



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 05:52 PM BST

PDB ID : 4CTF
EMDB ID: : EMD-2389
Title : The limits of structural plasticity in a picornavirus capsid revealed by a massively expanded equine rhinitis A virus particle
Authors : Bakker, S.E.; Groppelli, E.; Pearson, A.R.; Stockley, P.G.; Rowlands, D.J.; Ranson, N.A.
Deposited on : 2014-04-02
Resolution : 17.00 Å(reported)
Based on PDB ID : 2WFF

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

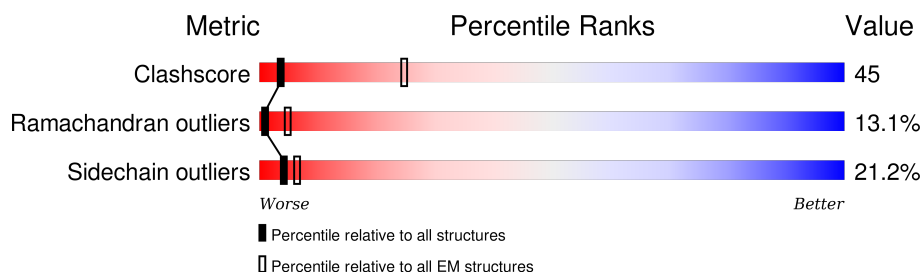
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 Å.

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



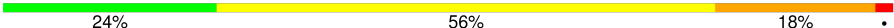
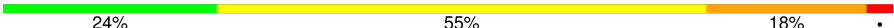
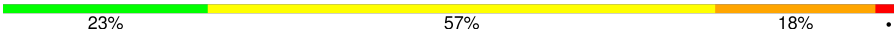
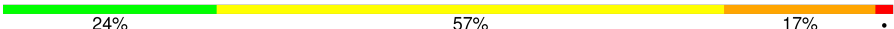
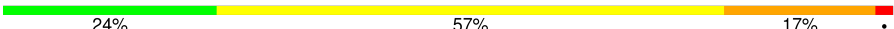
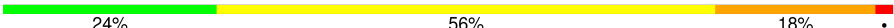
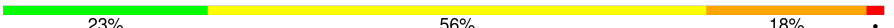
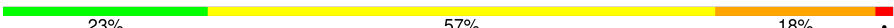
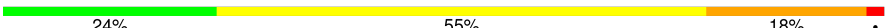
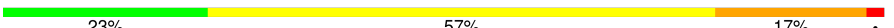
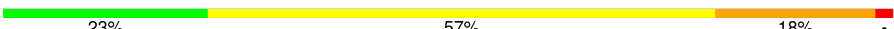
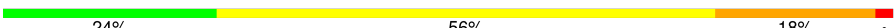
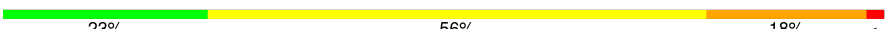
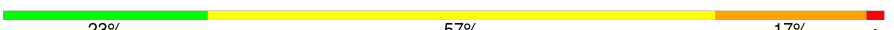
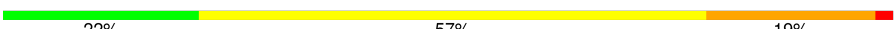
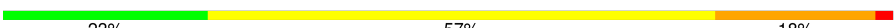
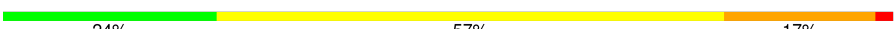







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A0	246	23% 57% 18% .
1	A1	246	24% 55% 19% .
1	A2	246	23% 57% 18% .
1	A3	246	25% 55% 18% .
1	A4	246	24% 56% 18% .
1	A5	246	23% 56% 18% .
1	A6	246	22% 58% 17% .
1	A7	246	24% 56% 18% .
1	A8	246	24% 56% 18% .

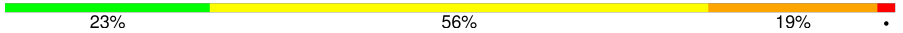
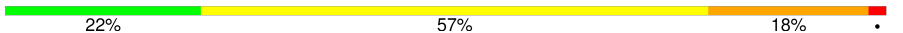
















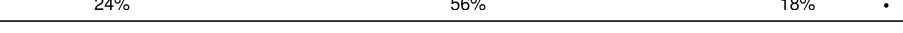
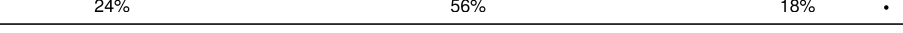
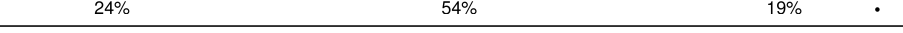
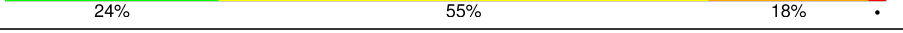
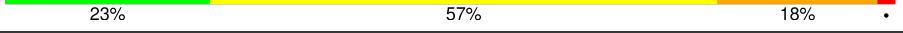
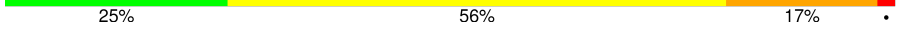
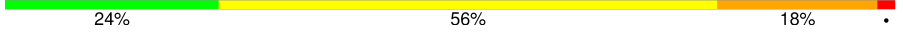
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	A9	246	 24% 56% 18% .
1	AA	246	 24% 55% 18% .
1	AB	246	 23% 57% 18% .
1	AC	246	 24% 57% 17% .
1	AD	246	 24% 57% 17% .
1	AE	246	 24% 56% 18% .
1	AF	246	 23% 56% 18% .
1	AG	246	 23% 57% 18% .
1	AH	246	 24% 55% 18% .
1	AI	246	 23% 57% 17% .
1	AJ	246	 23% 57% 18% .
1	AK	246	 24% 56% 18% .
1	AL	246	 23% 56% 18% .
1	AM	246	 23% 57% 17% .
1	AN	246	 22% 57% 19% .
1	AO	246	 23% 57% 18% .
1	AP	246	 24% 57% 17% .
1	AQ	246	 24% 56% 18% .
1	AR	246	 24% 56% 18% .
1	AS	246	 23% 57% 17% .
1	AT	246	 23% 57% 18% .
1	AU	246	 24% 56% 18% .
1	AV	246	 24% 57% 17% .
1	AW	246	 24% 56% 18% .
1	AX	246	 24% 56% 18% .

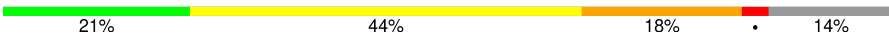
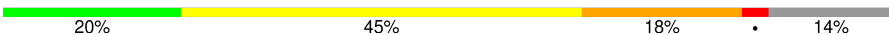
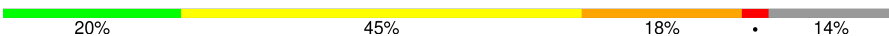
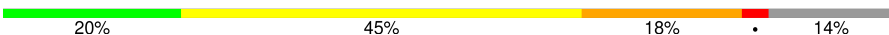
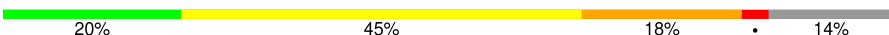


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AY	246	
1	AZ	246	
1	Aa	246	
1	Ab	246	
1	Ac	246	
1	Ad	246	
1	Ae	246	
1	Af	246	
1	Ag	246	
1	Ah	246	
1	Ai	246	
1	Aj	246	
1	Ak	246	
1	Al	246	
1	Am	246	
1	An	246	
1	Ao	246	
1	BA	246	
1	BB	246	
1	BC	246	
1	BD	246	
1	BE	246	
1	BF	246	
1	BG	246	
1	BH	246	


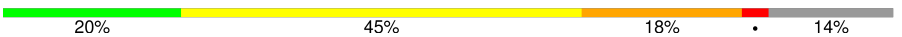



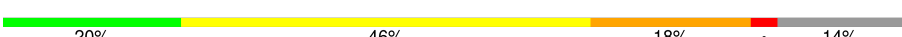
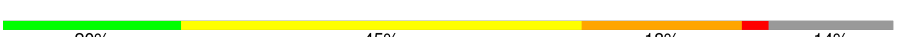
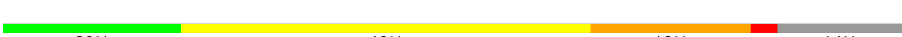
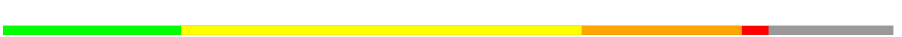

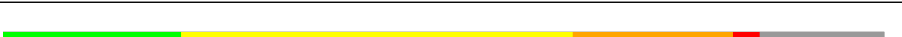
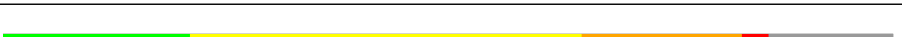

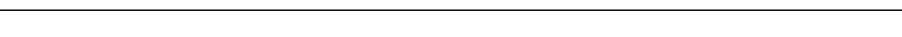
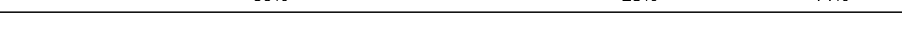
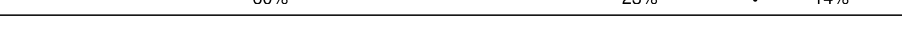



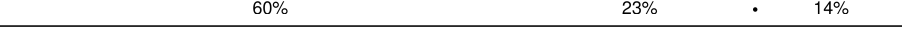





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	BI	246	
2	C0	230	
2	C1	230	
2	C2	230	
2	C3	230	
2	C4	230	
2	C5	230	
2	C6	230	
2	C7	230	
2	C8	230	
2	C9	230	
2	CA	230	
2	CB	230	
2	CC	230	
2	CD	230	
2	CE	230	
2	CF	230	
2	CG	230	
2	CH	230	
2	CI	230	
2	CJ	230	
2	CK	230	
2	CL	230	
2	CM	230	
2	CN	230	












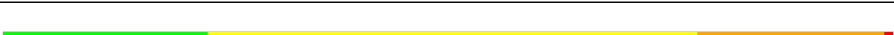

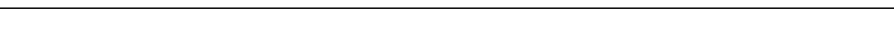
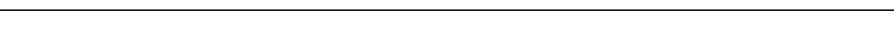
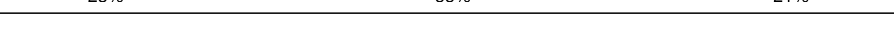
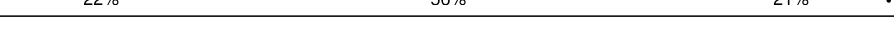
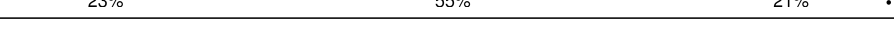
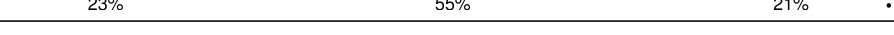
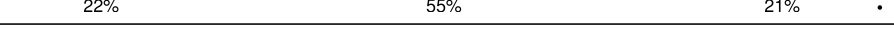
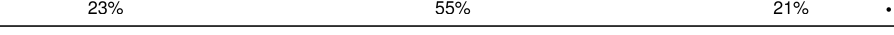
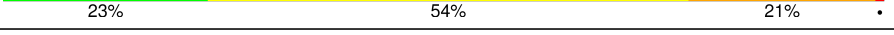
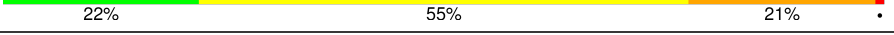
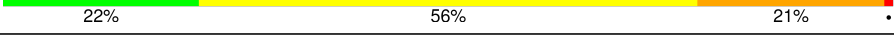
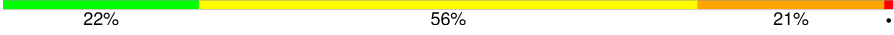
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	CO	230	
2	CP	230	
2	CQ	230	
2	CR	230	
2	CS	230	
2	CT	230	
2	CU	230	
2	CV	230	
2	CW	230	
2	CX	230	
2	CY	230	
2	CZ	230	
2	Ca	230	
2	Cb	230	
2	Cc	230	
2	Cd	230	
2	Ce	230	
2	Cf	230	
2	Cg	230	
2	Ch	230	
2	Ci	230	
2	Cj	230	
2	Ck	230	
2	Cl	230	
2	Cm	230	

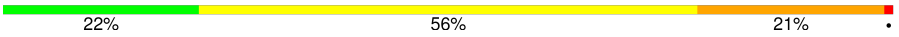
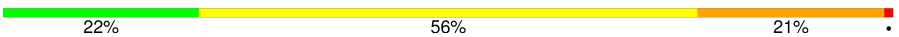
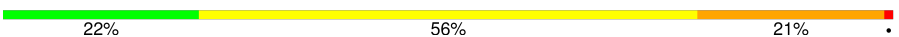
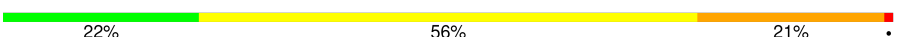
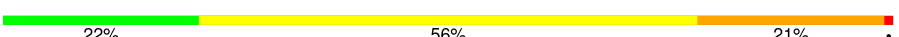
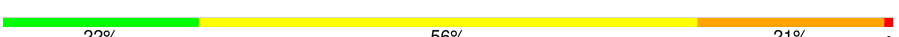
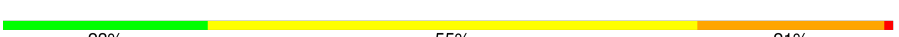

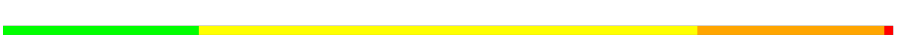

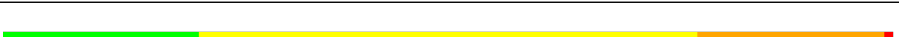
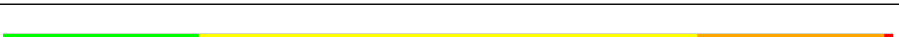

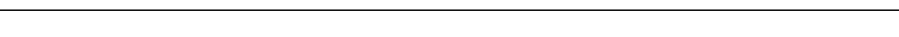
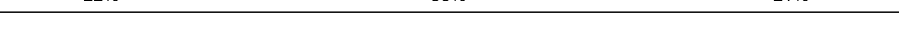
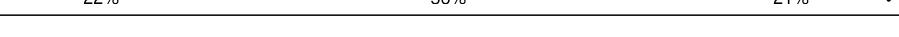
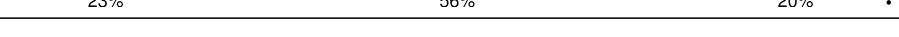
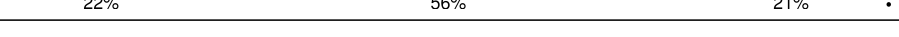
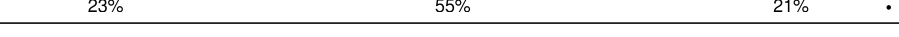
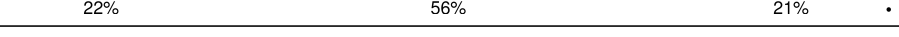
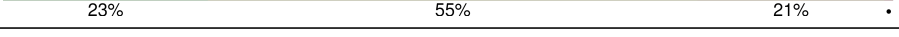
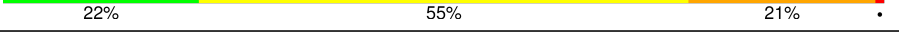
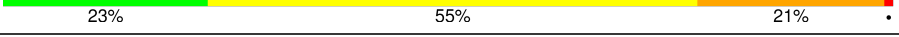


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Cn	230	
2	Co	230	
2	Cp	230	
2	Cq	230	
2	Cr	230	
2	Cs	230	
2	Ct	230	
2	Cu	230	
2	Cv	230	
2	Cw	230	
2	Cx	230	
3	D0	226	
3	D1	226	
3	D2	226	
3	D3	226	
3	D4	226	
3	D5	226	
3	D6	226	
3	D7	226	
3	D8	226	
3	D9	226	
3	DA	226	
3	DB	226	
3	DC	226	
3	DD	226	











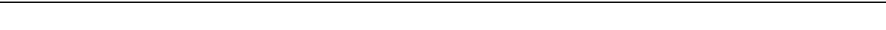

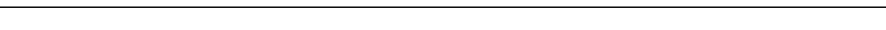
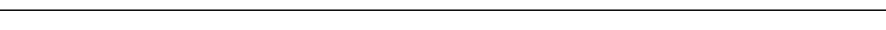



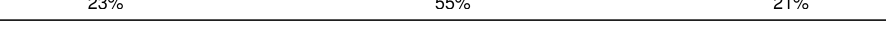
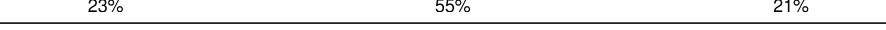
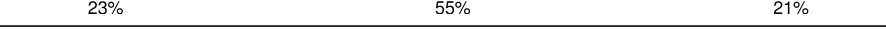
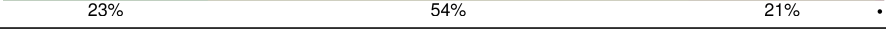
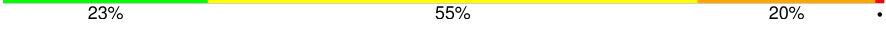



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	DE	226	 22% 56% 21% .
3	DF	226	 22% 56% 21% .
3	DG	226	 22% 56% 21% .
3	DH	226	 22% 56% 21% .
3	DI	226	 22% 56% 21% .
3	DJ	226	 22% 56% 21% .
3	DK	226	 23% 55% 21% .
3	DL	226	 23% 55% 21% .
3	DM	226	 22% 56% 21% .
3	DN	226	 23% 55% 21% .
3	DO	226	 22% 56% 21% .
3	DP	226	 22% 56% 21% .
3	DQ	226	 22% 56% 21% .
3	DR	226	 22% 56% 21% .
3	DS	226	 22% 56% 21% .
3	DT	226	 23% 56% 20% .
3	DU	226	 22% 56% 21% .
3	DV	226	 23% 55% 21% .
3	DW	226	 22% 56% 21% .
3	DX	226	 23% 55% 21% .
3	DY	226	 22% 55% 21% .
3	DZ	226	 23% 55% 21% .
3	Da	226	 69% 29% .
3	Db	226	 69% 29% .
3	Dc	226	 69% 29% .

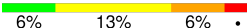
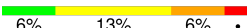
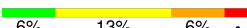
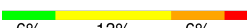
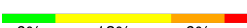
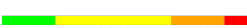







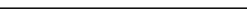

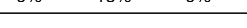
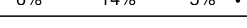
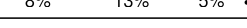
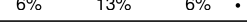
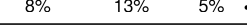
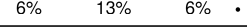
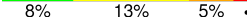
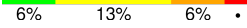
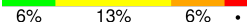
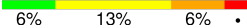
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Dd	226	 69% 29% .
3	De	226	 69% 29% .
3	Df	226	 69% 29% .
3	Dg	226	 69% 29% .
3	Dh	226	 69% 29% .
3	Di	226	 69% 29% .
3	Dj	226	 70% 28% .
3	Dk	226	 69% 29% .
3	Dl	226	 69% 29% .
3	Dm	226	 69% 29% .
3	Dn	226	 69% 29% .
3	Do	226	 69% 29% .
3	Dp	226	 69% 29% .
3	Dq	226	 70% 28% .
3	Dr	226	 69% 29% .
3	Ds	226	 69% 29% .
3	EA	226	 23% 55% 21% .
3	EB	226	 23% 55% 21% .
3	EC	226	 23% 55% 21% .
3	ED	226	 23% 54% 21% .
3	EE	226	 23% 55% 20% .
4	F0	80	 6% 13% 6% . 73%
4	F1	80	 6% 13% 6% . 73%
4	F2	80	 8% 13% 5% . 73%
4	F3	80	 8% 13% 5% . 73%

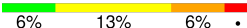
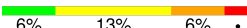
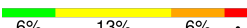
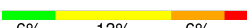
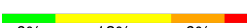
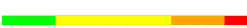







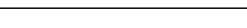











Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F4	80	 73%
4	F5	80	 73%
4	F6	80	 73%
4	F7	80	 73%
4	F8	80	 73%
4	F9	80	 73%
4	FA	80	 73%
4	FB	80	 73%
4	FC	80	 73%
4	FD	80	 73%
4	FE	80	 73%
4	FF	80	 73%
4	FG	80	 73%
4	FH	80	 73%
4	FI	80	 73%
4	FJ	80	 73%
4	FK	80	 73%
4	FL	80	 73%
4	FM	80	 73%
4	FN	80	 73%
4	FO	80	 73%
4	FP	80	 73%
4	FQ	80	 73%
4	FR	80	 73%
4	FS	80	 73%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	FT	80	 73%
4	FU	80	 73%
4	FV	80	 73%
4	FW	80	 73%
4	FX	80	 73%
4	FY	80	 73%
4	FZ	80	 73%
4	Fa	80	 73%
4	Fb	80	 73%
4	Fc	80	 73%
4	Fd	80	 73%
4	Fe	80	 73%
4	Ff	80	 73%
4	Fg	80	 73%
4	Fh	80	 73%
4	Fi	80	 73%
4	Fj	80	 73%
4	Fk	80	 73%
4	Fl	80	 73%
4	Fm	80	 73%
4	Fn	80	 73%
4	Fo	80	 73%
4	Fp	80	 73%
4	Fq	80	 73%
4	Fr	80	 73%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Fs	80	<div><div><div></div><div></div><div></div></div><div>19%6%•</div><div>73%</div></div>
4	Ft	80	<div><div><div></div><div></div><div></div></div><div>19%6%•</div><div>73%</div></div>
4	Fu	80	<div><div><div></div><div></div><div></div></div><div>19%6%•</div><div>73%</div></div>
4	Fv	80	<div><div><div></div><div></div><div></div></div><div>19%6%•</div><div>73%</div></div>
4	Fw	80	<div><div><div></div><div></div><div></div></div><div>19%6%•</div><div>73%</div></div>
4	Fx	80	<div><div><div></div><div></div><div></div></div><div>19%6%•</div><div>73%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 321060 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A1	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A2	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A3	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A4	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A5	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A6	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A7	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A8	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	A9	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AA	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AB	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AC	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AD	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AE	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AF	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AG	246	Total 1929	C 1240	N 329	O 352	S 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AH	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AI	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AJ	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AK	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AL	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AM	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AN	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AO	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AP	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AQ	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AR	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AS	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AT	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AU	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AV	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AW	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AX	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AY	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	AZ	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Aa	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Ab	246	Total 1929	C 1240	N 329	O 352	S 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ac	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Ad	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Ae	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Af	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Ag	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Ah	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Ai	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Aj	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Ak	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Al	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Am	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	An	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	Ao	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	BA	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	BB	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	BC	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	BD	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	BE	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	BF	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	BG	246	Total 1929	C 1240	N 329	O 352	S 8	0	0
1	BH	246	Total 1929	C 1240	N 329	O 352	S 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BI	246	Total	C	N	O	S	0	0
			1929	1240	329	352	8		

- Molecule 2 is a protein called EQUINE RHINITIS A VIRUS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C0	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C1	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C2	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C3	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C4	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C5	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C6	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C7	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C8	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	C9	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	CA	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	CB	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	CC	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	CD	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	CE	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	CF	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	CG	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		
2	CH	198	Total	C	N	O	S	0	0
			1537	986	261	286	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CI	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CJ	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CK	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CL	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CM	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CN	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CO	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CP	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CQ	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CR	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CS	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CT	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CU	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CV	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CW	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CX	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CY	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	CZ	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Ca	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cb	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cc	198	Total 1537	C 986	N 261	O 286	S 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Cd	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Ce	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cf	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cg	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Ch	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Ci	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cj	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Ck	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cl	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cm	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cn	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Co	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cp	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cq	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cr	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cs	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Ct	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cu	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cv	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cw	198	Total 1537	C 986	N 261	O 286	S 4	0	0
2	Cx	198	Total 1537	C 986	N 261	O 286	S 4	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	85	SER	GLY	CONFLICT	UNP Q91B42
C1	85	SER	GLY	CONFLICT	UNP Q91B42
C2	85	SER	GLY	CONFLICT	UNP Q91B42
C3	85	SER	GLY	CONFLICT	UNP Q91B42
C4	85	SER	GLY	CONFLICT	UNP Q91B42
C5	85	SER	GLY	CONFLICT	UNP Q91B42
C6	85	SER	GLY	CONFLICT	UNP Q91B42
C7	85	SER	GLY	CONFLICT	UNP Q91B42
C8	85	SER	GLY	CONFLICT	UNP Q91B42
C9	85	SER	GLY	CONFLICT	UNP Q91B42
CA	85	SER	GLY	CONFLICT	UNP Q91B42
CB	85	SER	GLY	CONFLICT	UNP Q91B42
CC	85	SER	GLY	CONFLICT	UNP Q91B42
CD	85	SER	GLY	CONFLICT	UNP Q91B42
CE	85	SER	GLY	CONFLICT	UNP Q91B42
CF	85	SER	GLY	CONFLICT	UNP Q91B42
CG	85	SER	GLY	CONFLICT	UNP Q91B42
CH	85	SER	GLY	CONFLICT	UNP Q91B42
CI	85	SER	GLY	CONFLICT	UNP Q91B42
CJ	85	SER	GLY	CONFLICT	UNP Q91B42
CK	85	SER	GLY	CONFLICT	UNP Q91B42
CL	85	SER	GLY	CONFLICT	UNP Q91B42
CM	85	SER	GLY	CONFLICT	UNP Q91B42
CN	85	SER	GLY	CONFLICT	UNP Q91B42
CO	85	SER	GLY	CONFLICT	UNP Q91B42
CP	85	SER	GLY	CONFLICT	UNP Q91B42
CQ	85	SER	GLY	CONFLICT	UNP Q91B42
CR	85	SER	GLY	CONFLICT	UNP Q91B42
CS	85	SER	GLY	CONFLICT	UNP Q91B42
CT	85	SER	GLY	CONFLICT	UNP Q91B42
CU	85	SER	GLY	CONFLICT	UNP Q91B42
CV	85	SER	GLY	CONFLICT	UNP Q91B42
CW	85	SER	GLY	CONFLICT	UNP Q91B42
CX	85	SER	GLY	CONFLICT	UNP Q91B42
CY	85	SER	GLY	CONFLICT	UNP Q91B42
CZ	85	SER	GLY	CONFLICT	UNP Q91B42
Ca	85	SER	GLY	CONFLICT	UNP Q91B42
Cb	85	SER	GLY	CONFLICT	UNP Q91B42
Cc	85	SER	GLY	CONFLICT	UNP Q91B42
Cd	85	SER	GLY	CONFLICT	UNP Q91B42
Ce	85	SER	GLY	CONFLICT	UNP Q91B42
Cf	85	SER	GLY	CONFLICT	UNP Q91B42

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	85	SER	GLY	CONFLICT	UNP Q91B42
Ch	85	SER	GLY	CONFLICT	UNP Q91B42
Ci	85	SER	GLY	CONFLICT	UNP Q91B42
Cj	85	SER	GLY	CONFLICT	UNP Q91B42
Ck	85	SER	GLY	CONFLICT	UNP Q91B42
Cl	85	SER	GLY	CONFLICT	UNP Q91B42
Cm	85	SER	GLY	CONFLICT	UNP Q91B42
Cn	85	SER	GLY	CONFLICT	UNP Q91B42
Co	85	SER	GLY	CONFLICT	UNP Q91B42
Cp	85	SER	GLY	CONFLICT	UNP Q91B42
Cq	85	SER	GLY	CONFLICT	UNP Q91B42
Cr	85	SER	GLY	CONFLICT	UNP Q91B42
Cs	85	SER	GLY	CONFLICT	UNP Q91B42
Ct	85	SER	GLY	CONFLICT	UNP Q91B42
Cu	85	SER	GLY	CONFLICT	UNP Q91B42
Cv	85	SER	GLY	CONFLICT	UNP Q91B42
Cw	85	SER	GLY	CONFLICT	UNP Q91B42
Cx	85	SER	GLY	CONFLICT	UNP Q91B42

- Molecule 3 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D0	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D1	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D2	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D3	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D4	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D5	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D6	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D7	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D8	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	D9	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DA	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DB	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DC	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DD	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DE	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DF	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DG	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DH	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DI	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DJ	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DK	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DL	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DM	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DN	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DO	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DP	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DQ	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DR	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DS	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DT	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DU	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DV	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DW	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DX	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DY	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	DZ	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Da	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Db	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dc	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dd	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	De	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Df	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dg	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dh	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Di	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dj	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dk	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dl	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dm	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dn	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Do	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dp	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Dq	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Dr	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	Ds	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	EA	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	EB	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	EC	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	ED	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		
3	EE	226	Total	C	N	O	S	0	0
			1719	1107	280	326	6		

- Molecule 4 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F0	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F1	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F2	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F3	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F4	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F5	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F6	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F7	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F8	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	F9	22	Total	C	N	O	S	0	1
			166	101	29	35	1		
4	FA	22	Total	C	N	O	S	0	1
			166	101	29	35	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	FB	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FC	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FD	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FE	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FF	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FG	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FH	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FI	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FJ	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FK	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FL	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FM	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FN	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FO	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FP	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FQ	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FR	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FS	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FT	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FU	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FV	22	Total 166	C 101	N 29	O 35	S 1	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	FW	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FX	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FY	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	FZ	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fa	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fb	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fc	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fd	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fe	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Ff	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fg	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fh	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fi	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fj	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fk	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fl	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fm	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fn	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fo	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fp	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fq	22	Total 166	C 101	N 29	O 35	S 1	0	1

Continued on next page...

