



wwPDB EM Validation Summary Report ⓘ

Sep 21, 2026 – 05:05 PM EDT

PDB ID : 12UT / pdb_000012ut
EMDB ID : EMD-76771
Title : The AAV2 capsid in complex with IgA-Fab#3-2
Authors : Zachery, J.; Mietzsch, M.; McKenna, R.
Deposited on : 2026-04-20
Resolution : 2.48 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:

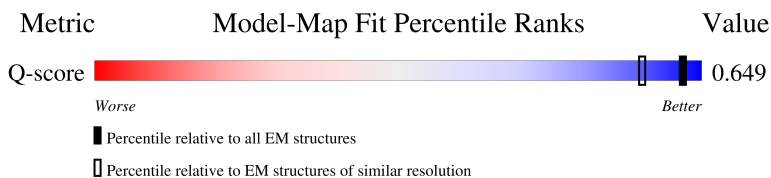
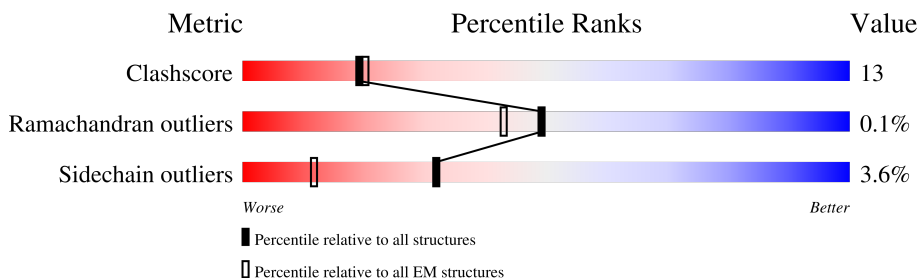
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.48 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.



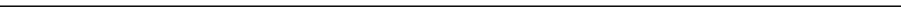
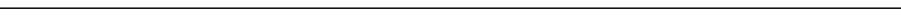
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6178 (1.98 - 2.98)

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

Mol	Chain	Length	Quality of chain
1	0	533	84% 12% ..
1	1	533	84% 12% ..
1	2	533	85% 12% ..
1	3	533	85% 12% ..

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Mol	Chain	Length	Quality of chain
1	4	533	 85% 12% ..
1	5	533	 84% 12% ..
1	6	533	 84% 12% ..
1	7	533	 85% 12% ..
1	A	533	 84% 12% ..
1	B	533	 85% 12% ..
1	C	533	 84% 12% ..
1	D	533	 85% 12% ..
1	E	533	 85% 12% ..
1	F	533	 84% 12% ..
1	G	533	 85% 12% ..
1	H	533	 84% 12% ..
1	I	533	 85% 12% ..
1	J	533	 85% 12% ..
1	K	533	 84% 12% ..
1	L	533	 85% 12% ..
1	M	533	 84% 12% ..
1	N	533	 84% 12% ..
1	O	533	 85% 12% ..
1	P	533	 84% 12% ..
1	Q	533	 85% 11% ..
1	R	533	 85% 12% ..
1	S	533	 85% 12% ..
1	T	533	 85% 12% ..
1	U	533	 85% 12% ..

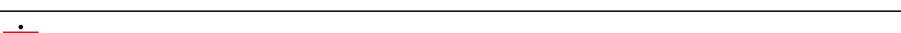
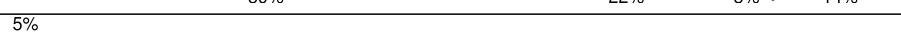
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Mol	Chain	Length	Quality of chain
1	V	533	 85% 12% ..
1	W	533	 85% 12% ..
1	X	533	 85% 12% ..
1	Y	533	 85% 12% ..
1	Z	533	 85% 11% ..
1	a	533	 85% 12% ..
1	b	533	 84% 12% ..
1	c	533	 84% 12% ..
1	d	533	 85% 12% ..
1	e	533	 84% 12% ..
1	f	533	 85% 12% ..
1	g	533	 85% 12% ..
1	h	533	 85% 12% ..
1	i	533	 85% 12% ..
1	j	533	 85% 12% ..
1	k	533	 85% 12% ..
1	l	533	 85% 12% ..
1	m	533	 84% 12% ..
1	n	533	 84% 13% ..
1	o	533	 85% 12% ..
1	p	533	 85% 11% ..
1	q	533	 85% 12% ..
1	r	533	 85% 11% ..
1	s	533	 85% 12% ..
1	t	533	 85% 12% ..

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Mol	Chain	Length	Quality of chain
1	u	533	 84% 12% . .
1	v	533	 85% 12% . .
1	w	533	 85% 12% . .
1	x	533	 84% 12% . .
1	y	533	 85% 11% . .
1	z	533	 85% 12% . .
2	0h	153	 5% 59% 22% 5% . 14%
2	1h	153	 5% 59% 22% 5% . 14%
2	2h	153	 5% 59% 22% 5% . 14%
2	3h	153	 5% 58% 24% 5% . 14%
2	4h	153	 5% 58% 24% 5% . 14%
2	5h	153	 5% 57% 24% 5% . 14%
2	6h	153	 5% 59% 22% 5% . 14%
2	7h	153	 5% 58% 23% 5% . 14%
2	Ah	153	 5% 59% 22% 5% . 14%
2	Bh	153	 5% 58% 24% 5% . 14%
2	Ch	153	 5% 57% 24% 5% . 14%
2	Dh	153	 5% 59% 22% 5% . 14%
2	Eh	153	 7% 59% 22% 5% . 14%
2	Fh	153	 7% 59% 22% 5% . 14%
2	Gh	153	 7% 57% 24% 5% . 14%
2	Hh	153	 5% 58% 23% 5% . 14%
2	Ih	153	 5% 58% 23% 5% . 14%
2	Jh	153	 5% 59% 22% 5% . 14%
2	Kh	153	 5% 59% 22% 5% . 14%

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Mol	Chain	Length	Quality of chain
2	Lh	153	
2	Mh	153	
2	Nh	153	
2	Oh	153	
2	Ph	153	
2	Qh	153	
2	Rh	153	
2	Sh	153	
2	Th	153	
2	Uh	153	
2	Vh	153	
2	Wh	153	
2	Xh	153	
2	Yh	153	
2	Zh	153	
2	ah	153	
2	bh	153	
2	ch	153	
2	dh	153	
2	eh	153	
2	fh	153	
2	gh	153	
2	hh	153	
2	ih	153	
2	jh	153	

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Mol	Chain	Length	Quality of chain
2	kh	153	
2	lh	153	
2	mh	153	
2	nh	153	
2	oh	153	
2	ph	153	
2	qh	153	
2	rh	153	
2	sh	153	
2	th	153	
2	uh	153	
2	vh	153	
2	wh	153	
2	xh	153	
2	yh	153	
2	zh	153	
3	0l	130	
3	1l	130	
3	2l	130	
3	3l	130	
3	4l	130	
3	5l	130	
3	6l	130	
3	7l	130	
3	Al	130	

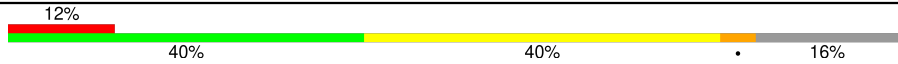
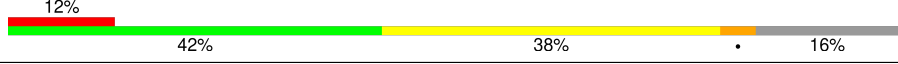
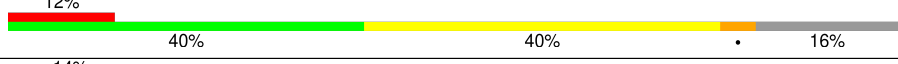
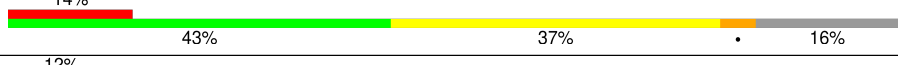
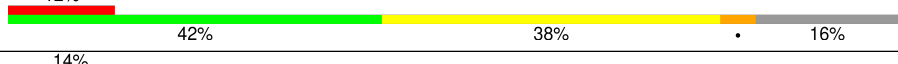
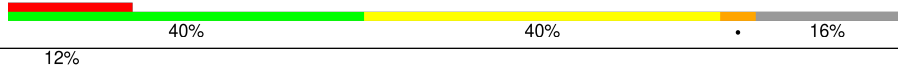
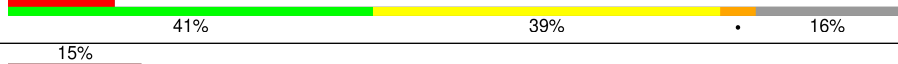
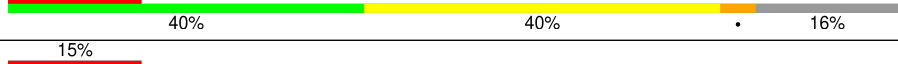
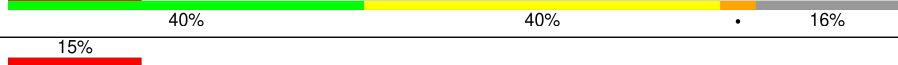
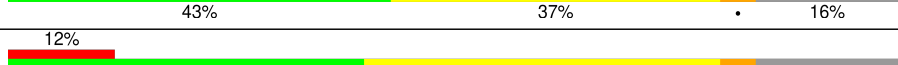
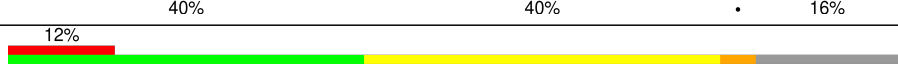
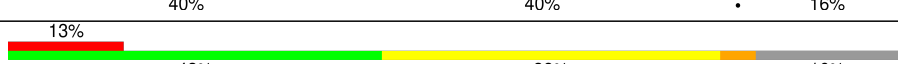
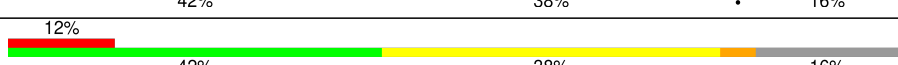
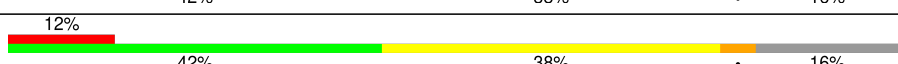
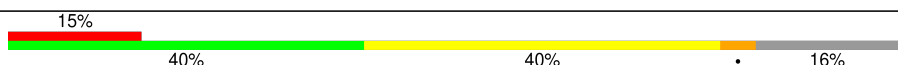
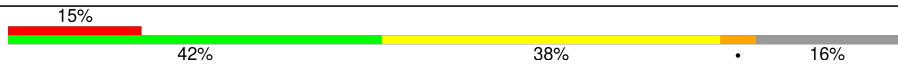
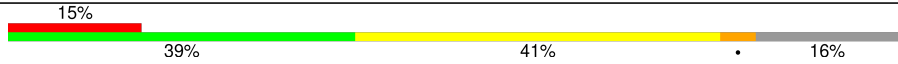
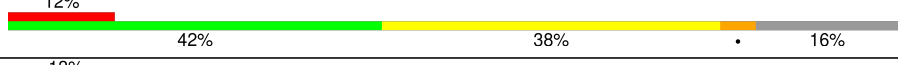
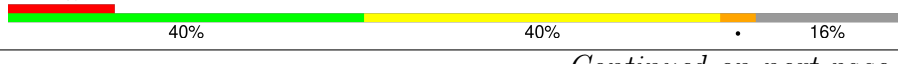
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Mol	Chain	Length	Quality of chain
3	B1	130	
3	C1	130	
3	D1	130	
3	E1	130	
3	F1	130	
3	G1	130	
3	H1	130	
3	I1	130	
3	J1	130	
3	K1	130	
3	L1	130	
3	M1	130	
3	N1	130	
3	O1	130	
3	P1	130	
3	Q1	130	
3	R1	130	
3	S1	130	
3	T1	130	
3	U1	130	
3	V1	130	
3	W1	130	
3	X1	130	
3	Y1	130	
3	Z1	130	

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Mol	Chain	Length	Quality of chain
3	al	130	
3	bl	130	
3	cl	130	
3	dl	130	
3	el	130	
3	fl	130	
3	gl	130	
3	hl	130	
3	il	130	
3	jl	130	
3	kl	130	
3	ll	130	
3	ml	130	
3	nl	130	
3	ol	130	
3	pl	130	
3	ql	130	
3	rl	130	
3	sl	130	
3	tl	130	
3	ul	130	
3	vl	130	
3	wl	130	
3	xl	130	
3	yl	130	

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Mol	Chain	Length	Quality of chain
3	zl	130	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 358500 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	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	B	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	C	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	D	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	E	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	F	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	G	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	H	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	I	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	J	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	K	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	L	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	M	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	N	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	O	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	P	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		
1	Q	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	S	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	T	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	U	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	V	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	W	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	X	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	Y	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	Z	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	a	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	b	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	c	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	d	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	e	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	f	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	g	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	h	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	i	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	j	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	k	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	l	518	Total 4148	C 2610	N 724	O 801	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	n	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	o	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	p	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	q	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	r	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	s	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	t	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	u	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	v	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	w	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	x	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	y	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	z	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	0	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	1	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	2	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	3	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	4	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	5	518	Total 4148	C 2610	N 724	O 801	S 13	0	0
1	6	518	Total 4148	C 2610	N 724	O 801	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	518	Total	C	N	O	S	0	0
			4148	2610	724	801	13		

- Molecule 2 is a protein called IgA-Fab3-2 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ah	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Bh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Ch	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Dh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Eh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Fh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Gh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Hh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Ih	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Jh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Kh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Lh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Mh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Nh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Oh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Ph	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Qh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Rh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Sh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Th	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Uh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Vh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Wh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Xh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Yh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	Zh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	ah	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	bh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	ch	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	dh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	eh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	fh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	gh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	hh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	ih	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	jh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	kh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	lh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	mh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	nh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	oh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	ph	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	qh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	rh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	sh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	th	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	uh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	vh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	wh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	xh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	yh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	zh	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	0h	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	1h	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	2h	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	3h	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	4h	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	5h	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	6h	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		
2	7h	132	Total	C	N	O	S	0	0
			1028	659	169	198	2		

- Molecule 3 is a protein called IgA-Fab3-2 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Al	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Bl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Cl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Dl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	El	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Fl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Gl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Hl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Il	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Jl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Kl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Ll	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Ml	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Nl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Ol	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Pl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Ql	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Rl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Sl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Tl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Ul	109	Total 799	C 494	N 134	O 167	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Vl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Wl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Xl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Yl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	Zl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	al	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	bl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	cl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	dl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	el	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	fl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	gl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	hl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	il	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	jl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	kl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	ll	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	ml	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	nl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	ol	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	pl	109	Total 799	C 494	N 134	O 167	S 4	0	0

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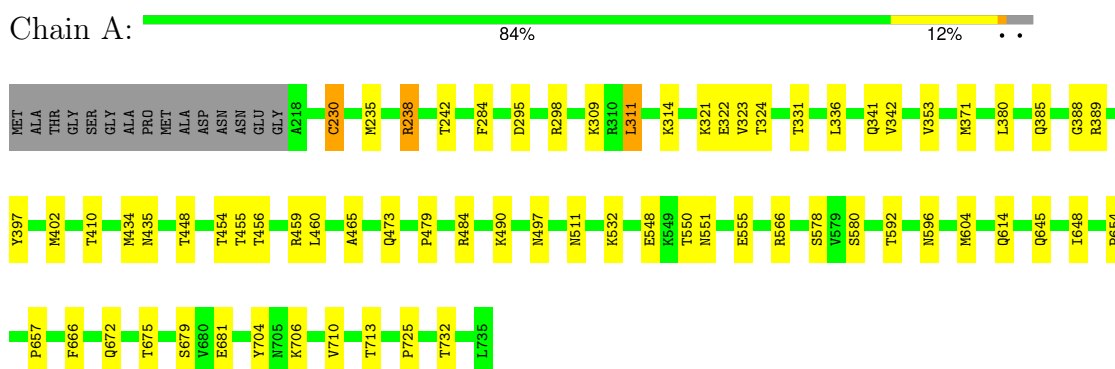
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Mol	Chain	Residues	Atoms					AltConf	Trace
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3	rl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	sl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	tl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	ul	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	vl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	wl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	xl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	yl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	zl	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	0l	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	1l	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	2l	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	3l	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	4l	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	5l	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	6l	109	Total 799	C 494	N 134	O 167	S 4	0	0
3	7l	109	Total 799	C 494	N 134	O 167	S 4	0	0

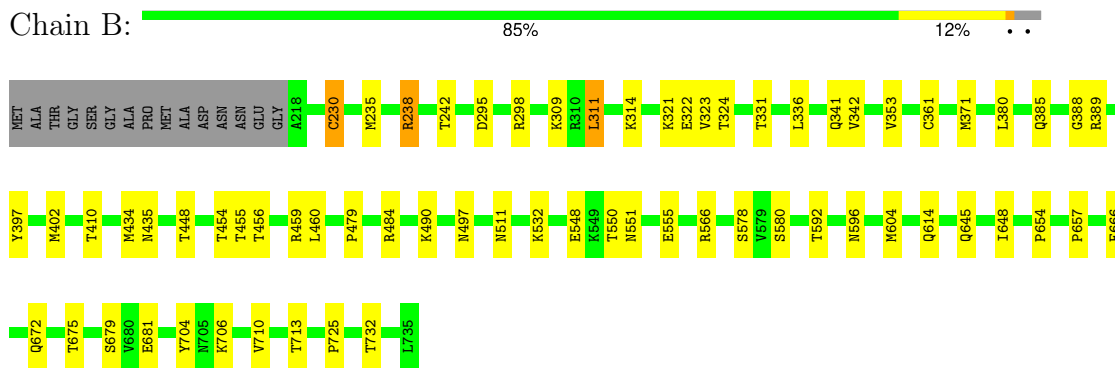
3 Residue-property plots

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.

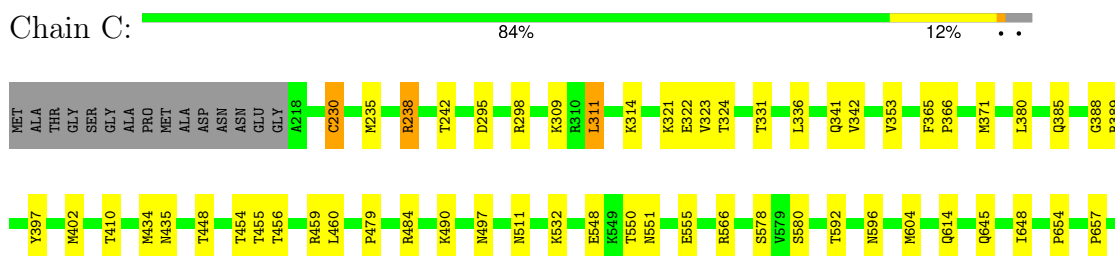
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



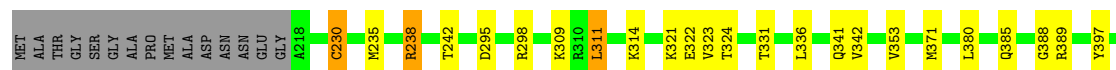
- Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1

Chain D: 85% 12% ..



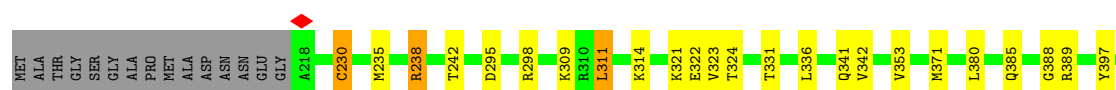
• Molecule 1: Capsid protein VP1

Chain E: 85% 12% ..



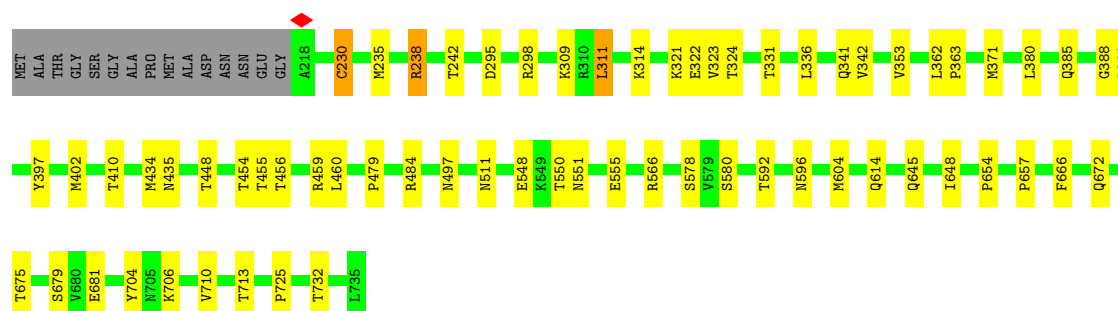
• Molecule 1: Capsid protein VP1

Chain F: 84% 12% ..



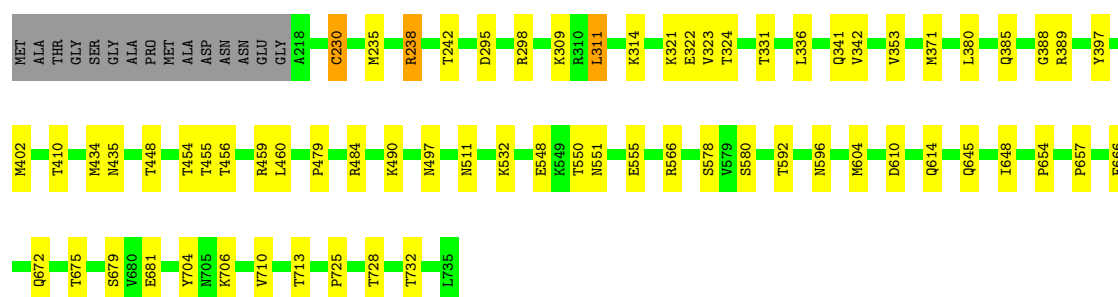
• Molecule 1: Capsid protein VP1

Chain G: 85% 12% ..



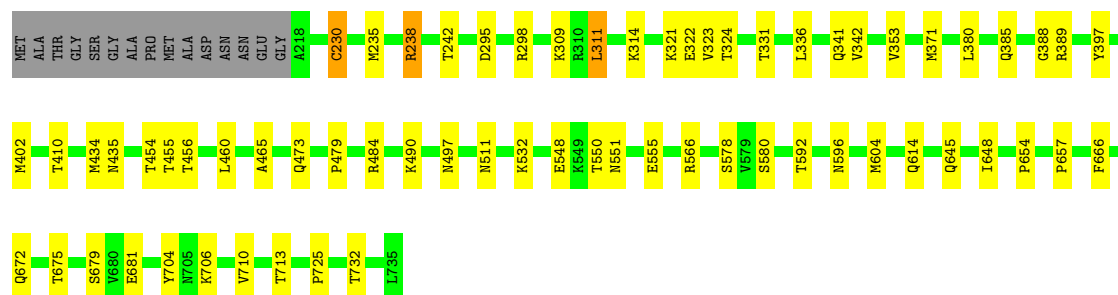
- Molecule 1: Capsid protein VP1

Chain H: 84% 12% ..



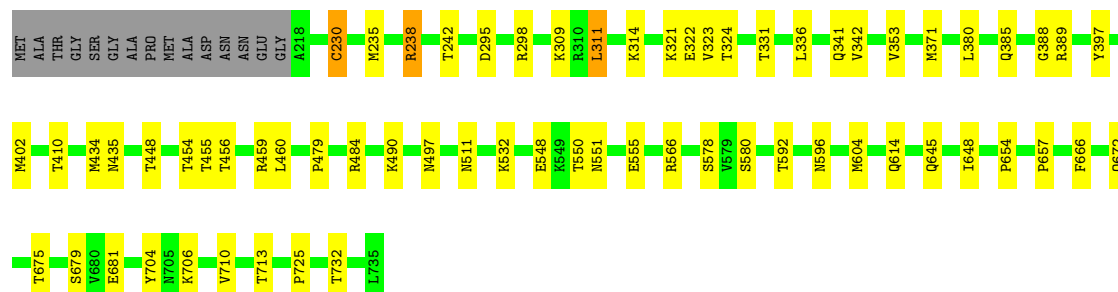
- Molecule 1: Capsid protein VP1

Chain I: 85% 12% ..

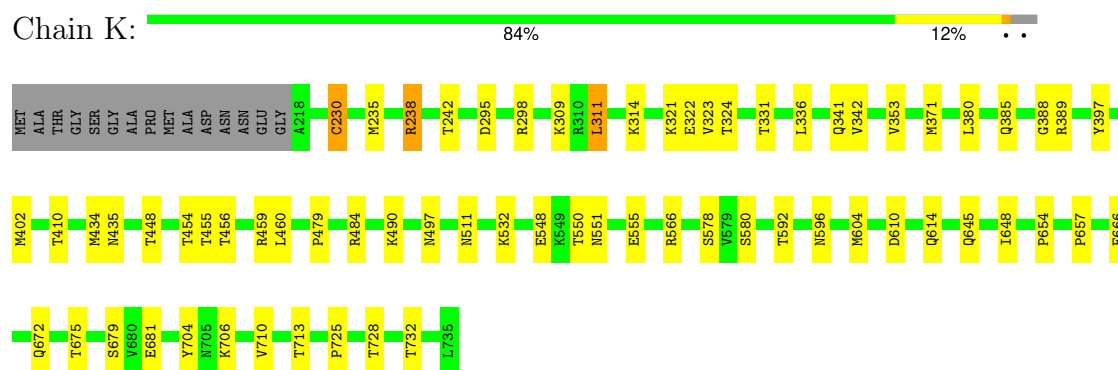


- Molecule 1: Capsid protein VP1

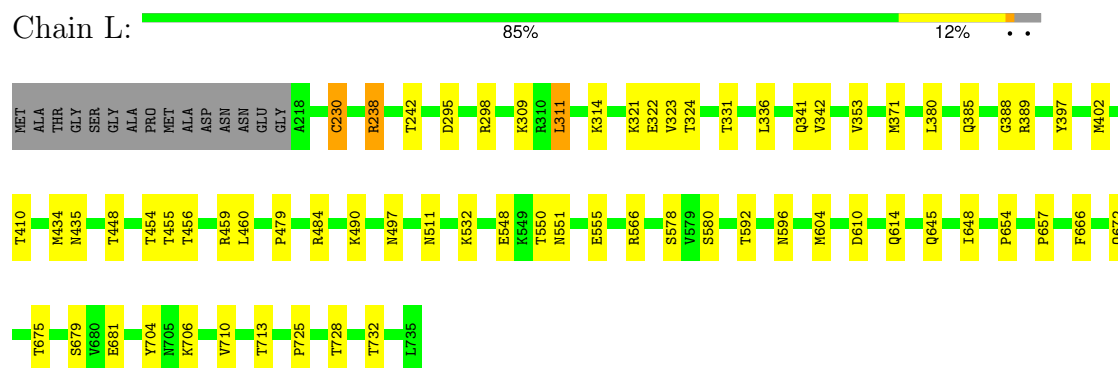
Chain J: 85% 12% ..



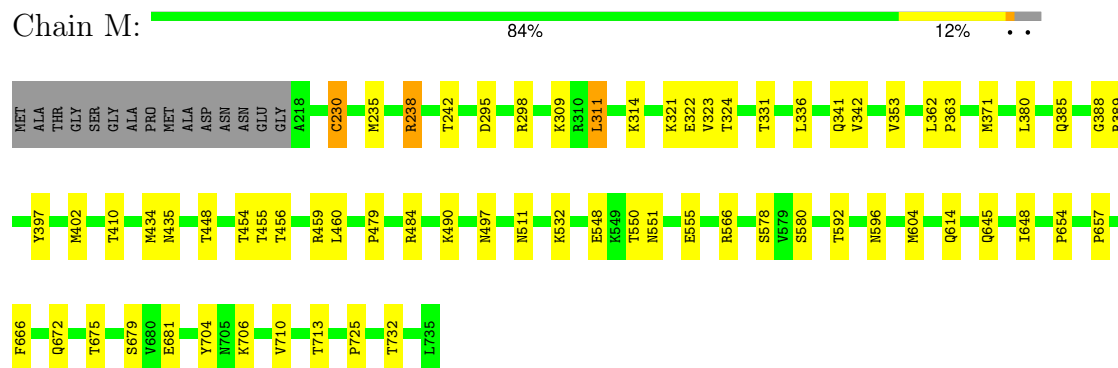
- Molecule 1: Capsid protein VP1



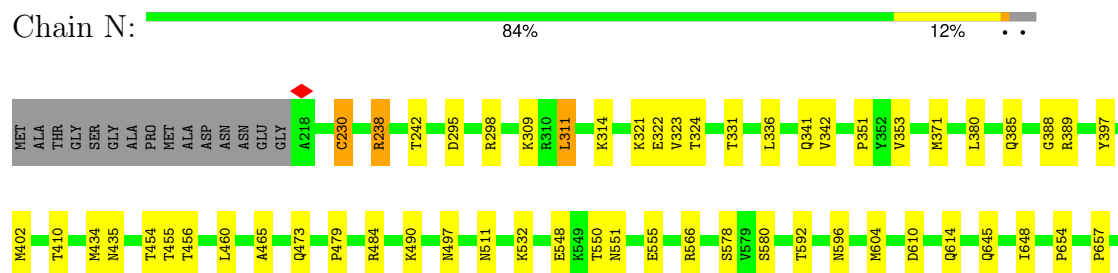
- Molecule 1: Capsid protein VP1

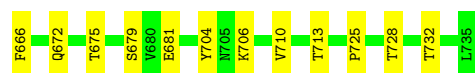


- Molecule 1: Capsid protein VP1



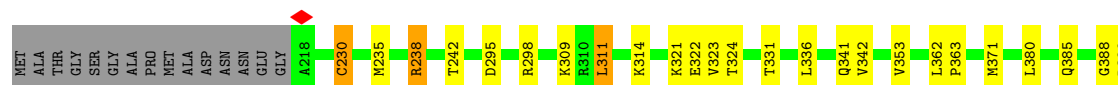
- Molecule 1: Capsid protein VP1





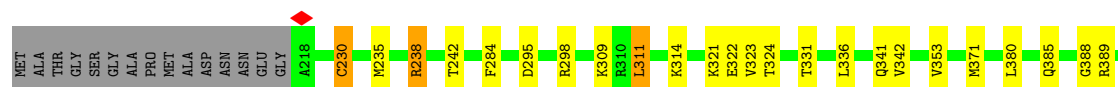
• Molecule 1: Capsid protein VP1

Chain O: 85% 12% ..



