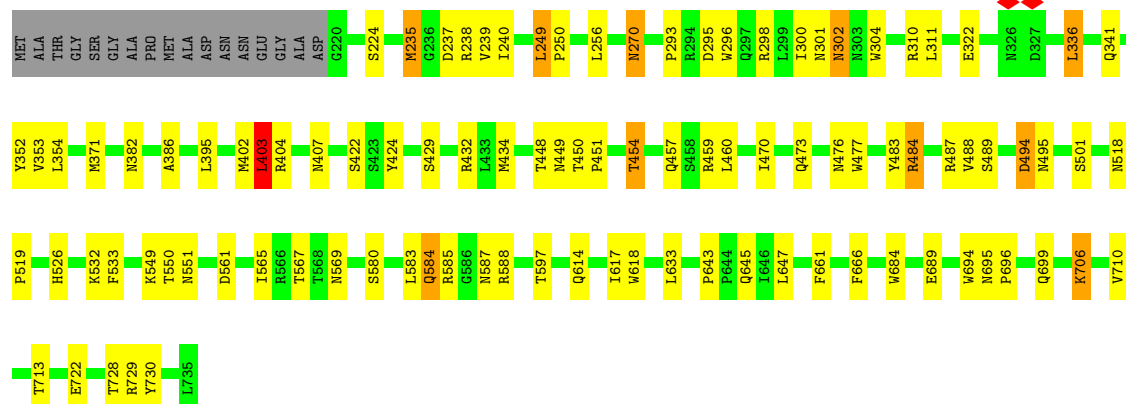
• Molecule 1: Capsid protein VP1





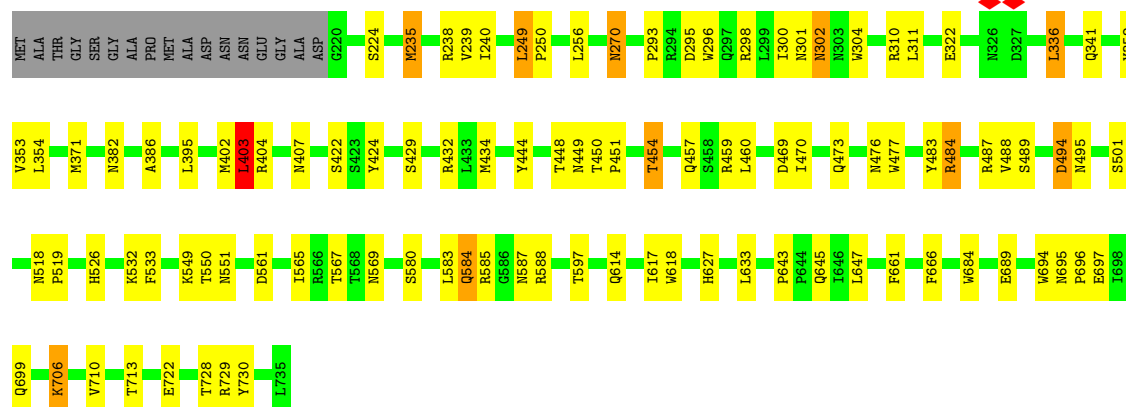
• Molecule 1: Capsid protein VP1

Chain 2: 78% 17%



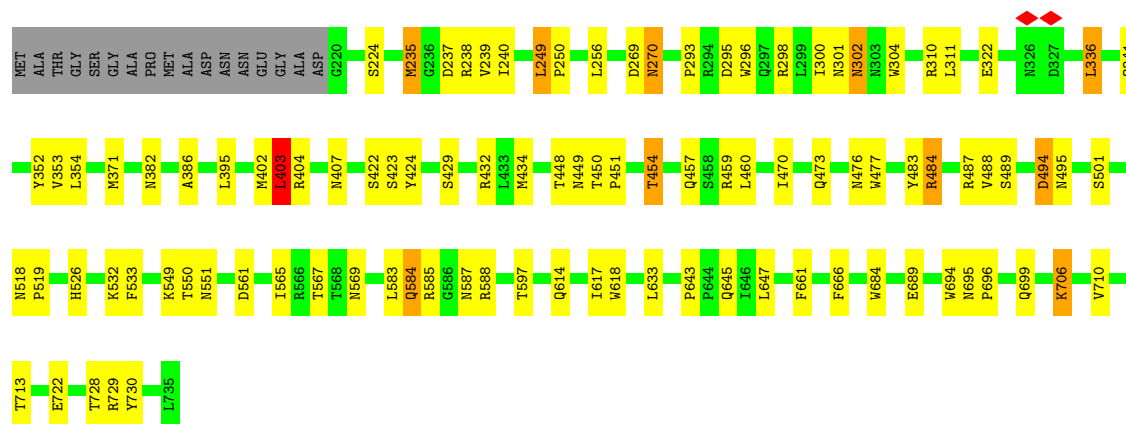
• Molecule 1: Capsid protein VP1

Chain 3: 77% 17%



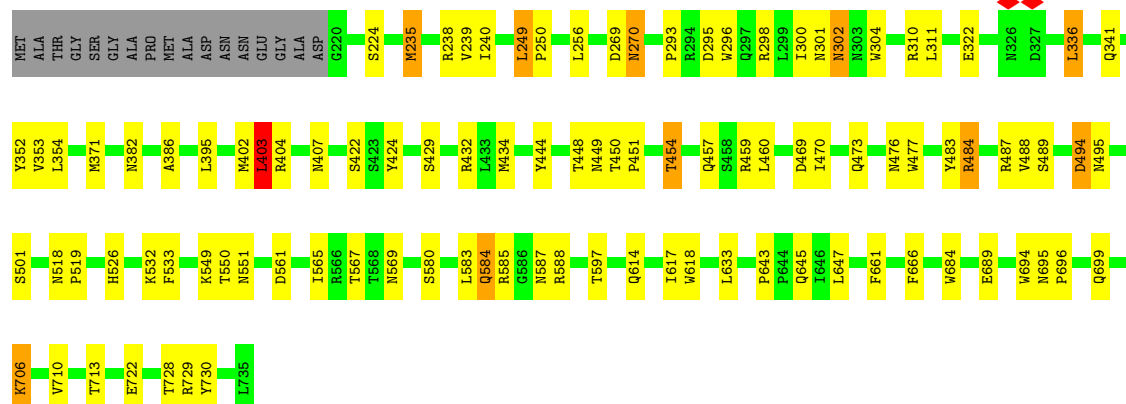
• Molecule 1: Capsid protein VP1

Chain 4: 78% 17%



• Molecule 1: Capsid protein VP1

Chain 5: 78% 17%



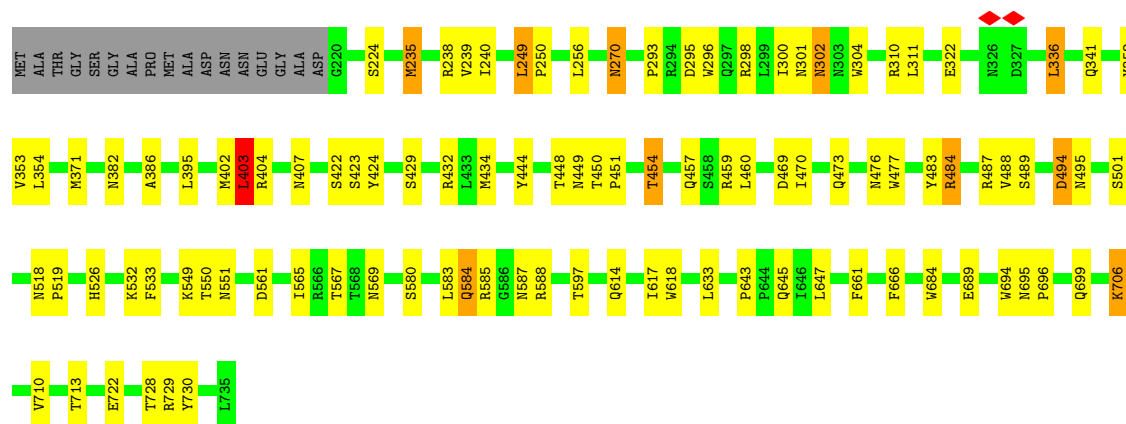
• Molecule 1: Capsid protein VP1

Chain 6: 77% 18%

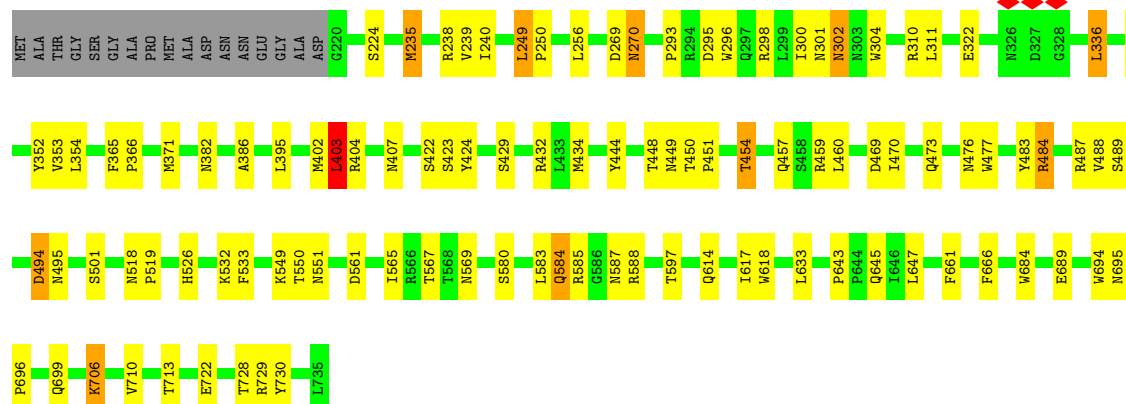
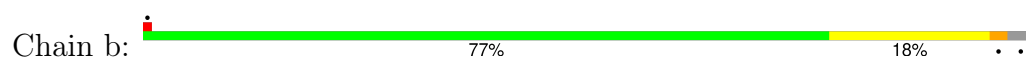


• Molecule 1: Capsid protein VP1

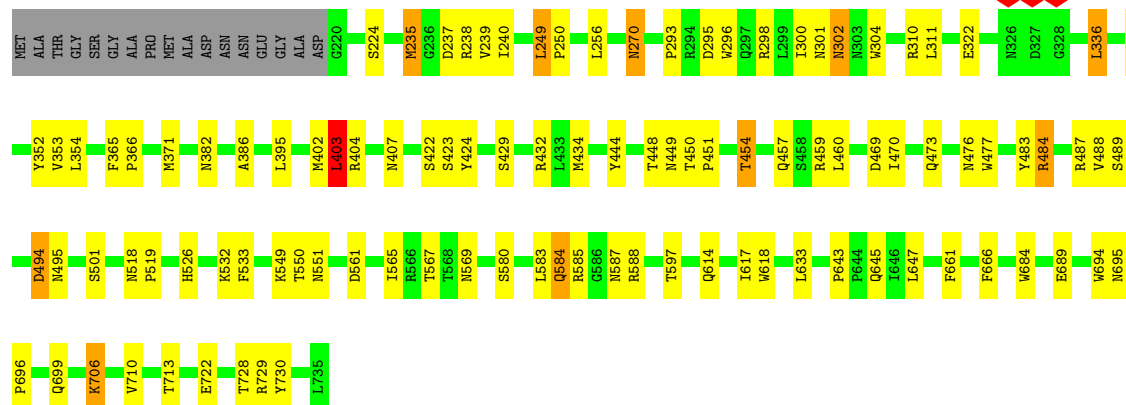
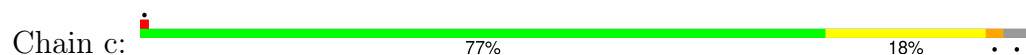
Chain a: 78% 17%



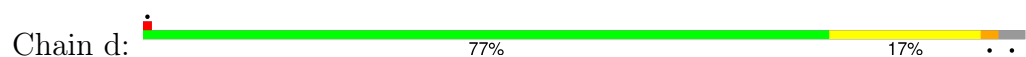
• Molecule 1: Capsid protein VP1

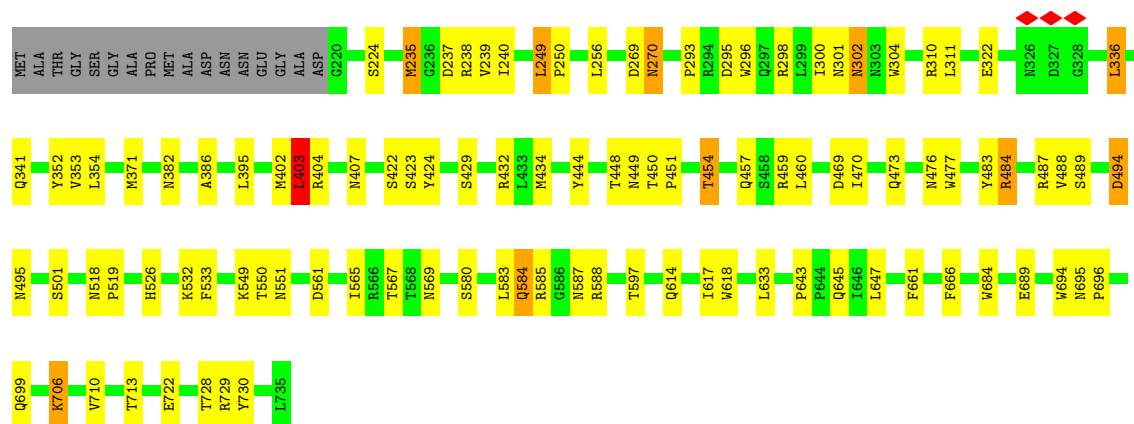


• Molecule 1: Capsid protein VP1

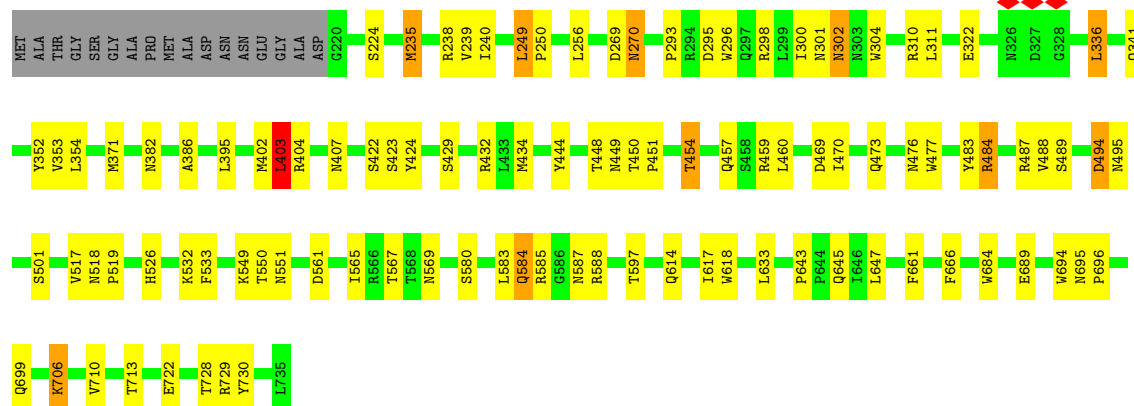
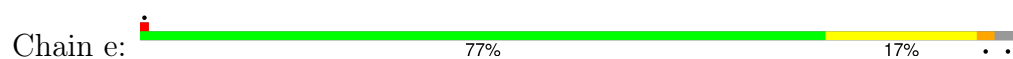


• Molecule 1: Capsid protein VP1

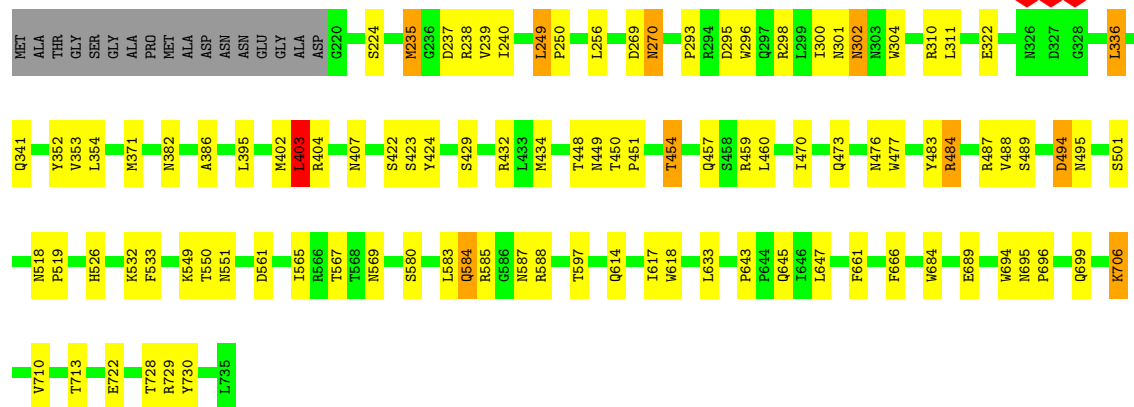
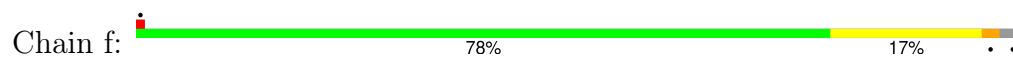




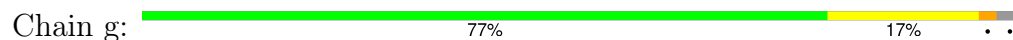
• Molecule 1: Capsid protein VP1

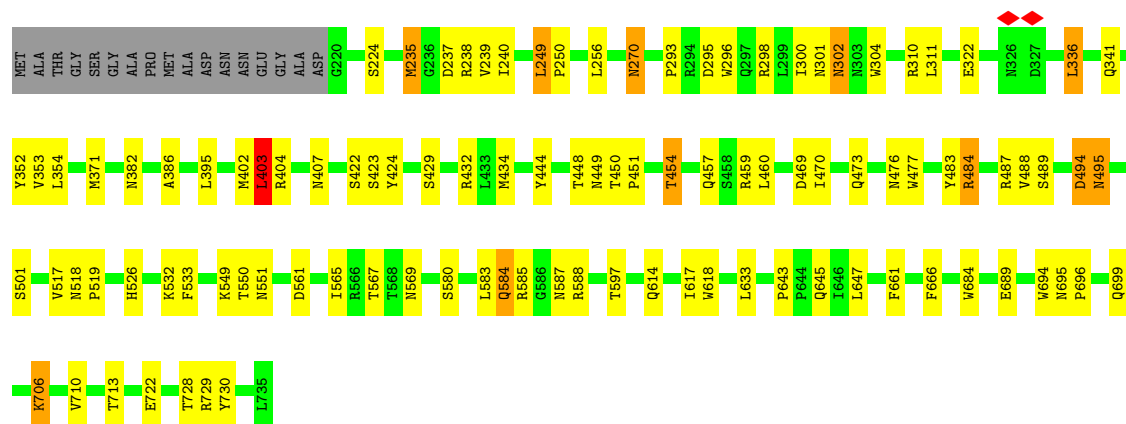


• Molecule 1: Capsid protein VP1



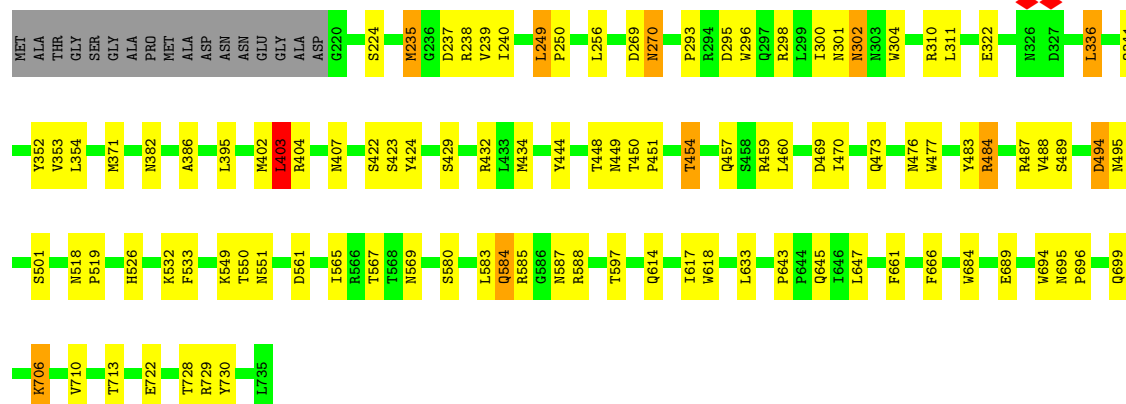
• Molecule 1: Capsid protein VP1





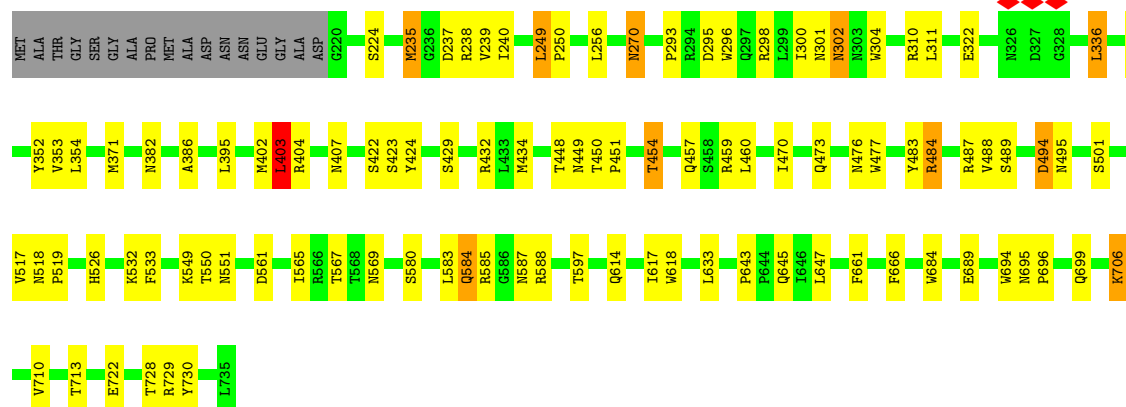
• Molecule 1: Capsid protein VP1

Chain h: 77% 17%



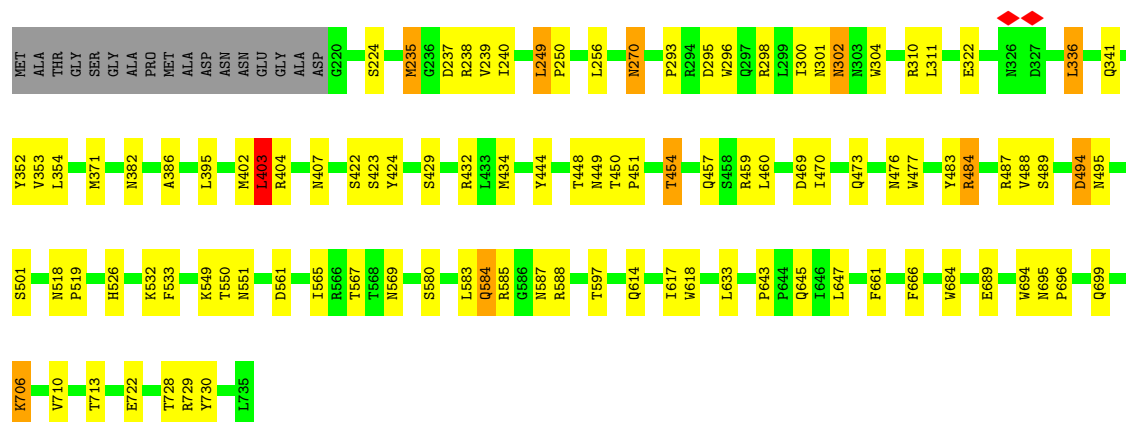
• Molecule 1: Capsid protein VP1

Chain i: 78% 17%



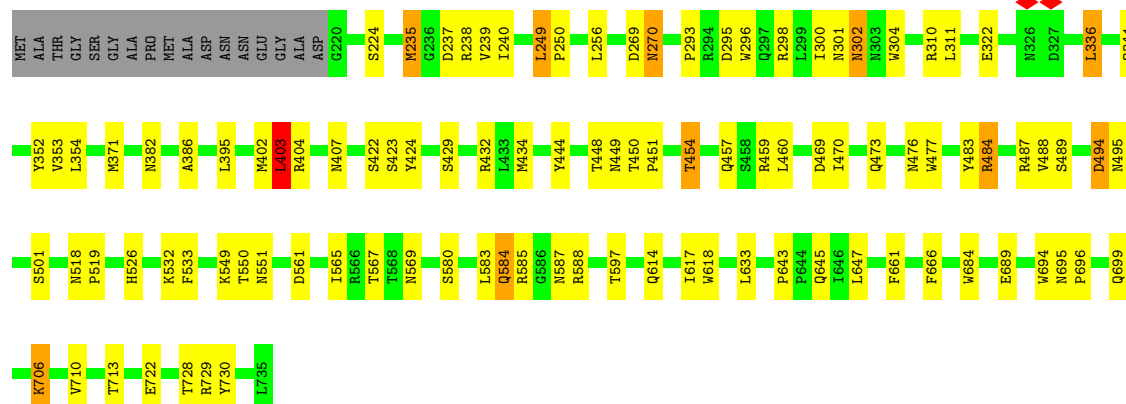
• Molecule 1: Capsid protein VP1

Chain j: 77% 17%



• Molecule 1: Capsid protein VP1

Chain k: 77% 17%



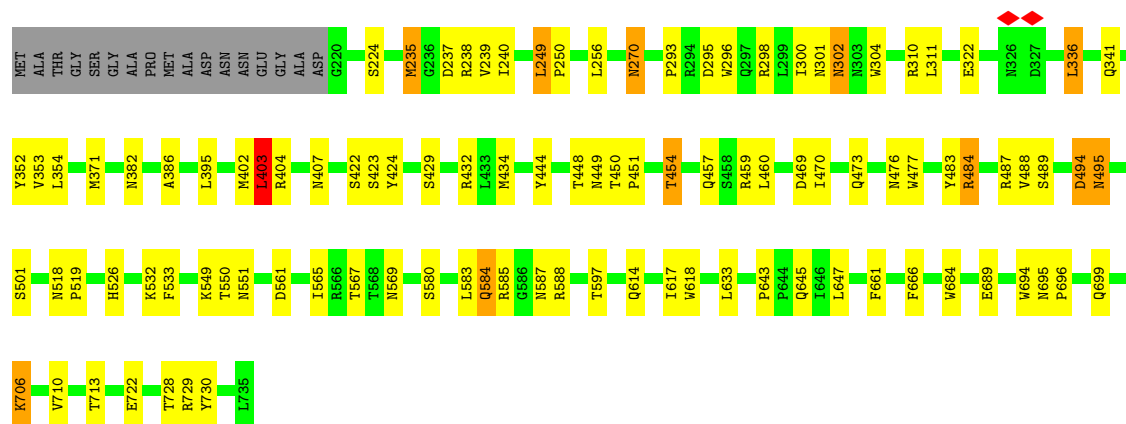
• Molecule 1: Capsid protein VP1

Chain l: 78% 17%

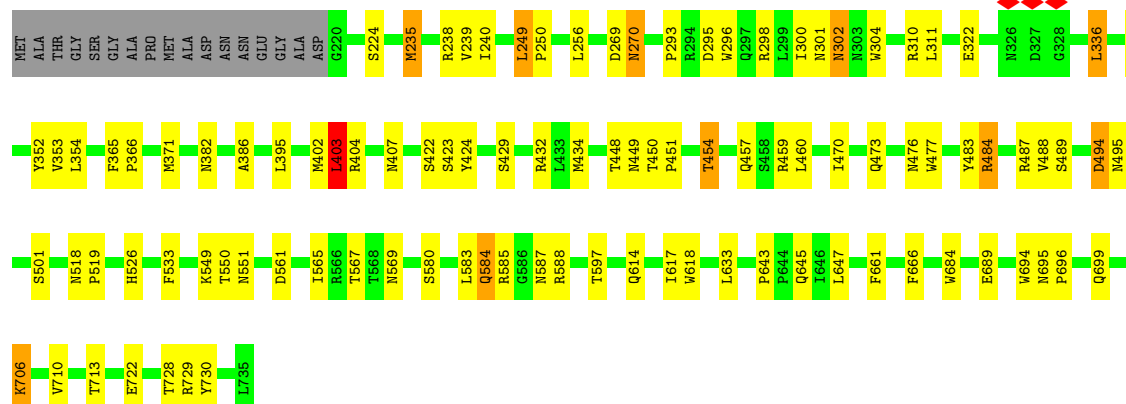
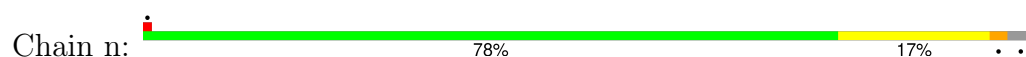