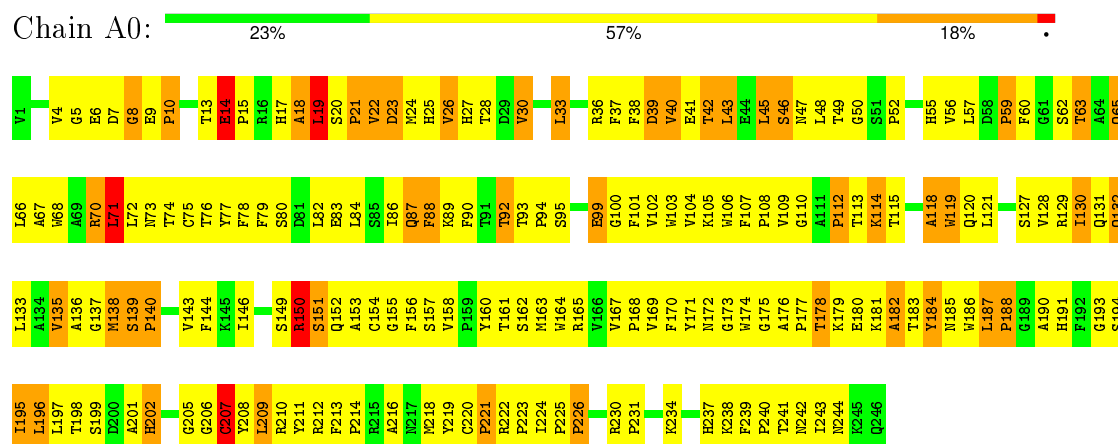
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Fr	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fs	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Ft	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fu	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fv	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fw	22	Total 166	C 101	N 29	O 35	S 1	0	1
4	Fx	22	Total 166	C 101	N 29	O 35	S 1	0	1

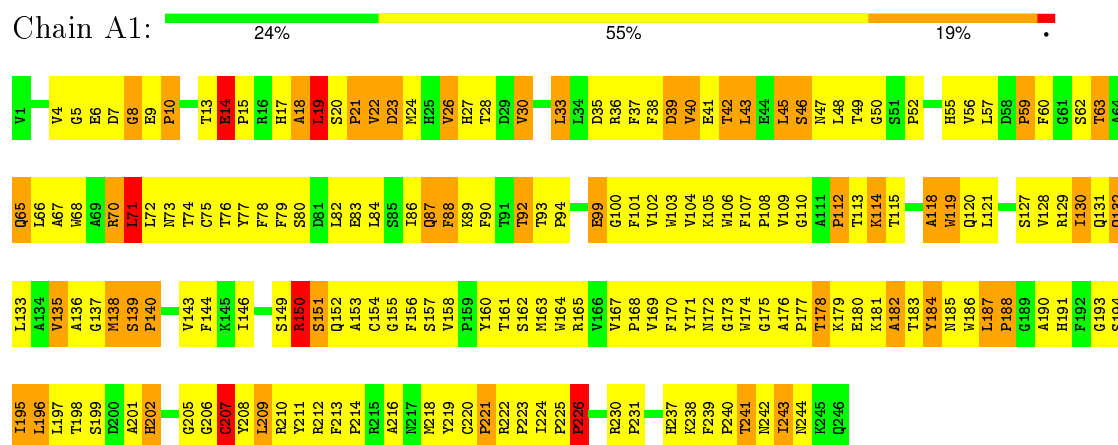
3 Residue-property plots

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

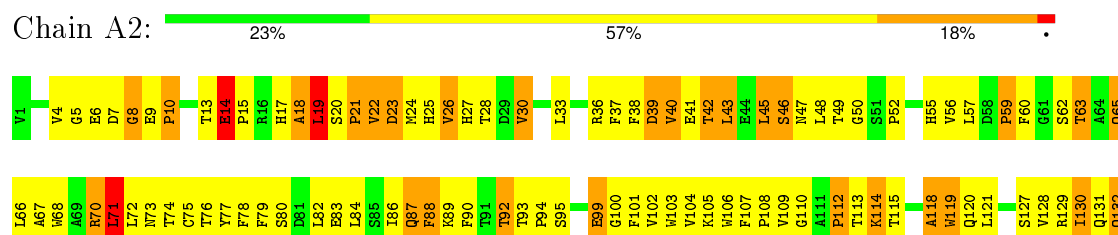
• Molecule 1: VP1

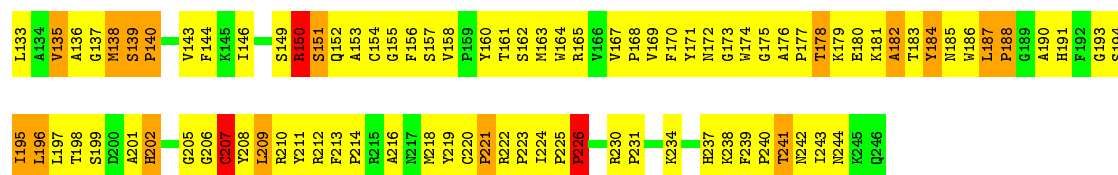


• Molecule 1: VP1



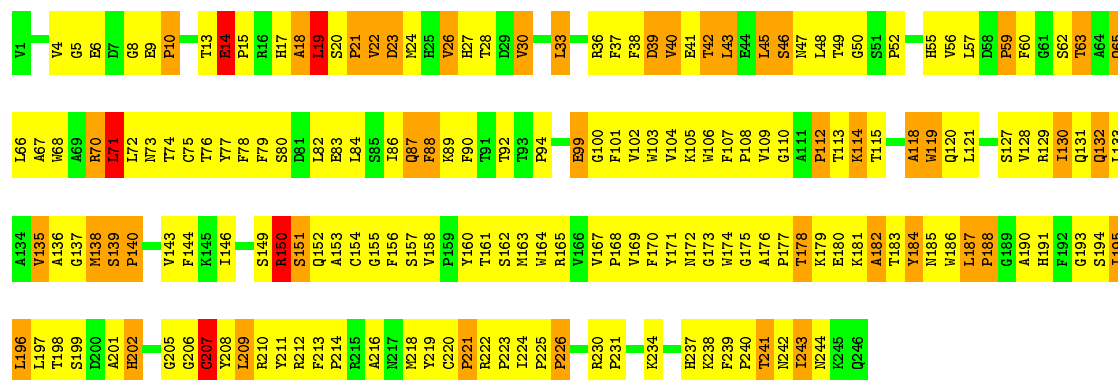
• Molecule 1: VP1





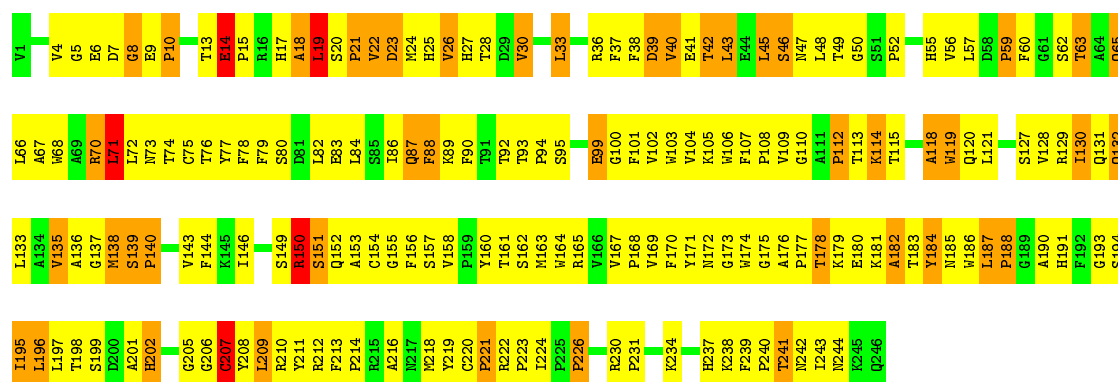
• Molecule 1: VP1

Chain A3: 25% 55% 18%



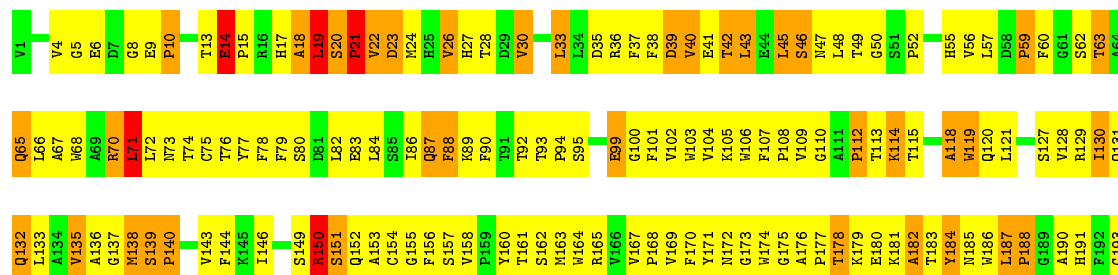
• Molecule 1: VP1

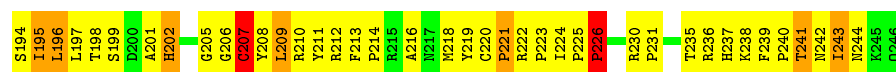
Chain A4: 24% 56% 18%



• Molecule 1: VP1

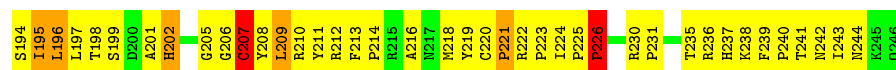
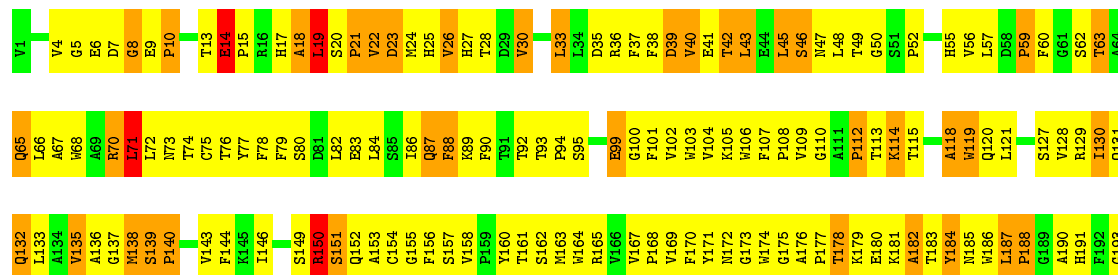
Chain A5: 23% 56% 18%





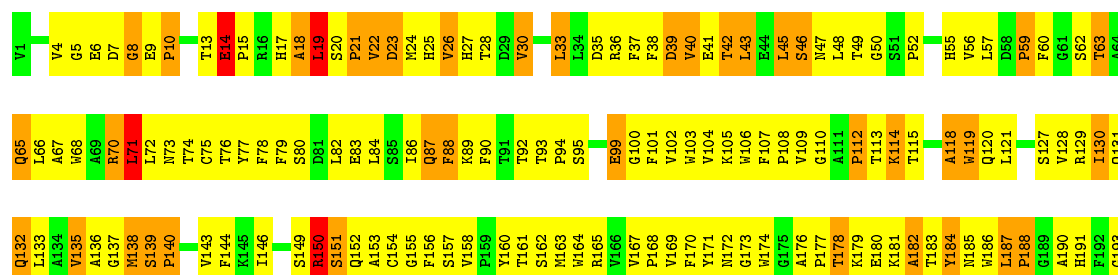
• Molecule 1: VP1

Chain A6: 22% 58% 17%



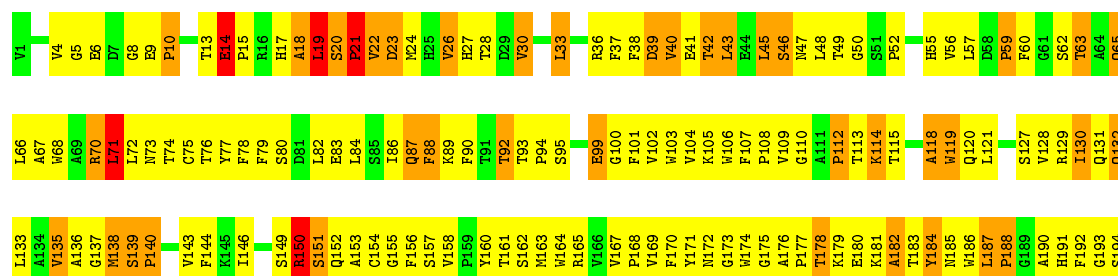
• Molecule 1: VP1

Chain A7: 24% 56% 18%

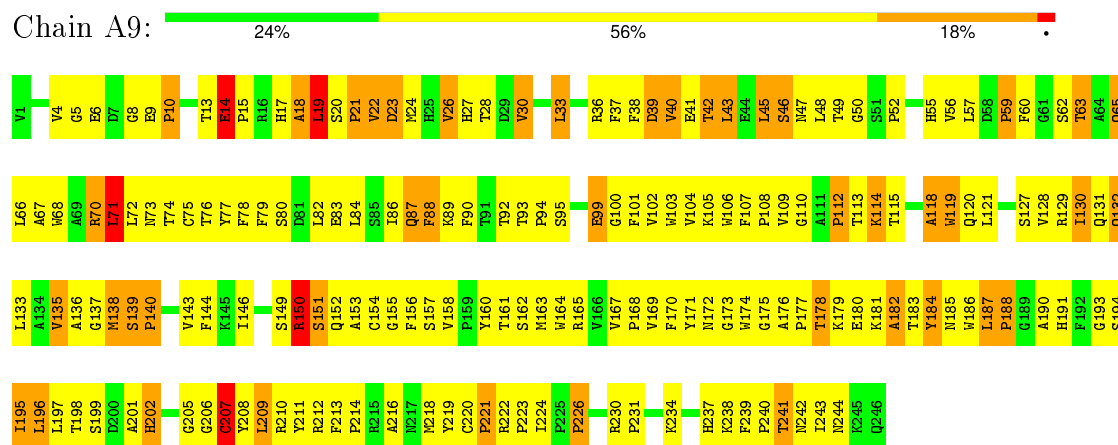


• Molecule 1: VP1

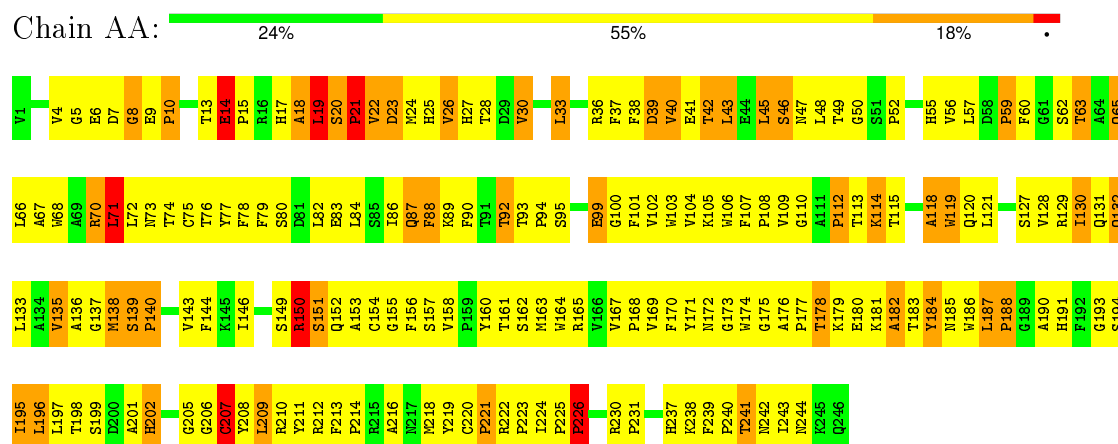
Chain A8: 24% 56% 18%



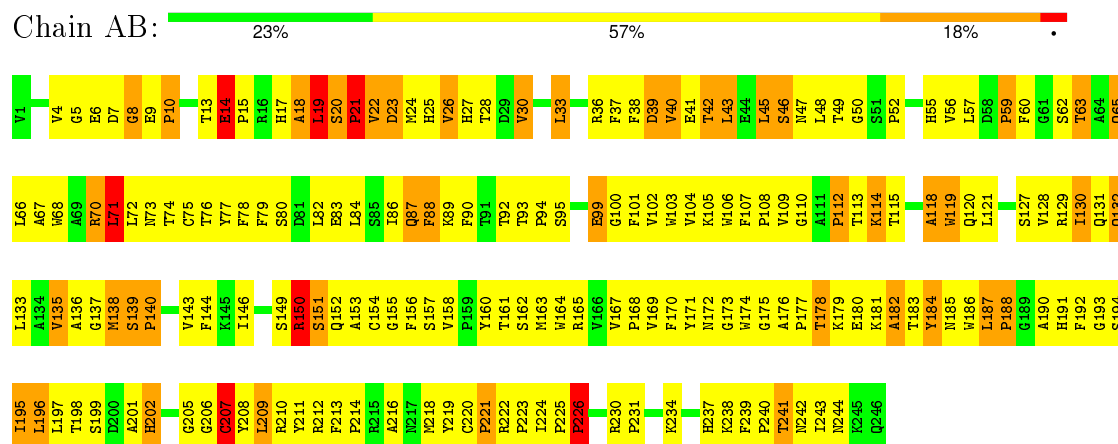
• Molecule 1: VP1



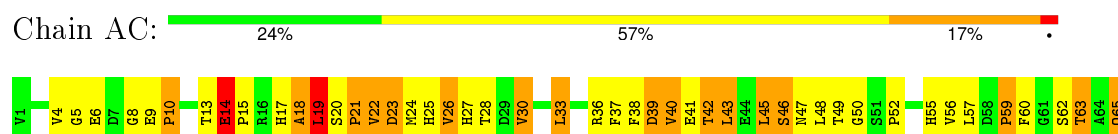
• Molecule 1: VP1

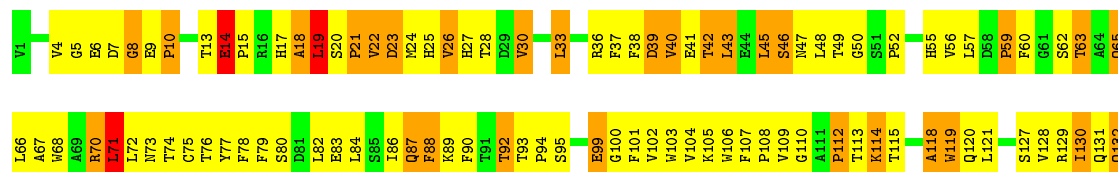


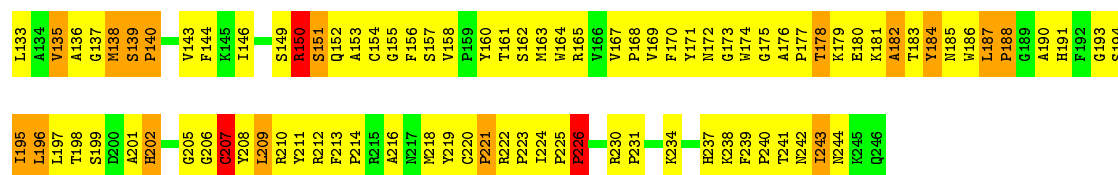
• Molecule 1: VP1



• Molecule 1: VP1

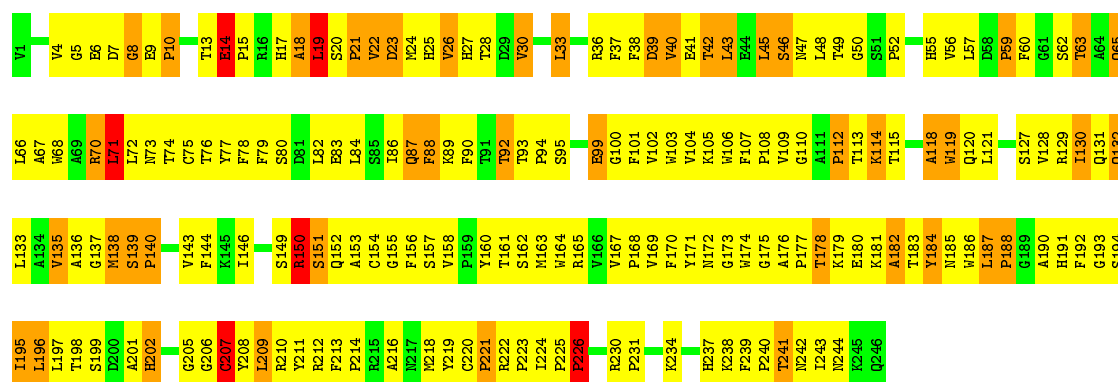






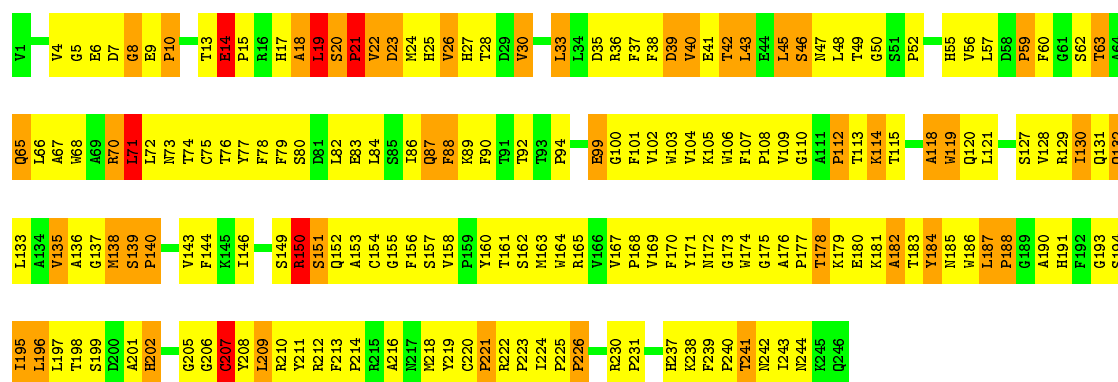
• Molecule 1: VP1

Chain AG: 23% 57% 18% •



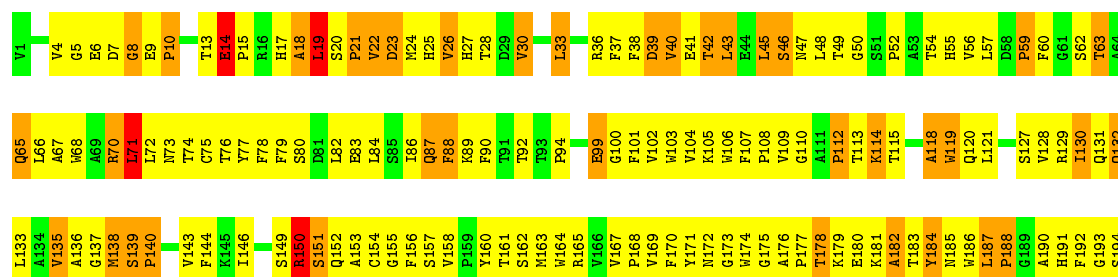
• Molecule 1: VP1

Chain AH: 24% 55% 18% •



• Molecule 1: VP1

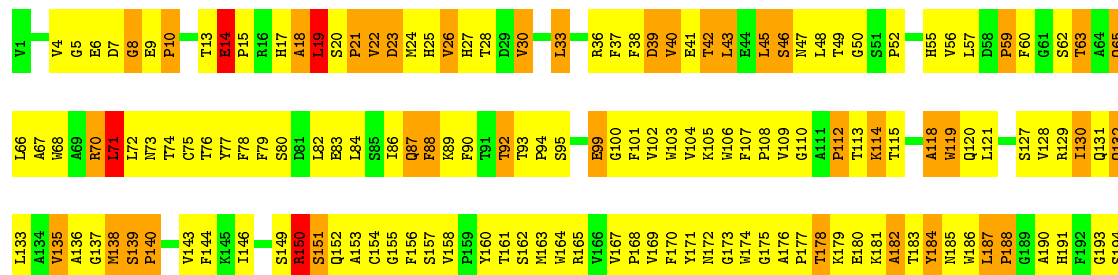
Chain AI: 23% 57% 17% •





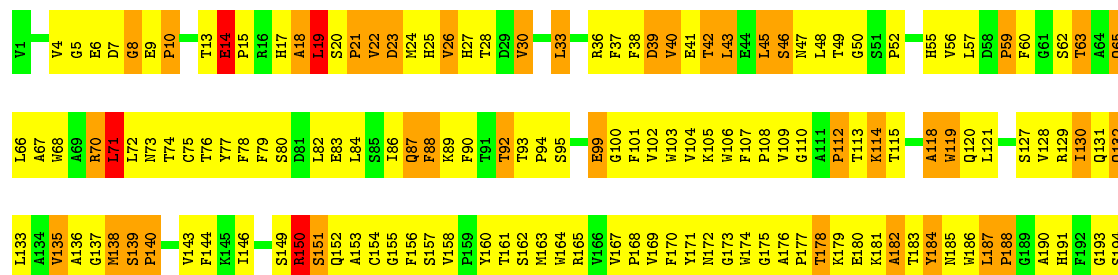
• Molecule 1: VP1

Chain AJ: 23% 57% 18%



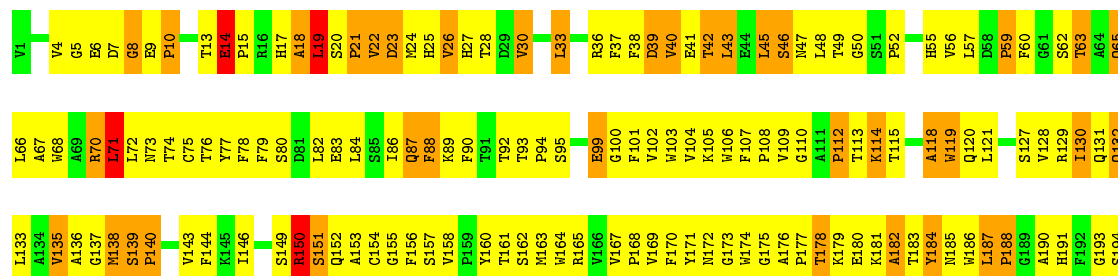
• Molecule 1: VP1

Chain AK: 24% 56% 18%



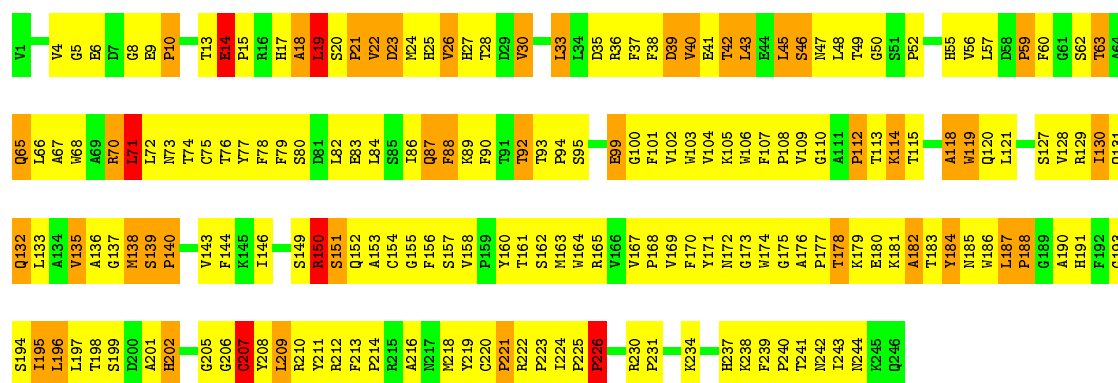
• Molecule 1: VP1

Chain AL: 23% 56% 18%

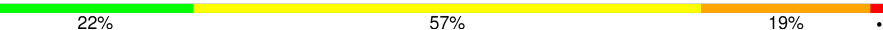


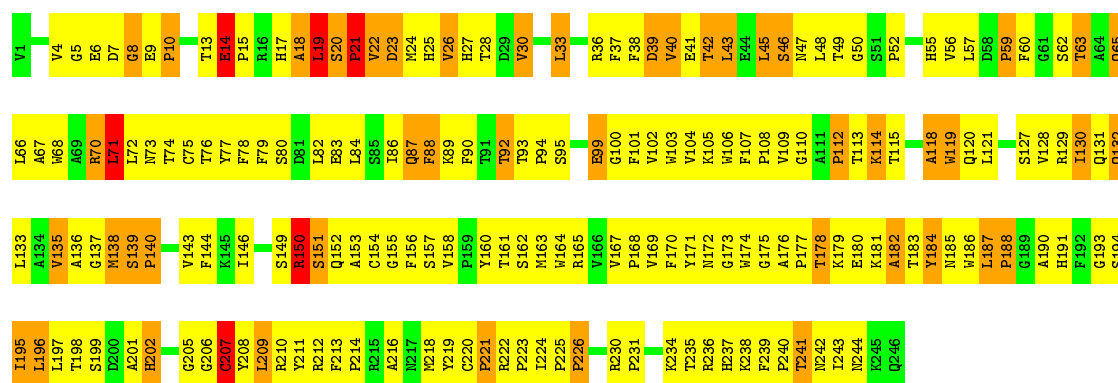
• Molecule 1: VP1

Chain AM: 



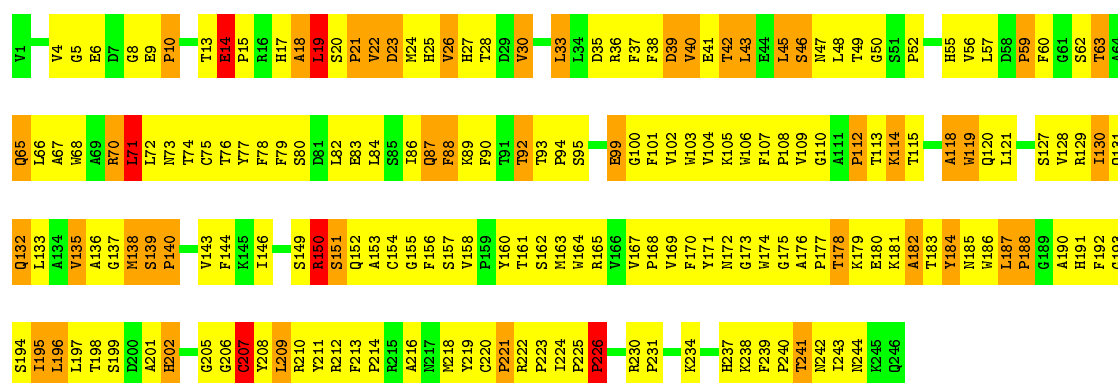
• Molecule 1: VP1

Chain AN: 



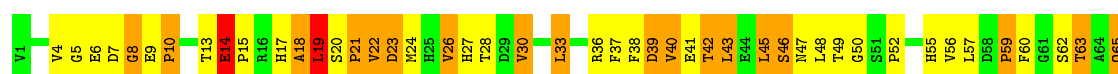
• Molecule 1: VP1

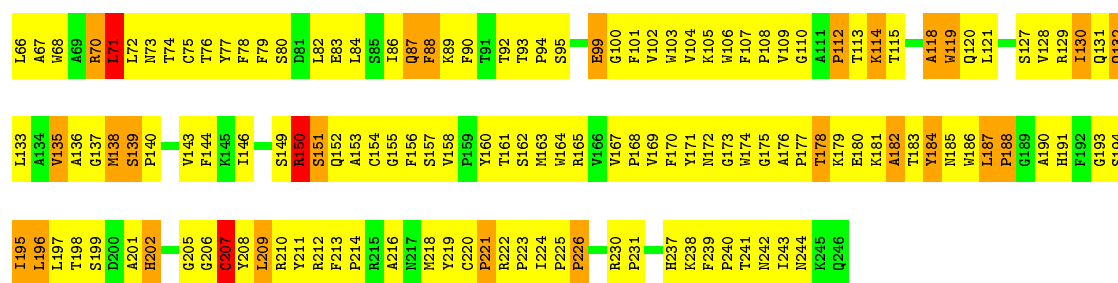
Chain AO: 



• Molecule 1: VP1

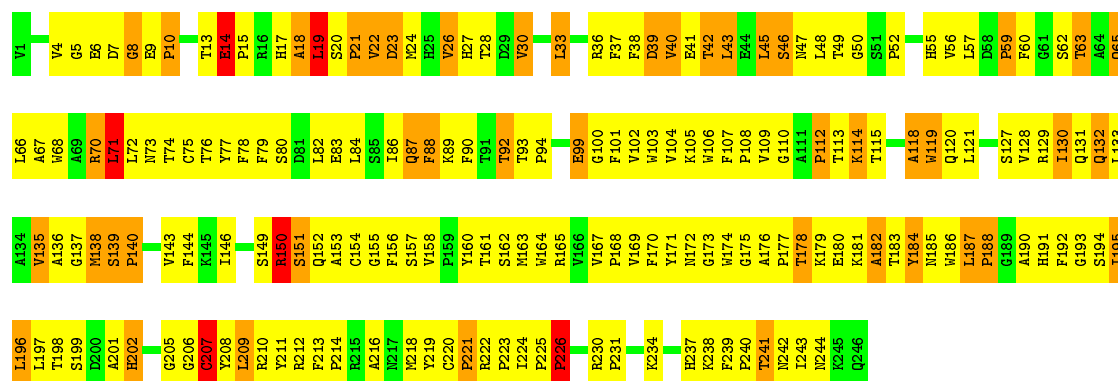
Chain AP: 