• Molecule 1: Capsid protein VP1

Chain P: 84% 12% ..



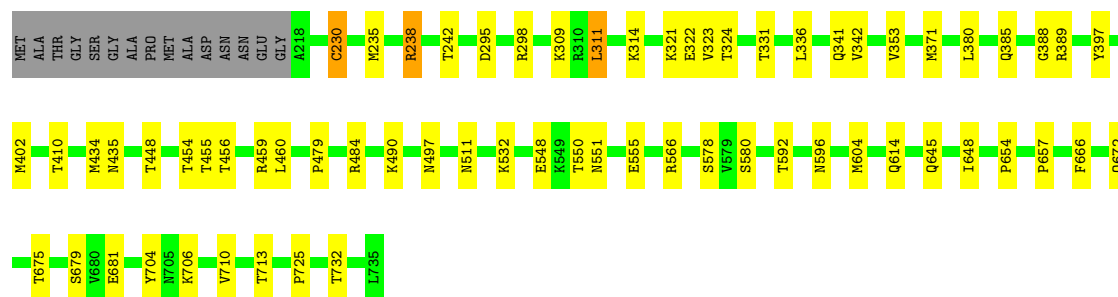
• Molecule 1: Capsid protein VP1

Chain Q: 85% 11% ..



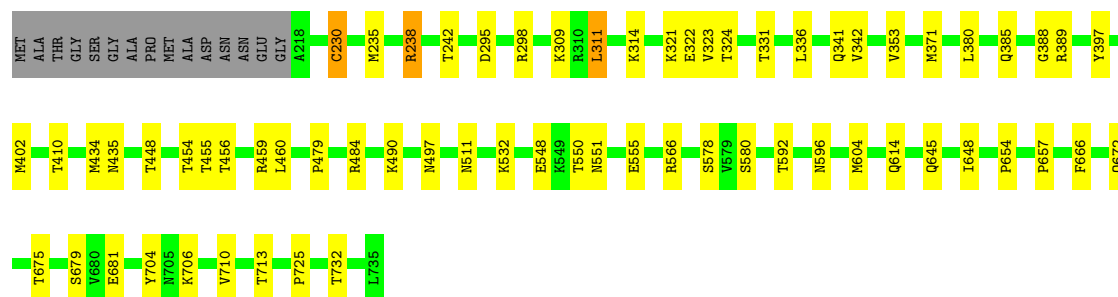
• Molecule 1: Capsid protein VP1

Chain R: 85% 12% ..



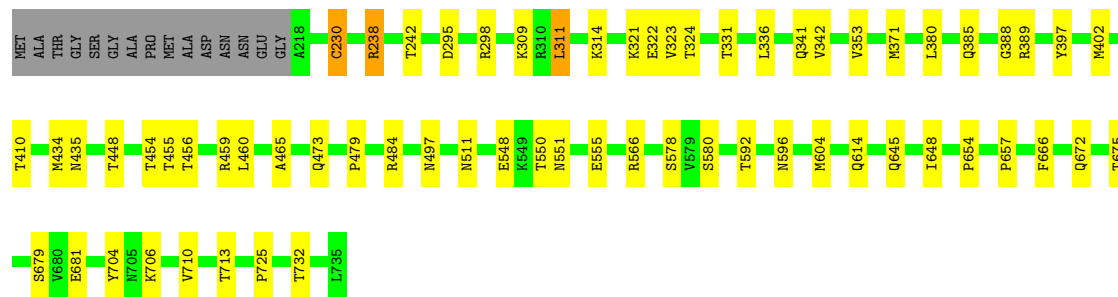
- Molecule 1: Capsid protein VP1

Chain S: 85% 12% ..



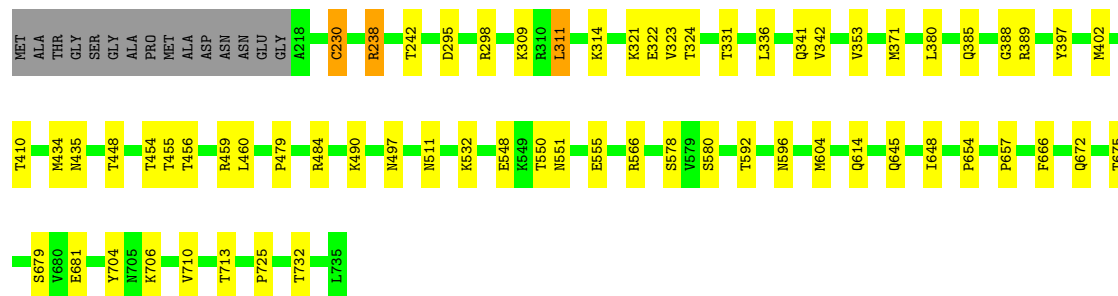
- Molecule 1: Capsid protein VP1

Chain T: 85% 12% ..



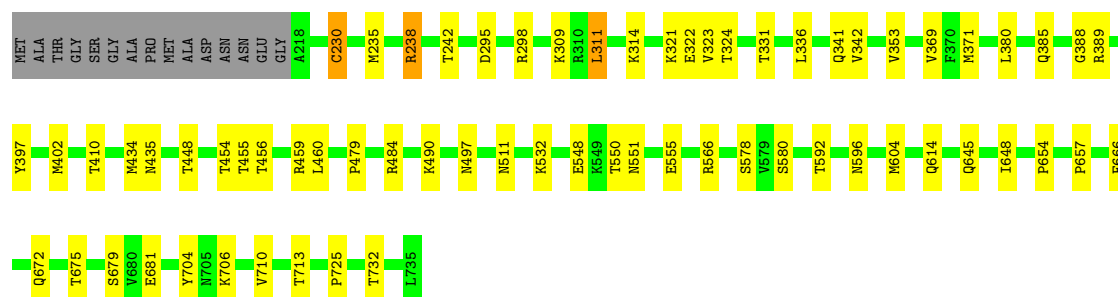
- Molecule 1: Capsid protein VP1

Chain U: 85% 12% ..



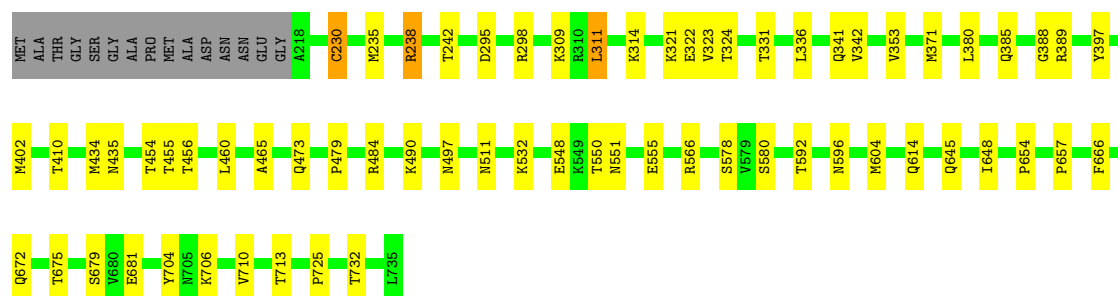
- Molecule 1: Capsid protein VP1

Chain V:  85% 12% ..



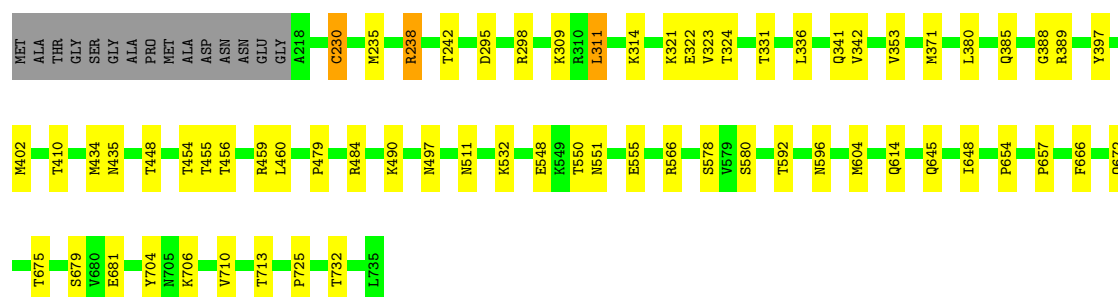
• Molecule 1: Capsid protein VP1

Chain W:  85% 12% ..



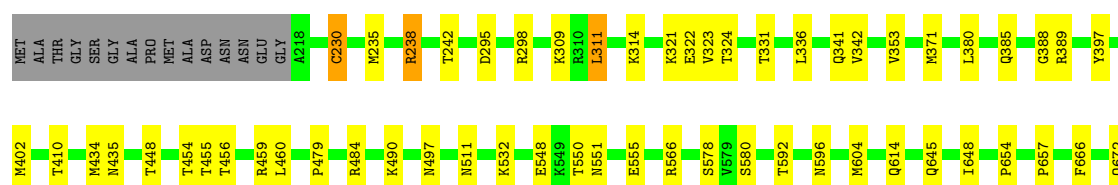
• Molecule 1: Capsid protein VP1

Chain X:  85% 12% ..



• Molecule 1: Capsid protein VP1

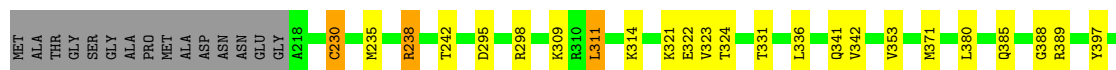
Chain Y:  85% 12% ..





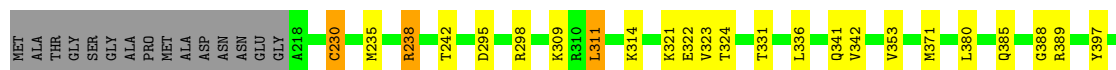
- Molecule 1: Capsid protein VP1

Chain Z: 85% 11% ..



- Molecule 1: Capsid protein VP1

Chain a: 85% 12% ..



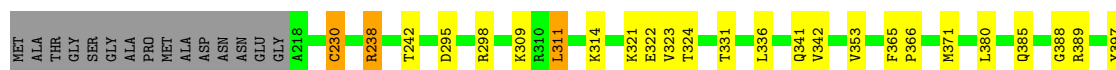
- Molecule 1: Capsid protein VP1

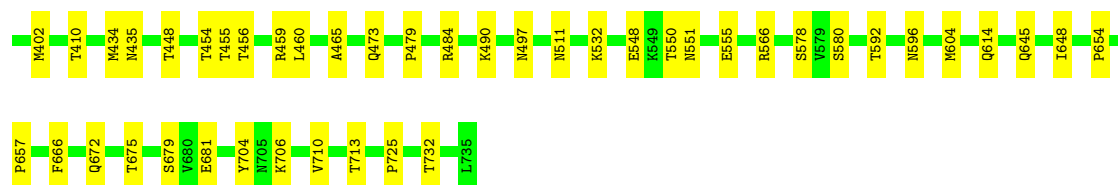
Chain b: 84% 12% ..



- Molecule 1: Capsid protein VP1

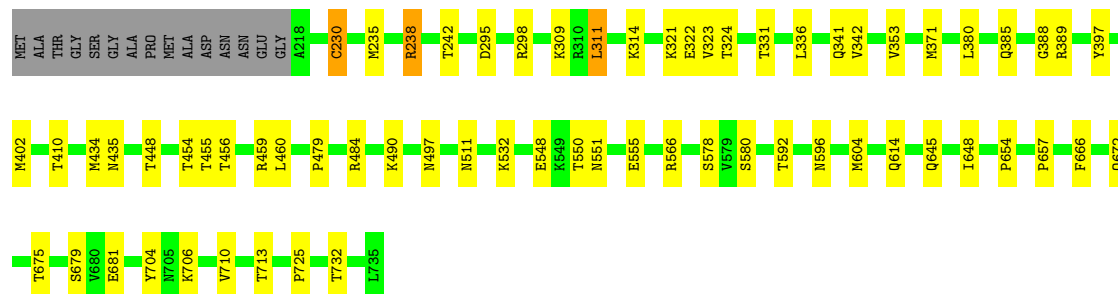
Chain c: 84% 12% ..





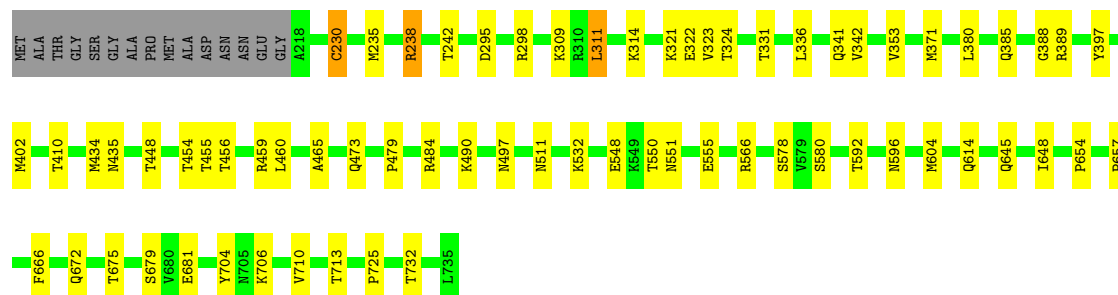
• Molecule 1: Capsid protein VP1

Chain d: 85% 12% ..



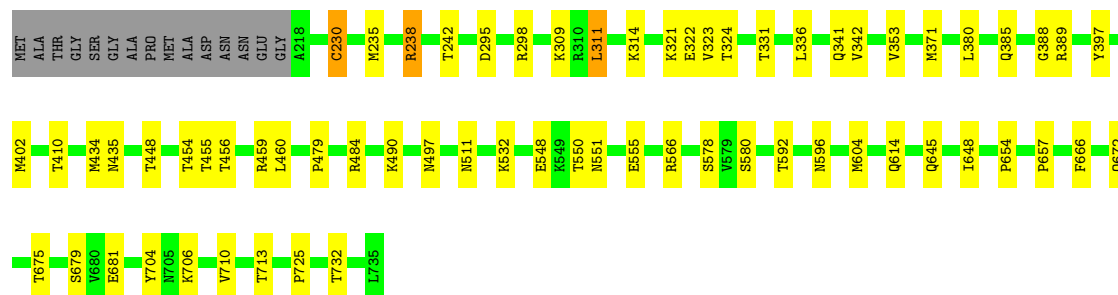
• Molecule 1: Capsid protein VP1

Chain e: 84% 12% ..



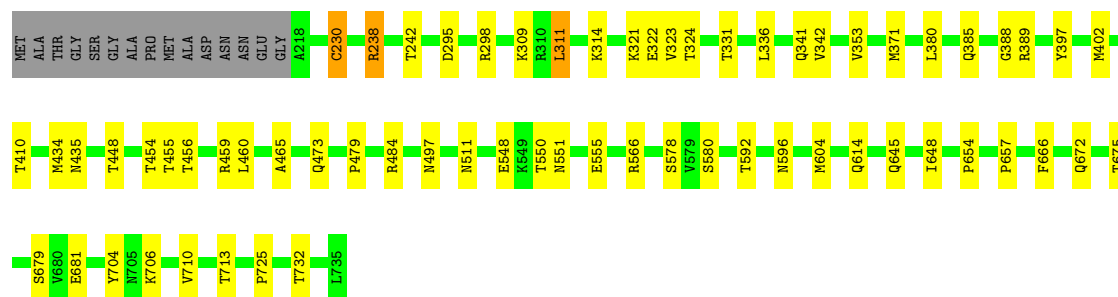
• Molecule 1: Capsid protein VP1

Chain f: 85% 12% ..



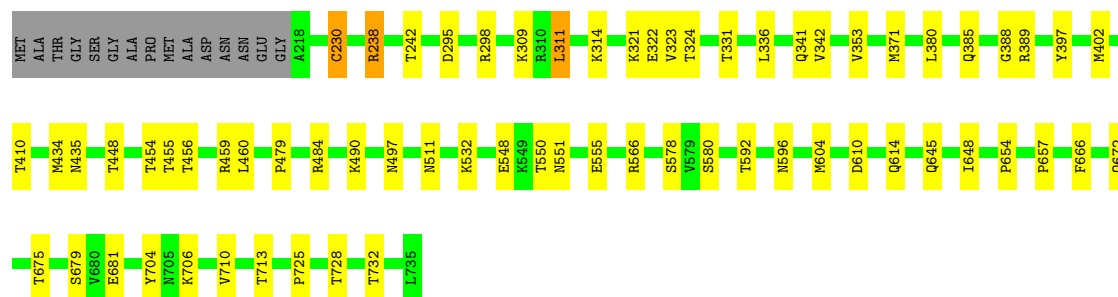
• Molecule 1: Capsid protein VP1

Chain g: 85% 12% ..



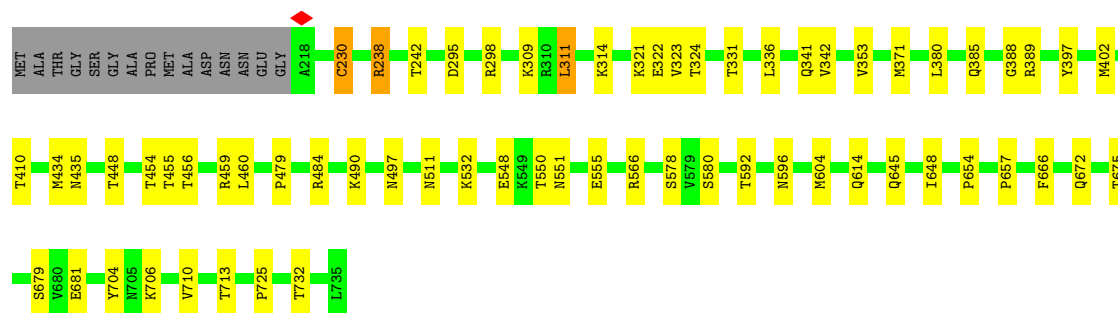
- Molecule 1: Capsid protein VP1

Chain h: 85% 12% ..



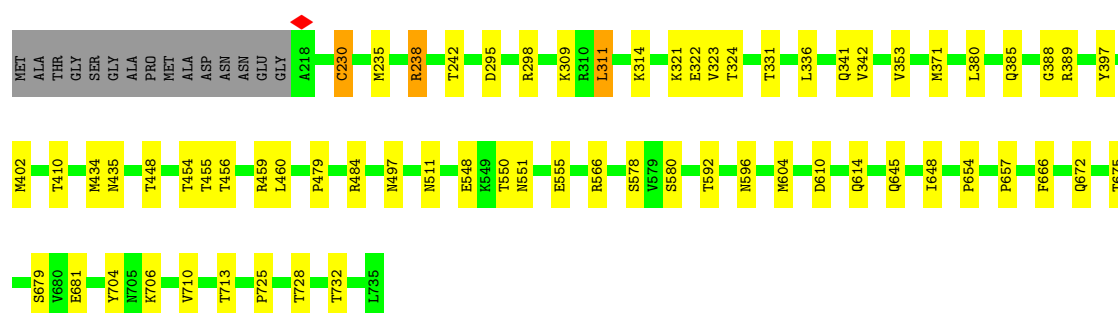
- Molecule 1: Capsid protein VP1

Chain i: 85% 12% ..

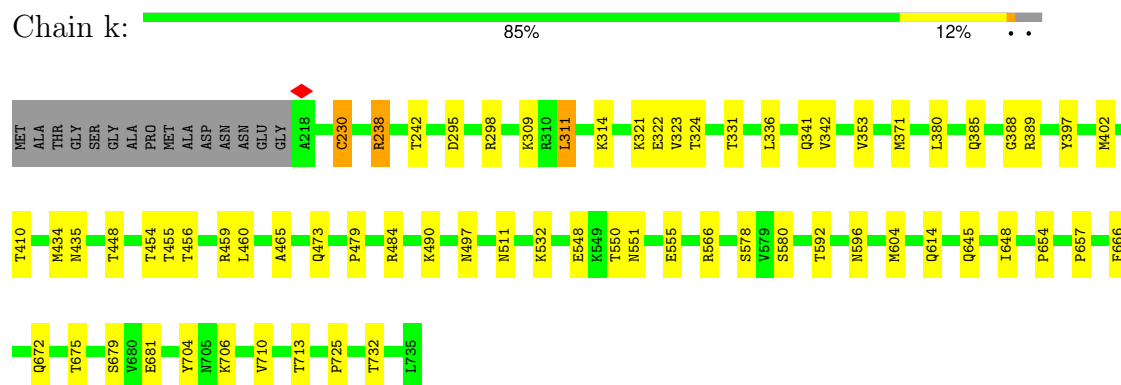


- Molecule 1: Capsid protein VP1

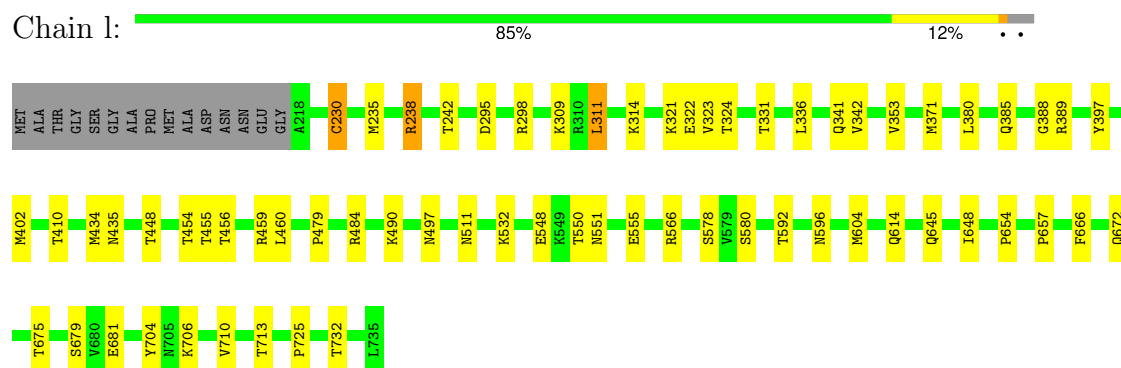
Chain j: 85% 12% ..



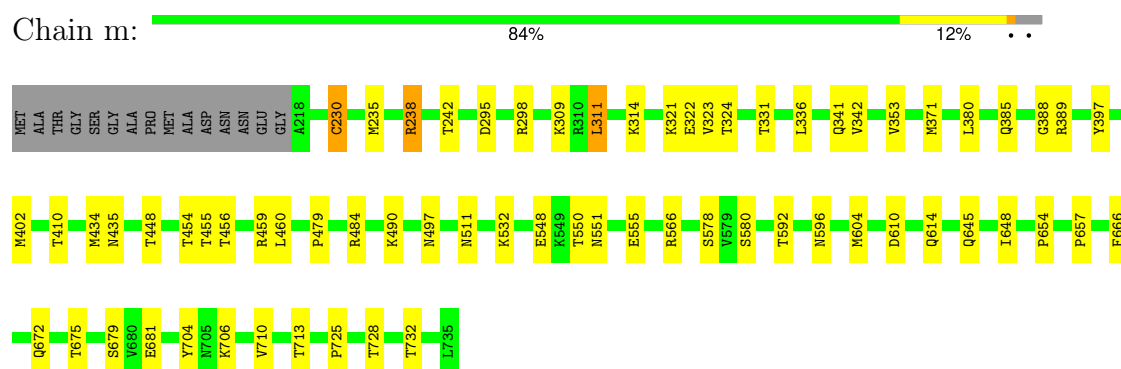
• Molecule 1: Capsid protein VP1



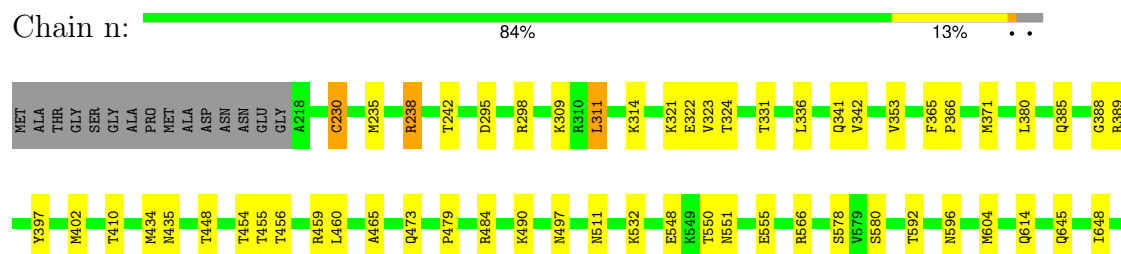
• Molecule 1: Capsid protein VP1

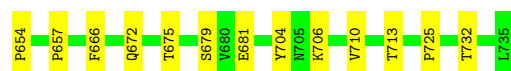


• Molecule 1: Capsid protein VP1



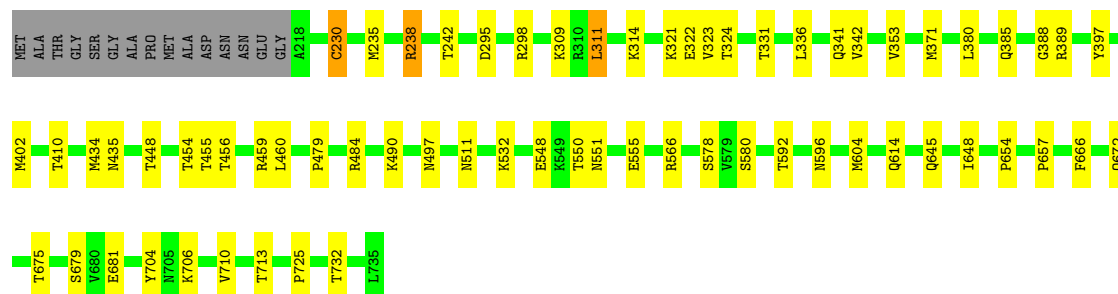
• Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1

Chain o: 85% 12% ..



• Molecule 1: Capsid protein VP1

Chain p: 85% 11% ..



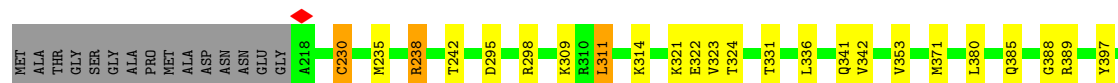
• Molecule 1: Capsid protein VP1

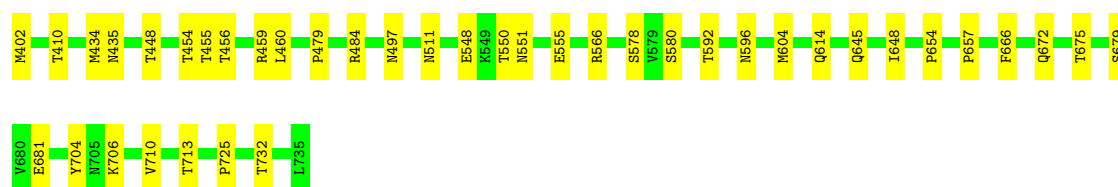
Chain q: 85% 12% ..



• Molecule 1: Capsid protein VP1

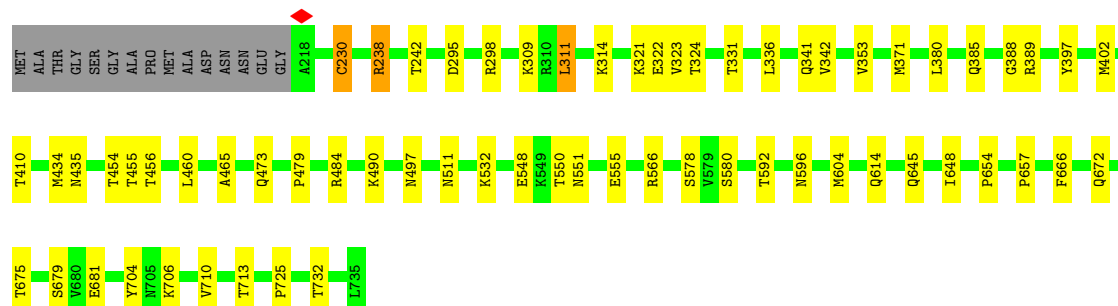
Chain r: 85% 11% ..