• Molecule 1: Capsid protein VP1

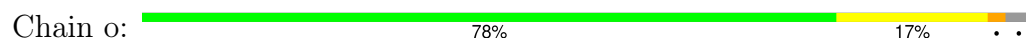
Chain m: 77% 17%



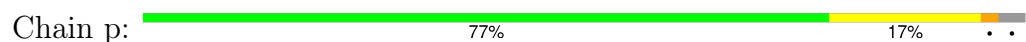
• Molecule 1: Capsid protein VP1

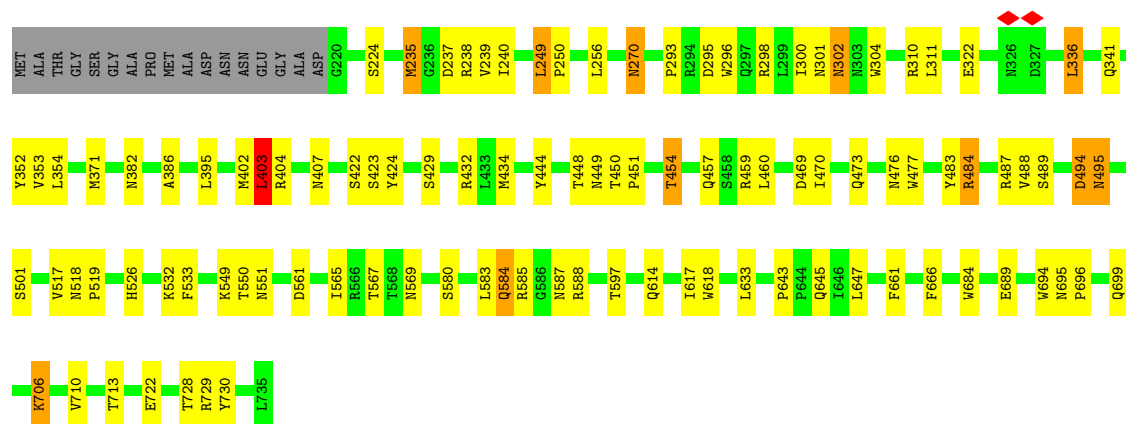


• Molecule 1: Capsid protein VP1

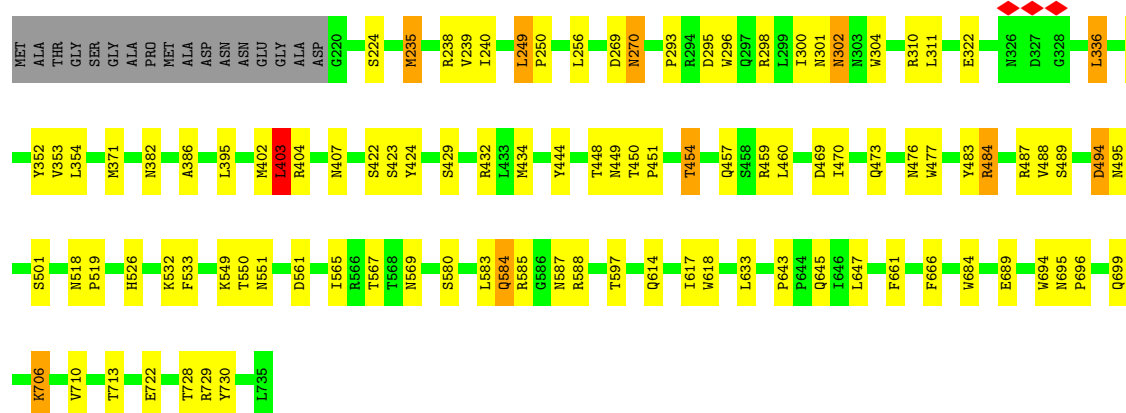
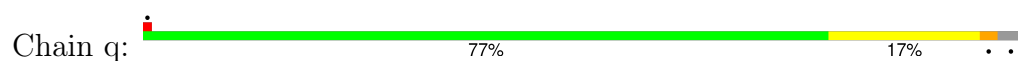


• Molecule 1: Capsid protein VP1

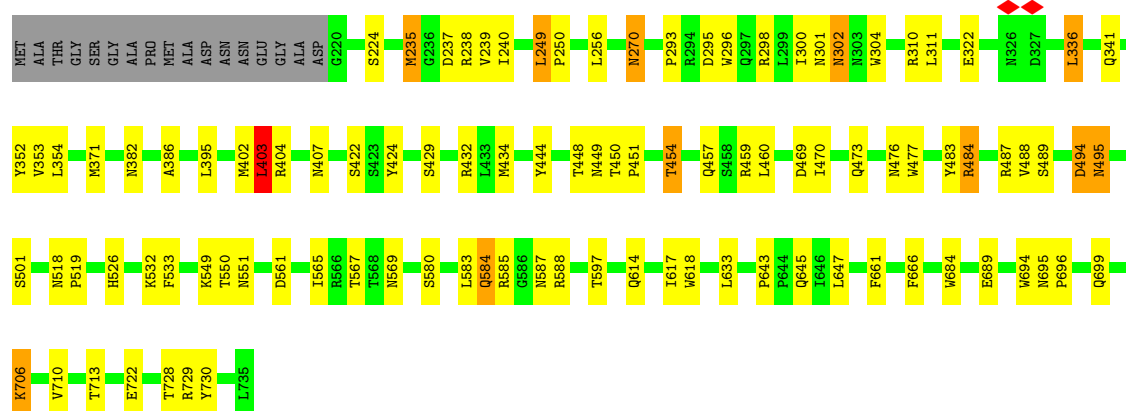
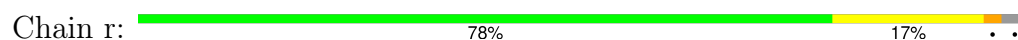




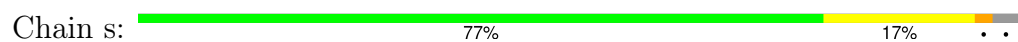
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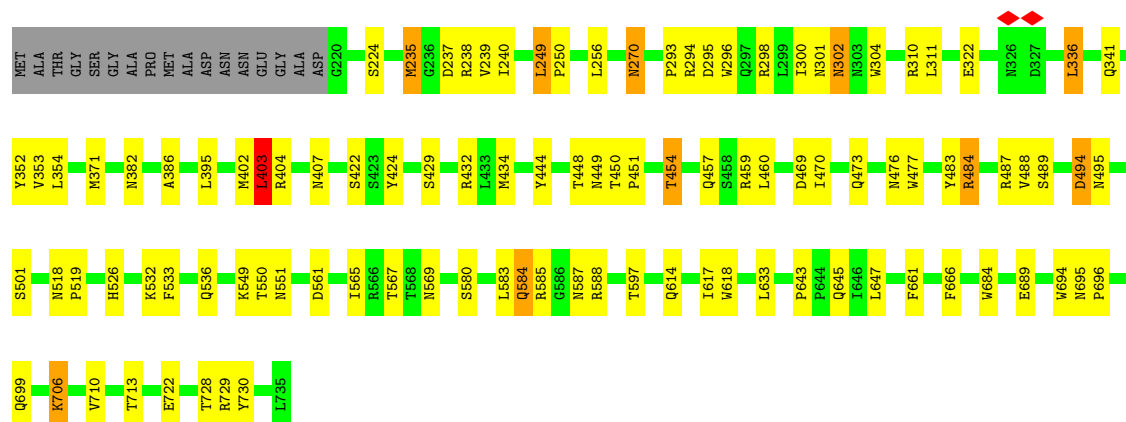


• Molecule 1: Capsid protein VP1



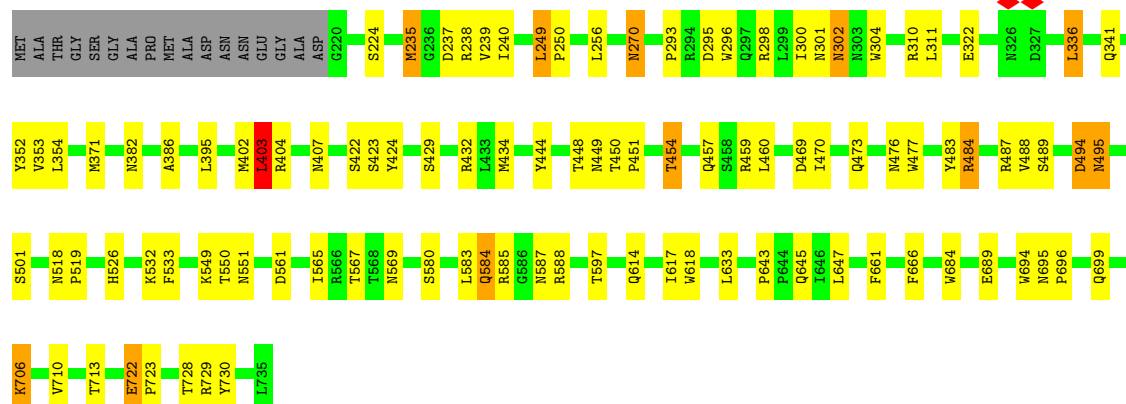
• Molecule 1: Capsid protein VP1





- Molecule 1: Capsid protein VP1

Chain t: 77% 17%



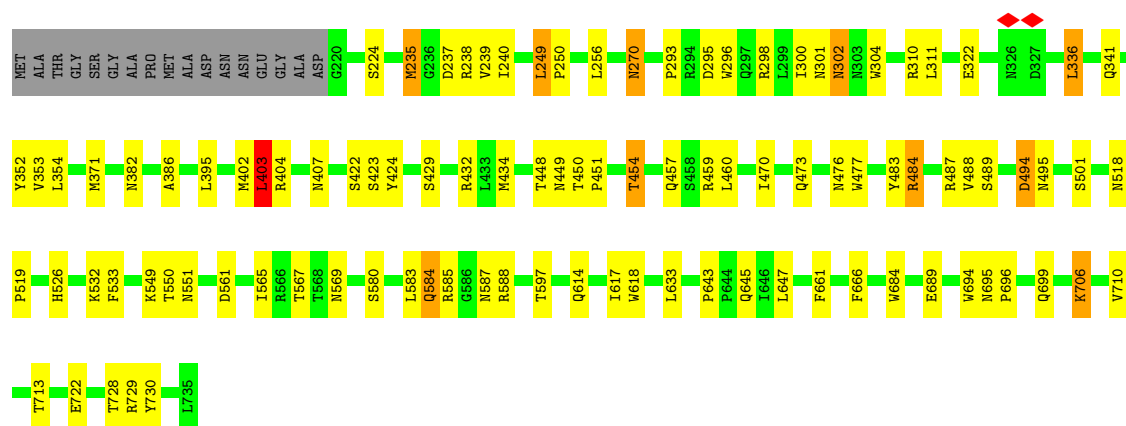
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Chain u: 77% 17%



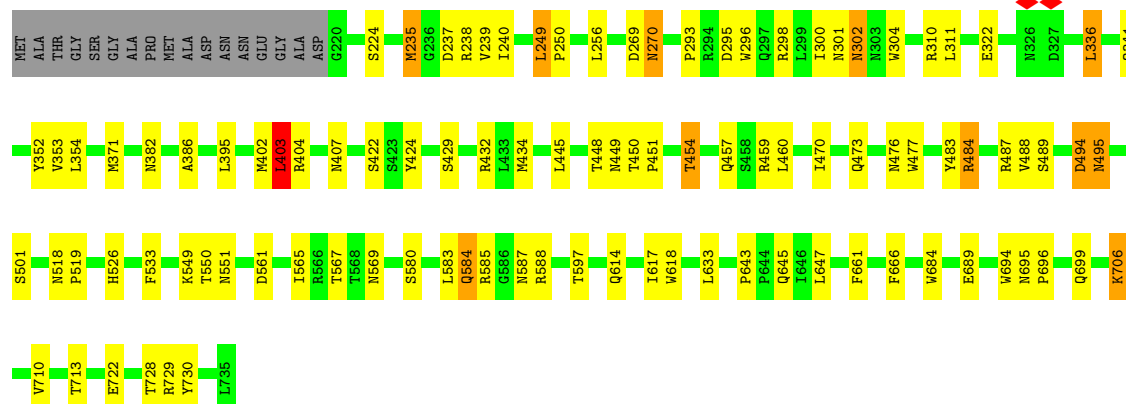
- Molecule 1: Capsid protein VP1

Chain v: 78% 17%



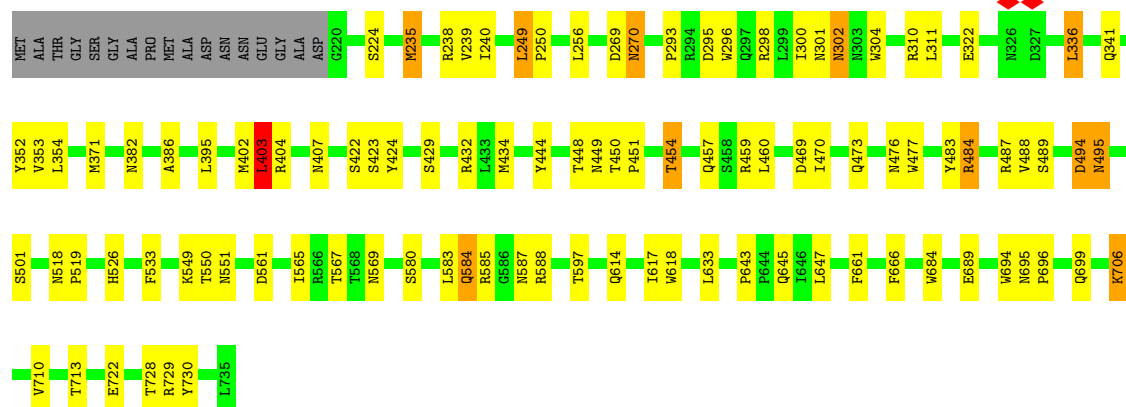
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Chain w: 78% 17%



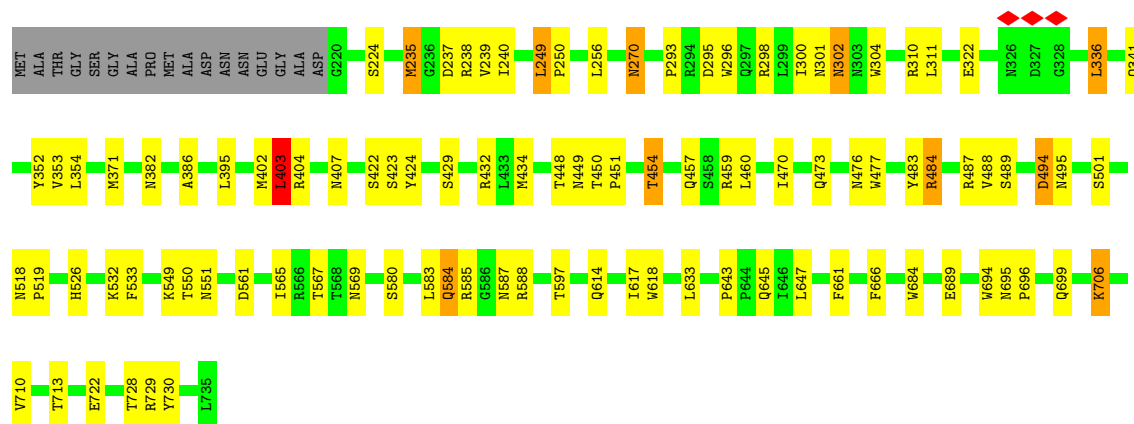
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Chain x: 78% 17%

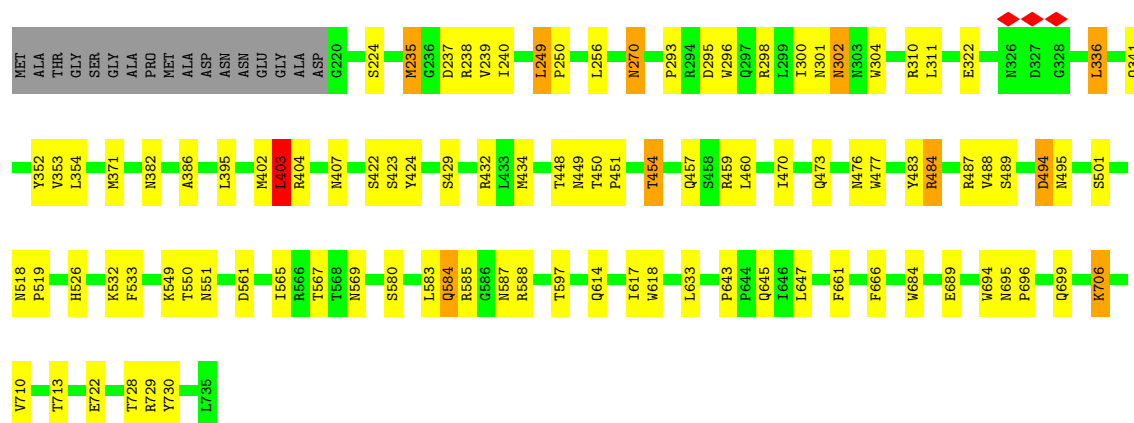
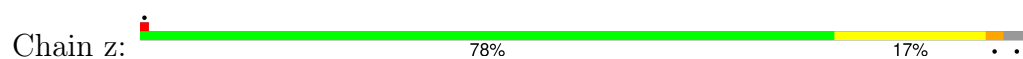


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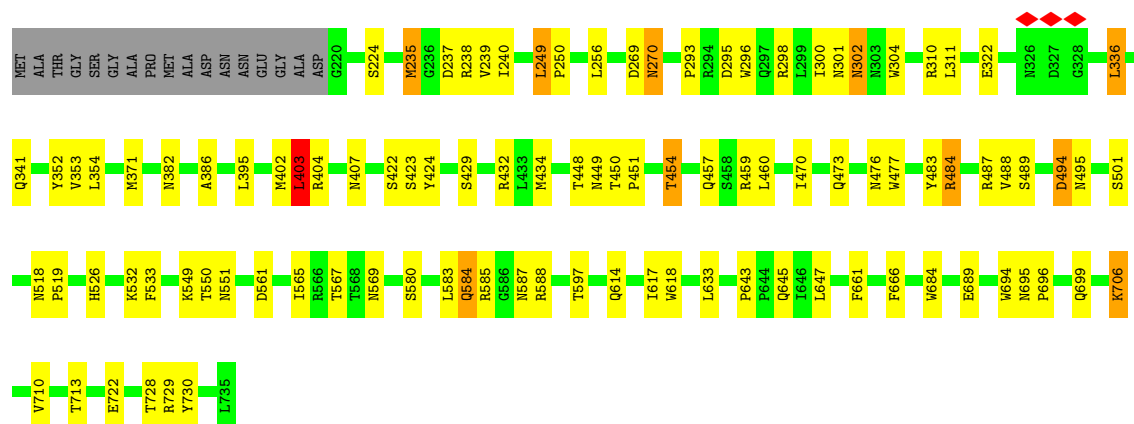
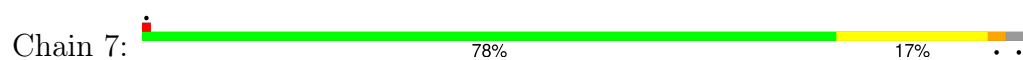
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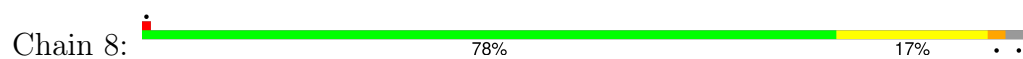
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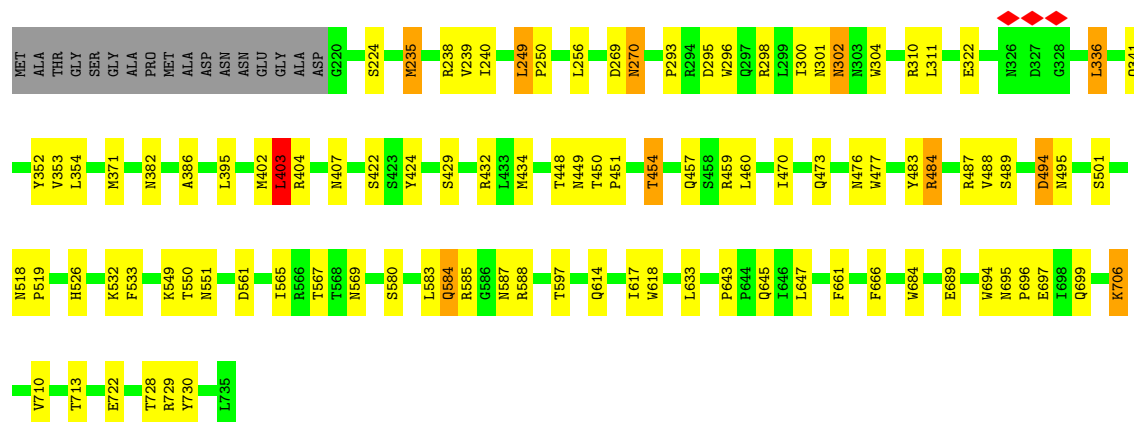


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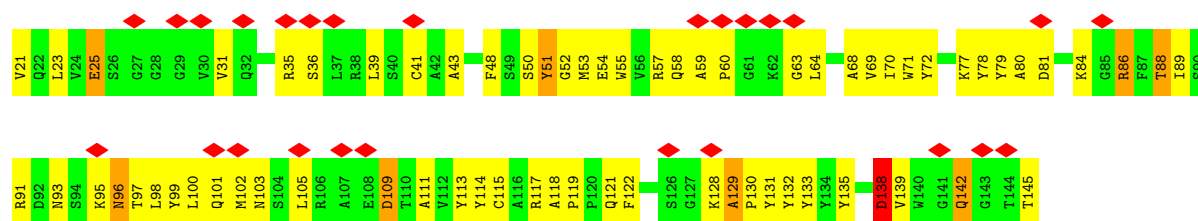


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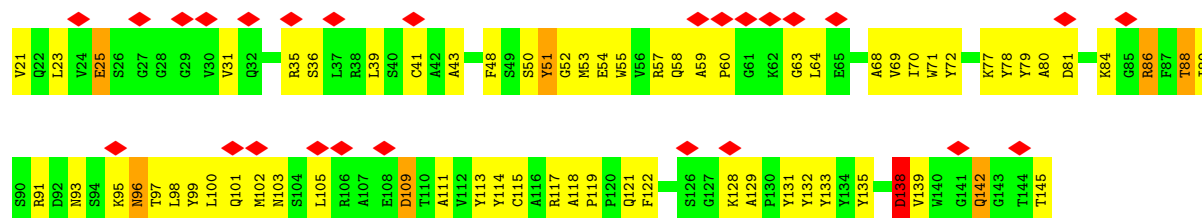




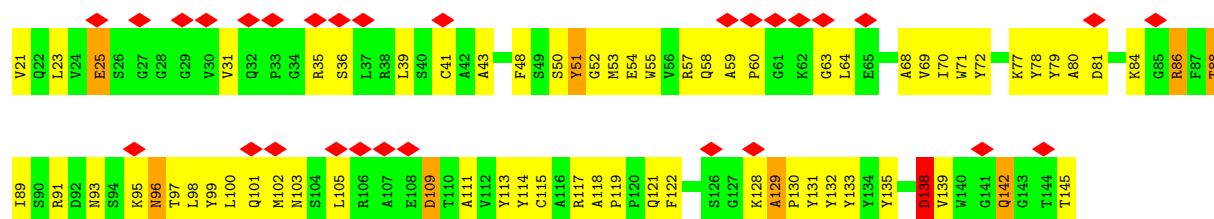
• Molecule 2: IgG Fab3-4 heavy chain



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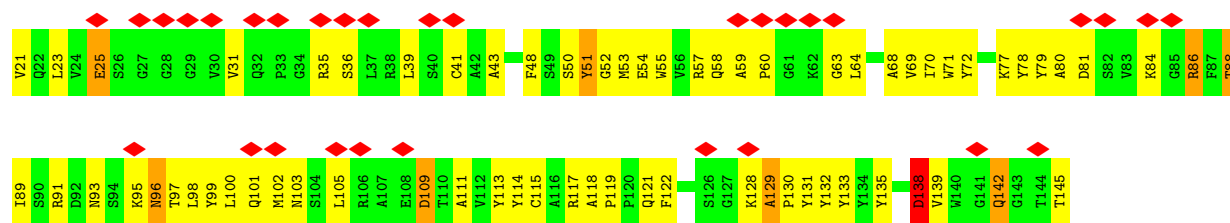