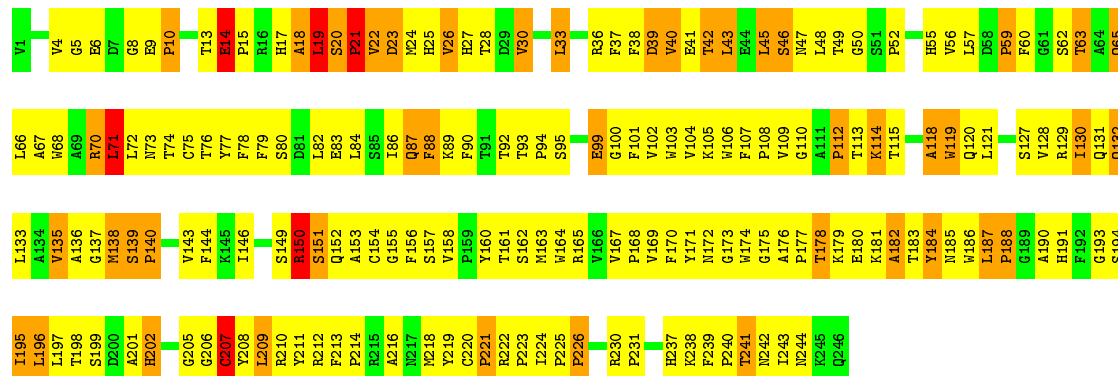
• Molecule 1: VP1

Chain AQ: 24% 56% 18%



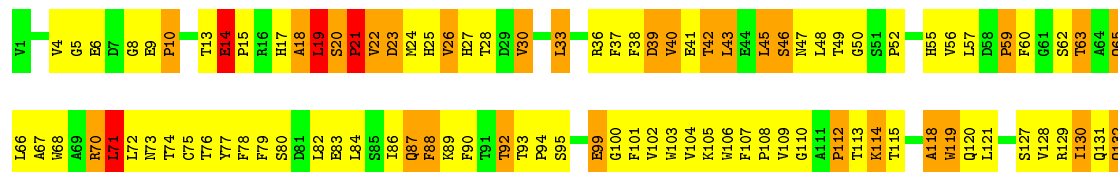
• Molecule 1: VP1

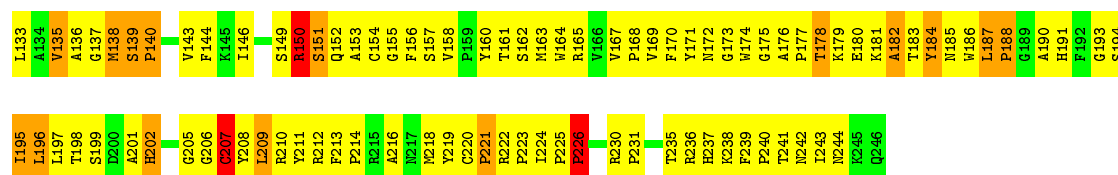
Chain AR: 24% 56% 18%



• Molecule 1: VP1

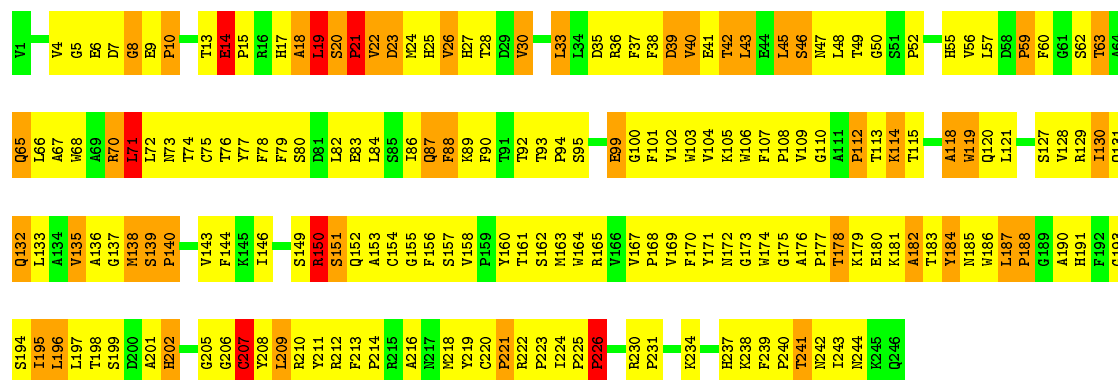
Chain AS: 23% 57% 17%





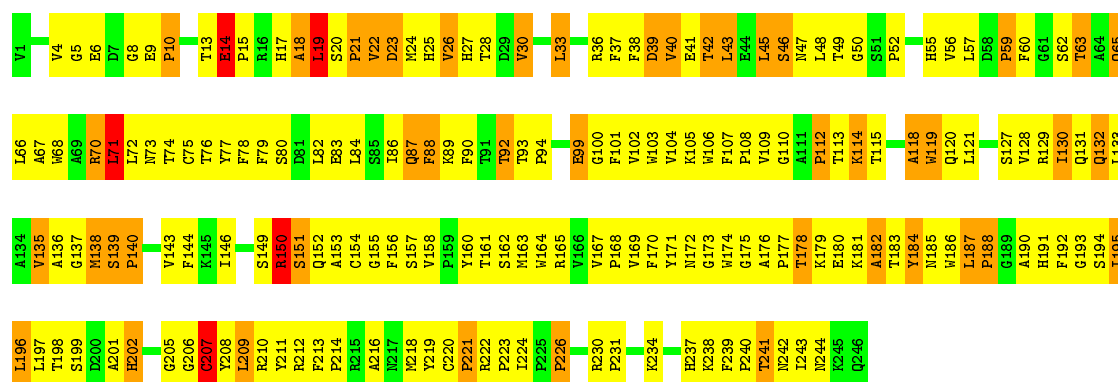
• Molecule 1: VP1

Chain AT: 23% 57% 18%



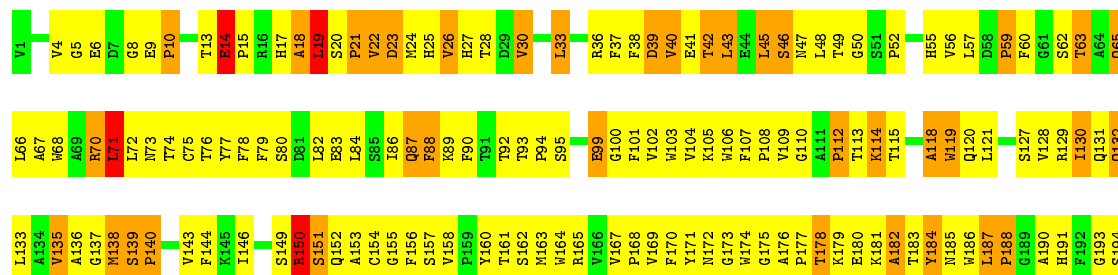
• Molecule 1: VP1

Chain AU: 24% 56% 18%



• Molecule 1: VP1

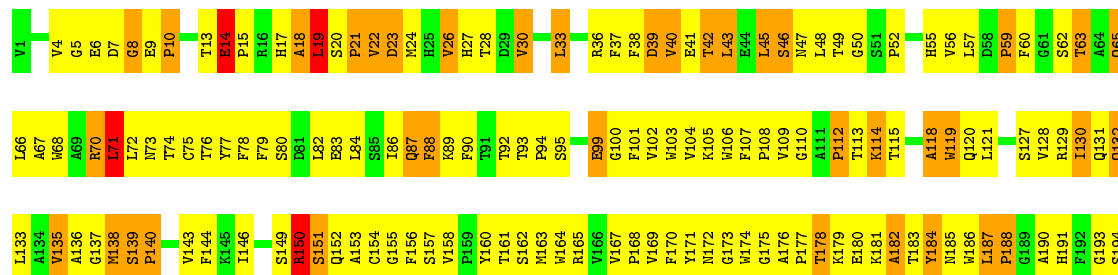
Chain AV: 24% 57% 17%





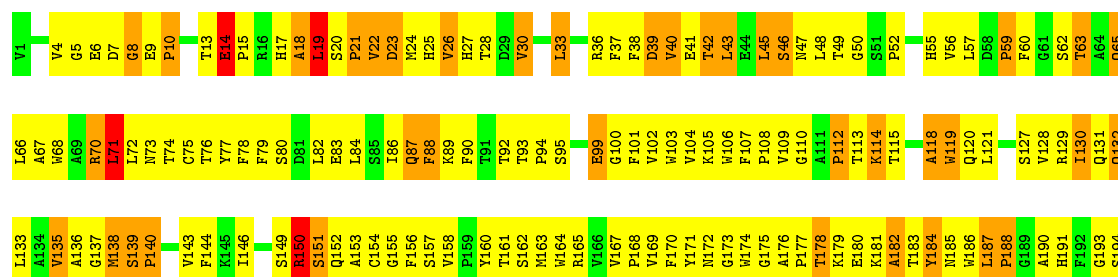
• Molecule 1: VP1

Chain AW: 24% 56% 18%



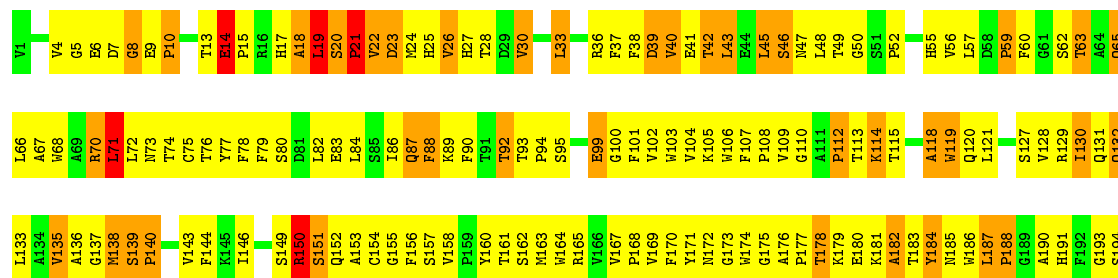
• Molecule 1: VP1

Chain AX: 24% 56% 18%

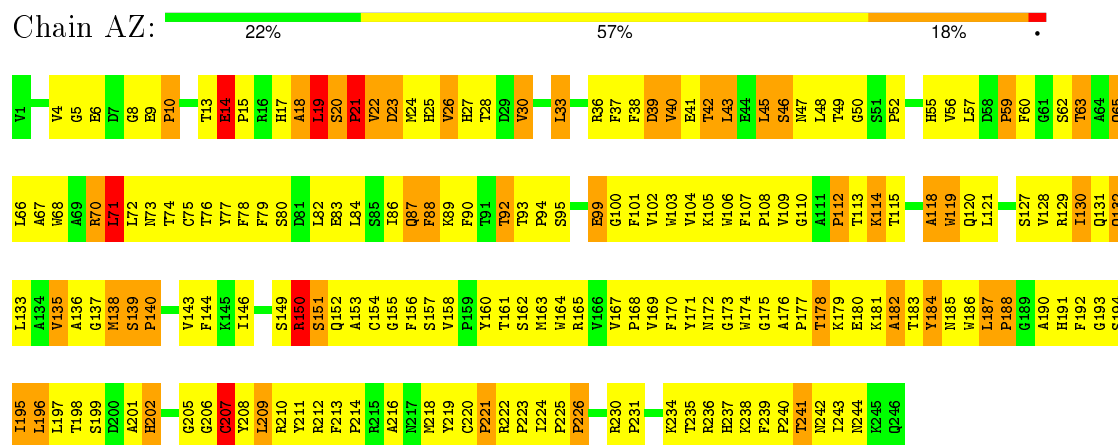


• Molecule 1: VP1

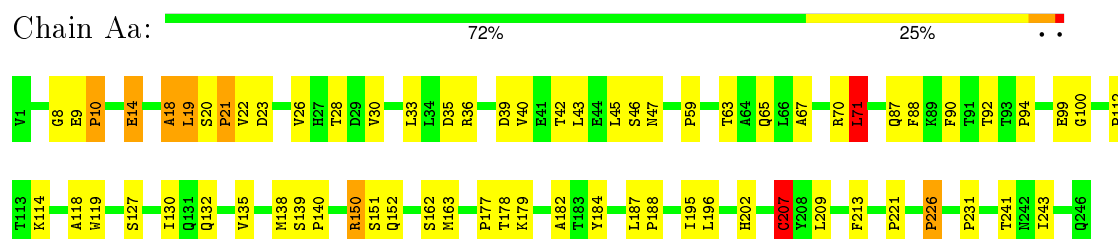
Chain AY: 23% 56% 19%



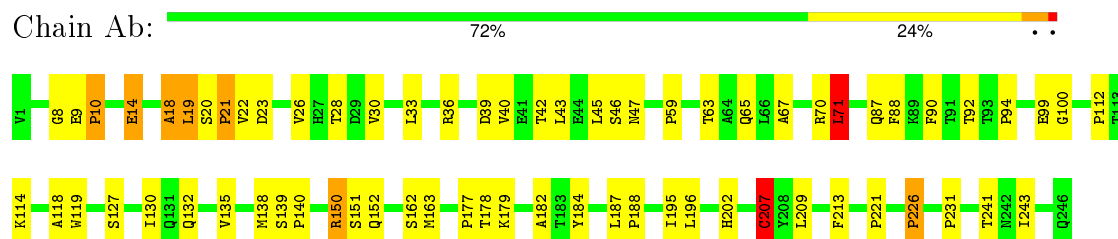
• Molecule 1: VP1



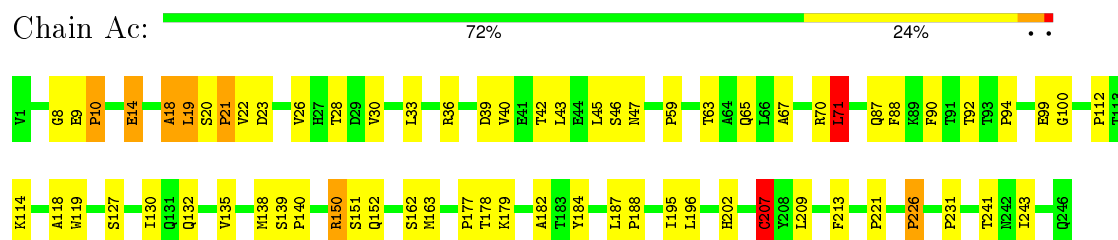
- Molecule 1: VP1



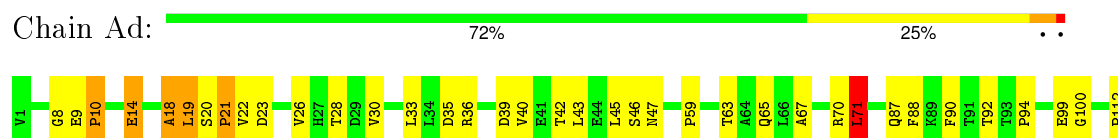
- Molecule 1: VP1

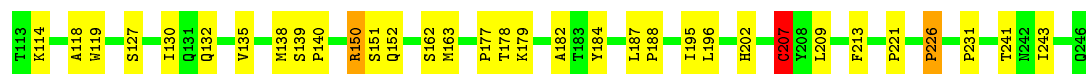


- Molecule 1: VP1



- Molecule 1: VP1





- Molecule 1: VP1

Chain Ae: 72% 24%



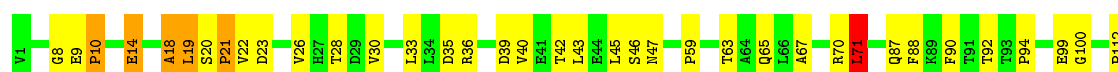
- Molecule 1: VP1

Chain Af: 72% 25%



- Molecule 1: VP1

Chain Ag: 72% 25%



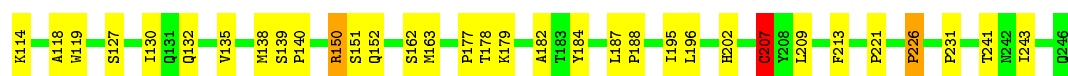
- Molecule 1: VP1

Chain Ah: 72% 25%

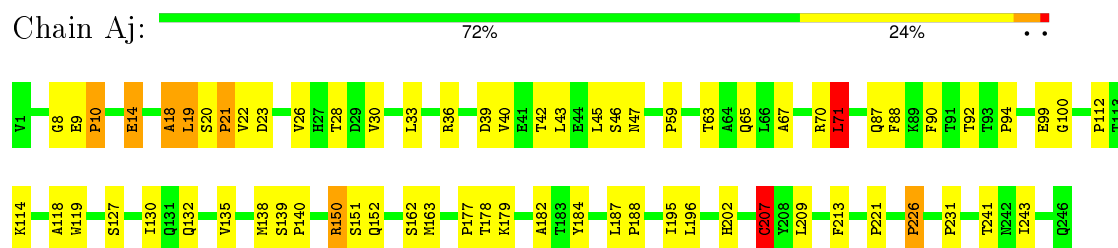


- Molecule 1: VP1

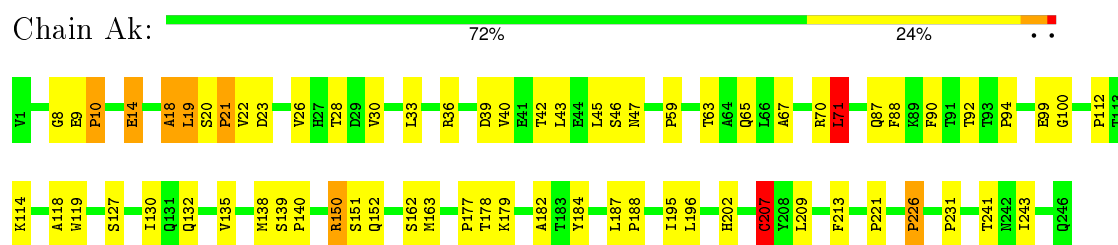
Chain Ai: 72% 24%



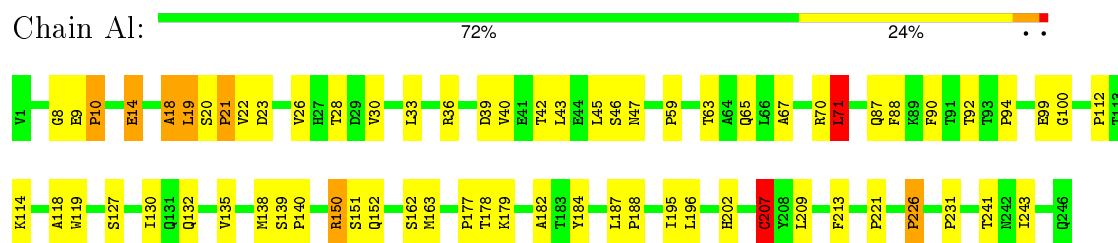
- Molecule 1: VP1



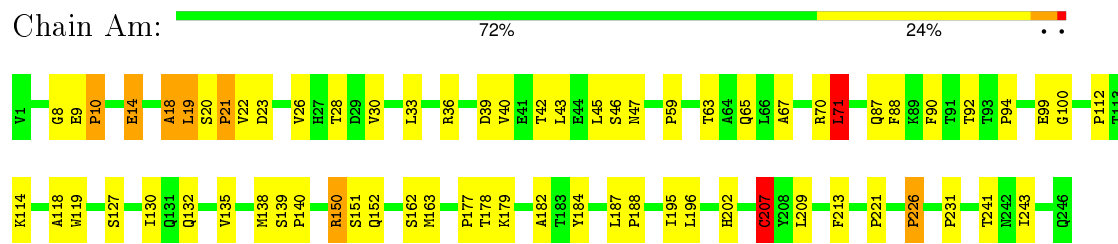
- Molecule 1: VP1



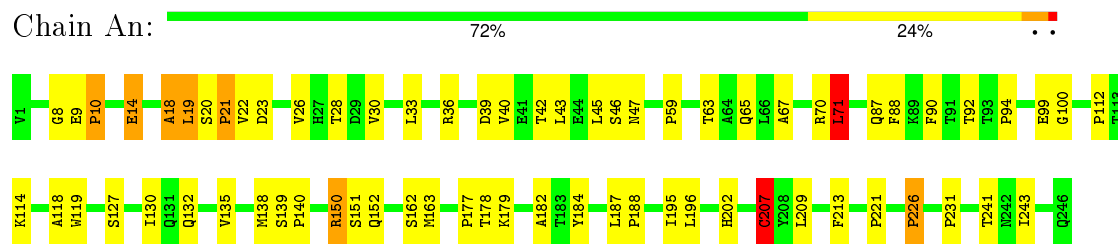
- Molecule 1: VP1



- Molecule 1: VP1



- Molecule 1: VP1

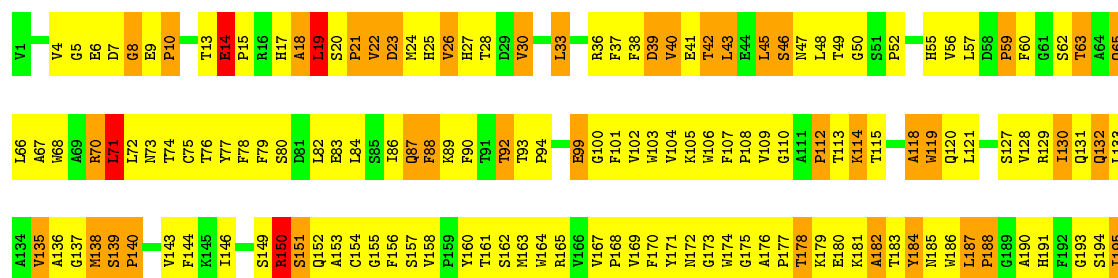


- Molecule 1: VP1



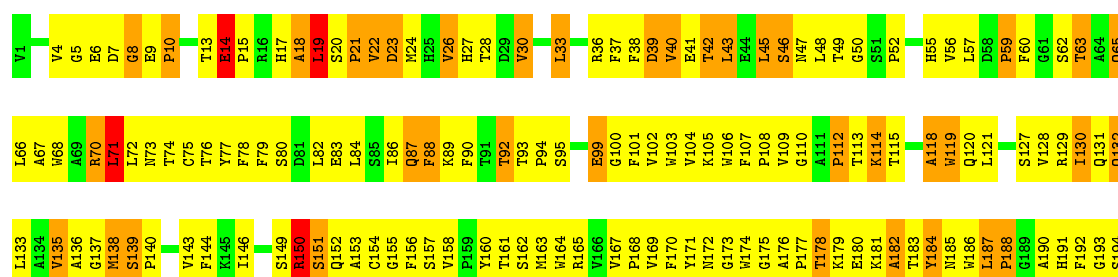
• Molecule 1: VP1

Chain BD: 24% 55% 18%



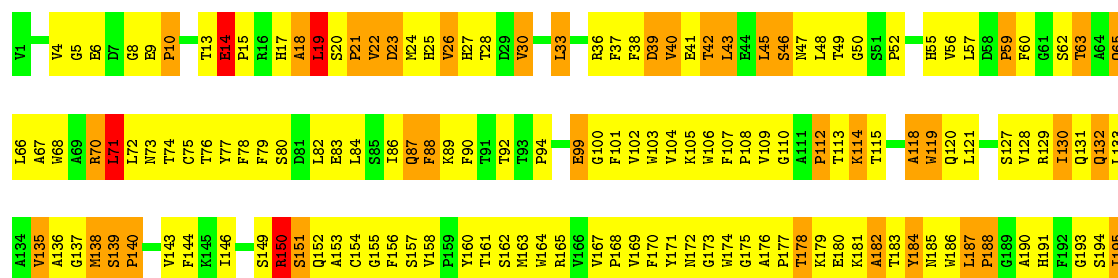
• Molecule 1: VP1

Chain BE: 23% 57% 18%



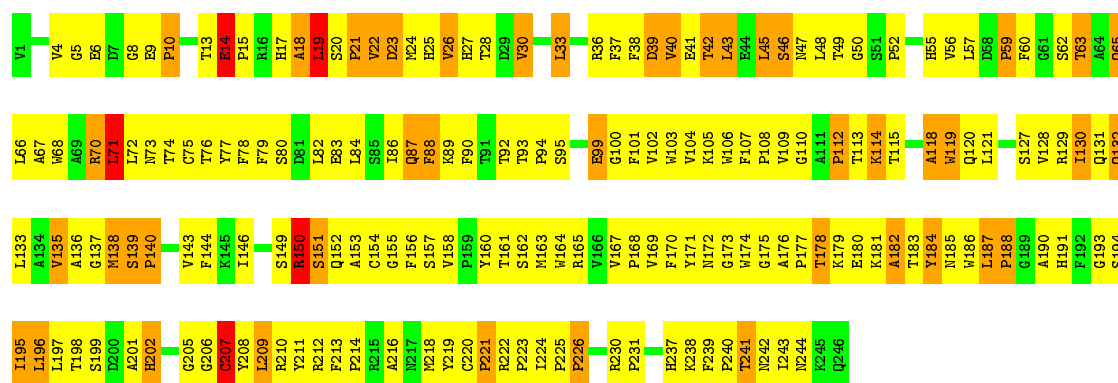
• Molecule 1: VP1

Chain BF: 25% 56% 17%



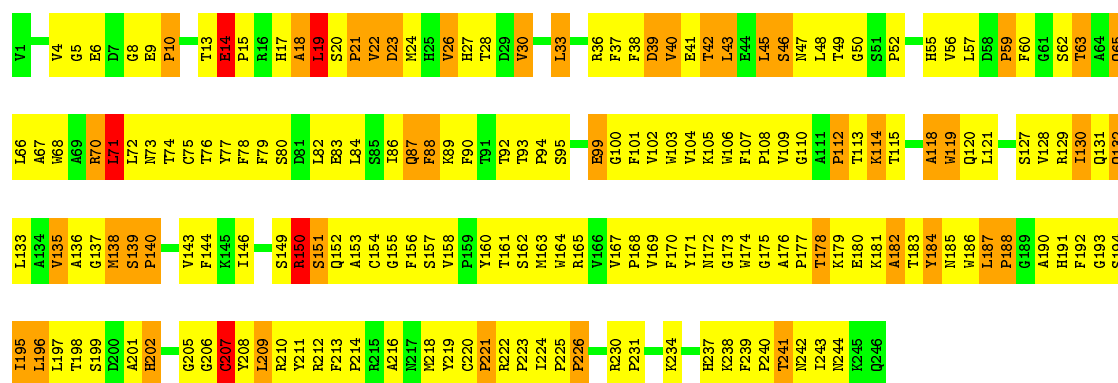
• Molecule 1: VP1

Chain BG: 

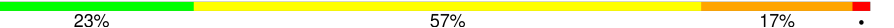


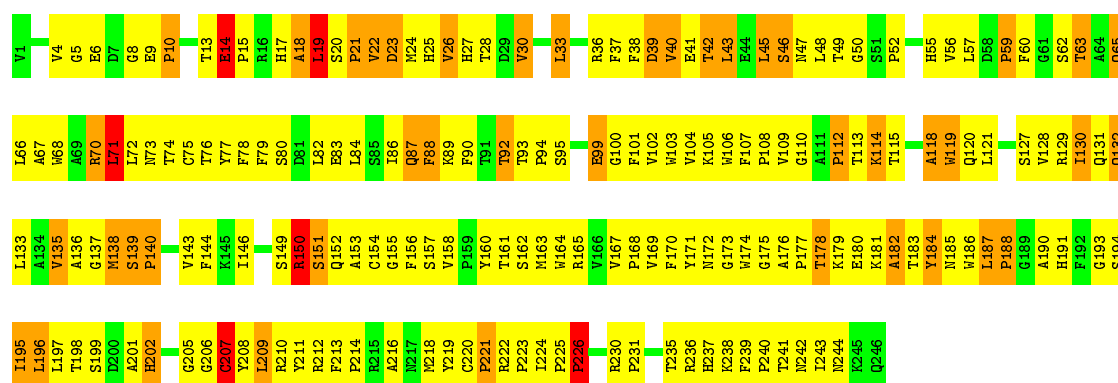
• Molecule 1: VP1

Chain BH: 




• Molecule 1: VP1

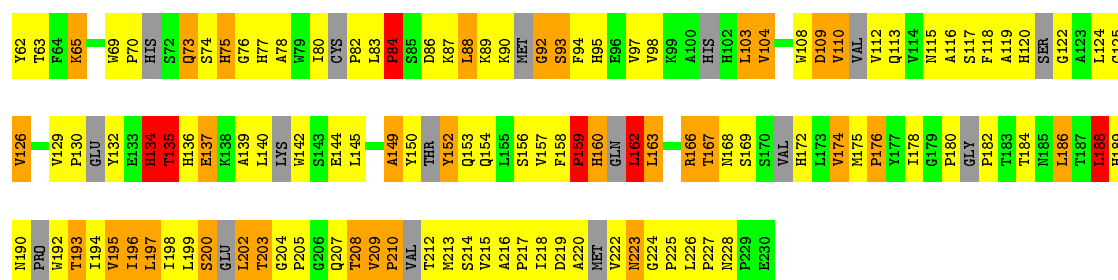
Chain BI: 



• Molecule 2: EQUINE RHINITIS A VIRUS

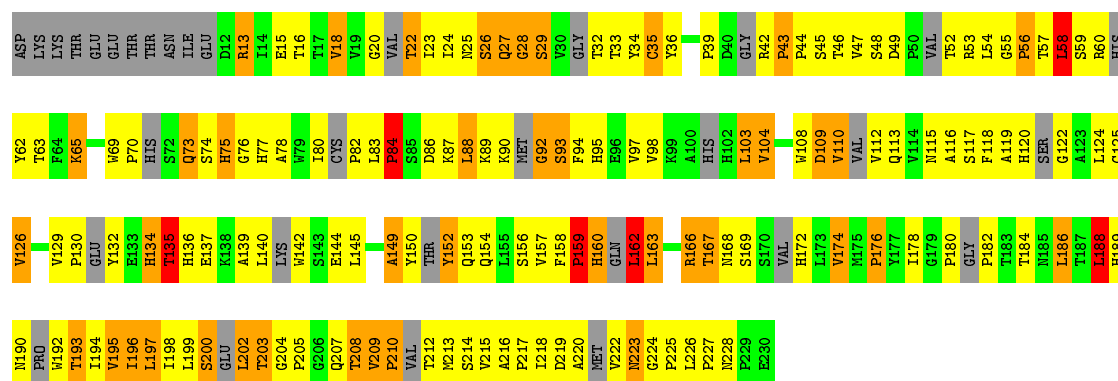
Chain C0: 





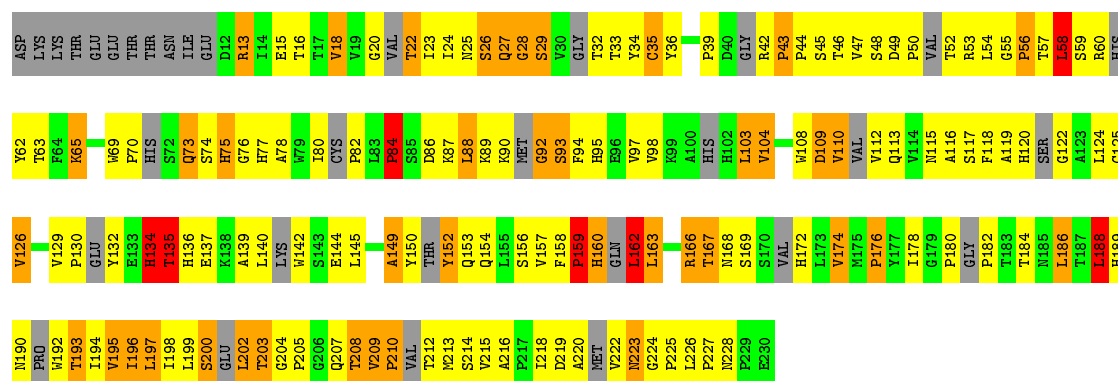
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain C1: 20% 45% 18% • 14%



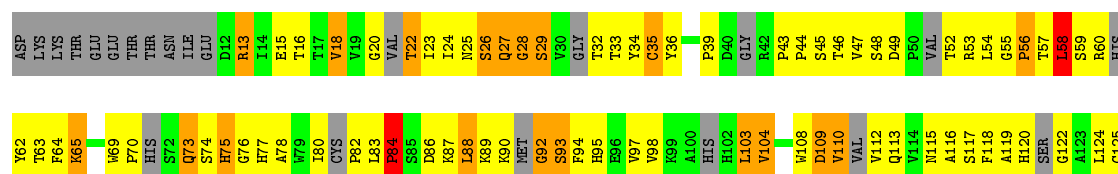
• Molecule 2: EQUINE RHINITIS A VIRUS

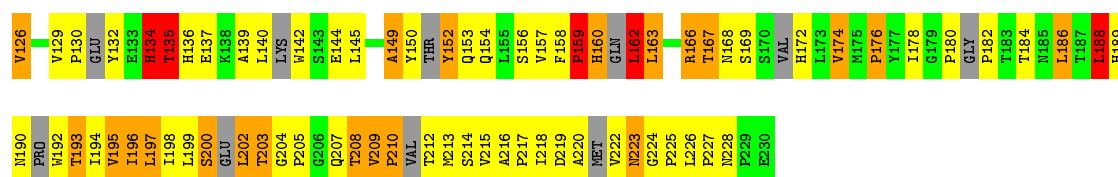
Chain C2: 21% 44% 18% • 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

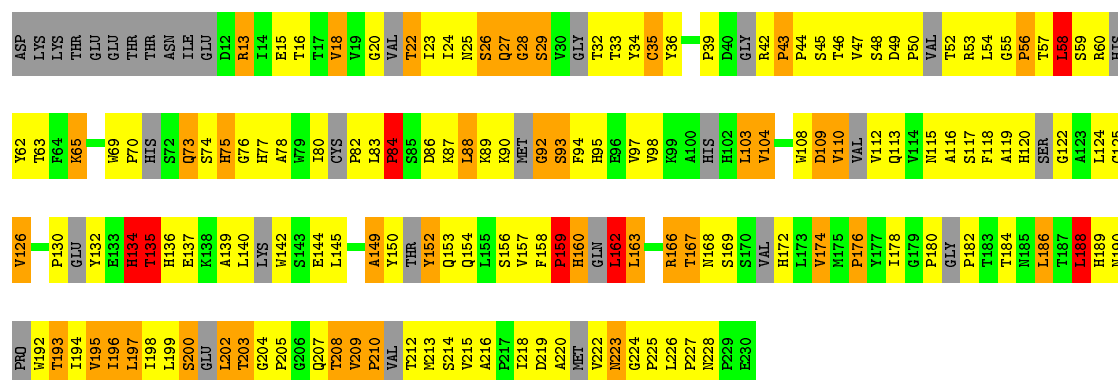
Chain C3: 20% 45% 17% • 14%





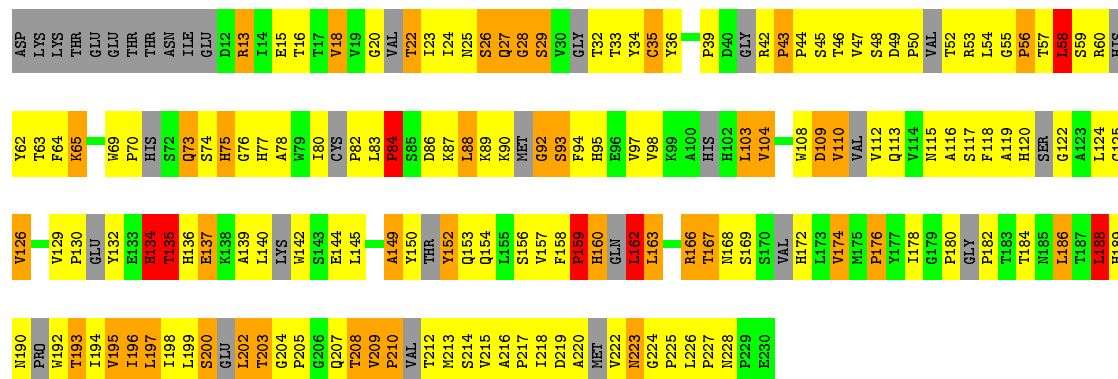
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain C4: 21% 44% 18% • 14%



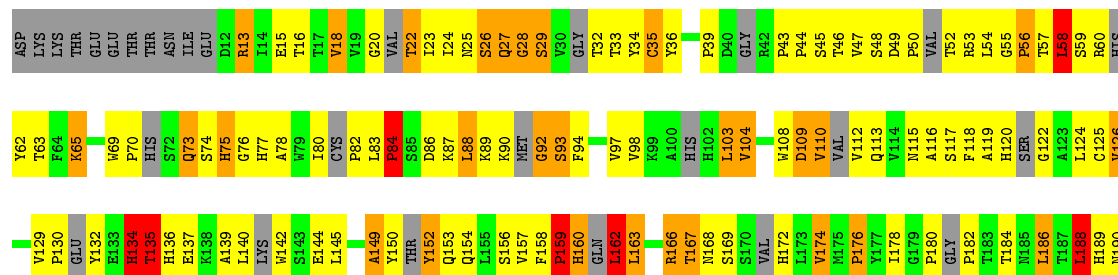
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain C5: 20% 45% 18% • 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