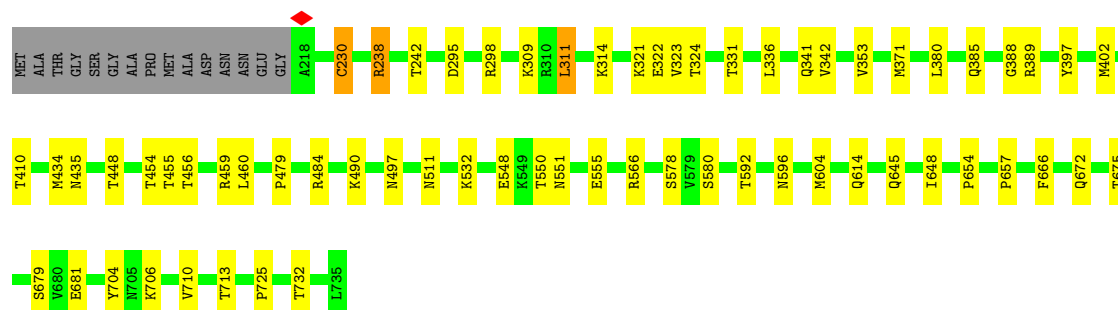
- Molecule 1: Capsid protein VP1

Chain s: 85% 12% ..



- Molecule 1: Capsid protein VP1

Chain t: 85% 12% ..



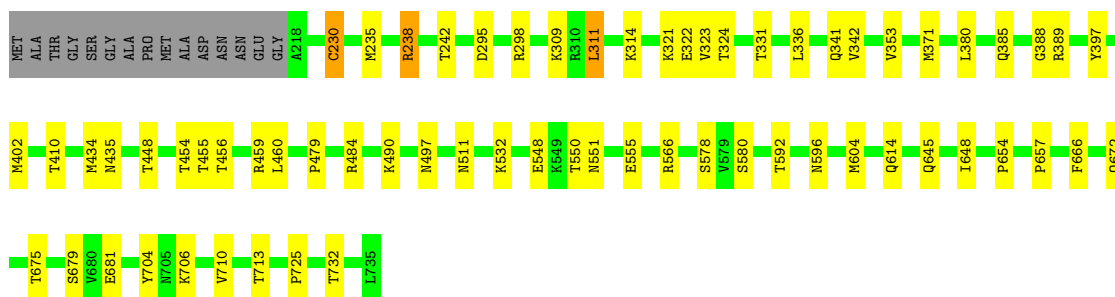
- Molecule 1: Capsid protein VP1

Chain u: 84% 12% ..



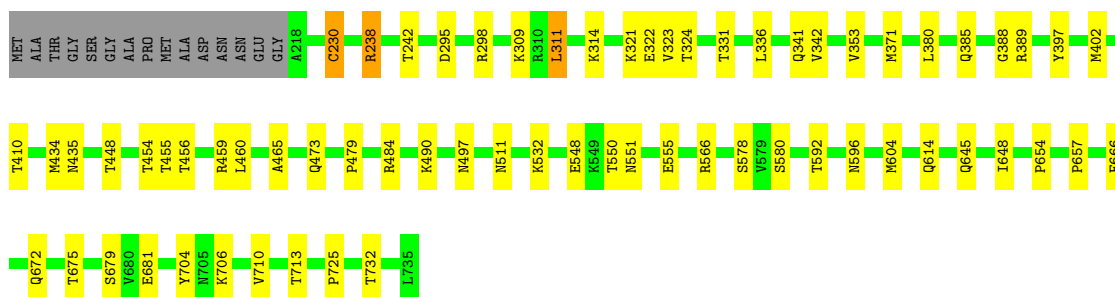
- Molecule 1: Capsid protein VP1

Chain v: 85% 12% ..



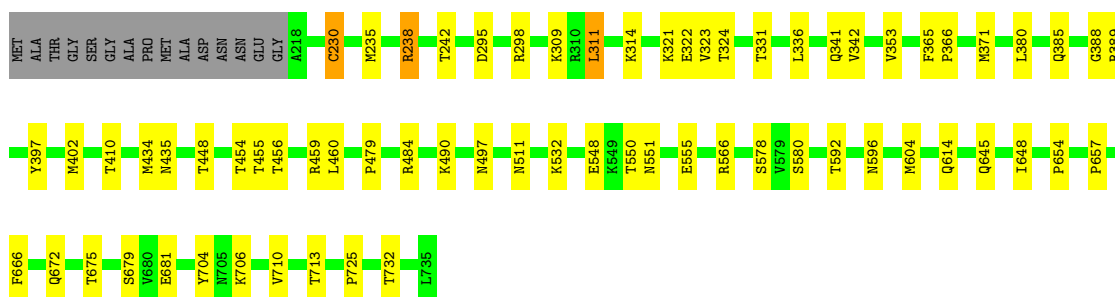
- Molecule 1: Capsid protein VP1

Chain w: 85% 12% . .



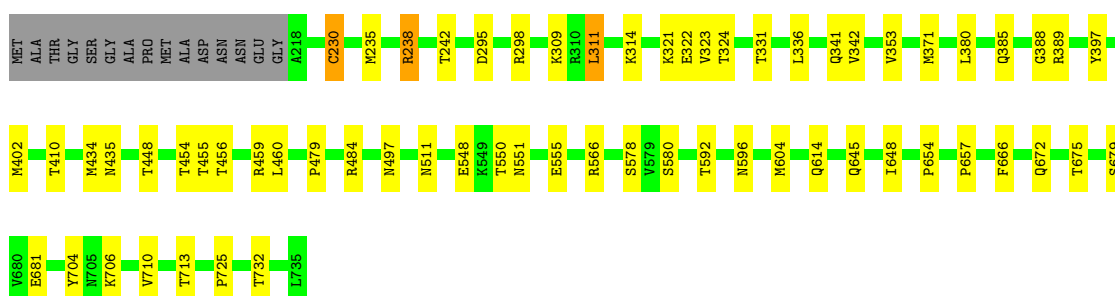
- Molecule 1: Capsid protein VP1

Chain x: 84% 12% . .



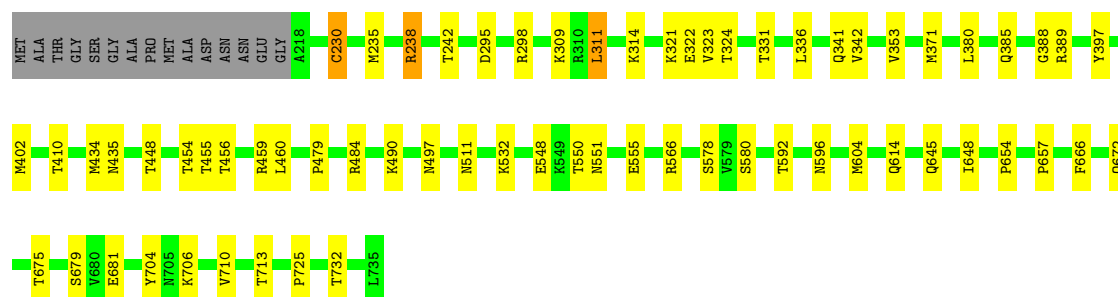
- Molecule 1: Capsid protein VP1

Chain y: 85% 11% . .



- Molecule 1: Capsid protein VP1

Chain z:  85% 12% ..



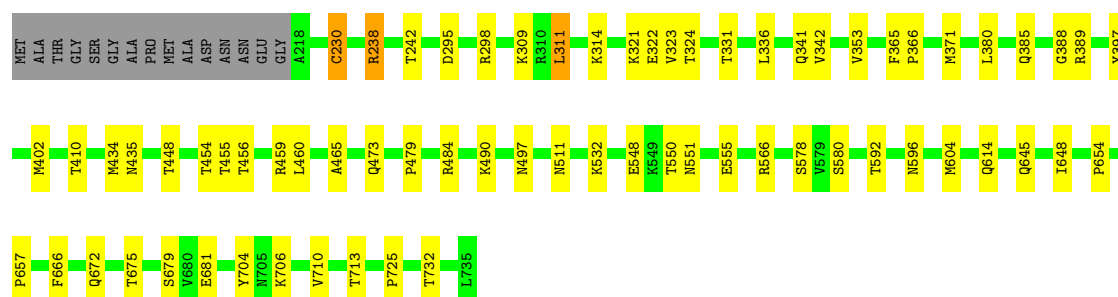
• Molecule 1: Capsid protein VP1

Chain 0:  84% 12% ..



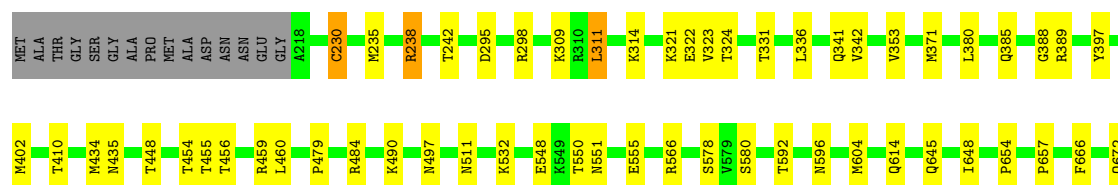
• Molecule 1: Capsid protein VP1

Chain 1:  84% 12% ..



• Molecule 1: Capsid protein VP1

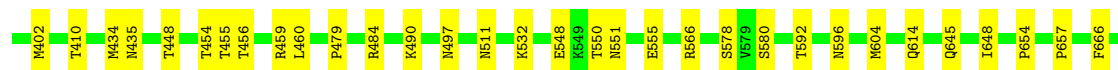
Chain 2:  85% 12% ..





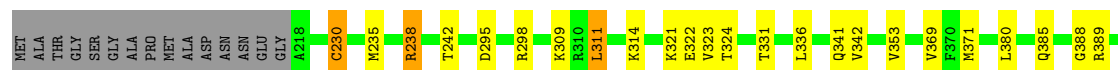
- Molecule 1: Capsid protein VP1

Chain 3: 85% 12% ..



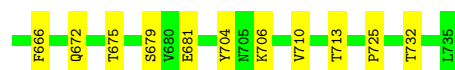
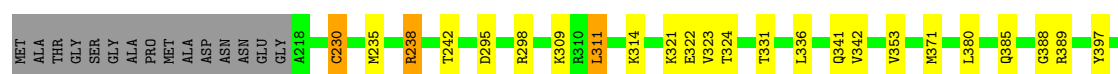
- Molecule 1: Capsid protein VP1

Chain 4: 85% 12% ..



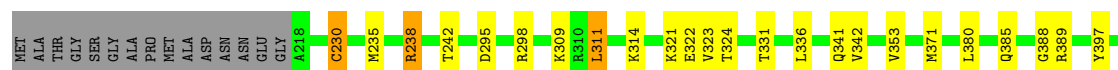
- Molecule 1: Capsid protein VP1

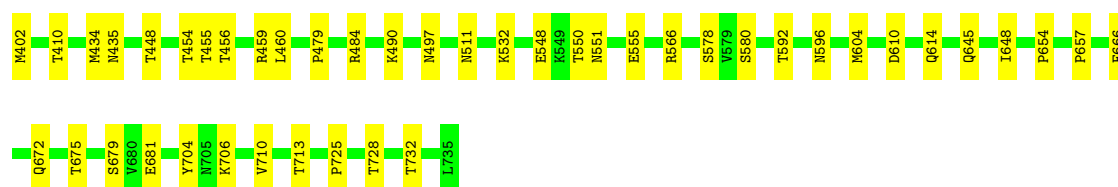
Chain 5: 84% 12% ..



- Molecule 1: Capsid protein VP1

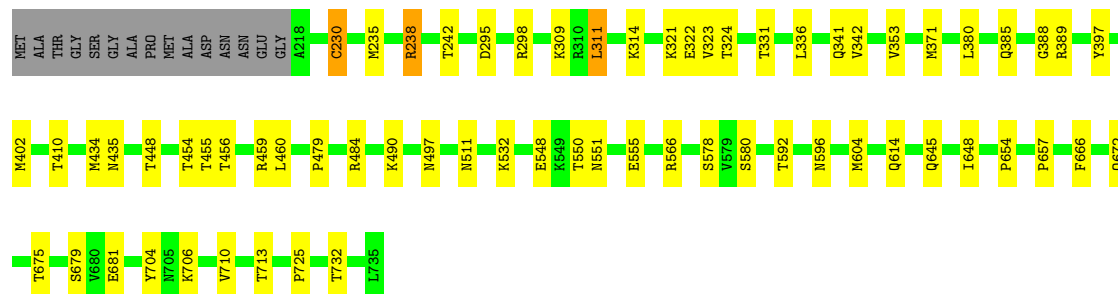
Chain 6: 84% 12% ..





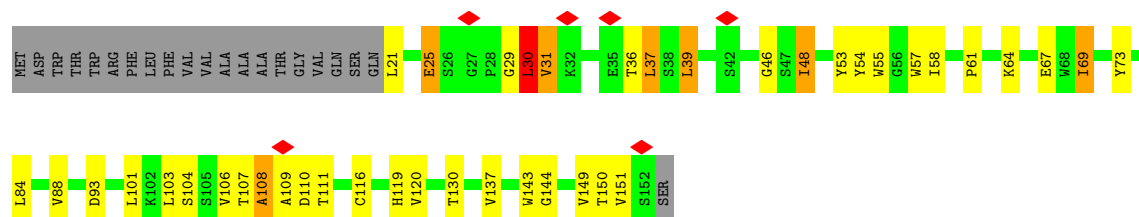
• Molecule 1: Capsid protein VP1

Chain 7: 85% 12% ..



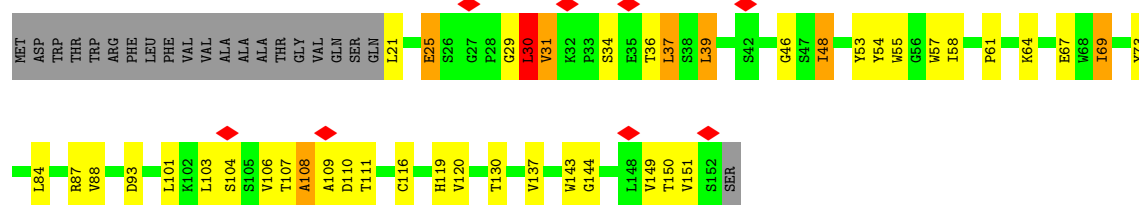
• Molecule 2: IgA-Fab3-2 Heavy chain

Chain Ah: 59% 22% 5% • 14%



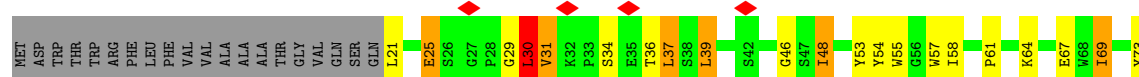
• Molecule 2: IgA-Fab3-2 Heavy chain

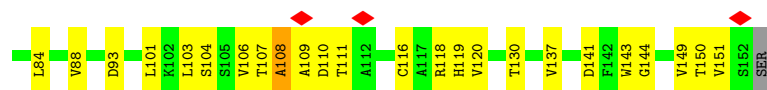
Chain Bh: 5% 58% 24% 5% • 14%



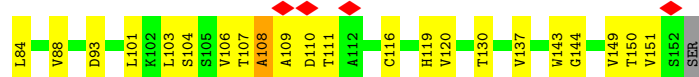
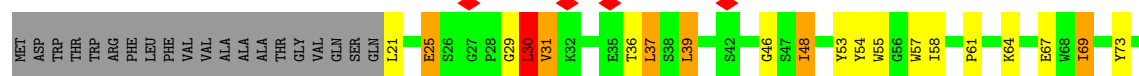
• Molecule 2: IgA-Fab3-2 Heavy chain

Chain Ch: 5% 57% 24% 5% • 14%

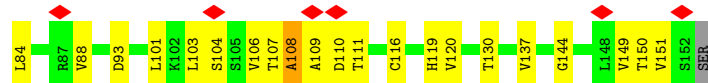




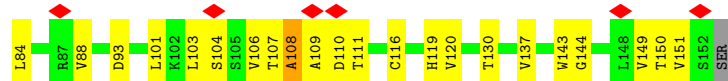
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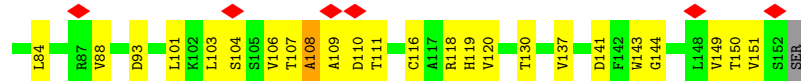
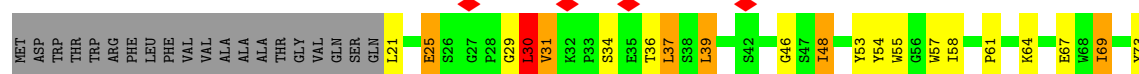
• Molecule 2: IgA-Fab3-2 Heavy chain



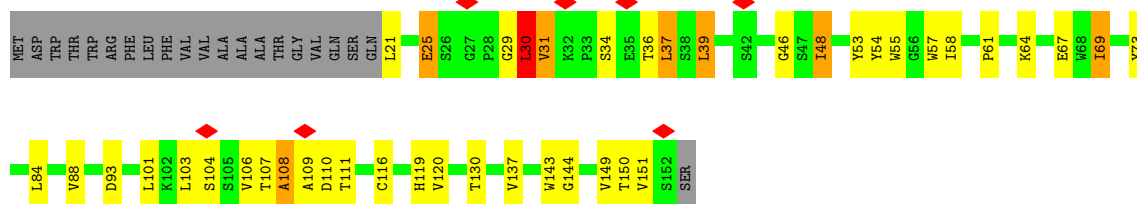
• Molecule 2: IgA-Fab3-2 Heavy chain



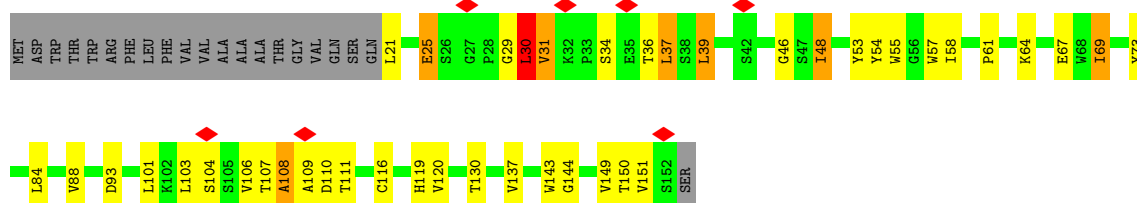
• Molecule 2: IgA-Fab3-2 Heavy chain



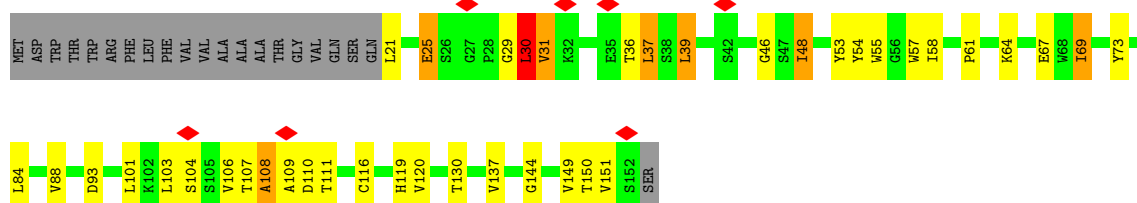
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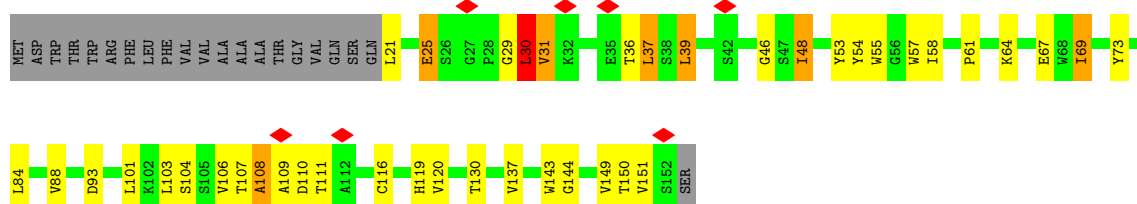
• Molecule 2: IgA-Fab3-2 Heavy chain



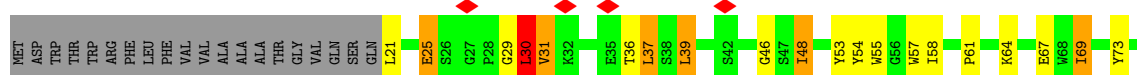
• Molecule 2: IgA-Fab3-2 Heavy chain

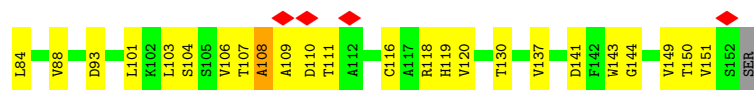


• Molecule 2: IgA-Fab3-2 Heavy chain

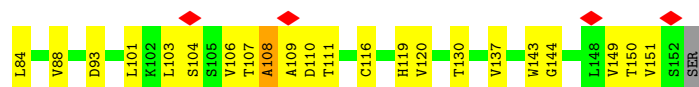


• Molecule 2: IgA-Fab3-2 Heavy chain

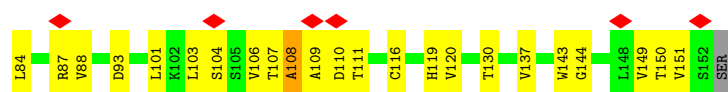




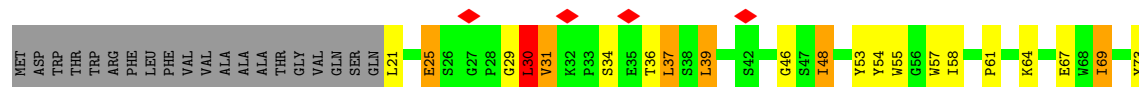
- Molecule 2: IgA-Fab3-2 Heavy chain



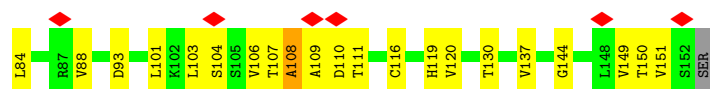
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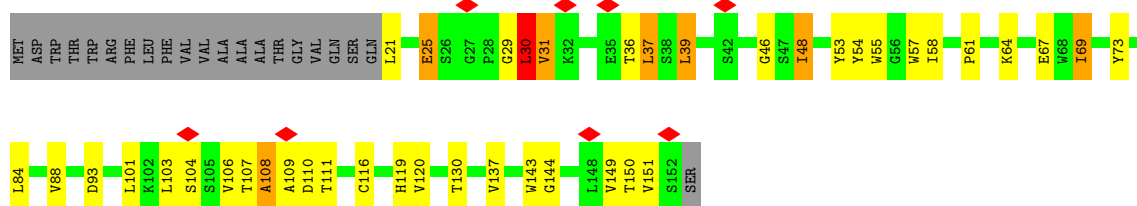
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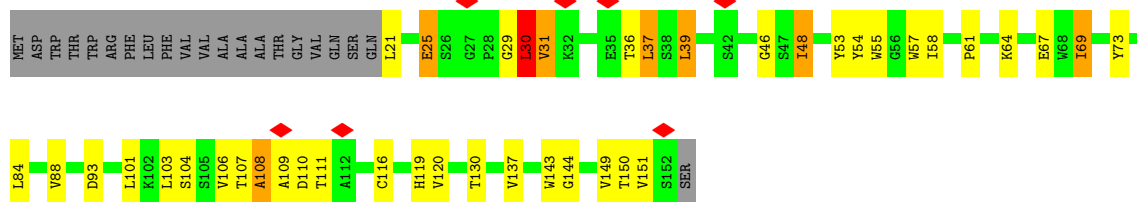
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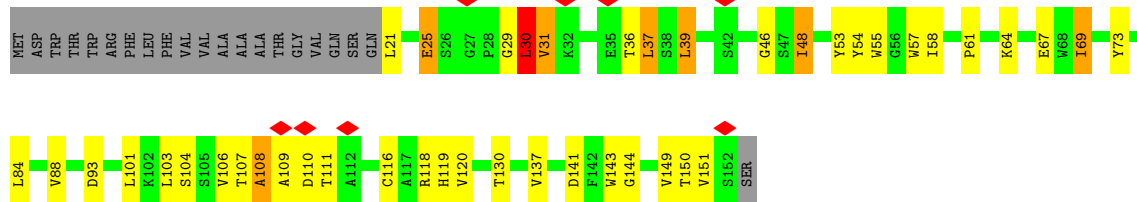
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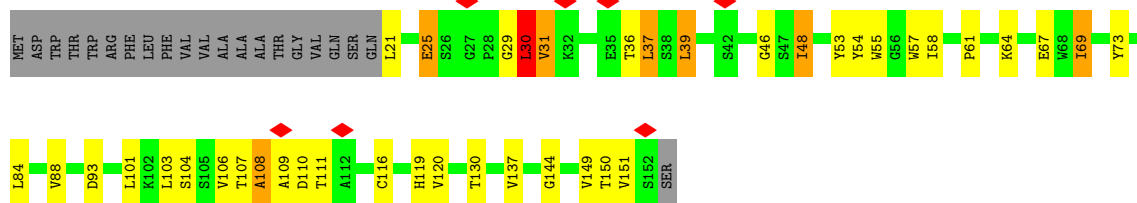
• Molecule 2: IgA-Fab3-2 Heavy chain



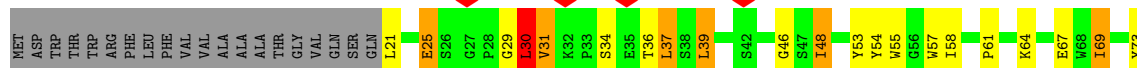
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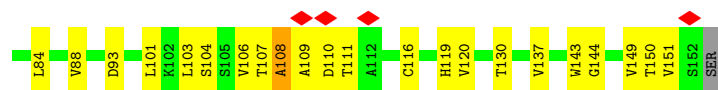


• Molecule 2: IgA-Fab3-2 Heavy chain

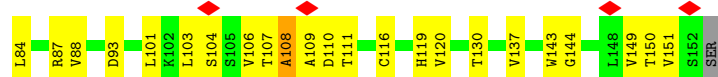
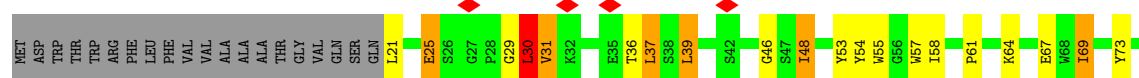


• Molecule 2: IgA-Fab3-2 Heavy chain

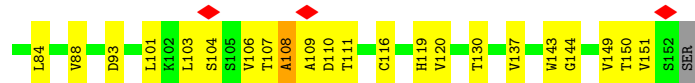
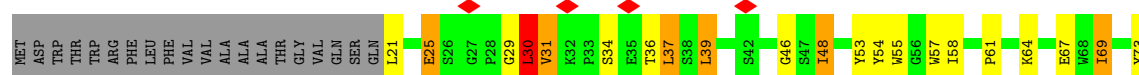