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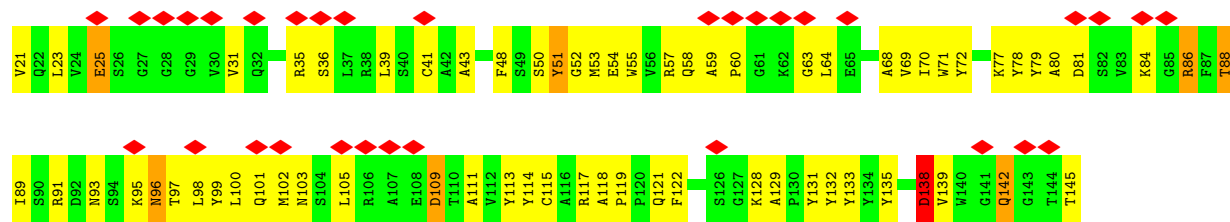


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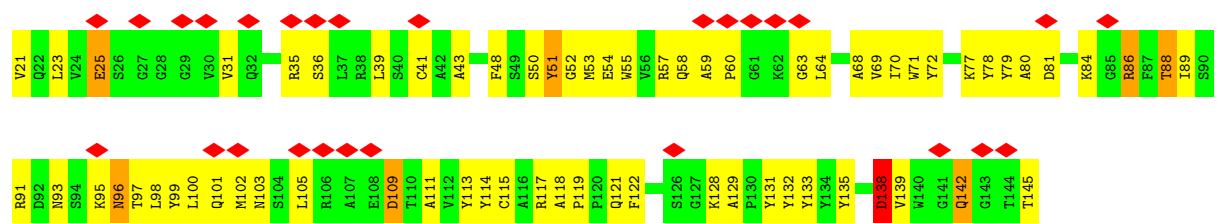




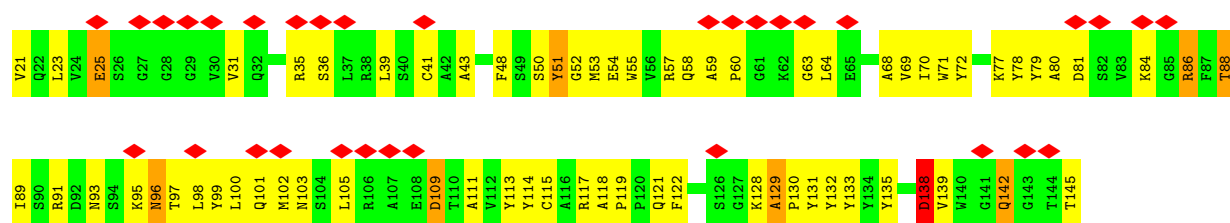
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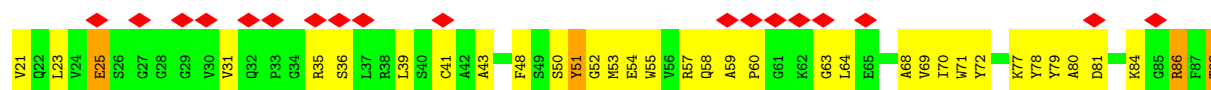


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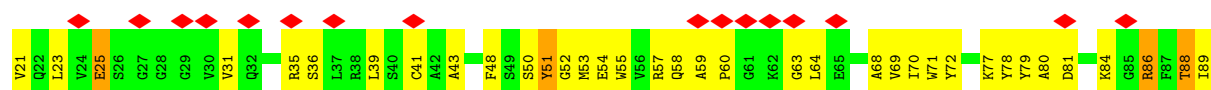




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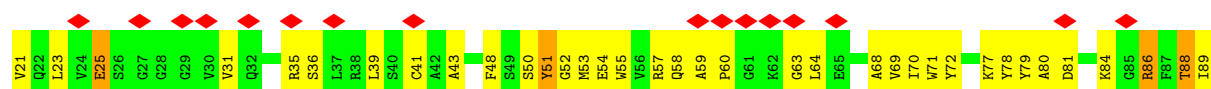
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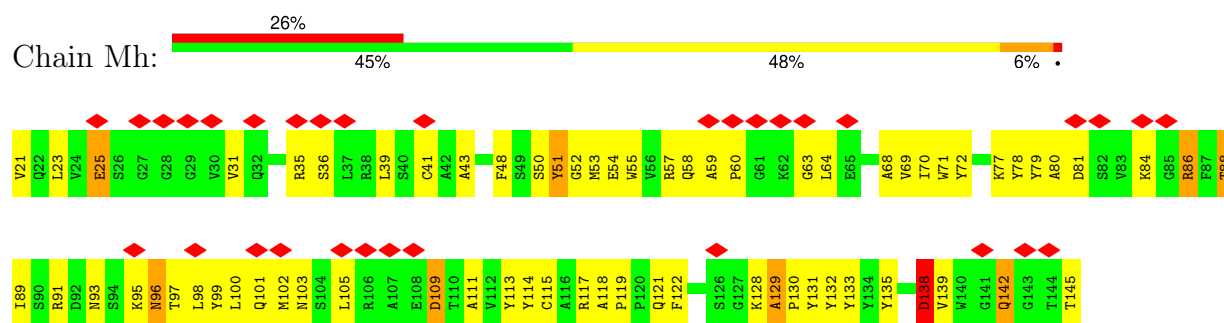
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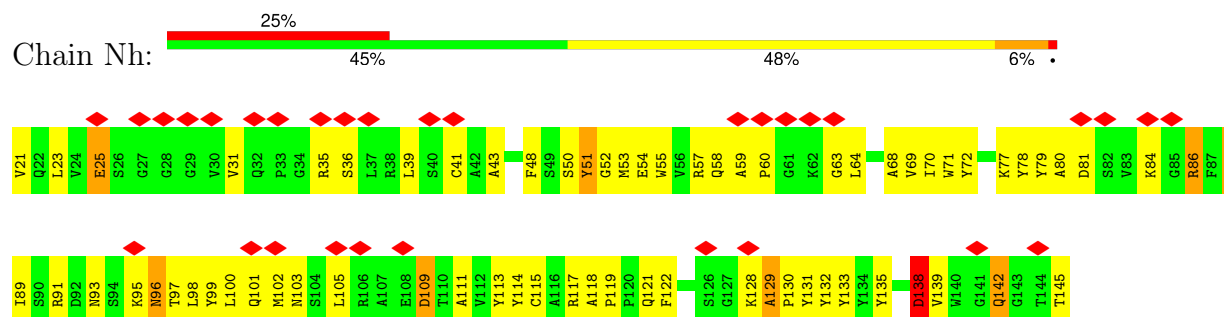
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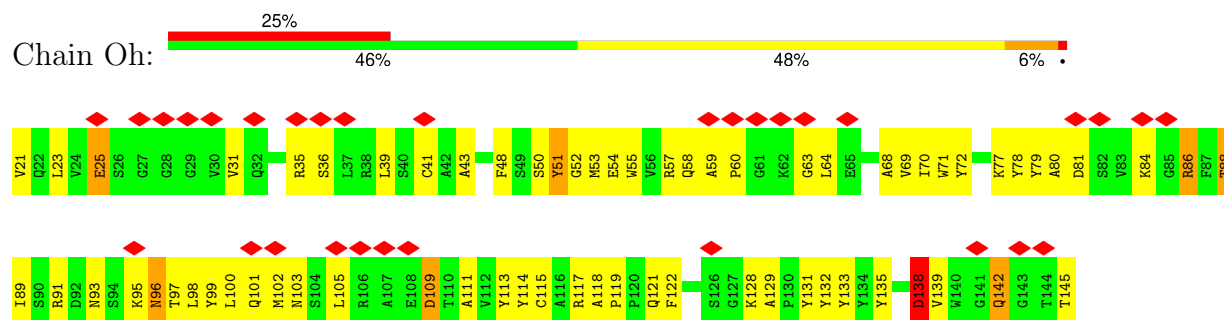
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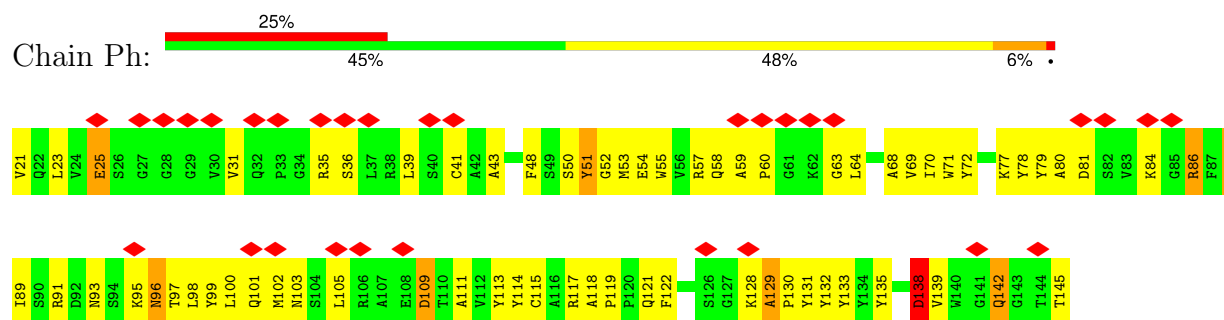
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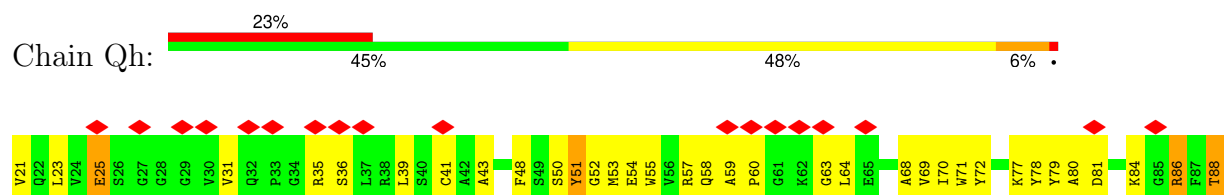
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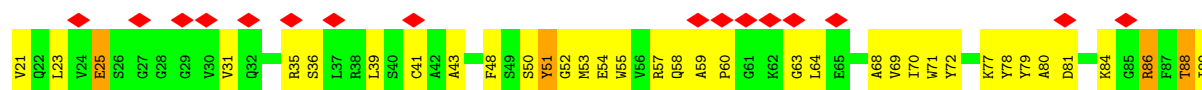


- Molecule 2: IgG Fab3-4 heavy chain

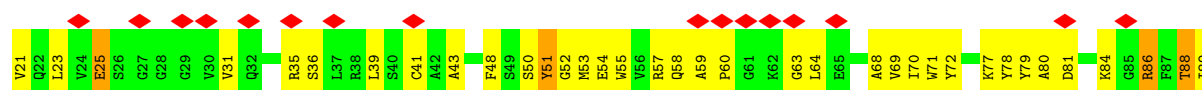




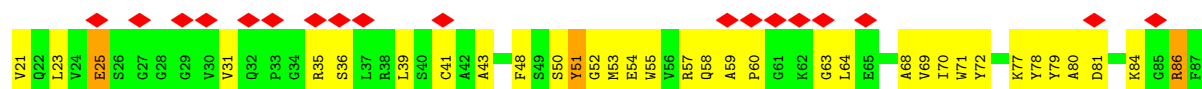
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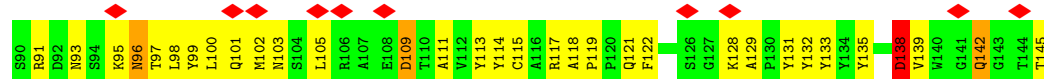
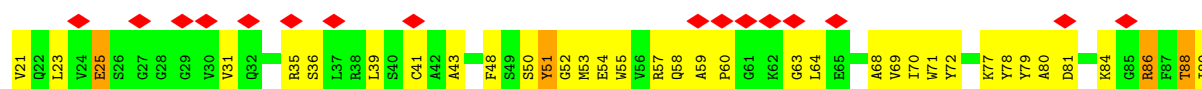
• Molecule 2: IgG Fab3-4 heavy chain



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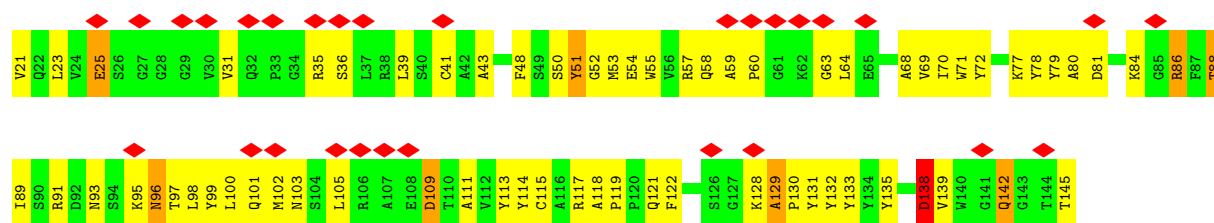


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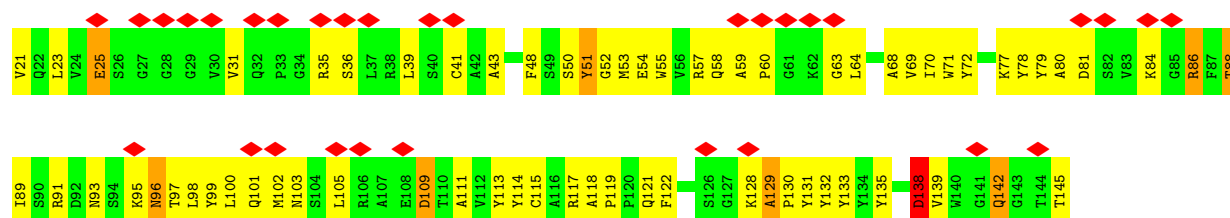
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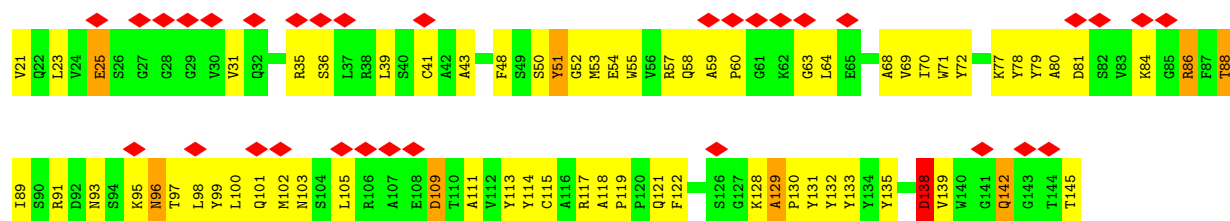
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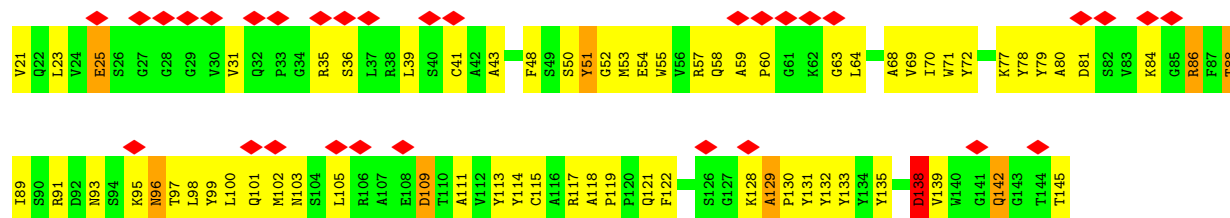
• Molecule 2: IgG Fab3-4 heavy chain

Chain Xh: 



• Molecule 2: IgG Fab3-4 heavy chain

Chain Yh: 



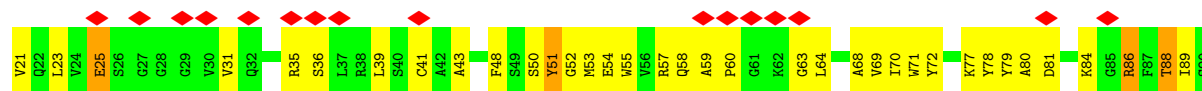
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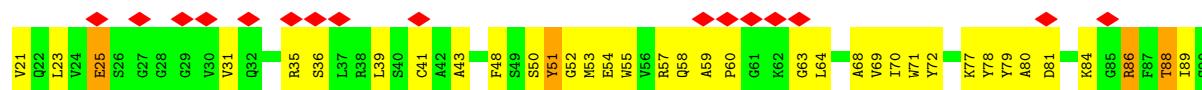




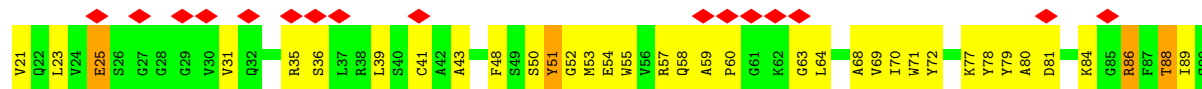
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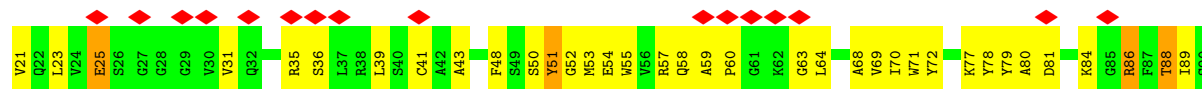
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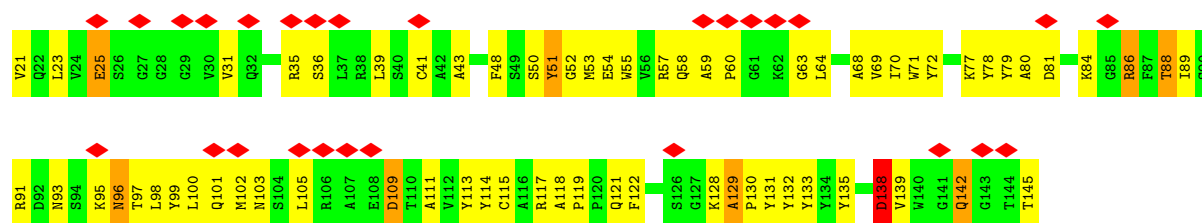
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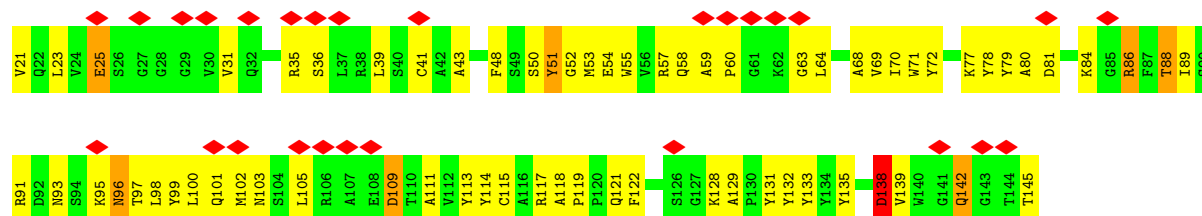


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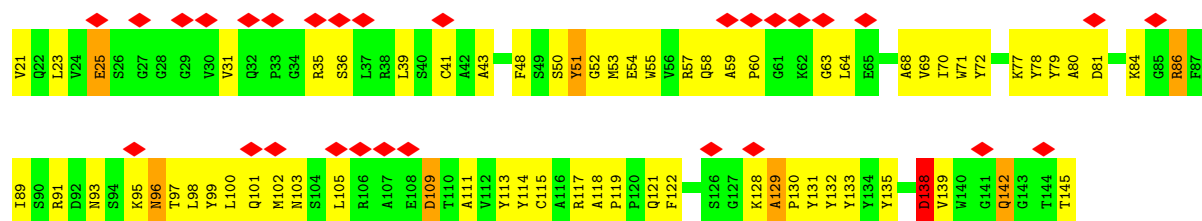
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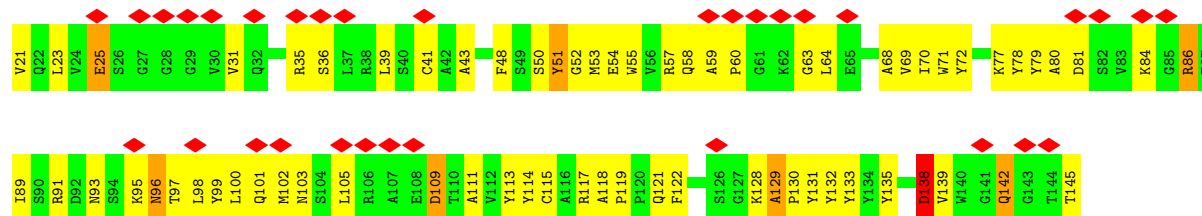
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Chain ah: 



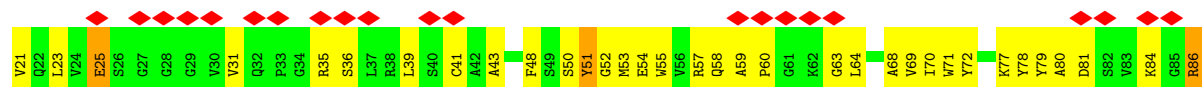
• Molecule 2: IgG Fab3-4 heavy chain

Chain bh: 



• Molecule 2: IgG Fab3-4 heavy chain

Chain ch: 





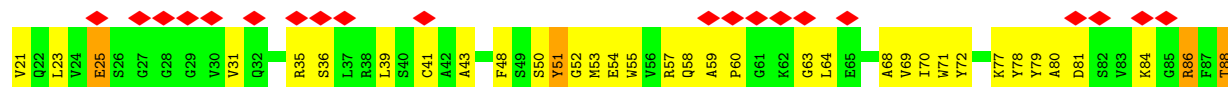
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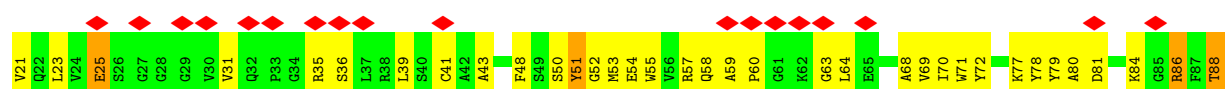
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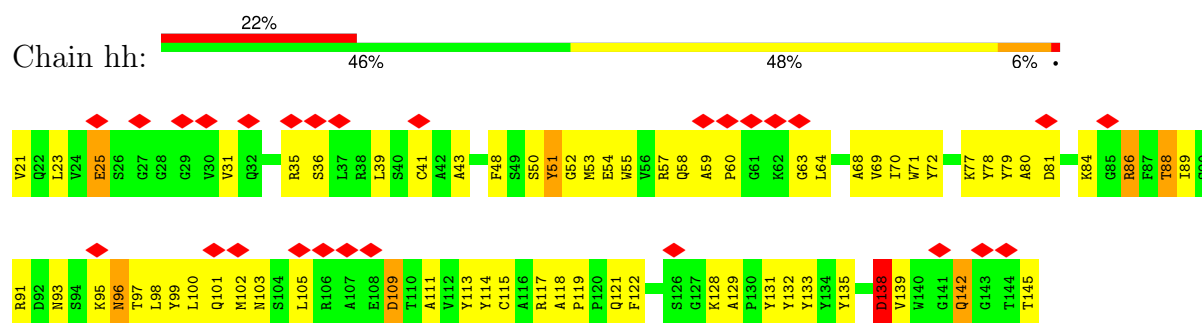
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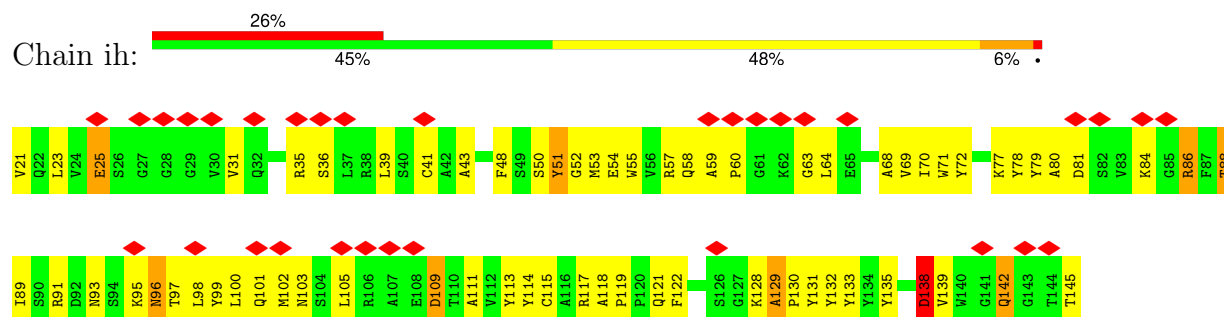
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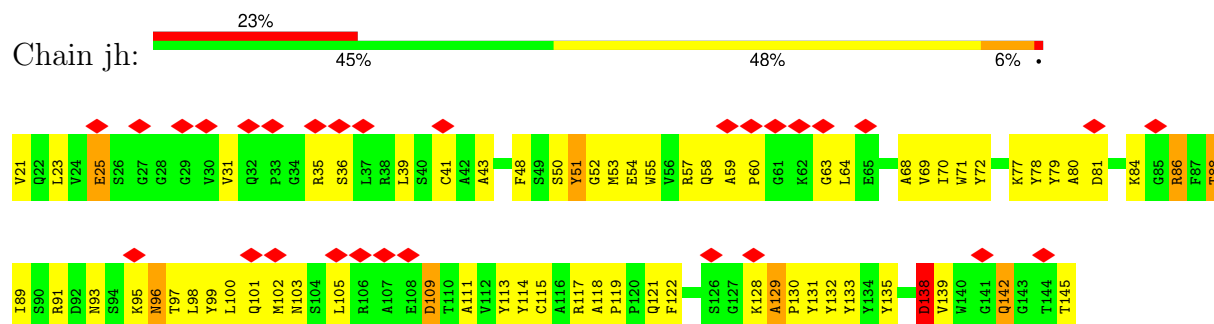
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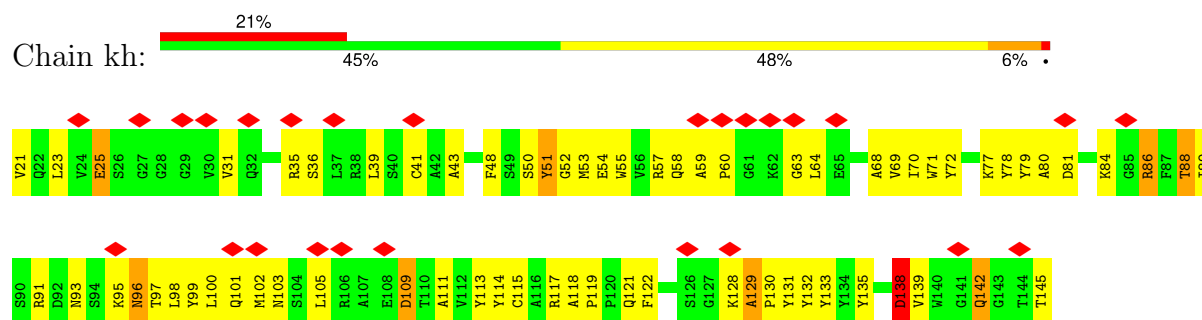
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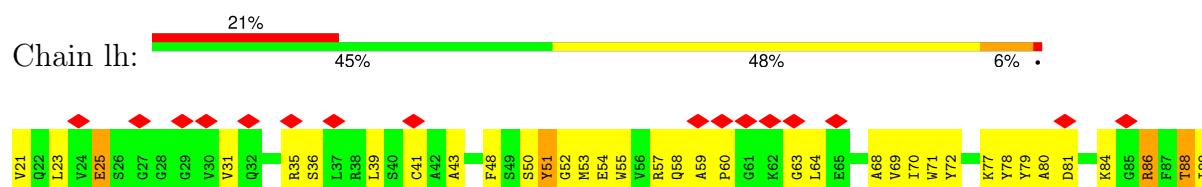
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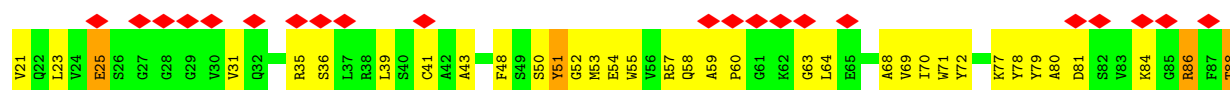