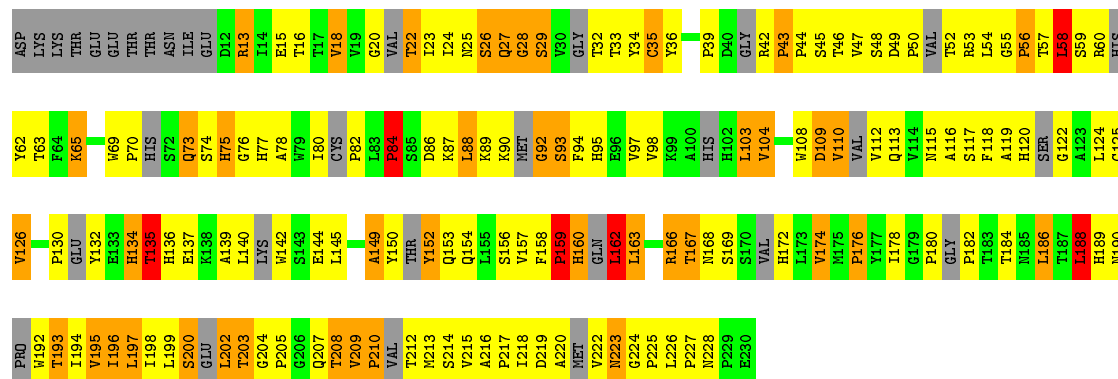
Chain C6: 21% 45% 17% • 14%





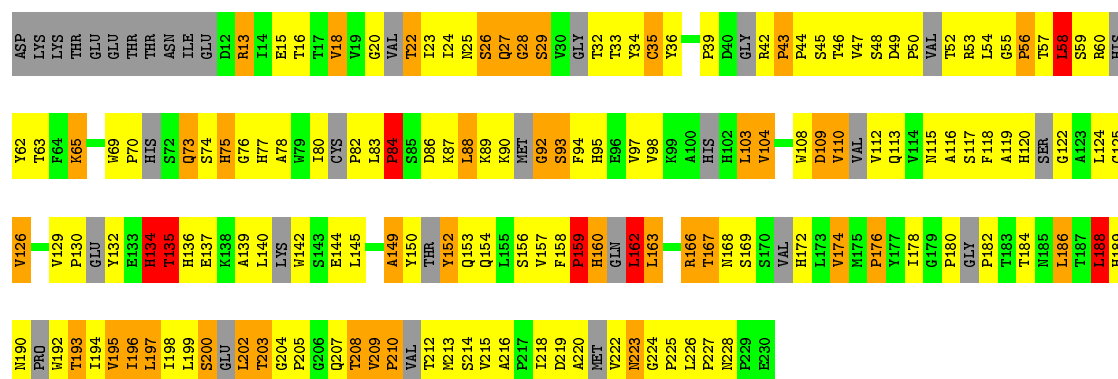
Molecule 2: EQUINE RHINITIS A VIRUS

Chain C7: 21% 44% 18% 14%



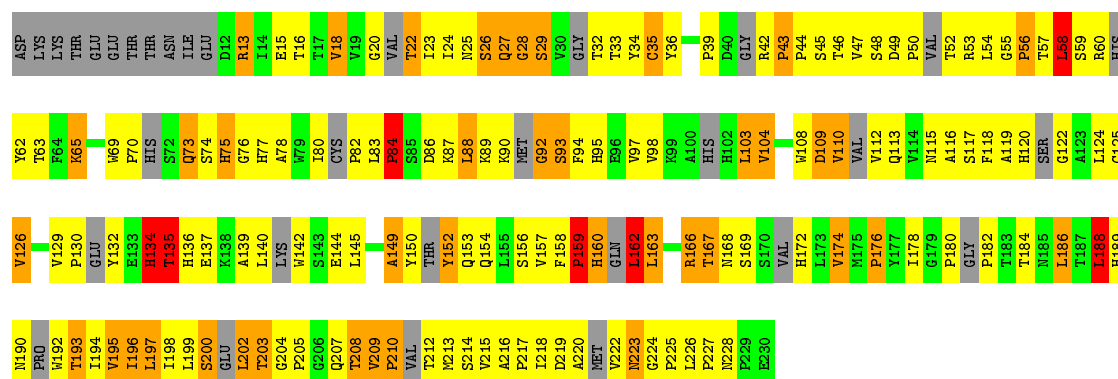
Molecule 2: EQUINE RHINITIS A VIRUS

Chain C8: 20% 45% 18% 14%

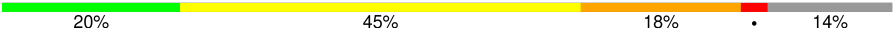


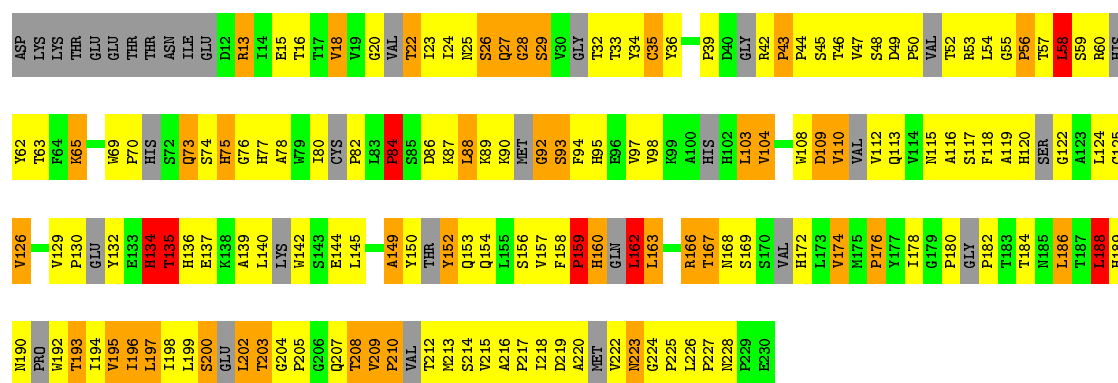
Molecule 2: EQUINE RHINITIS A VIRUS

Chain C9: 20% 45% 18% 14%




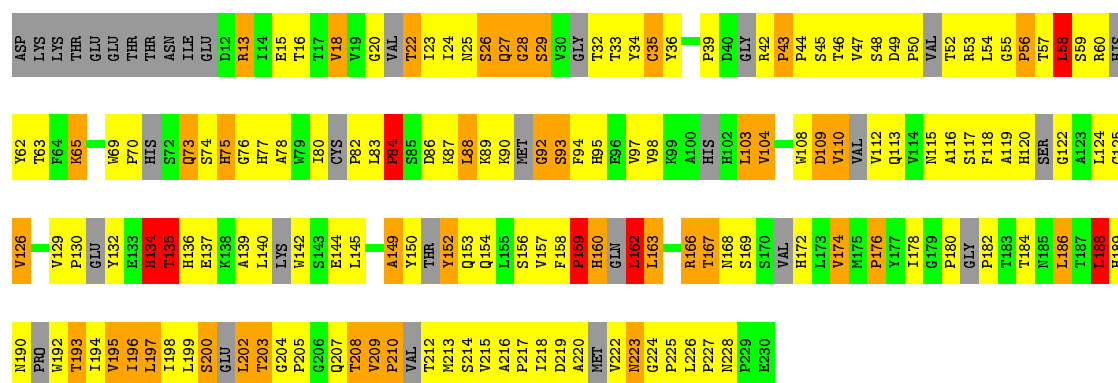
Molecule 2: EQUINE RHINITIS A VIRUS

Chain CA: 

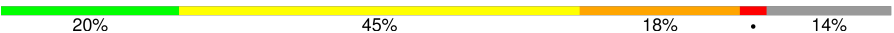


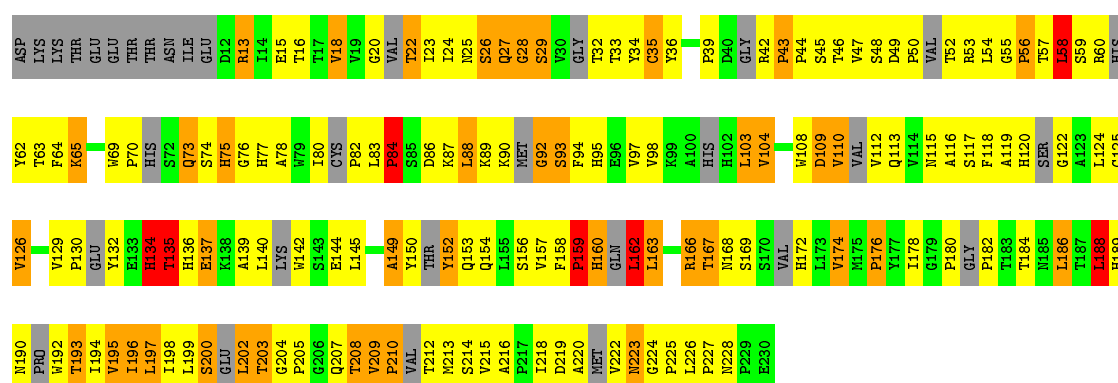
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CB: 

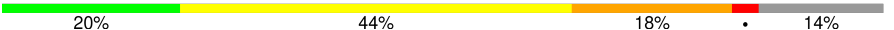


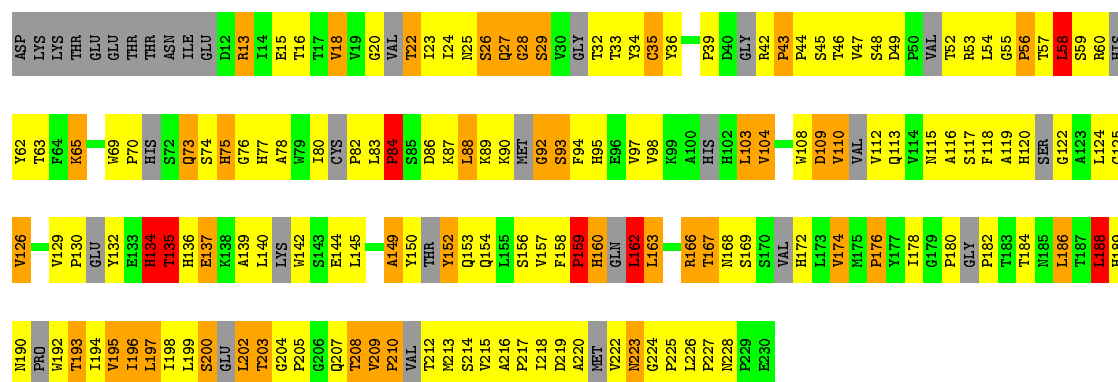
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CC: 



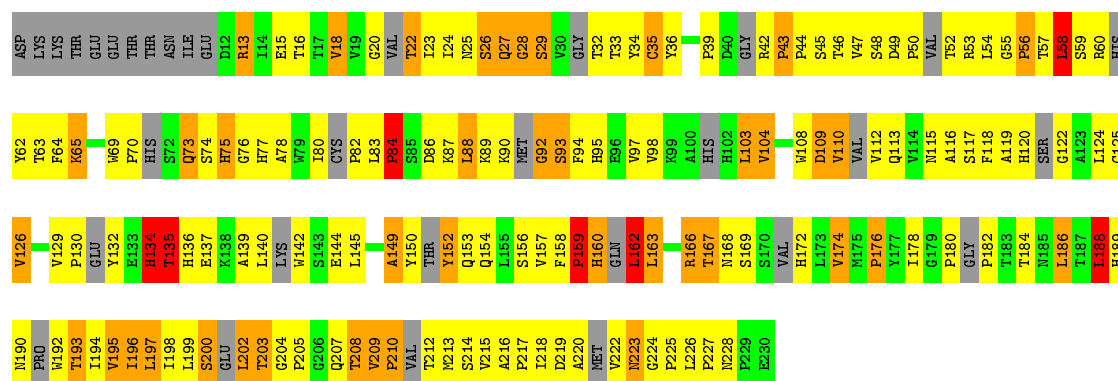
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CD: 



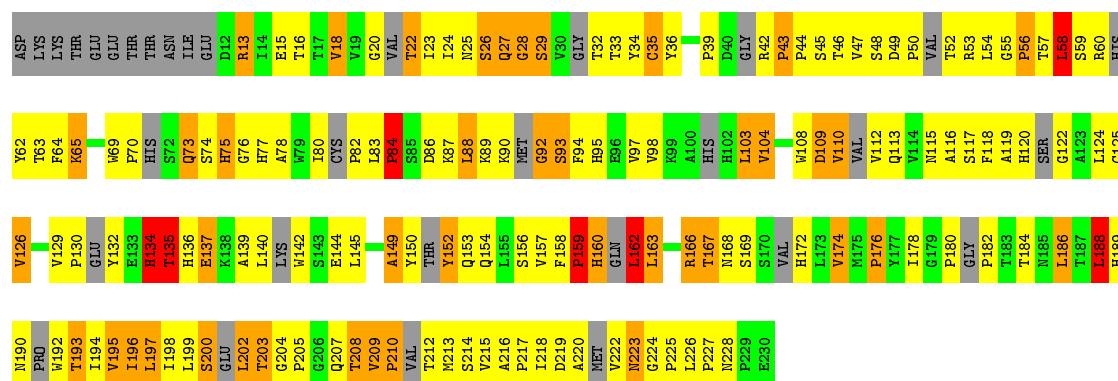
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CE: 20% 46% 18% • 14%



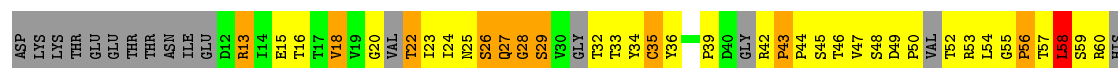
• Molecule 2: EQUINE RHINITIS A VIRUS

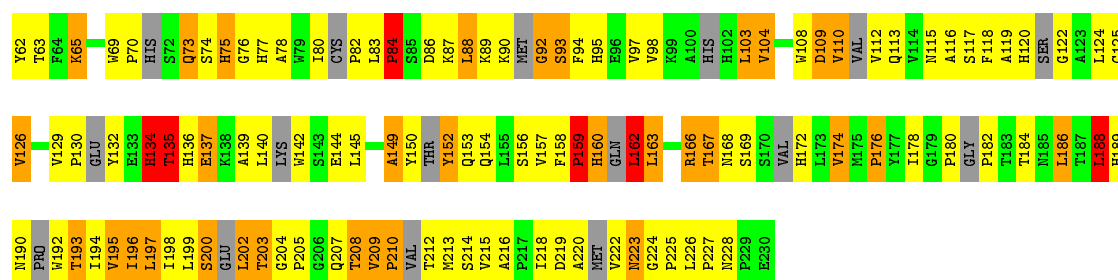
Chain CF: 20% 45% 18% • 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

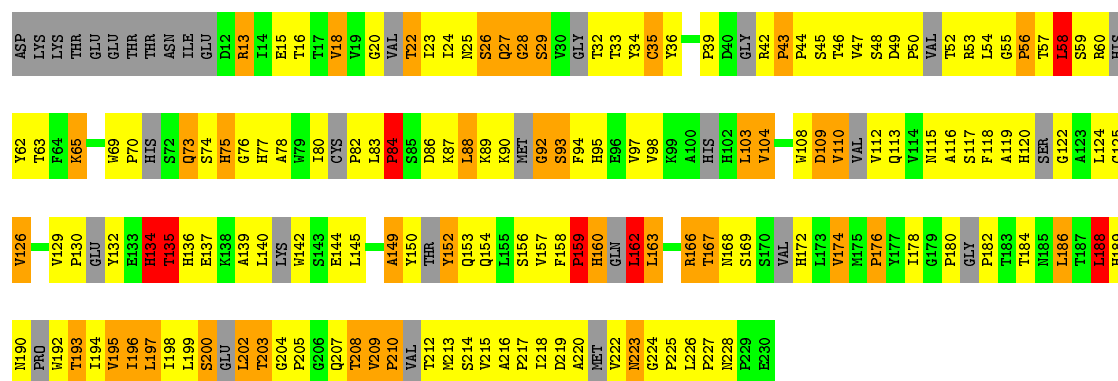
Chain CG: 20% 44% 18% • 14%





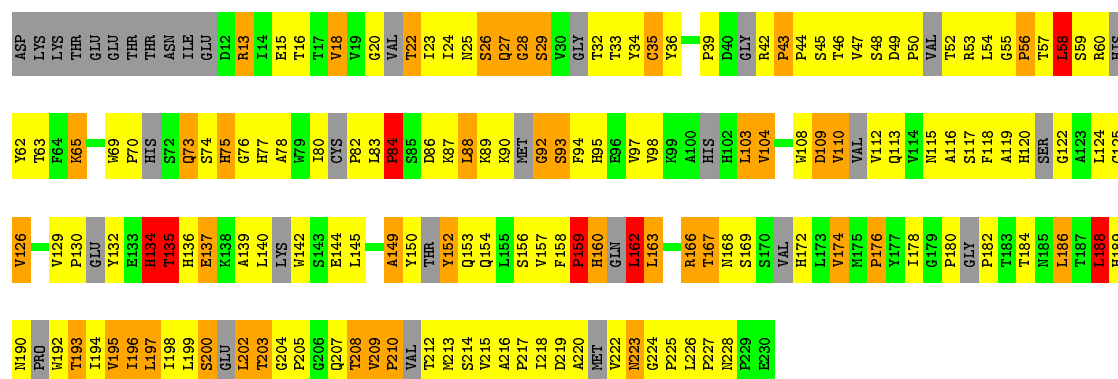
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CH: 20% 45% 18% • 14%



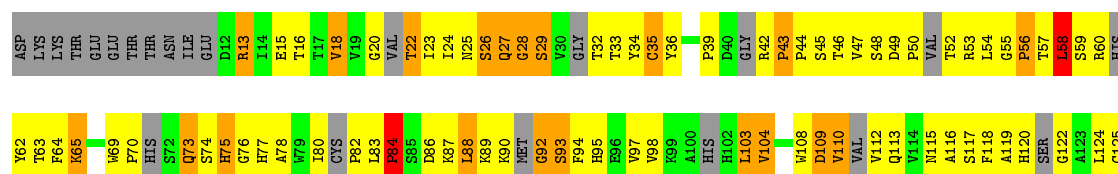
• Molecule 2: EQUINE RHINITIS A VIRUS

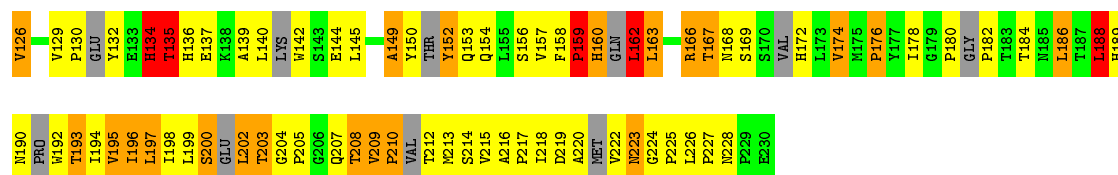
Chain CI: 20% 45% 18% • 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

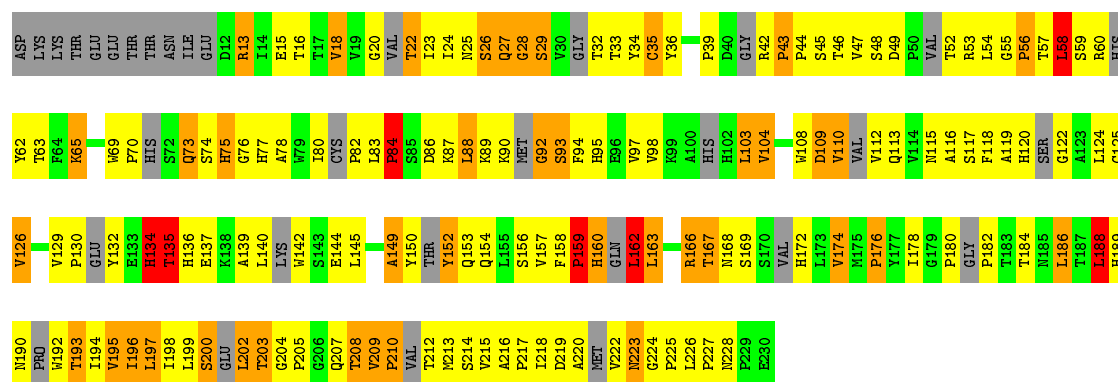
Chain CJ: 20% 46% 18% • 14%





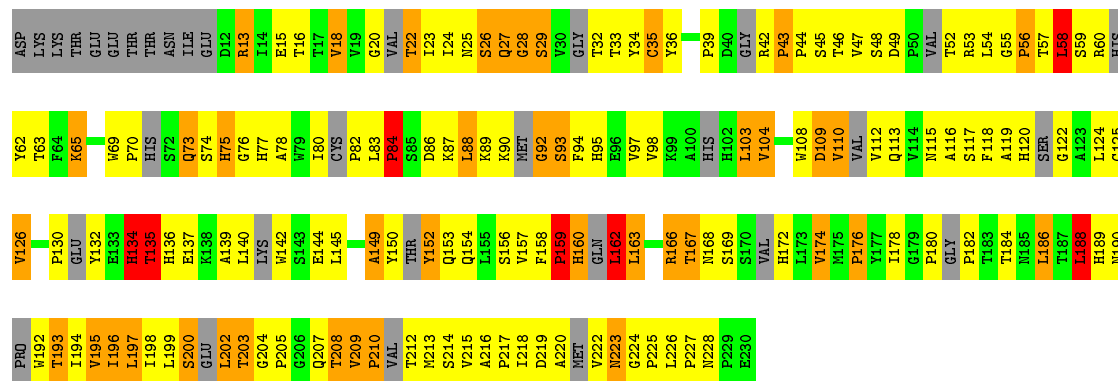
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CK: 20% 45% 18% 14%



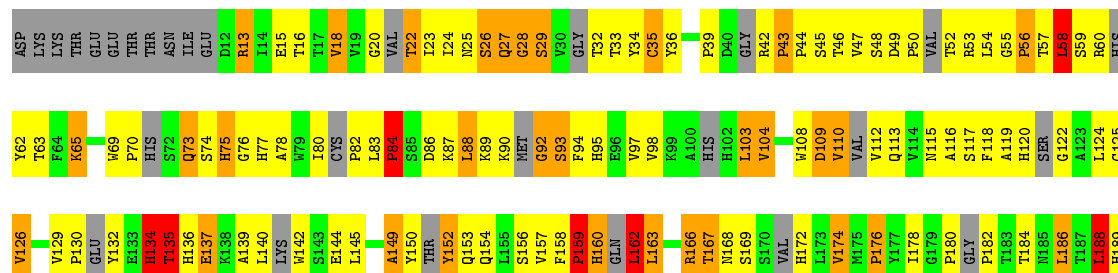
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CL: 21% 44% 18% 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

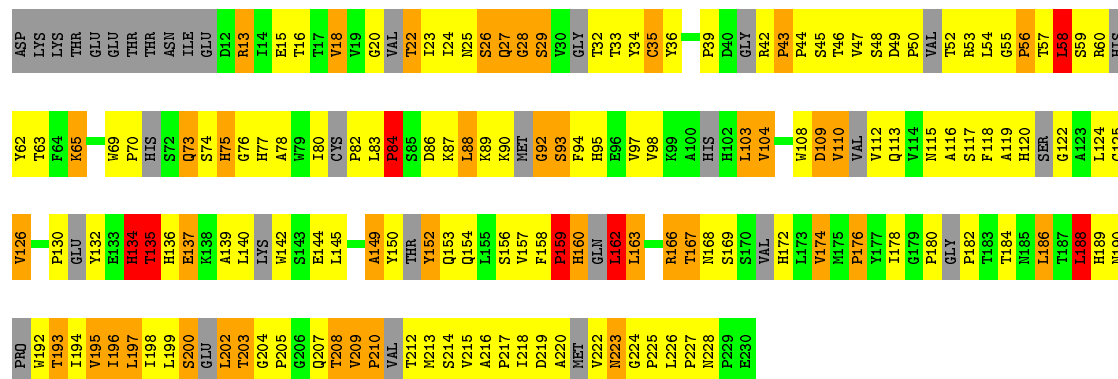
Chain CM: 20% 44% 18% 14%





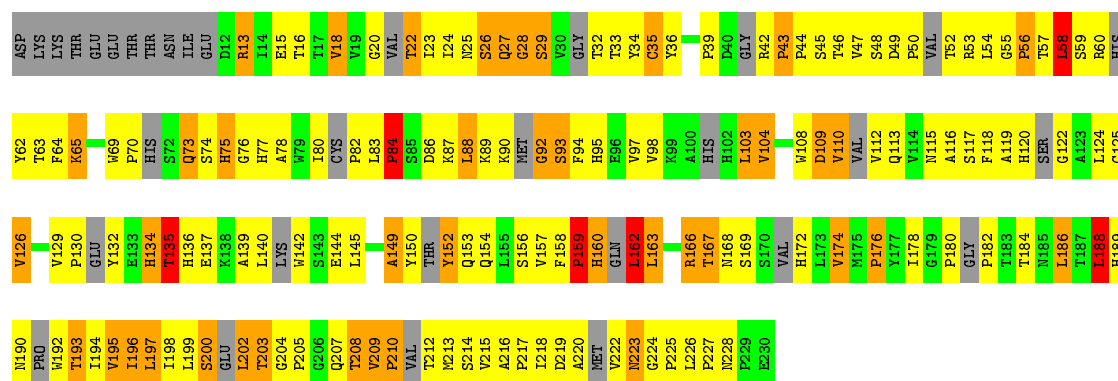
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CN: 20% 44% 18% • 14%



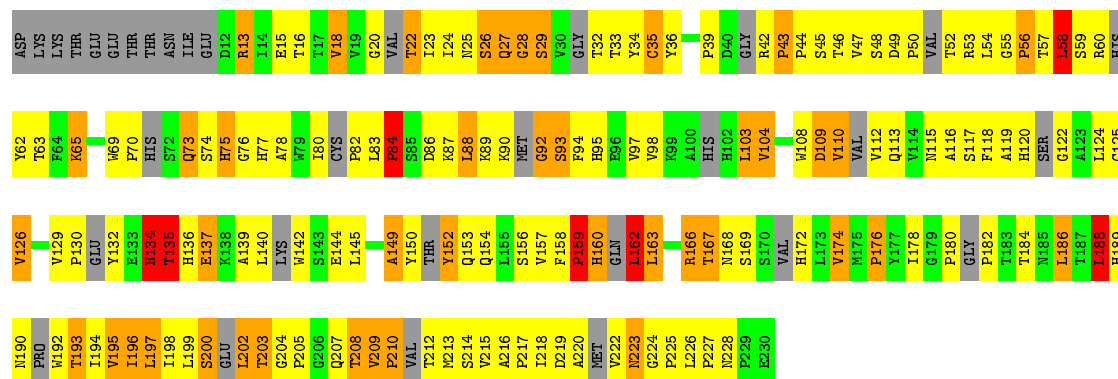
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CO: 20% 46% 18% • 14%

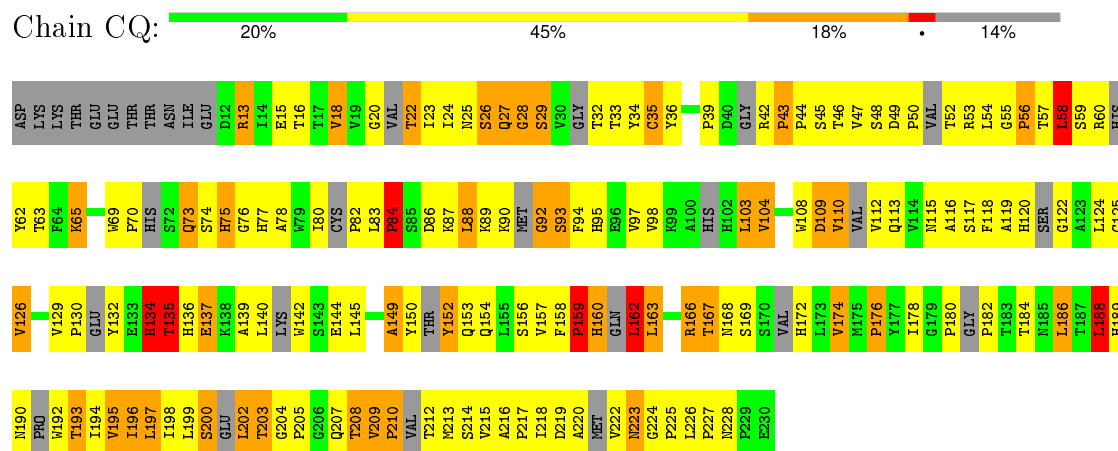


• Molecule 2: EQUINE RHINITIS A VIRUS

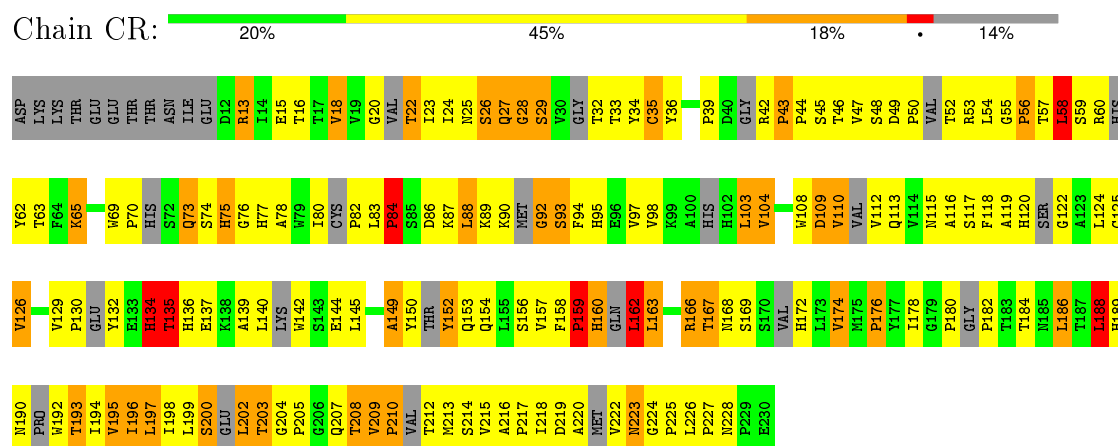
Chain CP: 20% 45% 18% • 14%



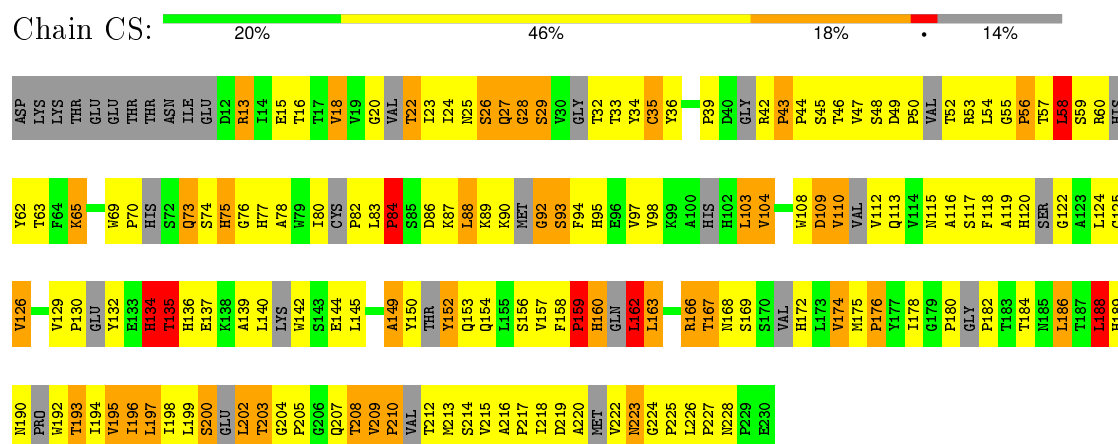
• Molecule 2: EQUINE RHINITIS A VIRUS



• Molecule 2: EQUINE RHINITIS A VIRUS

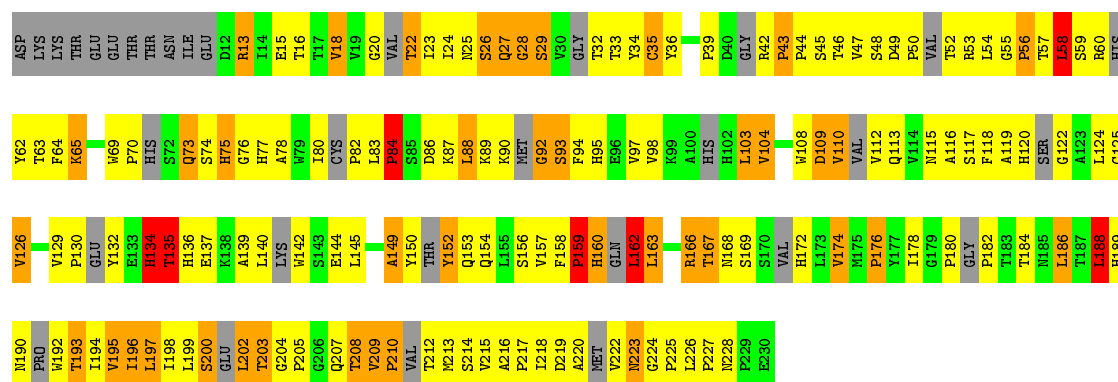


• Molecule 2: EQUINE RHINITIS A VIRUS



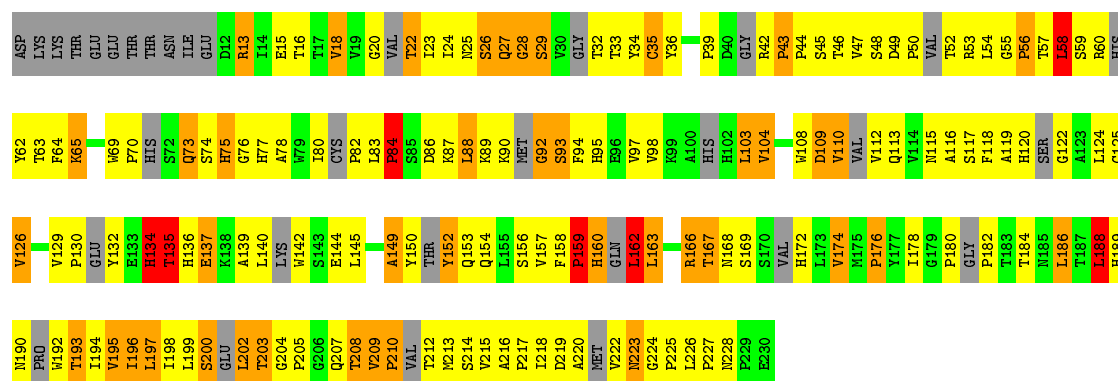
• Molecule 2: EQUINE RHINITIS A VIRUS





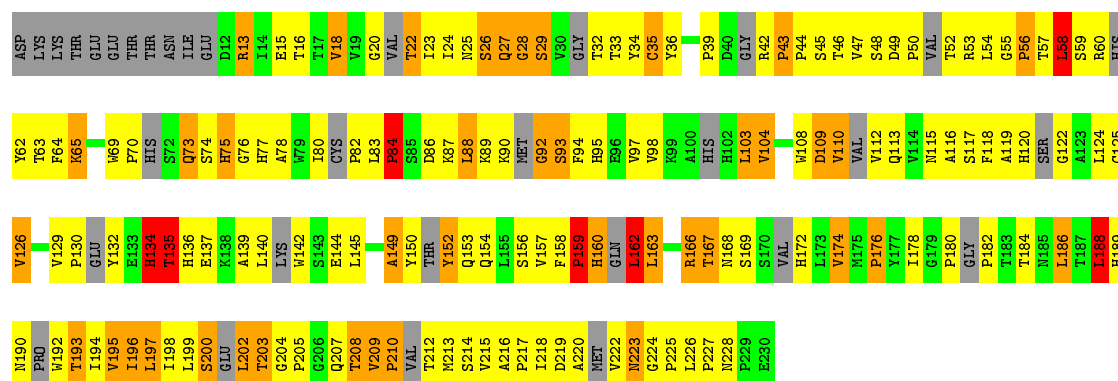
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CU: 20% 45% 18% 14%