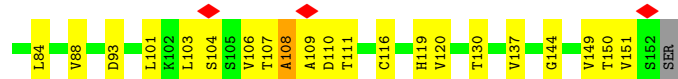
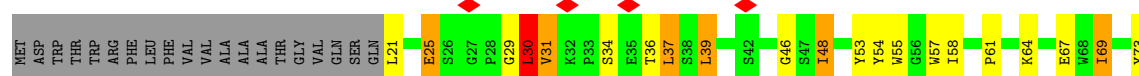
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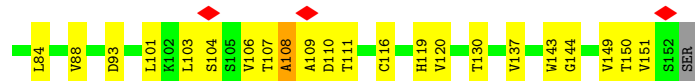
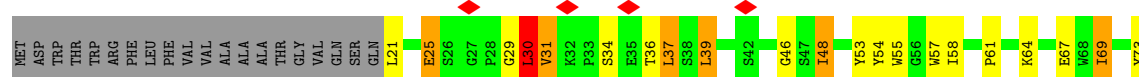
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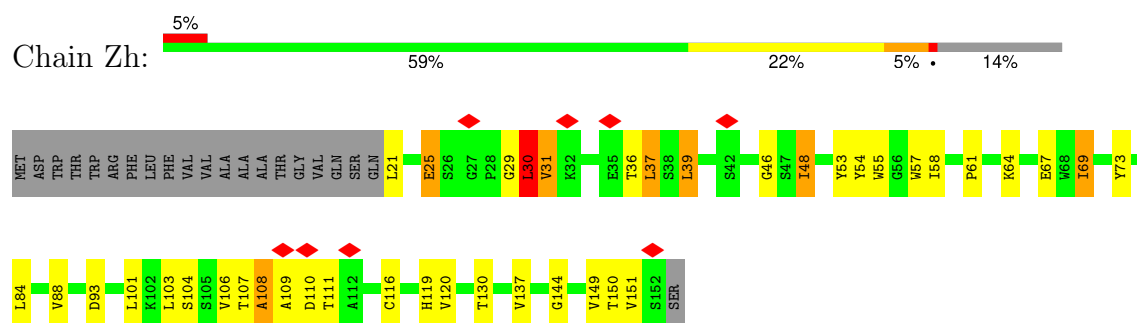
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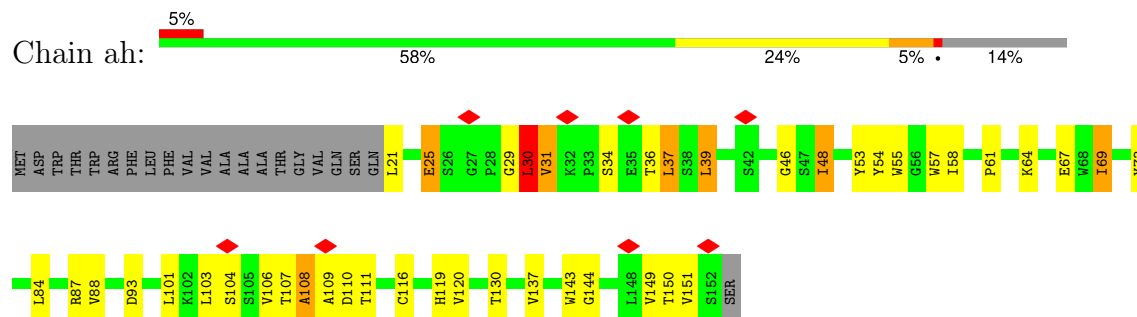
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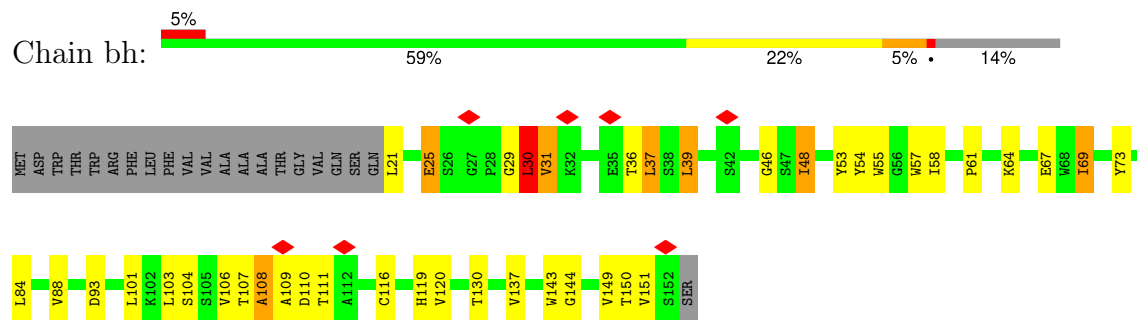
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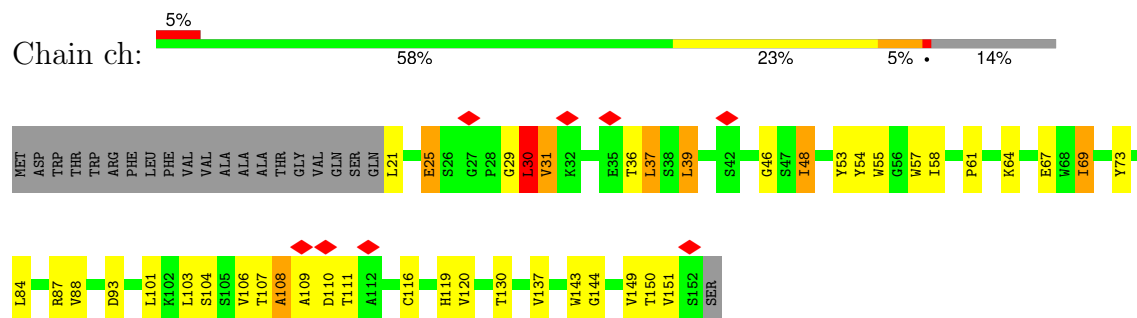
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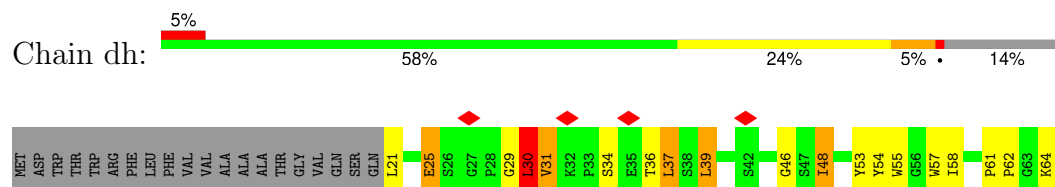
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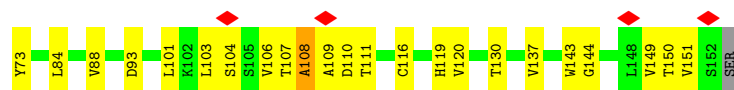


- Molecule 2: IgA-Fab3-2 Heavy chain

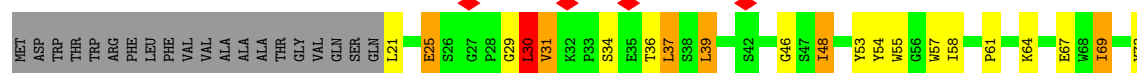


- Molecule 2: IgA-Fab3-2 Heavy chain





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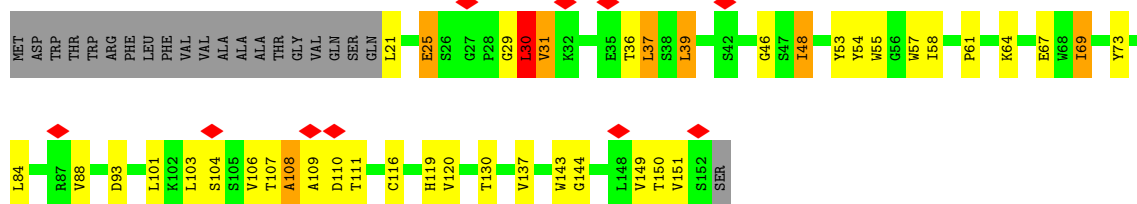
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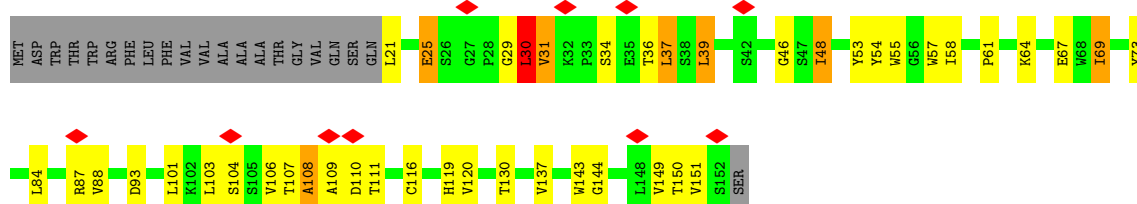
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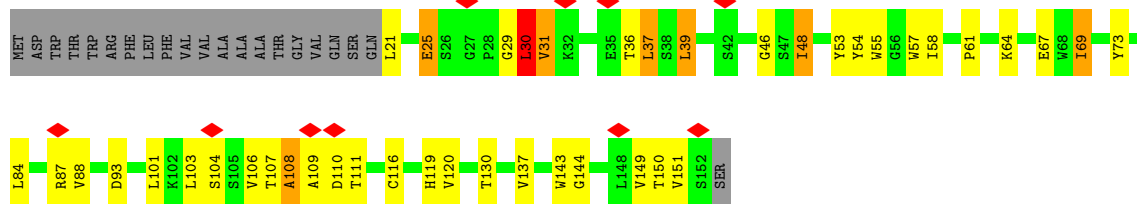
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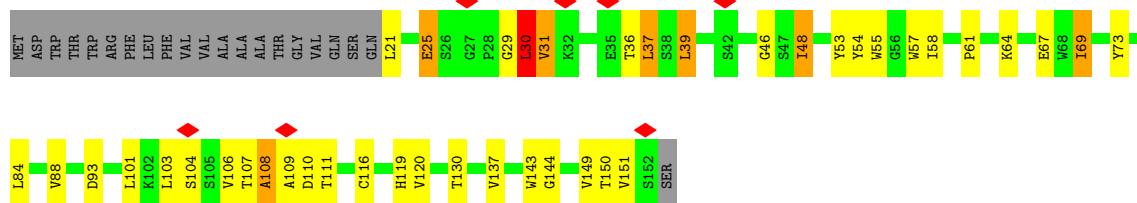
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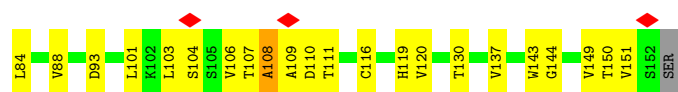


• Molecule 2: IgA-Fab3-2 Heavy chain

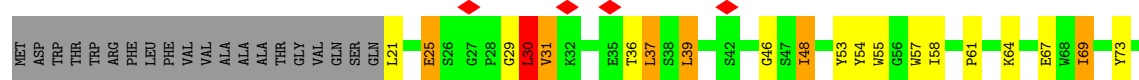


• Molecule 2: IgA-Fab3-2 Heavy chain

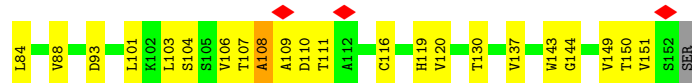




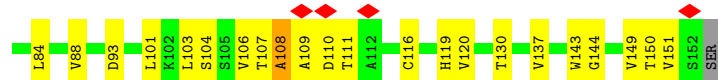
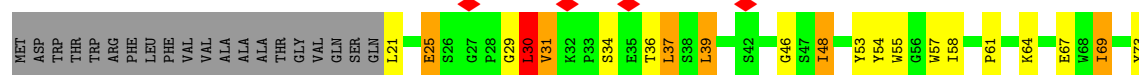
- Molecule 2: IgA-Fab3-2 Heavy chain



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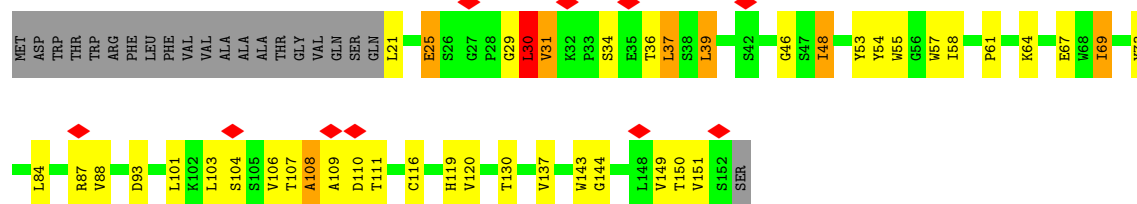
- Molecule 2: IgA-Fab3-2 Heavy chain



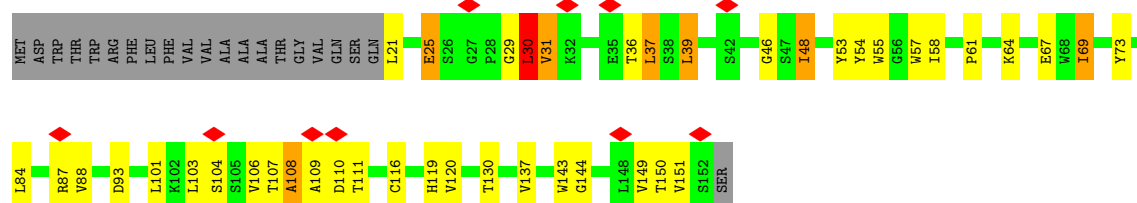
- Molecule 2: IgA-Fab3-2 Heavy chain



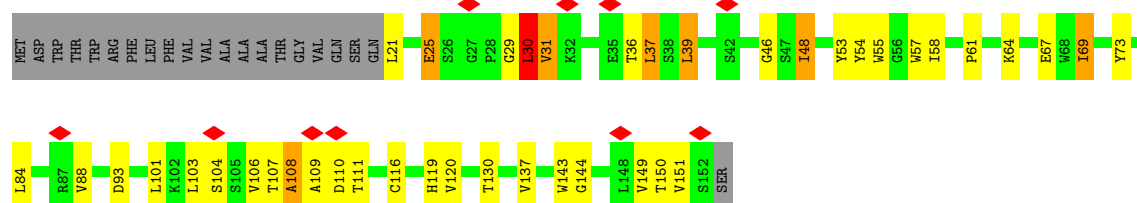
- Molecule 2: IgA-Fab3-2 Heavy chain



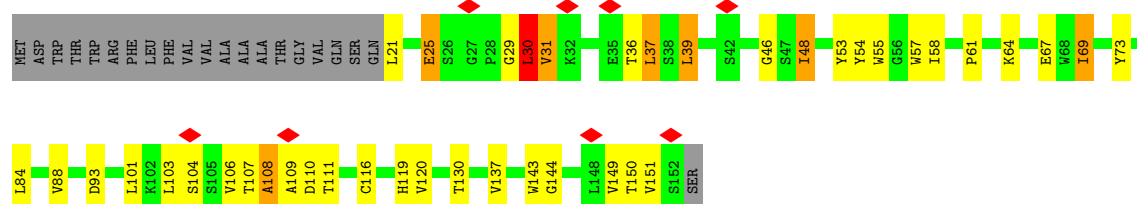
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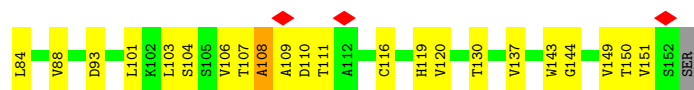


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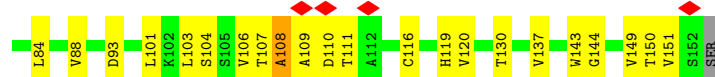
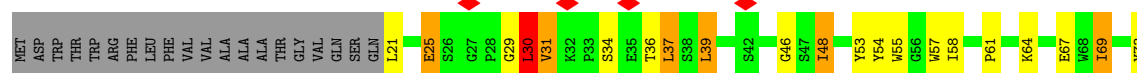


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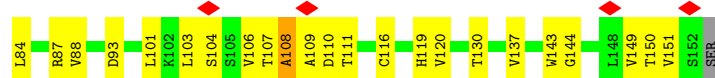
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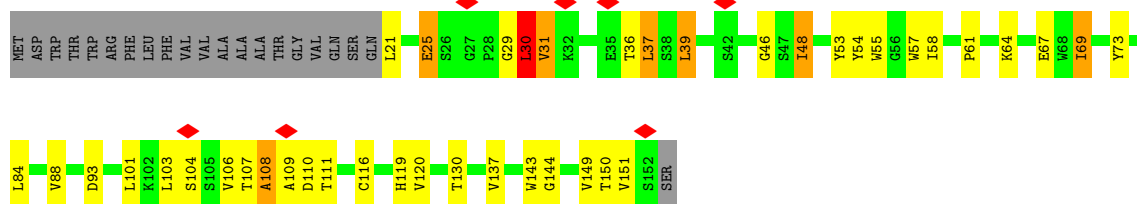
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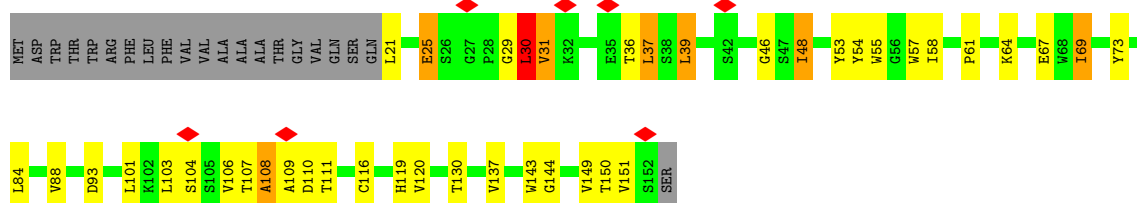
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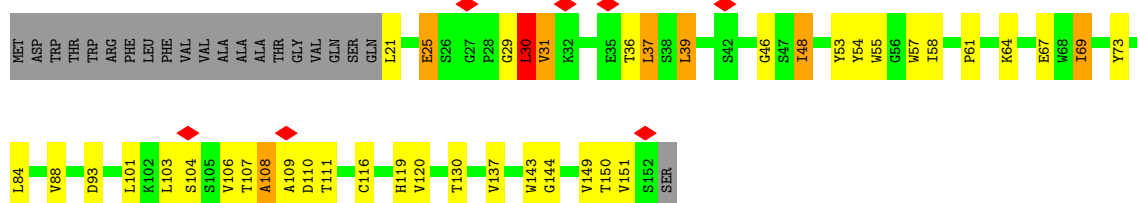
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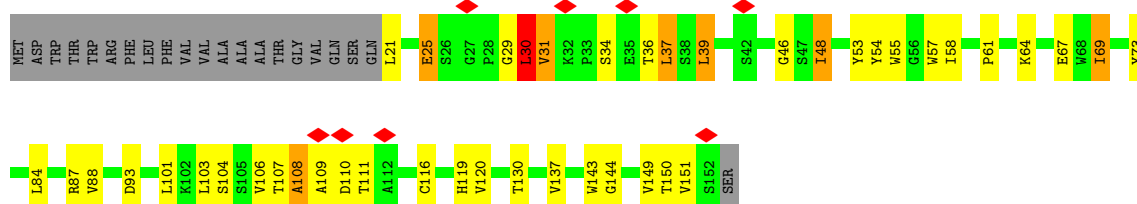
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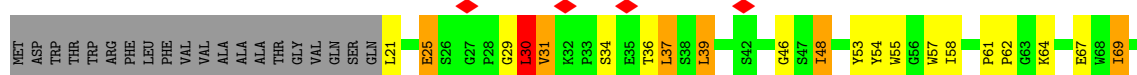
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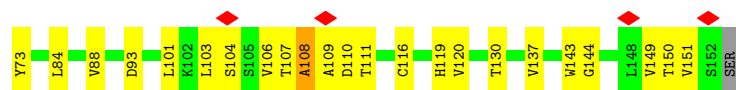


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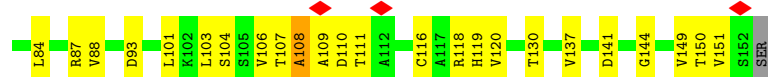
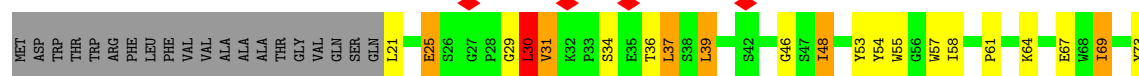


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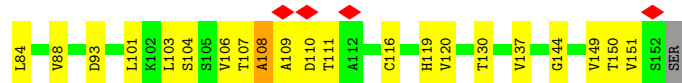




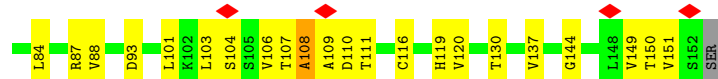
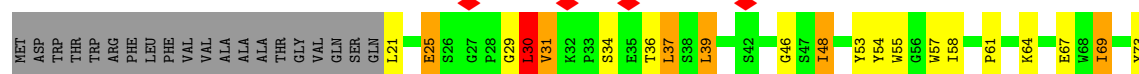
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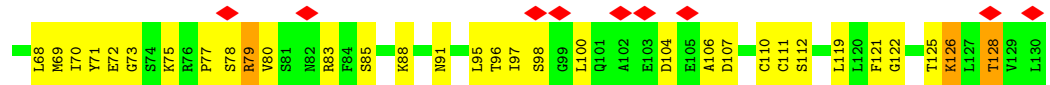
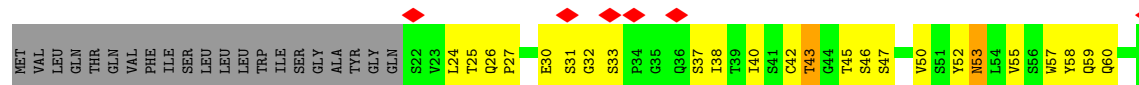
- Molecule 2: IgA-Fab3-2 Heavy chain



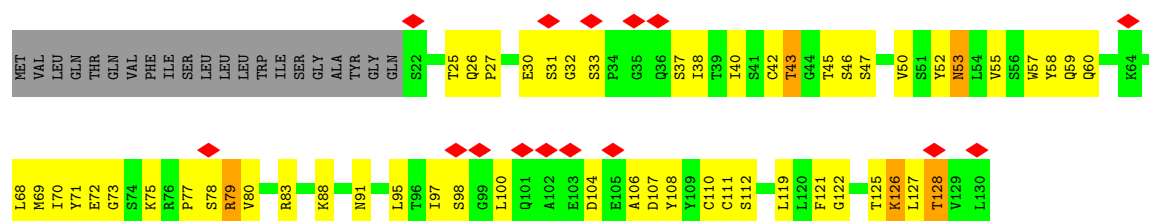
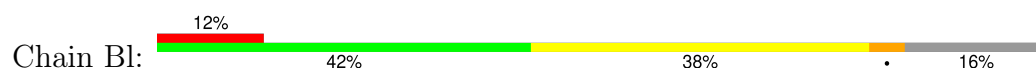
- Molecule 2: IgA-Fab3-2 Heavy chain



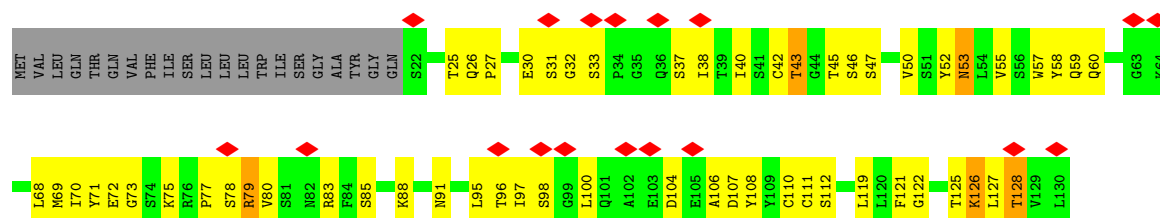
- Molecule 3: IgA-Fab3-2 Light chain



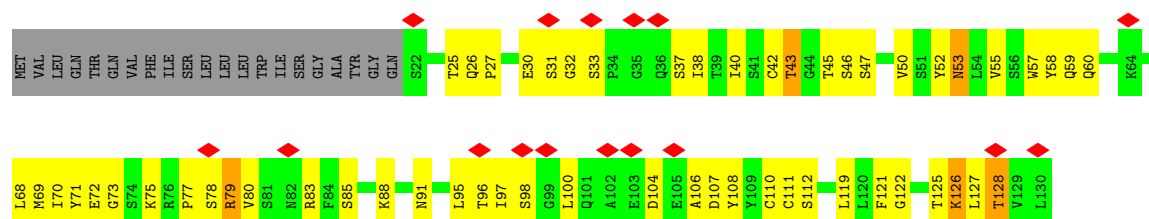
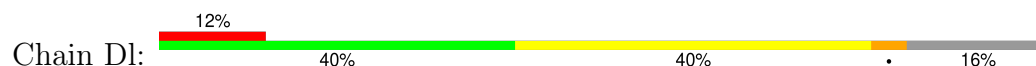
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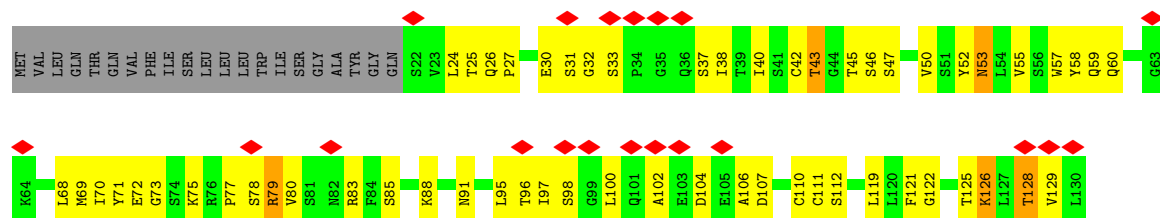
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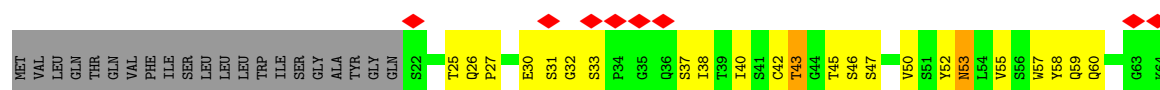
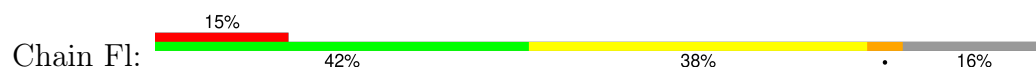
• Molecule 3: IgA-Fab3-2 Light chain



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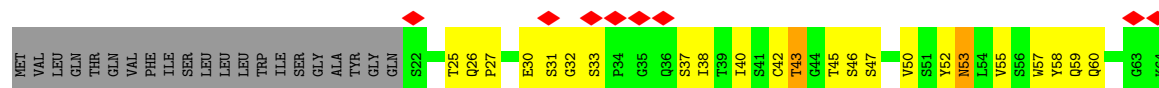
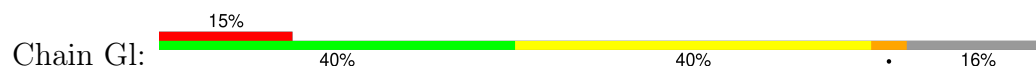


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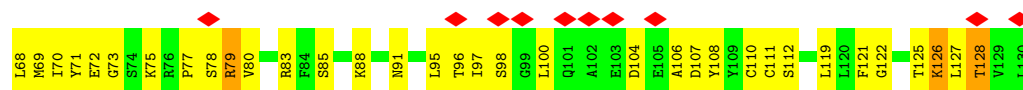
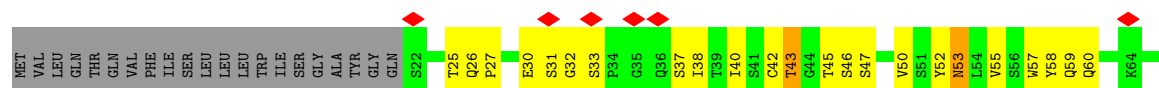