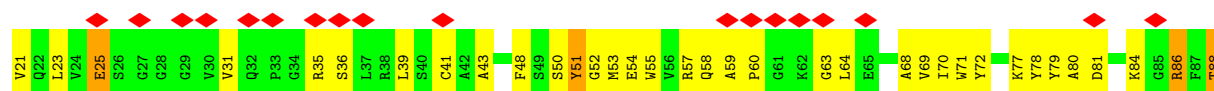
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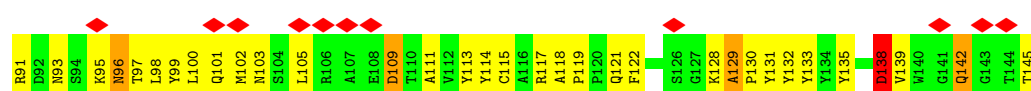
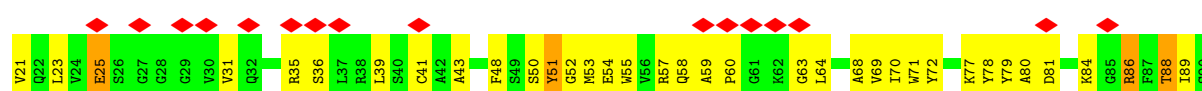
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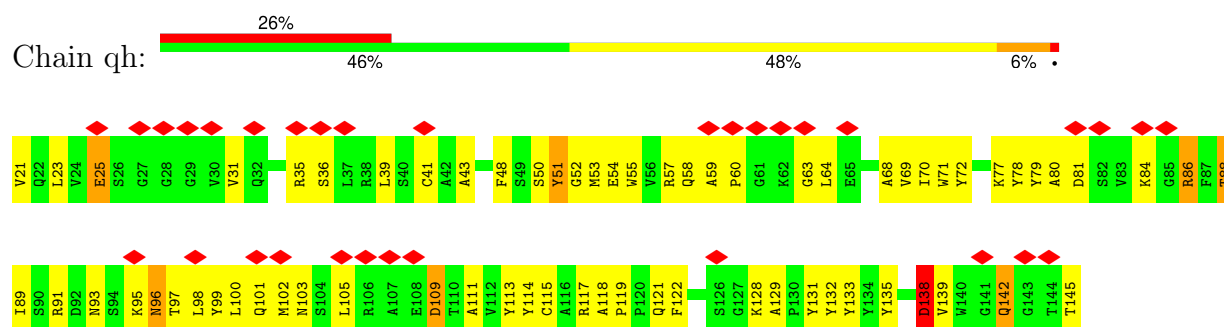
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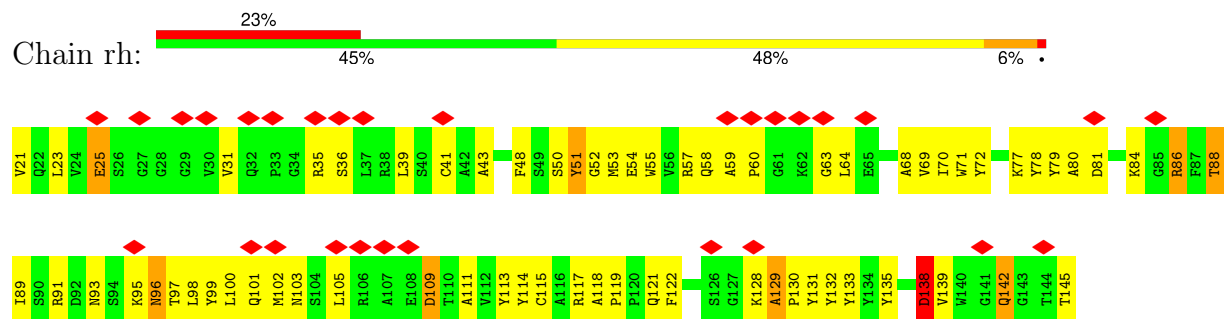
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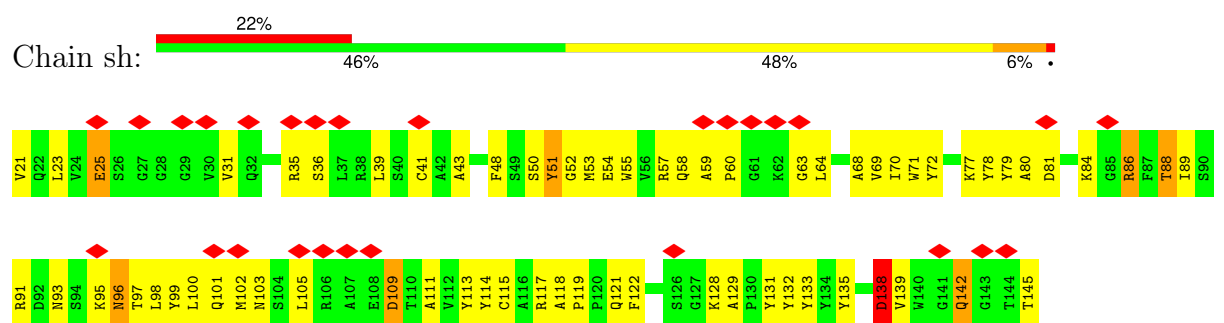
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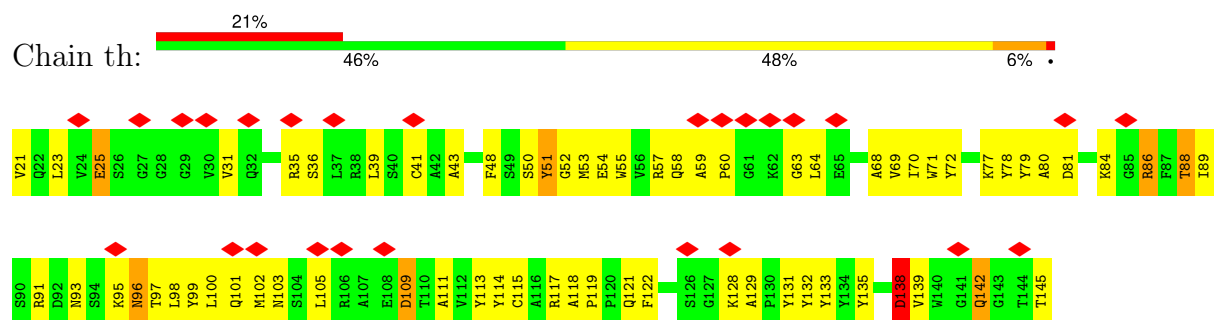
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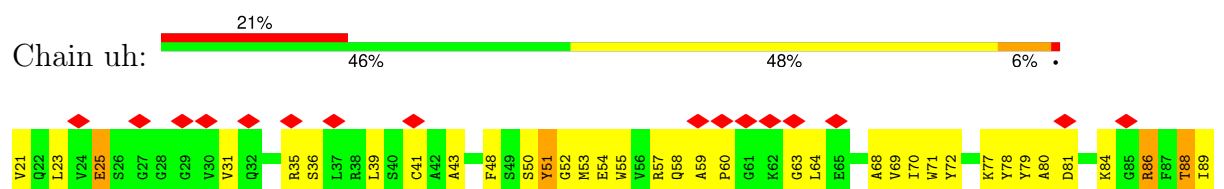
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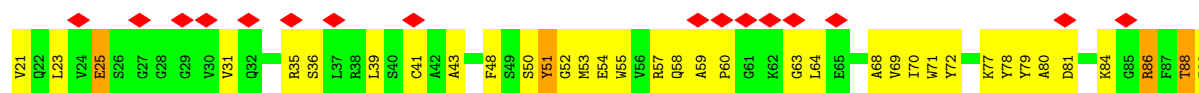


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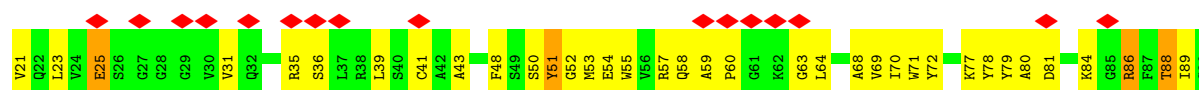




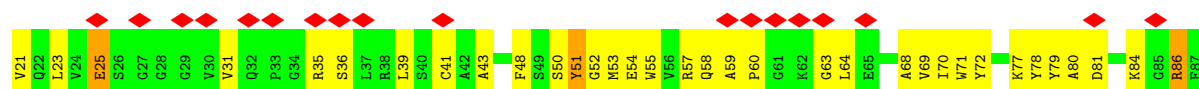
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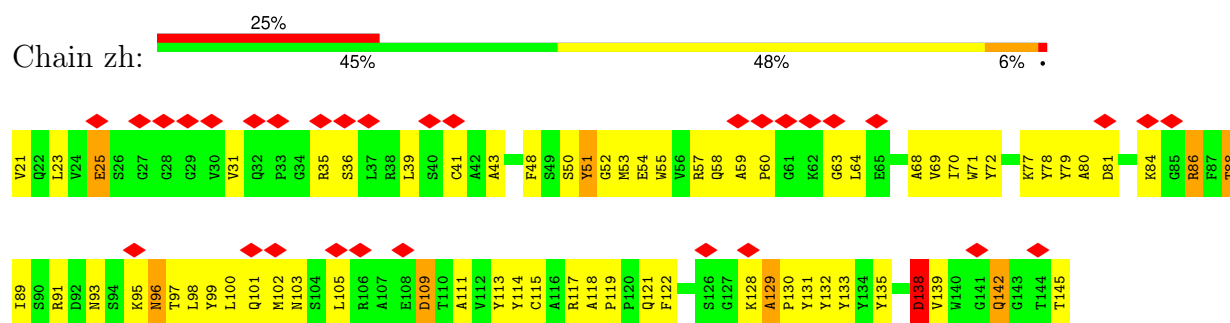
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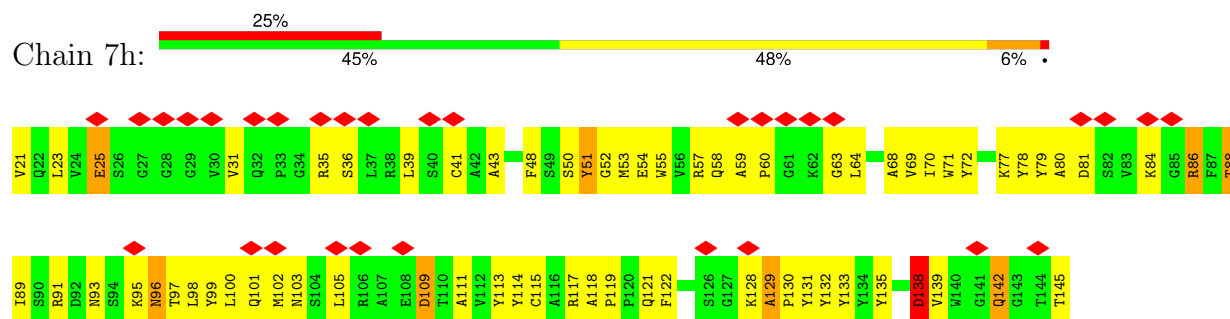
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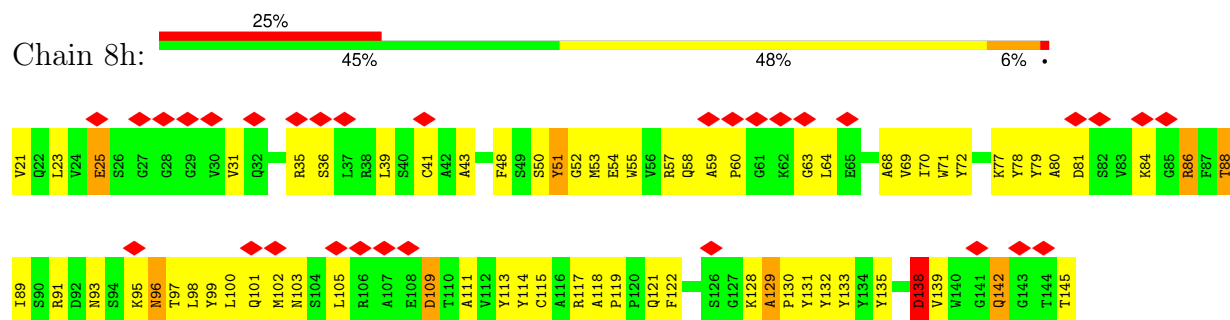
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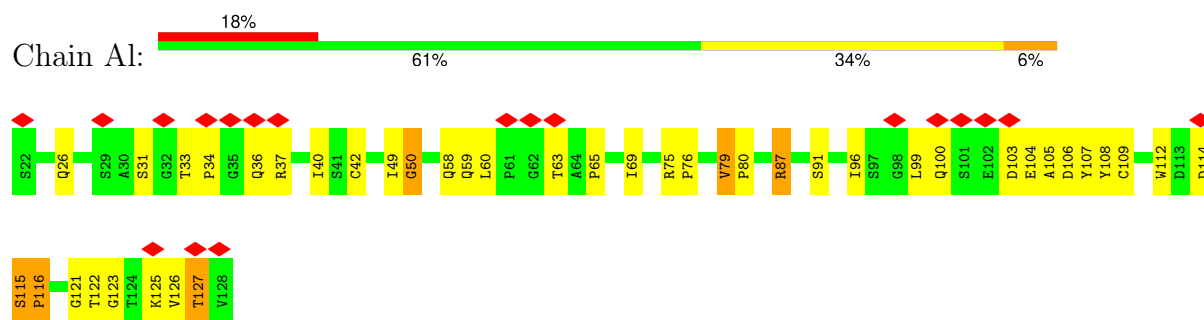
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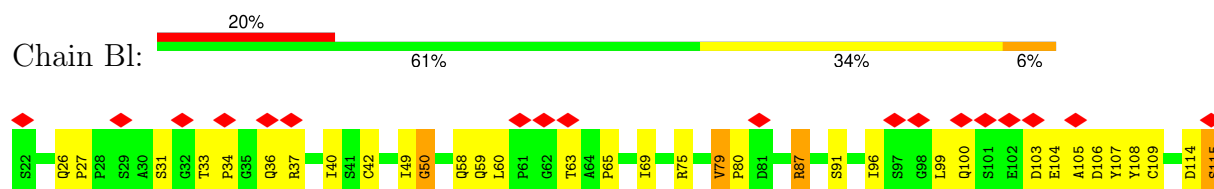
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• Molecule 3: IgG Fab3-4 light chain

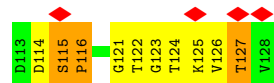
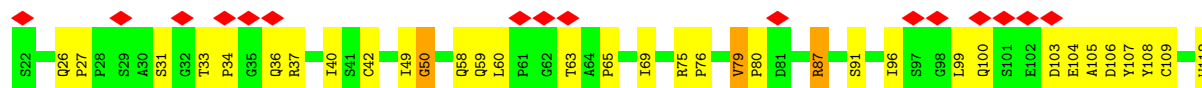


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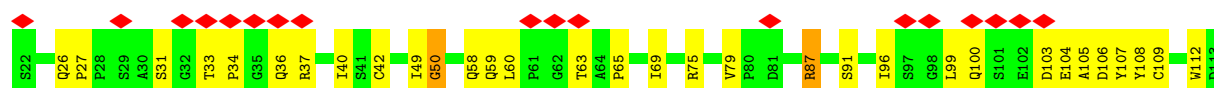




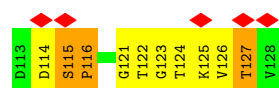
- Molecule 3: IgG Fab3-4 light chain



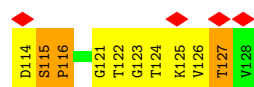
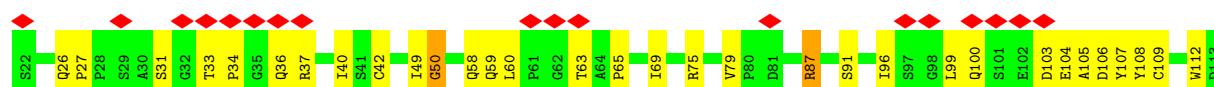
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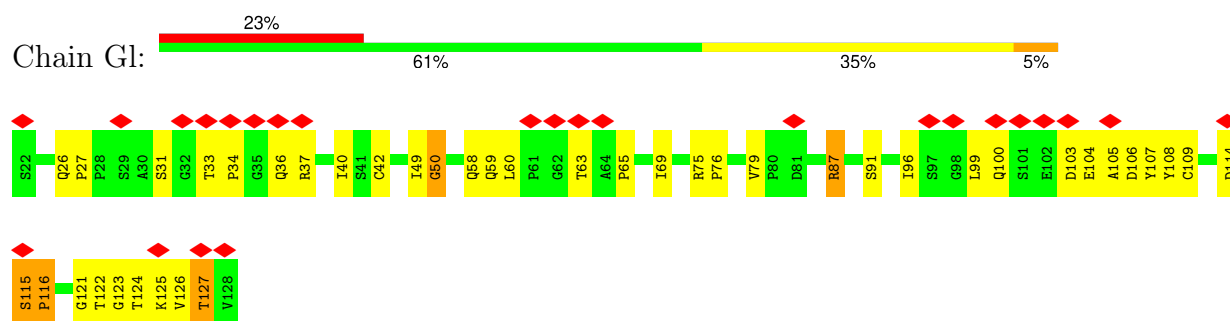
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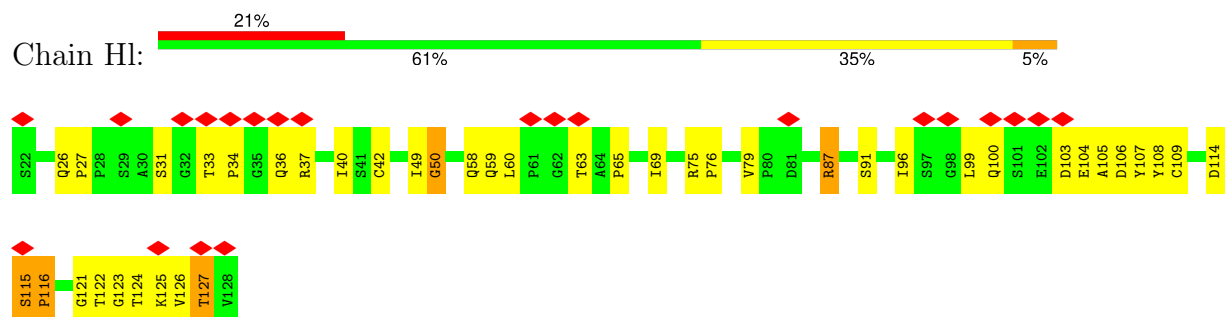
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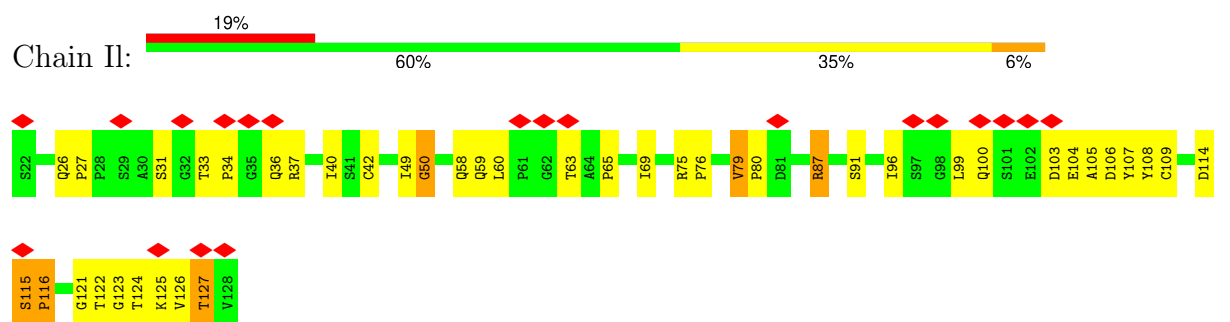
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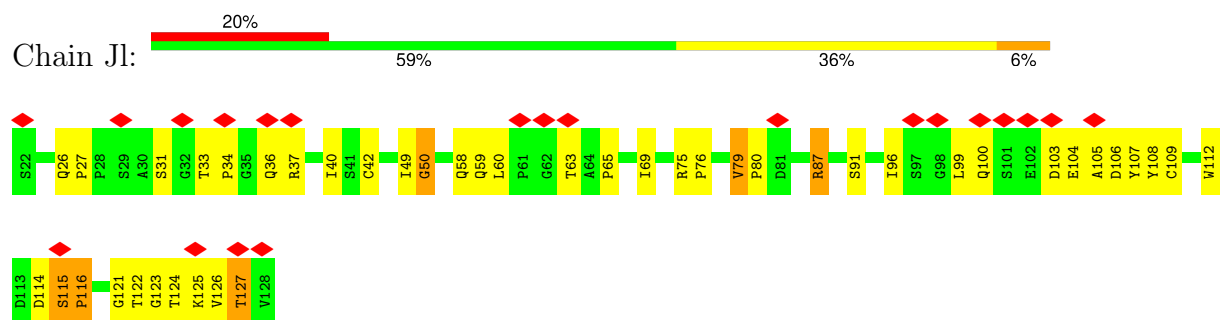
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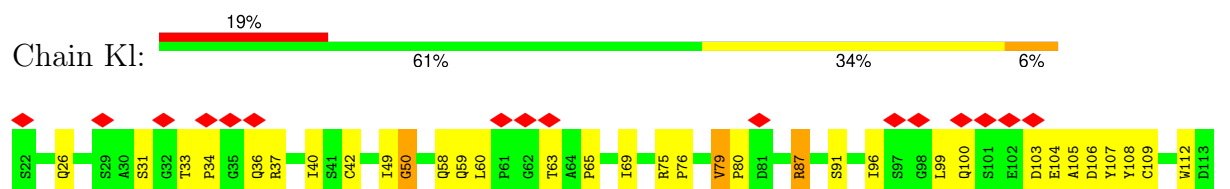
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- Molecule 3: IgG Fab3-4 light chain

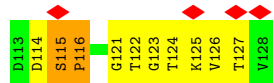
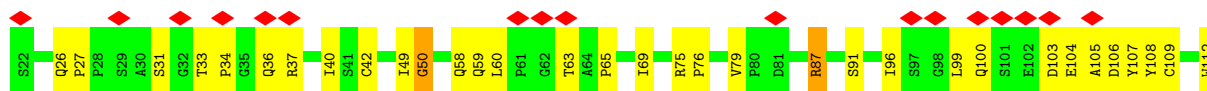


- Molecule 3: IgG Fab3-4 light chain

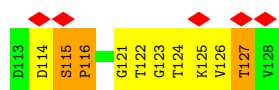
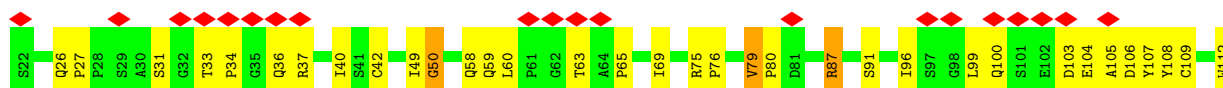