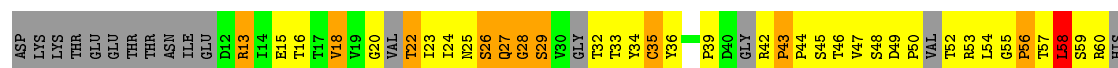
• Molecule 2: EQUINE RHINITIS A VIRUS

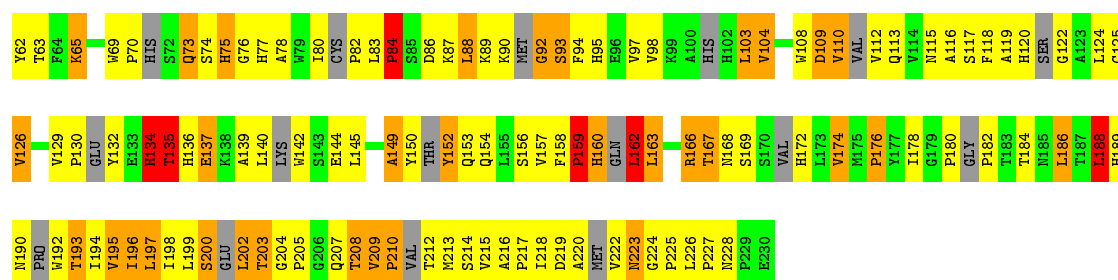
Chain CV: 20% 46% 18% 14%



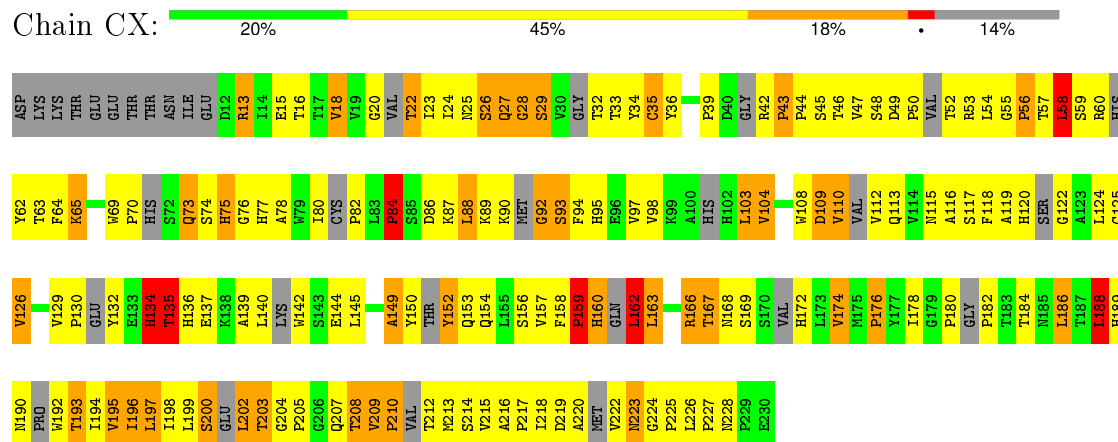
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain CW: 20% 45% 18% 14%

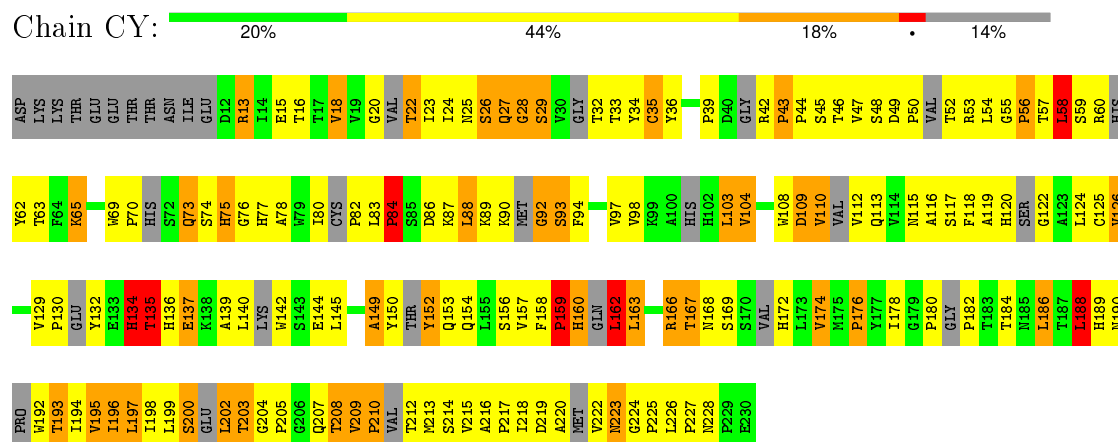




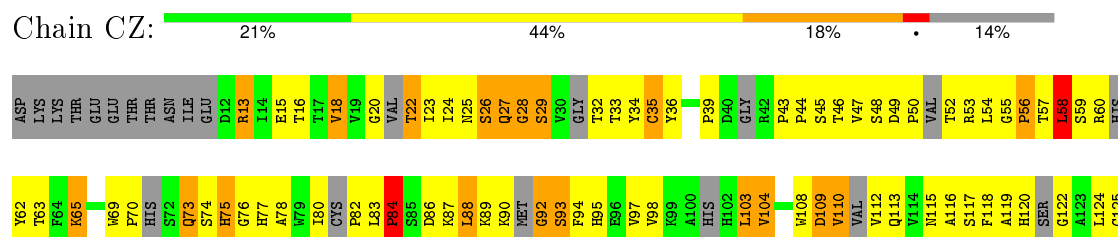
• Molecule 2: EQUINE RHINITIS A VIRUS

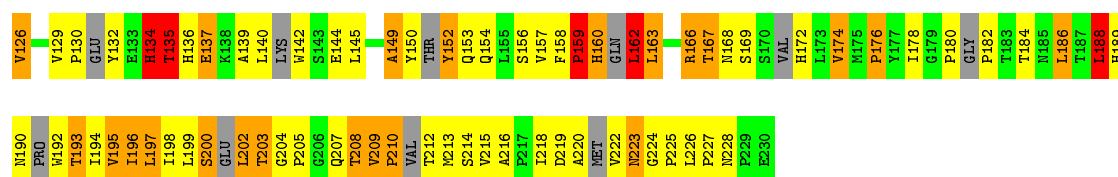


• Molecule 2: EQUINE RHINITIS A VIRUS

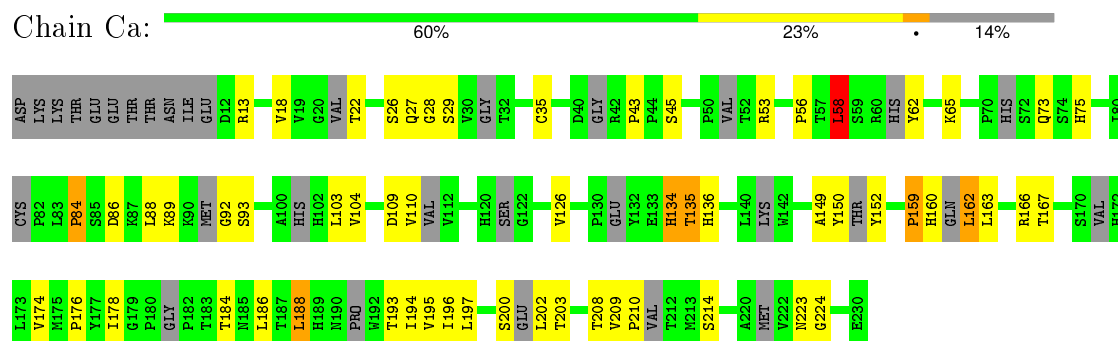


• Molecule 2: EQUINE RHINITIS A VIRUS

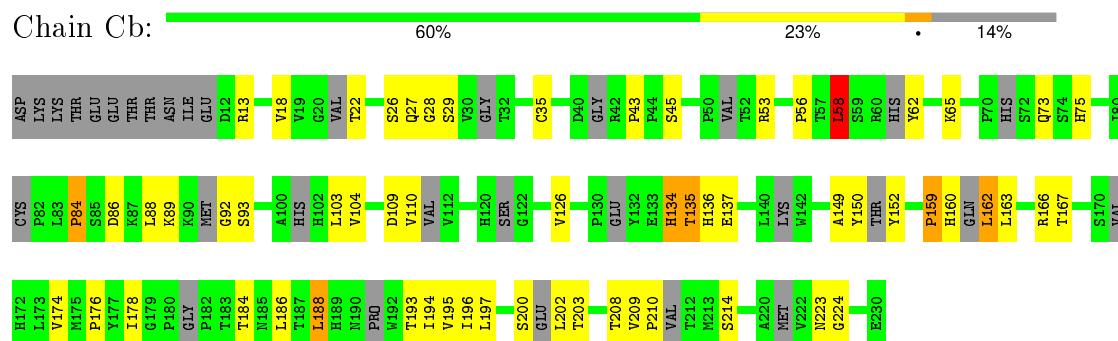




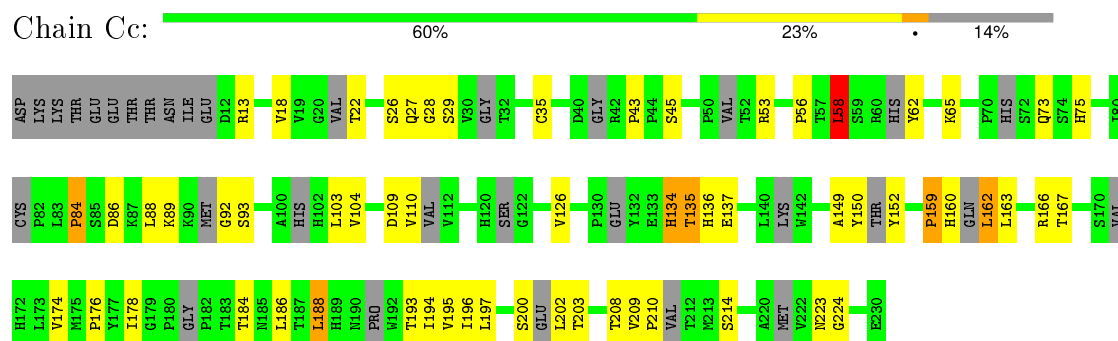
• Molecule 2: EQUINE RHINITIS A VIRUS



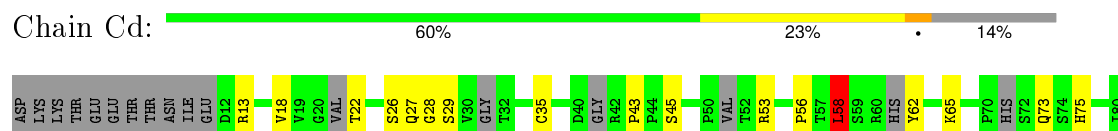
• Molecule 2: EQUINE RHINITIS A VIRUS

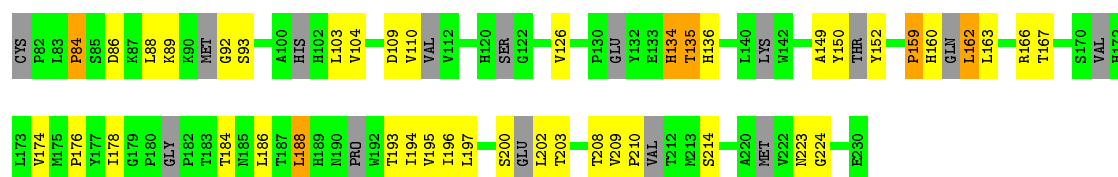


• Molecule 2: EQUINE RHINITIS A VIRUS



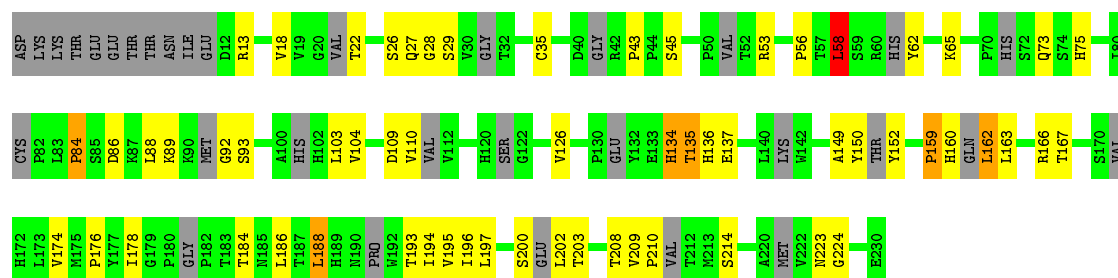
• Molecule 2: EQUINE RHINITIS A VIRUS





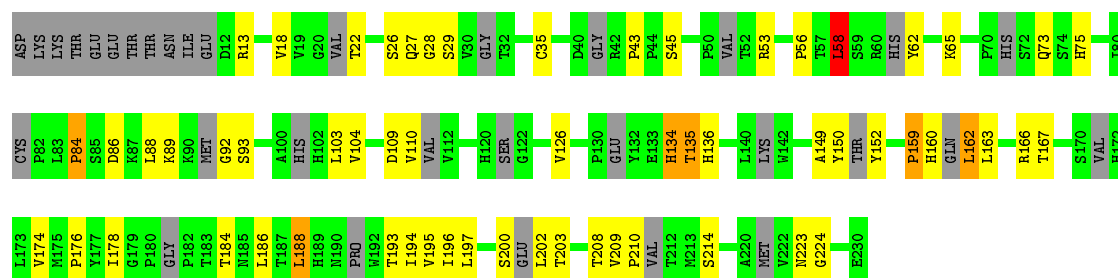
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain Ce: 60% 23% 14%



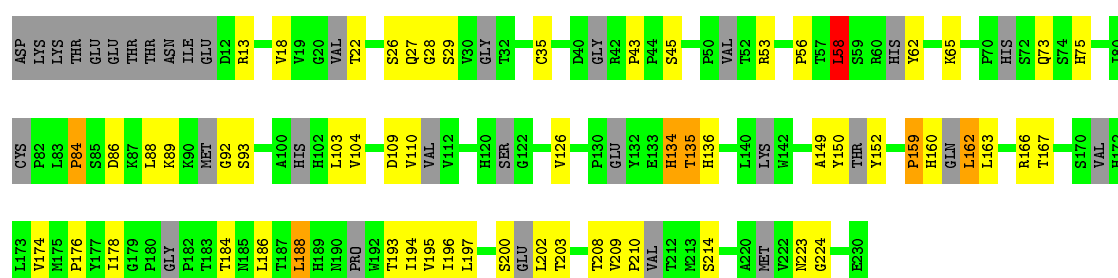
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain Cf: 60% 23% 14%



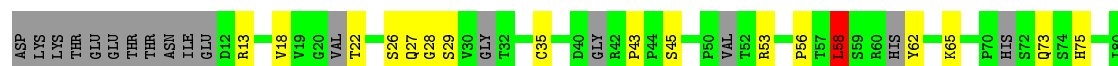
• Molecule 2: EQUINE RHINITIS A VIRUS

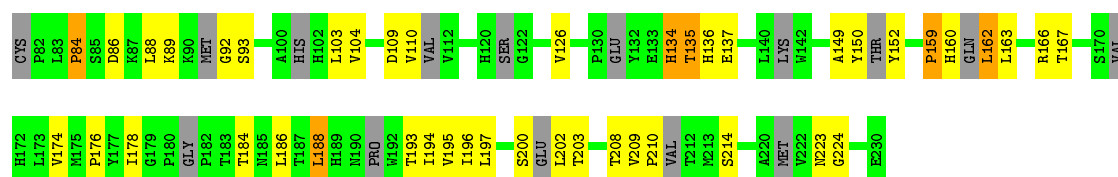
Chain Cg: 60% 23% 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

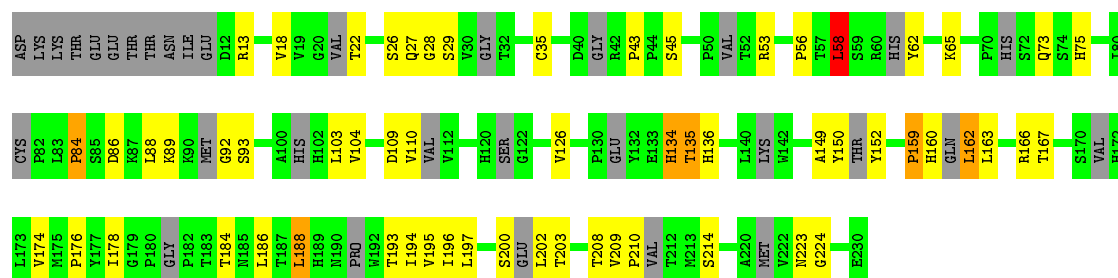
Chain Ch: 60% 23% 14%





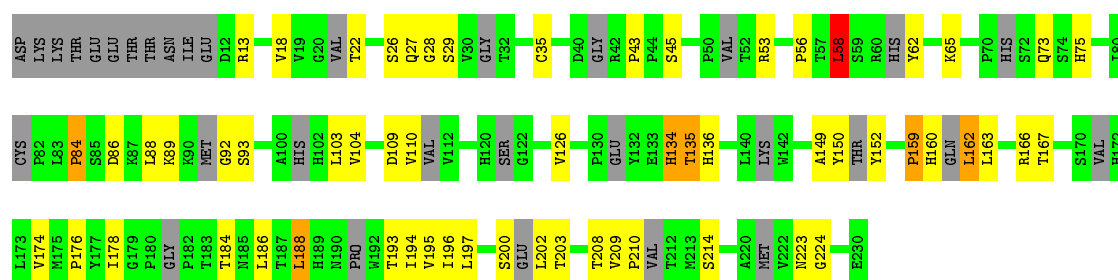
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain Ci: 60% 23% 14%



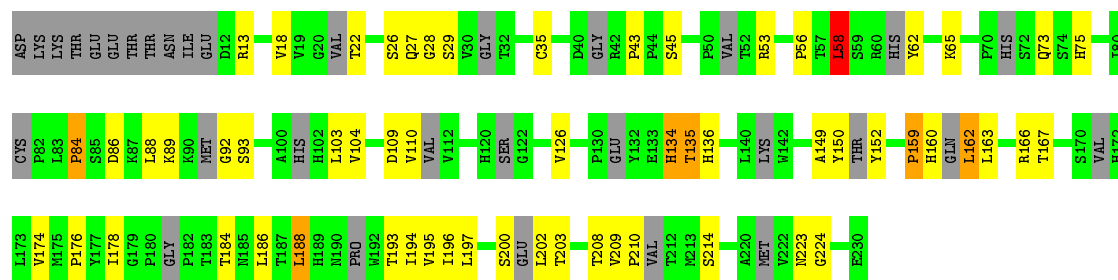
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain Cj: 60% 23% 14%



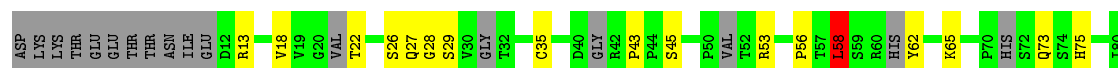
• Molecule 2: EQUINE RHINITIS A VIRUS

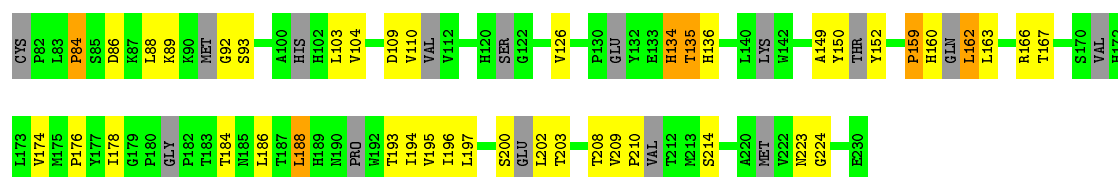
Chain Ck: 60% 23% 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

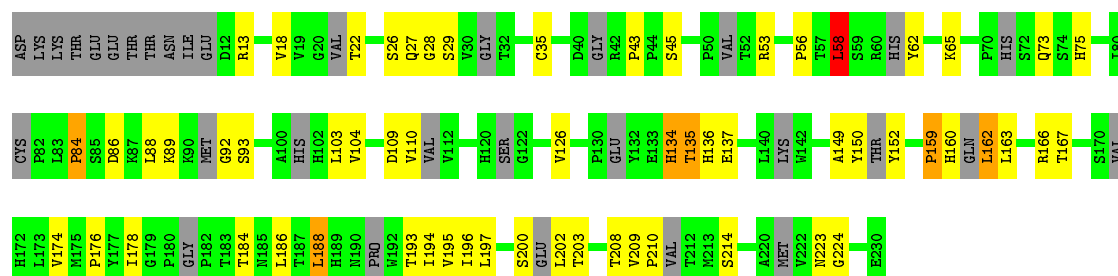
Chain Cl: 60% 23% 14%





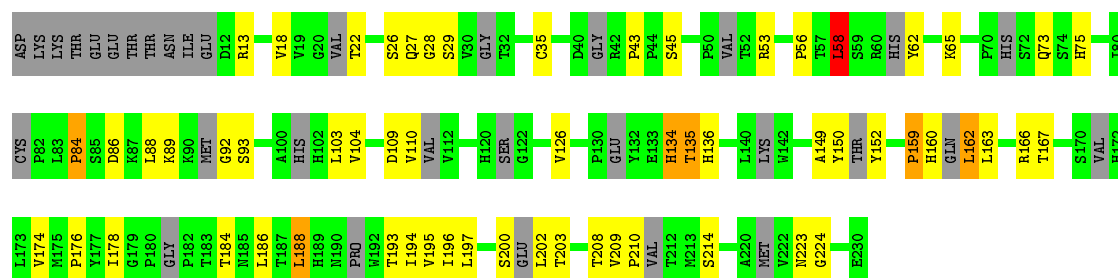
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain Cm: 60% 23% 14%



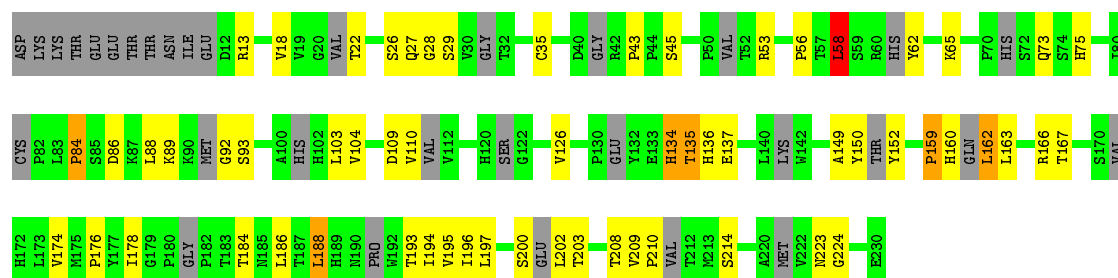
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain Cn: 60% 23% 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

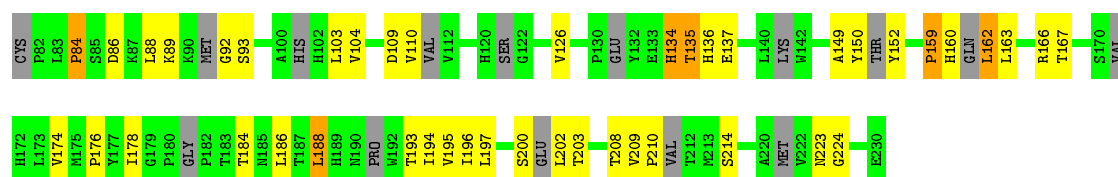
Chain Co: 60% 23% 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

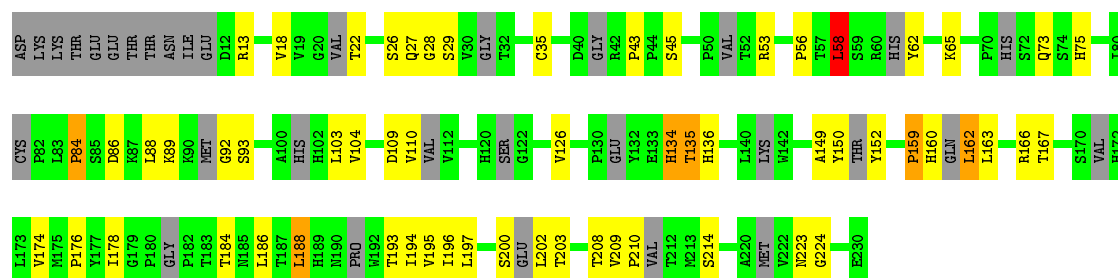
Chain Cp: 60% 23% 14%





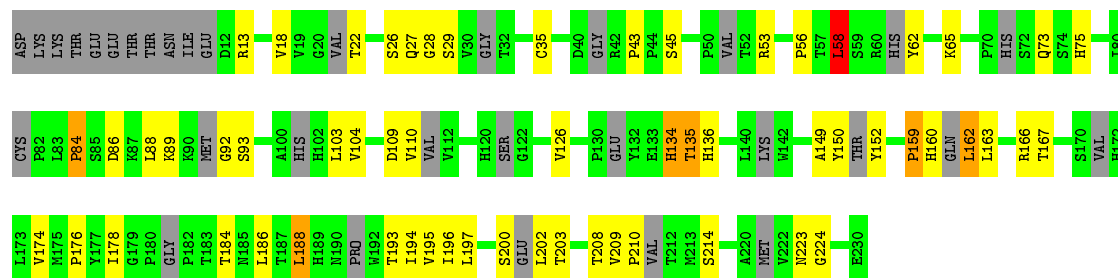
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain Cq: 60% 23% 14%