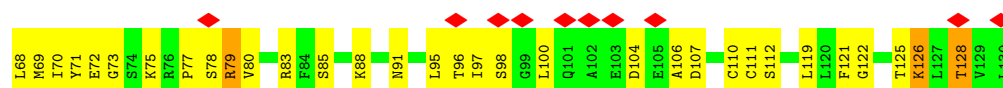
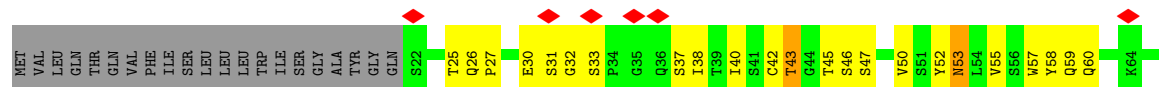
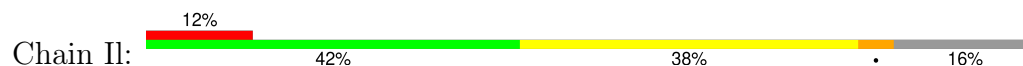
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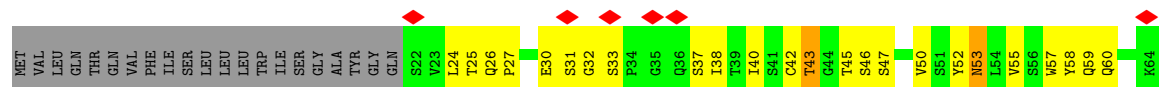
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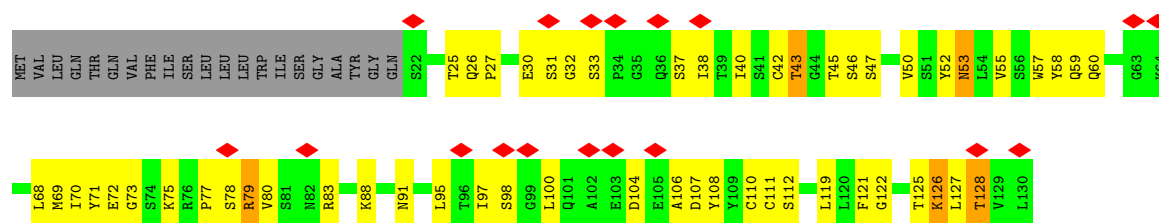
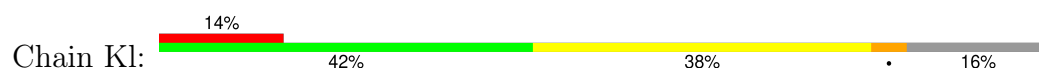
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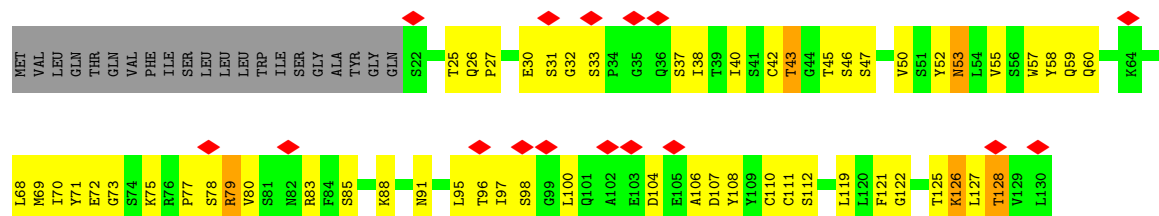
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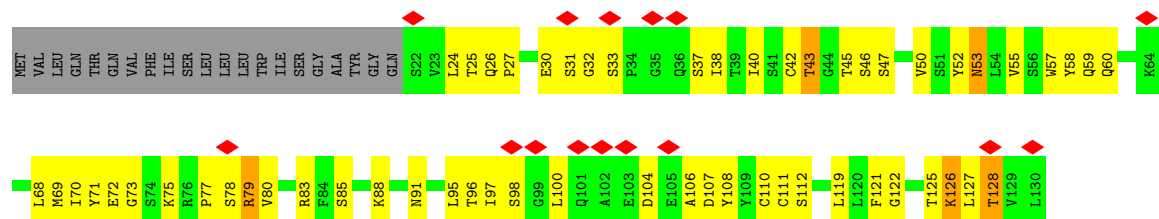
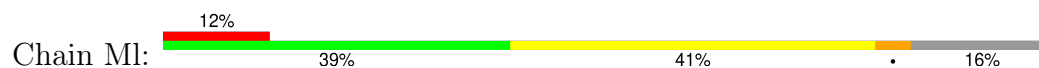
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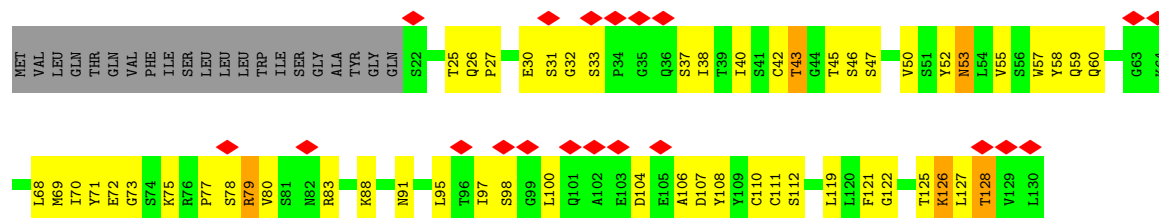
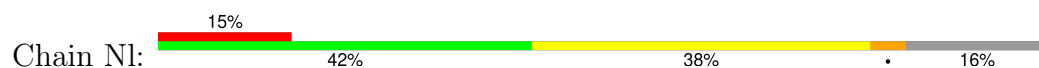
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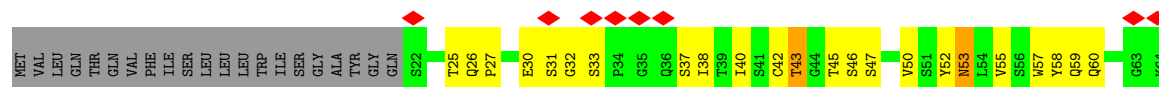
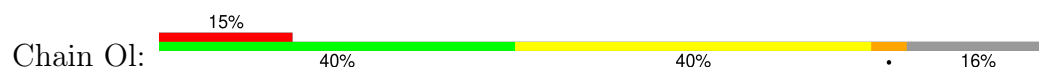
• Molecule 3: IgA-Fab3-2 Light chain



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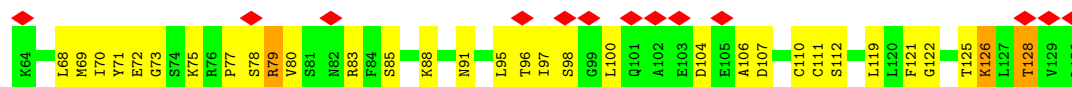
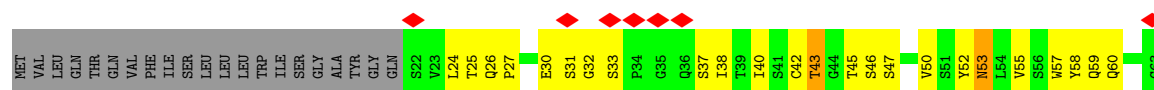
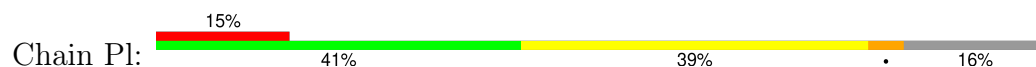


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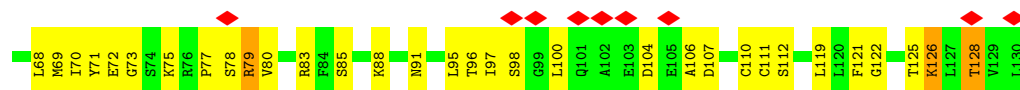
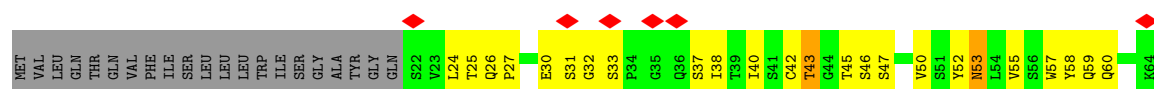
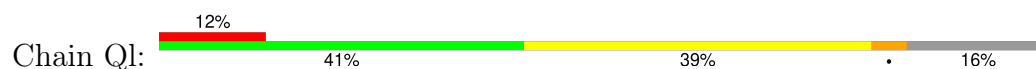




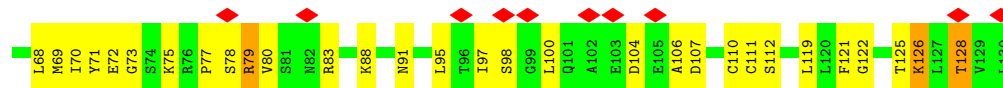
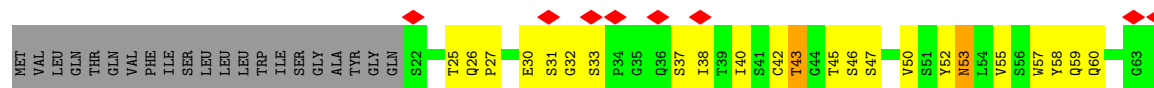
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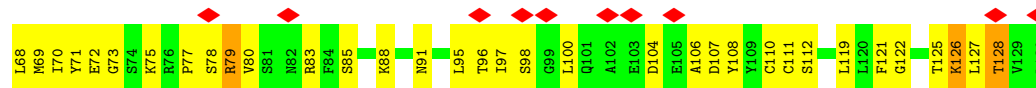
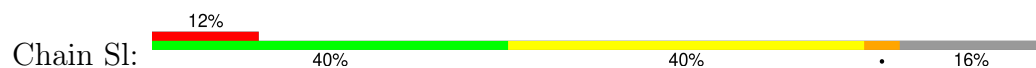
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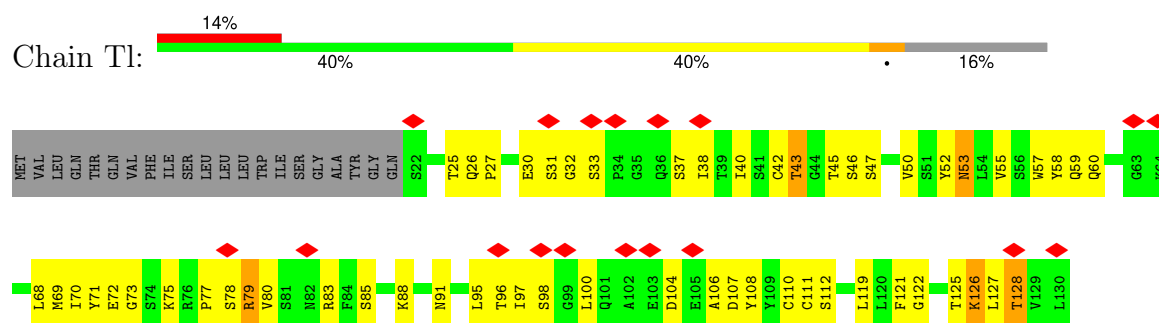
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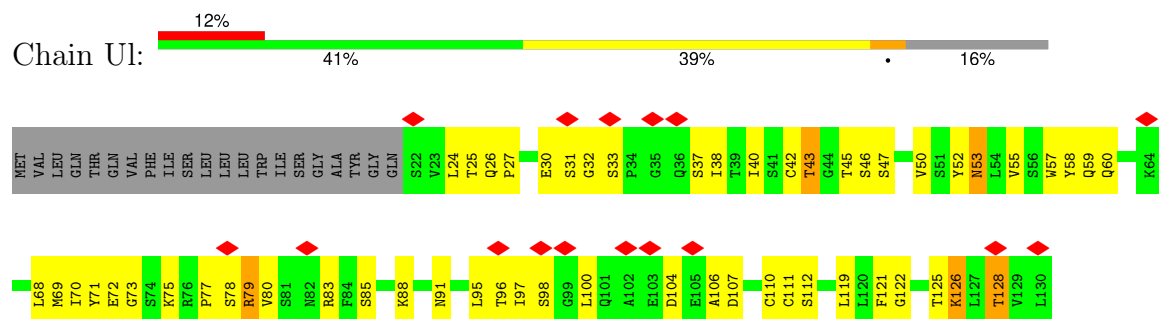
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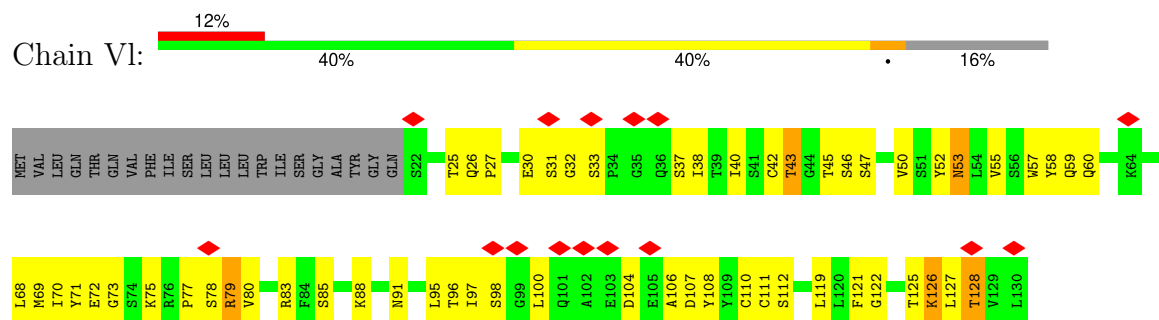
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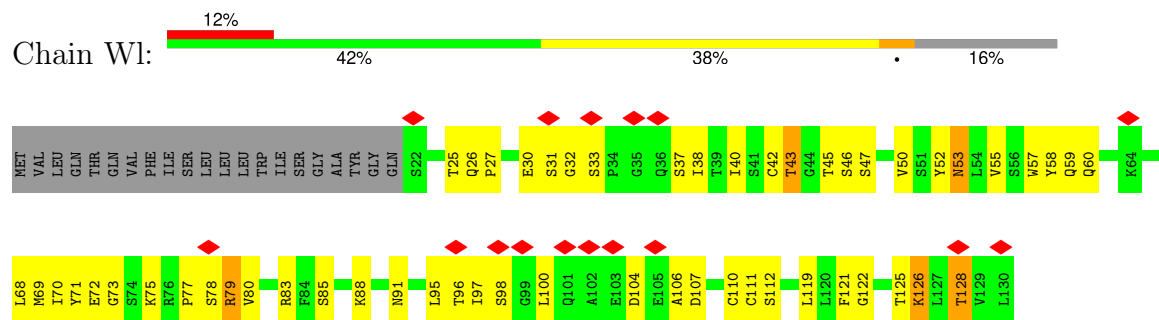
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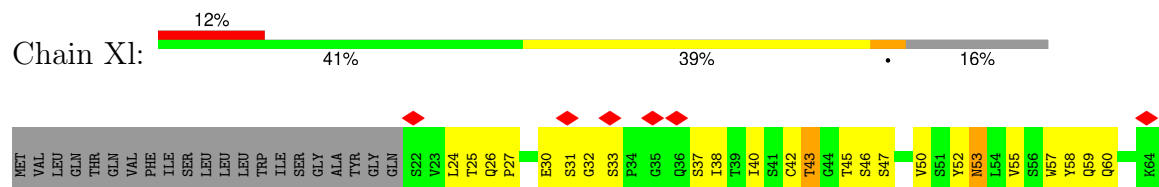
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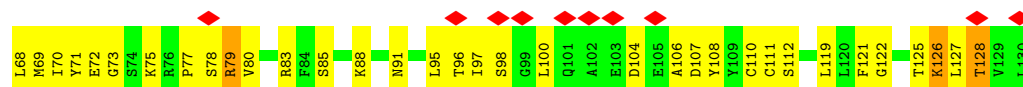
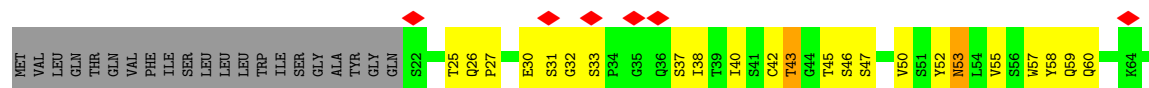
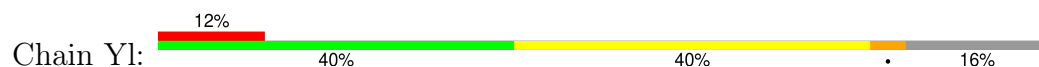


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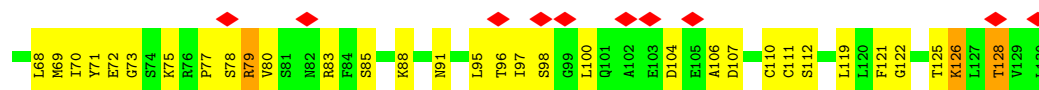
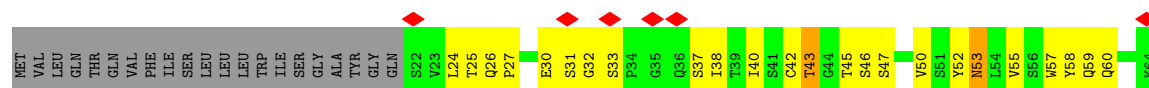
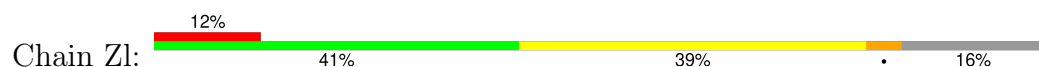




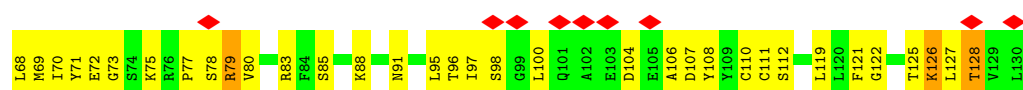
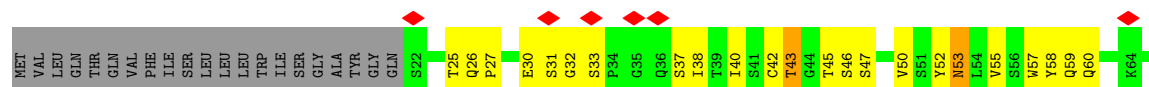
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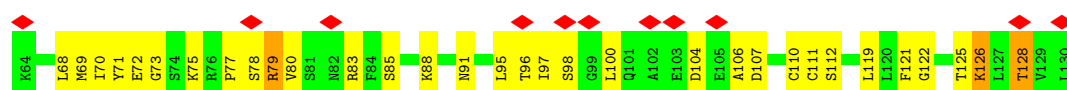
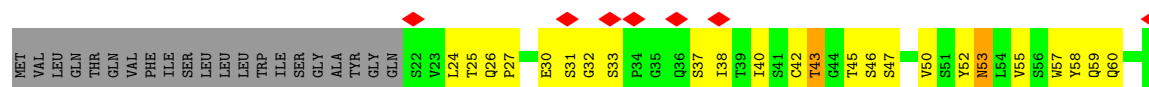
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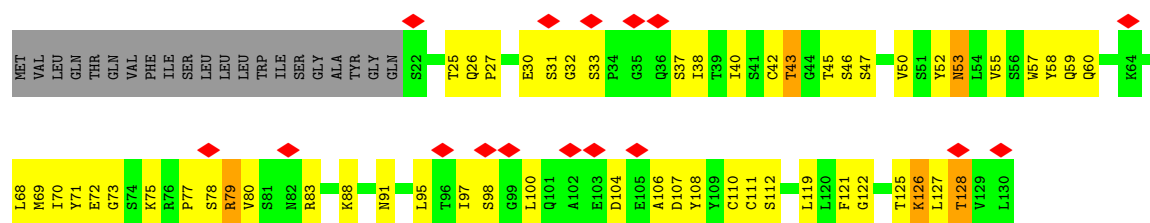
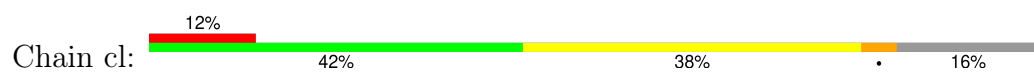
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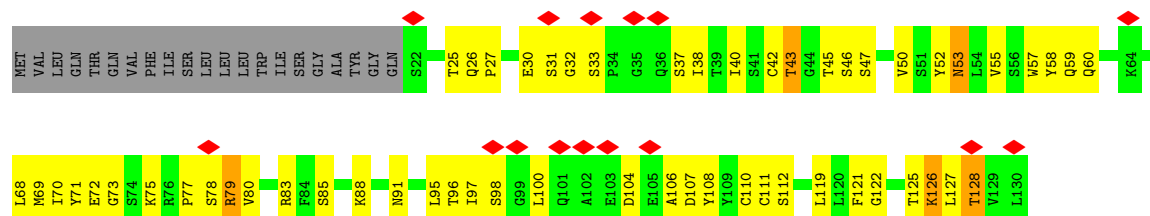
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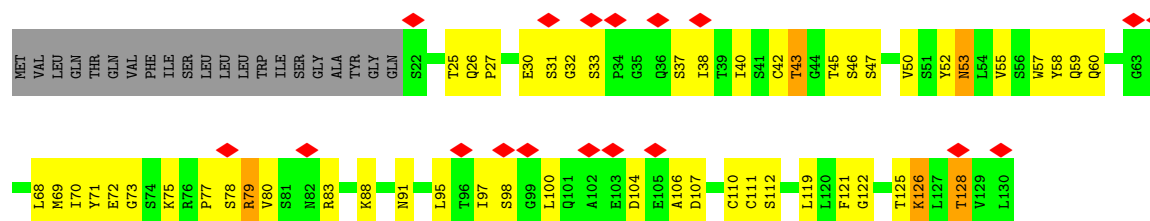
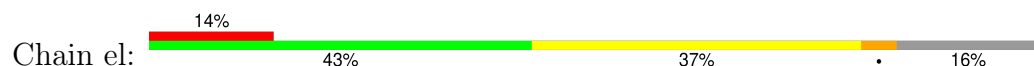
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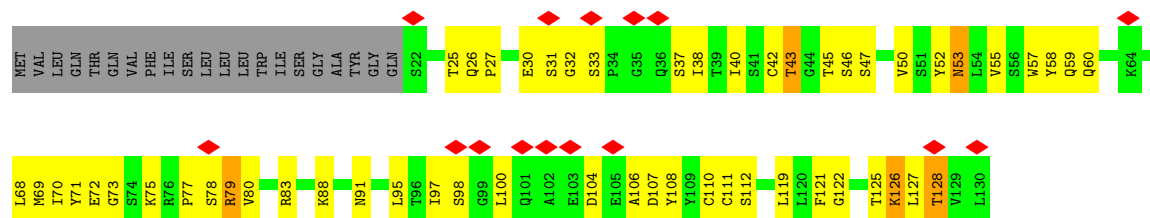
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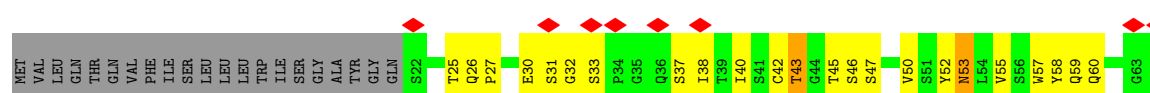
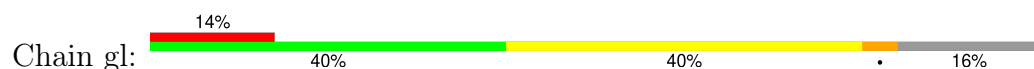
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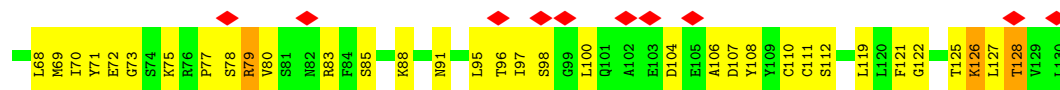


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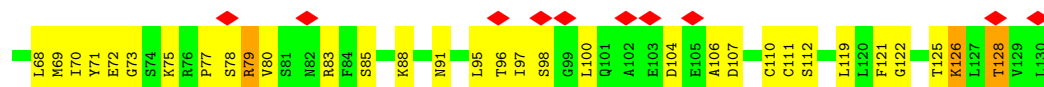
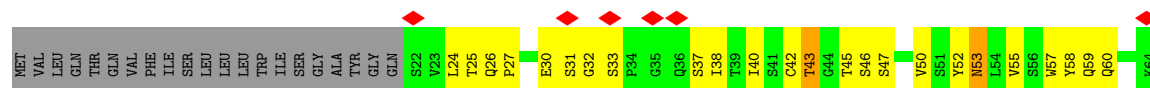
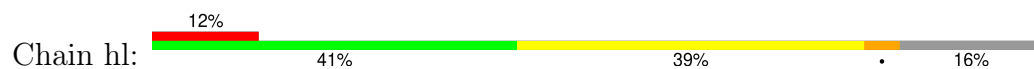


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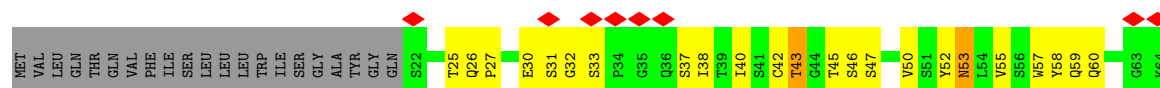




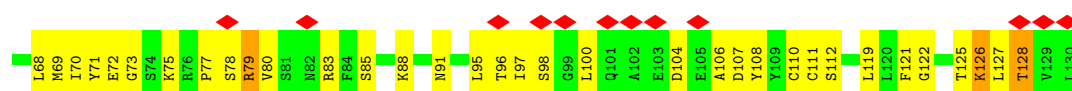
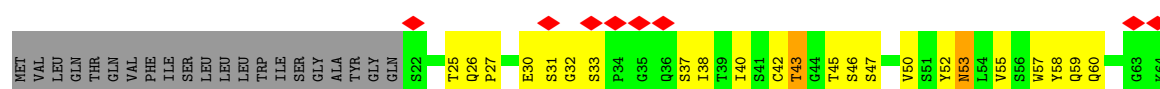
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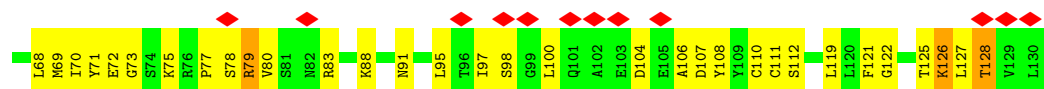
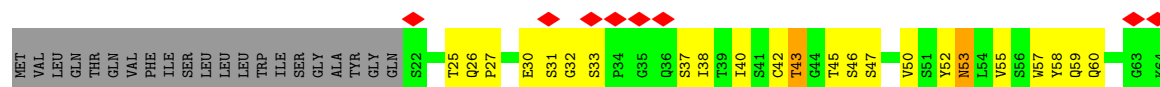
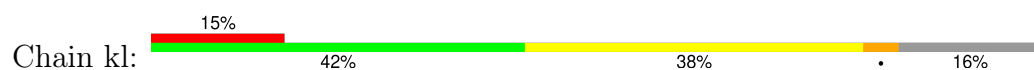
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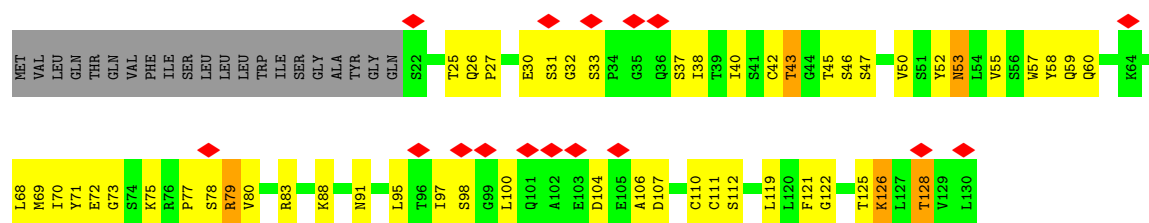
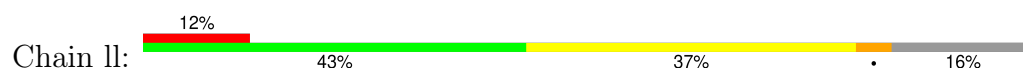
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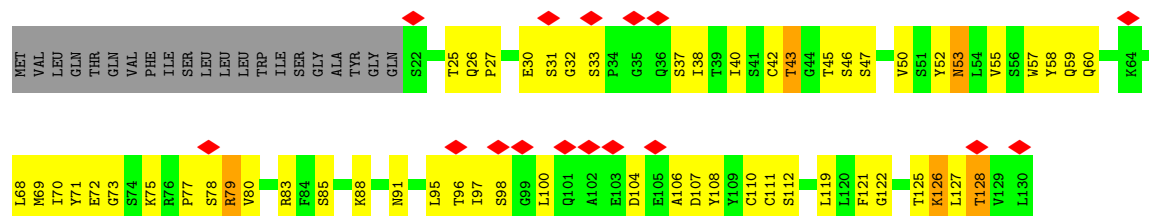
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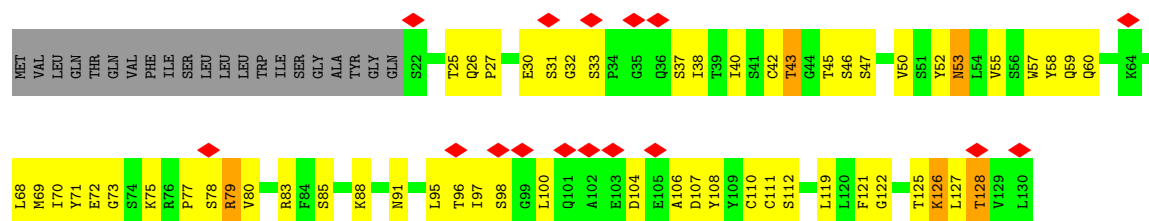
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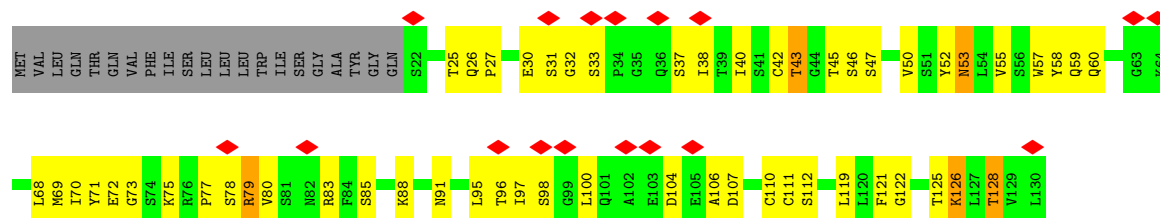
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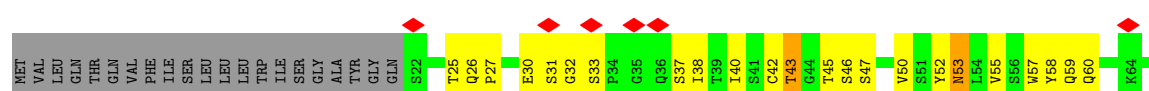
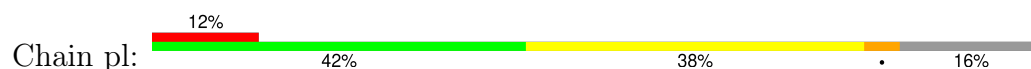
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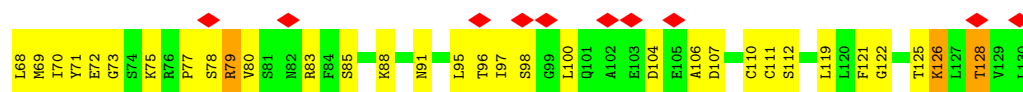