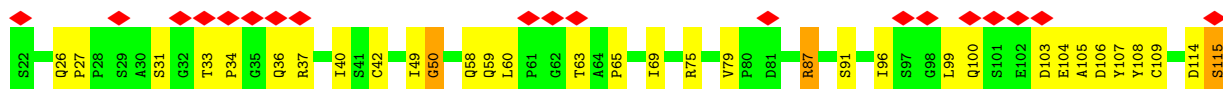
- Molecule 3: IgG Fab3-4 light chain



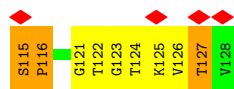
- Molecule 3: IgG Fab3-4 light chain



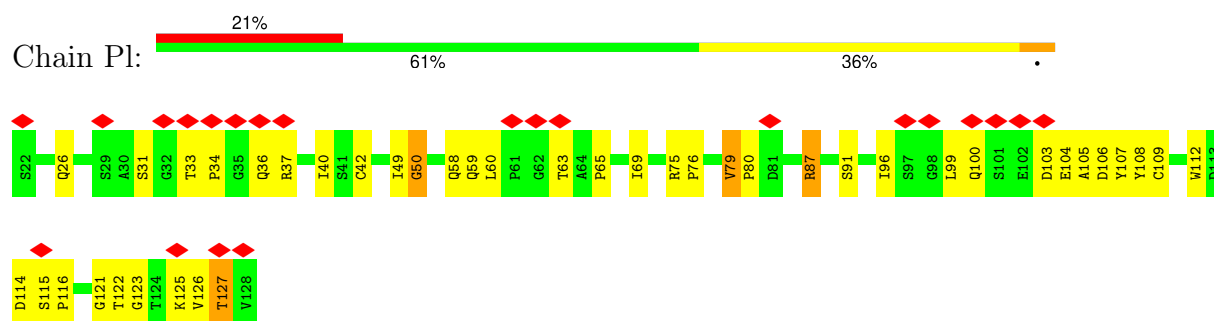
- Molecule 3: IgG Fab3-4 light chain



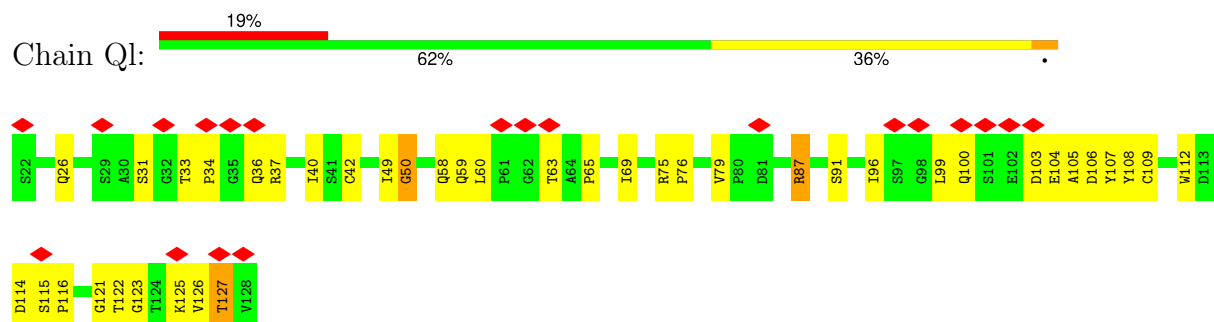
- Molecule 3: IgG Fab3-4 light chain



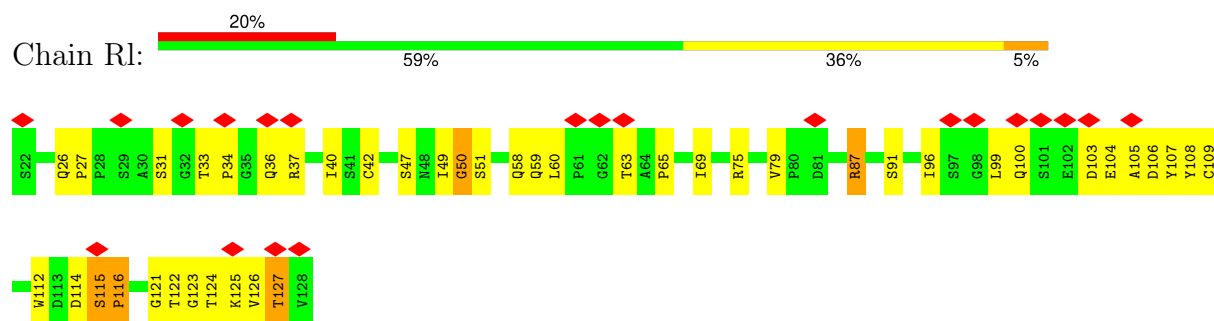
- Molecule 3: IgG Fab3-4 light chain



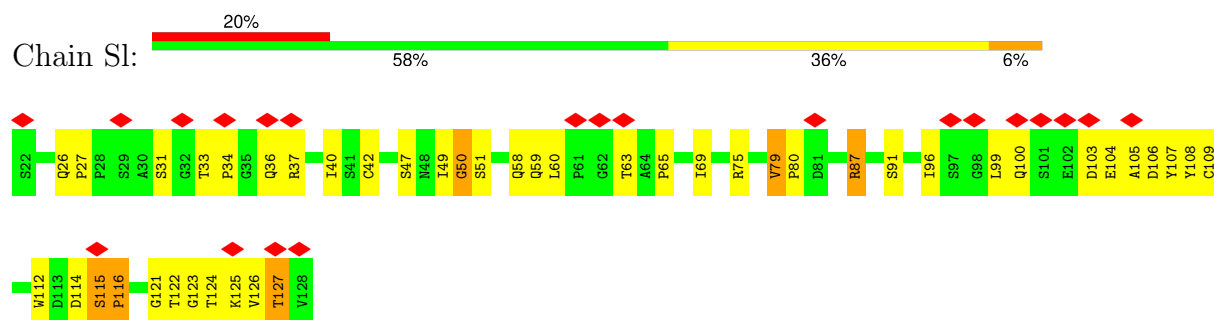
- Molecule 3: IgG Fab3-4 light chain



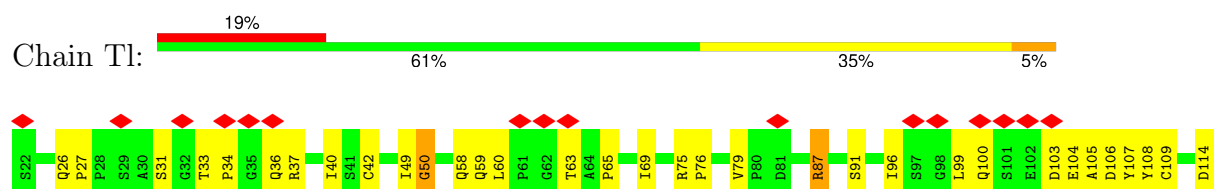
- Molecule 3: IgG Fab3-4 light chain



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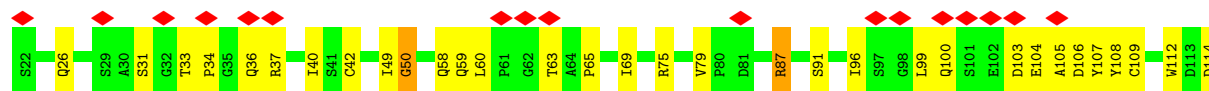


- Molecule 3: IgG Fab3-4 light chain

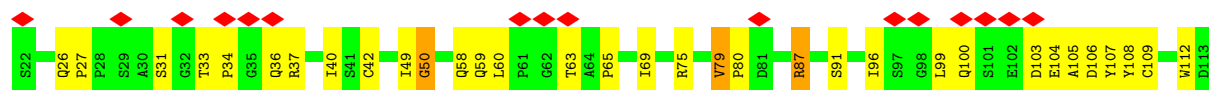




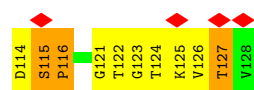
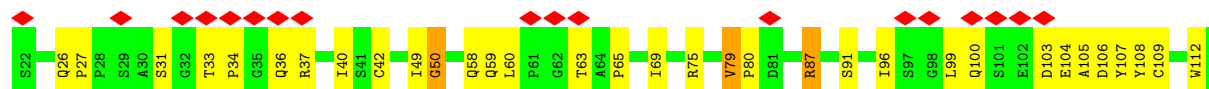
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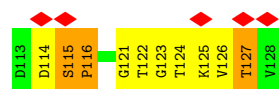
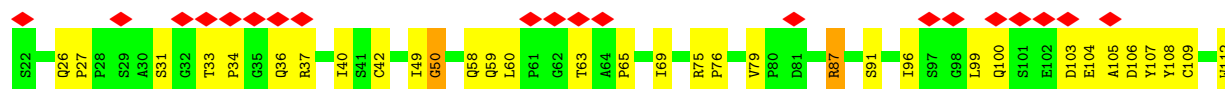
• Molecule 3: IgG Fab3-4 light chain



• Molecule 3: IgG Fab3-4 light chain

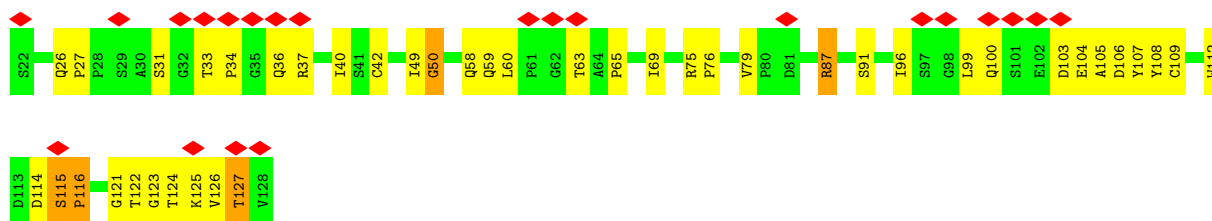


• Molecule 3: IgG Fab3-4 light chain



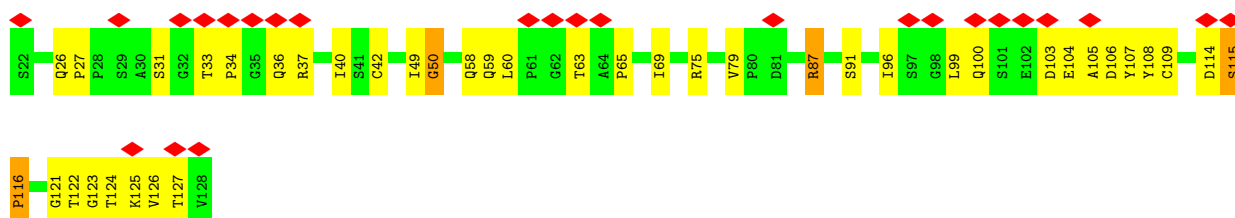
• Molecule 3: IgG Fab3-4 light chain

Chain Yl: 21% 60% 36% 5%



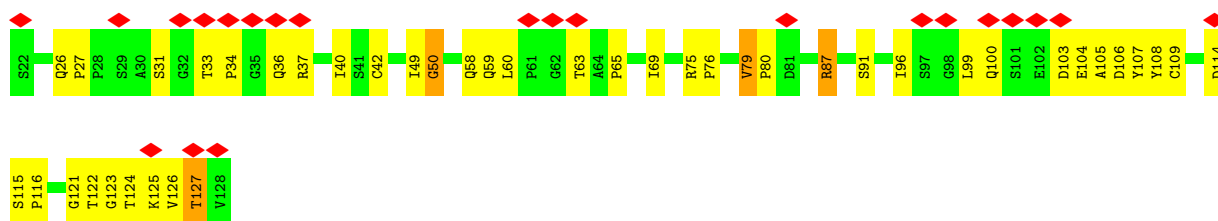
• Molecule 3: IgG Fab3-4 light chain

Chain Zl: 23% 62% 35%



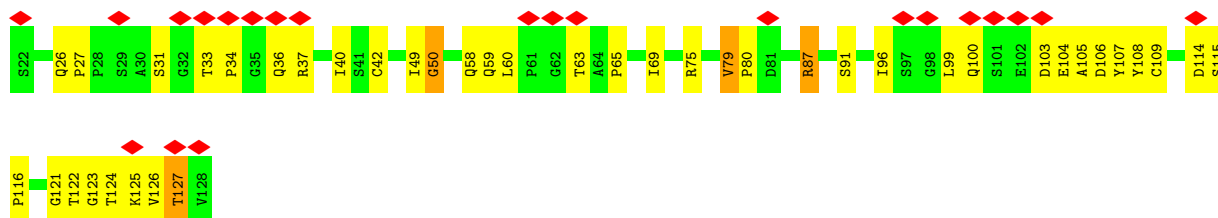
• Molecule 3: IgG Fab3-4 light chain

Chain 1l: 21% 60% 36%



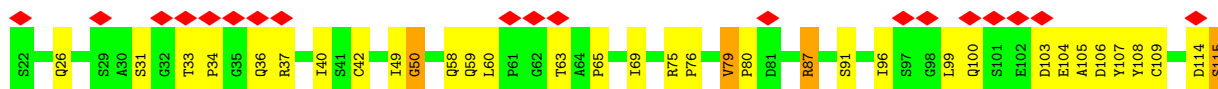
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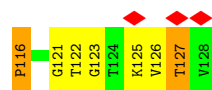
Chain 2l: 21% 61% 36%



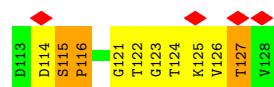
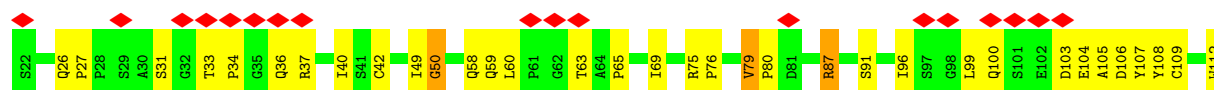
• Molecule 3: IgG Fab3-4 light chain

Chain 3l: 21% 62% 33% 6%

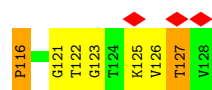
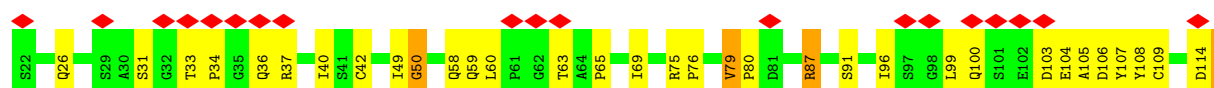




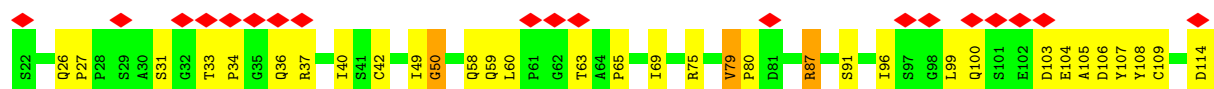
- Molecule 3: IgG Fab3-4 light chain



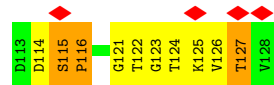
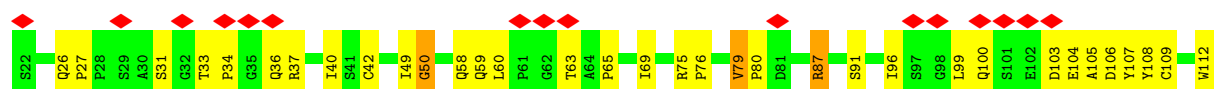
- Molecule 3: IgG Fab3-4 light chain



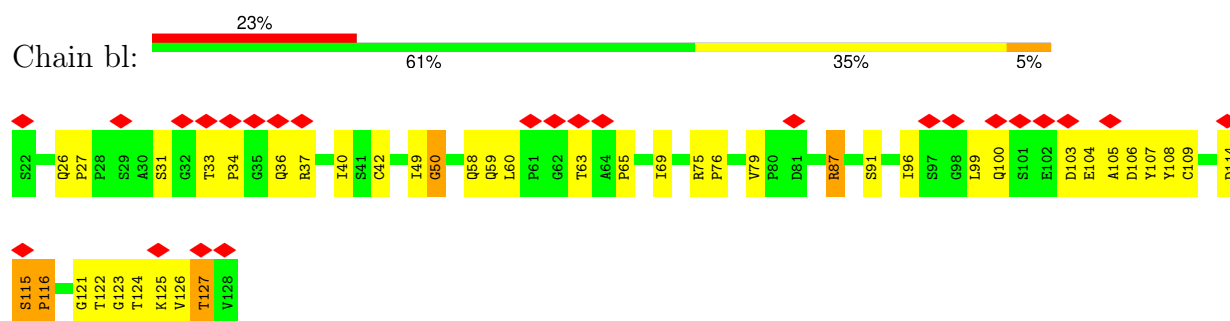
- Molecule 3: IgG Fab3-4 light chain



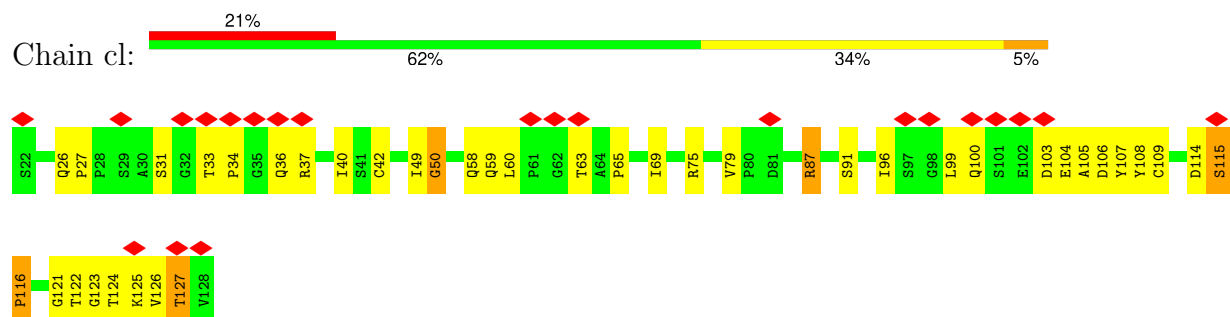
- Molecule 3: IgG Fab3-4 light chain



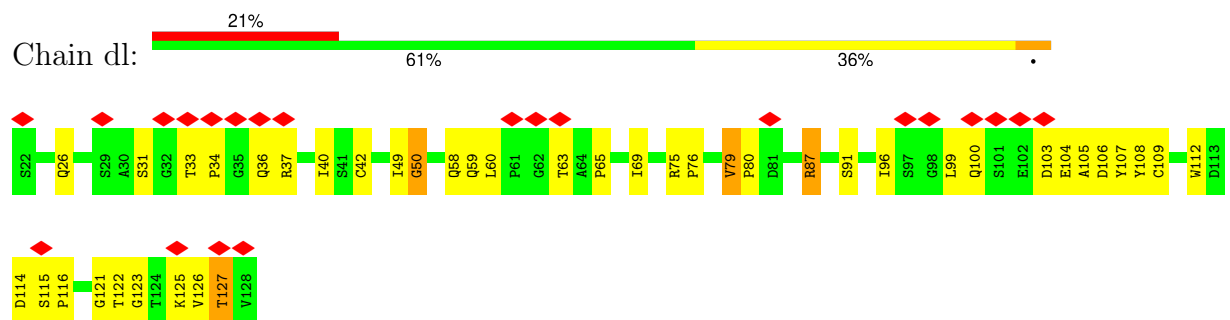
- Molecule 3: IgG Fab3-4 light chain



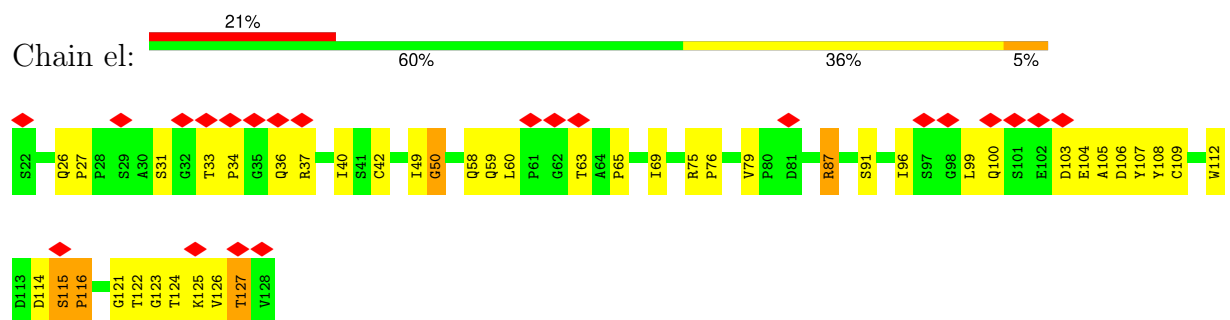
• Molecule 3: IgG Fab3-4 light chain



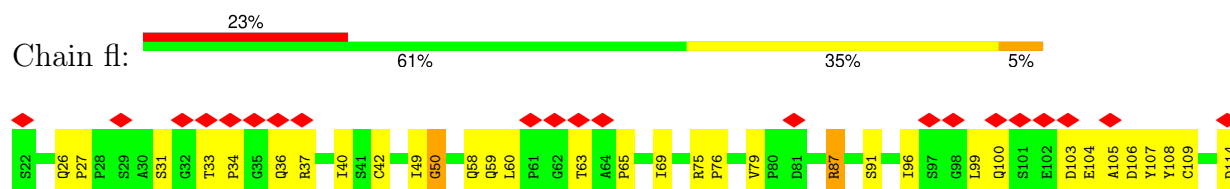
• Molecule 3: IgG Fab3-4 light chain



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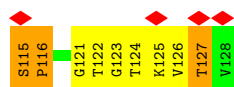
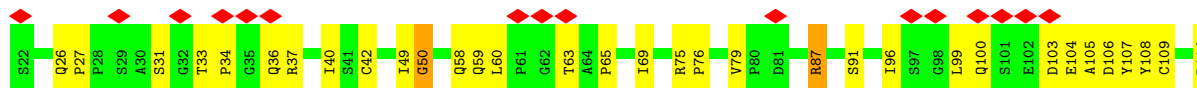


• Molecule 3: IgG Fab3-4 light chain

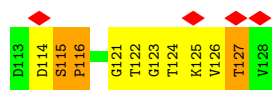
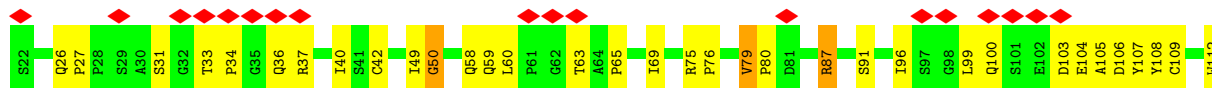




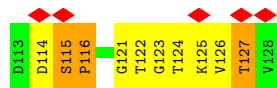
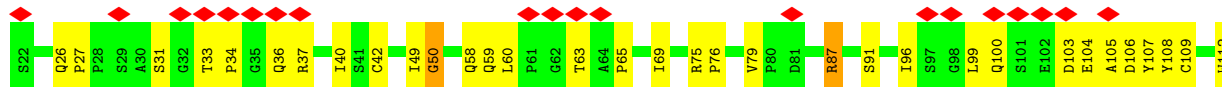
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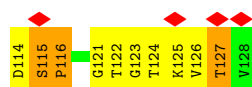
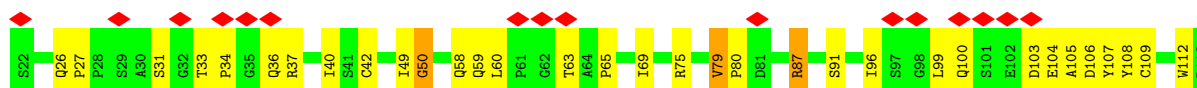
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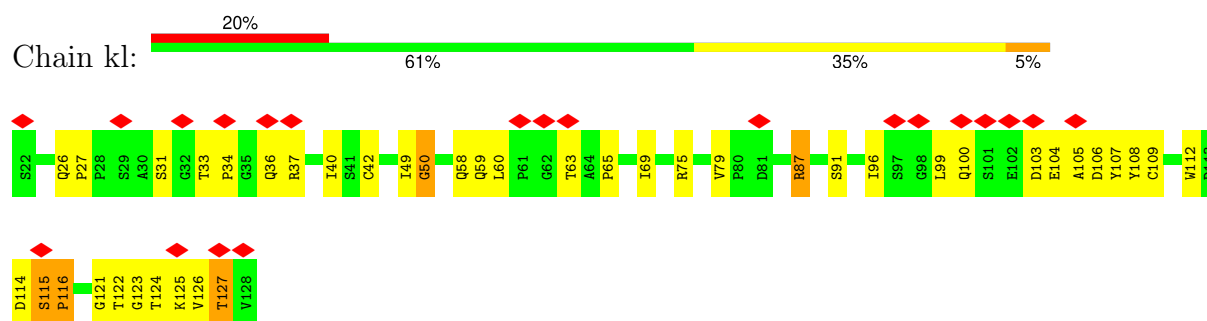
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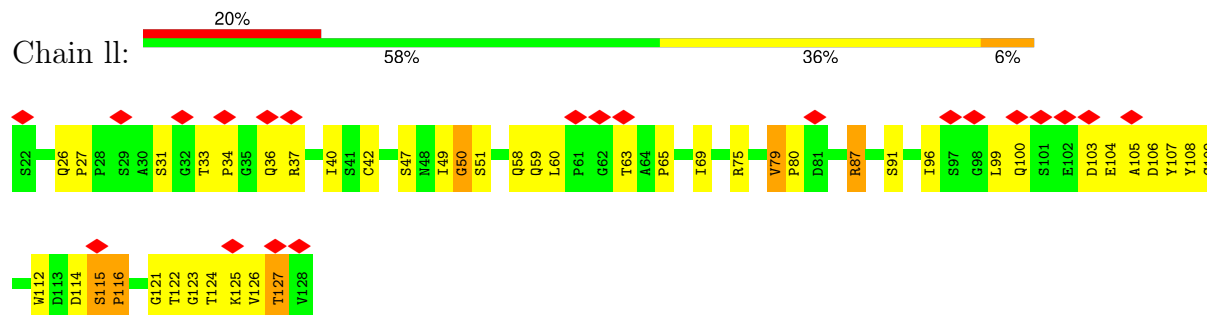
• Molecule 3: IgG Fab3-4 light chain



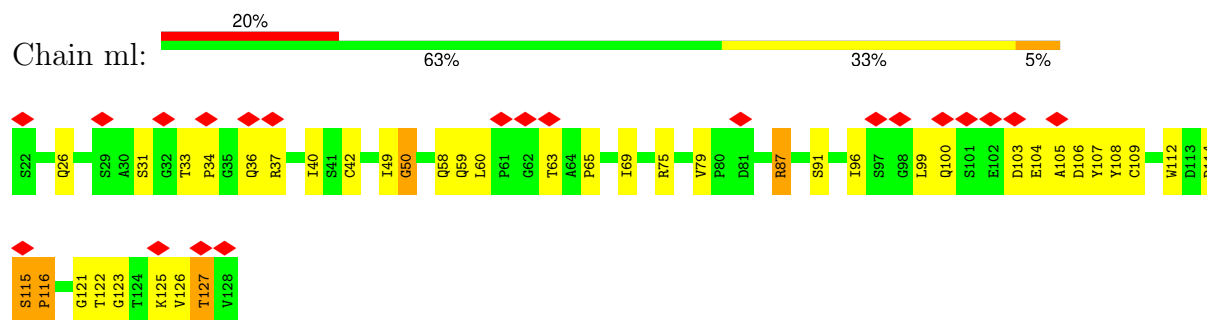
• Molecule 3: IgG Fab3-4 light chain



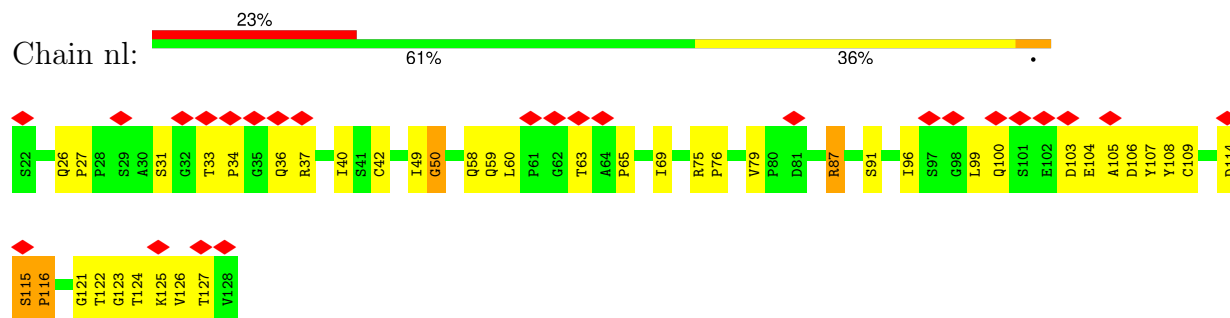
- Molecule 3: IgG Fab3-4 light chain



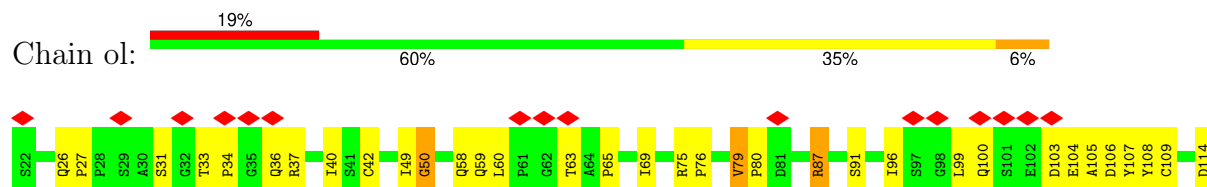
- Molecule 3: IgG Fab3-4 light chain



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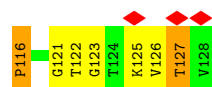
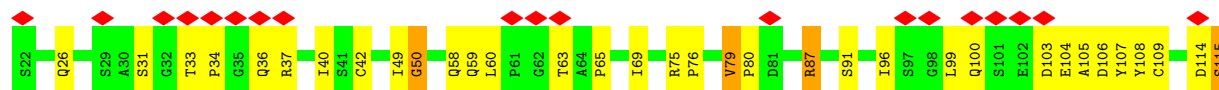