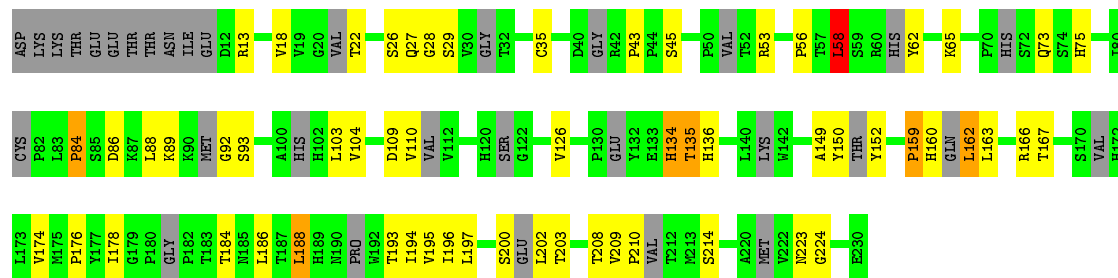
• Molecule 2: EQUINE RHINITIS A VIRUS

Chain Cr: 60% 23% 14%



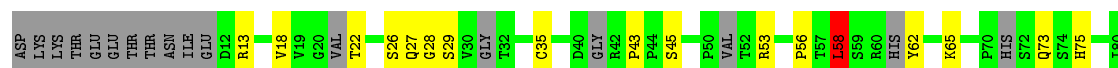
• Molecule 2: EQUINE RHINITIS A VIRUS

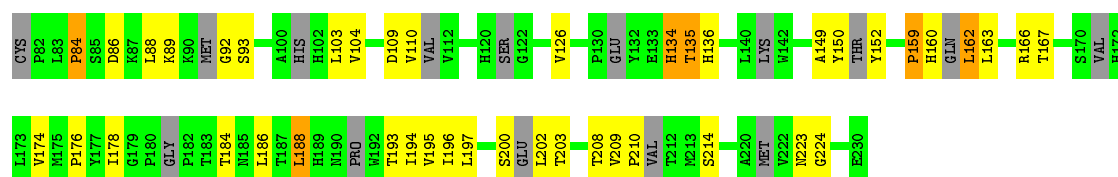
Chain Cs: 60% 23% 14%



• Molecule 2: EQUINE RHINITIS A VIRUS

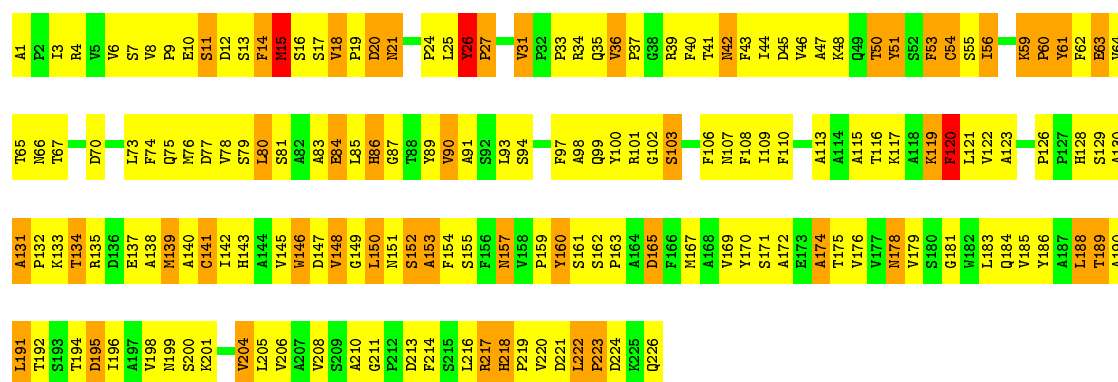
Chain Ct: 60% 23% 14%





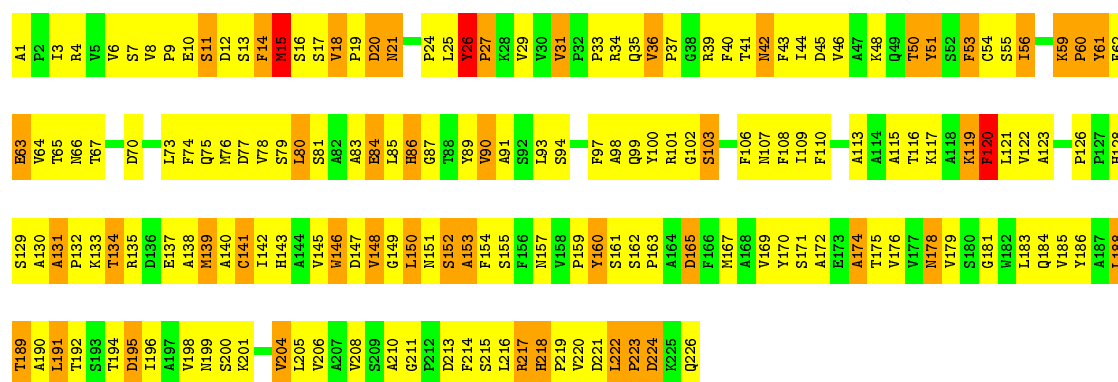
- Molecule 3: P1

Chain D0: 23% 55% 21%



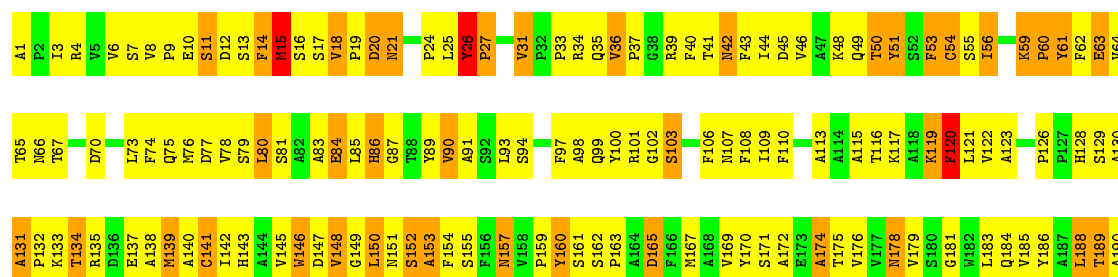
- Molecule 3: P1

Chain D1: 23% 56% 20%



- Molecule 3: P1

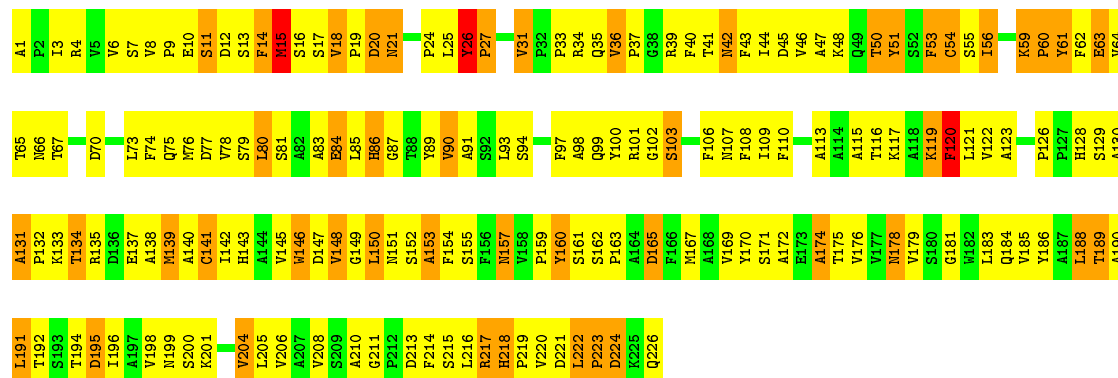
Chain D2: 23% 55% 21%





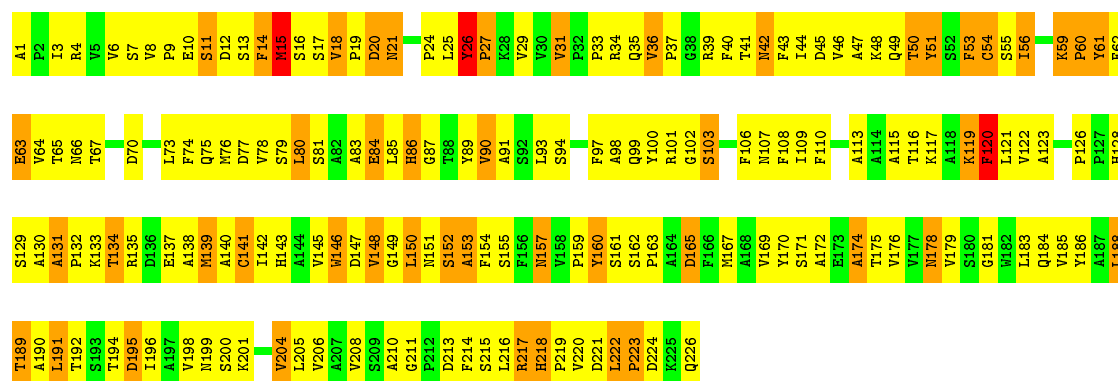
• Molecule 3: P1

Chain D3: 23% 55% 21%



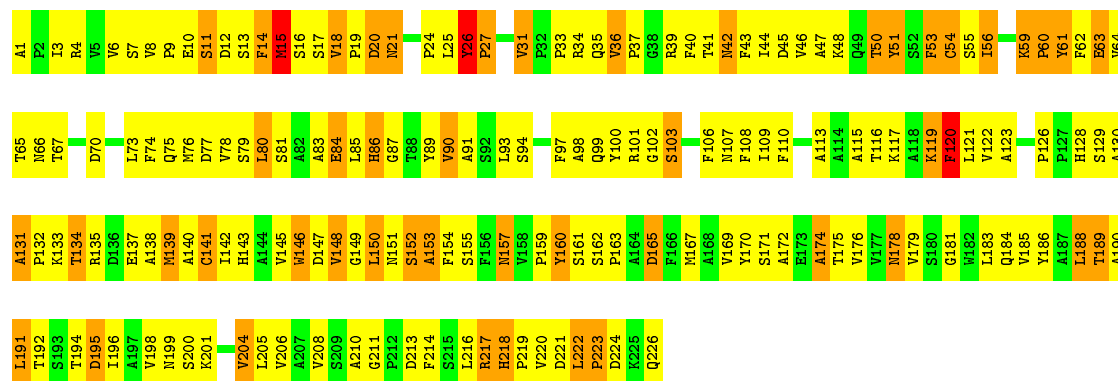
• Molecule 3: P1

Chain D4: 22% 56% 21%



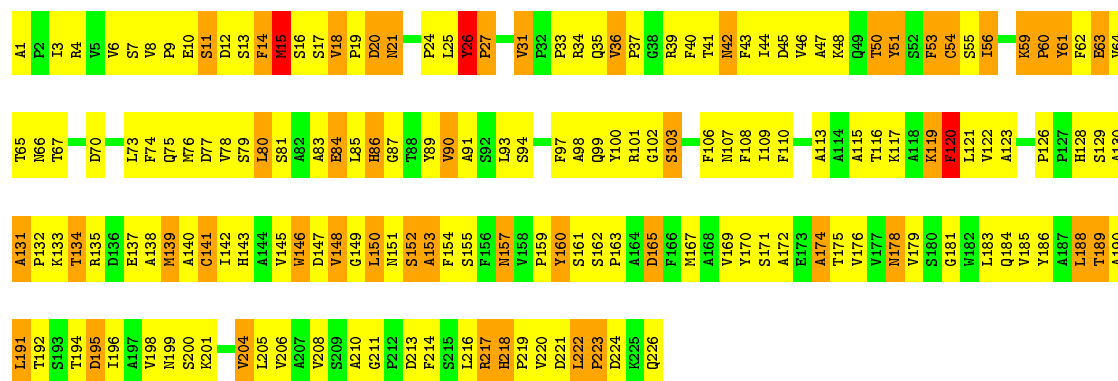
• Molecule 3: P1

Chain D5: 23% 55% 21%

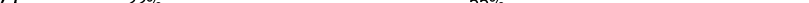


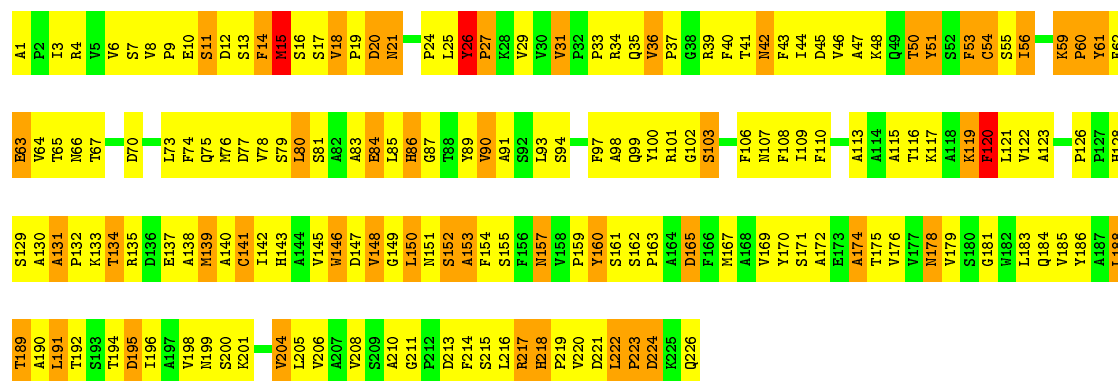
• Molecule 3: P1

Chain D6:  23% 55% 21%



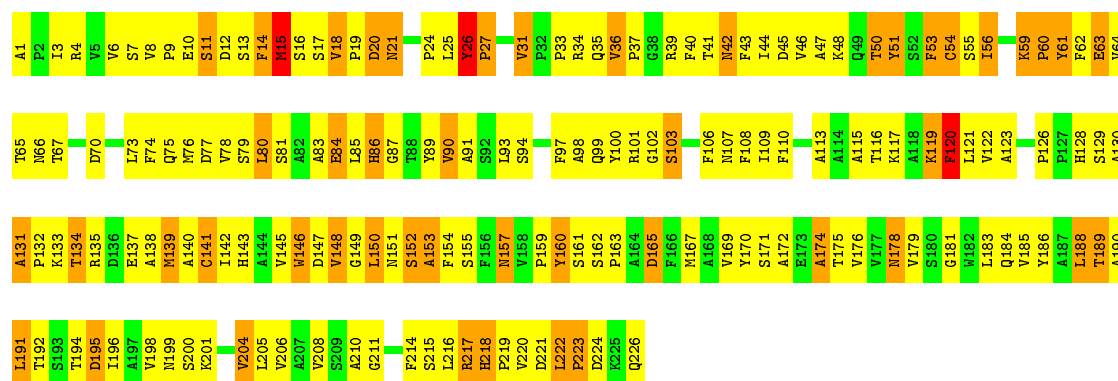
- Molecule 3: P1

Chain D7:  22% 55% 21%



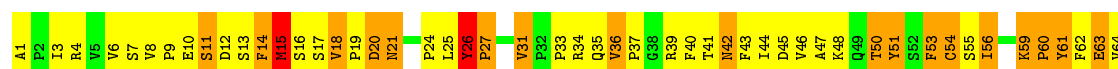
- Molecule 3: P1

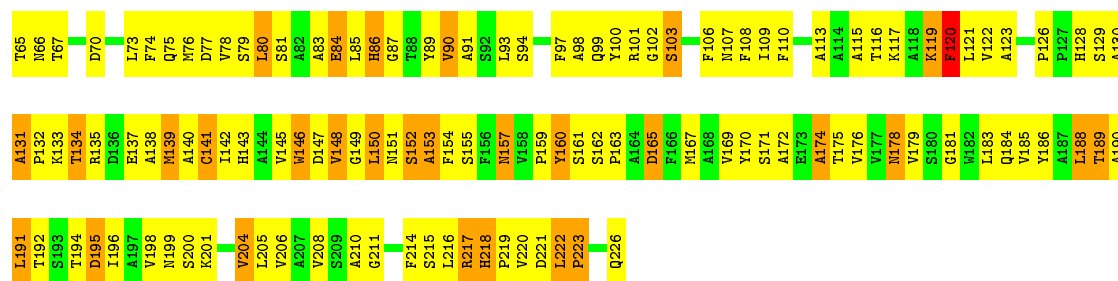
Chain D8:  23% 55% 21%



- Molecule 3: P1

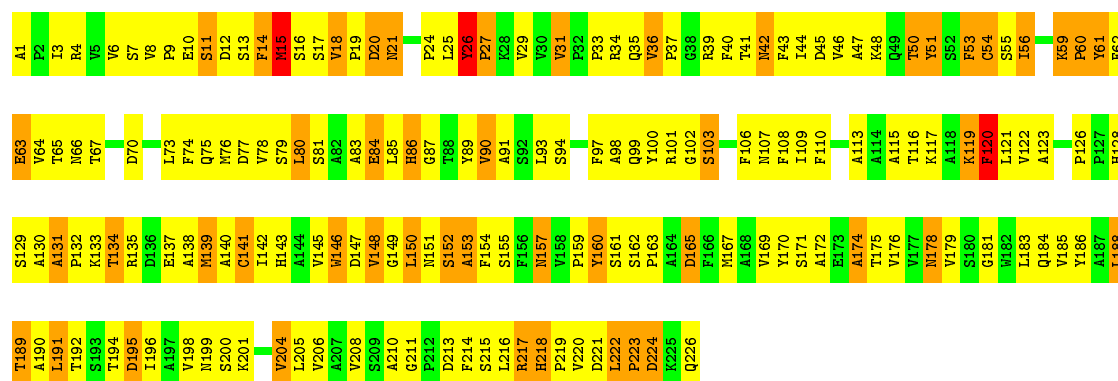
Chain D9:  23% 54% 21%





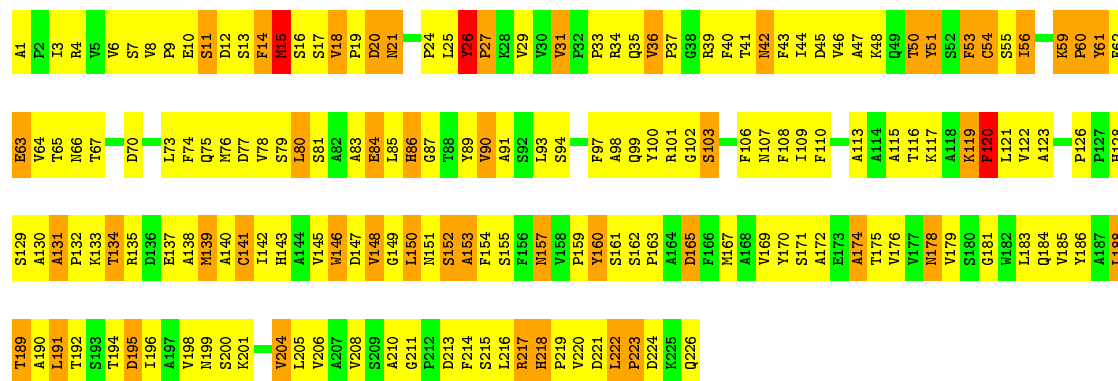
• Molecule 3: P1

Chain DA: 22% 55% 21%



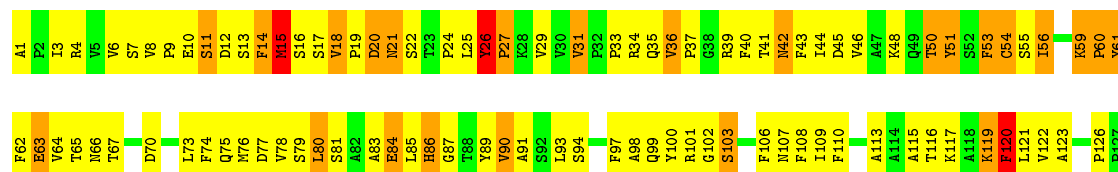
• Molecule 3: P1

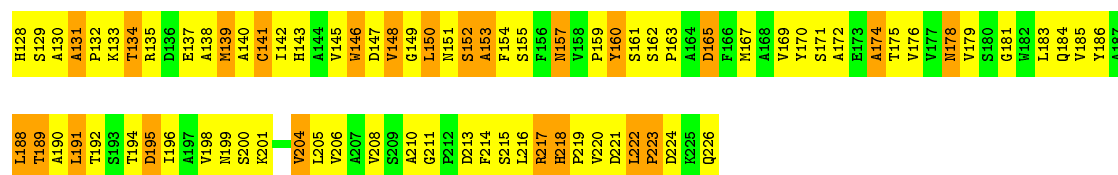
Chain DB: 22% 56% 21%



• Molecule 3: P1

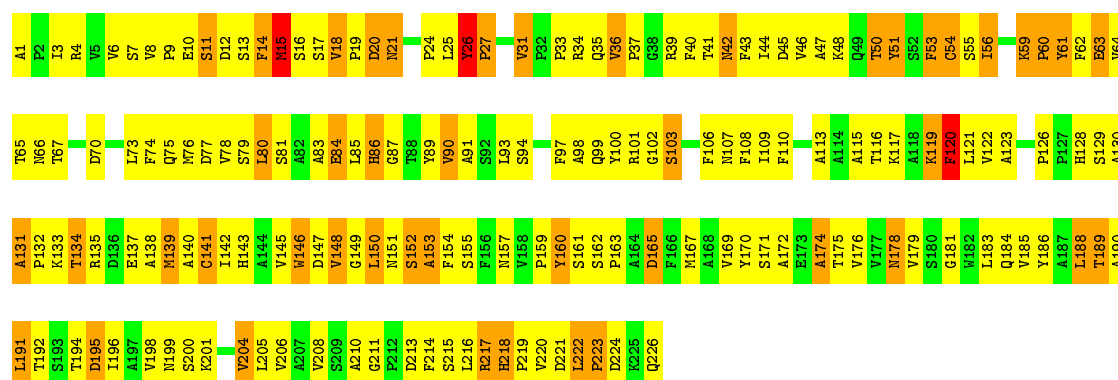
Chain DC: 22% 56% 21%





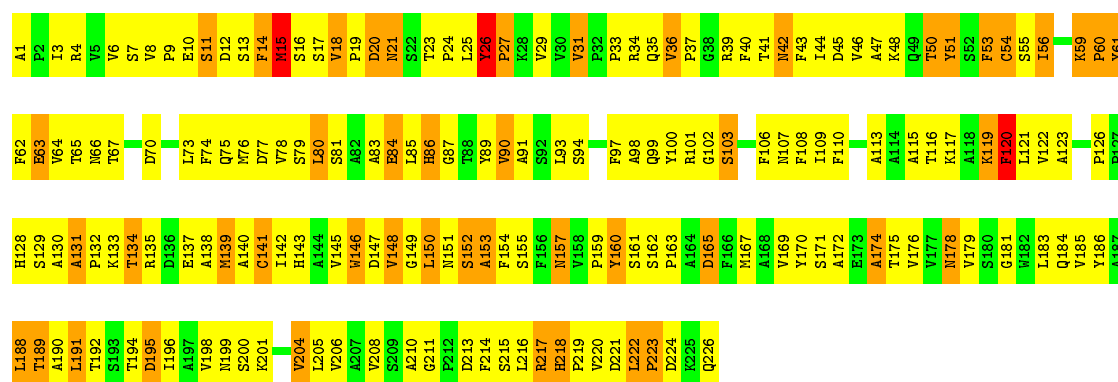
- Molecule 3: P1

Chain DD: 23% 56% 20%



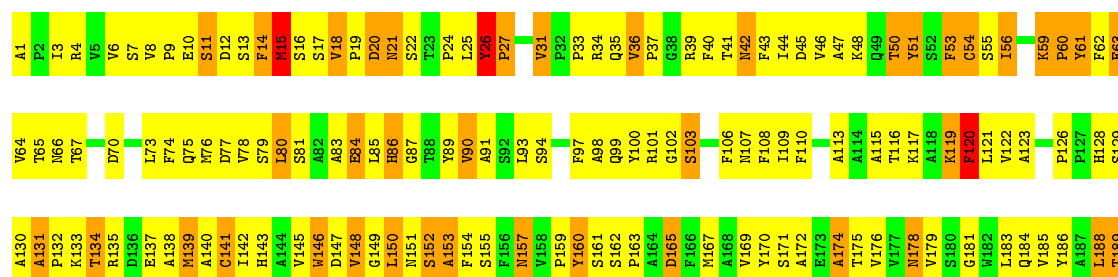
- Molecule 3: P1

Chain DE: 22% 56% 21%



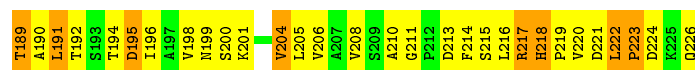
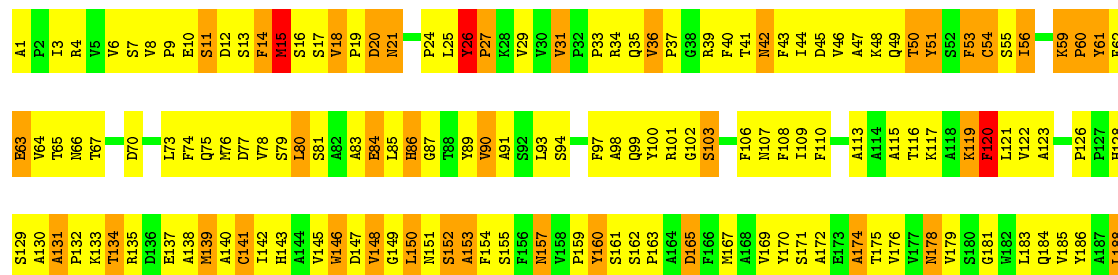
- Molecule 3: P1

Chain DF: 22% 56% 21%

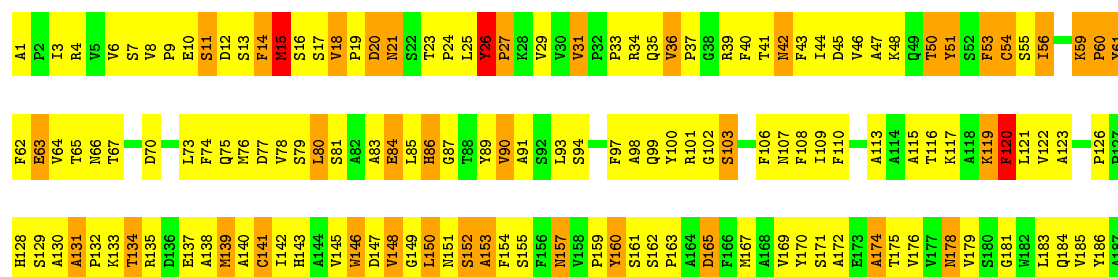




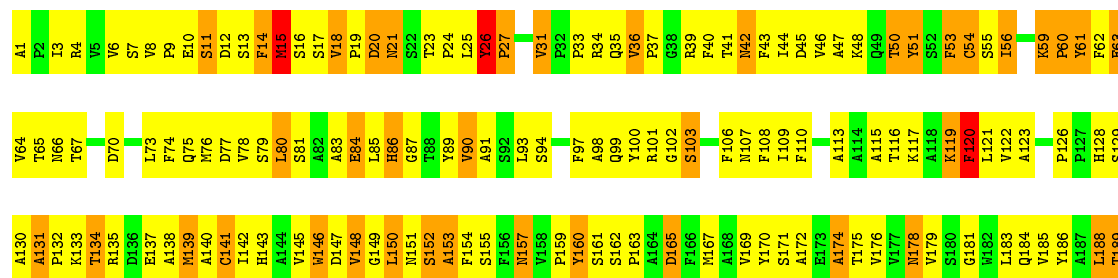
• Molecule 3: P1



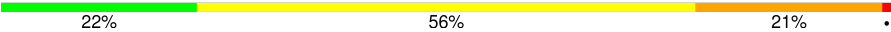
• Molecule 3: P1

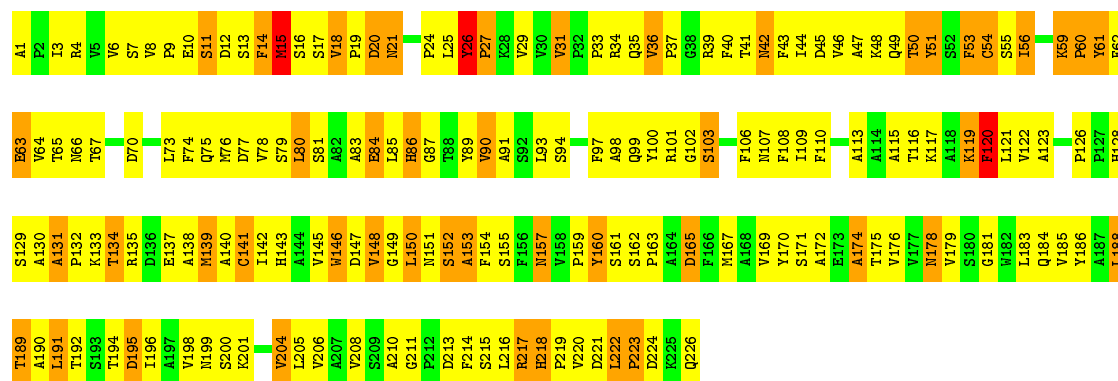


• Molecule 3: P1

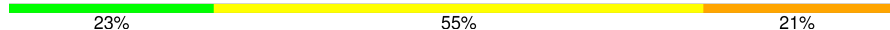


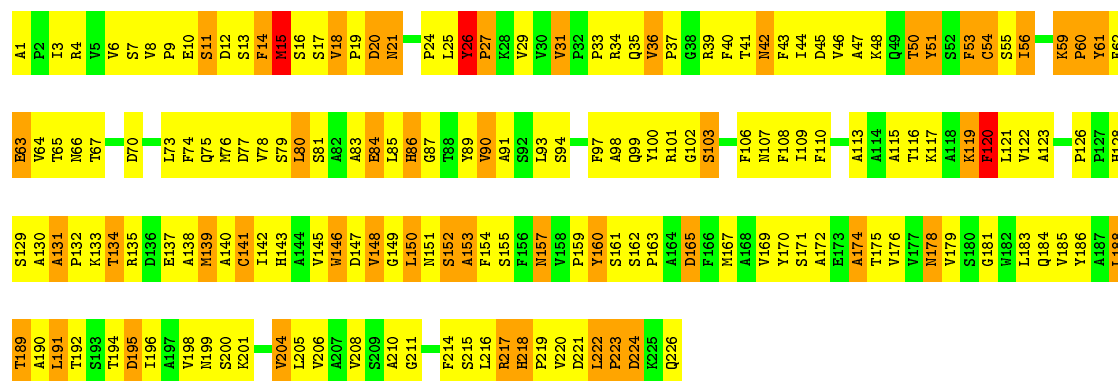
• Molecule 3: P1

Chain DJ:  22% 56% 21% .



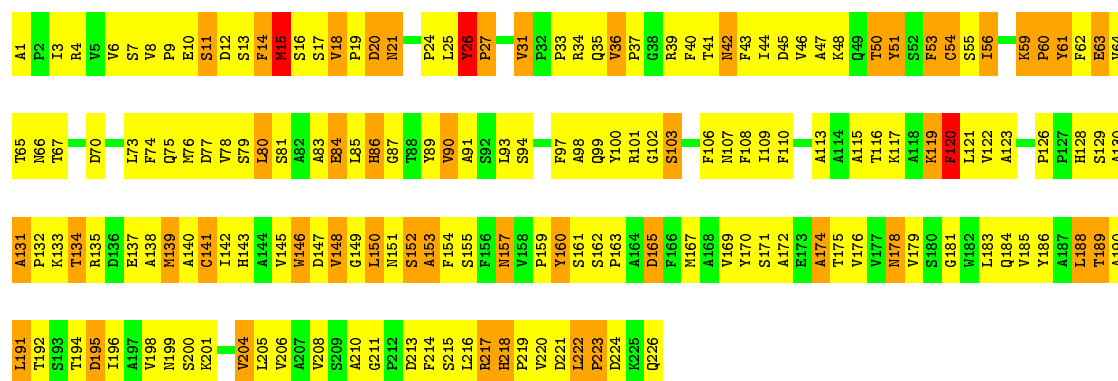
• Molecule 3: P1

Chain DK:  23% 55% 21% .



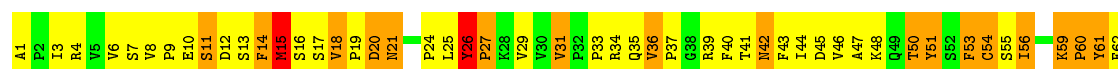
• Molecule 3: P1

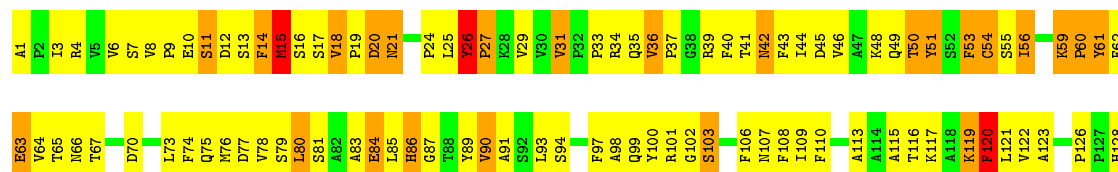
Chain DL:  23% 55% 21% .

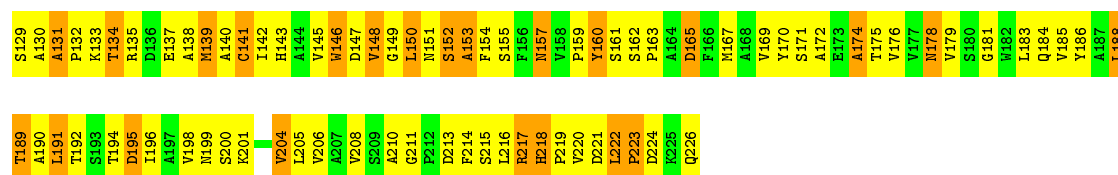


• Molecule 3: P1

Chain DM:  22% 56% 21% .