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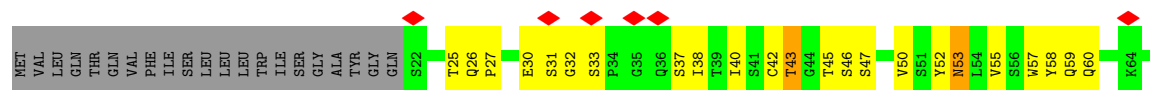
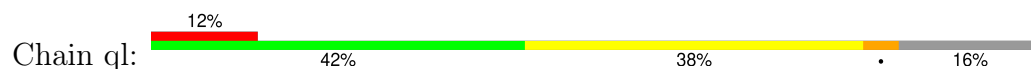


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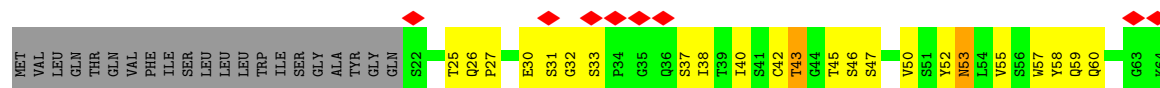
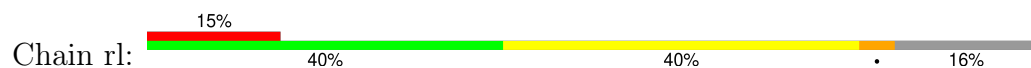




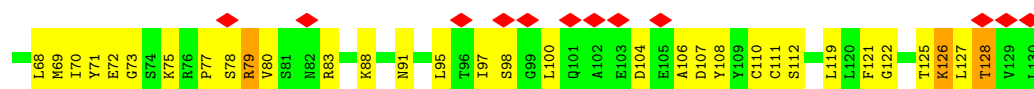
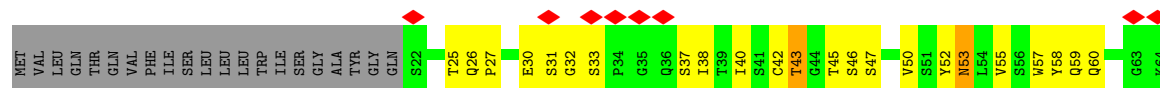
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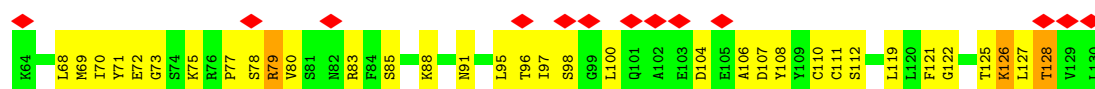
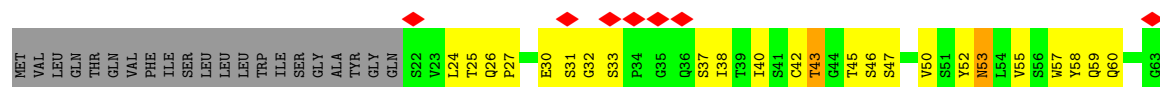
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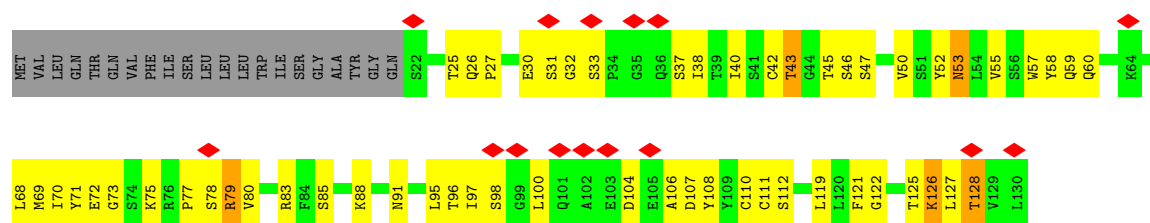
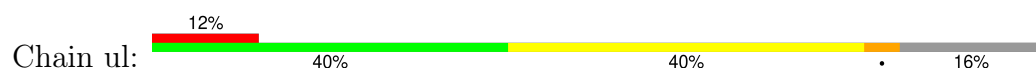
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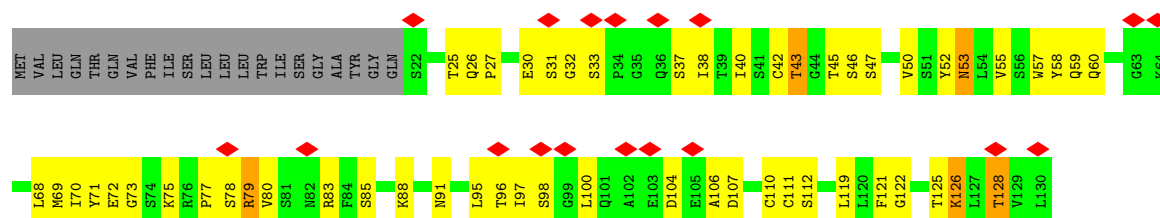
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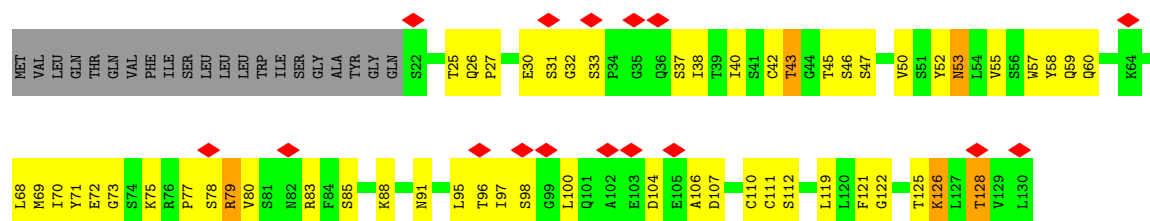
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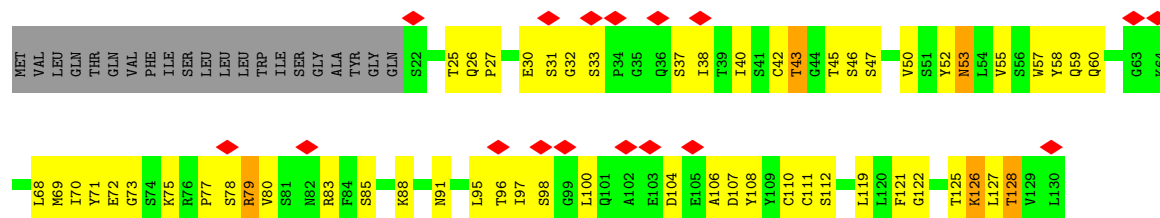
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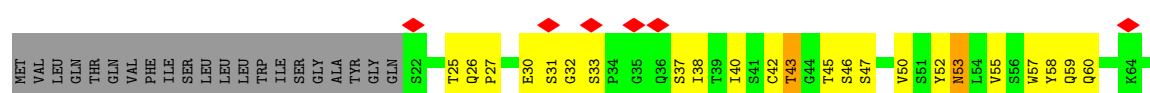
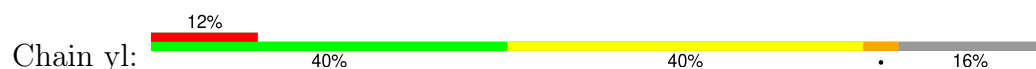
• Molecule 3: IgA-Fab3-2 Light chain

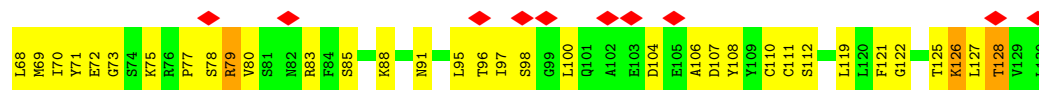


• Molecule 3: IgA-Fab3-2 Light chain

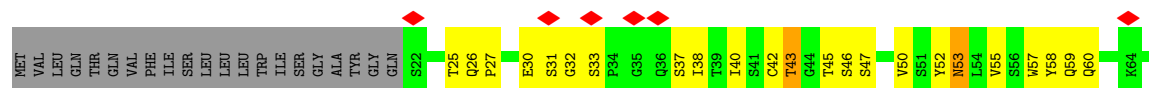
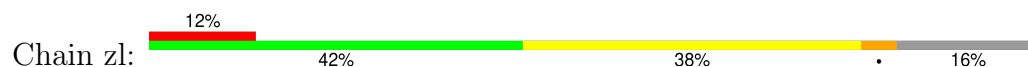


• Molecule 3: IgA-Fab3-2 Light chain

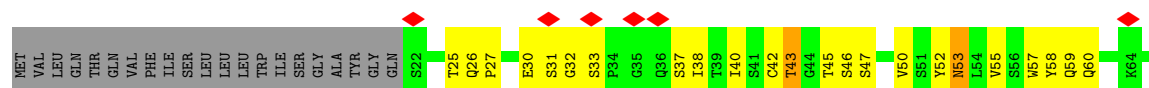




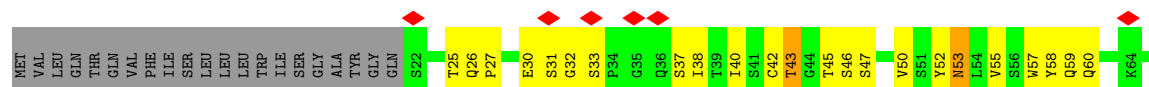
• Molecule 3: IgA-Fab3-2 Light chain



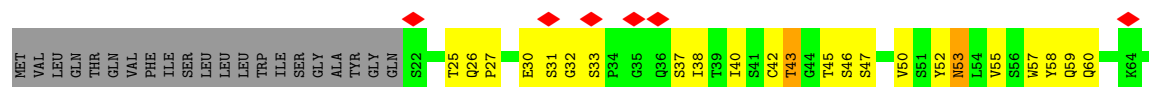
• Molecule 3: IgA-Fab3-2 Light chain



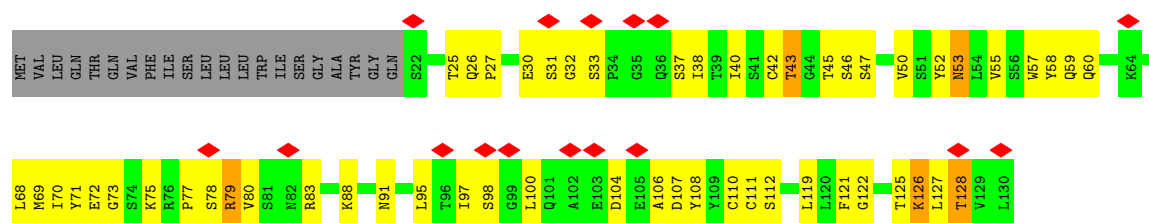
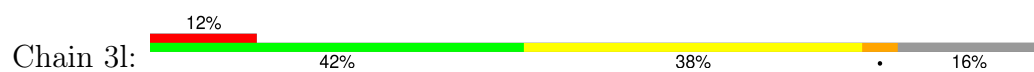
• Molecule 3: IgA-Fab3-2 Light chain



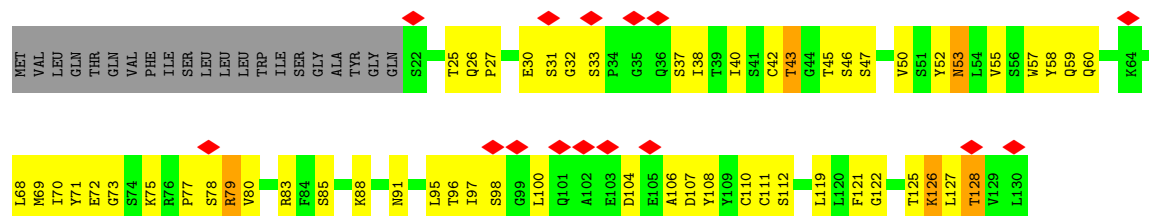
• Molecule 3: IgA-Fab3-2 Light chain



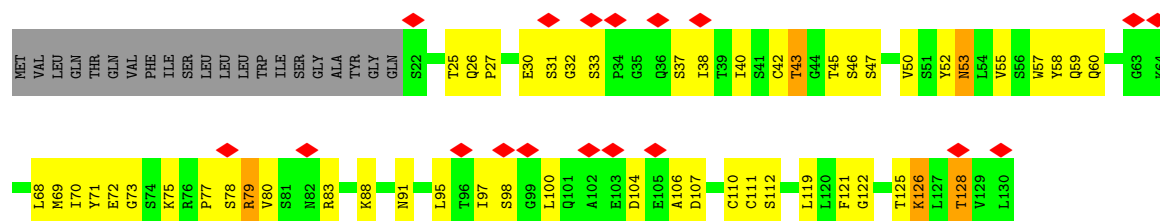
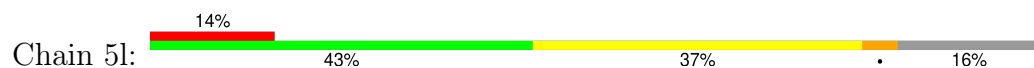
• Molecule 3: IgA-Fab3-2 Light chain



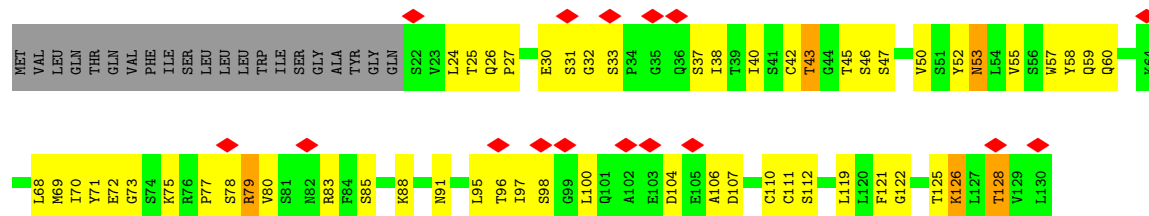
• Molecule 3: IgA-Fab3-2 Light chain



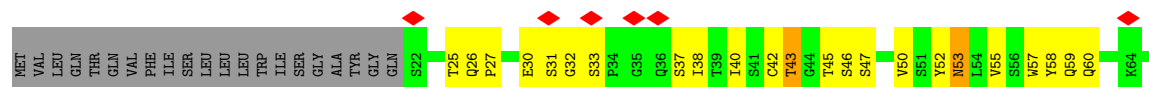
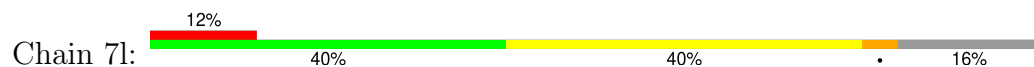
• Molecule 3: IgA-Fab3-2 Light chain

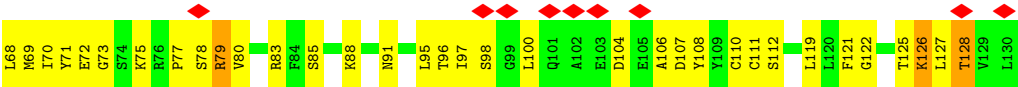


• Molecule 3: IgA-Fab3-2 Light chain



• Molecule 3: IgA-Fab3-2 Light chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10214	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	16.324	Depositor
Minimum map value	-17.105	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	441.0, 441.0, 441.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.735, 0.735, 0.735	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.50	0/4271	0.77	7/5822 (0.1%)
1	1	0.50	0/4271	0.77	7/5822 (0.1%)
1	2	0.50	0/4271	0.77	7/5822 (0.1%)
1	3	0.50	0/4271	0.77	7/5822 (0.1%)
1	4	0.50	0/4271	0.77	7/5822 (0.1%)
1	5	0.50	0/4271	0.77	7/5822 (0.1%)
1	6	0.50	0/4271	0.77	7/5822 (0.1%)
1	7	0.50	0/4271	0.77	7/5822 (0.1%)
1	A	0.50	0/4271	0.77	7/5822 (0.1%)
1	B	0.50	0/4271	0.90	8/5822 (0.1%)
1	C	0.50	0/4271	0.77	7/5822 (0.1%)
1	D	0.50	0/4271	0.77	7/5822 (0.1%)
1	E	0.50	0/4271	0.77	7/5822 (0.1%)
1	F	0.50	0/4271	0.77	7/5822 (0.1%)
1	G	0.50	0/4271	0.77	7/5822 (0.1%)
1	H	0.50	0/4271	0.77	7/5822 (0.1%)
1	I	0.50	0/4271	0.77	7/5822 (0.1%)
1	J	0.50	0/4271	0.77	7/5822 (0.1%)
1	K	0.50	0/4271	0.77	7/5822 (0.1%)
1	L	0.50	0/4271	0.77	7/5822 (0.1%)
1	M	0.50	0/4271	0.77	7/5822 (0.1%)
1	N	0.50	0/4271	0.77	7/5822 (0.1%)
1	O	0.50	0/4271	0.77	7/5822 (0.1%)
1	P	0.50	0/4271	0.77	7/5822 (0.1%)
1	Q	0.50	0/4271	0.77	7/5822 (0.1%)
1	R	0.50	0/4271	0.77	7/5822 (0.1%)
1	S	0.50	0/4271	0.77	7/5822 (0.1%)
1	T	0.50	0/4271	0.77	7/5822 (0.1%)
1	U	0.50	0/4271	0.77	7/5822 (0.1%)
1	V	0.50	0/4271	0.77	7/5822 (0.1%)
1	W	0.50	0/4271	0.77	7/5822 (0.1%)
1	X	0.50	0/4271	0.77	7/5822 (0.1%)
1	Y	0.50	0/4271	0.77	7/5822 (0.1%)
1	Z	0.50	0/4271	0.77	7/5822 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.50	0/4271	0.77	7/5822 (0.1%)
1	b	0.50	0/4271	0.77	7/5822 (0.1%)
1	c	0.50	0/4271	0.77	7/5822 (0.1%)
1	d	0.50	0/4271	0.77	7/5822 (0.1%)
1	e	0.50	0/4271	0.77	7/5822 (0.1%)
1	f	0.50	0/4271	0.77	7/5822 (0.1%)
1	g	0.50	0/4271	0.77	7/5822 (0.1%)
1	h	0.50	0/4271	0.77	7/5822 (0.1%)
1	i	0.50	0/4271	0.77	7/5822 (0.1%)
1	j	0.50	0/4271	0.77	7/5822 (0.1%)
1	k	0.50	0/4271	0.77	7/5822 (0.1%)
1	l	0.50	0/4271	0.77	7/5822 (0.1%)
1	m	0.50	0/4271	0.77	7/5822 (0.1%)
1	n	0.50	0/4271	0.77	7/5822 (0.1%)
1	o	0.50	0/4271	0.77	7/5822 (0.1%)
1	p	0.50	0/4271	0.77	7/5822 (0.1%)
1	q	0.50	0/4271	0.77	7/5822 (0.1%)
1	r	0.50	0/4271	0.77	7/5822 (0.1%)
1	s	0.50	0/4271	0.77	7/5822 (0.1%)
1	t	0.50	0/4271	0.77	7/5822 (0.1%)
1	u	0.50	0/4271	0.77	7/5822 (0.1%)
1	v	0.50	0/4271	0.77	7/5822 (0.1%)
1	w	0.50	0/4271	0.77	7/5822 (0.1%)
1	x	0.50	0/4271	0.77	7/5822 (0.1%)
1	y	0.50	0/4271	0.77	7/5822 (0.1%)
1	z	0.50	0/4271	0.77	7/5822 (0.1%)
2	0h	0.49	0/1058	0.83	3/1445 (0.2%)
2	1h	0.49	0/1058	0.84	3/1445 (0.2%)
2	2h	0.49	0/1058	0.83	3/1445 (0.2%)
2	3h	0.49	0/1058	0.83	3/1445 (0.2%)
2	4h	0.49	0/1058	0.83	3/1445 (0.2%)
2	5h	0.49	0/1058	0.83	3/1445 (0.2%)
2	6h	0.49	0/1058	0.83	3/1445 (0.2%)
2	7h	0.49	0/1058	0.83	3/1445 (0.2%)
2	Ah	0.49	0/1058	0.83	3/1445 (0.2%)
2	Bh	0.49	0/1058	0.84	3/1445 (0.2%)
2	Ch	0.49	0/1058	0.83	3/1445 (0.2%)
2	Dh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Eh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Fh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Gh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Hh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Ih	0.49	0/1058	0.83	3/1445 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Jh	0.49	0/1058	0.84	3/1445 (0.2%)
2	Kh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Lh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Mh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Nh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Oh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Ph	0.49	0/1058	0.83	3/1445 (0.2%)
2	Qh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Rh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Sh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Th	0.49	0/1058	0.83	3/1445 (0.2%)
2	Uh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Vh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Wh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Xh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Yh	0.49	0/1058	0.83	3/1445 (0.2%)
2	Zh	0.49	0/1058	0.83	3/1445 (0.2%)
2	ah	0.49	0/1058	0.83	3/1445 (0.2%)
2	bh	0.49	0/1058	0.83	3/1445 (0.2%)
2	ch	0.49	0/1058	0.83	3/1445 (0.2%)
2	dh	0.49	0/1058	0.83	3/1445 (0.2%)
2	eh	0.49	0/1058	0.83	3/1445 (0.2%)
2	fh	0.49	0/1058	0.84	3/1445 (0.2%)
2	gh	0.49	0/1058	0.83	3/1445 (0.2%)
2	hh	0.49	0/1058	0.83	3/1445 (0.2%)
2	ih	0.49	0/1058	0.83	3/1445 (0.2%)
2	jh	0.49	0/1058	0.83	3/1445 (0.2%)
2	kh	0.49	0/1058	0.83	3/1445 (0.2%)
2	lh	0.49	0/1058	0.83	3/1445 (0.2%)
2	mh	0.49	0/1058	0.83	3/1445 (0.2%)
2	nh	0.49	0/1058	0.84	3/1445 (0.2%)
2	oh	0.49	0/1058	0.83	3/1445 (0.2%)
2	ph	0.49	0/1058	0.83	3/1445 (0.2%)
2	qh	0.49	0/1058	0.83	3/1445 (0.2%)
2	rh	0.49	0/1058	0.83	3/1445 (0.2%)
2	sh	0.49	0/1058	0.83	3/1445 (0.2%)
2	th	0.49	0/1058	0.83	3/1445 (0.2%)
2	uh	0.49	0/1058	0.83	3/1445 (0.2%)
2	vh	0.49	0/1058	0.83	3/1445 (0.2%)
2	wh	0.49	0/1058	0.83	3/1445 (0.2%)
2	xh	0.49	0/1058	0.83	3/1445 (0.2%)
2	yh	0.49	0/1058	0.83	3/1445 (0.2%)
2	zh	0.49	0/1058	0.84	3/1445 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	0l	0.82	0/814	1.03	0/1103
3	1l	0.82	0/814	1.03	0/1103
3	2l	0.82	0/814	1.03	0/1103
3	3l	0.82	0/814	1.03	0/1103
3	4l	0.82	0/814	1.03	0/1103
3	5l	0.82	0/814	1.03	0/1103
3	6l	0.82	0/814	1.03	0/1103
3	7l	0.82	0/814	1.03	0/1103
3	Al	0.82	0/814	1.03	0/1103
3	Bl	0.82	0/814	1.03	0/1103
3	Cl	0.82	0/814	1.03	0/1103
3	Dl	0.82	0/814	1.03	0/1103
3	El	0.82	0/814	1.03	0/1103
3	Fl	0.82	0/814	1.03	0/1103
3	Gl	0.82	0/814	1.03	0/1103
3	Hl	0.82	0/814	1.03	0/1103
3	Il	0.82	0/814	1.03	0/1103
3	Jl	0.82	0/814	1.03	0/1103
3	Kl	0.82	0/814	1.03	0/1103
3	Ll	0.82	0/814	1.03	0/1103
3	Ml	0.82	0/814	1.03	0/1103
3	Nl	0.82	0/814	1.03	0/1103
3	Ol	0.82	0/814	1.03	0/1103
3	Pl	0.82	0/814	1.03	0/1103
3	Ql	0.82	0/814	1.03	0/1103
3	Rl	0.82	0/814	1.03	0/1103
3	Sl	0.82	0/814	1.03	0/1103
3	Tl	0.82	0/814	1.03	0/1103
3	Ul	0.82	0/814	1.03	0/1103
3	Vl	0.82	0/814	1.03	0/1103
3	Wl	0.82	0/814	1.03	0/1103
3	Xl	0.82	0/814	1.03	0/1103
3	Yl	0.82	0/814	1.03	0/1103
3	Zl	0.82	0/814	1.03	0/1103
3	al	0.82	0/814	1.03	0/1103
3	bl	0.82	0/814	1.03	0/1103
3	cl	0.82	0/814	1.03	0/1103
3	dl	0.82	0/814	1.03	0/1103
3	el	0.82	0/814	1.03	0/1103
3	fl	0.82	0/814	1.03	0/1103
3	gl	0.82	0/814	1.03	0/1103
3	hl	0.82	0/814	1.03	0/1103
3	il	0.82	0/814	1.03	0/1103

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	jl	0.82	0/814	1.03	0/1103
3	kl	0.82	0/814	1.03	0/1103
3	ll	0.82	0/814	1.03	0/1103
3	ml	0.82	0/814	1.03	0/1103
3	nl	0.82	0/814	1.03	0/1103
3	ol	0.82	0/814	1.03	0/1103
3	pl	0.82	0/814	1.03	0/1103
3	ql	0.82	0/814	1.03	0/1103
3	rl	0.82	0/814	1.03	0/1103
3	sl	0.82	0/814	1.03	0/1103
3	tl	0.82	0/814	1.03	0/1103
3	ul	0.82	0/814	1.03	0/1103
3	vl	0.82	0/814	1.03	0/1103
3	wl	0.82	0/814	1.03	0/1103
3	xl	0.82	0/814	1.03	0/1103
3	yl	0.82	0/814	1.03	0/1103
3	zl	0.82	0/814	1.03	0/1103
All	All	0.55	0/368580	0.82	601/502200 (0.1%)

There are no bond length outliers.