- Molecule 3: IgG Fab3-4 light chain

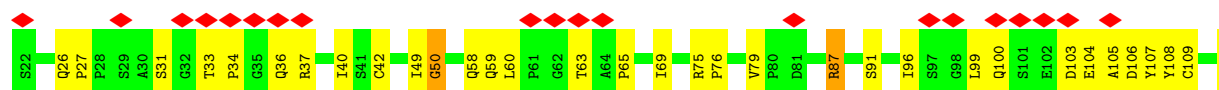




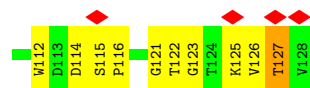
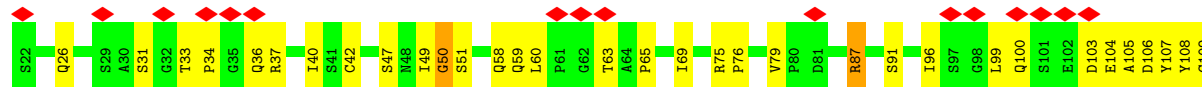
- Molecule 3: IgG Fab3-4 light chain



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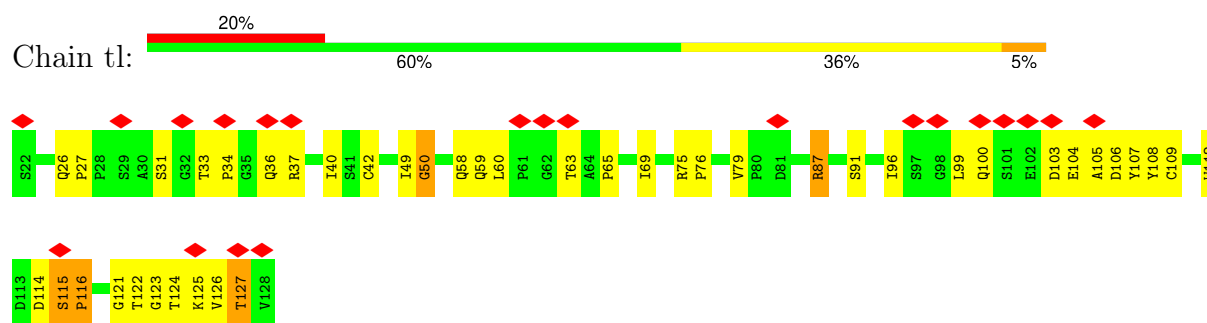
- Molecule 3: IgG Fab3-4 light chain



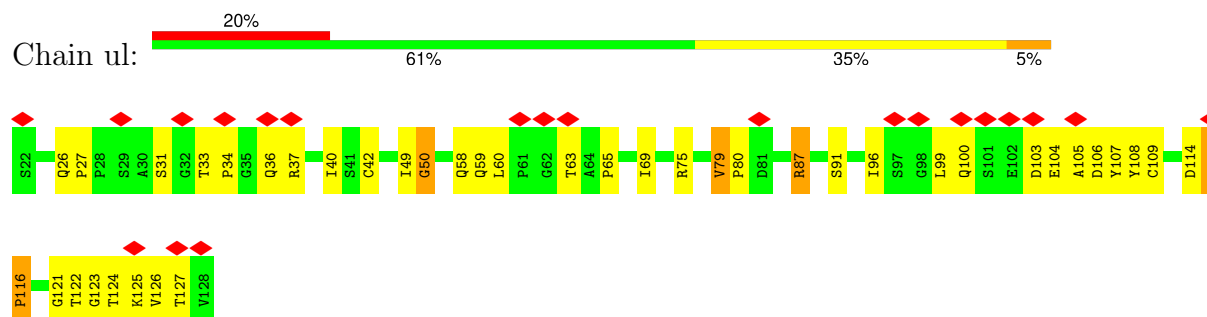
- Molecule 3: IgG Fab3-4 light chain



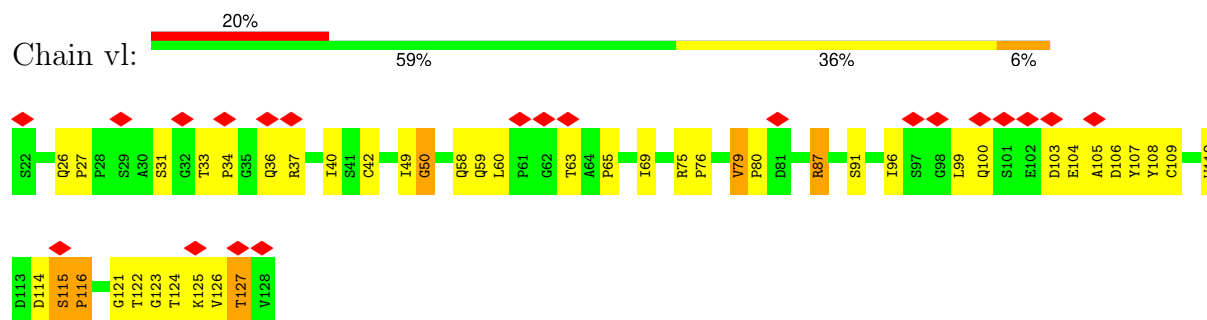
- Molecule 3: IgG Fab3-4 light chain



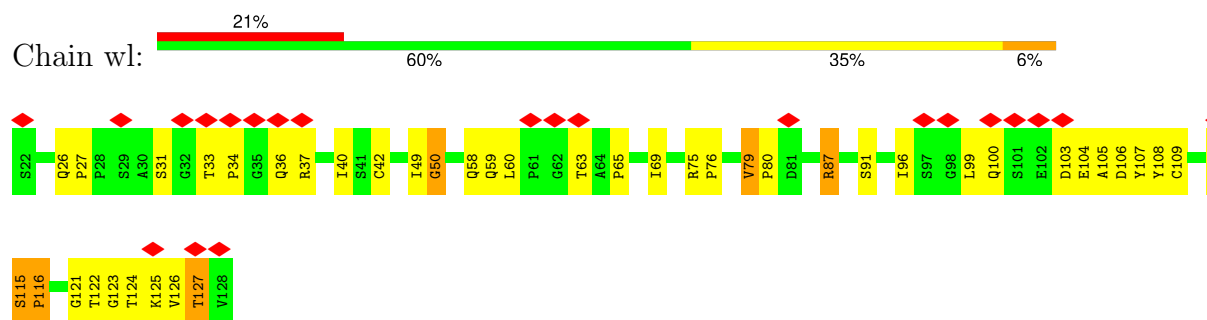
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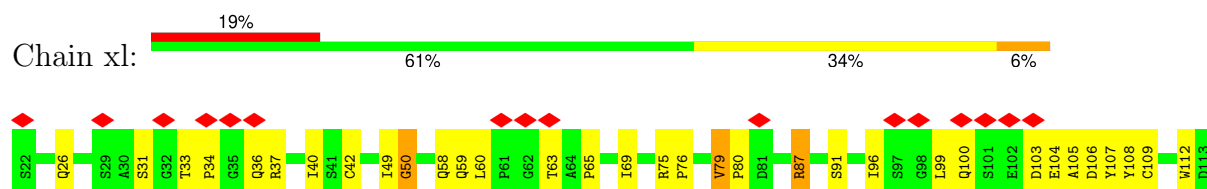
- Molecule 3: IgG Fab3-4 light chain



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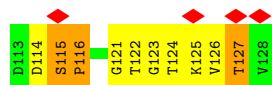
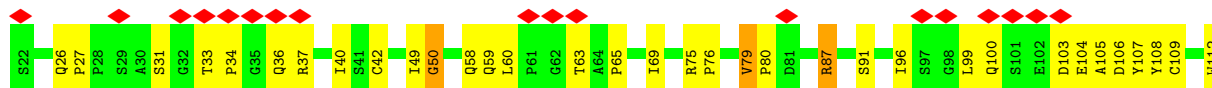


- Molecule 3: IgG Fab3-4 light chain

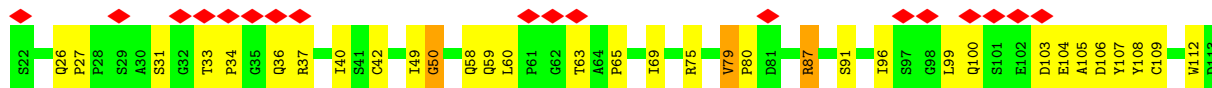




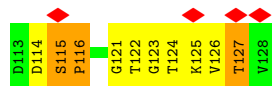
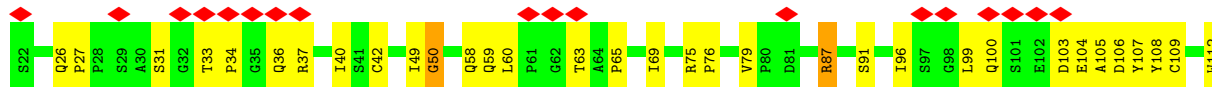
• Molecule 3: IgG Fab3-4 light chain



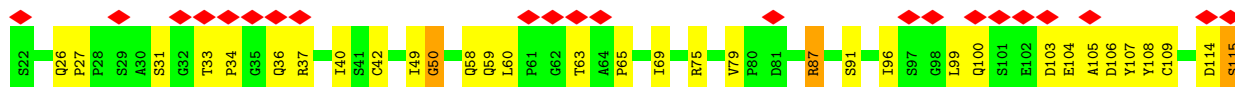
• Molecule 3: IgG Fab3-4 light chain



• Molecule 3: IgG Fab3-4 light chain



• Molecule 3: IgG Fab3-4 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.44	Depositor
Minimum defocus (nm)	320	Depositor
Maximum defocus (nm)	2450	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	16.151	Depositor
Minimum map value	-10.420	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	439.19998, 439.19998, 439.19998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.732, 0.732, 0.732	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	2	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	3	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	4	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	5	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	6	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	7	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	8	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	A	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	B	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	C	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	D	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	E	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	F	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	G	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	H	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	I	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	J	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	K	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	L	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	M	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	N	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	O	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	P	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	Q	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	R	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	S	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	T	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	U	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	V	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	W	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	X	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	Y	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	Z	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	b	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	c	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	d	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	e	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	f	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	g	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	h	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	i	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	j	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	k	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	l	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	m	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	n	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	o	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	p	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	q	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	r	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	s	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	t	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	u	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	v	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	w	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	x	0.72	3/4258 (0.1%)	0.91	21/5804 (0.4%)
1	y	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
1	z	0.72	3/4258 (0.1%)	0.91	20/5804 (0.3%)
2	1h	0.55	0/1018	1.03	5/1383 (0.4%)
2	2h	0.55	0/1018	1.03	5/1383 (0.4%)
2	3h	0.55	0/1018	1.03	5/1383 (0.4%)
2	4h	0.55	0/1018	1.03	5/1383 (0.4%)
2	5h	0.55	0/1018	1.03	5/1383 (0.4%)
2	6h	0.55	0/1018	1.03	5/1383 (0.4%)
2	7h	0.55	0/1018	1.03	5/1383 (0.4%)
2	8h	0.55	0/1018	1.03	5/1383 (0.4%)
2	Ah	0.55	0/1018	1.03	5/1383 (0.4%)
2	Bh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Ch	0.55	0/1018	1.03	5/1383 (0.4%)
2	Dh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Eh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Fh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Gh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Hh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Ih	0.55	0/1018	1.03	5/1383 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Jh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Kh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Lh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Mh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Nh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Oh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Ph	0.55	0/1018	1.03	5/1383 (0.4%)
2	Qh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Rh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Sh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Th	0.55	0/1018	1.03	5/1383 (0.4%)
2	Uh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Vh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Wh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Xh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Yh	0.55	0/1018	1.03	5/1383 (0.4%)
2	Zh	0.55	0/1018	1.03	5/1383 (0.4%)
2	ah	0.55	0/1018	1.03	5/1383 (0.4%)
2	bh	0.55	0/1018	1.03	5/1383 (0.4%)
2	ch	0.55	0/1018	1.03	5/1383 (0.4%)
2	dh	0.55	0/1018	1.03	5/1383 (0.4%)
2	eh	0.55	0/1018	1.03	5/1383 (0.4%)
2	fh	0.55	0/1018	1.03	5/1383 (0.4%)
2	gh	0.55	0/1018	1.03	5/1383 (0.4%)
2	hh	0.55	0/1018	1.03	5/1383 (0.4%)
2	ih	0.55	0/1018	1.03	5/1383 (0.4%)
2	jh	0.55	0/1018	1.03	5/1383 (0.4%)
2	kh	0.55	0/1018	1.03	5/1383 (0.4%)
2	lh	0.55	0/1018	1.03	5/1383 (0.4%)
2	mh	0.55	0/1018	1.03	5/1383 (0.4%)
2	nh	0.55	0/1018	1.03	5/1383 (0.4%)
2	oh	0.55	0/1018	1.03	5/1383 (0.4%)
2	ph	0.55	0/1018	1.03	5/1383 (0.4%)
2	qh	0.55	0/1018	1.03	5/1383 (0.4%)
2	rh	0.55	0/1018	1.03	5/1383 (0.4%)
2	sh	0.55	0/1018	1.03	5/1383 (0.4%)
2	th	0.55	0/1018	1.03	5/1383 (0.4%)
2	uh	0.55	0/1018	1.03	5/1383 (0.4%)
2	vh	0.55	0/1018	1.03	5/1383 (0.4%)
2	wh	0.55	0/1018	1.03	5/1383 (0.4%)
2	xh	0.55	0/1018	1.03	5/1383 (0.4%)
2	yh	0.55	0/1018	1.03	5/1383 (0.4%)
2	zh	0.55	0/1018	1.03	5/1383 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	1l	0.52	0/803	1.07	5/1098 (0.5%)
3	2l	0.52	0/803	1.07	5/1098 (0.5%)
3	3l	0.52	0/803	1.07	5/1098 (0.5%)
3	4l	0.52	0/803	1.07	5/1098 (0.5%)
3	5l	0.52	0/803	1.07	5/1098 (0.5%)
3	6l	0.52	0/803	1.07	5/1098 (0.5%)
3	7l	0.51	0/803	1.07	5/1098 (0.5%)
3	8l	0.52	0/803	1.07	5/1098 (0.5%)
3	Al	0.52	0/803	1.07	5/1098 (0.5%)
3	Bl	0.52	0/803	1.07	5/1098 (0.5%)
3	Cl	0.52	0/803	1.07	5/1098 (0.5%)
3	Dl	0.52	0/803	1.07	5/1098 (0.5%)
3	El	0.52	0/803	1.07	5/1098 (0.5%)
3	Fl	0.52	0/803	1.07	5/1098 (0.5%)
3	Gl	0.51	0/803	1.07	5/1098 (0.5%)
3	Hl	0.52	0/803	1.07	5/1098 (0.5%)
3	Il	0.52	0/803	1.07	5/1098 (0.5%)
3	Jl	0.52	0/803	1.07	5/1098 (0.5%)
3	Kl	0.52	0/803	1.07	5/1098 (0.5%)
3	Ll	0.52	0/803	1.07	4/1098 (0.4%)
3	Ml	0.52	0/803	1.07	5/1098 (0.5%)
3	Nl	0.52	0/803	1.07	5/1098 (0.5%)
3	Ol	0.52	0/803	1.07	5/1098 (0.5%)
3	Pl	0.52	0/803	1.07	5/1098 (0.5%)
3	Ql	0.52	0/803	1.07	5/1098 (0.5%)
3	Rl	0.52	0/803	1.07	5/1098 (0.5%)
3	Sl	0.52	0/803	1.07	5/1098 (0.5%)
3	Tl	0.52	0/803	1.07	5/1098 (0.5%)
3	Ul	0.52	0/803	1.07	5/1098 (0.5%)
3	Vl	0.52	0/803	1.07	5/1098 (0.5%)
3	Wl	0.52	0/803	1.07	5/1098 (0.5%)
3	Xl	0.52	0/803	1.07	5/1098 (0.5%)
3	Yl	0.51	0/803	1.07	5/1098 (0.5%)
3	Zl	0.52	0/803	1.07	4/1098 (0.4%)
3	al	0.52	0/803	1.07	5/1098 (0.5%)
3	bl	0.52	0/803	1.07	5/1098 (0.5%)
3	cl	0.51	0/803	1.07	5/1098 (0.5%)
3	dl	0.52	0/803	1.07	5/1098 (0.5%)
3	el	0.52	0/803	1.07	5/1098 (0.5%)
3	fl	0.52	0/803	1.07	5/1098 (0.5%)
3	gl	0.52	0/803	1.07	5/1098 (0.5%)
3	hl	0.52	0/803	1.07	5/1098 (0.5%)
3	il	0.52	0/803	1.07	5/1098 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	jl	0.52	0/803	1.07	5/1098 (0.5%)
3	kl	0.52	0/803	1.07	5/1098 (0.5%)
3	ll	0.52	0/803	1.07	5/1098 (0.5%)
3	ml	0.52	0/803	1.07	5/1098 (0.5%)
3	nl	0.52	0/803	1.07	4/1098 (0.4%)
3	ol	0.52	0/803	1.07	5/1098 (0.5%)
3	pl	0.52	0/803	1.07	5/1098 (0.5%)
3	ql	0.51	0/803	1.07	5/1098 (0.5%)
3	rl	0.52	0/803	1.07	5/1098 (0.5%)
3	sl	0.52	0/803	1.07	5/1098 (0.5%)
3	tl	0.52	0/803	1.07	5/1098 (0.5%)
3	ul	0.52	0/803	1.07	4/1098 (0.4%)
3	vl	0.52	0/803	1.07	5/1098 (0.5%)
3	wl	0.52	0/803	1.07	5/1098 (0.5%)
3	xl	0.52	0/803	1.07	5/1098 (0.5%)
3	yl	0.52	0/803	1.07	5/1098 (0.5%)
3	zl	0.52	0/803	1.07	5/1098 (0.5%)
All	All	0.67	180/364740 (0.0%)	0.95	1809/497100 (0.4%)

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	1	0	1
1	2	0	1
1	3	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1
1	U	0	1
1	V	0	1
1	W	0	1
1	X	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1
1	b	0	1
1	c	0	1
1	d	0	1
1	e	0	1
1	f	0	1
1	g	0	1
1	h	0	1
1	i	0	1
1	j	0	1
1	k	0	1
1	l	0	1
1	m	0	1
1	n	0	1
1	o	0	1
1	p	0	1
1	q	0	1
1	r	0	1
1	s	0	1
1	t	0	1
1	u	0	1
1	v	0	1
1	w	0	1
1	x	0	1
1	y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	z	0	1
All	All	0	60

The worst 5 of 180 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	310	ARG	C-N	8.49	1.46	1.33
1	J	310	ARG	C-N	8.47	1.46	1.33
1	S	310	ARG	C-N	8.47	1.46	1.33
1	l	310	ARG	C-N	8.47	1.46	1.33
1	v	310	ARG	C-N	8.47	1.46	1.33

The worst 5 of 1809 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	617	ILE	N-CA-C	9.68	120.50	110.72
1	L	617	ILE	N-CA-C	9.68	120.50	110.72
1	S	617	ILE	N-CA-C	9.68	120.50	110.72
1	U	617	ILE	N-CA-C	9.68	120.50	110.72
1	l	617	ILE	N-CA-C	9.68	120.50	110.72

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	518	ASN	Peptide
1	B	518	ASN	Peptide
1	C	518	ASN	Peptide
1	D	518	ASN	Peptide
1	E	518	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4135	0	3892	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4135	0	3892	89	0
1	3	4135	0	3892	91	0
1	4	4135	0	3892	91	0
1	5	4135	0	3892	92	0
1	6	4135	0	3892	90	0
1	7	4135	0	3892	93	0
1	8	4135	0	3892	93	0
1	A	4135	0	3892	94	0
1	B	4135	0	3892	93	0
1	C	4135	0	3892	93	0
1	D	4135	0	3892	95	0
1	E	4135	0	3892	93	0
1	F	4135	0	3892	91	0
1	G	4135	0	3892	92	0
1	H	4135	0	3892	92	0
1	I	4135	0	3892	92	0
1	J	4135	0	3892	92	0
1	K	4135	0	3892	92	0
1	L	4135	0	3892	93	0
1	M	4135	0	3892	95	0
1	N	4135	0	3892	93	0
1	O	4135	0	3892	91	0
1	P	4135	0	3892	92	0
1	Q	4135	0	3892	91	0
1	R	4135	0	3892	95	0
1	S	4135	0	3892	93	0
1	T	4135	0	3892	94	0
1	U	4135	0	3892	94	0
1	V	4135	0	3892	92	0
1	W	4135	0	3892	91	0
1	X	4135	0	3892	93	0
1	Y	4135	0	3892	94	0
1	Z	4135	0	3892	92	0
1	a	4135	0	3892	92	0
1	b	4135	0	3892	95	0
1	c	4135	0	3892	93	0
1	d	4135	0	3892	92	0
1	e	4135	0	3892	94	0
1	f	4135	0	3892	89	0
1	g	4135	0	3892	95	0
1	h	4135	0	3892	93	0
1	i	4135	0	3892	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4135	0	3892	92	0
1	k	4135	0	3892	97	0
1	l	4135	0	3892	92	0
1	m	4135	0	3892	94	0
1	n	4135	0	3892	91	0
1	o	4135	0	3892	91	0
1	p	4135	0	3892	95	0
1	q	4135	0	3892	93	0
1	r	4135	0	3892	91	0
1	s	4135	0	3892	92	0
1	t	4135	0	3892	94	0
1	u	4135	0	3892	93	0
1	v	4135	0	3892	92	0
1	w	4135	0	3892	91	0
1	x	4135	0	3892	94	0
1	y	4135	0	3892	90	0
1	z	4135	0	3892	91	0
2	1h	989	0	930	105	0
2	2h	989	0	930	106	0
2	3h	989	0	930	105	0
2	4h	989	0	930	107	0
2	5h	989	0	930	106	0
2	6h	989	0	930	106	0
2	7h	989	0	930	109	0
2	8h	989	0	930	106	0
2	Ah	989	0	930	110	0
2	Bh	989	0	930	104	0
2	Ch	989	0	930	109	0
2	Dh	989	0	930	109	0
2	Eh	989	0	930	106	0
2	Fh	989	0	930	105	0
2	Gh	989	0	930	105	0
2	Hh	989	0	930	107	0
2	Ih	989	0	930	107	0
2	Jh	989	0	930	106	0
2	Kh	989	0	930	106	0
2	Lh	989	0	930	107	0
2	Mh	989	0	930	107	0
2	Nh	989	0	930	105	0
2	Oh	989	0	930	106	0
2	Ph	989	0	930	105	0
2	Qh	989	0	930	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Rh	989	0	930	105	0
2	Sh	989	0	930	106	0
2	Th	989	0	930	107	0
2	Uh	989	0	930	107	0
2	Vh	989	0	930	109	0
2	Wh	989	0	930	105	0
2	Xh	989	0	930	108	0
2	Yh	989	0	930	109	0
2	Zh	989	0	930	106	0
2	ah	989	0	930	108	0
2	bh	989	0	930	106	0
2	ch	989	0	930	105	0
2	dh	989	0	930	104	0
2	eh	989	0	930	108	0
2	fh	989	0	930	107	0
2	gh	989	0	930	105	0
2	hh	989	0	930	106	0
2	ih	989	0	930	108	0
2	jh	989	0	930	109	0
2	kh	989	0	930	104	0
2	lh	989	0	930	106	0
2	mh	989	0	930	108	0
2	nh	989	0	930	105	0
2	oh	989	0	930	107	0
2	ph	989	0	930	106	0
2	qh	989	0	930	107	0
2	rh	989	0	930	110	0
2	sh	989	0	930	106	0
2	th	989	0	930	106	0
2	uh	989	0	930	105	0
2	vh	989	0	930	106	0
2	wh	989	0	930	105	0
2	xh	989	0	930	107	0
2	yh	989	0	930	107	0
2	zh	989	0	930	105	0
3	1l	785	0	741	55	0
3	2l	785	0	741	58	0
3	3l	785	0	741	58	0
3	4l	785	0	741	61	0
3	5l	785	0	741	57	0
3	6l	785	0	741	55	0
3	7l	785	0	741	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8l	785	0	741	59	0
3	Al	785	0	741	64	0
3	Bl	785	0	741	62	0
3	Cl	785	0	741	61	0
3	Dl	785	0	741	63	0
3	El	785	0	741	62	0
3	Fl	785	0	741	61	0
3	Gl	785	0	741	59	0
3	Hl	785	0	741	60	0
3	Il	785	0	741	61	0
3	Jl	785	0	741	64	0
3	Kl	785	0	741	62	0
3	Ll	785	0	741	58	0
3	Ml	785	0	741	65	0
3	Nl	785	0	741	60	0
3	Ol	785	0	741	61	0
3	Pl	785	0	741	62	0
3	Ql	785	0	741	57	0
3	Rl	785	0	741	62	0
3	Sl	785	0	741	64	0
3	Tl	785	0	741	59	0
3	Ul	785	0	741	57	0
3	Vl	785	0	741	59	0
3	Wl	785	0	741	58	0
3	Xl	785	0	741	62	0
3	Yl	785	0	741	63	0
3	Zl	785	0	741	59	0
3	al	785	0	741	60	0
3	bl	785	0	741	62	0
3	cl	785	0	741	60	0
3	dl	785	0	741	60	0
3	el	785	0	741	63	0
3	fl	785	0	741	61	0
3	gl	785	0	741	59	0
3	hl	785	0	741	61	0
3	il	785	0	741	63	0
3	jl	785	0	741	60	0
3	kl	785	0	741	61	0
3	ll	785	0	741	62	0
3	ml	785	0	741	57	0
3	nl	785	0	741	59	0
3	ol	785	0	741	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	pl	785	0	741	61	0
3	ql	785	0	741	63	0
3	rl	785	0	741	59	0
3	sl	785	0	741	63	0
3	tl	785	0	741	58	0
3	ul	785	0	741	62	0
3	vl	785	0	741	64	0
3	wl	785	0	741	57	0
3	xl	785	0	741	61	0
3	yl	785	0	741	62	0
3	zl	785	0	741	56	0
All	All	354540	0	333780	13529	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 20.