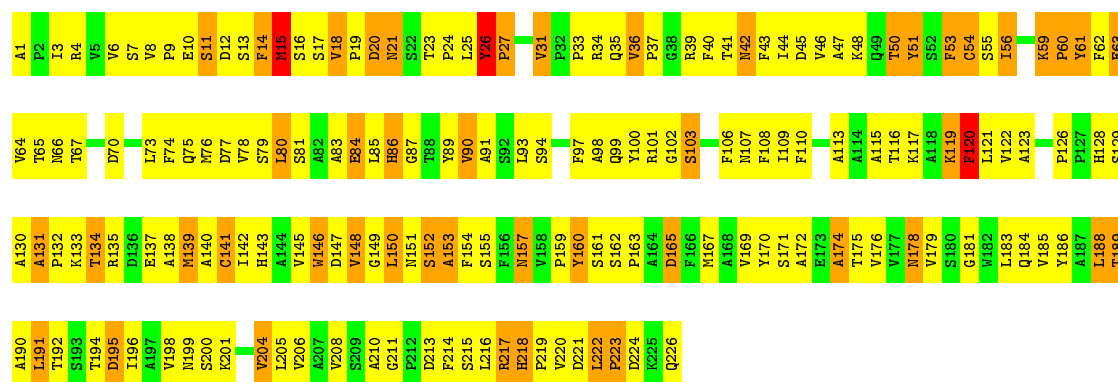






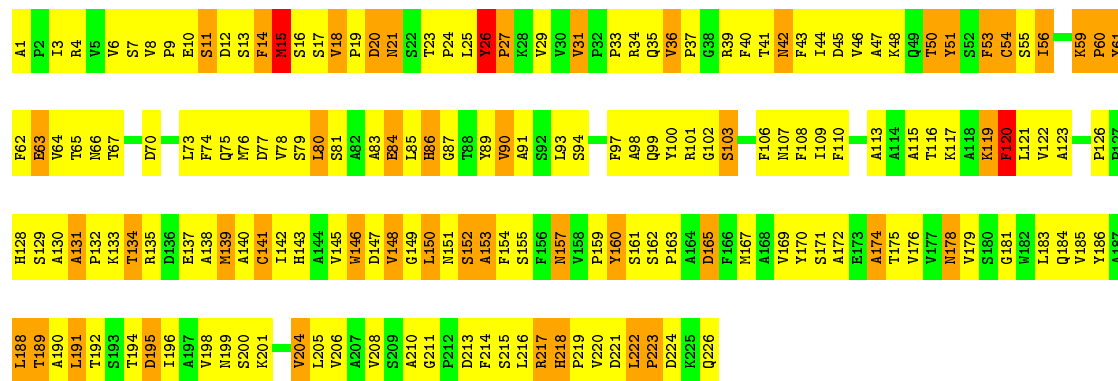
• Molecule 3: P1

Chain DQ: 22% 56% 21%



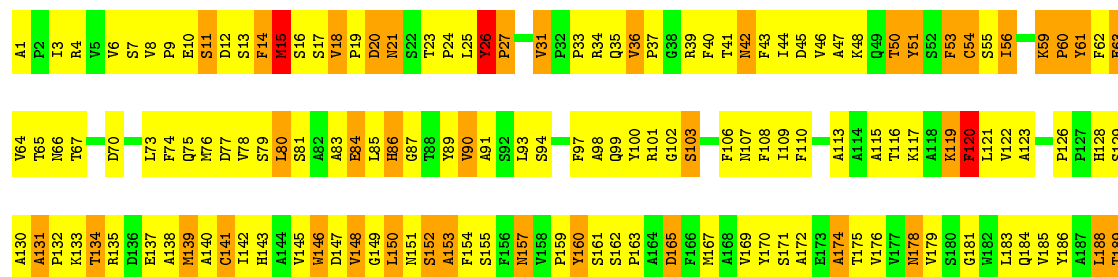
• Molecule 3: P1

Chain DR: 22% 56% 21%



• Molecule 3: P1

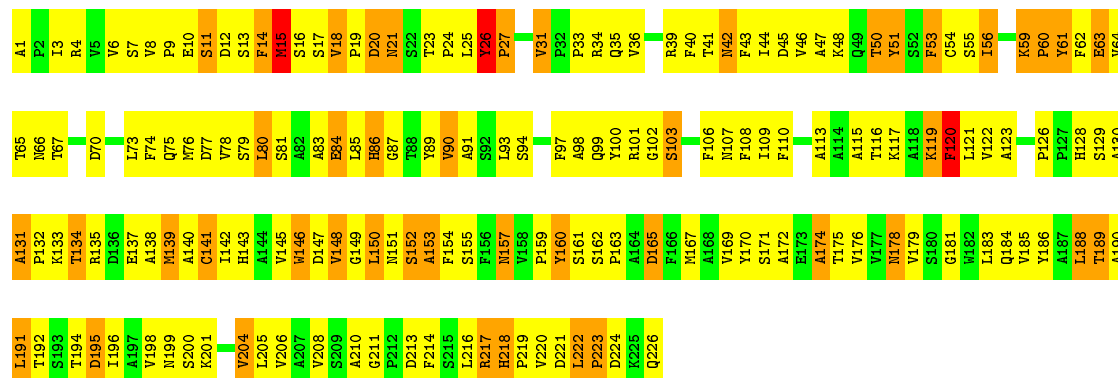
Chain DS: 22% 56% 21%





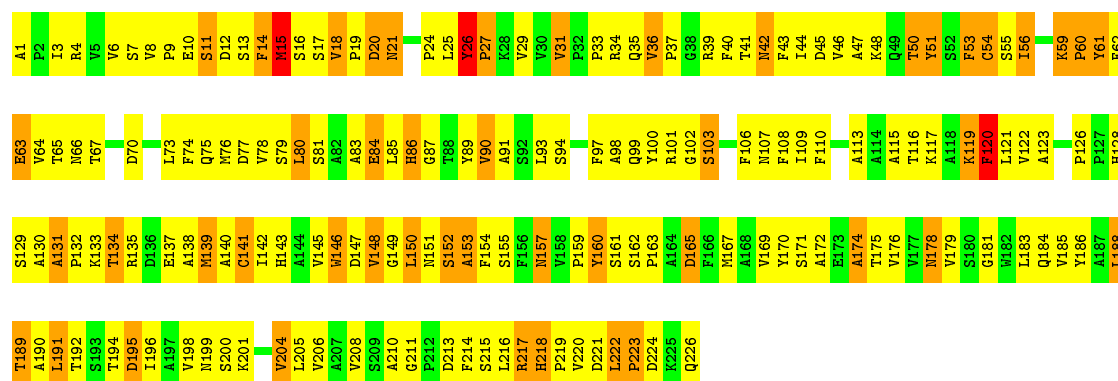
• Molecule 3: P1

Chain DT: 23% 56% 20%



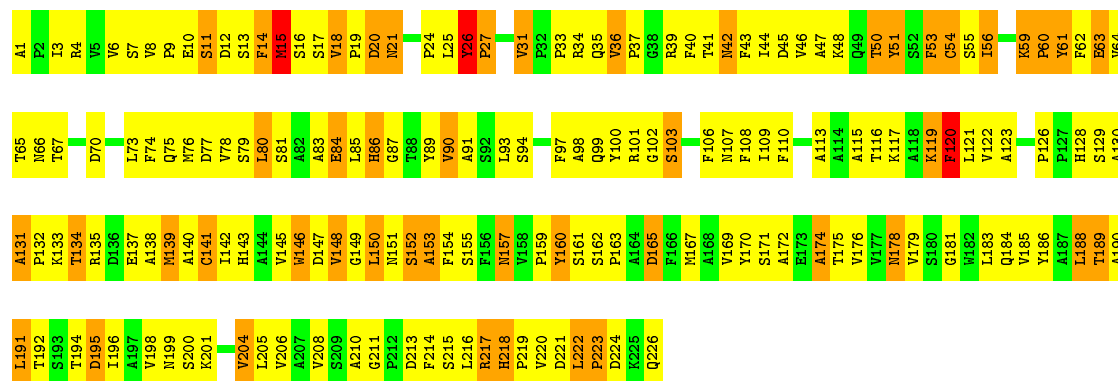
• Molecule 3: P1

Chain DU: 22% 56% 21%



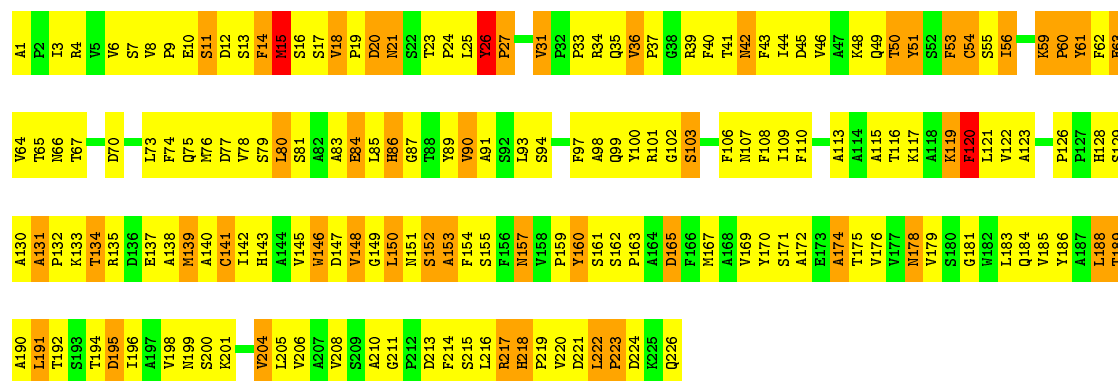
• Molecule 3: P1

Chain DV: 23% 55% 21%



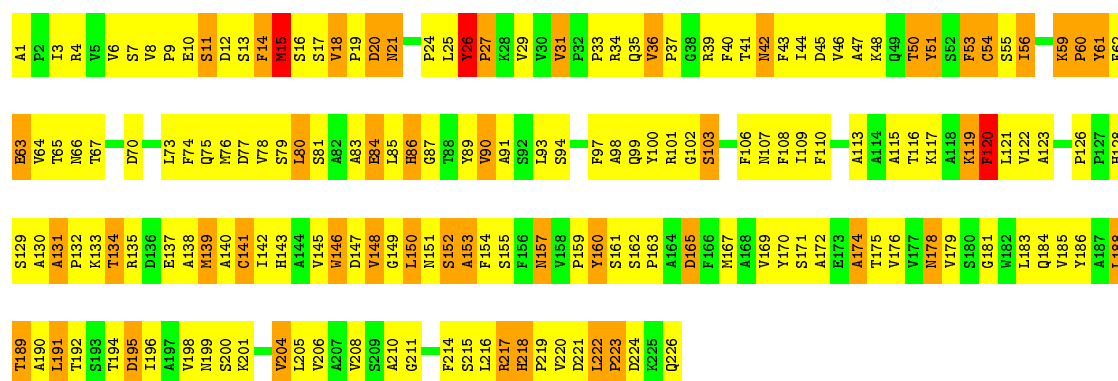
• Molecule 3: P1

Chain DW:  22% 56% 21%



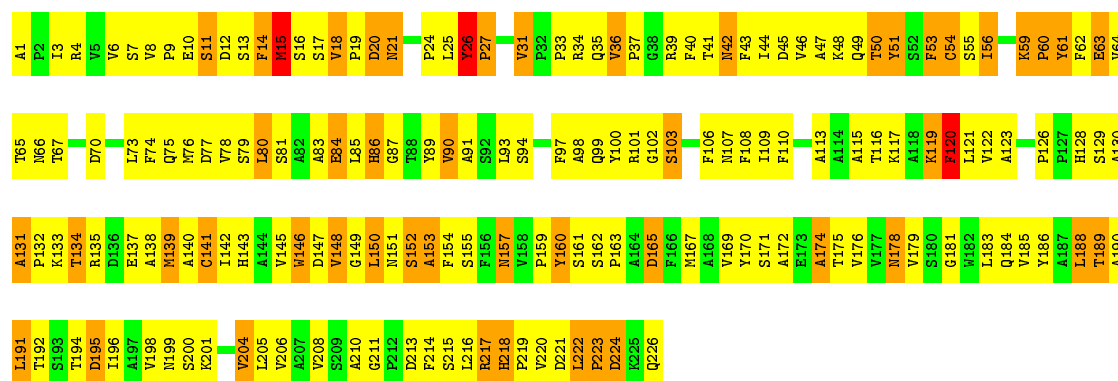
• Molecule 3: P1

Chain DX:  23% 55% 21%



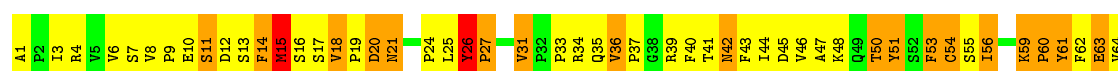
• Molecule 3: P1

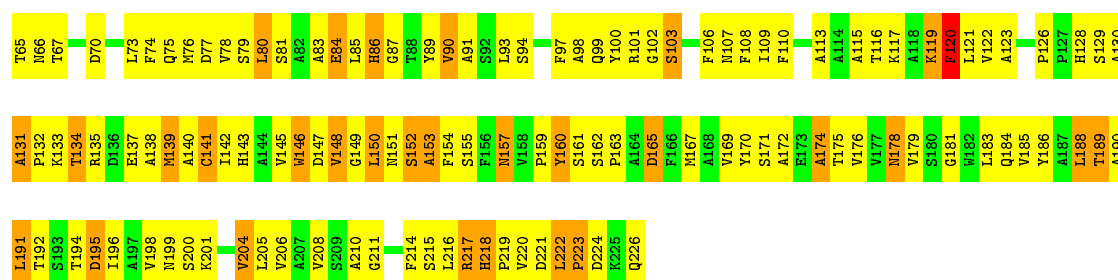
Chain DY:  22% 55% 21%



• Molecule 3: P1

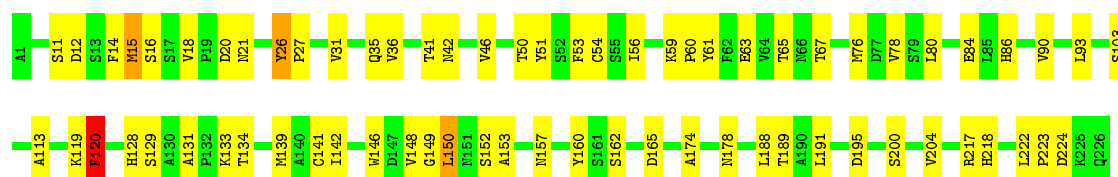
Chain DZ:  23% 55% 21%





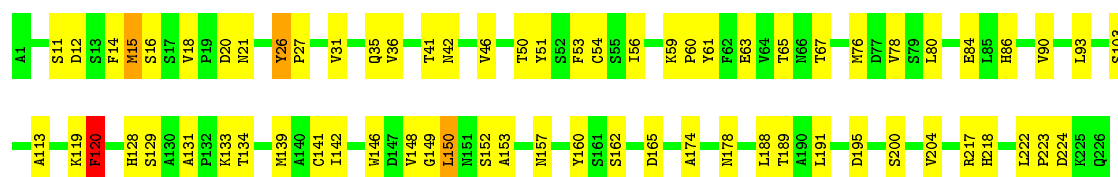
- Molecule 3: P1

Chain Da: 69% 29%



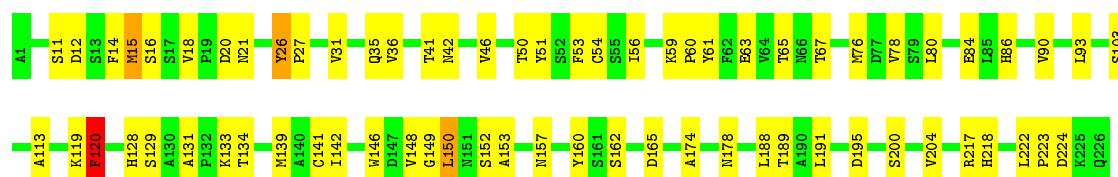
- Molecule 3: P1

Chain Db: 69% 29%



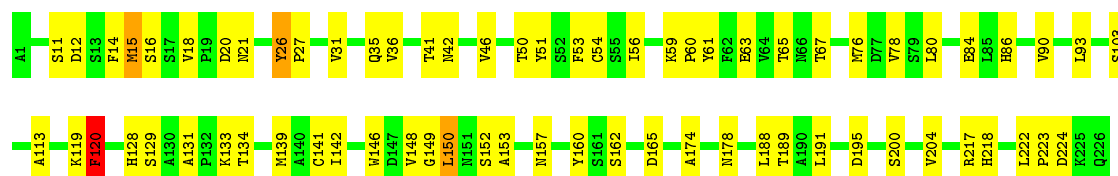
- Molecule 3: P1

Chain Dc: 69% 29%



- Molecule 3: P1

Chain Dd: 69% 29%



- Molecule 3: P1

Chain De: 69% 29%



- Molecule 3: P1

Chain Df: 69% 29%



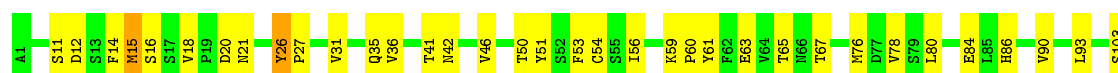
- Molecule 3: P1

Chain Dg: 69% 29%



- Molecule 3: P1

Chain Dh: 69% 29%



- Molecule 3: P1

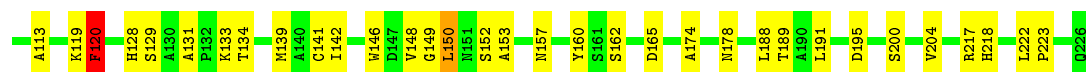
Chain Di: 69% 29%



- Molecule 3: P1

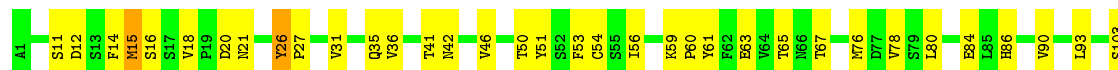
Chain Dj: 70% 28%





- Molecule 3: P1

Chain Dk: 69% 29%



- Molecule 3: P1

Chain Dl: 69% 29%



- Molecule 3: P1

Chain Dm: 69% 29%



- Molecule 3: P1

Chain Dn: 69% 29%



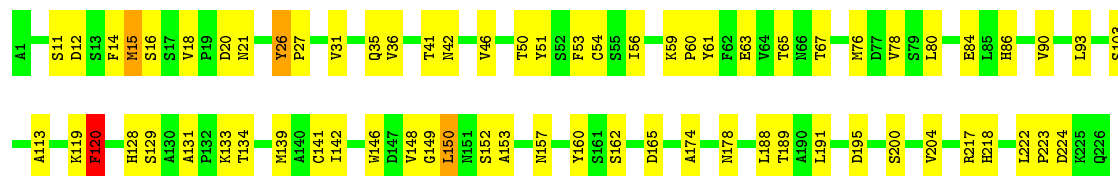
- Molecule 3: P1

Chain Do: 69% 29%



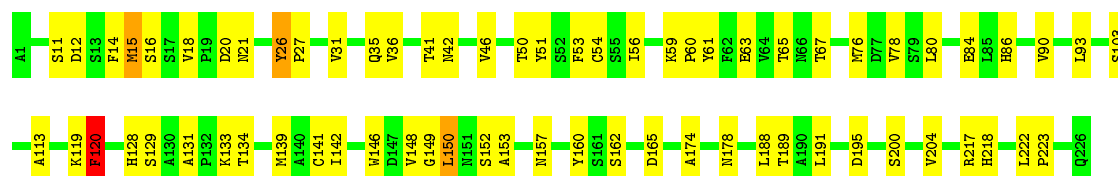
- Molecule 3: P1

Chain Dp: 



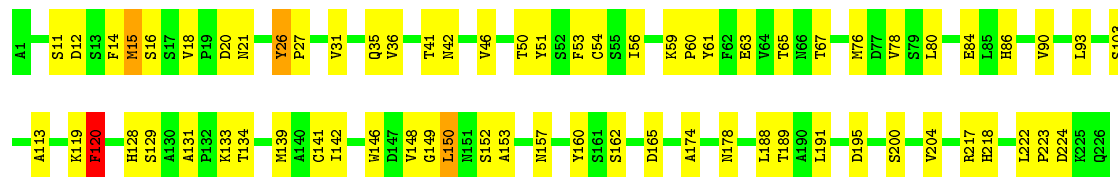
- Molecule 3: P1

Chain Dq: 



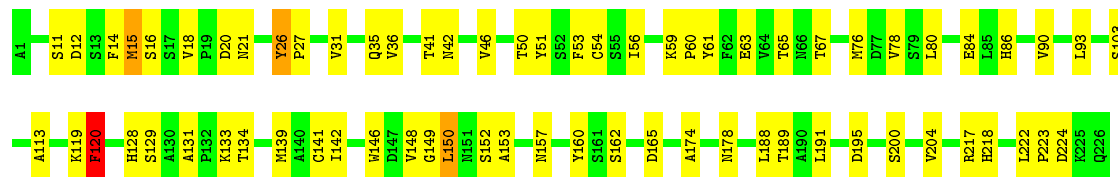
- Molecule 3: P1

Chain Dr: 

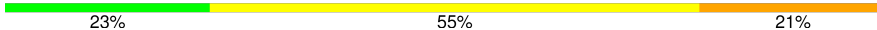


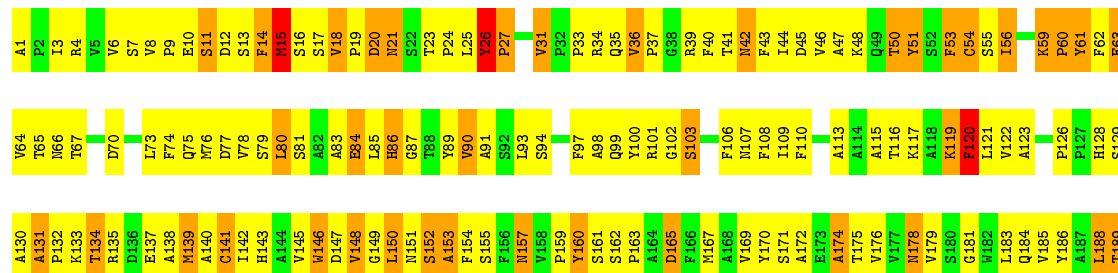
- Molecule 3: P1

Chain Ds: 



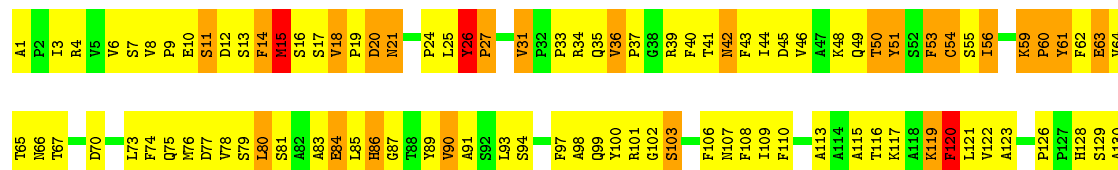
- Molecule 3: P1

Chain EA: 

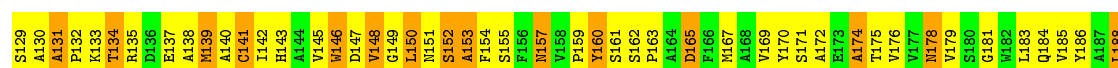
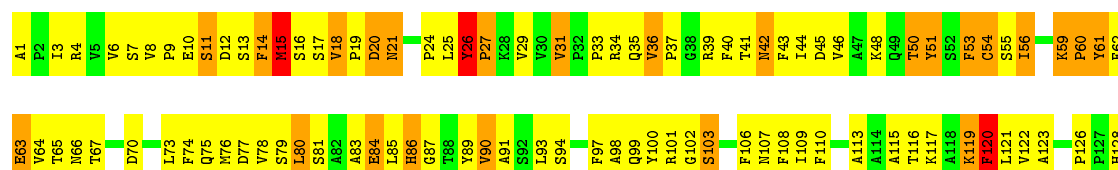




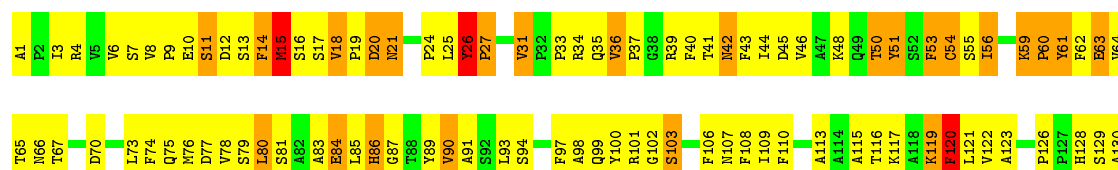
• Molecule 3: P1



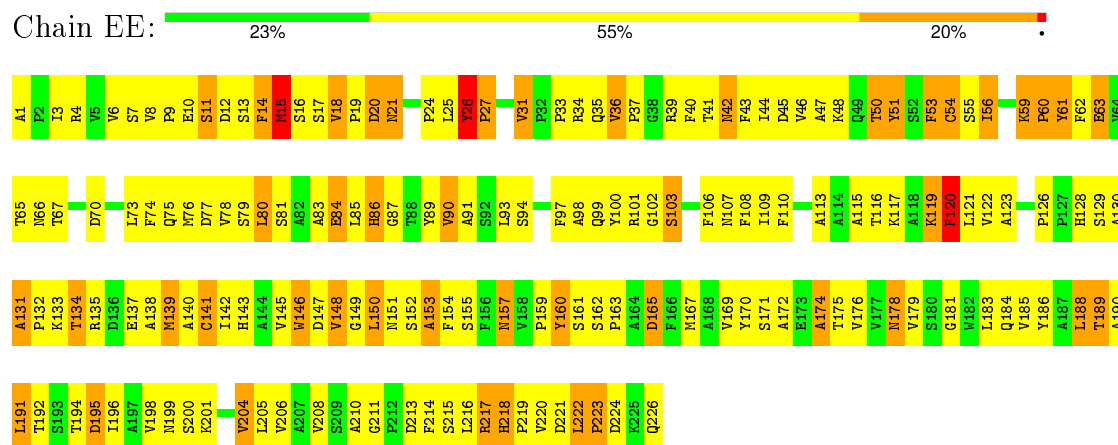
• Molecule 3: P1



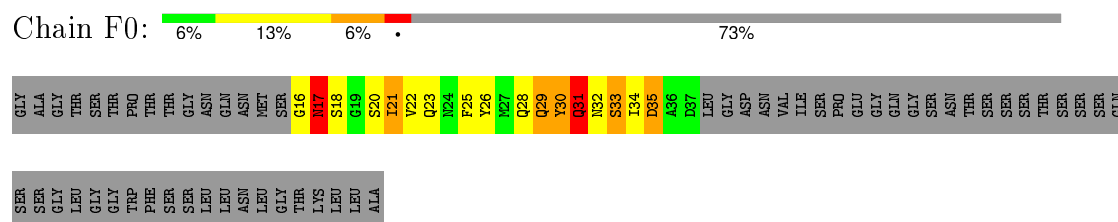
• Molecule 3: P1



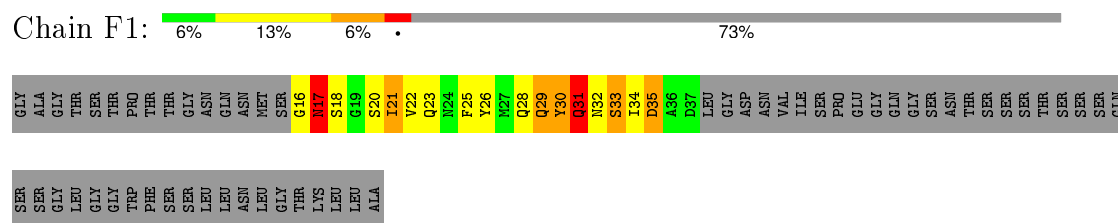
• Molecule 3: P1



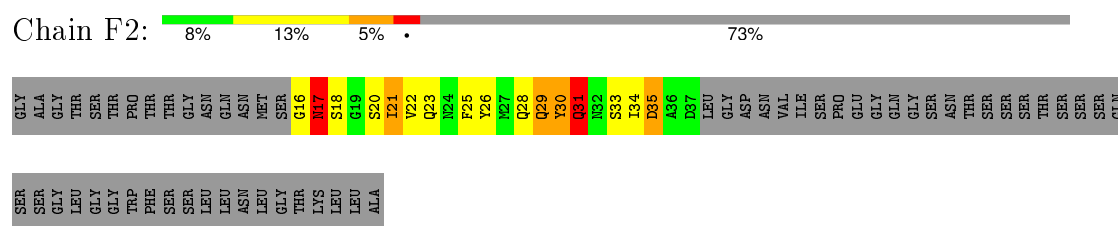
- Molecule 4: P1



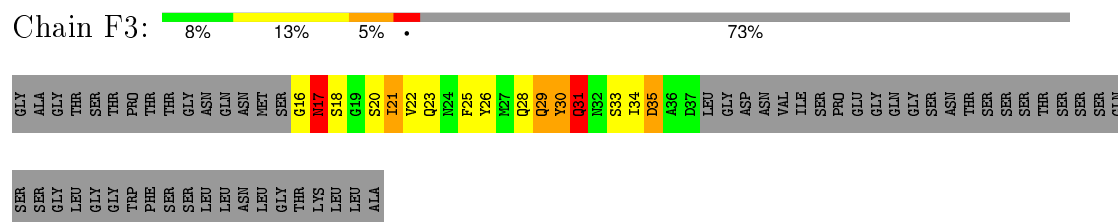
- Molecule 4: P1



- Molecule 4: P1

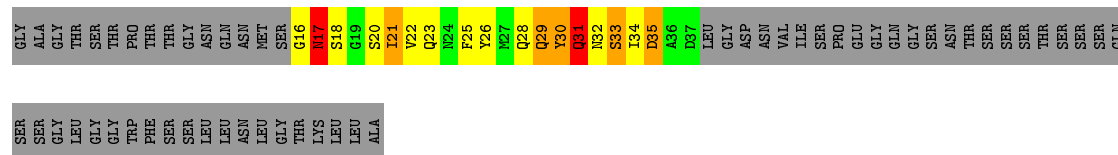


- Molecule 4: P1



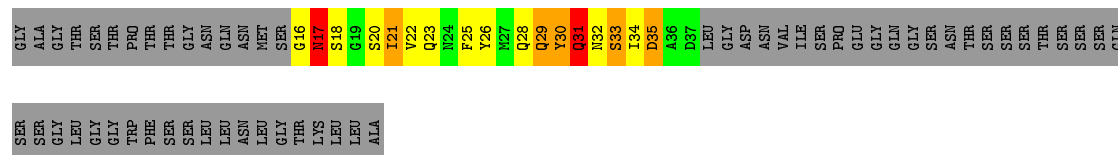
- Molecule 4: P1

Chain F4: 6% 13% 6% • 73%



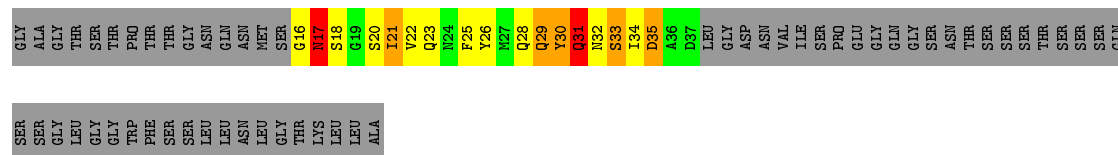
- Molecule 4: P1

Chain F5: 6% 13% 6% • 73%



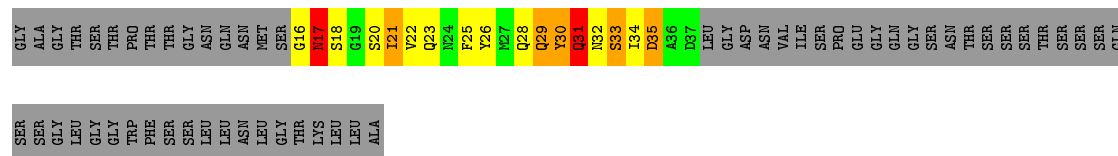
- Molecule 4: P1

Chain F6: 6% 13% 6% • 73%



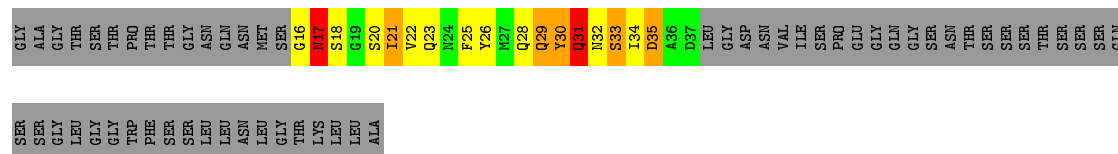
- Molecule 4: P1

Chain F7:  6% 13% 6% • 73%



- Molecule 4: P1

Chain F8:  6% 13% 6% 73%



- Molecule 4: P1

Chain F9: 6% 13% 6% • 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FA: 6% 13% 6% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FB: 6% 13% 6% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FC: 6% 13% 6% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FD: 8% 13% 5% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FE: 6% 13% 6% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain FF:  6% 13% 6% . 73%

GLY	ALA	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	N27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	SER	ASN	THR	SER	SER	THR	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain FG:  6% 13% 6% . 73%

GLY	ALA	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	N27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	SER	ASN	THR	SER	SER	THR	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain FH:  6% 13% 6% . 73%

GLY	ALA	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	N27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	SER	ASN	THR	SER	SER	THR	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain FI:  6% 13% 6% . 73%

GLY	ALA	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	N27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	SER	ASN	THR	SER	SER	THR	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

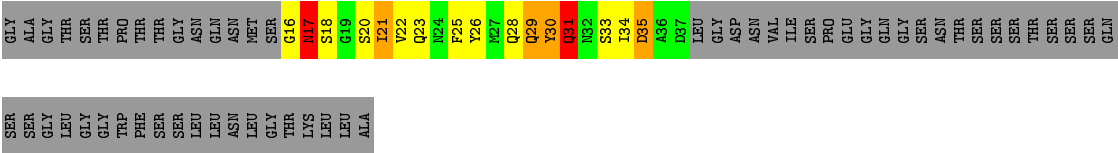
Chain FJ:  6% 14% 5% . 73%

GLY	ALA	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	N27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	SER	ASN	THR	SER	SER	THR	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

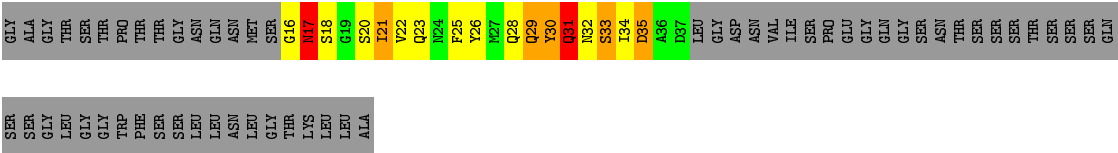
SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