The worst 5 of 601 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	CYS	CA-CB-SG	-35.18	30.33	104.20
2	Jh	29	GLY	N-CA-C	8.01	122.34	112.73
2	Xh	29	GLY	N-CA-C	8.01	122.34	112.73
2	nh	29	GLY	N-CA-C	8.01	122.34	112.73
2	lh	29	GLY	N-CA-C	8.01	122.34	112.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4148	0	3901	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4148	0	3901	56	0
1	2	4148	0	3901	56	0
1	3	4148	0	3901	56	0
1	4	4148	0	3901	56	0
1	5	4148	0	3901	57	0
1	6	4148	0	3901	56	0
1	7	4148	0	3901	55	0
1	A	4148	0	3901	58	0
1	B	4148	0	3901	56	0
1	C	4148	0	3901	57	0
1	D	4148	0	3901	56	0
1	E	4148	0	3901	55	0
1	F	4148	0	3901	56	0
1	G	4148	0	3901	56	0
1	H	4148	0	3901	57	0
1	I	4148	0	3901	56	0
1	J	4148	0	3901	56	0
1	K	4148	0	3901	56	0
1	L	4148	0	3901	55	0
1	M	4148	0	3901	57	0
1	N	4148	0	3901	56	0
1	O	4148	0	3901	56	0
1	P	4148	0	3901	58	0
1	Q	4148	0	3901	55	0
1	R	4148	0	3901	55	0
1	S	4148	0	3901	55	0
1	T	4148	0	3901	55	0
1	U	4148	0	3901	55	0
1	V	4148	0	3901	56	0
1	W	4148	0	3901	56	0
1	X	4148	0	3901	55	0
1	Y	4148	0	3901	56	0
1	Z	4148	0	3901	54	0
1	a	4148	0	3901	55	0
1	b	4148	0	3901	56	0
1	c	4148	0	3901	57	0
1	d	4148	0	3901	55	0
1	e	4148	0	3901	57	0
1	f	4148	0	3901	55	0
1	g	4148	0	3901	55	0
1	h	4148	0	3901	56	0
1	i	4148	0	3901	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4148	0	3901	55	0
1	k	4148	0	3901	55	0
1	l	4148	0	3901	56	0
1	m	4148	0	3901	57	0
1	n	4148	0	3901	57	0
1	o	4148	0	3901	55	0
1	p	4148	0	3901	54	0
1	q	4148	0	3901	54	0
1	r	4148	0	3901	54	0
1	s	4148	0	3901	55	0
1	t	4148	0	3901	54	0
1	u	4148	0	3901	57	0
1	v	4148	0	3901	56	0
1	w	4148	0	3901	56	0
1	x	4148	0	3901	57	0
1	y	4148	0	3901	55	0
1	z	4148	0	3901	56	0
2	0h	1028	0	988	56	0
2	1h	1028	0	988	57	0
2	2h	1028	0	988	56	0
2	3h	1028	0	988	58	0
2	4h	1028	0	988	59	0
2	5h	1028	0	988	58	0
2	6h	1028	0	988	55	0
2	7h	1028	0	988	58	0
2	Ah	1028	0	988	58	0
2	Bh	1028	0	988	58	0
2	Ch	1028	0	988	58	0
2	Dh	1028	0	988	56	0
2	Eh	1028	0	988	55	0
2	Fh	1028	0	988	55	0
2	Gh	1028	0	988	58	0
2	Hh	1028	0	988	58	0
2	Ih	1028	0	988	57	0
2	Jh	1028	0	988	56	0
2	Kh	1028	0	988	57	0
2	Lh	1028	0	988	57	0
2	Mh	1028	0	988	56	0
2	Nh	1028	0	988	57	0
2	Oh	1028	0	988	59	0
2	Ph	1028	0	988	55	0
2	Qh	1028	0	988	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Rh	1028	0	988	57	0
2	Sh	1028	0	988	57	0
2	Th	1028	0	988	56	0
2	Uh	1028	0	988	57	0
2	Vh	1028	0	988	58	0
2	Wh	1028	0	988	57	0
2	Xh	1028	0	988	57	0
2	Yh	1028	0	988	58	0
2	Zh	1028	0	988	55	0
2	ah	1028	0	988	59	0
2	bh	1028	0	988	57	0
2	ch	1028	0	988	58	0
2	dh	1028	0	988	59	0
2	eh	1028	0	988	58	0
2	fh	1028	0	988	58	0
2	gh	1028	0	988	57	0
2	hh	1028	0	988	56	0
2	ih	1028	0	988	57	0
2	jh	1028	0	988	58	0
2	kh	1028	0	988	57	0
2	lh	1028	0	988	56	0
2	mh	1028	0	988	56	0
2	nh	1028	0	988	57	0
2	oh	1028	0	988	57	0
2	ph	1028	0	988	57	0
2	qh	1028	0	988	56	0
2	rh	1028	0	988	58	0
2	sh	1028	0	988	58	0
2	th	1028	0	988	57	0
2	uh	1028	0	988	56	0
2	vh	1028	0	988	57	0
2	wh	1028	0	988	57	0
2	xh	1028	0	988	57	0
2	yh	1028	0	988	56	0
2	zh	1028	0	988	57	0
3	0l	799	0	776	46	0
3	1l	799	0	776	46	0
3	2l	799	0	776	43	0
3	3l	799	0	776	46	0
3	4l	799	0	776	47	0
3	5l	799	0	776	44	0
3	6l	799	0	776	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7l	799	0	776	46	0
3	Al	799	0	776	46	0
3	Bl	799	0	776	46	0
3	Cl	799	0	776	46	0
3	Dl	799	0	776	47	0
3	El	799	0	776	47	0
3	Fl	799	0	776	45	0
3	Gl	799	0	776	46	0
3	Hl	799	0	776	46	0
3	Il	799	0	776	45	0
3	Jl	799	0	776	47	0
3	Kl	799	0	776	45	0
3	Ll	799	0	776	47	0
3	Ml	799	0	776	47	0
3	Nl	799	0	776	45	0
3	Ol	799	0	776	46	0
3	Pl	799	0	776	46	0
3	Ql	799	0	776	46	0
3	Rl	799	0	776	43	0
3	Sl	799	0	776	45	0
3	Tl	799	0	776	47	0
3	Ul	799	0	776	46	0
3	Vl	799	0	776	46	0
3	Wl	799	0	776	45	0
3	Xl	799	0	776	46	0
3	Yl	799	0	776	46	0
3	Zl	799	0	776	47	0
3	al	799	0	776	46	0
3	bl	799	0	776	46	0
3	cl	799	0	776	46	0
3	dl	799	0	776	47	0
3	el	799	0	776	44	0
3	fl	799	0	776	45	0
3	gl	799	0	776	47	0
3	hl	799	0	776	46	0
3	il	799	0	776	46	0
3	jl	799	0	776	45	0
3	kl	799	0	776	46	0
3	ll	799	0	776	43	0
3	ml	799	0	776	45	0
3	nl	799	0	776	46	0
3	ol	799	0	776	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	pl	799	0	776	45	0
3	ql	799	0	776	44	0
3	rl	799	0	776	46	0
3	sl	799	0	776	46	0
3	tl	799	0	776	47	0
3	ul	799	0	776	45	0
3	vl	799	0	776	46	0
3	wl	799	0	776	45	0
3	xl	799	0	776	46	0
3	yl	799	0	776	47	0
3	zl	799	0	776	46	0
All	All	358500	0	339900	8788	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 13.

The worst 5 of 8788 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)
2:th:37:LEU:HD21	2:th:149:VAL:HG11	1.28	1.16
2:Sh:37:LEU:HD21	2:Sh:149:VAL:HG11	1.28	1.16
2:ih:37:LEU:HD21	2:ih:149:VAL:HG11	1.28	1.16
2:Lh:37:LEU:HD21	2:Lh:149:VAL:HG11	1.28	1.15
2:Ih:37:LEU:HD21	2:Ih:149:VAL:HG11	1.28	1.15

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	516/533 (97%)	506 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	2	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	3	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	4	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	5	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	6	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	7	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	A	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	B	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	C	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	D	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	E	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	F	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	G	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	H	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	I	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	J	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	K	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	L	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	M	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	N	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	O	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	P	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	Q	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	R	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	S	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	T	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	U	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	V	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	W	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	X	516/533 (97%)	506 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	Z	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	a	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	b	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	c	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	d	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	e	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	f	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	g	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	h	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	i	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	j	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	k	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	l	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	m	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	n	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	o	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	p	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	q	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	r	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	s	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	t	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	u	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	v	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	w	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	x	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	y	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
1	z	516/533 (97%)	506 (98%)	10 (2%)	0	100	100
2	0h	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	1h	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	2h	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3h	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	4h	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	5h	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	6h	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	7h	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Ah	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Bh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Ch	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Dh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Eh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Fh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Gh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Hh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Ih	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Jh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Kh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Lh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Mh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Nh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Oh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Ph	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Qh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Rh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Sh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Th	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Uh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Vh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Wh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Xh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Yh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	Zh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	ah	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	bh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	ch	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	dh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	eh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	fh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	gh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	hh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	ih	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	jh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	kh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	lh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	mh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	nh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	oh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	ph	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	qh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	rh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	sh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	th	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	uh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	vh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	wh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	xh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	yh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
2	zh	130/153 (85%)	128 (98%)	1 (1%)	1 (1%)	16	28
3	0l	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	1l	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	2l	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	3l	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	4l	107/130 (82%)	101 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	5l	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	6l	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	7l	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Al	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Bl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Cl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Dl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	El	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Fl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Gl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Hl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Il	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Jl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Kl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Ll	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Ml	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Nl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Ol	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Pl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Ql	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Rl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Sl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Tl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Ul	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Vl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Wl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Xl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Yl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	Zl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	al	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	bl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	cl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	dl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	el	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	fl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	gl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	hl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	il	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	jl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	kl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	ll	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	ml	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	nl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	ol	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	pl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	ql	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	rl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	sl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	tl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	ul	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	vl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	wl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	xl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	yl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
3	zl	107/130 (82%)	101 (94%)	6 (6%)	0	100	100
All	All	45180/48960 (92%)	44100 (98%)	1020 (2%)	60 (0%)	49	66

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Ah	108	ALA
2	Bh	108	ALA
2	Ch	108	ALA
2	Dh	108	ALA
2	Eh	108	ALA

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	0	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	1	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	2	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	3	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	4	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	5	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	6	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	7	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	A	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	B	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	C	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	D	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	E	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	F	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	G	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	H	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	I	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	J	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	K	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	L	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	M	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	N	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	O	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	P	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	Q	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	R	459/468 (98%)	451 (98%)	8 (2%)	53	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	T	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	U	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	V	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	W	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	X	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	Y	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	Z	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	a	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	b	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	c	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	d	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	e	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	f	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	g	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	h	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	i	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	j	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	k	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	l	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	m	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	n	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	o	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	p	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	q	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	r	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	s	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	t	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	u	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	v	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	w	459/468 (98%)	451 (98%)	8 (2%)	53	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	y	459/468 (98%)	451 (98%)	8 (2%)	53	75
1	z	459/468 (98%)	451 (98%)	8 (2%)	53	75
2	0h	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	1h	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	2h	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	3h	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	4h	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	5h	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	6h	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	7h	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Ah	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Bh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Ch	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Dh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Eh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Fh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Gh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Hh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Ih	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Jh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Kh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Lh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Mh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Nh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Oh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Ph	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Qh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Rh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Sh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Th	114/131 (87%)	106 (93%)	8 (7%)	14	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Uh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Vh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Wh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Xh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Yh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	Zh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	ah	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	bh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	ch	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	dh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	eh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	fh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	gh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	hh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	ih	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	jh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	kh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	lh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	mh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	nh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	oh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	ph	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	qh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	rh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	sh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	th	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	uh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	vh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	wh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	xh	114/131 (87%)	106 (93%)	8 (7%)	14	27
2	yh	114/131 (87%)	106 (93%)	8 (7%)	14	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	zh	114/131 (87%)	106 (93%)	8 (7%)	14	27
3	0l	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	1l	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	2l	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	3l	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	4l	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	5l	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	6l	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	7l	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Al	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Bl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Cl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Dl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	El	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Fl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Gl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Hl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Il	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Jl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Kl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Ll	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Ml	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Nl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Ol	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Pl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Ql	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Rl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Sl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Tl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Ul	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Vl	91/109 (84%)	83 (91%)	8 (9%)	9	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Wl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Xl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Yl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	Zl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	al	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	bl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	cl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	dl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	el	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	fl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	gl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	hl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	il	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	jl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	kl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	ll	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	ml	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	nl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	ol	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	pl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	ql	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	rl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	sl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	tl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	ul	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	vl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	wl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	xl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	yl	91/109 (84%)	83 (91%)	8 (9%)	9	18
3	zl	91/109 (84%)	83 (91%)	8 (9%)	9	18
All	All	39840/42480 (94%)	38400 (96%)	1440 (4%)	32	55

5 of 1440 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3h	93	ASP
3	Xl	79	ARG
2	7h	30	LEU
2	3h	48	ILE
3	Kl	43	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1231 such sidechains are listed below:

Mol	Chain	Res	Type
1	w	288	HIS
1	7	629	HIS
1	x	518	ASN
1	w	253	ASN
1	2	288	HIS

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.

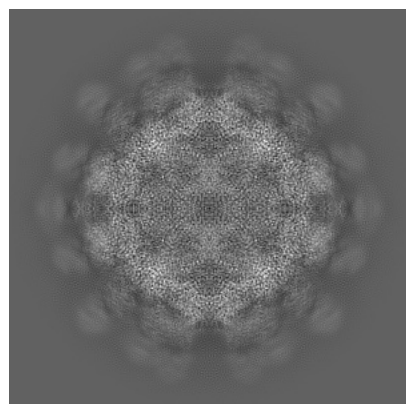
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76771. These allow visual inspection of the internal detail of the map and identification of artifacts.

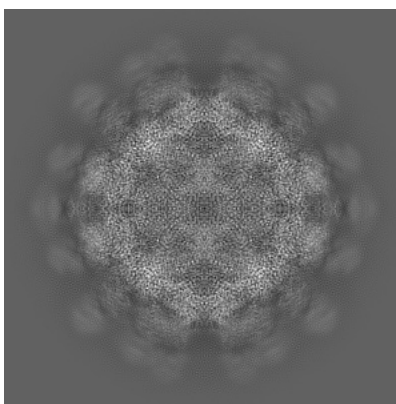
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

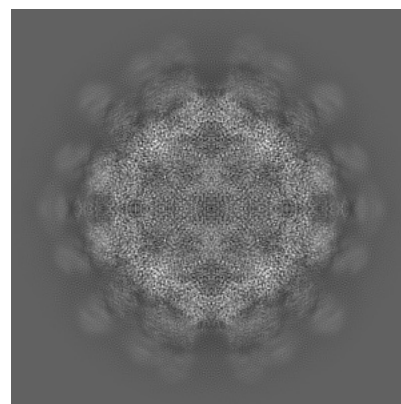
6.1.1 Primary map



X

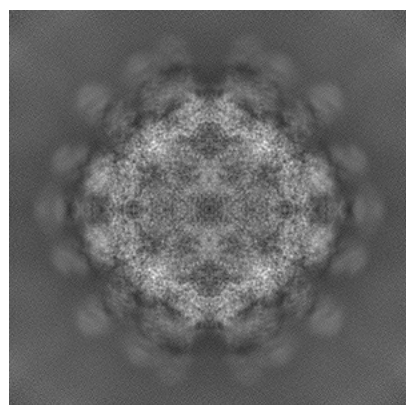


Y

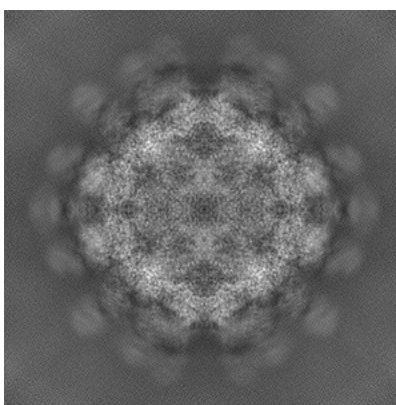


Z

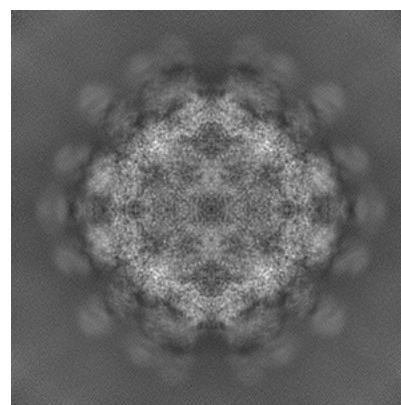
6.1.2 Raw map



X



Y

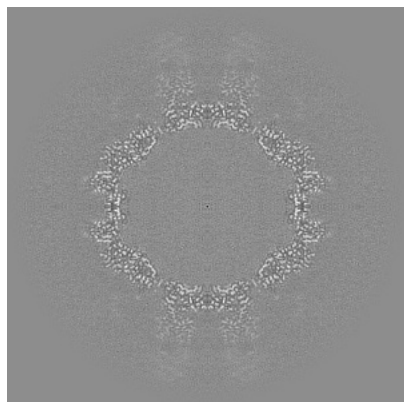


Z

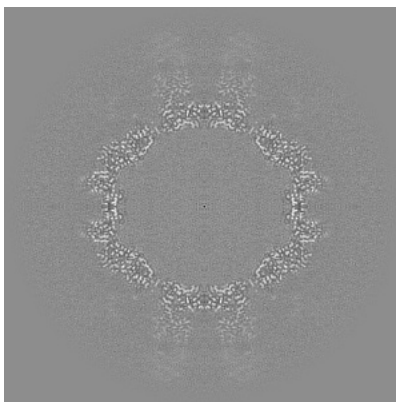
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

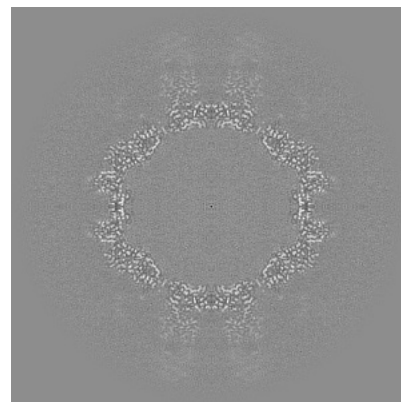
6.2.1 Primary map



X Index: 300

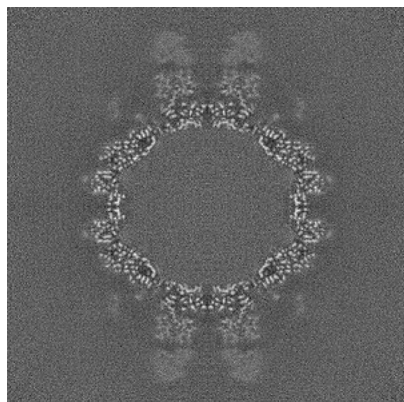


Y Index: 300

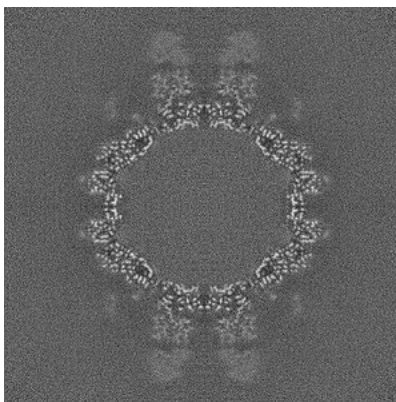


Z Index: 300

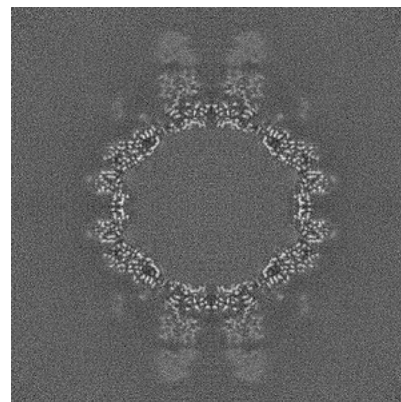
6.2.2 Raw map



X Index: 300



Y Index: 300

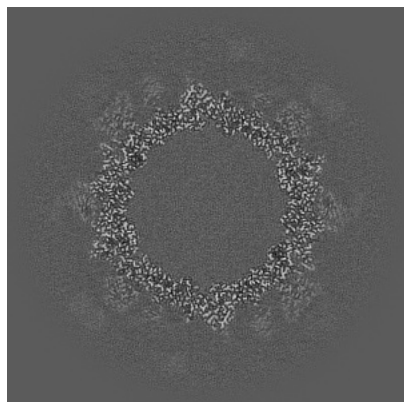


Z Index: 300

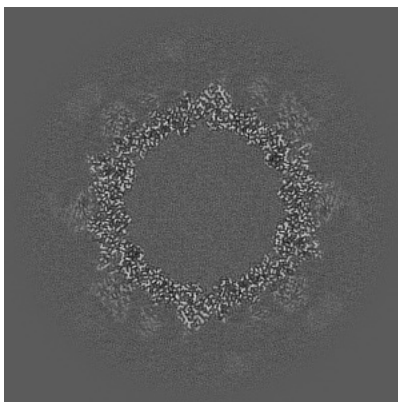
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

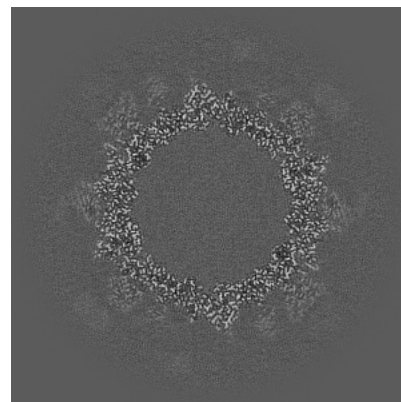
6.3.1 Primary map



X Index: 271

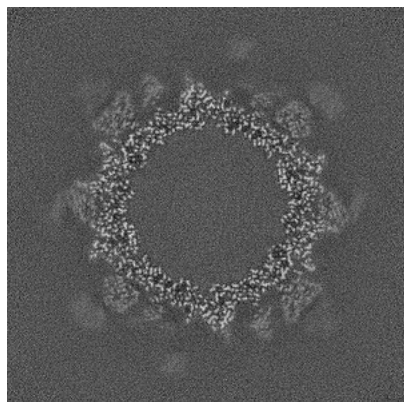


Y Index: 329

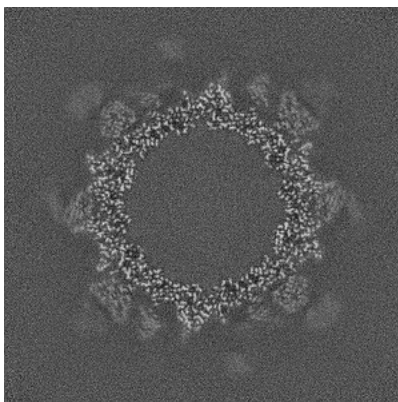


Z Index: 271

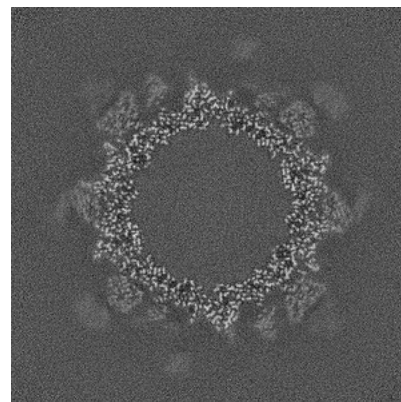
6.3.2 Raw map



X Index: 271



Y Index: 329

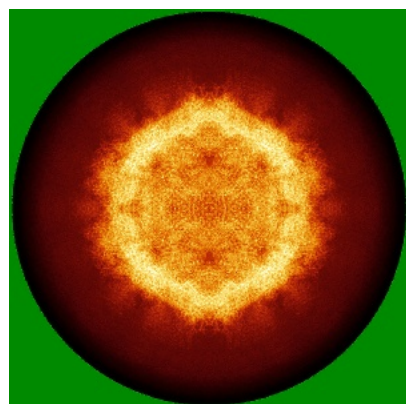


Z Index: 271

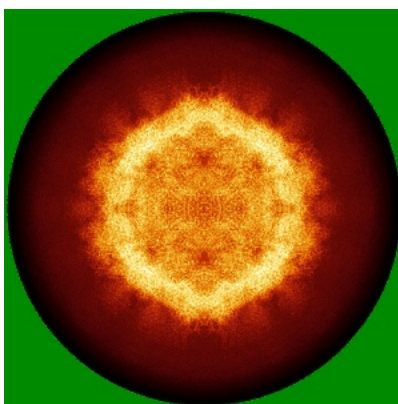
The images above show the largest variance slices of the map in three orthogonal directions.

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

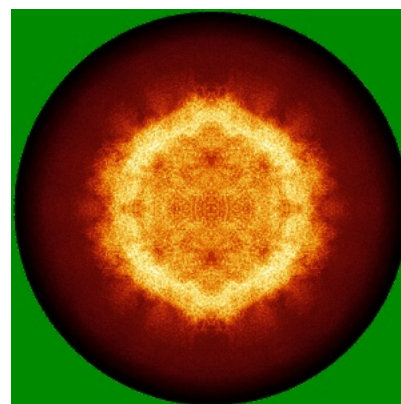
6.4.1 Primary map



X

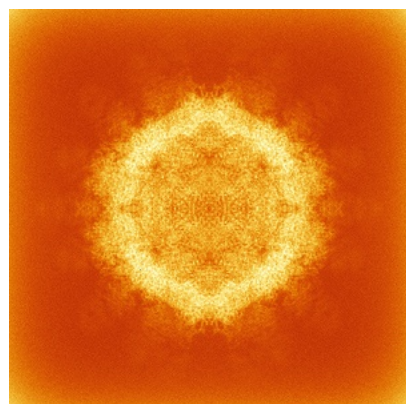


Y

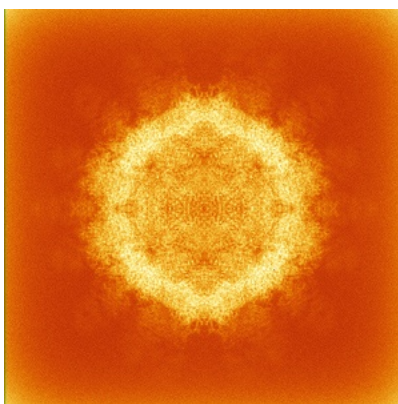


Z

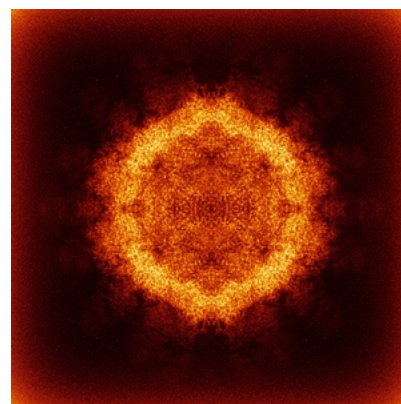
6.4.2 Raw map



X



Y

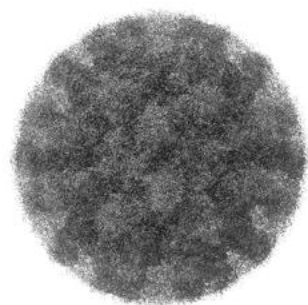


Z

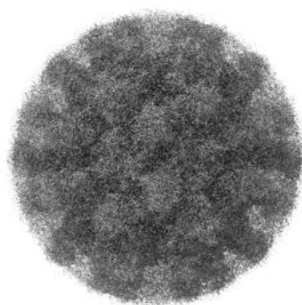
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

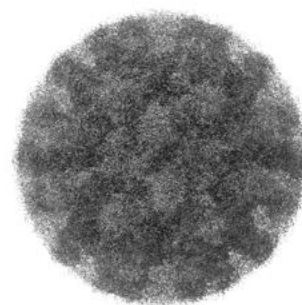
6.5.1 Primary map



X



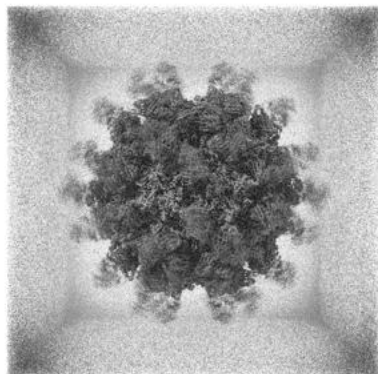
Y



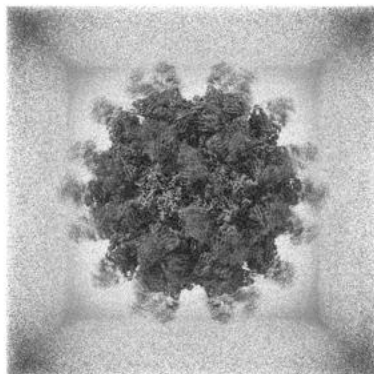
Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

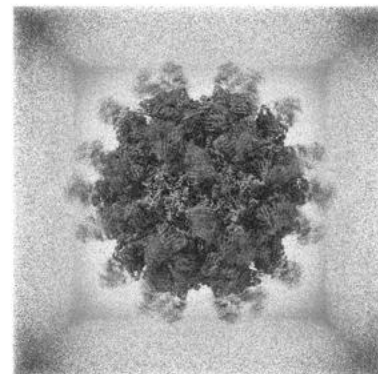
6.5.2 Raw map



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.