The worst 5 of 13529 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)
3:Vl:107:TYR:HE2	3:Vl:126:VAL:CG2	1.58	1.17
3:Sl:107:TYR:HE2	3:Sl:126:VAL:CG2	1.58	1.17
3:Zl:107:TYR:HE2	3:Zl:126:VAL:CG2	1.58	1.17
3:jl:107:TYR:HE2	3:jl:126:VAL:CG2	1.58	1.17
3:ll:107:TYR:HE2	3:ll:126:VAL:CG2	1.58	1.17

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	1	514/533 (96%)	502 (98%)	12 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	3	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	4	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	5	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	6	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	7	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	8	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	A	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	B	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	C	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	D	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	E	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	F	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	G	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	H	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	I	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	J	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	K	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	L	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	M	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	N	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	O	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	P	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	Q	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	R	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	S	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	T	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	U	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	V	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	W	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	X	514/533 (96%)	502 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	Z	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	a	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	b	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	c	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	d	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	e	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	f	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	g	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	h	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	i	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	j	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	k	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	l	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	m	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	n	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	o	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	p	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	q	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	r	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	s	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	t	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	u	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	v	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	w	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	x	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	y	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
1	z	514/533 (96%)	502 (98%)	12 (2%)	0	100	100
2	1h	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	2h	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	3h	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4h	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	5h	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	6h	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	7h	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	8h	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Ah	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Bh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Ch	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Dh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Eh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Fh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Gh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Hh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Ih	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Jh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Kh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Lh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Mh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Nh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Oh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Ph	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Qh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Rh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Sh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Th	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Uh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Vh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Wh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Xh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Yh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	Zh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	ah	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	bh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	ch	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	dh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	eh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	fh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	gh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	hh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	ih	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	jh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	kh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	lh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	mh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	nh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	oh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	ph	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	qh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	rh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	sh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	th	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	uh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	vh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	wh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	xh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	yh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
2	zh	123/125 (98%)	118 (96%)	3 (2%)	2 (2%)	7	25
3	1l	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	2l	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	3l	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	4l	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	5l	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	6l	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	7l	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	8l	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Al	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Bl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Cl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Dl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	El	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Fl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Gl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Hl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Il	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Jl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Kl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Ll	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Ml	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Nl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Ol	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Pl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Ql	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Rl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Sl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Tl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Ul	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Vl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Wl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Xl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Yl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	Zl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	al	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	bl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	cl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	dl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	el	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	fl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	gl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	hl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	il	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	jl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	kl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	ll	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	ml	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	nl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	ol	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	pl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	ql	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	rl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	sl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	tl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	ul	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	vl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	wl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	xl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	yl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
3	zl	105/107 (98%)	100 (95%)	3 (3%)	2 (2%)	6	22
All	All	44520/45900 (97%)	43200 (97%)	1080 (2%)	240 (0%)	26	53

5 of 240 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Al	115	SER
3	Al	116	PRO
3	Bl	115	SER
3	Bl	116	PRO
3	Cl	115	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	2	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	3	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	4	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	5	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	6	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	7	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	8	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	A	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	B	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	C	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	D	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	E	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	F	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	G	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	H	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	I	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	J	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	K	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	L	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	M	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	N	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	O	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	P	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	Q	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	R	458/468 (98%)	449 (98%)	9 (2%)	48	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	T	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	U	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	V	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	W	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	X	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	Y	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	Z	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	a	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	b	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	c	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	d	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	e	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	f	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	g	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	h	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	i	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	j	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	k	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	l	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	m	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	n	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	o	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	p	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	q	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	r	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	s	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	t	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	u	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	v	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	w	458/468 (98%)	449 (98%)	9 (2%)	48	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	y	458/468 (98%)	449 (98%)	9 (2%)	48	77
1	z	458/468 (98%)	449 (98%)	9 (2%)	48	77
2	1h	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	2h	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	3h	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	4h	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	5h	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	6h	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	7h	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	8h	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Ah	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Bh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Ch	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Dh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Eh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Fh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Gh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Hh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Ih	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Jh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Kh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Lh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Mh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Nh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Oh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Ph	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Qh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Rh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Sh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Th	101/101 (100%)	93 (92%)	8 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Uh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Vh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Wh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Xh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Yh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	Zh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	ah	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	bh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	ch	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	dh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	eh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	fh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	gh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	hh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	ih	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	jh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	kh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	lh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	mh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	nh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	oh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	ph	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	qh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	rh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	sh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	th	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	uh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	vh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	wh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	xh	101/101 (100%)	93 (92%)	8 (8%)	11	33
2	yh	101/101 (100%)	93 (92%)	8 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	zh	101/101 (100%)	93 (92%)	8 (8%)	11	33
3	1l	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	2l	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	3l	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	4l	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	5l	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	6l	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	7l	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	8l	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Al	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Bl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Cl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Dl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	El	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Fl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Gl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Hl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Il	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Jl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Kl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Ll	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Ml	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Nl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Ol	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Pl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Ql	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Rl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Sl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Tl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Ul	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Vl	89/89 (100%)	87 (98%)	2 (2%)	45	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Wl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Xl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Yl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	Zl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	al	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	bl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	cl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	dl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	el	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	fl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	gl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	hl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	il	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	jl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	kl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	ll	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	ml	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	nl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	ol	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	pl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	ql	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	rl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	sl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	tl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	ul	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	vl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	wl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	xl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	yl	89/89 (100%)	87 (98%)	2 (2%)	45	75
3	zl	89/89 (100%)	87 (98%)	2 (2%)	45	75
All	All	38880/39480 (98%)	37740 (97%)	1140 (3%)	38	69

5 of 1140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	qh	88	THR
2	th	109	ASP
2	qh	86	ARG
3	Kl	63	THR
1	l	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1631 such sidechains are listed below:

Mol	Chain	Res	Type
1	q	496	ASN
1	8	641	HIS
3	rl	58	GLN
1	r	687	GLN
1	q	495	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no chain breaks in this entry.

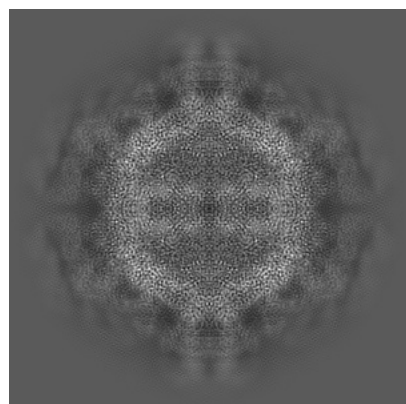
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76772. These allow visual inspection of the internal detail of the map and identification of artifacts.

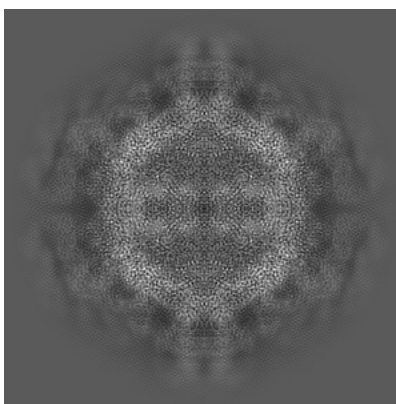
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

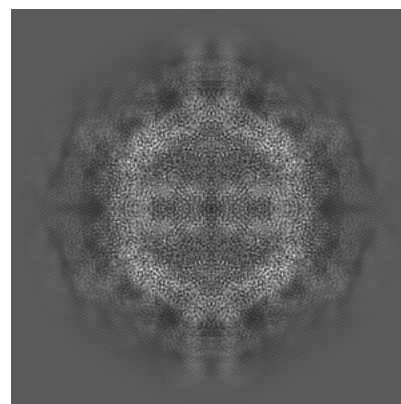
6.1.1 Primary map



X

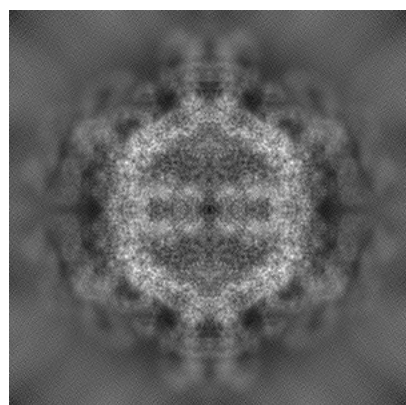


Y

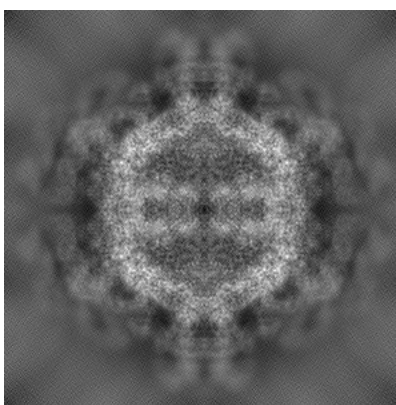


Z

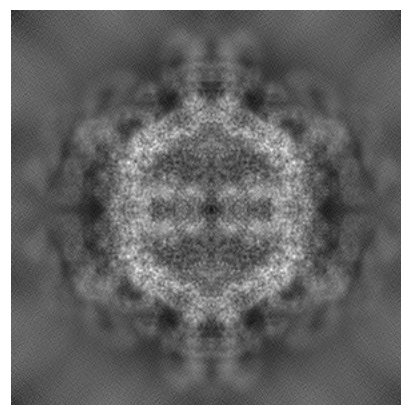
6.1.2 Raw map



X



Y

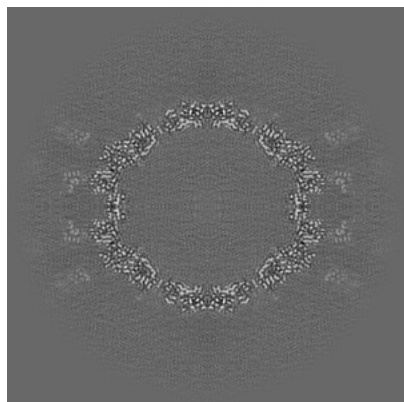


Z

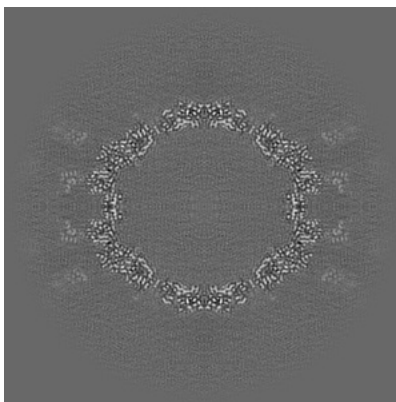
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

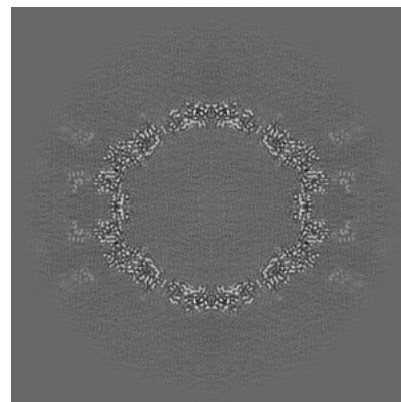
6.2.1 Primary map



X Index: 300

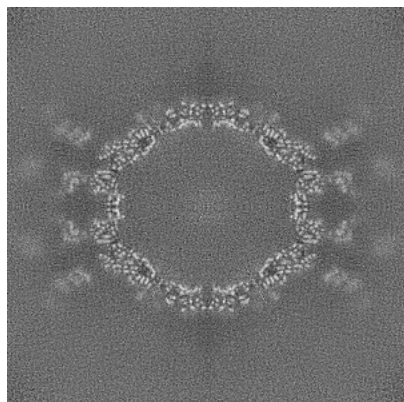


Y Index: 300

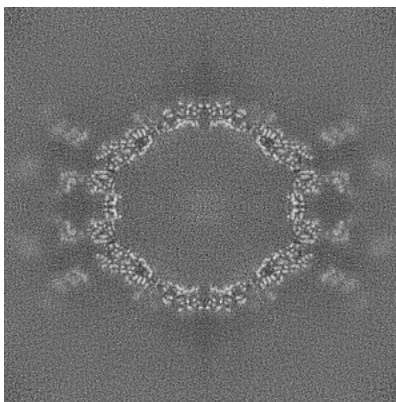


Z Index: 300

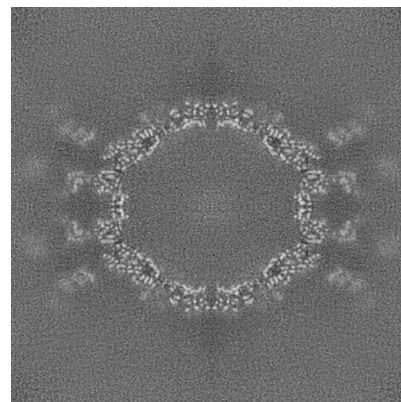
6.2.2 Raw map



X Index: 300



Y Index: 300

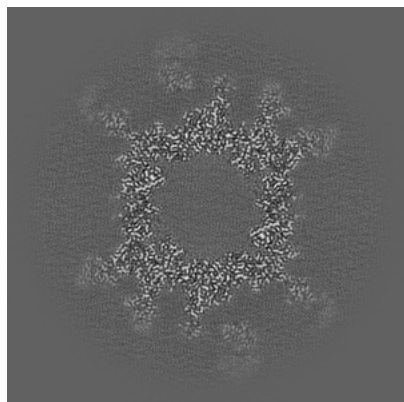


Z Index: 300

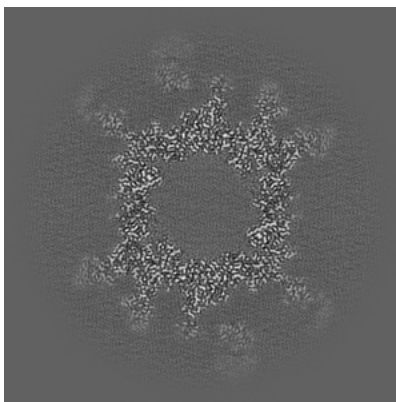
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

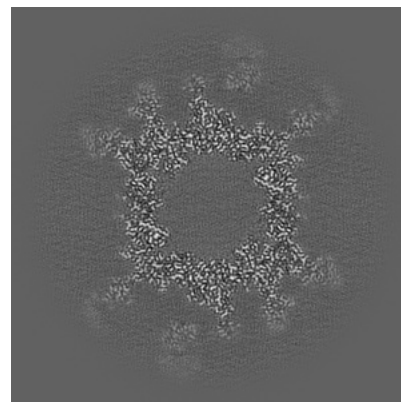
6.3.1 Primary map



X Index: 391

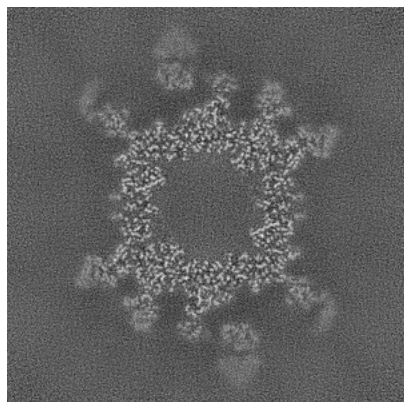


Y Index: 391

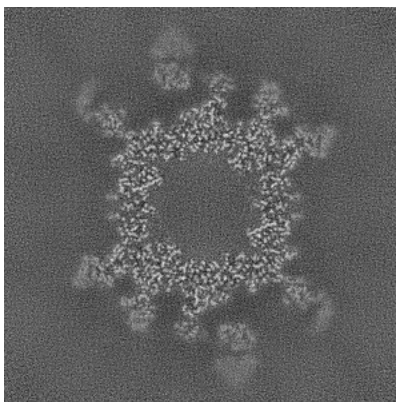


Z Index: 209

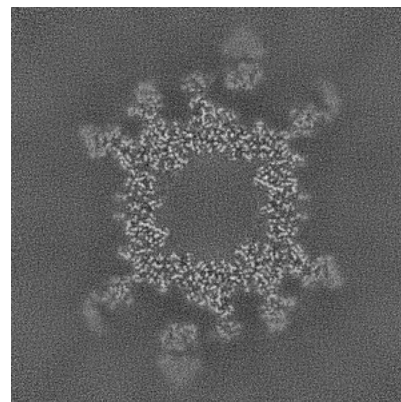
6.3.2 Raw map



X Index: 391



Y Index: 391

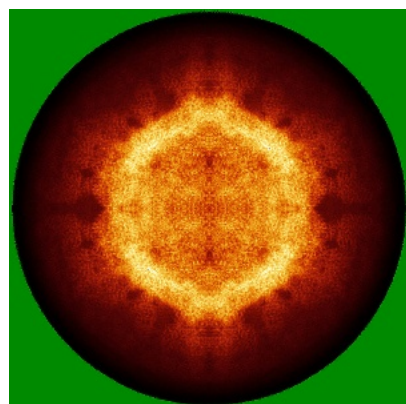


Z Index: 209

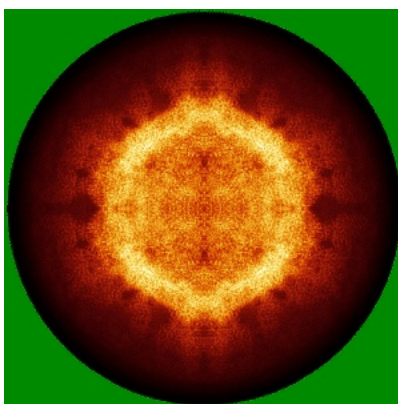
The images above show the largest variance slices of the map in three orthogonal directions.

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

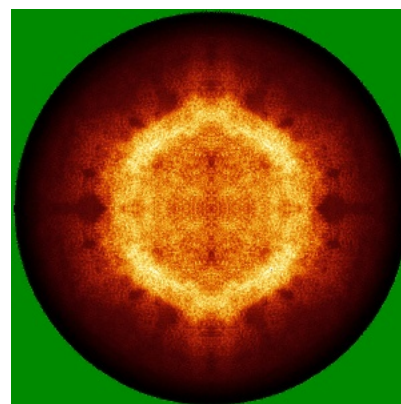
6.4.1 Primary map



X

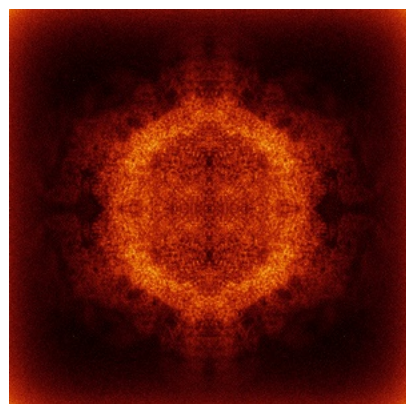


Y

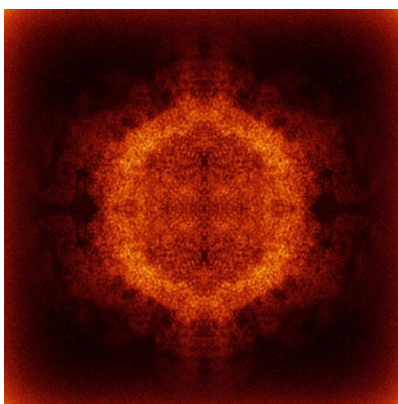


Z

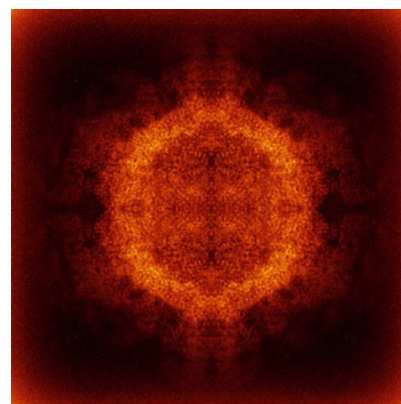
6.4.2 Raw map



X



Y



Z

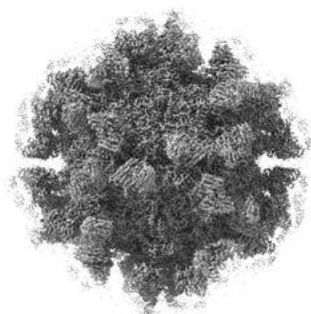
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



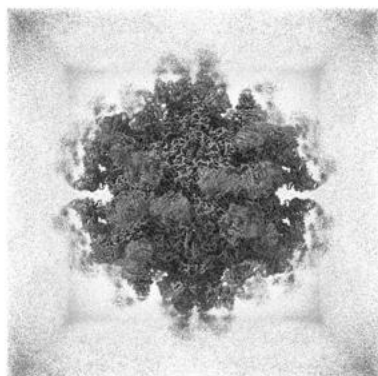
Y



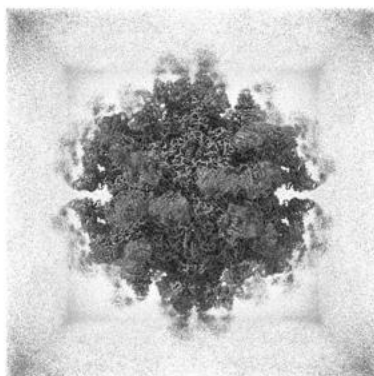
Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

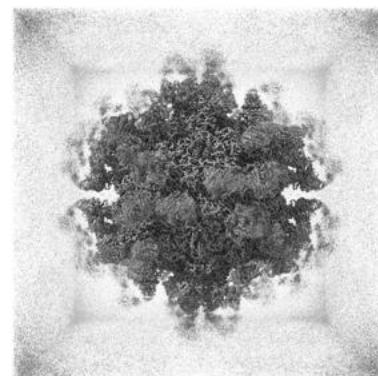
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

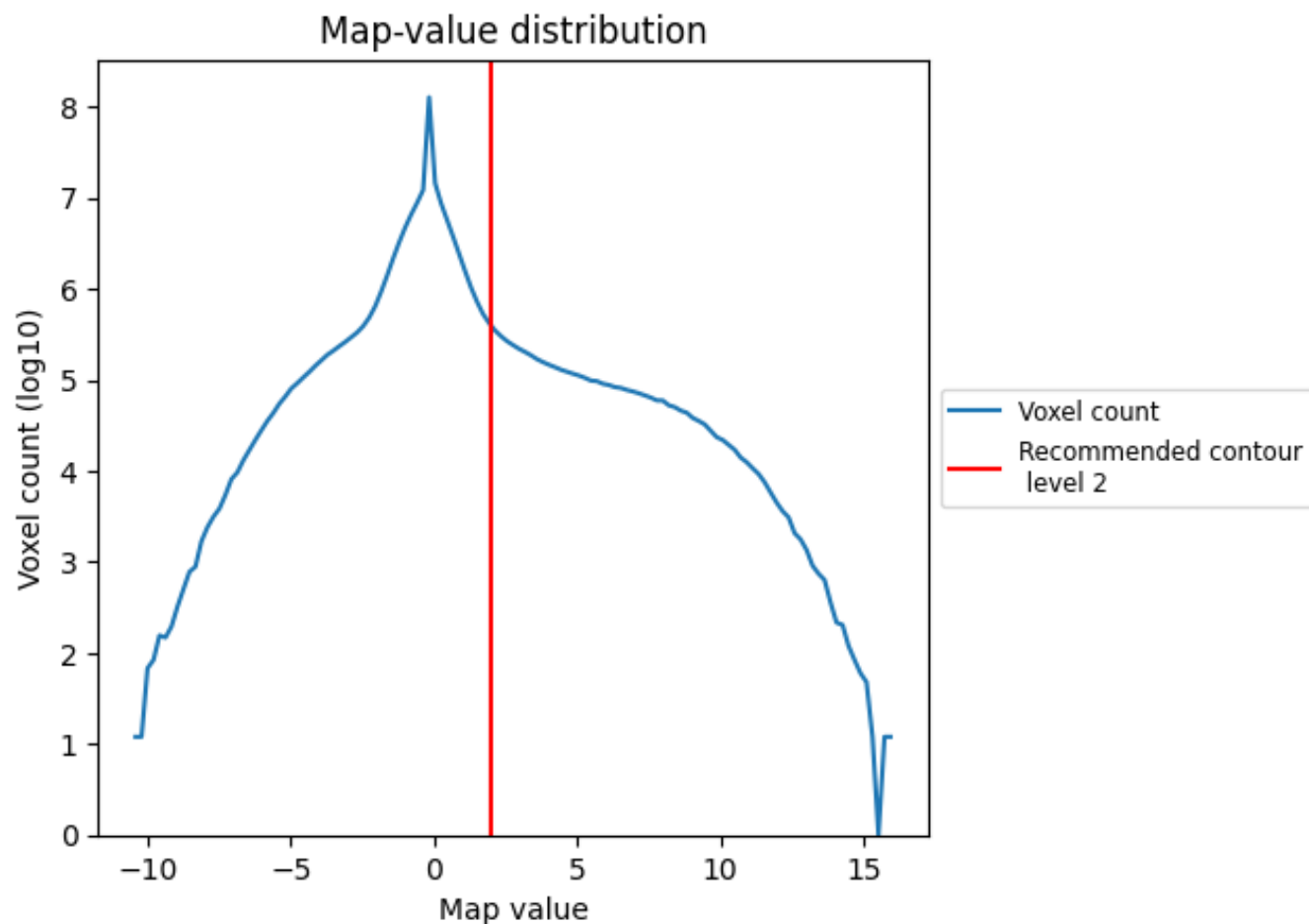
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

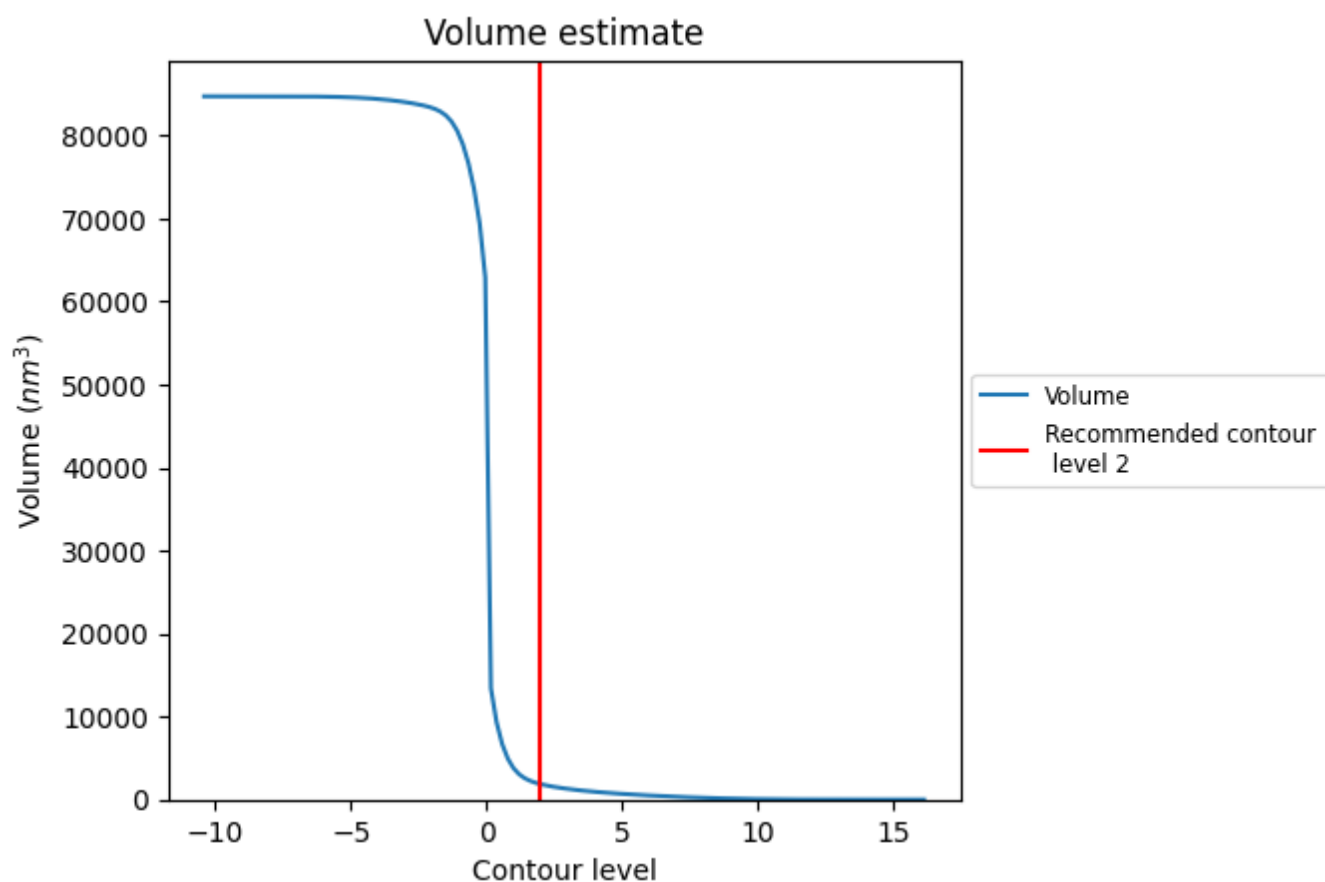
This section contains the results of statistical analysis of the map.