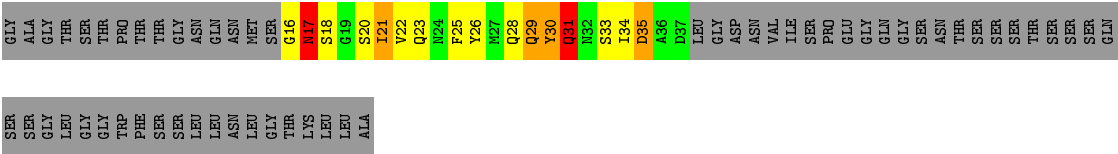
Chain FK:  8% 13% 5% . 73%



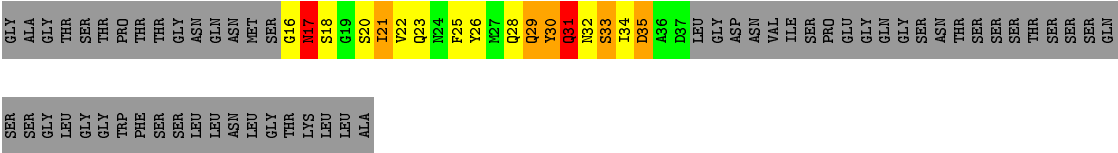
• Molecule 4: P1



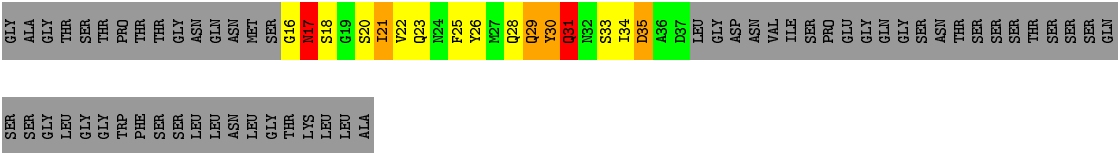
• Molecule 4: P1



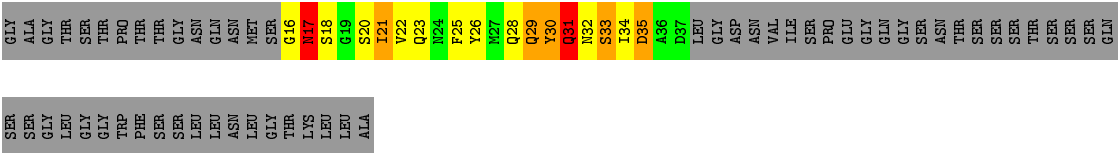
• Molecule 4: P1



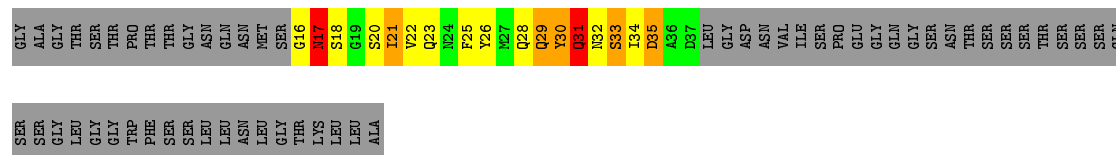
• Molecule 4: P1



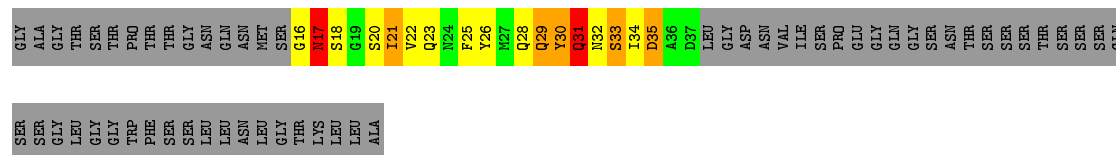
• Molecule 4: P1



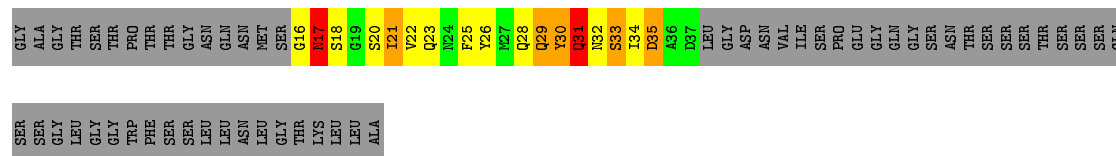
- Molecule 4: P1



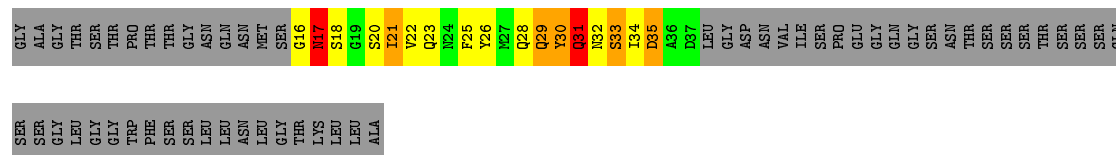
- Molecule 4: P1



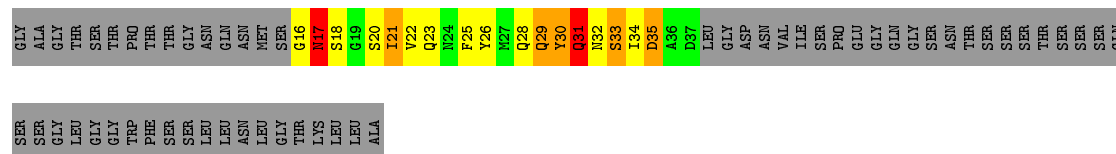
- Molecule 4: P1



- Molecule 4: P1



- Molecule 4: P1



- Molecule 4: P1



GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FW: 6% 13% 6% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FX: 6% 13% 6% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FY: 6% 13% 6% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain FZ: 8% 13% 5% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	S18	G19	S20	I21	V22	Q23	N24	F25	Y26	P27	Q28	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	SER	ASN	THR	SER	SER	SER	THR	SER	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLY	LEU	GLY	GLY	TRP	PHE	SER	SER	GLY	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 4: P1

Chain Fa: 19% 6% . 73%

GLY	ALA	GLY	THR	SER	GLY	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	SER	PRO	PRO	GLU	GLY	GLN	GLY	GLY	ASN	SER	SER	SER	THR	SER	SER	GLN	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	GLY	LYS	LEU	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 4: P1

Chain Fb:  19% 6% 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	LYS	PRO	PRO	GLU	GLY	GLN	GLY	SER	SER	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 4: P1

Chain Fc:  19% 6% 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	LYS	PRO	PRO	GLU	GLY	GLN	GLY	SER	SER	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 4: P1

Chain Fd:  19% 6% 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	LYS	PRO	PRO	GLU	GLY	GLN	GLY	SER	SER	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 4: P1

Chain Fe:  19% 6% 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	LYS	PRO	PRO	GLU	GLY	GLN	GLY	SER	SER	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 4: P1

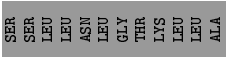
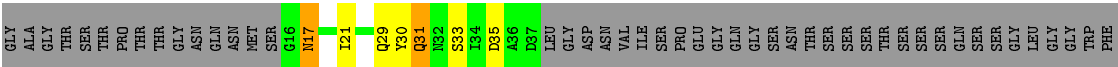
Chain Ff:  19% 6% 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	LYS	PRO	PRO	GLU	GLY	GLN	GLY	SER	SER	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 4: P1

Chain Fg:  19% 6% 73%



● Molecule 4: P1



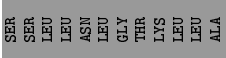
● Molecule 4: P1



● Molecule 4: P1



● Molecule 4: P1



● Molecule 4: P1



SER
SER
LEU
LEU
ASN
LEU
GLY
THR
LYS
LEU
LEU
ALA

• Molecule 4: P1



GLY	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER
SER
LEU
LEU
ASN
LEU
GLY
THR
LYS
LEU
LEU
ALA

• Molecule 4: P1



GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER
SER
LEU
LEU
ASN
LEU
GLY
THR
LYS
LEU
LEU
ALA

• Molecule 4: P1



GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER
SER
LEU
LEU
ASN
LEU
GLY
THR
LYS
LEU
LEU
ALA

• Molecule 4: P1



GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER
SER
LEU
LEU
ASN
LEU
GLY
THR
LYS
LEU
LEU
ALA

• Molecule 4: P1



GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	SER	GLY	LEU	GLY	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER
SER
LEU
LEU
ASN
LEU
GLY
THR
LYS
LEU
LEU
ALA

• Molecule 4: P1

Chain Fr:  19% 6% • 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain Fs:  19% 6% • 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain Ft:  19% 6% • 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain Fu:  19% 6% • 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain Fv:  19% 6% • 73%

GLY	ALA	GLY	THR	SER	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	SER	GLN	SER	SER	GLY	LEU	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 4: P1

Chain Fw:  19% 6% • 73%

GLY	SER	ALA	GLY	THR	SER	THR	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	THR	SER	SER	GLN	SER	SER	GLY	LEU	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 4: P1



GLY	ALA	GLY	THR	SER	THR	THR	PRO	THR	THR	GLY	ASN	GLN	ASN	MET	SER	G16	N17	I21	Q29	Y30	Q31	N32	S33	I34	D35	A36	D37	LEU	GLY	ASP	ASN	VAL	ILE	SER	PRO	GLU	GLY	GLN	GLY	ASN	THR	SER	SER	SER	THR	SER	SER	GLN	SER	SER	GLY	LEU	GLY	TRP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	LEU	LEU	ASN	LEU	GLY	THR	LYS	LEU	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING, EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN US4000SP	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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A0	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	A1	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	A2	0.84	1/1993 (0.1%)	1.07	5/2721 (0.2%)
1	A3	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	A4	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	A5	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	A6	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	A7	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	A8	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	A9	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AA	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AB	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AC	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AD	0.84	1/1993 (0.1%)	1.07	5/2721 (0.2%)
1	AE	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	AF	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AG	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AH	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	AI	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AJ	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AK	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AL	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AM	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	AN	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AO	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	AP	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AQ	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AR	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AS	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AT	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	AU	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AV	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AW	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AX	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	AY	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	AZ	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Aa	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	Ab	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Ac	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Ad	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	Ae	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Af	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	Ag	0.84	1/1993 (0.1%)	1.07	7/2721 (0.3%)
1	Ah	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Ai	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Aj	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Ak	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Al	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Am	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	An	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	Ao	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BA	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BB	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BC	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BD	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BE	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BF	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BG	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BH	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
1	BI	0.84	1/1993 (0.1%)	1.07	6/2721 (0.2%)
2	C0	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C1	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C2	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C3	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C4	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C5	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C6	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C7	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C8	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	C9	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CA	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CB	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CC	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CD	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CE	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CF	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CG	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	CH	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CI	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CJ	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CK	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CL	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CM	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CN	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CO	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CP	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CQ	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CR	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CS	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CT	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CU	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CV	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	CW	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CX	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CY	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	CZ	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Ca	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cb	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cc	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cd	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Ce	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cf	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cg	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Ch	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Ci	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cj	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Ck	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	Cl	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cm	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cn	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Co	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	Cp	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	Cq	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cr	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cs	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)
2	Ct	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cu	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cv	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cw	0.86	1/1566 (0.1%)	1.17	8/2117 (0.4%)
2	Cx	0.86	1/1566 (0.1%)	1.18	8/2117 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	D0	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D1	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D2	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D3	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D4	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D5	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D6	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D7	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D8	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	D9	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DA	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DB	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DC	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DD	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DE	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DF	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DG	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DH	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DI	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DJ	0.87	5/1769 (0.3%)	1.13	7/2420 (0.3%)
3	DK	0.86	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DL	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DM	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DN	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DO	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DP	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DQ	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DR	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DS	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DT	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DU	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DV	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DW	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DX	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DY	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	DZ	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Da	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Db	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dc	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dd	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	De	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Df	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dg	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	Dh	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Di	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dj	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dk	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Di	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dm	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dn	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Do	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dp	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dq	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Dr	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	Ds	0.86	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	EA	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	EB	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	EC	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	ED	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
3	EE	0.87	5/1769 (0.3%)	1.12	7/2420 (0.3%)
4	F0	0.78	0/168	1.03	0/226
4	F1	0.78	0/168	1.03	0/226
4	F2	0.78	0/168	1.03	0/226
4	F3	0.78	0/168	1.03	0/226
4	F4	0.78	0/168	1.03	0/226
4	F5	0.78	0/168	1.03	0/226
4	F6	0.77	0/168	1.03	0/226
4	F7	0.78	0/168	1.03	0/226
4	F8	0.78	0/168	1.03	0/226
4	F9	0.78	0/168	1.03	0/226
4	FA	0.78	0/168	1.03	0/226
4	FB	0.78	0/168	1.03	0/226
4	FC	0.78	0/168	1.03	0/226
4	FD	0.78	0/168	1.03	0/226
4	FE	0.78	0/168	1.03	0/226
4	FF	0.78	0/168	1.03	0/226
4	FG	0.78	0/168	1.03	0/226
4	FH	0.78	0/168	1.03	0/226
4	FI	0.78	0/168	1.03	0/226
4	FJ	0.78	0/168	1.03	0/226
4	FK	0.78	0/168	1.03	0/226
4	FL	0.78	0/168	1.03	0/226
4	FM	0.78	0/168	1.03	0/226
4	FN	0.78	0/168	1.03	0/226
4	FO	0.78	0/168	1.03	0/226
4	FP	0.78	0/168	1.03	0/226

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	FQ	0.78	0/168	1.03	0/226
4	FR	0.78	0/168	1.03	0/226
4	FS	0.77	0/168	1.03	0/226
4	FT	0.78	0/168	1.03	0/226
4	FU	0.78	0/168	1.03	0/226
4	FV	0.78	0/168	1.03	0/226
4	FW	0.78	0/168	1.03	0/226
4	FX	0.78	0/168	1.03	0/226
4	FY	0.78	0/168	1.03	0/226
4	FZ	0.77	0/168	1.03	0/226
4	Fa	0.78	0/168	1.03	0/226
4	Fb	0.78	0/168	1.03	0/226
4	Fc	0.78	0/168	1.03	0/226
4	Fd	0.77	0/168	1.03	0/226
4	Fe	0.78	0/168	1.03	0/226
4	Ff	0.78	0/168	1.03	0/226
4	Fg	0.78	0/168	1.03	0/226
4	Fh	0.78	0/168	1.03	0/226
4	Fi	0.78	0/168	1.03	0/226
4	Fj	0.78	0/168	1.03	0/226
4	Fk	0.78	0/168	1.03	0/226
4	Fl	0.78	0/168	1.03	0/226
4	Fm	0.78	0/168	1.03	0/226
4	Fn	0.77	0/168	1.03	0/226
4	Fo	0.78	0/168	1.03	0/226
4	Fp	0.78	0/168	1.03	0/226
4	Fq	0.78	0/168	1.03	0/226
4	Fr	0.78	0/168	1.03	0/226
4	Fs	0.78	0/168	1.03	0/226
4	Ft	0.78	0/168	1.03	0/226
4	Fu	0.78	0/168	1.03	0/226
4	Fv	0.78	0/168	1.03	0/226
4	Fw	0.78	0/168	1.03	0/226
4	Fx	0.78	0/168	1.03	0/226
All	All	0.85	420/329760 (0.1%)	1.12	1271/449040 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D0	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D1	0	2
3	D2	0	2
3	D3	0	2
3	D4	0	2
3	D5	0	2
3	D6	0	2
3	D7	0	2
3	D8	0	2
3	D9	0	2
3	DA	0	2
3	DB	0	2
3	DC	0	2
3	DD	0	2
3	DE	0	2
3	DF	0	2
3	DG	0	2
3	DH	0	2
3	DI	0	2
3	DJ	0	2
3	DK	0	2
3	DL	0	2
3	DM	0	2
3	DN	0	2
3	DO	0	2
3	DP	0	2
3	DQ	0	2
3	DR	0	2
3	DS	0	2
3	DT	0	2
3	DU	0	2
3	DV	0	2
3	DW	0	2
3	DX	0	2
3	DY	0	2
3	DZ	0	2
3	Da	0	2
3	Db	0	2
3	Dc	0	2
3	Dd	0	2
3	De	0	2
3	Df	0	2
3	Dg	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	Dh	0	2
3	Di	0	2
3	Dj	0	2
3	Dk	0	2
3	Di	0	2
3	Dm	0	2
3	Dn	0	2
3	Do	0	2
3	Dp	0	2
3	Dq	0	2
3	Dr	0	2
3	Ds	0	2
3	EA	0	2
3	EB	0	2
3	EC	0	2
3	ED	0	2
3	EE	0	2
All	All	0	120

The worst 5 of 420 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DO	119	LYS	CE-NZ	7.44	1.67	1.49
3	DS	119	LYS	CE-NZ	7.43	1.67	1.49
3	DG	119	LYS	CE-NZ	7.42	1.67	1.49
3	D3	119	LYS	CE-NZ	7.42	1.67	1.49
3	Dr	119	LYS	CE-NZ	7.42	1.67	1.49

The worst 5 of 1271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Cx	58	LEU	CA-CB-CG	9.46	137.05	115.30
2	C2	58	LEU	CA-CB-CG	9.45	137.04	115.30
2	CB	58	LEU	CA-CB-CG	9.46	137.05	115.30
2	Cn	58	LEU	CA-CB-CG	9.45	137.04	115.30
2	CC	58	LEU	CA-CB-CG	9.45	137.03	115.30

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D0	26	TYR	Sidechain
3	D0	53	PHE	Sidechain
3	D1	26	TYR	Sidechain
3	D1	53	PHE	Sidechain
3	D2	26	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	1929	0	1864	291	0
1	A1	1929	0	1864	288	0
1	A2	1929	0	1864	283	0
1	A3	1929	0	1864	283	0
1	A4	1929	0	1864	284	0
1	A5	1929	0	1864	290	0
1	A6	1929	0	1864	288	0
1	A7	1929	0	1864	288	0
1	A8	1929	0	1864	286	0
1	A9	1929	0	1864	288	0
1	AA	1929	0	1864	384	0
1	AB	1929	0	1864	386	0
1	AC	1929	0	1864	383	0
1	AD	1929	0	1864	360	0
1	AE	1929	0	1864	388	0
1	AF	1929	0	1864	387	0
1	AG	1929	0	1864	398	0
1	AH	1929	0	1864	382	0
1	AI	1929	0	1864	359	0
1	AJ	1929	0	1864	380	0
1	AK	1929	0	1864	386	0
1	AL	1929	0	1864	385	0
1	AM	1929	0	1864	413	0
1	AN	1929	0	1864	410	0
1	AO	1929	0	1864	413	0
1	AP	1929	0	1864	283	0
1	AQ	1929	0	1864	286	0
1	AR	1929	0	1864	282	0
1	AS	1929	0	1864	288	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AT	1929	0	1864	285	0
1	AU	1929	0	1864	289	0
1	AV	1929	0	1864	291	0
1	AW	1929	0	1864	285	0
1	AX	1929	0	1864	281	0
1	AY	1929	0	1864	288	0
1	AZ	1929	0	1864	289	0
1	Aa	1929	0	1864	0	0
1	Ab	1929	0	1864	0	0
1	Ac	1929	0	1864	0	0
1	Ad	1929	0	1864	0	0
1	Ae	1929	0	1864	0	0
1	Af	1929	0	1864	0	0
1	Ag	1929	0	1864	0	0
1	Ah	1929	0	1864	0	0
1	Ai	1929	0	1864	0	0
1	Aj	1929	0	1864	0	0
1	Ak	1929	0	1864	0	0
1	Al	1929	0	1864	0	0
1	Am	1929	0	1864	0	0
1	An	1929	0	1864	0	0
1	Ao	1929	0	1864	0	0
1	BA	1929	0	1864	293	0
1	BB	1929	0	1864	291	0
1	BC	1929	0	1864	289	0
1	BD	1929	0	1864	289	0
1	BE	1929	0	1864	292	0
1	BF	1929	0	1864	286	0
1	BG	1929	0	1864	289	0
1	BH	1929	0	1864	291	0
1	BI	1929	0	1864	298	0
2	C0	1537	0	1497	230	0
2	C1	1537	0	1497	226	0
2	C2	1537	0	1497	229	0
2	C3	1537	0	1497	227	0
2	C4	1537	0	1497	228	0
2	C5	1537	0	1497	230	0
2	C6	1537	0	1497	228	0
2	C7	1537	0	1497	226	0
2	C8	1537	0	1497	226	0
2	C9	1537	0	1497	230	0
2	CA	1537	0	1497	291	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CB	1537	0	1497	293	0
2	CC	1537	0	1497	290	0
2	CD	1537	0	1497	305	0
2	CE	1537	0	1497	301	0
2	CF	1537	0	1497	292	0
2	CG	1537	0	1497	287	0
2	CH	1537	0	1497	292	0
2	CI	1537	0	1497	304	0
2	CJ	1537	0	1497	301	0
2	CK	1537	0	1497	293	0
2	CL	1537	0	1497	285	0
2	CM	1537	0	1497	290	0
2	CN	1537	0	1497	303	0
2	CO	1537	0	1497	301	0
2	CP	1537	0	1497	293	0
2	CQ	1537	0	1497	293	0
2	CR	1537	0	1497	292	0
2	CS	1537	0	1497	296	0
2	CT	1537	0	1497	328	0
2	CU	1537	0	1497	327	0
2	CV	1537	0	1497	326	0
2	CW	1537	0	1497	327	0
2	CX	1537	0	1497	325	0
2	CY	1537	0	1497	225	0
2	CZ	1537	0	1497	228	0
2	Ca	1537	0	1497	0	0
2	Cb	1537	0	1497	0	0
2	Cc	1537	0	1497	0	0
2	Cd	1537	0	1497	0	0
2	Ce	1537	0	1497	0	0
2	Cf	1537	0	1497	0	0
2	Cg	1537	0	1497	0	0
2	Ch	1537	0	1497	0	0
2	Ci	1537	0	1497	0	0
2	Cj	1537	0	1497	0	0
2	Ck	1537	0	1497	0	0
2	Cl	1537	0	1497	0	0
2	Cm	1537	0	1497	0	0
2	Cn	1537	0	1497	0	0
2	Co	1537	0	1497	0	0
2	Cp	1537	0	1497	0	0
2	Cq	1537	0	1497	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Cr	1537	0	1497	0	0
2	Cs	1537	0	1497	0	0
2	Ct	1537	0	1497	0	0
2	Cu	1537	0	1497	0	0
2	Cv	1537	0	1497	0	0
2	Cw	1537	0	1497	0	0
2	Cx	1537	0	1497	0	0
3	D0	1719	0	1677	263	0
3	D1	1719	0	1677	263	0
3	D2	1719	0	1677	269	0
3	D3	1719	0	1677	266	0
3	D4	1719	0	1677	266	0
3	D5	1719	0	1677	265	0
3	D6	1719	0	1677	263	0
3	D7	1719	0	1677	267	0
3	D8	1719	0	1677	264	0
3	D9	1719	0	1677	263	0
3	DA	1719	0	1677	362	0
3	DB	1719	0	1677	345	0
3	DC	1719	0	1677	350	0
3	DD	1719	0	1677	351	0
3	DE	1719	0	1677	374	0
3	DF	1719	0	1677	363	0
3	DG	1719	0	1677	350	0
3	DH	1719	0	1677	354	0
3	DI	1719	0	1677	349	0
3	DJ	1719	0	1677	373	0
3	DK	1719	0	1677	365	0
3	DL	1719	0	1677	346	0
3	DM	1719	0	1677	343	0
3	DN	1719	0	1677	349	0
3	DO	1719	0	1677	376	0
3	DP	1719	0	1677	360	0
3	DQ	1719	0	1677	351	0
3	DR	1719	0	1677	350	0
3	DS	1719	0	1677	353	0
3	DT	1719	0	1677	260	0
3	DU	1719	0	1677	267	0
3	DV	1719	0	1677	264	0
3	DW	1719	0	1677	263	0
3	DX	1719	0	1677	266	0
3	DY	1719	0	1677	267	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DZ	1719	0	1677	260	0
3	Da	1719	0	1677	0	0
3	Db	1719	0	1677	0	0
3	Dc	1719	0	1677	0	0
3	Dd	1719	0	1677	0	0
3	De	1719	0	1677	0	0
3	Df	1719	0	1677	0	0
3	Dg	1719	0	1677	0	0
3	Dh	1719	0	1677	0	0
3	Di	1719	0	1677	0	0
3	Dj	1719	0	1677	0	0
3	Dk	1719	0	1677	0	0
3	Dl	1719	0	1677	0	0
3	Dm	1719	0	1677	0	0
3	Dn	1719	0	1677	0	0
3	Do	1719	0	1677	0	0
3	Dp	1719	0	1677	0	0
3	Dq	1719	0	1677	0	0
3	Dr	1719	0	1677	0	0
3	Ds	1719	0	1677	0	0
3	EA	1719	0	1677	264	0
3	EB	1719	0	1677	262	0
3	EC	1719	0	1677	268	0
3	ED	1719	0	1677	266	0
3	EE	1719	0	1677	263	0
4	F0	166	0	146	26	0
4	F1	166	0	146	26	0
4	F2	166	0	146	26	0
4	F3	166	0	146	26	0
4	F4	166	0	146	26	0
4	F5	166	0	146	25	0
4	F6	166	0	146	26	0
4	F7	166	0	146	25	0
4	F8	166	0	146	25	0
4	F9	166	0	146	27	0
4	FA	166	0	146	31	0
4	FB	166	0	146	26	0
4	FC	166	0	146	28	0
4	FD	166	0	146	31	0
4	FE	166	0	146	35	0
4	FF	166	0	146	29	0
4	FG	166	0	146	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	FH	166	0	146	26	0
4	FI	166	0	146	31	0
4	FJ	166	0	146	36	0
4	FK	166	0	146	29	0
4	FL	166	0	146	27	0
4	FM	166	0	146	25	0
4	FN	166	0	146	32	0
4	FO	166	0	146	35	0
4	FP	166	0	146	30	0
4	FQ	166	0	146	27	0
4	FR	166	0	146	26	0
4	FS	166	0	146	31	0
4	FT	166	0	146	42	0
4	FU	166	0	146	39	0
4	FV	166	0	146	33	0
4	FW	166	0	146	34	0
4	FX	166	0	146	38	0
4	FY	166	0	146	25	0
4	FZ	166	0	146	25	0
4	Fa	166	0	146	0	0
4	Fb	166	0	146	0	0
4	Fc	166	0	146	0	0
4	Fd	166	0	146	0	0
4	Fe	166	0	146	0	0
4	Ff	166	0	146	0	0
4	Fg	166	0	146	0	0
4	Fh	166	0	146	0	0
4	Fi	166	0	146	0	0
4	Fj	166	0	146	0	0
4	Fk	166	0	146	0	0
4	Fl	166	0	146	0	0
4	Fm	166	0	146	0	0
4	Fn	166	0	146	0	0
4	Fo	166	0	146	0	0
4	Fp	166	0	146	0	0
4	Fq	166	0	146	0	0
4	Fr	166	0	146	0	0
4	Fs	166	0	146	0	0
4	Ft	166	0	146	0	0
4	Fu	166	0	146	0	0
4	Fv	166	0	146	0	0
4	Fw	166	0	146	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Fx	166	0	146	0	0
All	All	321060	0	311040	28399	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 45.

The worst 5 of 28399 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D9:119:LYS:CE	3:D9:119:LYS:NZ	1.67	1.58
3:DS:119:LYS:CE	3:DS:119:LYS:NZ	1.67	1.58
3:DD:119:LYS:NZ	3:DD:119:LYS:CE	1.67	1.57
3:DI:119:LYS:CE	3:DI:119:LYS:NZ	1.67	1.57
3:DN:119:LYS:CE	3:DN:119:LYS:NZ	1.67	1.57

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	A1	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	A2	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	A3	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	A4	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	A5	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	A6	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	A7	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A8	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	A9	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AA	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AB	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AC	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AD	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AE	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AF	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AG	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AH	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	AI	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	AJ	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AK	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	AL	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AM	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	AN	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AO	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AP	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AQ	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AR	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AS	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	AT	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AU	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AV	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AW	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AX	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AY	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	AZ	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	Aa	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Ab	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	Ac	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ad	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Ae	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Af	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Ag	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Ah	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Ai	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Aj	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Ak	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	Al	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	Am	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	An	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	Ao	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	BA	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	BB	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	BC	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	BD	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	BE	244/246 (99%)	144 (59%)	60 (25%)	40 (16%)	0	5
1	BF	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	BG	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	BH	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
1	BI	244/246 (99%)	145 (59%)	59 (24%)	40 (16%)	0	5
2	C0	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C1	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C2	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C3	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C4	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C5	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C6	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C7	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C8	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	C9	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CA	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CB	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CC	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CD	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CE	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CF	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CG	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CH	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CI	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CJ	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CK	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CL	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CM	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CN	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CO	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CP	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CQ	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CR	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CS	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CT	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CU	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CV	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CW	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CX	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CY	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	CZ	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Ca	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cb	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cc	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cd	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Ce	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Cf	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cg	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Ch	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Ci	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cj	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Ck	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cl	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cm	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cn	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Co	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cp	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cq	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cr	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cs	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Ct	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cu	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cv	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cw	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
2	Cx	154/230 (67%)	104 (68%)	33 (21%)	17 (11%)	0	11
3	D0	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	D1	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	D2	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	D3	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	D4	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	D5	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	D6	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	D7	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	D8	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	D9	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DA	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DB	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	DC	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DD	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DE	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DF	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DG	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DH	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DI	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DJ	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DK	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DL	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DM	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DN	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DO	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DP	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DQ	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DR	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DS	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DT	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DU	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DV	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DW	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DX	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DY	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	DZ	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	Da	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	Db	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	Dc	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	Dd	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	De	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	Df	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	Dg	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Dh	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	Di	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	Dj	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	Dk	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	DI	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	Dm	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	Dn	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	Do	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	Dp	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	Dq	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	Dr	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	Ds	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	EA	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	EB	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	EC	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
3	ED	224/226 (99%)	156 (70%)	45 (20%)	23 (10%)	1	12
3	EE	224/226 (99%)	155 (69%)	46 (20%)	23 (10%)	1	12
4	F0	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F1	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F2	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F3	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F4	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F5	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F6	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F7	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F8	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	F9	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FA	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FB	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FC	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FD	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	FE	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FF	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FG	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FH	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FI	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FJ	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FK	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FL	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FM	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FN	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FO	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FP	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FQ	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FR	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FS	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FT	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FU	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FV	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FW	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FX	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FY	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	FZ	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fa	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fb	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fc	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fd	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fe	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Ff	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fg	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fh	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fi	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Fj	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fk	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fl	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fm	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fn	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fo	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fp	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fq	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fr	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fs	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Ft	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fu	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fv	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fw	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
4	Fx	20/80 (25%)	9 (45%)	7 (35%)	4 (20%)	0	3
All	All	38520/46920 (82%)	24801 (64%)	8679 (22%)	5040 (13%)	1	7

5 of 5040 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	10	PRO
1	A0	18	ALA
1	A0	22	VAL
1	A0	26	VAL
1	A0	63	THR

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	A0	208/208 (100%)	174 (84%)	34 (16%)	3	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	A2	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	A3	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	A4	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	A5	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	A6	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	A7	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	A8	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	A9	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AA	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AB	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AC	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AD	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AE	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AF	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AG	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AH	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AI	208/208 (100%)	173 (83%)	35 (17%)	2	19
1	AJ	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AK	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AL	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AM	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AN	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AO	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AP	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AQ	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AR	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AS	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AT	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AU	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AV	208/208 (100%)	174 (84%)	34 (16%)	3	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AW	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AX	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AY	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	AZ	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Aa	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Ab	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Ac	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Ad	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Ae	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Af	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Ag	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Ah	208/208 (100%)	173 (83%)	35 (17%)	2	19
1	Ai	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Aj	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Ak	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Al	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Am	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	An	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	Ao	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BA	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BB	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BC	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BD	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BE	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BF	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BG	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BH	208/208 (100%)	174 (84%)	34 (16%)	3	20
1	BI	208/208 (100%)	174 (84%)	34 (16%)	3	20
2	C0	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	C1	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	C2	175/204 (86%)	133 (76%)	42 (24%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C3	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	C4	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	C5	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	C6	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	C7	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	C8	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	C9	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CA	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CB	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CC	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CD	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CE	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CF	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CG	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CH	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CI	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CJ	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CK	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CL	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CM	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CN	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CO	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CP	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CQ	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CR	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CS	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CT	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CU	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CV	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	CW	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CX	175/204 (86%)	133 (76%)	42 (24%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CY	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	CZ	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Ca	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Cb	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cc	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cd	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Ce	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cf	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Cg	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Ch	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Ci	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Cj	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Ck	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Cl	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Cm	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cn	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Co	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cp	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cq	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Cr	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Cs	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Ct	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cu	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cv	175/204 (86%)	133 (76%)	42 (24%)	1	7
2	Cw	175/204 (86%)	132 (75%)	43 (25%)	1	6
2	Cx	175/204 (86%)	133 (76%)	42 (24%)	1	7
3	D0	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	D1	190/190 (100%)	147 (77%)	43 (23%)	1	8
3	D2	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	D3	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	D4	190/190 (100%)	146 (77%)	44 (23%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D5	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	D6	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	D7	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	D8	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	D9	190/190 (100%)	147 (77%)	43 (23%)	1	8
3	DA	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DB	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DC	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DD	190/190 (100%)	147 (77%)	43 (23%)	1	8
3	DE	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DF	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DG	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DH	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DI	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DJ	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DK	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DL	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DM	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DN	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DO	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DP	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DQ	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DR	190/190 (100%)	147 (77%)	43 (23%)	1	8
3	DS	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DT	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DU	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DV	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DW	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DX	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DY	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	DZ	190/190 (100%)	146 (77%)	44 (23%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Da	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Db	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dc	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dd	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	De	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Df	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dg	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dh	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Di	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dj	190/190 (100%)	147 (77%)	43 (23%)	1	8
3	Dk	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dl	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dm	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dn	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Do	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dp	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Dq	190/190 (100%)	147 (77%)	43 (23%)	1	8
3	Dr	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	Ds	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	EA	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	EB	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	EC	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	ED	190/190 (100%)	146 (77%)	44 (23%)	1	7
3	EE	190/190 (100%)	146 (77%)	44 (23%)	1	7
4	F0	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	F1	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	F2	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	F3	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	F4	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	F5	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	F6	18/65 (28%)	13 (72%)	5 (28%)	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F7	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	F8	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	F9	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FA	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FB	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FC	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FD	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FE	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FF	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FG	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FH	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FI	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FJ	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FK	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FL	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FM	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FN	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FO	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FP	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FQ	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FR	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FS	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FT	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FU	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FV	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FW	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FX	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FY	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	FZ	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fa	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fb	18/65 (28%)	13 (72%)	5 (28%)	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Fc	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fd	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fe	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Ff	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fg	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fh	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fi	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fj	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fk	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fl	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fm	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fn	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fo	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fp	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fq	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fr	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fs	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Ft	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fu	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fv	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fw	18/65 (28%)	13 (72%)	5 (28%)	0	4
4	Fx	18/65 (28%)	13 (72%)	5 (28%)	0	4
All	All	35460/40020 (89%)	27939 (79%)	7521 (21%)	4	9

5 of 7521 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CW	45	SER
2	Cp	53	ARG
3	Dr	188	LEU
2	CY	137	GLU
2	Cf	202	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1352 such sidechains are listed below:

Mol	Chain	Res	Type
2	CQ	134	HIS
2	CI	189	HIS
4	FV	24	ASN
2	CT	73	GLN
2	Cb	136	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.