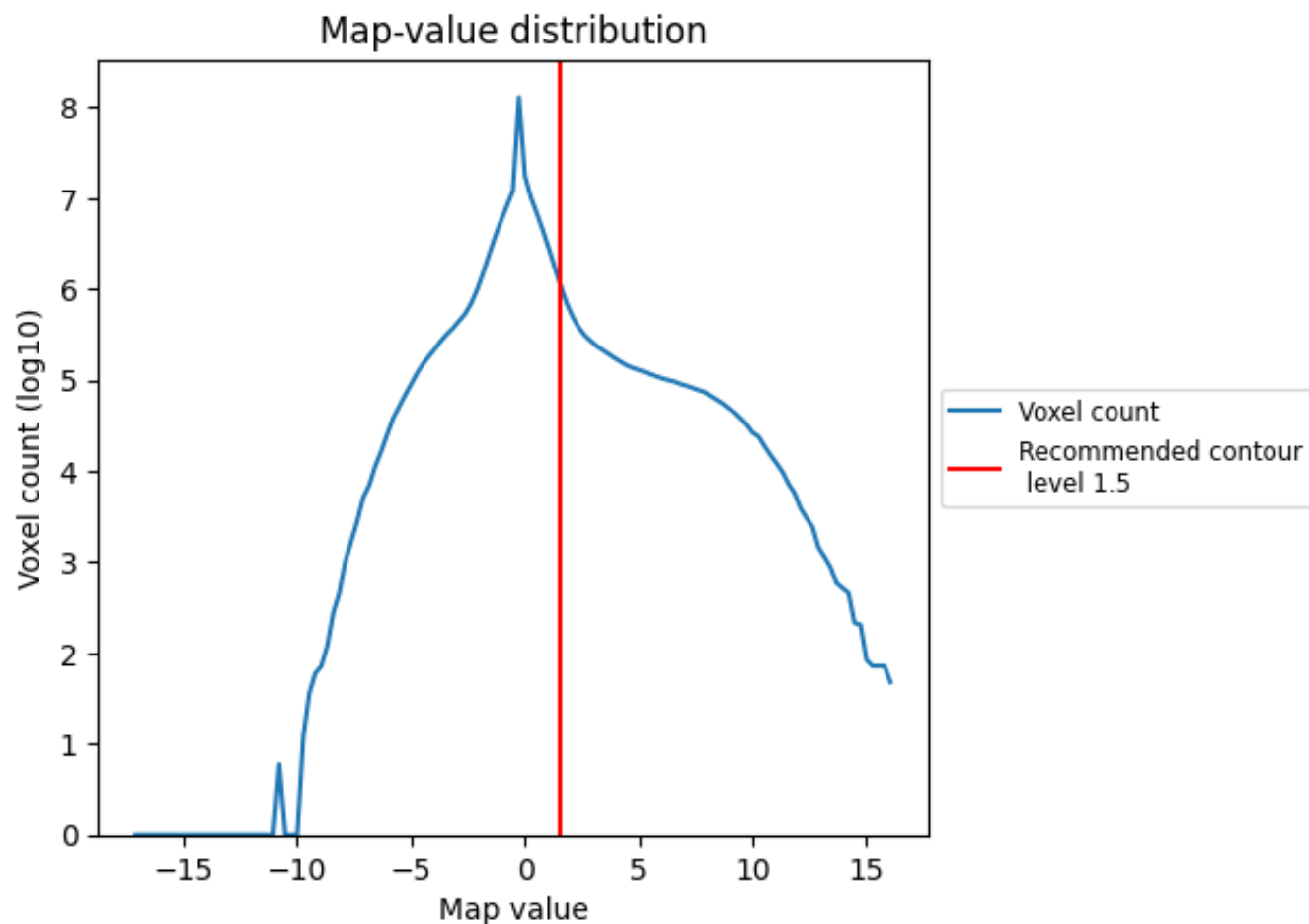
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

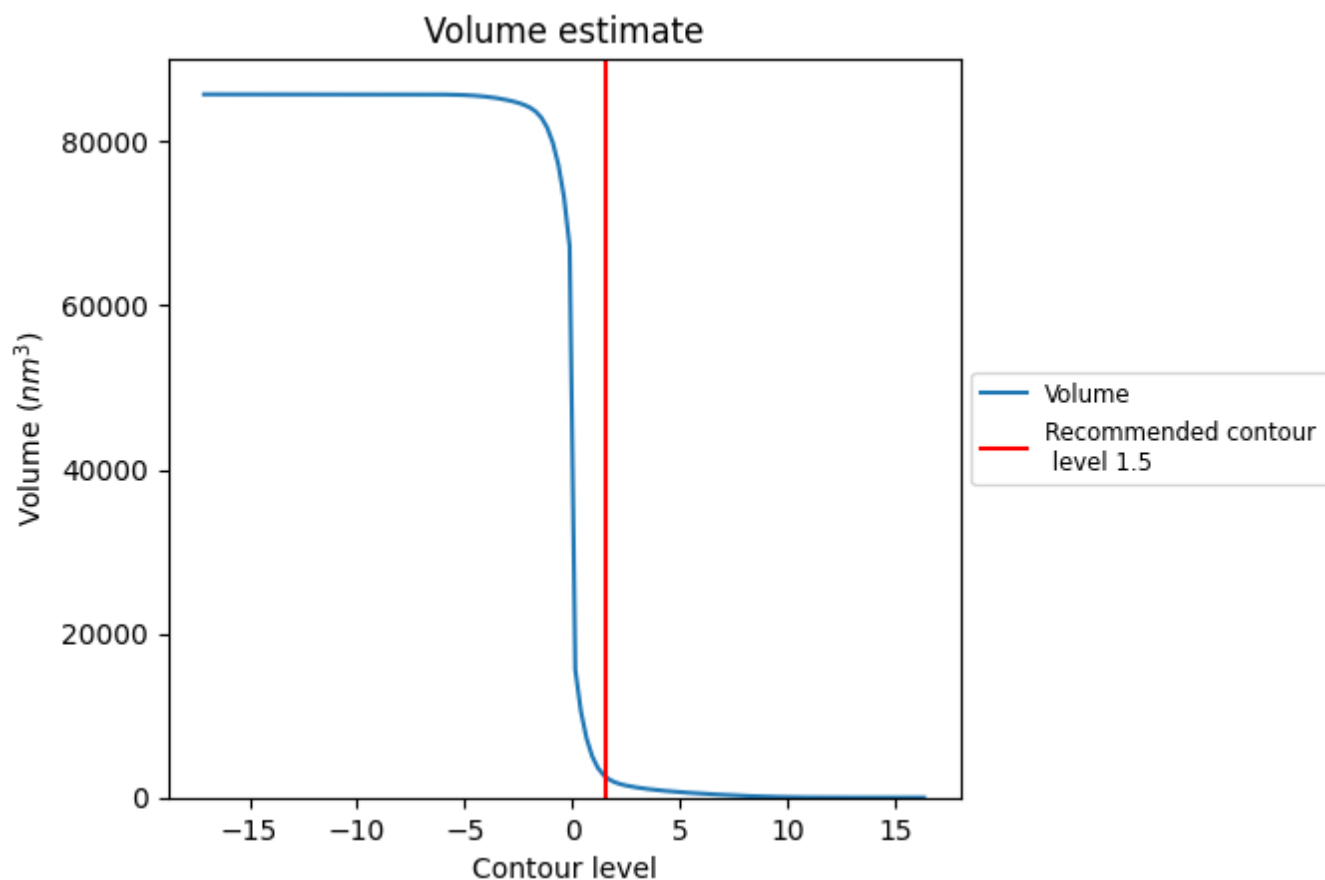
This section contains the results of statistical analysis of the map.

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.

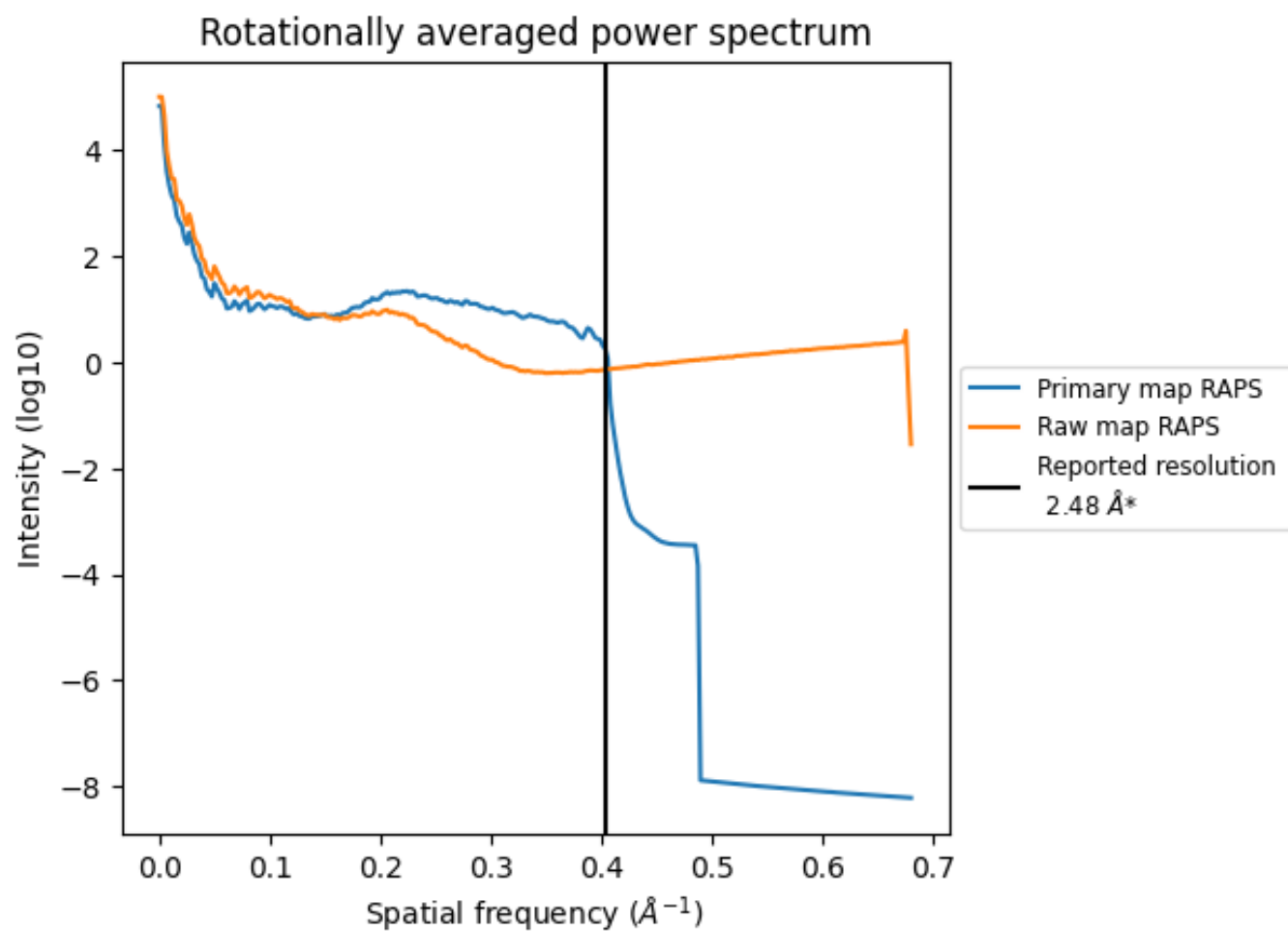
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2635 nm³; this corresponds to an approximate mass of 2380 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 ⓘ

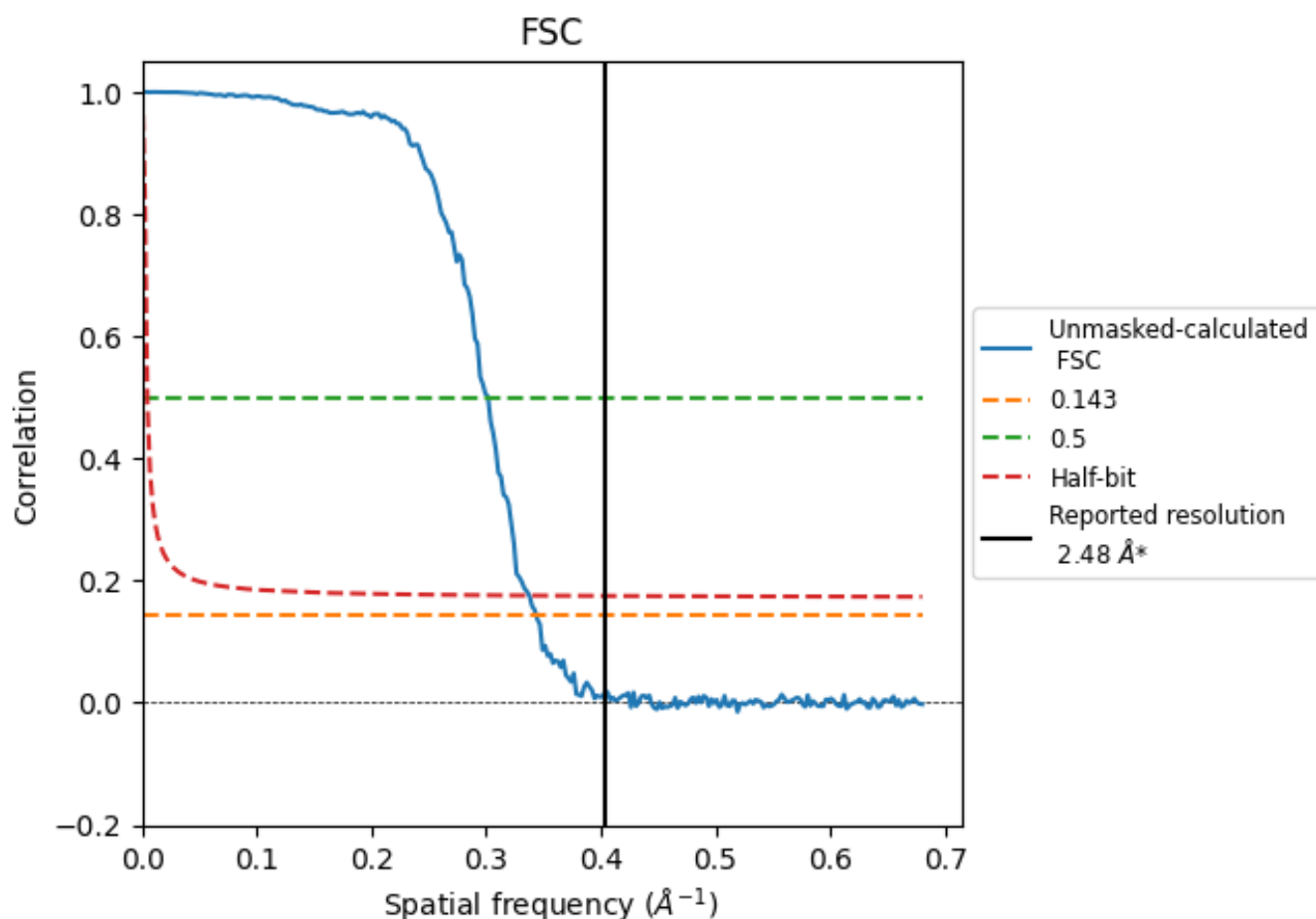


*Reported resolution corresponds to spatial frequency of 0.403 Å⁻¹

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 0.403 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

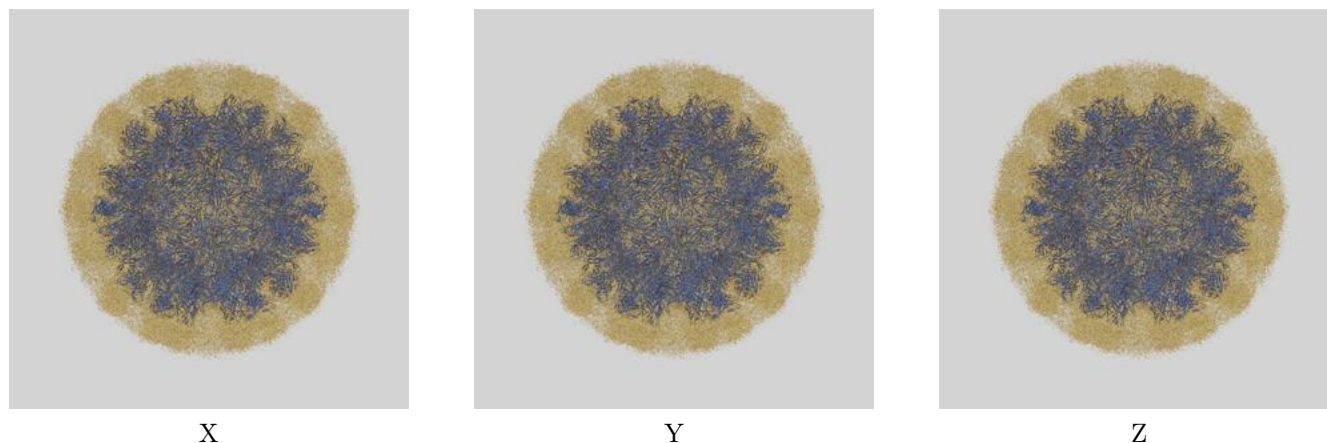
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.91	3.32	2.96

*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 2.91 differs from the reported value 2.48 by more than 10 %

9 Map-model fit [i](#)

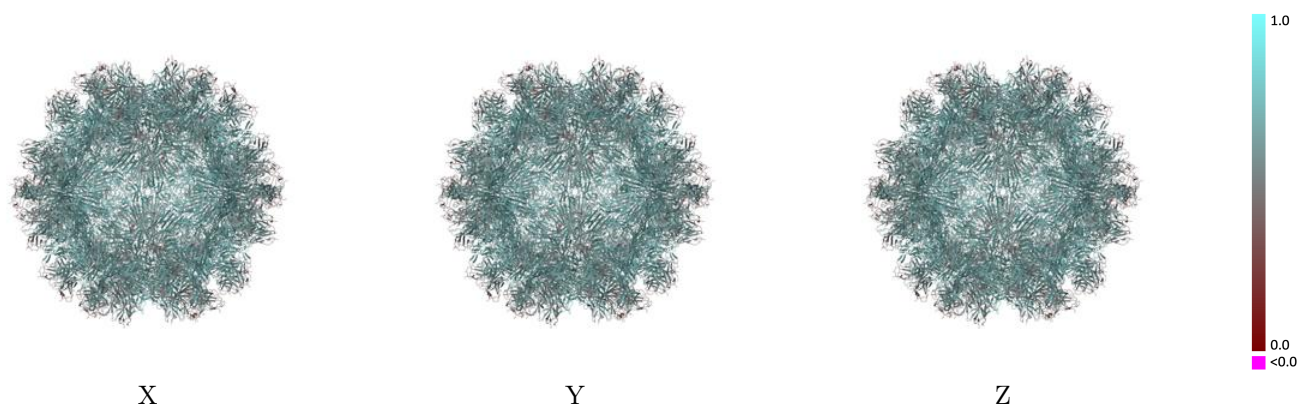
This section contains information regarding the fit between EMDB map EMD-76771 and PDB model 12UT. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



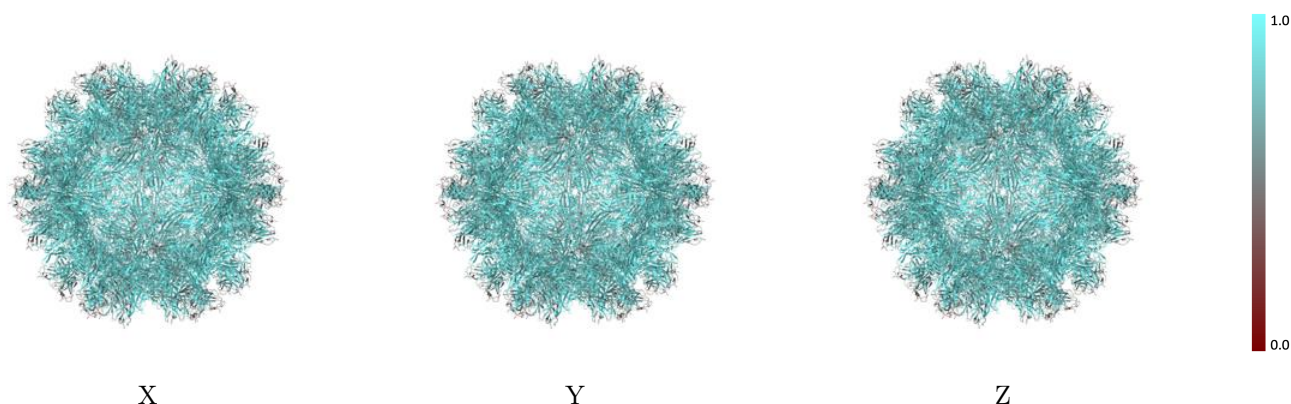
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



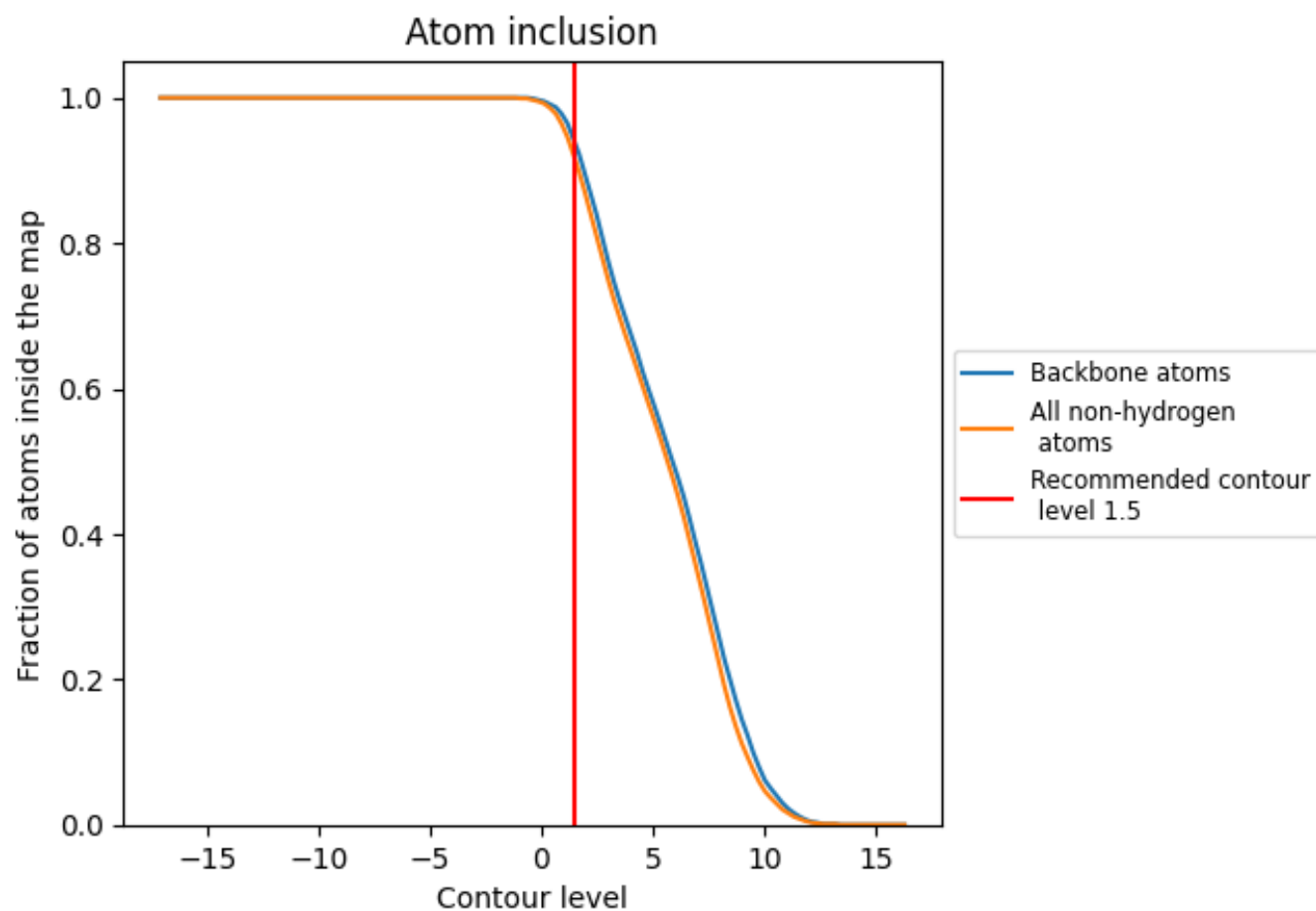
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.6490
0	 0.9860	 0.6930
0h	 0.8040	 0.5670
0l	 0.7070	 0.5230
1	 0.9860	 0.6940
1h	 0.8040	 0.5710
1l	 0.7070	 0.5220
2	 0.9860	 0.6930
2h	 0.8050	 0.5700
2l	 0.7070	 0.5230
3	 0.9880	 0.6940
3h	 0.8050	 0.5660
3l	 0.6970	 0.5200
4	 0.9870	 0.6930
4h	 0.8090	 0.5730
4l	 0.6970	 0.5260
5	 0.9860	 0.6930
5h	 0.8060	 0.5710
5l	 0.7040	 0.5270
6	 0.9880	 0.6940
6h	 0.8050	 0.5690
6l	 0.6970	 0.5210
7	 0.9870	 0.6930
7h	 0.8090	 0.5720
7l	 0.6970	 0.5230
A	 0.9860	 0.6940
Ah	 0.8160	 0.5750
Al	 0.7090	 0.5290
B	 0.9870	 0.6940
Bh	 0.8090	 0.5720
Bl	 0.6970	 0.5230
C	 0.9860	 0.6940
Ch	 0.8060	 0.5700
Cl	 0.7040	 0.5250
D	 0.9880	 0.6930



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Chain	Atom inclusion	Q-score
Dh	 0.8050	 0.5700
DI	 0.6970	 0.5210
E	 0.9880	 0.6940
Eh	 0.8020	 0.5720
El	 0.7000	 0.5210
F	 0.9880	 0.6930
Fh	 0.8020	 0.5690
Fl	 0.7000	 0.5240
G	 0.9880	 0.6930
Gh	 0.8020	 0.5720
Gl	 0.6990	 0.5250
H	 0.9860	 0.6940
Hh	 0.8050	 0.5740
HI	 0.7070	 0.5230
I	 0.9860	 0.6920
Ih	 0.8040	 0.5660
Il	 0.7070	 0.5200
J	 0.9860	 0.6930
Jh	 0.8040	 0.5710
JI	 0.7070	 0.5200
K	 0.9860	 0.6930
Kh	 0.8060	 0.5740
KI	 0.7040	 0.5250
L	 0.9880	 0.6940
Lh	 0.8050	 0.5650
LI	 0.6970	 0.5200
M	 0.9870	 0.6930
Mh	 0.8090	 0.5720
MI	 0.6970	 0.5240
N	 0.9880	 0.6920
Nh	 0.8020	 0.5730
NI	 0.7000	 0.5240
O	 0.9880	 0.6940
Oh	 0.8020	 0.5720
OI	 0.6990	 0.5220
P	 0.9880	 0.6940
Ph	 0.8020	 0.5690
PI	 0.7000	 0.5180
Q	 0.9870	 0.6920
Qh	 0.8090	 0.5730
QI	 0.6970	 0.5240
R	 0.9860	 0.6940

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Chain	Atom inclusion	Q-score
Rh	 0.8060	 0.5730
Rl	 0.7040	 0.5230
S	 0.9880	 0.6940
Sh	 0.8050	 0.5670
Sl	 0.6970	 0.5200
T	 0.9860	 0.6940
Th	 0.8060	 0.5730
Tl	 0.7020	 0.5250
U	 0.9880	 0.6930
Uh	 0.8050	 0.5700
Ul	 0.6970	 0.5210
V	 0.9870	 0.6940
Vh	 0.8090	 0.5680
Vl	 0.6970	 0.5210
W	 0.9860	 0.6930
Wh	 0.8040	 0.5660
Wl	 0.7070	 0.5210
X	 0.9860	 0.6930
Xh	 0.8040	 0.5710
Xl	 0.7070	 0.5220
Y	 0.9860	 0.6930
Yh	 0.8050	 0.5710
Yl	 0.7070	 0.5230
Z	 0.9880	 0.6940
Zh	 0.8050	 0.5680
Zl	 0.6970	 0.5190
a	 0.9870	 0.6930
ah	 0.8090	 0.5720
al	 0.6970	 0.5260
b	 0.9860	 0.6930
bh	 0.8060	 0.5720
bl	 0.7040	 0.5270
c	 0.9880	 0.6940
ch	 0.8050	 0.5670
cl	 0.6990	 0.5200
d	 0.9870	 0.6940
dh	 0.8090	 0.5730
dl	 0.6970	 0.5260
e	 0.9860	 0.6940
eh	 0.8060	 0.5710
el	 0.7040	 0.5260
f	 0.9870	 0.6940

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Chain	Atom inclusion	Q-score
fh	 0.8090	 0.5730
fl	 0.6970	 0.5230
g	 0.9860	 0.6930
gh	 0.8060	 0.5690
gl	 0.7040	 0.5240
h	 0.9880	 0.6930
hh	 0.8050	 0.5690
hl	 0.6970	 0.5200
i	 0.9880	 0.6930
ih	 0.8020	 0.5700
il	 0.7000	 0.5250
j	 0.9880	 0.6930
jh	 0.8020	 0.5690
jl	 0.7000	 0.5210
k	 0.9880	 0.6930
kh	 0.8020	 0.5740
kl	 0.6990	 0.5210
l	 0.9860	 0.6930
lh	 0.8050	 0.5730
ll	 0.7070	 0.5230
m	 0.9860	 0.6930
mh	 0.8040	 0.5650
ml	 0.7070	 0.5190
n	 0.9860	 0.6940
nh	 0.8040	 0.5700
nl	 0.7070	 0.5200
o	 0.9860	 0.6940
oh	 0.8070	 0.5760
ol	 0.7000	 0.5290
p	 0.9880	 0.6940
ph	 0.8050	 0.5640
pl	 0.6970	 0.5170
q	 0.9870	 0.6930
qh	 0.8090	 0.5730
ql	 0.6970	 0.5230
r	 0.9880	 0.6930
rh	 0.8020	 0.5720
rl	 0.7000	 0.5220
s	 0.9880	 0.6940
sh	 0.8020	 0.5720
sl	 0.6990	 0.5200
t	 0.9880	 0.6940

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Chain	Atom inclusion	Q-score
th	 0.8020	 0.5680
tl	 0.7000	 0.5210
u	 0.9870	 0.6930
uh	 0.8090	 0.5740
ul	 0.6970	 0.5240
v	 0.9860	 0.6940
vh	 0.8060	 0.5750
vl	 0.7040	 0.5260
w	 0.9880	 0.6940
wh	 0.8050	 0.5660
wl	 0.6970	 0.5170
x	 0.9860	 0.6940
xh	 0.8080	 0.5730
xl	 0.7020	 0.5240
y	 0.9880	 0.6940
yh	 0.8050	 0.5700
yl	 0.6970	 0.5230
z	 0.9870	 0.6930
zh	 0.8090	 0.5680
zl	 0.6970	 0.5210