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.

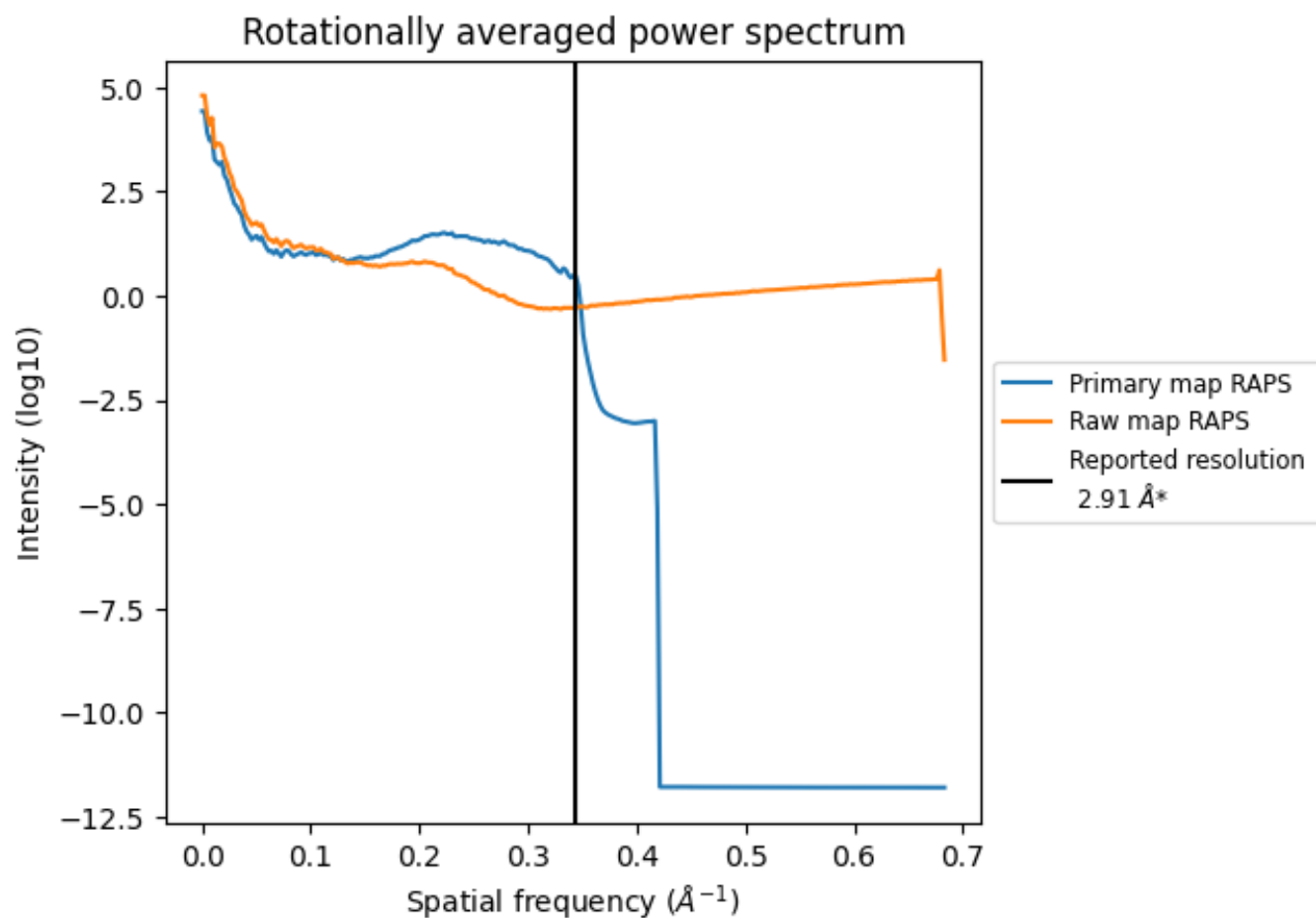
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1860 nm³; this corresponds to an approximate mass of 1680 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

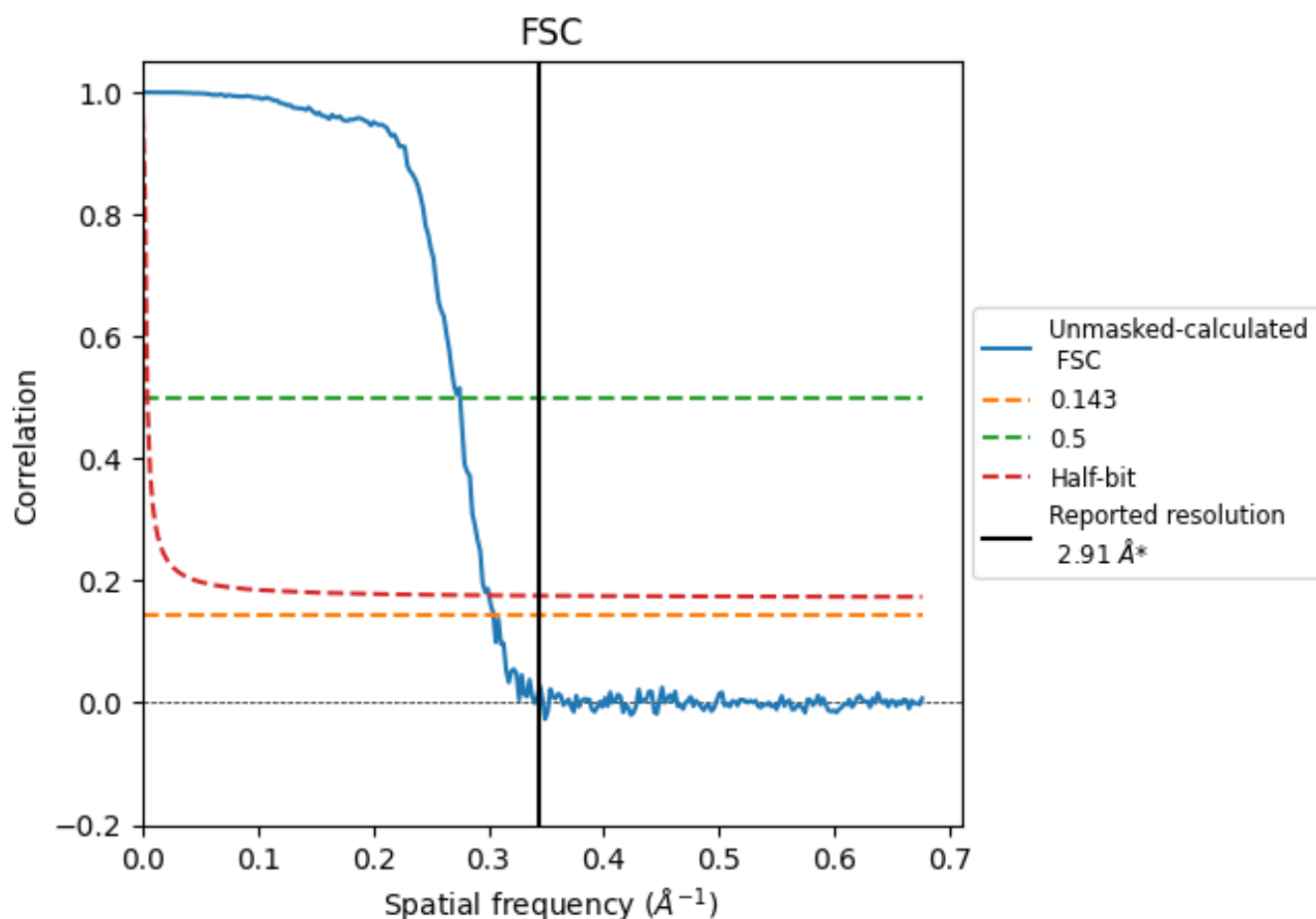


*Reported resolution corresponds to spatial frequency of $0.344 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

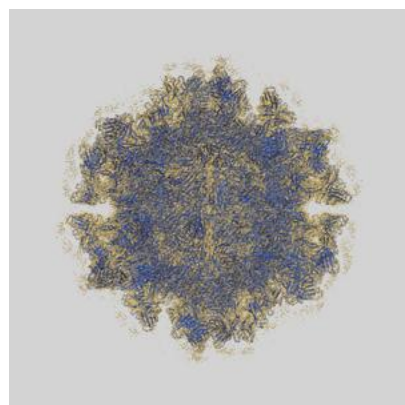
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.29	3.63	3.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.91 by more than 10 %

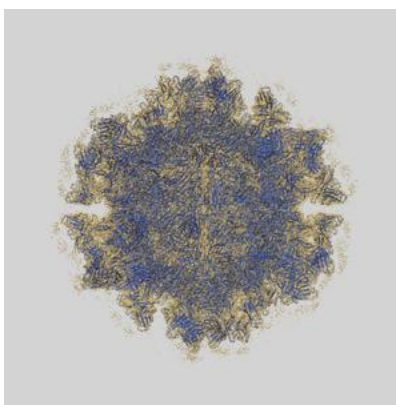
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-76772 and PDB model 12UU. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

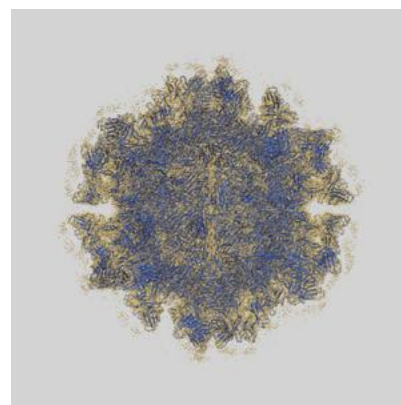
9.1 Map-model overlay [i](#)



X



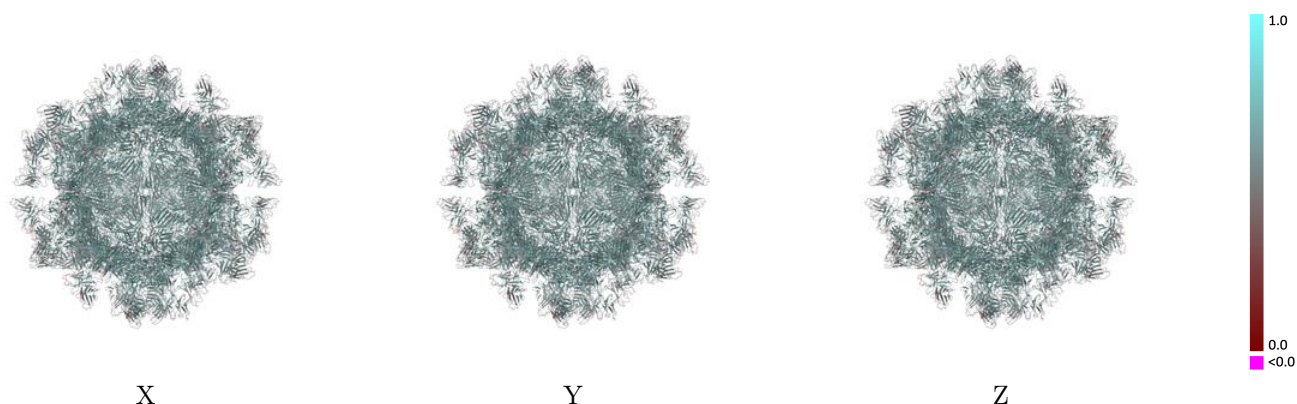
Y



Z

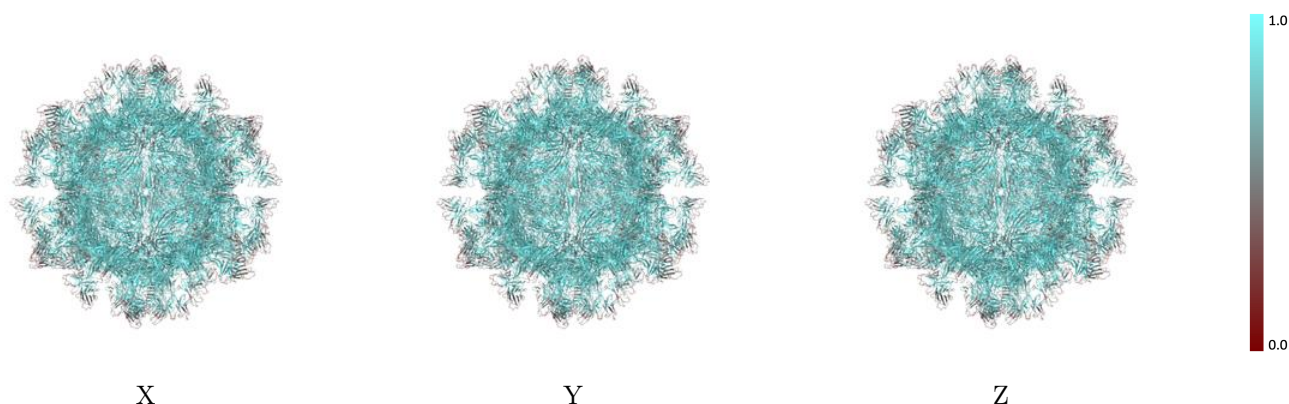
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



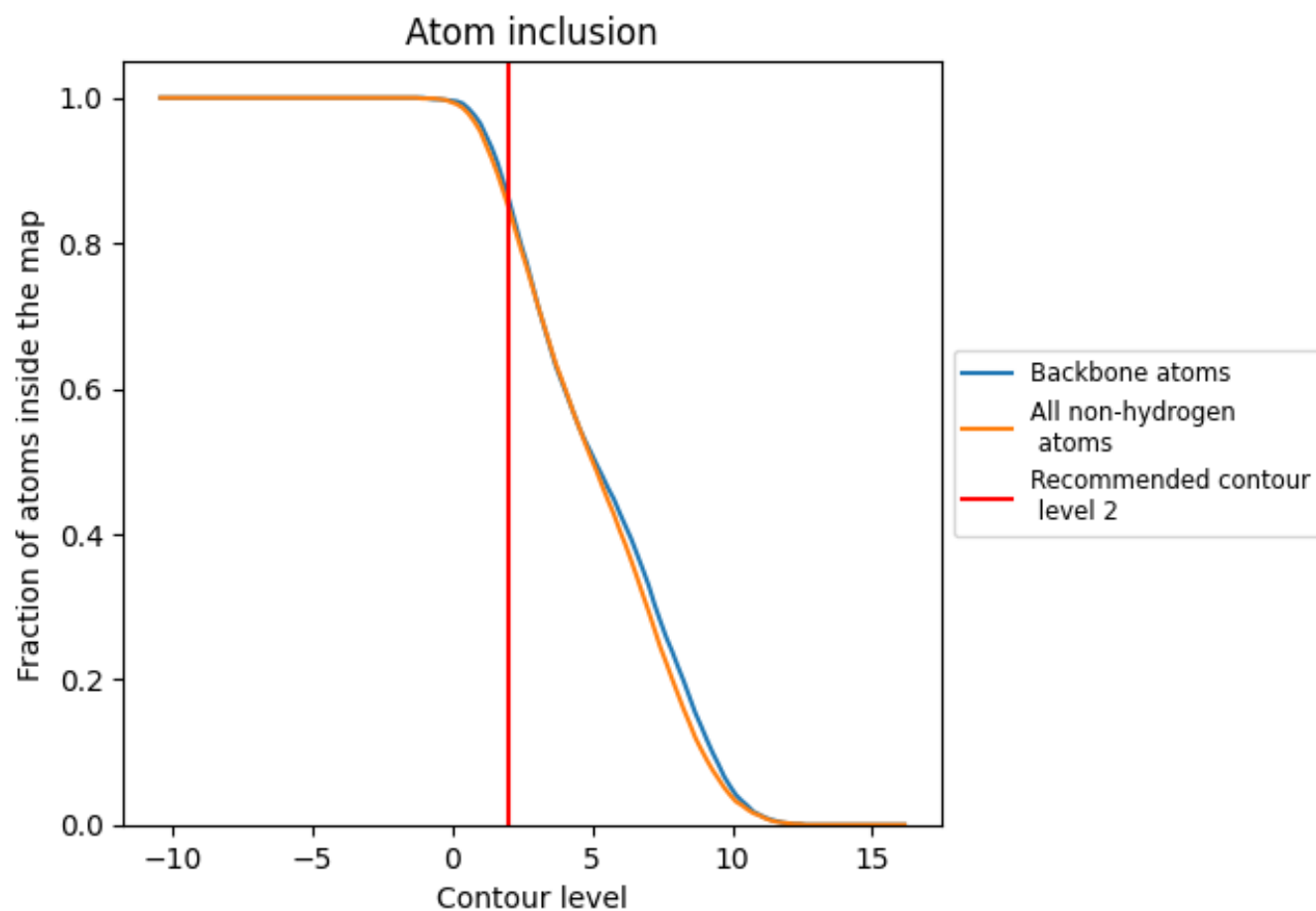
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.5940
1	 0.9370	 0.6220
1h	 0.6440	 0.5280
1l	 0.6710	 0.5390
2	 0.9370	 0.6210
2h	 0.6440	 0.5260
2l	 0.6710	 0.5370
3	 0.9370	 0.6230
3h	 0.6440	 0.5240
3l	 0.6710	 0.5380
4	 0.9370	 0.6230
4h	 0.6440	 0.5260
4l	 0.6710	 0.5380
5	 0.9370	 0.6230
5h	 0.6440	 0.5250
5l	 0.6710	 0.5390
6	 0.9370	 0.6240
6h	 0.6440	 0.5260
6l	 0.6710	 0.5400
7	 0.9360	 0.6220
7h	 0.6350	 0.5230
7l	 0.6640	 0.5350
8	 0.9360	 0.6210
8h	 0.6260	 0.5250
8l	 0.6540	 0.5380
A	 0.9380	 0.6240
Ah	 0.6440	 0.5290
Al	 0.6740	 0.5400
B	 0.9350	 0.6220
Bh	 0.6380	 0.5250
Bl	 0.6610	 0.5320
C	 0.9390	 0.6210
Ch	 0.6490	 0.5240
Cl	 0.6770	 0.5350
D	 0.9360	 0.6220



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Chain	Atom inclusion	Q-score
Dh	 0.6350	 0.5250
DI	 0.6640	 0.5350
E	 0.9350	 0.6220
Eh	 0.6260	 0.5260
El	 0.6530	 0.5360
F	 0.9370	 0.6220
Fh	 0.6440	 0.5270
Fl	 0.6710	 0.5360
G	 0.9350	 0.6220
Gh	 0.6260	 0.5250
Gl	 0.6530	 0.5360
H	 0.9370	 0.6210
Hh	 0.6350	 0.5210
HI	 0.6640	 0.5340
I	 0.9380	 0.6210
Ih	 0.6490	 0.5250
Il	 0.6770	 0.5330
J	 0.9360	 0.6220
Jh	 0.6380	 0.5280
JI	 0.6610	 0.5330
K	 0.9380	 0.6220
Kh	 0.6490	 0.5220
KI	 0.6770	 0.5350
L	 0.9360	 0.6220
Lh	 0.6380	 0.5270
LI	 0.6610	 0.5330
M	 0.9350	 0.6240
Mh	 0.6260	 0.5270
MI	 0.6530	 0.5370
N	 0.9360	 0.6230
Nh	 0.6350	 0.5220
NI	 0.6640	 0.5350
O	 0.9360	 0.6230
Oh	 0.6260	 0.5260
OI	 0.6540	 0.5350
P	 0.9370	 0.6240
Ph	 0.6350	 0.5210
PI	 0.6640	 0.5340
Q	 0.9380	 0.6240
Qh	 0.6490	 0.5220
QI	 0.6770	 0.5320
R	 0.9350	 0.6210

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Chain	Atom inclusion	Q-score
Rh	 0.6380	 0.5260
Rl	 0.6610	 0.5340
S	 0.9360	 0.6230
Sh	 0.6380	 0.5270
Sl	 0.6610	 0.5320
T	 0.9380	 0.6220
Th	 0.6490	 0.5240
Tl	 0.6770	 0.5330
U	 0.9360	 0.6220
Uh	 0.6380	 0.5270
Ul	 0.6610	 0.5310
V	 0.9390	 0.6230
Vh	 0.6490	 0.5250
Vl	 0.6770	 0.5330
W	 0.9360	 0.6240
Wh	 0.6350	 0.5270
Wl	 0.6640	 0.5340
X	 0.9350	 0.6220
Xh	 0.6260	 0.5220
Xl	 0.6530	 0.5340
Y	 0.9360	 0.6220
Yh	 0.6350	 0.5220
Yl	 0.6640	 0.5350
Z	 0.9350	 0.6210
Zh	 0.6260	 0.5240
Zl	 0.6540	 0.5410
a	 0.9390	 0.6200
ah	 0.6490	 0.5270
al	 0.6770	 0.5330
b	 0.9350	 0.6230
bh	 0.6260	 0.5240
bl	 0.6530	 0.5320
c	 0.9360	 0.6230
ch	 0.6350	 0.5220
cl	 0.6640	 0.5350
d	 0.9370	 0.6210
dh	 0.6350	 0.5210
dl	 0.6640	 0.5340
e	 0.9360	 0.6210
eh	 0.6350	 0.5250
el	 0.6640	 0.5370
f	 0.9360	 0.6200

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Chain	Atom inclusion	Q-score
fh	 0.6260	 0.5240
fl	 0.6540	 0.5380
g	 0.9380	 0.6220
gh	 0.6490	 0.5210
gl	 0.6770	 0.5300
h	 0.9370	 0.6220
hh	 0.6440	 0.5300
hl	 0.6710	 0.5400
i	 0.9350	 0.6220
ih	 0.6260	 0.5260
il	 0.6530	 0.5380
j	 0.9390	 0.6210
jh	 0.6490	 0.5220
jl	 0.6770	 0.5330
k	 0.9350	 0.6190
kh	 0.6380	 0.5250
kl	 0.6610	 0.5310
l	 0.9360	 0.6230
lh	 0.6380	 0.5290
ll	 0.6610	 0.5340
m	 0.9360	 0.6230
mh	 0.6380	 0.5240
ml	 0.6610	 0.5330
n	 0.9350	 0.6220
nh	 0.6220	 0.5280
nl	 0.6540	 0.5370
o	 0.9380	 0.6220
oh	 0.6490	 0.5230
ol	 0.6770	 0.5340
p	 0.9370	 0.6220
ph	 0.6440	 0.5260
pl	 0.6710	 0.5370
q	 0.9350	 0.6220
qh	 0.6260	 0.5250
ql	 0.6530	 0.5360
r	 0.9380	 0.6240
rh	 0.6490	 0.5220
rl	 0.6770	 0.5330
s	 0.9370	 0.6220
sh	 0.6440	 0.5300
sl	 0.6710	 0.5370
t	 0.9360	 0.6220

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Chain	Atom inclusion	Q-score
th	 0.6380	 0.5280
tl	 0.6610	 0.5330
u	 0.9350	 0.6200
uh	 0.6380	 0.5280
ul	 0.6610	 0.5330
v	 0.9360	 0.6210
vh	 0.6380	 0.5260
vl	 0.6610	 0.5340
w	 0.9370	 0.6220
wh	 0.6440	 0.5270
wl	 0.6710	 0.5370
x	 0.9380	 0.6220
xh	 0.6490	 0.5230
xl	 0.6770	 0.5330
y	 0.9370	 0.6220
yh	 0.6350	 0.5220
yl	 0.6640	 0.5340
z	 0.9360	 0.6220
zh	 0.6350	 0.5260
zl	 0.6620	 0.5340